

# Quantum mechanical simulations of the radical-radical chemistry on icy surfaces: XYZ data

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# 1 Radical interaction with a single water molecule

8  
CH2OH\_H2O\_HtoW  
O -0.88398448 1.36893957 0.24398678  
H -0.59082250 1.81323687 1.03113301  
H -0.72407316 1.96446597 -0.47907888  
O -0.14332012 -1.31640640 -0.14041386  
H -0.37894872 -0.39818257 -0.00236791  
C -1.23129069 -2.03424869 -0.46888104  
H -2.20265615 -1.63245916 -0.24795193  
H -1.07074915 -3.09070210 -0.53819345

8  
CH2OH\_H2O\_WtoO  
O -3.08234404 0.75088309 -0.11813682  
H -2.29572278 0.21210826 -0.16526030  
H -3.25153544 1.04162370 -1.00510403  
O -0.59942745 -0.79036905 -0.14030057  
H 0.09246818 -0.37044048 0.35700840  
C -0.51053786 -2.14027374 -0.05702843  
H 0.43952546 -2.57809146 0.17891072  
H -1.24783240 -2.66255639 -0.62903630

8  
CH3O\_H2O\_WtoO  
O -1.13681741 1.94686608 -0.13192875  
H -0.35978965 1.40131219 -0.02640705  
H -0.84705627 2.84602096 -0.04688898  
C -0.46685616 -1.20481205 -0.27443102  
H -1.25135182 -0.72919191 -0.85595747  
H -0.13894652 -2.13983680 -0.71730949  
H -0.89393558 -1.42761842 0.70789817  
O 0.57268540 -0.35147706 -0.03120941

7  
CH3\_H2O\_WtoC  
C -1.70344346 0.00175808 -0.00127890  
O 1.59557002 -0.09664865 0.00767879  
H 1.94404862 0.78622461 -0.00511158  
H 0.64749903 -0.00061283 0.00399049  
H -1.93812363 1.04564890 -0.05279969  
H -1.65303308 -0.48724216 0.95063779  
H -1.63920649 -0.57543795 -0.90158891

6  
HCO\_H2O\_HtoW  
O 2.17017937 0.05251990 0.00016808  
C -1.10237411 -0.44695912 0.00000151  
O -2.01297829 0.27516599 -0.00010647  
H 2.65823825 0.86746126 0.00010687  
H 2.81681858 -0.64333531 0.00033300  
H -0.03548378 -0.15075872 0.00005401

6  
HCO\_H2O\_WtoO  
O 2.09533287 -0.19257648 -0.00003298  
H 1.17081280 0.03446784 -0.00003512  
H 2.56330066 0.63285716 -0.00007223  
O -0.89081265 0.42423129 -0.00005134  
C -1.76330056 -0.34132252 0.00006783  
H -2.84275312 -0.08801228 0.00001483

6  
NH2\_H2O\_WtoN  
O 1.50005122 -0.00000119 -0.11078488  
H 1.86316654 0.00024911 0.76532935

H	0.54848494	0.00002096	-0.00204794
N	-1.46672393	0.00000820	0.03308427
H	-2.07521412	-0.80609887	-0.05468212
H	-2.07524467	0.80604979	-0.05507068

## 2 W18 geometries

### 2.1 Adsorption geometries

59  
ch2oh W18

O	4.06319300	-0.76398000	-1.38292300
O	1.35615200	-0.32504300	-1.12836400
O	-0.90558100	-1.74962000	-0.98467800
O	-2.17920500	0.40624500	-2.10998400
O	-4.37927500	-0.98381400	-2.81555700
O	1.67480600	-0.54794100	1.60386700
O	4.23164300	0.53554100	0.98465400
O	3.16903700	2.85139300	0.42708800
O	0.20547300	1.33215000	2.97034500
O	0.81993900	3.57273900	1.83940100
O	-0.82177300	3.70937800	-0.30923300
O	0.19966900	1.90959500	-2.22003700
O	2.50022100	3.40164800	-2.20364800
O	-0.77308500	-2.00762600	1.76114900
O	-2.18622000	-0.10974500	3.16689900
O	-4.11342700	0.34977700	1.49908500
O	-3.25724400	2.20887600	-0.26788900
O	-2.66378200	-3.58158200	0.18629900
O	-4.71765900	-1.90837100	-0.17975300
H	5.04928800	0.68707200	1.45095700
H	3.84099600	1.42485900	0.79014000
H	2.39441700	3.13658600	0.92556900
H	3.00541600	3.06496700	-0.50390600
H	-2.53796800	2.82544400	-0.10942800
H	-2.93305700	1.61676100	-0.95823900
H	0.15953200	-1.82901000	1.91647500
H	-1.26497800	-1.39933000	2.33329800
H	2.61640600	-0.38935900	1.71865900
H	1.52900500	-0.40494600	0.65394400
H	-0.81596200	4.57518500	-0.70979200
H	-0.25024200	3.75177100	0.47808500
H	0.53700600	2.74770600	2.31271800
H	0.91552700	4.25808100	2.49548600
H	1.70251800	2.88578300	-2.40454000
H	3.10050600	3.30226100	-2.93645200
H	0.62183000	1.14344100	-1.79771900
H	-0.17673000	2.45520700	-1.51624400
H	-0.68429800	0.97029100	3.06673900
H	0.73943200	0.64789300	2.53760200
H	0.70013700	-1.02965200	-1.26202100
H	2.22472300	-0.60754500	-1.44238900
H	-4.35851700	-0.38080400	0.92161400
H	-3.87524800	1.09830100	0.92266900
H	-2.14608600	-3.40963400	0.97733100
H	-2.08999000	-3.26562800	-0.52116800
H	-4.01800200	-2.56864100	0.01311300
H	-5.55248000	-2.30138700	0.06235500
H	-2.87691200	0.04650700	-2.67523600
H	-1.51841500	0.89766600	-2.60785500
H	-4.54100500	-1.69953300	-3.42257600
H	-4.56724100	-1.31426600	-1.92552600
H	-2.94599400	0.07824900	2.55600000
H	-2.54726800	-0.24276600	4.03908800
H	-1.42943400	-1.01472600	-1.34160200

H	-0.91461600	-1.66959200	-0.01870700
C	4.70404100	-1.95464200	-1.45240400
H	4.24004300	-0.31631400	-0.53688300
H	4.62780700	-2.44776600	-2.40392300
H	5.55808600	-2.10850500	-0.81406800

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ch3 W18

C	-3.92126700	3.44164400	-2.08668000
O	-1.33911400	1.64893900	-1.61906100
O	1.29646500	2.01843000	-1.46310700
O	1.52734000	-0.59705800	-2.14539200
O	3.95693400	-1.75998700	-2.10867700
O	-1.22323000	-1.05543600	-2.15020800
O	-3.41766200	-2.57520400	-1.73435400
O	-1.56587100	2.02958200	1.14842600
O	-0.87894000	0.02445500	2.90658000
O	-2.18758100	-2.11115600	2.26549400
O	-1.02216900	-2.92363200	-0.06220600
O	-4.27439400	1.64294800	0.83645400
O	-4.17333900	-1.04488300	0.57006000
O	1.27765700	2.43665600	1.26313100
O	1.88697500	0.40340600	3.03291600
O	3.36456200	-1.27129900	1.69651700
O	1.79466300	-2.55033900	-0.15657100
O	3.81101000	2.57443600	-0.30318200
O	4.93465700	0.12604200	-0.20305600
H	-5.05393800	1.84326500	1.34608200
H	-4.27189500	0.67653100	0.69695100
H	-3.57339200	-1.44058600	1.21300900
H	-4.05592800	-1.53842800	-0.24821700
H	0.94503500	-2.97705600	-0.01045900
H	1.59625800	-1.80564400	-0.73814700
H	0.35484100	2.65616400	1.42304800
H	1.51059500	1.76027900	1.91614600
H	-2.52403500	2.09922100	1.26300400
H	-1.47009900	1.82059300	0.20907800
H	-1.73054600	-3.36104900	-0.53777200
H	-1.38690000	-2.70829100	0.81145900
H	-1.66786600	-1.32555000	2.57269300
H	-2.38388700	-2.64881500	3.02748800
H	-2.76080000	-1.99521600	-2.15407700
H	-3.99099200	-2.91905300	-2.41320500
H	-1.36222200	-0.11143700	-1.98051000
H	-1.01834400	-1.47143100	-1.30224900
H	0.07956800	0.04570600	3.01200400
H	-1.11250800	0.73588500	2.28955700
H	-0.42914700	1.97630000	-1.75242000
H	-1.96425500	2.26852200	-1.99938600
H	3.98459700	-0.82905200	1.10529900
H	2.80649800	-1.83526500	1.13828300
H	3.27958600	2.81278600	0.45923600
H	3.17959700	2.59206800	-1.03009200
H	4.55356200	1.02719300	-0.24212500
H	5.87844300	0.22945100	-0.11154000
H	2.34020500	-0.99777900	-2.49078900
H	0.74614600	-0.89422900	-2.62063900
H	3.68028600	-2.48328700	-1.54524200
H	4.39367700	-1.12313000	-1.53024100
H	2.46409900	-0.24968100	2.56357700
H	2.27091400	0.56399000	3.89061100
H	1.47459000	1.09959800	-1.72105300
H	1.27049500	2.03938500	-0.49353000
H	-4.12977800	2.87601500	-1.19338600
H	-4.29389100	3.10675900	-3.03898100
H	-3.48627100	4.42323300	-2.01316900

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ch3o W18

C	-4.24421900	1.31884700	-2.49708100
O	-1.06048900	1.09634400	-1.71984400
O	1.55305300	1.43116100	-1.30055000
O	2.00513100	-1.18046800	-2.01594600
O	4.60431600	-0.84210000	-2.62848600
O	-1.53055800	1.56903100	0.99028400
O	-4.25054600	1.06206500	0.75370700
O	-4.02768200	-1.59657100	0.45347600
O	-0.85299500	-0.36261100	2.83695700
O	-2.07650200	-2.55381500	2.23146900
O	-0.75391900	-3.36590200	-0.01007200
O	-0.77287500	-1.58867400	-2.16382500
O	-3.08626500	-2.95135700	-1.86693000
O	1.27103200	2.11676700	1.33673000
O	1.88770600	0.09003400	3.09143900
O	3.47719700	-1.40865100	1.70171100
O	2.10412400	-3.07331600	0.05100300
O	3.81027600	2.56936100	-0.12746800
O	5.06935500	0.20675000	-0.07098500
H	-4.96653700	1.23668400	1.35768700
H	-4.20354800	0.09135600	0.63976800
H	-3.43734200	-1.97541300	1.11611600
H	-3.82273800	-2.03880400	-0.37788600
H	1.19915800	-3.37994100	0.14941400
H	2.09420000	-2.48623300	-0.71439800
H	0.32562100	2.27865000	1.41244100
H	1.49640500	1.47147400	2.02349600
H	-2.49327600	1.59732200	1.07600300
H	-1.38175200	1.36227700	0.05610200
H	-1.41254900	-3.85315800	-0.50547700
H	-1.17429100	-3.13934000	0.83512500
H	-1.59162500	-1.74200400	2.52997300
H	-2.25641600	-3.08827400	2.99972700
H	-2.33399900	-2.44174800	-2.21497500
H	-3.57074200	-3.31260600	-2.60328900
H	-0.93048800	-0.64245700	-2.01349100
H	-0.61056200	-1.99157400	-1.29977700
H	0.10008100	-0.31726600	2.98215100
H	-1.07425100	0.31643300	2.18045800
H	-0.14409900	1.41935100	-1.77846600
H	-1.64513400	1.63171200	-2.26779900
H	4.03566000	-0.93536300	1.07637600
H	2.99995100	-2.09367400	1.20081400
H	3.23356400	2.76783300	0.61351200
H	3.19056900	2.38807400	-0.84447400
H	4.66990800	1.10106900	-0.02351300
H	5.96471500	0.27854200	0.25018700
H	2.83094800	-1.18293600	-2.52169300
H	1.24843600	-1.42776000	-2.55398100
H	5.05589100	-0.31797200	-3.28294600
H	4.85090700	-0.49382900	-1.75958400
H	2.50578200	-0.50071700	2.58707000
H	2.24971100	0.20685900	3.96540300
H	1.77894300	0.50669900	-1.49169300
H	1.43027700	1.51091900	-0.34065700
O	-3.30357900	2.21376100	-2.93966400
H	-3.87718500	0.29287900	-2.55177200
H	-4.38180400	1.53306400	-1.42780900
H	-5.19755200	1.43581600	-3.00854500

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hco W18

C	-0.70740200	4.91745700	-0.25557100
O	0.45769800	4.90247600	-0.08257800
O	2.06135500	2.50881500	0.19931900
O	1.29356000	1.32787800	2.50965900
O	2.65309200	-0.87446000	2.40540400
O	1.13508700	-2.87771700	1.42947600

O	4.32806000	1.33008700	-0.92358200
O	4.80014300	-0.88716600	0.47478700
O	4.10061500	-2.78741800	-1.44382300
O	1.54565500	-1.98349200	-1.21424600
O	1.62546500	0.67609000	-1.83113900
O	-0.88475700	0.62903500	-2.62870700
O	-1.22096100	-1.97050300	-1.62774200
O	-3.57036500	-3.19993800	-0.99308900
O	-2.12202800	2.17457700	-0.64543500
O	-1.46543900	1.36557100	1.89993000
O	-2.99140600	-0.66925400	2.43968200
O	-1.65020400	-2.59295200	1.05595500
O	-4.70456600	1.41668600	-0.98305100
O	-4.79321600	-0.94667400	0.28248400
H	-5.51270400	1.89670300	-0.83155300
H	-4.79978400	0.54235700	-0.55835400
H	-4.25571900	-0.86267700	1.07868400
H	-4.48413600	-1.73028600	-0.18375800
H	0.17675700	-2.91491700	1.50324400
H	1.30298100	-2.65184800	0.50719400
H	1.65416000	3.37014400	0.08042700
H	1.80424000	2.18755600	1.08050000
H	-3.07800400	2.01600300	-0.73152800
H	-1.71376100	1.67188600	-1.36171700
H	-2.32382700	-3.18880100	0.72269200
H	-2.09871000	-1.97374700	1.65272200
H	-2.42067700	0.12564300	2.29136800
H	-3.25987600	-0.67079000	3.35403100
H	-2.82517900	-2.84268500	-1.50185500
H	-4.01250200	-3.85340900	-1.52715900
H	-1.23773600	-1.07185600	-1.98392900
H	-1.23384800	-1.90789900	-0.66214100
H	-0.51640000	1.31047300	2.06244500
H	-1.61732500	1.66819800	0.99037800
H	0.08027800	0.71657600	-2.46199700
H	-1.05341600	0.84883000	-3.54096800
H	3.39950700	-0.90547700	1.79783000
H	2.08977400	-1.64060700	2.18998900
H	3.76560000	1.93575100	-0.42483300
H	3.77036300	1.06755300	-1.65929300
H	4.69512400	-0.04083000	-0.01090800
H	5.65918700	-0.87494500	0.88919700
H	2.34032800	-2.43723400	-1.53127400
H	0.75253700	-2.29158600	-1.66381500
H	4.76423100	-2.84297100	-2.12422900
H	4.44014400	-2.20438900	-0.74939000
H	1.80537600	0.47615100	2.48935100
H	1.44057700	1.72089900	3.36616700
H	1.67008700	-0.23988400	-1.50845900
H	1.65060400	1.27047700	-1.06684700
H	-1.34571600	4.02315000	-0.41807300

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nh2 W18

H	-5.10458100	1.97251200	1.11054900
O	-4.38728600	1.74104900	0.52710800
H	-4.33529700	0.76151500	0.52715800
H	-4.21426300	2.45179000	-1.38329000
N	-3.74480700	2.63339700	-2.27255300
H	-4.38167800	3.17326000	-2.85049300
H	-2.03300300	1.88535900	-2.20875100
O	-1.31030600	1.37113900	-1.81469700
H	-0.44774100	1.74791900	-2.04663300
H	0.02315400	0.45143400	2.98485100
O	-0.93483700	0.41358400	2.87613700
H	-1.16166000	1.02857400	2.16033200
H	-1.47210200	1.78569600	-0.06221800
O	-1.60900200	2.12458800	0.83659100

H	-2.56581400	2.22555800	0.90596600
H	-3.96603400	-3.11510500	-2.10023100
O	-3.40706200	-2.70315200	-1.44791300
H	-2.71253700	-2.20388300	-1.91271600
H	1.27436100	1.99988900	-0.78544300
O	1.36110800	1.86229300	-1.74072100
H	1.51515900	0.91401700	-1.87246100
H	3.29801400	2.89079400	0.12400000
O	3.82414600	2.54373500	-0.59861700
H	3.18375300	2.44835200	-1.31407800
H	4.56272200	1.02748200	-0.31693700
O	4.94431700	0.14059900	-0.14873600
H	5.88644500	0.25827200	-0.05809000
H	4.43082900	-1.26951400	-1.31274800
O	4.00994000	-1.97972900	-1.81224700
H	3.71756600	-2.62132100	-1.16421700
H	2.39561300	-1.27532400	-2.32717100
O	1.57467300	-0.84087600	-2.04939100
H	0.80552900	-1.20367600	-2.49793700
H	2.20276800	1.10521900	3.79117500
O	1.82484300	0.82291800	2.96275300
H	2.41360400	0.11953300	2.59018000
H	3.96752000	-0.63434100	1.25177500
O	3.33579800	-0.99989000	1.88202200
H	2.78944400	-1.63161100	1.38840200
H	0.30325400	2.83237300	1.03925500
O	1.23093400	2.60712500	0.92585100
H	1.45660100	2.02014000	1.66181100
H	-1.71337300	-0.96685200	2.68819900
O	-2.23629700	-1.77896700	2.46442300
H	-2.45090200	-2.22254700	3.28023600
H	-1.39829500	-2.57402400	1.12395200
O	-1.01278500	-2.91457200	0.30087400
H	-1.71483400	-3.40461600	-0.12982300
H	0.95517100	-2.92379700	0.36840800
O	1.80493300	-2.51418400	0.18083500
H	1.61676000	-1.85481900	-0.49944200
H	-3.59216100	-1.23284200	1.31977300
O	-4.18974600	-0.92321100	0.62821300
H	-4.05344900	-1.50726400	-0.12663500
H	-1.28544100	-0.37264200	-1.97574800
H	-0.95906100	-1.64340600	-1.13509000
O	-1.16531900	-1.33666400	-2.02714700

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O	4.26065089	-2.24498765	-0.70511413
O	1.55708433	-2.52204486	-0.54840484
O	4.54272317	0.23420951	0.36065593
O	1.25517291	-1.65517446	2.05729746
O	2.77327444	0.38013929	2.55030315
O	1.54930759	2.30986802	1.06567865
O	-1.50779618	-1.89945144	2.40178421
O	-2.85193772	0.32961257	2.34806046
O	-1.28096593	2.27726614	1.21859690
O	-1.28859873	-2.75976679	-0.21367822
O	-1.51030940	-0.96592684	-2.26689484
O	1.08534118	-0.81060965	-2.74901270
O	-1.42508859	1.62528191	-1.50010946
O	-3.66080850	2.78720353	-0.55603322
O	1.35982960	1.75072680	-1.68305822
O	3.73549380	2.73170533	-0.82326760
O	-4.74914680	0.27183765	0.24312403
O	-3.98138105	-1.84881497	-1.23806854
H	5.03627575	-2.75271022	-0.48839129
H	4.40453733	-1.34209703	-0.36742747
H	4.03472890	0.28702224	1.17830154
H	4.39886226	1.06600240	-0.10134362

H	-0.37099948	2.49744854	1.44015436
H	-1.22935529	1.92969502	0.31950205
H	-0.38267471	-3.06882419	-0.31433337
H	-1.38882630	-2.51253390	0.71720387
H	2.51360121	-2.68270551	-0.54711449
H	1.43046935	-1.90753441	-1.28198765
H	2.26590875	2.87730976	0.77534847
H	1.95071359	1.67323215	1.67878510
H	2.18977587	-0.41137621	2.43459212
H	3.04484929	0.41628003	3.46295871
H	2.99899341	2.47549066	-1.40150064
H	4.29195637	3.34114531	-1.29946868
H	1.37693575	0.86112683	-2.06283574
H	1.27886878	1.65974679	-0.72432860
H	0.31627182	-1.68208560	2.27542202
H	1.34486147	-1.93887173	1.13436223
H	0.11291253	-0.92201694	-2.79610267
H	1.47057689	-1.12218079	-3.56367302
H	-3.57554562	0.31739113	1.71126254
H	-2.27009945	1.06163253	2.08955792
H	-3.45458066	-2.50951699	-0.78507872
H	-3.39789080	-1.53538537	-1.93747560
H	-4.50135001	-0.50563900	-0.29734386
H	-5.68880669	0.21367984	0.39589607
H	-2.19803972	2.21120952	-1.48224638
H	-0.64907489	2.05682761	-1.86827886
H	-3.24756959	3.08834655	0.25383164
H	-4.13880667	1.98083132	-0.32767901
H	-2.03139336	-1.05988907	2.42256982
H	-1.81793861	-2.45223210	3.11381336
H	-1.57892565	-0.03948545	-1.98280850
H	-1.40077186	-1.50605981	-1.46630768

## 2.2 PES geometries

### 2.2.1 CH2OH + CH2OH

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i0\_dHa2\_ch2oh\_ch2oh W18

O	3.48808326	-2.81887394	-1.19286171
O	1.47383803	-0.86030453	-1.37946415
O	-0.98634724	-1.80654249	-1.04280878
O	-2.09620361	0.35919101	-2.28868955
O	-4.40245167	-0.79524608	-3.05735353
O	2.22991841	-0.36109134	1.19374969
O	4.41914766	1.15691139	0.92230327
O	3.17526654	3.41482932	0.21872939
O	0.49169158	1.15644256	2.74070577
O	0.87469782	3.57086648	1.85287509
O	-0.38843455	3.47589543	-0.56673864
O	0.47192184	1.51797496	-2.37842387
O	1.90147177	3.82442823	-2.30298185
O	-1.13580366	-2.44345363	1.63422325
O	-1.95664161	-0.18897700	2.94770385
O	-3.78492988	0.53546817	1.25925697
O	-3.00393644	2.36970980	-0.57064224
O	-3.07948863	-3.51243640	-0.10915628
O	-4.86850493	-1.55802887	-0.40478925
H	5.09902807	1.37122749	1.55396706
H	4.03561488	2.00327084	0.61489380
H	2.42959339	3.54288794	0.81669494
H	2.85063288	3.58151980	-0.67306728
H	-2.23854707	2.94542975	-0.48742990
H	-2.75468600	1.72823681	-1.24691588
H	-0.24380517	-2.73014724	1.85627585
H	-1.38306323	-1.72634606	2.23769011



H	3.07279240	0.13098267	1.19841589
H	1.95567476	-0.43256362	0.26187108
H	0.11177930	4.06874426	-1.13031823
H	-0.01704167	3.57027591	0.32378332
H	0.69709438	2.68354352	2.25152839
H	0.75105389	4.22752283	2.53237938
H	1.53592753	2.96668138	-2.57737066
H	2.28767367	4.24255656	-3.06705364
H	0.94848933	0.72131731	-2.10302618
H	0.11898656	1.93356208	-1.57996280
H	-0.37709073	0.73971409	2.80806533
H	1.06250778	0.57269435	2.22248625
H	0.61462039	-1.32594904	-1.32025231
H	2.14144199	-1.51772443	-1.60158040
H	-4.18433203	-0.13384431	0.69404236
H	-3.53841697	1.28290654	0.68408403
H	-2.56878444	-3.39794720	0.70035135
H	-2.44779156	-3.27786402	-0.79525643
H	-4.27855152	-2.32629223	-0.24546662
H	-5.74544935	-1.80648552	-0.12349272
H	-2.80576423	0.03022165	-2.85918435
H	-1.36179412	0.71792320	-2.79505968
H	-4.64183376	-1.50520856	-3.64506734
H	-4.66317915	-1.05841977	-2.16296605
H	-2.66424665	0.10399780	2.31589194
H	-2.33711642	-0.17308064	3.82192300
H	-1.47343870	-1.03722826	-1.37985799
H	-1.05886317	-1.82828342	-0.07746746
C	4.67239367	-2.18246065	-0.98054277
H	3.18692453	-3.24650527	-0.38255517
H	5.05845904	-1.69013977	-1.85370660
H	4.86631995	-1.78628686	0.00244581
O	1.66377170	-2.79618271	1.94413569
C	2.66790844	-3.66382184	1.72739432
H	1.95506239	-1.87248822	1.77827587
H	2.40927023	-4.69600196	1.88689570
H	3.67282279	-3.32622645	1.94008124

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O	4.21276889	-1.45178854	-1.11295071
O	1.55136318	-0.97008745	-0.97311334
O	-0.83648217	-2.21651117	-0.90059740
O	-1.89126521	-0.10493992	-2.33787652
O	-4.21707710	-1.10044598	-3.26835518
O	2.22520048	-0.36069161	1.62226288
O	4.50894575	0.84145255	0.48423333
O	3.27416136	3.07056620	-0.16121795
O	0.39060154	1.37285162	2.66944243
O	0.99499072	3.58262100	1.42834121
O	-0.29763678	3.40150351	-0.98237841
O	0.58336328	1.15029645	-2.38898454
O	2.07568343	3.36354693	-2.68828538
O	-1.47884938	-2.33428341	1.81163030
O	-2.15543178	0.18024737	2.69324248
O	-3.93733514	0.73275883	0.89719067
O	-2.88840793	2.21621051	-1.09825016
O	-3.27354928	-3.48456190	0.02368587
O	-4.94193414	-1.51409015	-0.60465007
H	5.35089358	1.09044546	0.85569422
H	4.07108640	1.67575121	0.19362616
H	2.54323046	3.28622537	0.43121650
H	2.96097661	3.22227131	-1.06169819
H	-2.13595559	2.80948463	-1.02615563
H	-2.57042359	1.45070619	-1.59264707
H	-0.72771787	-2.69031567	2.30240173
H	-1.71902338	-1.48884772	2.21957911
H	3.07323248	0.06339989	1.44814635

H	1.90101535	-0.61835305	0.74329437
H	0.25019818	3.89214265	-1.59719377
H	0.07821064	3.54806325	-0.10126377
H	0.72631072	2.77971309	1.94083993
H	0.95263957	4.32899598	2.01980116
H	1.67348811	2.48560710	-2.81598464
H	2.49715438	3.62286035	-3.50241780
H	1.00496766	0.41781096	-1.90710247
H	0.17999690	1.72528001	-1.72493989
H	-0.50000828	1.00193356	2.61557256
H	1.01511022	0.72326561	2.30732008
H	0.83950422	-1.62970057	-1.04016444
H	2.41259348	-1.34041099	-1.22000398
H	-4.30661536	-0.00166087	0.39472349
H	-3.61674130	1.38108364	0.24414864
H	-2.81879701	-3.26805697	0.84771912
H	-2.56785176	-3.44750674	-0.62757424
H	-4.38067392	-2.27645342	-0.34037189
H	-5.84074528	-1.72478276	-0.36479678
H	-2.57819995	-0.42534082	-2.94039185
H	-1.12707222	0.23580484	-2.81336161
H	-4.43859010	-1.87085878	-3.78238014
H	-4.58145530	-1.23038580	-2.38064572
H	-2.83400707	0.41150709	2.00417992
H	-2.57349421	0.31568893	3.53986106
H	-1.28155050	-1.47791082	-1.34492778
H	-0.99777348	-2.12334309	0.04894175
C	4.65979300	-2.51792074	-0.30538543
H	4.42030949	-0.61684939	-0.67522830
H	5.73855133	-2.48175287	-0.16460487
H	4.17096154	-2.51313733	0.66794336
O	0.93427849	-3.02758570	3.03673253
C	1.57186273	-2.12037494	3.50453249
H	4.41090813	-3.44143008	-0.81541707
H	2.64894761	-2.20661272	3.66319616
H	1.10570173	-1.18263100	3.81254353

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O	3.29605414	2.16017122	1.58636847
O	1.14986595	0.44522107	1.28714308
O	-1.43572835	0.21456815	1.87129850
O	-1.14092907	-2.51995936	1.97105829
O	-3.35698214	-3.30798826	3.28133574
O	1.05015149	1.62776753	-1.16027807
O	3.84989395	1.53602461	-1.01711518
O	3.92481437	-1.00599529	-1.62130863
O	-0.06328796	-0.07932479	-3.04754862
O	1.77241143	-1.90144050	-3.19101387
O	1.30995575	-3.59669319	-1.09768348
O	1.56307640	-2.26648371	1.33986810
O	3.89425210	-3.08867315	0.26778431
O	-2.73237725	1.35384876	-0.29507850
O	-2.77277172	-0.37637728	-2.42910039
O	-3.53951328	-2.52127713	-1.18822340
O	-1.43442826	-4.02529627	-0.38476228
O	-4.32116004	0.52703192	1.83988105
O	-4.87289524	-2.02635152	1.32214758
H	4.55251727	1.96007277	-1.50280615
H	3.91209153	0.56802001	-1.21055494
H	3.22797612	-1.29147572	-2.22638699
H	4.02967308	-1.70623388	-0.96454854
H	-0.55643133	-4.07374353	-0.77077534
H	-1.32282221	-3.57410027	0.46090239
H	-2.24789167	2.16654343	-0.49297990
H	-2.78757742	0.83719323	-1.11314523
H	1.98159367	1.79967656	-1.33942935
H	1.04837389	1.14473598	-0.31327625

H	2.16226067	-3.98844541	-0.90365455
H	1.43131170	-3.06960577	-1.90296256
H	1.03653748	-1.23768330	-3.18180343
H	1.89567290	-2.17986491	-4.09444613
H	3.20579428	-2.79510618	0.89010906
H	4.63267695	-3.41842398	0.77156633
H	1.49972453	-1.29774428	1.33200375
H	1.26349136	-2.57115780	0.47195166
H	-0.99514931	-0.24515969	-2.85145046
H	0.25869245	0.58127330	-2.41974533
H	0.25656315	0.51829487	1.67650012
H	1.76789813	1.04620190	1.71824479
H	-3.99989433	-2.40033928	-0.35096993
H	-2.80418573	-3.13608906	-1.01751726
H	-4.04246379	0.97782209	1.03256221
H	-3.51712547	0.50667603	2.36492439
H	-4.74135546	-1.06947036	1.50102359
H	-5.81202024	-2.17557310	1.24686896
H	-1.72804123	-2.89870048	2.64195145
H	-0.21353083	-2.64128643	2.19589766
H	-3.71807550	-3.13083196	4.14443892
H	-3.96804827	-2.93623144	2.62848634
H	-3.06766721	-1.20893668	-1.97575404
H	-3.34779798	-0.24756435	-3.17895093
H	-1.42621827	-0.75591121	1.85987540
H	-1.81028055	0.51597666	1.03000730
C	3.08603229	3.49260432	1.70478435
H	3.60082949	1.93888745	0.69096986
H	2.87060687	3.82266323	2.70451541
H	3.56594911	4.14729357	0.99631952
O	-0.92173395	3.40856251	-0.77323820
C	-0.59822636	4.34719956	0.14907748
H	-0.14387917	2.86850985	-0.99603029
H	-1.43529243	4.88438280	0.55493452
H	0.31767851	4.21999413	0.70224066

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r_dHa2_ch2oh_ch2oh W18			
O	4.22705397	-1.14185603	-1.42989627
O	1.51264372	-0.91234309	-1.05923168
O	-0.87490664	-2.08349150	-0.94552878
O	-1.96545689	0.10938872	-2.21384171
O	-4.32634631	-0.84769090	-3.08452706
O	2.10706068	-0.66359887	1.57558816
O	4.44941666	0.58452953	0.66913666
O	3.32162764	2.89334731	0.19453575
O	0.37316257	1.12380952	2.82010822
O	1.05157441	3.39032451	1.76708478
O	-0.26355178	3.45739032	-0.62931127
O	0.53589057	1.34712313	-2.26829979
O	2.18082260	3.47799506	-2.30660678
O	-1.35526262	-2.39003805	1.77117138
O	-2.16963325	-0.02726061	2.91321712
O	-3.95443854	0.68364079	1.17167037
O	-2.88596837	2.30450211	-0.71703558
O	-3.23082874	-3.47155604	0.01527170
O	-4.94713625	-1.48998952	-0.44325745
H	5.28629232	0.74075645	1.09887692
H	4.05162934	1.46772568	0.46878447
H	2.59252271	3.10616623	0.79177759
H	3.03294150	3.13335197	-0.69530597
H	-2.13090011	2.89135960	-0.62865539
H	-2.59236890	1.58625308	-1.29070660
H	-0.53615216	-2.71314301	2.16943248
H	-1.63575501	-1.61025595	2.27348360
H	2.99775836	-0.29542466	1.53962755
H	1.83276858	-0.72670237	0.64178442
H	0.27787378	4.01247805	-1.19173298

H	0.12796973	3.50610903	0.25673009
H	0.75418976	2.55400100	2.20814786
H	1.03044598	4.08342277	2.42132514
H	1.71092339	2.65536098	-2.53157352
H	2.61851358	3.79766486	-3.09012292
H	0.94650116	0.57049241	-1.85454855
H	0.15114606	1.87412652	-1.55431367
H	-0.52966749	0.77867681	2.83725315
H	0.94702526	0.44168933	2.44667041
H	0.77122517	-1.54315032	-1.13492040
H	2.33358846	-1.27933816	-1.40561984
H	-4.32157092	-0.01534522	0.61997979
H	-3.62443348	1.37260898	0.56807158
H	-2.73319952	-3.30329468	0.82559469
H	-2.56209130	-3.38966803	-0.66953872
H	-4.36615165	-2.25533936	-0.23776422
H	-5.83456831	-1.73005178	-0.18884259
H	-2.68811556	-0.17246085	-2.79428632
H	-1.22984523	0.47856540	-2.71107186
H	-4.57334202	-1.56409275	-3.66119639
H	-4.65224495	-1.06291182	-2.19824141
H	-2.85897756	0.26485734	2.26089422
H	-2.57027114	0.00682542	3.77796768
H	-1.33832087	-1.32182109	-1.32817323
H	-1.00485435	-2.05255179	0.01408199
C	5.01052008	-0.83464679	-2.48988969
H	4.39521163	-0.53828521	-0.68785156
H	4.80203987	-1.39763053	-3.38046848
H	5.44142820	0.15169761	-2.53602778
O	1.22900203	-2.97324207	2.62755312
C	1.85746035	-4.06075620	2.11994802
H	1.65599395	-2.15420749	2.32043208
H	1.50527509	-5.00067868	2.50280536
H	2.86824383	-3.94248144	1.76732785

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	ts1_dHa2_ch2oh_ch2oh W18		
O	-0.02091326	0.25709051	0.07667393
O	0.01135849	0.12202409	2.85314992
O	2.45514870	0.00041937	3.91610170
O	1.47873527	-0.94126420	6.29048130
O	3.75854844	-2.06785317	7.17596789
O	-0.41697364	2.79132859	2.53706234
O	-3.02663269	2.65835865	1.90536359
O	-3.85998940	2.35965211	4.42163199
O	-0.03287776	4.43185665	4.72539362
O	-2.16224139	3.87363467	6.11253378
O	-1.60615372	1.39705260	7.12401227
O	-1.11779078	-0.63231384	5.25282810
O	-3.71367087	-0.11281232	5.82448627
O	3.45015741	2.51235963	3.37599805
O	2.66683632	4.14405355	5.43482379
O	3.13307279	2.45429094	7.34707976
O	0.99699267	1.03176978	8.20885697
O	5.25519727	0.47339285	4.14001339
O	5.06470189	0.38177612	6.79825820
H	-3.59256278	3.28928827	1.47031639
H	-3.40263837	2.50418424	2.79676561
H	-3.34565415	2.93336139	5.00163184
H	-3.91094574	1.49888010	4.85249447
H	0.07560630	1.26231368	8.06093078
H	1.15479776	0.27119839	7.63631101
H	3.05833613	2.71158871	2.51993653
H	3.21131477	3.21825098	3.99572893
H	-1.33575686	2.88324713	2.22609945
H	-0.31250255	1.84973281	2.76782332
H	-2.45879088	0.96823200	7.21496830
H	-1.78895071	2.31117987	6.85766734

H	-1.33927919	4.14490928	5.63599354
H	-2.46978330	4.62451289	6.61248678
H	-2.89849195	-0.53934061	5.50974349
H	-4.39755721	-0.77439132	5.87309689
H	-0.84912209	-0.43526309	4.34292949
H	-1.03793029	0.18889883	5.75688630
H	0.87527286	4.34626301	5.04265338
H	-0.11299479	3.88818526	3.92900948
H	0.94173774	-0.00746116	3.12372998
H	-0.04271866	-0.07546539	1.90942858
H	3.77937264	1.75411361	7.20938965
H	2.34121821	2.03836712	7.73441856
H	4.96505201	1.32787356	3.80188732
H	4.52709360	-0.10867510	3.90223214
H	5.22771560	0.45155859	5.83281946
H	5.89118724	0.55429727	7.24214004
H	2.09905231	-1.61515142	6.60309674
H	0.63195121	-1.31811473	6.03410035
H	4.31848837	-2.77830453	6.87843958
H	4.27262255	-1.24980050	7.11637228
H	2.84302677	3.51272088	6.18006053
H	3.09516019	4.96608504	5.65897302
H	2.19046601	-0.24141506	4.81825369
H	2.68557935	0.94019502	3.89670002
C	-1.23317912	0.51249972	-0.39023943
H	0.69809121	1.04937745	-0.02655536
H	-1.44002279	0.30390456	-1.42871188
H	-1.95084514	1.01010860	0.24553155
O	1.76227371	2.85596350	1.09200939
C	1.50826722	2.35751849	-0.13648510
H	0.92002788	2.99408932	1.57790349
H	2.40677643	2.14245297	-0.69549321
H	0.69705179	2.83547074	-0.68376058

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	ts_dHal_ch2oh_ch2oh W18		
O	3.82568075	-1.80108450	0.01861660
O	1.33269900	-0.76270294	-0.65976242
O	-1.03253575	-1.97556143	-0.68011799
O	-2.15971559	0.09641664	-2.08186272
O	-4.44436226	-1.14566698	-2.78479543
O	1.84067290	-0.07599172	2.04675493
O	4.31826528	0.71386471	0.96184284
O	3.10029307	2.90064371	0.18637177
O	0.13481254	1.65041977	3.22244338
O	0.84828383	3.64486373	1.73418158
O	-0.47804229	3.47927078	-0.64540399
O	0.36228144	1.30442338	-2.17622041
O	1.97776843	3.44976602	-2.33456653
O	-1.12865597	-2.20835292	2.02753785
O	-2.16740802	0.05225586	3.22613484
O	-3.94905444	0.58654758	1.40613857
O	-3.07532412	2.25483285	-0.55291210
O	-3.08980266	-3.56342780	0.49541617
O	-4.90468893	-1.69384694	-0.07790502
H	5.17117140	0.97765340	1.29599037
H	3.89440403	1.52237085	0.58466522
H	2.37961788	3.16374542	0.77325070
H	2.82085875	3.11661370	-0.71226405
H	-2.33597836	2.86670999	-0.51930770
H	-2.80174253	1.55463406	-1.15807311
H	-0.22626741	-2.46750745	2.24492198
H	-1.38171992	-1.45023779	2.57431303
H	2.72997329	0.27048193	1.94399764
H	1.54260825	-0.27654545	1.14899563
H	0.03212254	4.02461785	-1.24488738
H	-0.07187454	3.58964224	0.22946052
H	0.51233762	2.92519754	2.32976080

H	0.87531860	4.44725760	2.24842956
H	1.50995216	2.61625759	-2.52031567
H	2.43729313	3.71830171	-3.12472898
H	0.81236557	0.58717154	-1.70148302
H	-0.03414102	1.86953390	-1.49808916
H	-0.73506339	1.23270609	3.24040726
H	0.74771874	0.97498066	2.88699959
H	0.56380650	-1.36001174	-0.74102245
H	2.13805149	-1.27994105	-0.74714103
H	-4.29661073	-0.14168810	0.88103124
H	-3.67655133	1.28201237	0.78207153
H	-2.57550315	-3.32925896	1.27630744
H	-2.46311417	-3.42972306	-0.22169148
H	-4.29863450	-2.42048278	0.18393643
H	-5.78033165	-1.93350903	0.21485636
H	-2.85896961	-0.27295601	-2.63957157
H	-1.41546917	0.42199269	-2.59631460
H	-4.65006743	-1.91466162	-3.30738929
H	-4.69289340	-1.34336268	-1.87013443
H	-2.85563752	0.26474420	2.54573533
H	-2.61475151	0.00217571	4.06679395
H	-1.51964051	-1.25532319	-1.11066129
H	-1.13078320	-1.87663926	0.27968653
C	3.70336344	-2.70250661	1.02363276
H	4.06337826	-0.91757259	0.34920133
H	3.75305887	-3.72034430	0.66309400
H	4.26910651	-2.48455878	1.92594537
O	1.59756147	-3.03927508	2.48175054
C	1.85955406	-2.74418712	3.73684235
H	2.37130814	-2.76326091	1.76964075
H	2.18100712	-3.53581671	4.39688601
H	1.86592205	-1.70840954	4.03848809

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O	-3.16265646	2.35955714	-1.39892952
O	-1.20966436	0.44117478	-1.48684827
O	1.33537358	1.24722069	-1.36974426
O	2.07376446	-1.34241949	-1.89772056
O	4.64065711	-0.92579291	-2.60704218
O	-1.94660424	0.88041749	1.12332543
O	-4.56076027	0.54601998	0.29645826
O	-3.82419622	-1.99962592	0.32305107
O	-0.79698845	-0.46948731	3.19088926
O	-1.91641191	-2.65720453	2.34084578
O	-0.45658333	-3.65544295	0.25753884
O	-0.60733961	-2.13904706	-2.08382372
O	-2.76133079	-3.71441305	-1.65967290
O	1.43049316	2.47458365	1.08877529
O	1.79928411	0.58009552	3.07833938
O	3.48525525	-0.92315387	1.78574514
O	2.33691963	-2.94732323	0.37798530
O	3.67603095	2.70206729	-0.58160337
O	5.05172343	0.44803472	-0.20969688
H	-5.41797728	0.61766925	0.70689480
H	-4.36944573	-0.41286595	0.19722603
H	-3.23154894	-2.19955689	1.05780042
H	-3.57006173	-2.58255321	-0.40295293
H	1.48642140	-3.37803038	0.49003467
H	2.27483064	-2.46574880	-0.45612960
H	0.58928573	2.95370942	1.08309316
H	1.47535383	1.92410455	1.88373132
H	-2.90767172	0.80716843	1.08932037
H	-1.63426464	0.52771356	0.27314553
H	-1.04498698	-4.27589704	-0.17313605
H	-0.93213572	-3.33964657	1.04266345
H	-1.43507756	-1.88066591	2.72155381
H	-2.18251536	-3.20948113	3.07109407

H	-2.06840566	-3.17238314	-2.07537701
H	-3.25118200	-4.15102635	-2.35045662
H	-0.92601584	-1.22925806	-1.96601297
H	-0.41886725	-2.47323171	-1.19566017
H	0.13895360	-0.23645068	3.23224477
H	-1.18972491	0.12507783	2.53583786
H	-0.32744884	0.85256755	-1.55953139
H	-1.87088224	1.10592426	-1.72333671
H	4.03268522	-0.51795141	1.10540852
H	3.08398298	-1.71839004	1.39438853
H	3.08307100	2.87281385	0.16032713
H	3.07160738	2.44157001	-1.28213409
H	4.61154510	1.32065044	-0.30457631
H	5.93553199	0.60720275	0.11186212
H	2.89234097	-1.33562672	-2.41465921
H	1.33577080	-1.70808808	-2.39532855
H	5.06352498	-0.46417855	-3.32456183
H	4.88125338	-0.47011587	-1.78727850
H	2.45105257	0.00492155	2.60341371
H	2.18743130	0.80402228	3.92010051
H	1.68953347	0.34922777	-1.47118840
H	1.36626779	1.48725871	-0.43134348
C	-2.92810886	3.70082349	-1.00758709
H	-3.79518212	1.90797161	-0.83244069
H	-3.15168257	4.34022174	-1.85955689
H	-3.58797765	3.98172535	-0.18933659
C	-1.17234993	3.44666954	0.68794865
O	-1.48761636	3.92682926	-0.59849647
H	-1.52817092	2.55517505	0.82590959
H	-1.29365452	4.99583013	-0.58348568
H	-0.83243886	3.48086018	-1.34945186

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p\_dHa2\_ch2oh\_ch2oh W18

O	-1.85460738	-2.08955643	-4.03074073
O	-0.68542389	-1.21189580	-1.66111313
O	1.79765422	-1.29095532	-0.71118355
O	0.88471707	-2.29374055	1.68009197
O	3.11335346	-3.45684494	2.64348240
O	-0.95620343	1.47638866	-2.06081308
O	-3.66171467	1.35251973	-2.58325593
O	-4.46522384	0.98798857	-0.07741242
O	-0.63616353	2.93167869	0.28318345
O	-2.78097195	2.43437017	1.64515089
O	-2.27246236	-0.02699698	2.71053441
O	-1.74200248	-1.96281924	0.76708098
O	-4.35262244	-1.50279961	1.27803228
O	2.80255830	1.26551422	-0.86513512
O	1.96422748	2.74128847	1.29573830
O	2.48279319	1.01577706	3.16707908
O	0.32636261	-0.50700124	3.7725899
O	4.59828426	-0.75500016	-0.22335568
O	4.41436842	-0.99869943	2.42137970
H	-4.21161936	2.03772994	-2.95276858
H	-3.99785791	1.18322784	-1.67657410
H	-3.95276533	1.54137824	0.52528043
H	-4.53700820	0.11945874	0.33490628
H	-0.59167840	-0.25877227	3.63907575
H	0.50791798	-1.18463388	3.11499819
H	2.43904551	1.60720890	-1.70013923
H	2.56739196	1.88854134	-0.16254966
H	-1.87653709	1.60650040	-2.33212648
H	-0.87558446	0.52448484	-1.87881181
H	-3.13179401	-0.44717419	2.77014977
H	-2.43643042	0.8888911	2.43684695
H	-1.95117296	2.67051056	1.15674023
H	-3.06490932	3.20722475	2.12522601
H	-3.51522465	-1.90223358	0.98443916

H	-5.01407664	-2.18724745	1.31769134
H	-1.45209090	-1.70757302	-0.12329570
H	-1.67807656	-1.17547118	1.32509315
H	0.24885764	2.84825709	0.66167000
H	-0.66170536	2.44361394	-0.55218609
H	0.26521856	-1.34860924	-1.47576764
H	-0.93267123	-1.66599347	-2.47567291
H	3.13165405	0.33496986	2.96045480
H	1.68647884	0.55554145	3.48751711
H	4.25285554	0.10340251	-0.50223294
H	3.93663491	-1.36827735	-0.55326061
H	4.55545134	-0.87803007	1.45655317
H	5.25032433	-0.84281837	2.85348517
H	1.50280658	-2.96572693	2.00297645
H	0.02932454	-2.67017618	1.45397738
H	3.68619631	-4.15490646	2.34138794
H	3.63073658	-2.63808728	2.64714167
H	2.15377851	2.10094510	2.02916694
H	2.34349445	3.57894573	1.54773168
H	1.55304887	-1.58193692	0.18185305
H	2.02964400	-0.34981916	-0.66498779
C	-2.78651255	-1.37419087	-4.29813819
H	1.45889042	-0.00029680	-3.88206819
H	-3.38832710	-1.56332844	-5.19401098
H	-3.06824255	-0.52144882	-3.67438015
O	1.50705971	1.94363608	-3.15873517
C	1.70647647	1.01262612	-4.19757142
H	0.58201051	1.91077346	-2.87617842
H	2.75497277	1.04430730	-4.47133888
H	1.11183588	1.26604893	-5.07326851

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r_dHa1_ch2oh_ch2oh W18			
O	4.27148311	-1.23557516	-1.42101928
O	1.56111230	-1.03504181	-1.08595635
O	-0.82405413	-2.22267388	-0.95771200
O	-1.89032176	-0.09819051	-2.35557844
O	-4.23207121	-1.09753965	-3.23115744
O	2.09816772	-0.58310938	1.53458446
O	4.45415877	0.60904250	0.59517788
O	3.31414341	2.88146975	-0.01606669
O	0.34469295	1.24252657	2.65988643
O	1.01624992	3.46450583	1.49659884
O	-0.24584817	3.36053775	-0.93209731
O	0.59668807	1.15672410	-2.42395483
O	2.20666416	3.31156363	-2.56400801
O	-1.35565064	-2.33493825	1.76726386
O	-2.20710412	0.10083568	2.70881271
O	-3.97473200	0.70484039	0.91502361
O	-2.85889149	2.19775065	-1.04526939
O	-3.20859261	-3.52275886	0.04603844
O	-4.91984362	-1.57796446	-0.57020296
H	5.27680582	0.80421560	1.03623422
H	4.05080995	1.47476635	0.33803193
H	2.57673598	3.12607567	0.55768723
H	3.03710997	3.06734798	-0.92247714
H	-2.10504982	2.78796390	-0.96701509
H	-2.54681805	1.44159752	-1.55700716
H	-0.56546623	-2.59586208	2.25750635
H	-1.66742053	-1.51152003	2.17383371
H	2.99429903	-0.23072564	1.47561336
H	1.84244174	-0.74977785	0.60856356
H	0.30980660	3.87440289	-1.51977269
H	0.12221488	3.47405655	-0.04243606
H	0.71933388	2.65504845	1.98348281
H	0.97847153	4.19767936	2.10472305
H	1.76178490	2.46590126	-2.75029417
H	2.67228542	3.58434602	-3.34926088



H	1.00760928	0.40620305	-1.96488751
H	0.19944014	1.71839987	-1.74447737
H	-0.55860167	0.89799358	2.65194726
H	0.92559661	0.56429840	2.28822890
H	0.82832174	-1.67532565	-1.15241913
H	2.39335287	-1.40661650	-1.40031885
H	-4.32813045	-0.03062942	0.40308844
H	-3.63378078	1.35406734	0.27412347
H	-2.72586735	-3.31525279	0.85577067
H	-2.52604511	-3.48343177	-0.62901713
H	-4.34115976	-2.32588326	-0.30414110
H	-5.81238957	-1.80756675	-0.32415082
H	-2.59721312	-0.41085166	-2.93946871
H	-1.14370438	0.25059301	-2.85169501
H	-4.47172577	-1.84311061	-3.77286687
H	-4.58146086	-1.25941664	-2.34266008
H	-2.88919517	0.35671626	2.03303683
H	-2.62296348	0.17018837	3.56430912
H	-1.27881557	-1.48250218	-1.39030031
H	-0.96361234	-2.13241462	-0.00338260
C	5.24348551	-2.17799250	-1.43011605
H	4.43093959	-0.57028480	-0.73208678
H	5.16448062	-2.89061050	-2.23022987
H	6.20227219	-1.91974505	-1.01172106
O	1.08791999	-2.52136323	3.10956462
C	1.07094882	-2.09670856	4.39616108
H	1.58415309	-1.89533035	2.55494267
H	0.48287636	-2.70406628	5.05909899
H	1.23807541	-1.04966898	4.58820378

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ts0_dHa2_ch2oh_ch2oh W18			
O	3.81909787	-2.32219818	-1.01765847
O	1.38080995	-0.94924059	-1.22672046
O	-1.04401947	-1.96235251	-0.89831453
O	-2.16468622	0.23329118	-2.10243812
O	-4.51986520	-0.81991043	-2.86516560
O	2.23252460	-0.64607973	1.34775157
O	4.38790601	0.93980105	1.05897342
O	3.16636652	3.18898363	0.33971418
O	0.46560706	0.96240161	2.83999272
O	0.88506321	3.38172877	1.97912195
O	-0.41948123	3.40030370	-0.42279695
O	0.38364434	1.42029491	-2.23039735
O	1.89850705	3.66709795	-2.16096702
O	-1.28482025	-2.51333346	1.79461555
O	-2.05389143	-0.21820064	3.07326215
O	-3.90353425	0.54203311	1.42699003
O	-3.04661290	2.30703933	-0.43641835
O	-3.24268904	-3.54808277	0.07627821
O	-4.99625114	-1.56356894	-0.21438148
H	5.03479435	1.16160636	1.72259934
H	4.00226454	1.78415539	0.74245954
H	2.42385565	3.33553515	0.93788517
H	2.84901621	3.37541348	-0.55125354
H	-2.28003194	2.88130262	-0.35791536
H	-2.79216850	1.63868780	-1.08416973
H	-0.41923244	-2.81892707	2.09307922
H	-1.54611733	-1.77595161	2.36670680
H	3.04105320	-0.10158249	1.35092991
H	1.89805571	-0.65615598	0.43357648
H	0.09932379	3.98482984	-0.97794525
H	-0.03552589	3.45756622	0.46544137
H	0.70051233	2.48750514	2.35818177
H	0.78528735	4.02141999	2.67858278
H	1.49372384	2.82586461	-2.43273209
H	2.28954174	4.07253147	-2.92942986
H	0.83973223	0.61903728	-1.93252916

H	0.03212490	1.85921968	-1.44378060
H	-0.42028625	0.58126824	2.90654652
H	1.02890819	0.34168680	2.36133083
H	0.55092226	-1.46866145	-1.18531143
H	2.09558039	-1.52303570	-1.51712700
H	-4.30689005	-0.13211272	0.87003546
H	-3.63537494	1.27113255	0.83867535
H	-2.71329530	-3.42713727	0.87384094
H	-2.61183361	-3.37836981	-0.62842239
H	-4.41031556	-2.33659952	-0.06100979
H	-5.87255510	-1.80778532	0.07263082
H	-2.89602519	-0.06807832	-2.66129825
H	-1.44303244	0.59949923	-2.62156156
H	-4.78569633	-1.51951297	-3.45392342
H	-4.79099732	-1.07354550	-1.97092346
H	-2.76784549	0.09372522	2.45712685
H	-2.41268845	-0.19112076	3.95633880
H	-1.53079476	-1.19012061	-1.22829774
H	-1.12083090	-1.98680613	0.06742889
C	4.85678461	-1.47766255	-1.29013270
H	3.65700034	-2.35824652	-0.07549186
H	5.09524466	-1.42762790	-2.33602823
H	5.02723489	-0.65171764	-0.62032728
O	1.40125652	-2.91782619	2.45200403
C	2.30412691	-3.91636858	2.32284318
H	1.78040526	-2.07260397	2.15080703
H	1.94516646	-4.88499011	2.61885838
H	3.34788899	-3.66508036	2.43129476

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O	3.15977380	2.37587393	1.45547328
O	1.21614033	0.41398001	1.29723434
O	-1.39347562	0.25072973	1.80058524
O	-1.13249220	-2.47760153	1.97721251
O	-3.37674498	-3.19908531	3.27630650
O	1.05122123	1.52038928	-1.18772328
O	3.84398703	1.55409913	-1.07268930
O	3.92311932	-1.01309336	-1.59374465
O	-0.05587818	-0.12031264	-3.11576338
O	1.78838703	-1.94022100	-3.17970410
O	1.31826952	-3.60099784	-1.06134326
O	1.59117803	-2.29733132	1.38987142
O	3.91534916	-3.11214878	0.28774967
O	-2.66999097	1.40045671	-0.38668408
O	-2.77364060	-0.34586825	-2.50082489
O	-3.53171779	-2.45803888	-1.20090222
O	-1.44276620	-3.97581874	-0.37900789
O	-4.26783486	0.63809325	1.76915088
O	-4.86505207	-1.91437692	1.29858197
H	4.54144119	1.96887647	-1.57338034
H	3.91983863	0.58120207	-1.22496696
H	3.23185401	-1.30731841	-2.20065717
H	4.03464180	-1.71141760	-0.93649347
H	-0.56252176	-4.04591931	-0.75636955
H	-1.32745085	-3.52817037	0.46799673
H	-2.17513021	2.20941775	-0.56644094
H	-2.73598829	0.89306495	-1.20981526
H	1.97082556	1.73320289	-1.38425548
H	1.08982696	1.02464429	-0.35016172
H	2.16622392	-4.00441306	-0.87240058
H	1.44183663	-3.08003390	-1.87043905
H	1.04752335	-1.28262245	-3.20382186
H	1.93302896	-2.24106199	-4.07272287
H	3.23367047	-2.82998114	0.92213285
H	4.66152050	-3.44440920	0.77833025
H	1.55486120	-1.32750640	1.38308817
H	1.29029350	-2.59105855	0.51854607

H	-0.99303040	-0.27371487	-2.93726190
H	0.26146921	0.52706909	-2.47126430
H	0.31131663	0.50227998	1.65427390
H	1.80207698	1.08119025	1.67429523
H	-3.99216888	-2.32339315	-0.36586132
H	-2.80032098	-3.07536863	-1.02268011
H	-3.98410209	1.06887819	0.95293191
H	-3.46198184	0.60991763	2.29094840
H	-4.71841596	-0.95680831	1.46090743
H	-5.80621645	-2.04986120	1.22268121
H	-1.73598979	-2.83553521	2.64517231
H	-0.21072683	-2.61723378	2.21490277
H	-3.73818387	-3.01064003	4.13686872
H	-3.97946232	-2.82264618	2.61841949
H	-3.06885147	-1.16513243	-2.02412491
H	-3.35708132	-0.22977289	-3.24616670
H	-1.39913379	-0.72020019	1.81450220
H	-1.75785171	0.53748693	0.95040708
C	2.75247405	3.67015408	1.39539040
H	3.51698340	2.09236654	0.59935571
H	2.49568428	4.10034511	2.34525216
H	3.12621720	4.28226885	0.59234486
O	-0.73420068	3.43810498	-0.53551392
C	-0.52052451	3.79675322	0.75606252
H	-0.03747425	2.82569574	-0.82955993
H	-1.18029568	4.56693132	1.11311986
H	-0.13629633	3.05171830	1.43155217

## 2.2.2 CH3O + CH3O

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C	2.87915135	3.42373952	-1.69967445
O	-0.66250208	1.08291059	-2.15160351
O	1.72674804	0.24739249	-1.33379937
O	0.92876809	-2.36192274	-1.46069519
O	3.27348180	-3.65310185	-1.75124350
O	-1.72828658	2.33282619	0.15737355
O	-4.35538929	2.36131314	-0.63923552
O	-5.12225026	-0.14116675	-0.01949249
O	-1.59630588	0.84990377	2.43153729
O	-3.54934329	-0.83930622	2.22157418
O	-2.52143474	-2.62207259	0.44494508
O	-1.68016690	-1.50738067	-1.97266177
O	-4.29489754	-2.24176843	-1.78365203
O	2.26857948	1.39811503	1.12128706
O	1.02594142	0.00273833	3.08990194
O	1.86761440	-2.35846041	2.39611204
O	0.06115789	-3.66859362	0.87926535
O	4.34277287	0.07652198	-0.17489401
O	4.15865663	-2.46396112	0.62035421
O	1.71857503	3.95516108	0.16933773
C	0.56019099	4.74035713	0.38697574
H	-5.04497151	2.97148495	-0.39708089
H	-4.69066700	1.46253121	-0.45968655
H	-4.65988313	-0.37696340	0.79345838
H	-4.94132848	-0.83904679	-0.65743618
H	-0.88157645	-3.47656625	0.89064871
H	0.37426641	-3.30542449	0.04255737
H	2.01575778	2.32281137	1.02380219
H	1.83598804	1.02782246	1.90658445
H	-2.66639752	2.44376743	-0.06211009
H	-1.33415391	1.91823349	-0.61857971
H	-3.27103804	-2.93805058	-0.06294920
H	-2.88171581	-2.07025858	1.15740053
H	-2.81013430	-0.18999532	2.35145952
H	-3.92902436	-1.02208756	3.07623690

H	-3.43804855	-1.96026246	-2.14313232
H	-4.81091824	-2.61186870	-2.49379355
H	-1.45279184	-0.57375839	-2.08561611
H	-1.77801965	-1.67255041	-1.02428608
H	-0.70631821	0.52924559	2.61577098
H	-1.56923260	1.41094255	1.63585768
H	0.28006018	0.90588827	-1.95199499
H	-0.70009885	1.72058775	-2.85908346
H	2.64567739	-2.42060828	1.83298693
H	1.17349906	-2.89031889	1.96441171
H	3.86988109	0.62082318	0.46770071
H	3.75580895	0.09324055	-0.93665429
H	4.31295805	-1.52832255	0.36814865
H	4.93915653	-2.77221569	1.07368301
H	1.62553487	-2.90468575	-1.85547307
H	0.13886017	-2.32793932	-2.00959190
H	3.98583736	-3.69588763	-2.38137673
H	3.64271062	-3.33497829	-0.91478092
H	1.33423831	-0.90672401	2.84175426
H	1.18752686	0.10650282	4.02382450
H	1.49453527	-0.69507849	-1.28563514
H	1.74511517	0.59984712	-0.43113048
H	0.67288614	5.11907065	1.39742330
O	1.59067023	3.39762679	-1.13541939
H	2.76908131	2.94470692	-2.66608532
H	3.22854486	4.44577870	-1.81926383
H	3.57975107	2.85637120	-1.09387326
H	-0.33303373	4.12984179	0.30911366
H	0.53587297	5.56569019	-0.31870837

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C	2.89329207	4.25403894	1.33281882
O	1.52779491	0.92399569	1.40468418
O	-0.99208847	0.30735516	2.09665729
O	-0.55820334	-2.38971164	1.98334936
O	-2.52223802	-3.02073697	3.71526859
O	1.47005163	1.86997539	-1.18748243
O	4.01808443	1.54173608	-2.04744320
O	3.86256001	-1.01530005	-2.80419999
O	-0.21968396	0.69223743	-2.96072940
O	1.20685277	-1.34934690	-3.75643682
O	1.09005334	-2.90117512	-1.50367699
O	1.98509607	-1.76861435	0.91655629
O	3.83391291	-2.92859021	-0.69388325
O	-2.47087293	1.94199368	0.43669207
O	-2.79729021	0.46390915	-1.84271041
O	-3.38690117	-1.72950904	-0.59749249
O	-1.41563789	-3.56041342	-0.39980585
O	-3.67541228	0.92629357	2.78944066
O	-4.32483746	-1.56956058	2.12561766
O	-0.40346067	3.88481278	0.11188748
C	0.05833353	3.91528749	-1.00503082
H	4.51604007	2.03918136	-2.68862514
H	4.04575359	0.60391460	-2.32392100
H	2.99701872	-1.14266559	-3.20895992
H	3.95057130	-1.67687048	-2.10906262
H	-0.62228098	-3.49215827	-0.94014491
H	-1.12651815	-3.29053166	0.48034671
H	-1.88467561	2.70061719	0.34120934
H	-2.63942018	1.57032112	-0.44183838
H	2.38110472	1.82231047	-1.52476677
H	1.48186622	1.48321592	-0.29665373
H	1.93467861	-3.35401383	-1.46137280
H	1.07170443	-2.42822558	-2.34890582
H	0.62784750	-0.58190835	-3.52817053
H	1.00048478	-1.61771942	-4.64723243
H	3.39669743	-2.50919598	0.06647423

H	4.58424994	-3.42076280	-0.37383472
H	2.01666351	-0.82101663	1.11218647
H	1.46845654	-1.87881787	0.10773101
H	-1.09083804	0.54900276	-2.57010022
H	0.34862692	1.10675743	-2.28977489
H	0.62975322	0.76138276	1.75015729
H	1.81350930	1.76321358	1.79136651
H	-3.72262727	-1.70329798	0.30457843
H	-2.71029312	-2.43233669	-0.62781664
H	-3.58499427	1.47401089	2.00206352
H	-2.76111642	0.77050205	3.04639571
H	-4.19211705	-0.62902046	2.37417073
H	-5.25836308	-1.75512015	2.18833200
H	-0.98712756	-2.74560795	2.77403445
H	0.40059058	-2.42749728	2.04119390
H	-2.69671557	-2.83351178	4.63254488
H	-3.20970524	-2.58002122	3.19563976
H	-3.02023093	-0.38715983	-1.38123790
H	-3.47764467	0.60755295	-2.49541689
H	-0.96296378	-0.65499991	1.97633766
H	-1.48040833	0.70511720	1.36312976
H	-0.46215983	3.46941138	-1.85304550
O	1.81649284	3.60938358	1.97732818
H	3.78768997	4.04009722	1.90595966
H	3.03379498	3.88019288	0.31946507
H	2.74984885	5.33264592	1.30609043
H	0.99668134	3.83191984	1.52833943
H	0.99333561	4.43133886	-1.22047949

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r\_dHa1\_ch3o\_ch3o W18

C	2.20704140	2.29384518	3.80346700
O	1.32623781	-0.35558360	1.89794072
O	-1.34614816	-0.37467826	1.86205268
O	-1.38211775	-2.68971383	0.40775003
O	-3.80281257	-3.65103716	1.08667407
O	2.07737881	1.79412410	0.31319790
O	4.65279572	1.16340525	-0.28063280
O	4.32333353	-0.61321427	-2.25493864
O	0.73703805	1.96084807	-2.06975667
O	1.99510983	0.26841262	-3.60599867
O	1.05371554	-2.09978906	-2.62445628
O	1.40046150	-2.49230530	0.13179230
O	3.44166632	-3.22177100	-1.50484501
O	-2.22899184	2.06556872	0.89703277
O	-2.07955141	1.88519597	-1.81241545
O	-3.34558207	-0.36124309	-2.05500362
O	-1.72448708	-2.48918661	-2.36988779
O	-4.10889155	0.38844716	2.12865515
O	-4.92667674	-1.24746326	0.19417635
O	-0.29828977	3.84187921	1.99942269
C	0.52458826	4.45650251	1.09208960
H	5.39223158	1.73048809	-0.47562035
H	4.60810217	0.49066317	-0.98806275
H	3.58377364	-0.29937692	-2.78787431
H	4.12580580	-1.52225761	-2.00462972
H	-0.81865954	-2.40804523	-2.68404016
H	-1.63842250	-2.66712763	-1.42556272
H	-1.66703906	2.74798891	1.27864842
H	-2.19682489	2.14907849	-0.06917168
H	3.01525814	1.65677932	0.09735075
H	1.80736632	1.02265591	0.83300771
H	1.78397472	-2.71755834	-2.69671291
H	1.33195853	-1.28601638	-3.07139843
H	1.50813159	0.94549385	-3.07426237
H	2.00073966	0.55871299	-4.51363115
H	2.87615513	-3.11164205	-0.72235306
H	3.99975191	-3.98140965	-1.36639216

H	1.52357861	-1.77881966	0.77544194
H	1.13081893	-2.08775820	-0.70364323
H	-0.21808837	1.87628448	-1.96388361
H	1.15413145	1.91720088	-1.19308619
H	0.35703417	-0.34256525	2.02391746
H	1.73124914	-0.16044834	2.74849377
H	-3.90503007	-0.66352214	-1.33189622
H	-2.77443849	-1.11456035	-2.29717300
H	-3.72210918	1.18303140	1.74223104
H	-3.34358795	-0.07157403	2.48480756
H	-4.71194979	-0.61023690	0.90950978
H	-5.86257805	-1.18210964	0.02210255
H	-2.05903469	-3.27565624	0.77522760
H	-0.49381165	-3.03607417	0.53730975
H	-4.22897517	-3.92391760	1.89327461
H	-4.28128810	-2.87884774	0.75226424
H	-2.55583250	1.01980092	-1.92326841
H	-2.47992396	2.49802607	-2.42366675
H	-1.45195417	-1.14175645	1.27553855
H	-1.57144195	0.42608947	1.36808093
H	-0.01456572	4.78875615	0.20526377
O	2.30859244	0.98642352	4.21563123
H	2.59262341	2.40544934	2.78950420
H	1.13562510	2.51730047	3.73905819
H	2.67611082	2.98696592	4.49819106
H	1.22299884	3.66596252	0.77477157
H	1.09796021	5.26418530	1.54455166

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C	-3.03002364	2.95186743	2.36195524
O	0.06682447	0.16794442	3.05179425
O	-2.02106568	-0.05332546	1.41907664
O	-1.41597576	-2.67372214	0.92747252
O	-3.80139103	-3.69843868	0.21229710
O	1.79286819	1.84147477	1.56725630
O	4.09222299	1.31653276	2.95746969
O	4.90099086	-0.97472921	1.80834581
O	2.21924376	1.10504619	-1.01666851
O	3.98142477	-0.79446806	-0.85948001
O	2.41140545	-2.85514770	-0.02460904
O	0.98284206	-2.36392523	2.32583989
O	3.50620863	-3.35534203	2.57955591
O	-1.78761944	1.77431422	-0.65192684
O	-0.13093665	0.77107412	-2.56181837
O	-1.23741400	-1.55858134	-2.87411212
O	0.00915447	-3.42861652	-1.38346742
O	-4.18999472	0.40371040	-0.40823509
O	-3.93442795	-1.82183816	-1.85347731
O	-1.09874594	4.21917807	0.58422020
C	0.22441605	4.55910624	0.77088854
H	4.84326995	1.87989118	3.11540940
H	4.43206778	0.47498718	2.59832839
H	4.67385817	-0.90821385	0.87344446
H	4.51364017	-1.79371510	2.13399837
H	0.92570682	-3.35381840	-1.10034767
H	-0.50700047	-3.25495457	-0.58758281
H	-1.51320015	2.62922197	-0.29880832
H	-1.19221289	1.53860573	-1.38052011
H	2.63710676	1.76609316	2.03962309
H	1.17078758	1.30217960	2.06938964
H	2.97187060	-3.39369868	0.53728047
H	2.98367780	-2.18094812	-0.42355299
H	3.33416882	-0.05063800	-0.96431706
H	4.57169506	-0.77446937	-1.60727814
H	2.59882661	-3.07655458	2.78339324
H	3.78505259	-3.97825080	3.24424694
H	0.77662350	-1.48155678	2.66474519

H	1.33336022	-2.26094158	1.43004593
H	1.40415446	0.94401470	-1.50547441
H	1.99468752	1.39610696	-0.11520348
H	-0.78559805	0.18457212	2.56927098
H	-0.06860445	0.56128122	3.90948287
H	-2.14566900	-1.66950615	-2.57515534
H	-0.72009323	-2.26909078	-2.45138711
H	-3.52963567	1.04441503	-0.70292754
H	-3.85547626	0.13841872	0.45328551
H	-4.09519331	-0.97704312	-1.38044404
H	-4.57736518	-1.88552054	-2.55508502
H	-2.22164351	-3.20927523	0.94702407
H	-0.81316181	-2.90065135	1.64273333
H	-4.66228432	-3.83176325	0.59622384
H	-3.91169597	-3.12836763	-0.56236928
H	-0.53729175	-0.12480720	-2.69259102
H	-0.01133830	1.15014617	-3.42851714
H	-1.82674301	-0.96144552	1.13307008
H	-1.76311552	0.55131983	0.70632092
H	0.68137205	4.69522870	-0.21245667
O	-1.65932705	2.84255472	2.34347054
H	-3.36698669	2.14855289	3.02521893
H	-3.36437551	3.90462263	2.76801337
H	-3.46694799	2.76552384	1.38300215
H	0.74091651	3.70825378	1.22332271
H	0.33741429	5.45419987	1.37761685

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	ts_dHa2_ch3o_ch3o W18		
C	3.18708975	3.36955675	0.82315248
O	1.21718398	0.44688295	1.30326808
O	-1.24020023	-0.12780603	2.13518022
O	-0.80666149	-2.82661010	2.09991685
O	-2.79915135	-3.54434401	3.76118864
O	0.99387362	1.39521705	-1.32500253
O	3.67336323	1.24981444	-1.96293448
O	3.64910898	-1.36431686	-2.50533655
O	-0.54007065	-0.03210049	-3.05142018
O	1.09592590	-1.97535521	-3.56409114
O	0.99250060	-3.52950568	-1.32972917
O	1.74614574	-2.26692071	1.04999604
O	3.73843100	-3.32802080	-0.44731705
O	-2.72096135	1.29054200	0.32554247
O	-3.10319861	-0.24507377	-1.90552117
O	-3.64402470	-2.43761319	-0.61382778
O	-1.56005609	-4.12938977	-0.26287752
O	-4.01580157	0.35588785	2.64933188
O	-4.59883726	-2.18411699	2.10116665
O	-1.10928803	3.65795362	0.62647387
C	0.09468586	4.01668306	0.20552379
H	4.08974443	1.68010716	-2.70424702
H	3.74960301	0.28718712	-2.12488547
H	2.81009335	-1.57143708	-2.93451379
H	3.78889965	-2.03053337	-1.82343486
H	-0.75207296	-4.10015053	-0.78341033
H	-1.30457966	-3.78537912	0.60145141
H	-2.21437180	2.10409668	0.24428749
H	-2.86337979	0.90692349	-0.55290138
H	1.90707541	1.39018289	-1.64576403
H	1.01989959	0.98258917	-0.45106398
H	1.85411598	-3.94629521	-1.27474627
H	0.97320037	-3.04769926	-2.17178507
H	0.43359169	-1.25187261	-3.41321830
H	0.98643164	-2.28428770	-4.45903316
H	3.23365900	-2.93989553	0.28735618
H	4.51270047	-3.75186037	-0.08898381
H	1.72314888	-1.30481968	1.15415275
H	1.27297612	-2.47631525	0.23265673

H	-1.42244284	-0.16954080	-2.68609020
H	-0.05653055	0.54573568	-2.43664954
H	0.33819129	0.32568778	1.71670132
H	1.59941090	1.24941383	1.66626204
H	-3.98243196	-2.38429105	0.28581473
H	-2.92466079	-3.09519001	-0.60253588
H	-3.89103611	0.85493740	1.83388367
H	-3.11959294	0.27000650	2.98683760
H	-4.47782982	-1.23131458	2.30523052
H	-5.53232531	-2.37270285	2.15474011
H	-1.25323403	-3.20230689	2.87174535
H	0.15062505	-2.87617680	2.17213128
H	-3.01828260	-3.36956242	4.67122506
H	-3.48820343	-3.13835569	3.21537099
H	-3.31268079	-1.08967835	-1.43053035
H	-3.80521299	-0.09877705	-2.53405445
H	-1.19786097	-1.09541613	2.06979111
H	-1.73096124	0.21322586	1.37268269
H	0.41786491	3.53464521	-0.71592178
O	2.11802300	3.14400418	1.68553812
H	4.06925257	3.09835774	1.40945344
H	3.16020855	2.73007800	-0.05477653
H	3.27209119	4.42099649	0.55674847
H	0.82551550	3.55311914	0.99920598
H	0.29496275	5.08687849	0.27932575

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C	1.59575017	1.83394799	4.29950434
O	1.42745393	-0.44975413	1.85412235
O	-1.23381047	-0.38845019	1.79902927
O	-1.35119853	-2.74692224	0.42026586
O	-3.79275582	-3.52540736	1.24802174
O	1.98857331	1.71472225	0.28914277
O	4.56453184	1.34411521	-0.38138398
O	4.29998469	-0.55274587	-2.25369580
O	0.70727873	1.88304158	-2.15679661
O	1.97067687	0.18336231	-3.67387760
O	1.06404613	-2.17993708	-2.64072542
O	1.44151368	-2.59903803	0.10966851
O	3.51538862	-3.20790154	-1.53513094
O	-1.92327440	2.08458142	0.82397734
O	-2.08640226	1.87200540	-1.90321223
O	-3.34566046	-0.38988051	-2.01747587
O	-1.72934440	-2.53113890	-2.34586959
O	-3.88170937	0.59930020	2.18761134
O	-4.83773655	-1.08550656	0.35440493
O	0.36153164	3.44688124	1.53013713
C	0.51417203	4.80788387	1.19399245
H	5.27530716	1.93315151	-0.61347785
H	4.54295704	0.63075048	-1.04925087
H	3.56359898	-0.29158943	-2.81862944
H	4.14283805	-1.46706083	-1.99418775
H	-0.82778741	-2.46468942	-2.67456490
H	-1.63151427	-2.72043804	-1.40494974
H	-1.18767524	2.65410307	1.09978872
H	-2.00612279	2.15458824	-0.13826051
H	2.93810059	1.72084603	0.07050489
H	1.83492502	0.90307542	0.80267096
H	1.80553355	-2.78321074	-2.71924120
H	1.32603800	-1.36490398	-3.09510255
H	1.47772634	0.86571409	-3.15492235
H	1.96731894	0.45106131	-4.58841104
H	2.93691057	-3.14057706	-0.75708395
H	4.10602433	-3.94405111	-1.40484467
H	1.58036065	-1.88512850	0.74970344
H	1.15241977	-2.19409911	-0.71899622
H	-0.25399022	1.83617411	-2.07858823



H	1.09090868	1.82512775	-1.26917277
H	0.45587406	-0.42328475	1.96566244
H	1.81344868	-0.26255929	2.71718908
H	-3.86444867	-0.65483406	-1.25094352
H	-2.78251374	-1.14961616	-2.25587413
H	-3.45741926	1.35998837	1.77291605
H	-3.13239214	0.08887311	2.50832286
H	-4.57186591	-0.41873025	1.02414876
H	-5.77552098	-0.98819053	0.20977532
H	-2.04342606	-3.28345486	0.83179919
H	-0.47478786	-3.11889203	0.55635240
H	-4.18812397	-3.76111325	2.08156493
H	-4.24103651	-2.72889813	0.92911448
H	-2.56675742	1.00568492	-1.97140330
H	-2.52645202	2.48267387	-2.48829224
H	-1.37365177	-1.16708019	1.23590455
H	-1.42245589	0.40993228	1.28225690
H	-0.27519685	5.36179940	1.68961718
O	2.10329287	0.74287251	4.31038432
H	1.04315178	2.21453258	3.43591163
H	1.03740122	2.91656466	1.07217910
H	1.67691361	2.49454850	5.16964977
H	0.43145456	4.96420517	0.11980766
H	1.47460240	5.19199875	1.53286066

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r Rc_ch3o_ch3o W18			
C	2.01171129	3.33099079	-2.75213430
O	-0.43486655	1.15605798	-2.04484375
O	1.91744597	0.20681573	-1.15166031
O	1.02342912	-2.35045037	-1.42532469
O	3.33922109	-3.69974847	-1.65199088
O	-1.61980645	2.38693268	0.15197197
O	-4.23713199	2.49463825	-0.59216247
O	-5.04690917	-0.01502297	-0.08792072
O	-1.53874447	0.87977943	2.42630324
O	-3.52517078	-0.78245118	2.17257221
O	-2.49053278	-2.53065309	0.35775091
O	-1.53973098	-1.39083194	-2.01668342
O	-4.17981932	-2.05173007	-1.90597641
O	2.47603774	1.36493680	1.28759780
O	1.05451178	-0.02054334	3.13611880
O	1.81166357	-2.40181409	2.44126753
O	0.03567077	-3.66527612	0.85893595
O	4.53619687	-0.07007176	0.04916122
O	4.17468854	-2.60706679	0.78840782
O	1.55133980	3.95698880	0.60812033
C	0.45307407	4.51956647	1.20117759
H	-4.92611552	3.11505109	-0.37665316
H	-4.59621151	1.59765382	-0.45310076
H	-4.60731602	-0.28061901	0.72798672
H	-4.84370522	-0.68550898	-0.74851849
H	-0.90115982	-3.44632042	0.83666765
H	0.38812289	-3.30935913	0.03484319
H	2.22695952	2.29071980	1.19761981
H	1.99429989	0.98647793	2.04096184
H	-2.55631446	2.52577894	-0.06629496
H	-1.22855184	1.96476846	-0.62576430
H	-3.23014300	-2.80809336	-0.18636680
H	-2.85946236	-1.99649768	1.07824933
H	-2.78043388	-0.14853577	2.32687097
H	-3.91917538	-0.98132034	3.01710016
H	-3.30761440	-1.78528979	-2.23947254
H	-4.68915781	-2.38912827	-2.63702764
H	-1.28930707	-0.46025323	-2.11316077
H	-1.66877576	-1.56283304	-1.07386574
H	-0.65637725	0.54113652	2.61636540
H	-1.49892030	1.42891204	1.62435182

H	0.45405931	0.86490518	-1.76626089
H	-0.28883043	1.82120209	-2.72354382
H	2.61524202	-2.50200484	1.92072700
H	1.11976013	-2.91335689	1.98120605
H	4.08605055	0.52010498	0.66558805
H	3.99748429	-0.00602290	-0.74361206
H	4.39154312	-1.67666562	0.56587262
H	4.91638592	-2.96918289	1.26645421
H	1.71446252	-2.90474751	-1.81362432
H	0.25753775	-2.26471187	-2.00248521
H	4.07561145	-3.78185521	-2.24973447
H	3.68773015	-3.41770216	-0.79433121
H	1.32942988	-0.94038904	2.88159079
H	1.16879709	0.05005628	4.08025541
H	1.66248273	-0.73166060	-1.14777599
H	1.96584946	0.51735415	-0.23560544
H	0.47301671	4.41207649	2.28553380
O	0.84103353	3.27861136	-3.47053584
H	2.37772513	2.33067339	-2.51902786
H	2.76933402	3.93985903	-3.24127315
H	1.75490803	3.79429177	-1.79111232
H	-0.39848015	3.92325025	0.82959279
H	0.30947590	5.55459628	0.89562169

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C	4.60225643	2.01348914	1.07266285
O	1.42181105	1.25453390	1.21940561
O	-1.08266975	0.82810322	2.03841101
O	-0.54601779	-1.86945994	2.07495431
O	-2.39265816	-2.87824490	3.75265617
O	1.06144710	2.27724650	-1.33846805
O	3.74020181	2.11415228	-2.08430944
O	3.82695869	-0.49033258	-2.63296585
O	-0.39160551	0.56978519	-2.91582603
O	1.29457880	-1.28038751	-3.56548631
O	1.33417608	-2.84893594	-1.34275231
O	1.98442778	-1.42112964	0.96115349
O	4.07643775	-2.33969395	-0.48549706
O	-2.88488791	1.75944311	0.14549062
O	-2.97226756	-0.00510394	-1.92490689
O	-3.43693952	-2.20162444	-0.61925340
O	-1.13701294	-3.53101856	-0.12800967
O	-3.96080379	0.75838402	2.50191328
O	-4.37153431	-1.83685553	2.08924991
O	-2.08530225	4.33481879	-0.66494727
C	-0.83138933	4.60606539	-0.18346685
H	4.15499210	2.59509644	-2.79474987
H	3.82529403	1.16098808	-2.29598602
H	2.99201428	-0.76850954	-3.02993814
H	4.02574571	-1.11703269	-1.92876284
H	-0.34552070	-3.49471972	-0.67229960
H	-0.92340020	-3.02319229	0.66363788
H	-2.72648926	2.66634431	-0.14246779
H	-2.97383472	1.20891801	-0.64950739
H	1.95434477	2.33393028	-1.70567566
H	1.17703322	1.90472851	-0.45292767
H	2.22901285	-3.18876153	-1.29501203
H	1.26328189	-2.37852911	-2.18872571
H	0.62191696	-0.58059441	-3.35696515
H	1.14614705	-1.56634268	-4.46247816
H	3.52074704	-1.98654388	0.23013918
H	4.85625665	-2.72777809	-0.09984326
H	1.85497283	-0.46071442	1.01873374
H	1.53658550	-1.72564127	0.15927271
H	-1.25382873	0.35065773	-2.54277407
H	0.04265532	1.22406214	-2.34391951
H	0.55228114	1.24604144	1.66360387

H	2.03825433	1.82399251	1.69110227
H	-3.78124288	-2.11710403	0.27608964
H	-2.64396393	-2.76419981	-0.55653213
H	-3.87192190	1.21460839	1.65475968
H	-3.08224483	0.83404280	2.88194866
H	-4.29679803	-0.87030225	2.24706578
H	-5.29058420	-2.07272331	2.18660588
H	-0.96439745	-2.29167858	2.84001056
H	0.41328943	-1.92267918	2.11898757
H	-2.62384202	-2.73457546	4.66510304
H	-3.15173738	-2.61023575	3.21419423
H	-3.14814956	-0.85692559	-1.44675344
H	-3.61837967	0.06054398	-2.62333228
H	-0.99448796	-0.13840785	2.00948232
H	-1.60970570	1.10050699	1.27306000
H	-0.14684020	3.98499011	-0.78145945
O	3.71913211	2.70087239	1.86544773
H	4.44897376	0.93568561	1.14194962
H	4.35874845	2.29250726	0.03711632
H	5.63572844	2.28897966	1.27445068
H	-0.71873814	4.27799197	0.85095571
H	-0.56065661	5.65290028	-0.30696115

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C	1.84973086	2.44470729	3.46952831
O	1.25945354	-0.63143220	1.90048190
O	-1.40334055	-0.75279660	1.78034079
O	-1.41768591	-3.03457904	0.28366254
O	-3.85968406	-3.87887627	1.03844242
O	2.04998037	1.49823244	0.28407333
O	4.63511338	0.86396632	-0.29481466
O	4.29734121	-0.84278051	-2.32929945
O	0.74757597	1.80747790	-2.08525035
O	1.97098969	0.10826068	-3.63940929
O	1.00538916	-2.24943830	-2.65601868
O	1.38011456	-2.74383038	0.08464218
O	3.38199025	-3.45089705	-1.61299723
O	-2.07643653	1.79093074	0.98504830
O	-2.05761454	1.76571659	-1.73443207
O	-3.32140629	-0.48046456	-1.98849580
O	-1.77405738	-2.63597196	-2.46137211
O	-4.05833999	0.17112470	2.20671920
O	-4.91353357	-1.40400163	0.23515458
O	-0.13721298	3.58123697	2.15752396
C	0.60582908	4.26958364	1.20092138
H	5.37111998	1.44089495	-0.47323790
H	4.59007507	0.21718814	-1.02584287
H	3.55889898	-0.50323595	-2.84784543
H	4.08486853	-1.75288755	-2.09597705
H	-0.86384624	-2.53811918	-2.75835524
H	-1.69459758	-2.90016446	-1.53687319
H	-1.42553852	2.36881704	1.39387932
H	-2.06680861	1.94377466	0.02708353
H	2.98780895	1.34704462	0.08025085
H	1.75733587	0.72620104	0.78869080
H	1.72201337	-2.87978375	-2.75270282
H	1.29129050	-1.43428561	-3.09574367
H	1.49632501	0.79114388	-3.10311222
H	1.96869006	0.39657599	-4.54767794
H	2.83437456	-3.35250380	-0.81651086
H	3.92959959	-4.22316645	-1.50625895
H	1.51553970	-2.06300189	0.75830551
H	1.10115321	-2.29828685	-0.72643214
H	-0.20857349	1.74094101	-1.97739926
H	1.16118041	1.71453798	-1.20941866
H	0.28585380	-0.67377986	1.97754408
H	1.57877351	-0.28738260	2.73809154

H	-3.88039959	-0.79943003	-1.27239266
H	-2.77483917	-1.23639867	-2.27616272
H	-3.66104270	0.97421217	1.85330972
H	-3.29339401	-0.33652863	2.49516546
H	-4.69435189	-0.78118385	0.96140962
H	-5.84766918	-1.32414172	0.05950867
H	-2.09851711	-3.60477939	0.66726675
H	-0.53045796	-3.37296722	0.43479937
H	-4.26780522	-4.14366248	1.85704474
H	-4.30439225	-3.07209133	0.74161291
H	-2.53541969	0.90241060	-1.85200791
H	-2.49146246	2.39906227	-2.30007562
H	-1.50197498	-1.50234957	1.17092838
H	-1.58825531	0.06820749	1.30328123
H	-0.13533877	4.70132309	0.52357362
O	1.61346845	1.26751604	4.02798127
H	2.51112537	2.41960710	2.60376305
H	0.82226866	2.75363311	2.99036756
H	2.04594616	3.25139398	4.17686564
H	1.22553512	3.58522396	0.62712047
H	1.18709364	5.07497699	1.64367791

## 2.2.3 CH3 + CH2OH

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i\_dHa\_ch3\_ch2oh W18

C	0.52096817	2.68549091	4.01312473
O	1.34389065	-0.23023234	2.40010151
O	-1.29165684	-0.15181479	2.28173806
O	-1.16179601	-2.44760830	0.82810220
O	-3.18564390	-3.83465363	-0.31091958
O	2.03173061	2.06870237	0.93081929
O	4.69825709	1.52022797	0.64729095
O	4.69234149	-0.40534224	-1.23833021
O	1.02603315	1.86933801	-1.61156082
O	2.51853741	0.21035819	-2.93103704
O	1.61965894	-2.21479247	-2.10345019
O	1.63792501	-2.40659436	0.69636063
O	3.91808016	-3.09872907	-0.61385040
O	-2.37412195	1.94243041	0.81443479
O	-1.79452977	1.74353703	-1.84282161
O	-2.93700780	-0.51549062	-2.47236704
O	-1.15169024	-2.52894193	-1.98865179
O	-4.28626171	0.10817217	1.58362760
O	-4.75808644	-1.48439571	-0.51509828
C	-0.16554004	4.63334350	0.72145325
O	-1.00087994	4.20664552	1.71439180
H	5.44872932	2.09025194	0.51193743
H	4.75915539	0.80148510	-0.00922640
H	4.01326967	-0.17470493	-1.88295571
H	4.55274713	-1.32843602	-1.00483436
H	-0.24342391	-2.56177455	-2.30793164
H	-1.06977172	-2.34110178	-1.04548057
H	-2.06196120	2.78911191	1.15628499
H	-2.18865052	1.93853532	-0.13884520
H	2.99499782	2.02801127	0.82074683
H	1.81082176	1.27209388	1.42793716
H	2.39870166	-2.77191956	-2.04565164
H	1.90428972	-1.38125636	-2.51226811
H	1.94256577	0.86749774	-2.46291303
H	2.64624640	0.52031621	-3.82316582
H	3.25370547	-3.00701508	0.08777209
H	4.50330401	-3.81388407	-0.38160234
H	1.65769261	-1.63771013	1.28452267
H	1.48004218	-2.08560259	-0.20150548
H	0.06566808	1.79596321	-1.64107234
H	1.31142995	1.97827432	-0.68848527

H	0.36543027	-0.16752433	2.47629894
H	1.70952043	-0.22537011	3.28090531
H	-3.64506086	-0.79815355	-1.88190527
H	-2.28915028	-1.23746503	-2.47451402
H	-3.79167375	0.89371038	1.30999809
H	-3.76298258	-0.27288320	2.28765373
H	-4.62047750	-0.92118922	0.27455343
H	-5.69847279	-1.52300279	-0.66930127
H	-1.83881023	-3.12940071	0.68774558
H	-0.29792914	-2.84172414	0.98583566
H	-2.74776265	-3.85554118	-1.16338692
H	-3.83941750	-3.12737329	-0.37143867
H	-2.22295973	0.89248823	-2.11203606
H	-2.08887121	2.40946741	-2.45897303
H	-1.38028053	-0.96769842	1.76334181
H	-1.57058376	0.58046569	1.71289297
H	-0.48719090	3.86031194	2.44904699
H	0.55717293	3.35339591	4.85518574
H	1.30862643	2.69471765	3.27899969
H	-0.24023007	1.92530724	3.97150788
H	-0.68406354	5.04364283	-0.12487294
H	0.79288735	4.15236922	0.63331525

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p\_dHa\_ch3\_ch2oh W18

C	0.24308504	2.66380997	4.22322143
O	1.35373275	-0.08565202	2.38274405
O	-1.27264092	-0.06016045	2.21875396
O	-1.12342261	-2.40963658	0.85382012
O	-3.17294467	-3.83682265	-0.17902915
O	1.98047683	2.08396849	0.71861427
O	4.65343407	1.59592183	0.44961239
O	4.69488931	-0.41517291	-1.33729796
O	1.00397392	1.79624528	-1.82349912
O	2.51733692	0.08921637	-3.06099892
O	1.62428877	-2.27781257	-2.06003976
O	1.67747571	-2.31833317	0.75306389
O	3.94054780	-3.06648463	-0.54742630
O	-2.27232128	1.99321557	0.66112099
O	-1.80560575	1.65806791	-2.01406053
O	-2.95126061	-0.63331134	-2.49990454
O	-1.14776153	-2.61426928	-1.94766483
O	-4.21503807	0.22500252	1.53191948
O	-4.73176215	-1.48572057	-0.45680462
C	-0.02932493	4.57280695	1.37210195
O	-1.23178784	4.48099903	1.36871211
H	5.39395062	2.17255607	0.28999098
H	4.73059293	0.84729692	-0.17168155
H	4.01614135	-0.22762006	-1.99612962
H	4.56137194	-1.32423343	-1.05046591
H	-0.24118453	-2.65400904	-2.27020241
H	-1.05803168	-2.39289177	-1.01221070
H	-2.01601179	2.88115634	0.94411464
H	-2.12691848	1.94594780	-0.29695290
H	2.94510948	2.05474771	0.61205525
H	1.77417776	1.34662856	1.30681603
H	2.40445358	-2.82910089	-1.97001595
H	1.90575400	-1.47480899	-2.52681888
H	1.93456341	0.76618502	-2.63206985
H	2.63326433	0.34057506	-3.97290922
H	3.28281940	-2.93575335	0.15478795
H	4.52893071	-3.76703348	-0.28122871
H	1.68709006	-1.53198298	1.31798391
H	1.50051297	-2.03016975	-0.15193562
H	0.04444075	1.70744496	-1.85838891
H	1.27989261	1.91158927	-0.89864948
H	0.37304132	-0.03850524	2.45319709
H	1.71547856	-0.01525509	3.26213922

H	-3.64608328	-0.88437807	-1.88003066
H	-2.29906551	-1.35103091	-2.47395642
H	-3.72143097	0.99151028	1.20747027
H	-3.67252364	-0.12182369	2.23985640
H	-4.57483414	-0.87628124	0.29480911
H	-5.67540122	-1.52735673	-0.58866175
H	-1.80180351	-3.09828997	0.76347900
H	-0.26075375	-2.79021517	1.04522770
H	-2.75361119	-3.90080903	-1.03848205
H	-3.82053686	-3.12535222	-0.25663579
H	-2.24000221	0.79417968	-2.22750064
H	-2.12691191	2.29551108	-2.64661755
H	-1.34976087	-0.88788949	1.71852240
H	-1.51917129	0.66309403	1.62320200
H	-0.18913645	3.63763335	4.42725953
H	0.62417208	2.24483975	5.14916837
H	1.05514818	2.76396077	3.51033392
H	-0.51913149	2.00924088	3.81530220
H	0.44798106	5.51901098	1.65069699
H	0.62478616	3.73841493	1.10745079

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r\_dHa\_ch3\_ch2oh W18

C	-0.03354012	2.00391151	4.62435779
O	1.30618540	0.13470294	2.26846251
O	-1.32200396	0.02587990	2.07689262
O	-1.09892939	-2.41545000	0.92133945
O	-3.21431256	-3.79490505	-0.01877149
O	1.82724696	2.16910996	0.48629924
O	4.48107112	1.88272318	0.18973586
O	4.63147458	-0.32356205	-1.33350339
O	0.93513606	1.63659679	-2.09552967
O	2.49806497	-0.13506209	-3.16476854
O	1.65073986	-2.41358897	-1.93657227
O	1.70659354	-2.24953933	0.87495379
O	4.01916881	-2.94886254	-0.36019736
O	-2.15503040	2.08180804	0.44491529
O	-1.85956598	1.58916041	-2.24151448
O	-2.95603862	-0.76021814	-2.51238658
O	-1.14363253	-2.71239511	-1.86105093
O	-4.19427180	0.45949711	1.46063345
O	-4.72101028	-1.41229516	-0.38653789
C	0.12387686	4.83833858	1.97448044
O	-0.12875184	3.87400190	1.06138281
H	5.17967260	2.48177032	-0.05416982
H	4.59852805	1.06682650	-0.33453045
H	3.97545101	-0.25054823	-2.03655821
H	4.54911027	-1.21109575	-0.96945115
H	-0.24003144	-2.79043309	-2.18273313
H	-1.04206736	-2.47121151	-0.93160320
H	-1.60289345	2.82938492	0.71024310
H	-2.07329948	1.99550142	-0.51698808
H	2.79235060	2.23363789	0.36733392
H	1.68930428	1.43824114	1.10918754
H	2.44391215	-2.93648290	-1.80352756
H	1.91774825	-1.64863712	-2.47062313
H	1.88960525	0.56151750	-2.81241141
H	2.61727280	0.02426317	-4.09675381
H	3.34374270	-2.81051387	0.32374551
H	4.64608953	-3.58933543	-0.03666159
H	1.69235451	-1.42334153	1.37865901
H	1.51279582	-2.03584640	-0.04711895
H	-0.02763065	1.59751278	-2.15206253
H	1.18263822	1.84035266	-1.18272765
H	0.32272097	0.13341330	2.30650898
H	1.61196129	0.36806994	3.14290887
H	-3.63920391	-0.96176863	-1.86237494
H	-2.29629630	-1.46761933	-2.43988958

H	-3.71074477	1.20887673	1.09029810
H	-3.61577221	0.13298250	2.15088603
H	-4.56094153	-0.73646631	0.30492414
H	-5.66512389	-1.46053177	-0.51332055
H	-1.79047524	-3.09507860	0.87724662
H	-0.24751911	-2.78576847	1.17058507
H	-2.81933473	-3.91183099	-0.88392191
H	-3.83523471	-3.06170175	-0.10975477
H	-2.28155173	0.70430367	-2.37859992
H	-2.21504495	2.17876852	-2.90135756
H	-1.36806570	-0.84137948	1.64411871
H	-1.54597655	0.69964198	1.41618723
H	0.67101434	3.35283834	0.85552159
H	0.28833631	2.00450757	5.65048016
H	0.24684309	2.81497402	3.97551901
H	-0.74759585	1.27543428	4.28322022
H	-0.70133406	5.49876864	2.16850448
H	1.14170290	5.17648851	2.07991501

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ts2\_dHa\_ch3\_ch2oh W18

C	-0.23260973	2.55808989	3.81049434
O	0.85489902	-0.46705588	2.35248458
O	-1.77761197	-0.43750581	2.22360985
O	-1.62987406	-2.73968051	0.78747310
O	-3.66912289	-4.12014375	-0.32942103
O	1.49751237	1.79533248	0.79530455
O	4.17330672	1.26090288	0.54192644
O	4.20283475	-0.67906749	-1.32887806
O	0.52845204	1.56322686	-1.74670919
O	2.03213605	-0.10412711	-3.03815326
O	1.13072882	-2.50827387	-2.15373357
O	1.16773601	-2.64924911	0.64947072
O	3.43886150	-3.36406587	-0.66094869
O	-2.77641290	1.65151647	0.71231215
O	-2.28531343	1.43999885	-1.96362999
O	-3.43983661	-0.82995273	-2.53859516
O	-1.64104054	-2.82835010	-2.02935341
O	-4.73480470	-0.12026200	1.52618671
O	-5.22917588	-1.75906756	-0.53206232
C	-0.53795680	4.43660767	0.95027495
O	-1.36197525	3.79529229	1.77349824
H	4.91817080	1.83754799	0.40367663
H	4.24435079	0.53759406	-0.10865384
H	3.52611599	-0.46191149	-1.98074066
H	4.06764126	-1.59981033	-1.08376099
H	-0.73364329	-2.86033520	-2.35114878
H	-1.55597188	-2.63518578	-1.08760680
H	-2.41015936	2.47531744	1.05806568
H	-2.61689575	1.64745661	-0.24516613
H	2.46160025	1.75614290	0.69527998
H	1.27876753	1.02909362	1.33794349
H	1.90882689	-3.06582907	-2.08824828
H	1.41565095	-1.68461915	-2.58197315
H	1.45160140	0.55847351	-2.58250244
H	2.15580735	0.18753584	-3.93696372
H	2.77846963	-3.25701401	0.04235729
H	4.02531266	-4.07419045	-0.41676280
H	1.18011309	-1.87505341	1.23063795
H	1.00168472	-2.33909773	-0.25068660
H	-0.43163228	1.48839101	-1.78708191
H	0.80271696	1.66847908	-0.81927100
H	-0.12473583	-0.42687551	2.43275891
H	1.22589005	-0.47338197	3.23080063
H	-4.13755625	-1.10021946	-1.93037055
H	-2.78803685	-1.54818956	-2.53005576
H	-4.23437914	0.65348886	1.23117031
H	-4.20116811	-0.49450345	2.22658109

H	-5.08142134	-1.17773856	0.24276074
H	-6.17144687	-1.79881450	-0.67403206
H	-2.30507712	-3.42477091	0.65569920
H	-0.76264983	-3.12648136	0.94337625
H	-3.24040895	-4.14637437	-1.18634134
H	-4.31599510	-3.40595675	-0.38378005
H	-2.72264120	0.58898542	-2.21614828
H	-2.59881656	2.10762524	-2.56829986
H	-1.85462487	-1.26197659	1.71695941
H	-2.03198530	0.28507612	1.62993382
H	-0.89500108	3.29447363	2.56134947
H	-0.34014970	3.28851676	4.59584152
H	0.73552085	2.45817236	3.34483843
H	-0.85399805	1.67773740	3.86461655
H	-0.58569055	5.51348693	0.94105028
H	0.25983201	3.88476209	0.48141661

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p_Rc_ch3_ch2oh W18			
C	-0.00038353	4.70371234	-1.27756746
O	-1.05513782	1.21487329	-2.17343902
O	1.51226413	1.18077204	-1.64920005
O	1.50267405	-1.51557308	-1.96044854
O	3.64916190	-3.09881816	-1.56773589
O	-1.99284157	2.04279946	0.31599379
O	-4.61774219	1.48180964	-0.01318469
O	-4.65006433	-1.20407069	0.15000091
O	-1.30623437	0.26090371	2.33574380
O	-2.75086683	-1.87597394	2.11713147
O	-1.51627310	-3.17794424	0.07317788
O	-1.29153702	-1.56974673	-2.21820272
O	-3.62216248	-2.92400327	-1.90200715
O	1.94437010	2.02640827	0.92629066
O	1.43620024	0.18005018	2.90378298
O	2.79294269	-1.89447364	2.08124453
O	1.28978289	-3.25420854	0.23219802
O	4.24475390	1.32714189	-0.46249638
O	4.81239383	-1.20709205	0.20221271
C	-0.02445389	5.02121255	0.20428492
O	-0.04529304	3.85862386	1.00685765
H	-5.40615959	1.82395507	0.39649599
H	-4.68184788	0.50772975	0.00318401
H	-4.08039475	-1.46769670	0.88225905
H	-4.42599857	-1.77433460	-0.59241156
H	0.37193655	-3.52557856	0.33384230
H	1.25867089	-2.55158865	-0.42901533
H	1.31570439	2.76507050	1.01322496
H	1.79041743	1.43470731	1.67708721
H	-2.96336441	1.97723984	0.30391216
H	-1.70847718	1.75023309	-0.56106940
H	-2.22609305	-3.59308743	-0.42077979
H	-1.92443910	-2.80299764	0.87027986
H	-2.19747472	-1.06532002	2.25232127
H	-2.98628477	-2.21507332	2.97608835
H	-2.89819344	-2.41493786	-2.30142088
H	-4.12297259	-3.33273199	-2.60199296
H	-1.31917665	-0.60253203	-2.20407629
H	-1.22539207	-1.87589417	-1.30384156
H	-0.35838103	0.22467412	2.51312131
H	-1.47289940	0.91563080	1.64215933
H	-0.07907397	1.30946089	-2.06609296
H	-1.32327152	1.73705755	-2.92482199
H	3.55122085	-1.67362617	1.52811772
H	2.23175692	-2.47851554	1.54795527
H	3.62100599	1.72185026	0.16222041
H	3.79664938	1.39551513	-1.30613488
H	4.63689739	-0.27778900	-0.05607180
H	5.73817529	-1.26202790	0.42495145



H	2.26012977	-2.08744899	-2.16434805
H	0.72532295	-1.75660266	-2.47206060
H	3.18078170	-3.67450672	-0.96158538
H	4.16616298	-2.49953960	-1.01519931
H	1.94910544	-0.62036273	2.63163248
H	1.64299018	0.35495036	3.81799527
H	1.62958951	0.22157863	-1.73761400
H	1.58536436	1.39487704	-0.70482011
H	-0.84033405	3.33757888	0.82133131
H	-0.90729335	4.18132780	-1.57182453
H	0.06655604	5.61931421	-1.86094660
H	0.85059909	4.07444720	-1.52455704
H	0.86889440	5.56796676	0.49058681
H	-0.88246900	5.64843918	0.44518507

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r\_Rc\_ch3\_ch2oh W18

C	0.32525138	4.23558581	-2.75900829
O	-1.03157536	1.31990011	-2.04754659
O	1.55578182	1.22352493	-1.54552740
O	1.49607594	-1.45578176	-1.94927542
O	3.64409791	-3.04343201	-1.59394874
O	-1.97324010	2.00666866	0.44825285
O	-4.59177052	1.50446025	0.12765476
O	-4.64701688	-1.17986026	0.16865526
O	-1.30794631	0.17167897	2.43210856
O	-2.75885604	-1.95397768	2.11210057
O	-1.52602404	-3.13874723	-0.00796184
O	-1.29858811	-1.45009248	-2.25121318
O	-3.63248335	-2.80391152	-1.96420502
O	1.96451592	2.06378845	1.04483943
O	1.44248479	0.15842669	2.95398437
O	2.76783447	-1.90547419	2.07085028
O	1.27583018	-3.23887241	0.19596915
O	4.27542570	1.35315582	-0.36110072
O	4.81494580	-1.20597904	0.23246739
C	-0.44755635	5.11768110	0.94181918
O	-0.17912291	3.81786958	1.19854357
H	-5.37805620	1.84190975	0.54511617
H	-4.66906624	0.53098177	0.10101279
H	-4.08312951	-1.48276154	0.88995473
H	-4.42356738	-1.71436472	-0.60036325
H	0.35830349	-3.51645309	0.28060973
H	1.24699554	-2.52805570	-0.45693712
H	1.36109925	2.81192435	1.14618382
H	1.79105573	1.45738146	1.78075513
H	-2.94646322	1.95833666	0.43251298
H	-1.68477348	1.74774253	-0.44109067
H	-2.23455931	-3.52996734	-0.52293094
H	-1.93536496	-2.80746747	0.80710492
H	-2.20149238	-1.15633276	2.29285863
H	-2.99538548	-2.34189045	2.94982013
H	-2.90857855	-2.28467144	-2.35084243
H	-4.14202950	-3.18263138	-2.67472952
H	-1.32687590	-0.48335588	-2.21740061
H	-1.23048547	-1.77463190	-1.34376856
H	-0.35886545	0.14494093	2.60576173
H	-1.47798993	0.83612895	1.74977637
H	-0.05620966	1.37761316	-1.92935768
H	-1.26805041	1.98729601	-2.68883841
H	3.53556877	-1.68786833	1.52948132
H	2.20624909	-2.47882770	1.52603329
H	3.67138078	1.75371668	0.27701654
H	3.81563897	1.44082306	-1.19695245
H	4.65256539	-0.26725926	0.00240233
H	5.73909181	-1.28034059	0.45646411
H	2.25342632	-2.01957543	-2.17436154
H	0.72550852	-1.65874077	-2.48701526

H	3.17437504	-3.63351587	-1.00289471
H	4.16232865	-2.45986799	-1.02624332
H	1.94667824	-0.63806513	2.65200748
H	1.65579023	0.29819451	3.87287494
H	1.65576125	0.26417799	-1.65140216
H	1.62762675	1.42697107	-0.59995782
H	-0.93016519	3.24007042	0.96250488
H	0.11725030	4.79560672	-3.65323784
H	-0.11571596	4.53649364	-1.82497609
H	1.07850155	3.46780330	-2.76616770
H	0.31129671	5.80484714	1.26850513
H	-1.48163814	5.41668786	0.88995674

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ts1\_dHa\_ch3\_ch2oh W18

C	0.54071881	2.67846227	4.03040317
O	1.33942418	-0.23078136	2.40034834
O	-1.29563330	-0.15978528	2.28025421
O	-1.16041422	-2.45365542	0.82500821
O	-3.18733201	-3.83666643	-0.31225949
O	2.01229012	2.07577976	0.93501421
O	4.68043578	1.53530711	0.65268036
O	4.68603424	-0.39097603	-1.23213541
O	1.01657927	1.87239561	-1.61134548
O	2.51440373	0.21737656	-2.92949601
O	1.61944810	-2.21048495	-2.10463427
O	1.63886913	-2.40527699	0.69495314
O	3.92132564	-3.08860639	-0.61504166
O	-2.36478868	1.94046953	0.81329653
O	-1.80195306	1.74240667	-1.84815688
O	-2.94173713	-0.51902245	-2.47278049
O	-1.15246204	-2.52967121	-1.99128624
O	-4.28297577	0.11203199	1.58719187
O	-4.75752904	-1.48386450	-0.50886734
C	-0.15716255	4.65120220	0.69653087
O	-0.95921839	4.18861802	1.70020833
H	5.43016365	2.10670920	0.51901607
H	4.74485900	0.81608511	-0.00301070
H	4.00806658	-0.16284150	-1.87882142
H	4.55023571	-1.31513959	-1.00061496
H	-0.24437867	-2.56063022	-2.31116736
H	-1.07009085	-2.34419389	-1.04767488
H	-2.03906462	2.78268880	1.15370721
H	-2.18564440	1.93563361	-0.14111119
H	2.97570925	2.03835379	0.82495062
H	1.79456182	1.27700135	1.43007403
H	2.39981128	-2.76580825	-2.04737158
H	1.90247959	-1.37582836	-2.51225263
H	1.93658130	0.87309402	-2.46166516
H	2.64236702	0.52798045	-3.82136345
H	3.25612242	-2.99989956	0.08620879
H	4.50856431	-3.80228066	-0.38332693
H	1.65656084	-1.63675088	1.28365356
H	1.47962965	-2.08405126	-0.20259652
H	0.05637930	1.79822872	-1.64507432
H	1.29763359	1.98150526	-0.68700250
H	0.36072427	-0.17241615	2.47750580
H	1.70595611	-0.22607092	3.28078513
H	-3.64780520	-0.80122407	-1.87972336
H	-2.29265701	-1.23991412	-2.47499003
H	-3.78945551	0.89779684	1.31269662
H	-3.75667093	-0.26914766	2.28900376
H	-4.61835942	-0.91925997	0.27954163
H	-5.69824561	-1.52259631	-0.66104846
H	-1.83732738	-3.13560189	0.68504640
H	-0.29633722	-2.84707523	0.98314279
H	-2.75177796	-3.85716411	-1.16589714
H	-3.83982570	-3.12793956	-0.36970449

H	-2.22959827	0.89052237	-2.11600096
H	-2.10022932	2.40822989	-2.46249993
H	-1.38179907	-0.97544925	1.76106806
H	-1.57102172	0.57290622	1.71008328
H	-0.42238422	3.83385653	2.41384024
H	0.56326571	3.35489790	4.86599990
H	1.33922803	2.68103168	3.30827316
H	-0.22376031	1.92214420	3.98069373
H	-0.70375113	5.07081577	-0.12727339
H	0.80644928	4.18887500	0.57448361

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C	-1.81499585	3.13765351	3.60358887
O	0.30566591	0.87248105	2.27846163
O	-2.05635151	0.67539603	1.12007330
O	-1.84966280	-2.02391375	1.21682189
O	-3.67515584	-3.66586757	0.10694367
O	1.80596917	1.90684573	0.21461983
O	4.29281273	1.54840529	1.16542241
O	4.58977914	-1.09863033	0.81932532
O	1.83350936	0.35947925	-2.08916455
O	3.32997061	-1.70825227	-1.62872559
O	1.71011712	-3.22708211	-0.05155917
O	0.76813675	-1.88196528	2.23798647
O	3.21459660	-3.04534862	2.41233557
O	-1.87084207	1.84519880	-1.36218905
O	-0.69507274	0.27907413	-3.28988935
O	-2.00433313	-1.96035999	-3.02686980
O	-0.92416717	-3.45951318	-1.00019957
O	-4.38993618	0.81804190	-0.71173881
O	-4.51154188	-1.66088125	-1.72835155
C	-0.29973861	4.50303401	0.60146895
O	-0.02165619	3.72129712	-0.46803856
H	5.12171818	1.98622057	0.99898617
H	4.44968148	0.58691038	1.09445561
H	4.25409979	-1.33006019	-0.05458313
H	4.22523411	-1.74245447	1.43540430
H	0.00628681	-3.66878186	-0.87152361
H	-1.12957179	-2.85049644	-0.27964824
H	-1.32460356	2.61729685	-1.16018479
H	-1.45064063	1.37467011	-2.09770272
H	2.74283542	1.92767241	0.48170961
H	1.33134597	1.50234677	0.95774118
H	2.29770933	-3.64480729	0.58130004
H	2.28083782	-2.76703082	-0.68749355
H	2.77087504	-0.92637091	-1.86508106
H	3.80693579	-1.97387821	-2.40986068
H	2.37317556	-2.62592801	2.65537239
H	3.56181684	-3.48773876	3.18152106
H	0.71157875	-0.92008454	2.32586960
H	0.96103083	-2.08174422	1.31259735
H	0.96303952	0.30390041	-2.50243282
H	1.76714262	0.92624189	-1.30736638
H	-0.60770511	0.88571157	1.91226392
H	0.30866234	1.47613170	3.01862701
H	-2.90219486	-1.86914812	-2.68723761
H	-1.54884338	-2.57081986	-2.42623471
H	-3.68104825	1.33508387	-1.11504478
H	-4.16746413	0.81288555	0.22001133
H	-4.50588805	-0.75565916	-1.35289832
H	-5.33555446	-1.76075102	-2.19823889
H	-2.58201778	-2.65851515	1.16183535
H	-1.22582599	-2.25420824	1.91081479
H	-3.01592378	-4.13464669	-0.40675736
H	-4.08494459	-3.03851638	-0.50123970
H	-1.18444080	-0.57871273	-3.22303310
H	-0.68720663	0.53016846	-4.20985370

H	-2.08994473	-0.29395093	1.09050399
H	-1.90858181	0.99493590	0.21642678
H	0.75095048	3.15601457	-0.27900118
H	-1.55485561	2.73522560	4.56733250
H	-1.75431024	4.19766183	3.44078377
H	-2.24326680	2.50188033	2.84977621
H	-1.10008804	5.20371574	0.44713926
H	0.50329798	4.72060666	1.28584323

## 2.2.4 CH3 + CH3

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p\_ch3\_ch3 W18

C	-2.04475109	4.57521336	-0.96088142
O	-1.46263520	0.85847587	-1.30099454
O	1.13558147	1.55853092	-1.18744176
O	1.68099176	-1.00957312	-2.00366014
O	4.30417917	-0.74032131	-2.56177402
O	-1.71940017	1.56086104	1.38655592
O	-3.98924795	1.42657276	-0.38315448
O	-4.16572710	-1.23689332	-0.04538224
O	-1.20632066	-0.51312094	3.13682362
O	-2.53741559	-2.41418553	1.96358930
O	-1.09768552	-3.44536490	-0.12641148
O	-1.00684160	-1.65205955	-2.26021929
O	-3.32799180	-3.02462851	-2.09808373
O	1.08238050	2.02730698	1.55677424
O	1.56324175	-0.10751595	3.22385267
O	3.16439909	-1.48935679	1.72995807
O	1.75795501	-3.00832944	-0.02188959
O	3.45742515	2.59716914	0.04241315
O	4.72391547	0.23826563	0.02788015
C	-0.64357045	4.62696413	-0.36951990
H	-4.85131866	1.79043651	-0.56217440
H	-4.10468176	0.46072271	-0.27006004
H	-3.68239309	-1.59793487	0.70700064
H	-4.00374173	-1.84011905	-0.77980164
H	0.86742804	-3.35894187	0.05424643
H	1.73470941	-2.36750949	-0.74278508
H	0.15458017	2.25370461	1.66732228
H	1.26890133	1.32767930	2.20193765
H	-2.62133695	1.87104259	1.28782353
H	-1.54097616	1.15616524	0.52495183
H	-1.74563839	-3.94125194	-0.62754754
H	-1.56393919	-3.12590660	0.66308626
H	-2.00426177	-1.73776725	2.45036200
H	-2.94335073	-2.97652030	2.61793365
H	-2.56688072	-2.52340057	-2.43679525
H	-3.83851122	-3.33129986	-2.84171903
H	-1.23839377	-0.75138418	-1.98165331
H	-0.87687909	-2.14838904	-1.43956711
H	-0.24434864	-0.51593695	3.21984364
H	-1.43138979	0.27691025	2.62584448
H	-0.67257885	1.38800717	-1.48638548
H	-2.27208863	1.36146249	-1.42464677
H	3.70700270	-0.96610418	1.13077128
H	2.68056489	-2.13569551	1.18631926
H	2.85036875	2.69186532	0.78250441
H	2.86572890	2.50255802	-0.71142371
H	4.31178419	1.12690758	0.08445036
H	5.61282713	0.31732572	0.36493656
H	2.51899959	-1.02449841	-2.48808095
H	0.94042214	-1.29771856	-2.54623284
H	4.78689189	-0.21636253	-3.19363870
H	4.54020566	-0.41974315	-1.67938698
H	2.18105986	-0.66337024	2.68046400
H	1.94973306	-0.01864007	4.09088070

H	1.38801857	0.66334250	-1.46627570
H	1.10007947	1.54655720	-0.22007720
H	-0.67328748	4.57505183	0.71584779
H	-2.56727159	3.66899414	-0.66604089
H	-2.01490755	4.60339655	-2.04793791
H	-2.64490894	5.41940496	-0.62938180
H	-0.13657675	5.54971530	-0.64053555
H	-0.03170757	3.80291412	-0.72423540

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C	-3.60610614	3.08194816	-2.79003070
O	-1.09788820	1.41100539	-1.76426124
O	1.53785198	1.51661830	-1.37705605
O	1.68685832	-1.16311535	-1.90699868
O	4.25980013	-1.47774939	-2.63472753
O	-2.00059990	1.99121475	0.83440626
O	-4.58438747	1.37592157	0.06186332
O	-4.43270765	-1.29599024	0.27802663
O	-1.14837182	0.23439963	2.73048799
O	-2.52484877	-1.91146611	2.26933908
O	-1.21457752	-3.02503330	0.15932487
O	-1.08515318	-1.33696481	-2.05482434
O	-3.31351691	-2.86734191	-1.83029340
O	1.93001928	2.35788294	1.25032396
O	1.67596576	0.27075006	2.95033997
O	3.13342672	-1.51119786	1.76523050
O	1.62149744	-3.07223444	0.16778943
O	4.18519623	2.08977765	-0.42118073
O	5.00577874	-0.43404550	-0.15170738
C	-0.23568431	4.59495429	1.99586974
H	-5.41865982	1.65564799	0.42684469
H	-4.57445262	0.39919028	0.09578282
H	-3.84757278	-1.52254038	1.01071093
H	-4.16585451	-1.84009498	-0.47031403
H	0.68559986	-3.25632918	0.29029838
H	1.66521357	-2.47733021	-0.59004548
H	1.35548245	3.08732529	1.49418225
H	1.83626154	1.67602655	1.93873016
H	-2.95609549	1.88946712	0.72011588
H	-1.63849293	1.78838183	-0.03676693
H	-1.88916695	-3.49136608	-0.33750316
H	-1.63906056	-2.71564941	0.97544889
H	-1.99386198	-1.10470397	2.49550639
H	-2.76626948	-2.33771723	3.08681374
H	-2.61881206	-2.29351265	-2.19320624
H	-3.78122920	-3.26918747	-2.55648323
H	-1.20537590	-0.37928992	-1.96947569
H	-0.99820848	-1.69731391	-1.16084971
H	-0.18633097	0.19993880	2.77488551
H	-1.40361437	0.91119629	2.07907836
H	-0.14501041	1.62334597	-1.78536782
H	-1.58102921	2.01208779	-2.33217759
H	3.78841391	-1.19344425	1.13497861
H	2.59064258	-2.16978122	1.29383207
H	3.65410127	2.36339255	0.33495124
H	3.54253590	2.05783768	-1.13588583
H	4.77354315	0.51732527	-0.21478477
H	5.90583943	-0.48876035	0.15927179
H	2.47068700	-1.35838260	-2.44068353
H	0.87013017	-1.35755298	-2.37837709
H	4.81986170	-1.12813272	-3.32080561
H	4.61621474	-1.17719322	-1.78630913
H	2.22898854	-0.42898960	2.51161980
H	1.94328987	0.30436419	3.86512572
H	1.65807755	0.55878887	-1.49312187
H	1.54876255	1.70142922	-0.42744410
H	-0.93263691	3.84898135	1.64935867

H	-3.96343247	2.49953763	-1.95682402
H	-3.76602573	2.74105219	-3.79804827
H	-3.23661248	4.07978558	-2.62895084
H	-0.02747519	4.69334869	3.04720603
H	0.12380494	5.35556537	1.32429029

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C	3.47235714	3.14233490	1.33597393
O	1.40625442	0.73404136	1.29966044
O	-1.10492054	0.46794790	2.16224535
O	-0.76772919	-2.23992609	2.18963551
O	-2.75305763	-2.96212638	3.85631331
O	0.67956222	1.86280361	-1.17884275
O	3.35928582	1.82322986	-1.85636814
O	3.50627047	-0.80102867	-2.43563866
O	-0.65354521	0.28752454	-2.95621192
O	1.02309252	-1.60594665	-3.50976233
O	0.98446175	-3.21852078	-1.31385448
O	1.76971038	-1.98553141	1.06270254
O	3.76896121	-2.91396402	-0.51884862
O	-2.53627310	1.63767768	0.10701109
O	-3.22995755	-0.06445119	-1.87914789
O	-3.75188556	-2.19061227	-0.49948453
O	-1.54379240	-3.69521565	-0.09562914
O	-3.88334847	0.92615662	2.52607249
O	-4.58528812	-1.63300550	2.20583854
C	-0.41657933	3.92957114	1.30370979
H	3.86271588	2.28959249	-2.51708368
H	3.47506601	0.86999833	-2.03632627
H	2.69612738	-1.07400116	-2.88239001
H	3.71583739	-1.49096219	-1.79754381
H	-0.75549322	-3.71806518	-0.64548721
H	-1.27123957	-3.26483518	0.72318184
H	-2.01550995	2.38006101	-0.19644162
H	-2.80368465	1.12065212	-0.67222887
H	1.55295873	2.02510385	-1.56253479
H	0.87811874	1.39454295	-0.35850197
H	1.85533548	-3.61888248	-1.29557722
H	0.93692724	-2.71331208	-2.14137611
H	0.35253132	-0.89416229	-3.34384095
H	0.92865967	-1.88730266	-4.41541498
H	3.27299406	-2.58993709	0.25099364
H	4.58043254	-3.30554825	-0.20927963
H	1.76213746	-1.01905760	1.13139359
H	1.30026549	-2.21437511	0.24798423
H	-1.53705433	0.08800610	-2.62660302
H	-0.22975079	0.89031706	-2.32076214
H	0.56923301	0.78598002	1.79719860
H	2.00986743	1.40690010	1.61898737
H	-4.04855643	-2.05839870	0.40687803
H	-2.99590873	-2.80461131	-0.46121517
H	-3.76610466	1.38091658	1.68627467
H	-2.98271828	0.84809814	2.85664190
H	-4.41231151	-0.67436917	2.32113686
H	-5.52283705	-1.76904319	2.31724560
H	-1.22123206	-2.62338527	2.95393485
H	0.18377132	-2.38178744	2.21928346
H	-2.96488308	-2.81274384	4.77251172
H	-3.45771039	-2.56342472	3.32584946
H	-3.44098773	-0.89353573	-1.37353817
H	-3.94452981	0.08402366	-2.49261667
H	-1.06704616	-0.50397689	2.16346897
H	-1.53235830	0.73990995	1.33703432
H	0.06276671	3.59084149	0.40151423
H	2.71735287	3.88722249	1.51724676
H	3.57793906	2.71270945	0.35338633
H	4.20976610	2.94731601	2.09492624

H	-0.60131734	4.97674145	1.46194718
H	-0.69631530	3.22225047	2.06432361

## 2.2.5 CH3 + CH3O

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p\_Rc\_ch3\_ch3o W18

C	-0.37168756	4.70022087	0.66818811
O	-0.90979815	0.31288899	-2.56955476
O	1.61132515	0.30575514	-1.81307904
O	1.46778893	-2.34114829	-1.12739909
O	4.01473427	-3.16896818	-1.39055318
O	-2.05614540	1.98960688	-0.60669790
O	-4.69026816	1.29944186	-0.92354422
O	-4.81893505	-1.01658152	0.43769938
O	-1.39925840	1.28380744	1.94468091
O	-2.95846743	-0.70413819	2.53887414
O	-1.70632077	-2.73141539	1.22193835
O	-1.30451938	-2.23890130	-1.49388642
O	-3.68235521	-3.35329695	-0.76970130
O	2.07351630	2.16259506	0.15319810
O	1.35537611	1.08363449	2.55286894
O	2.66285392	-1.15525641	2.44235435
O	1.06914546	-3.14091331	1.54748721
O	4.31748869	0.98235478	-0.96731888
O	4.76405884	-1.21994573	0.46012441
O	0.58129896	4.39283599	-0.32566449
C	0.06447183	4.50228569	-1.63192884
H	-5.48071726	1.80571612	-0.76468582
H	-4.79833190	0.44392652	-0.46654924
H	-4.25508006	-0.91230610	1.21313261
H	-4.53967129	-1.82460982	-0.00479820
H	0.11163875	-3.12389041	1.63909909
H	1.23112710	-2.95102967	0.61602940
H	1.59359746	2.99006869	-0.01298420
H	1.84680762	1.87347492	1.05051674
H	-3.01481250	1.86386212	-0.68464520
H	-1.67470172	1.43856249	-1.29935965
H	-2.41027943	-3.31073611	0.92406460
H	-2.11925782	-2.06537757	1.79392469
H	-2.37287754	0.07564478	2.35998151
H	-3.21397414	-0.67255679	3.45635141
H	-2.93341629	-3.04035999	-1.30220223
H	-4.15192244	-4.01327906	-1.27125079
H	-1.29840556	-1.35189133	-1.87967528
H	-1.29241563	-2.14151126	-0.53116643
H	-0.45334742	1.17577617	2.09650552
H	-1.54810116	1.55706748	1.02252837
H	0.05988944	0.37713329	-2.41983718
H	-1.08876047	0.51932307	-3.48272309
H	3.38740604	-1.20480723	1.81015726
H	2.07760059	-1.91163814	2.25287176
H	3.75436348	1.59371149	-0.47358458
H	3.74818814	0.69810507	-1.68605214
H	4.66712658	-0.37788281	-0.03588796
H	5.62751341	-1.21524824	0.86533710
H	2.24667254	-2.81621988	-1.45111378
H	0.66005272	-2.63553629	-1.55948333
H	4.66094514	-3.23377283	-2.08670571
H	4.36549845	-2.56293152	-0.72164850
H	1.84148152	0.21840535	2.52963778
H	1.54371037	1.48409679	3.39739684
H	1.63648456	-0.60526653	-1.47624281
H	1.65409942	0.90987522	-1.05402907
H	-0.80374664	3.85874293	-1.75269213
H	0.10288494	4.54481331	1.62997106
H	-0.67792962	5.74312089	0.58693269

H	-1.23894410	4.05193039	0.57932305
H	-0.21240653	5.53506152	-1.84433629
H	0.84934129	4.19966703	-2.31578162

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p\_dHa\_ch3\_ch3o W18

C	0.66924921	4.07989720	-2.47164859
O	-0.87359822	0.93299714	-2.39126596
O	1.62191904	0.62074440	-1.60822273
O	1.28717607	-2.09518889	-1.52468775
O	3.75905833	-3.07619475	-1.93436898
O	-1.88253162	2.25247617	-0.12577532
O	-4.55020781	1.88302464	-0.56313354
O	-4.90296462	-0.66287102	0.21499863
O	-1.36407825	0.93765465	2.22521387
O	-3.09806829	-0.99358481	2.36082153
O	-1.97613908	-2.77646453	0.63258429
O	-1.46410575	-1.75001999	-1.91118033
O	-3.94512496	-2.77889429	-1.46155625
O	2.21954984	1.94633383	0.73139736
O	1.34819300	0.41117928	2.80092382
O	2.47555018	-1.85578014	2.23797361
O	0.75664321	-3.44513111	0.89540622
O	4.36691437	0.81514288	-0.60830374
O	4.61860034	-1.66829143	0.31179252
O	1.17782596	4.51151464	1.09539467
C	-0.00596296	4.68057388	0.93920157
H	-5.30826645	2.39964181	-0.30865850
H	-4.73766069	0.95547054	-0.32255403
H	-4.36309667	-0.78960853	1.00396975
H	-4.68356226	-1.37665897	-0.39271652
H	-0.19995922	-3.38469898	0.97592016
H	0.95696304	-3.05914326	0.03471244
H	1.93593460	2.86537977	0.82512934
H	1.94498597	1.47941751	1.53700529
H	-2.84906566	2.23471598	-0.21898862
H	-1.54626540	1.82221645	-0.92152761
H	-2.71541637	-3.21725698	0.20945917
H	-2.34988995	-2.22255602	1.33559310
H	-2.44626207	-0.24779084	2.36420080
H	-3.37394111	-1.14443959	3.26039264
H	-3.15662802	-2.43185426	-1.90922374
H	-4.45623589	-3.27389802	-2.09512065
H	-1.38783894	-0.80445001	-2.10081710
H	-1.47112908	-1.85875875	-0.94976565
H	-0.43303740	0.72781987	2.36535293
H	-1.46255844	1.41195345	1.38310461
H	0.09269986	0.90909470	-2.21291398
H	-1.01227178	1.38851083	-3.21715025
H	3.21569008	-1.83164957	1.62246830
H	1.83698588	-2.49808780	1.87741004
H	3.84226548	1.35168411	0.00141358
H	3.80572577	0.75648530	-1.38436326
H	4.59321855	-0.73503549	0.00701256
H	5.47242307	-1.81594358	0.71048450
H	2.04040789	-2.55035727	-1.92887642
H	0.47523904	-2.23570329	-2.02174299
H	4.41526080	-3.04145022	-2.62331405
H	4.14508031	-2.67516584	-1.14191308
H	1.76727669	-0.46727063	2.60383930
H	1.54187658	0.61393806	3.71236635
H	1.58089759	-0.34049002	-1.47217818
H	1.69491508	1.04857898	-0.74086469
H	-0.67142888	3.88142740	0.60393736
H	-0.30041000	3.92816275	-2.00918830
H	1.10637948	5.00493208	-2.11173244
H	0.55319221	4.13638021	-3.54940357
H	-0.44897726	5.66435905	1.13145325



H	1.32229259	3.25177735	-2.22007579
63			
r_Rc_ch3_ch3o W18			
C	0.10591569	4.25333475	2.94113429
O	-0.92360614	0.04494022	-2.79478481
O	1.61716940	0.14054919	-2.10768793
O	1.48083123	-2.36942775	-1.03292231
O	3.99612397	-3.32351573	-1.09639745
O	-2.09002259	1.92596874	-1.05325793
O	-4.70163723	1.17379460	-1.29115223
O	-4.83213332	-0.99841031	0.28483318
O	-1.43587813	1.41090438	1.55418019
O	-3.02558742	-0.46575384	2.38559980
O	-1.72407376	-2.60437438	1.31757972
O	-1.28833753	-2.37069720	-1.42335261
O	-3.66450123	-3.44572060	-0.63714049
O	2.12801993	2.18751189	-0.33306659
O	1.31198060	1.33110533	2.08569684
O	2.68262787	-0.84688185	2.47410948
O	1.06461420	-2.87981778	1.72003489
O	4.35491854	0.79845055	-1.22306665
O	4.78304448	-1.18415571	0.50899299
O	0.59759499	4.55278676	-0.53457447
C	-0.42011304	4.65341916	-1.44553389
H	-5.50255846	1.67956459	-1.19549536
H	-4.80491288	0.36436364	-0.75502518
H	-4.29465835	-0.81651160	1.06461095
H	-4.54406212	-1.84939582	-0.06116279
H	0.10655635	-2.88839488	1.80257568
H	1.23137116	-2.76537361	0.77744583
H	1.73907766	3.05165211	-0.50490795
H	1.85863396	1.93894883	0.56981412
H	-3.04879531	1.78440499	-1.11763662
H	-1.70164642	1.30714750	-1.68352770
H	-2.41020428	-3.22763103	1.07169873
H	-2.16107753	-1.89355195	1.81223252
H	-2.43115497	0.27944605	2.11583716
H	-3.28233574	-0.32257027	3.29204433
H	-2.90776638	-3.17982679	-1.18375396
H	-4.11824506	-4.15752889	-1.07884999
H	-1.29082208	-1.52913186	-1.89992221
H	-1.29849551	-2.17599244	-0.47538168
H	-0.48600879	1.29136628	1.67921027
H	-1.60505480	1.62014739	0.61985536
H	0.04923342	0.12841393	-2.67573977
H	-1.11963893	0.11910924	-3.72477834
H	3.41637229	-0.98013904	1.86529902
H	2.08917013	-1.61000346	2.35473290
H	3.79000747	1.47961685	-0.83446251
H	3.81780126	0.44565058	-1.93520063
H	4.68582049	-0.42322826	-0.10275064
H	5.65079748	-1.12589942	0.90064271
H	2.25616866	-2.90309748	-1.26055763
H	0.67416032	-2.72852093	-1.41588151
H	4.65956466	-3.51550390	-1.75163330
H	4.36194227	-2.65904420	-0.49449633
H	1.83610741	0.51429489	2.28637226
H	1.41228356	1.94493126	2.81100352
H	1.64629458	-0.71153420	-1.64083608
H	1.67696216	0.84721675	-1.44659276
H	-1.10812218	3.82455951	-1.21504887
H	0.60578831	4.68294232	2.09105774
H	0.30016584	4.63686369	3.92705869
H	-0.67528787	3.53037233	2.78334352
H	-0.95715560	5.59622474	-1.36176812
H	-0.06280769	4.47999315	-2.46162540

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r_dHa_ch3_ch3o W18			
C	0.74842436	3.76037350	-3.21574214
O	-0.92239253	1.03681960	-2.22230771
O	1.60756592	0.75604984	-1.49196060
O	1.29256476	-1.95767622	-1.55571016
O	3.75160042	-2.95623483	-1.99795025
O	-1.89034260	2.31533774	0.09161509
O	-4.56649261	1.96237889	-0.33652858
O	-4.88650157	-0.64755873	0.23586515
O	-1.36010572	0.80412903	2.32677787
O	-3.08926861	-1.12644852	2.35459771
O	-1.98608581	-2.84329444	0.55834653
O	-1.46349017	-1.67461061	-1.91358015
O	-3.96007773	-2.70237632	-1.53997197
O	2.23090694	1.91983290	0.93153224
O	1.35941685	0.27239513	2.89592017
O	2.48514795	-1.96992392	2.23439853
O	0.76563335	-3.45940507	0.78333934
O	4.36902810	0.85435845	-0.47195697
O	4.62918193	-1.67753774	0.31848786
O	1.01457832	4.41165715	1.39116799
C	0.12112555	4.82442667	0.43789811
H	-5.32221354	2.44259773	-0.01291756
H	-4.73754778	1.01492762	-0.17684610
H	-4.34725282	-0.82780269	1.01493772
H	-4.68011552	-1.33014044	-0.41065818
H	-0.19232263	-3.42996950	0.86406084
H	0.96080409	-3.01042190	-0.04717219
H	1.92001307	2.82212661	1.07399326
H	1.95292191	1.39935472	1.70419544
H	-2.85883799	2.31165117	0.02344543
H	-1.58494902	1.89501189	-0.72130410
H	-2.72902369	-3.26016173	0.11805319
H	-2.35569807	-2.31552606	1.28408786
H	-2.43523885	-0.38241574	2.39143353
H	-3.37188556	-1.30998864	3.24596832
H	-3.16391574	-2.34553836	-1.96516777
H	-4.47778835	-3.15110036	-2.20201991
H	-1.40521476	-0.71619385	-2.03350142
H	-1.48370279	-1.85187114	-0.96214331
H	-0.42625677	0.60763630	2.46278893
H	-1.46029258	1.37379274	1.54645865
H	0.04271307	1.01759458	-2.04580609
H	-1.05483701	1.50510576	-3.04274988
H	3.22691333	-1.91459727	1.62310203
H	1.84405361	-2.58551656	1.83438393
H	3.84236393	1.35742079	0.16384710
H	3.81460596	0.84053626	-1.25445507
H	4.60139311	-0.73054228	0.06265759
H	5.48409057	-1.84391137	0.70735397
H	2.04071900	-2.40538011	-1.97694705
H	0.47415101	-2.09030160	-2.04542099
H	4.41735434	-2.92912772	-2.67790436
H	4.14553737	-2.60535416	-1.18609227
H	1.77808532	-0.59758261	2.66474770
H	1.53665614	0.43312874	3.81905382
H	1.58003652	-0.21343671	-1.42127190
H	1.69008067	1.12180063	-0.59765700
H	-0.68358611	4.07292473	0.43435369
H	-0.21735519	3.98415114	-2.79916336
H	1.12416378	4.34950076	-4.03225664
H	1.34638239	2.97043155	-2.79757512
H	-0.29759513	5.80417888	0.65910784
H	0.56834661	4.79140872	-0.55729663
63			
ts_Rc_ch3_ch3o W18			
C	0.06930234	4.39122310	2.46476515

O	-0.92611325	0.09153451	-2.75852842
O	1.60411047	0.19175059	-2.03290774
O	1.47830929	-2.35725797	-1.05569427
O	4.00149850	-3.28499752	-1.15640374
O	-2.08890369	1.90635201	-0.94493451
O	-4.70977171	1.18357046	-1.19239494
O	-4.83824790	-1.03948247	0.31376297
O	-1.43373410	1.33101338	1.63754945
O	-3.02778340	-0.56160815	2.42510185
O	-1.72471421	-2.66391737	1.28866497
O	-1.29057948	-2.35723337	-1.44618235
O	-3.66502584	-3.45641425	-0.68383272
O	2.09733076	2.19661960	-0.20402845
O	1.31018958	1.27826010	2.21129950
O	2.66986433	-0.91927715	2.47564522
O	1.06383134	-2.94208381	1.68023007
O	4.33247335	0.84699937	-1.14080201
O	4.77791584	-1.19306465	0.51539268
O	0.75822300	4.63142775	-0.69759920
C	-0.27878078	4.51174698	-1.58917771
H	-5.50586544	1.69184802	-1.07271384
H	-4.81445073	0.35751321	-0.68293347
H	-4.29905956	-0.87902859	1.09700462
H	-4.54801668	-1.87840271	-0.05868024
H	0.10576058	-2.95609445	1.76281293
H	1.22991133	-2.80689604	0.74023313
H	1.72348057	3.06660165	-0.38739921
H	1.82957614	1.94978814	0.69829564
H	-3.04946207	1.77758473	-1.00579475
H	-1.71306518	1.30912424	-1.60246139
H	-2.40945936	-3.28181857	1.02587002
H	-2.16260513	-1.97014555	1.80620220
H	-2.43366483	0.19033909	2.17490082
H	-3.28406582	-0.44275707	3.33518851
H	-2.91055503	-3.17527308	-1.22571829
H	-4.11975285	-4.15650326	-1.14293953
H	-1.29455102	-1.50436416	-1.90202068
H	-1.30170258	-2.18602022	-0.49372668
H	-0.48568774	1.21463736	1.77518931
H	-1.59525603	1.55386477	0.70416476
H	0.04407831	0.18076074	-2.62518736
H	-1.11268740	0.18730501	-3.68842960
H	3.40624768	-1.03430079	1.86615067
H	2.07937633	-1.68183872	2.33724436
H	3.76375736	1.50889854	-0.72534104
H	3.79284754	0.51317718	-1.86026222
H	4.67681916	-0.41099665	-0.06875135
H	5.64471840	-1.14421703	0.91042535
H	2.25721191	-2.87698421	-1.30262866
H	0.67353596	-2.70774126	-1.45046402
H	4.66554150	-3.45581574	-1.81686365
H	4.36475203	-2.63672625	-0.53560415
H	1.83130830	0.44615121	2.35338766
H	1.41920068	1.83108740	2.98175872
H	1.63614823	-0.67728694	-1.59840967
H	1.65371852	0.87357219	-1.34550642
H	-1.00435210	3.81349323	-1.15173939
H	0.98299617	4.48137133	1.90618493
H	-0.22308947	5.18902168	3.12357369
H	-0.59692815	3.56487068	2.29074044
H	-0.75672309	5.46529741	-1.80143526
H	0.06874711	4.02790634	-2.50458770
63			
ts_dHa_ch3_ch3o W18			
C	0.67325251	4.06504140	-2.67440017
O	-0.95950009	1.00277179	-2.24847653
O	1.57048769	0.78944852	-1.51288819

O	1.29374047	-1.93002563	-1.53952888
O	3.73390320	-2.98893220	-1.94177741
O	-1.94761284	2.24796575	0.08767901
O	-4.62602599	1.88045966	-0.36408280
O	-4.91679620	-0.72872881	0.24046805
O	-1.40688084	0.77130701	2.32866865
O	-3.11710053	-1.17305737	2.36618474
O	-1.99036486	-2.88319680	0.58212397
O	-1.46903819	-1.71187258	-1.88486793
O	-3.95383939	-2.77817519	-1.52566354
O	2.22300149	1.90276419	0.92767768
O	1.31934717	0.28762112	2.90860690
O	2.46977745	-1.95481074	2.28231029
O	0.77099867	-3.44068044	0.80566364
O	4.35157050	0.81601745	-0.44532928
O	4.61787353	-1.70474164	0.36638793
O	1.42746938	4.56632898	1.06454974
C	0.28192264	4.70777577	0.36216585
H	-5.38560014	2.35714945	-0.04426360
H	-4.78715146	0.93387223	-0.19138958
H	-4.37577447	-0.89473918	1.02149127
H	-4.69857305	-1.41240009	-0.40080719
H	-0.18782011	-3.43012606	0.88119110
H	0.96456164	-2.97909988	-0.01800632
H	2.00392160	2.83444971	1.06517883
H	1.92055355	1.40683142	1.70650925
H	-2.91486511	2.24514071	0.01494928
H	-1.63889896	1.85164248	-0.73441077
H	-2.72588547	-3.31242023	0.14131054
H	-2.36907577	-2.35795655	1.30529158
H	-2.46904402	-0.42297279	2.40036474
H	-3.40067148	-1.35389641	3.25778723
H	-3.16152798	-2.40978795	-1.94771642
H	-4.46180836	-3.23565828	-2.18925127
H	-1.42046812	-0.75324122	-2.00551896
H	-1.49545490	-1.88911133	-0.93342591
H	-0.47085677	0.58682946	2.46601190
H	-1.51392849	1.32848326	1.53909167
H	0.00672557	1.01117011	-2.07410302
H	-1.11333282	1.40970439	-3.09659160
H	3.21878895	-1.90693410	1.67921780
H	1.83325797	-2.57141716	1.87697835
H	3.79865159	1.30827427	0.17853415
H	3.83403823	0.81821202	-1.25185673
H	4.58559475	-0.76171364	0.09600204
H	5.47433899	-1.86166440	0.75569345
H	2.03975741	-2.39680642	-1.94373308
H	0.47239392	-2.08870848	-2.01655544
H	4.40903634	-2.99577747	-2.61286926
H	4.12966344	-2.64244756	-1.12879053
H	1.74953900	-0.57941573	2.68853794
H	1.48583841	0.45560618	3.83243923
H	1.56147245	-0.18053030	-1.44209971
H	1.66030374	1.15098150	-0.61739989
H	-0.44670762	3.91875635	0.55460826
H	-0.39825989	4.02738441	-2.76020730
H	1.19495132	4.94799979	-2.99815170
H	1.22427733	3.16137330	-2.48041230
H	-0.14731769	5.70635843	0.43390552
H	0.57094172	4.54228052	-0.71472125

## 2.2.6 CH3 + NH2

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p_ch3_nh2	W18		
H	3.92524945	2.89832305	-1.51813377
O	3.38398609	2.33970905	-0.96917635

H	3.30630925	1.47851433	-1.42132481
H	1.91404762	1.13683876	3.02122086
O	1.25760195	0.92647095	2.36258566
H	0.37180968	0.92719913	2.79596689
H	-1.72470982	1.79532019	-1.30838922
O	-0.82787188	1.90681217	-1.64582289
H	-0.25508900	2.22725292	-0.92998941
H	1.10484676	2.12631476	0.97573655
O	0.97571241	2.74893675	0.24909071
H	1.82340290	2.75998279	-0.22375840
H	3.61653096	-3.08228192	-0.64390705
O	2.89135463	-2.47917636	-0.77867540
H	2.52973086	-2.23706488	0.08938345
H	-1.74355940	1.33253617	2.62016716
O	-1.21562173	0.77899832	3.21975516
H	-1.36800367	-0.14483656	2.96604966
H	-3.88888148	1.69210891	3.05759947
O	-4.17307020	1.02002590	3.69482834
H	-3.37445820	0.81162152	4.17978837
H	-4.85136595	-0.33286411	2.92772817
O	-5.21550510	-1.10101356	2.43843265
H	-6.13096763	-1.18215169	2.69331112
H	-4.17228566	-2.67267636	2.55042586
O	-3.50919447	-3.37128870	2.48670377
H	-3.45849067	-3.59819137	1.55706768
H	-1.91573871	-2.50156179	2.67227702
O	-1.31687074	-1.80038794	2.36986427
H	-0.41420393	-2.11756262	2.27559444
H	-4.09303237	2.13276274	-1.30182591
O	-3.47924242	1.64930706	-0.75546817
H	-3.86592262	0.75173204	-0.60717942
H	-4.82895167	-0.83215837	0.60919099
O	-4.46829567	-0.72340755	-0.27842756
H	-3.78147713	-1.40163365	-0.37278180
H	-2.24715572	3.29428222	1.74323095
O	-2.81533149	2.48912590	1.79776833
H	-3.08196080	2.26351705	0.89597858
H	-0.16540611	0.75701776	-2.53767203
O	0.28161216	0.02032779	-3.02894695
H	0.01875072	0.07921078	-3.94307235
H	0.08335203	-1.41670269	-2.03303759
O	0.08693250	-2.12425539	-1.36814187
H	0.89939180	-2.61661136	-1.50205679
H	-1.68185003	-2.58782662	-0.76546671
O	-2.39544659	-2.50982598	-0.12381274
H	-1.97533696	-2.12015079	0.65308229
H	2.09228212	0.00727918	-2.59608545
O	2.98454494	-0.00734648	-2.23017250
H	3.07820707	-0.84390888	-1.76351155
H	1.32434013	-0.70474476	1.51941564
H	0.66120687	-1.51403352	0.35977000
O	1.20487311	-1.59335747	1.15481814
C	-0.41209023	4.56945713	3.07929994
H	-0.18453481	3.56321988	3.41736141
N	-0.96434078	4.50365332	1.73048945
H	-0.27333556	4.13139028	1.09049253
H	-1.22162515	5.42105673	1.40537392
H	-1.15218127	4.98232972	3.75802809
H	0.49589063	5.16782807	3.15275117

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r_ch3_nh2 W18			
H	3.70293087	3.06234479	-1.96319118
O	3.18577306	2.55265018	-1.34752536
H	3.17636527	1.63162147	-1.66985157
H	1.61248002	1.81965610	2.80233007
O	1.03552620	1.47364784	2.12357202
H	0.13309253	1.45769578	2.51312788

H	-1.85714894	1.59568963	-1.60023230
O	-0.96863011	1.71874791	-1.95468067
H	-0.42481549	2.18581116	-1.30005710
H	0.89247062	2.47845685	0.60624179
O	0.74854064	2.97956308	-0.20806033
H	1.60390776	2.96880504	-0.66809823
H	3.78046141	-2.72132432	-0.21900480
O	3.01604272	-2.20275269	-0.45257032
H	2.61310031	-1.86701818	0.36474498
H	-2.01060543	1.69330065	2.35286071
O	-1.45042224	1.24320545	3.00502291
H	-1.53088904	0.28876770	2.85045016
H	-4.21031972	1.89761302	2.71880698
O	-4.43446796	1.26443323	3.41474891
H	-3.62869997	1.18745973	3.92581097
H	-4.97921282	-0.22450986	2.79838134
O	-5.26248058	-1.07316863	2.39813291
H	-6.17531210	-1.20292651	2.64219555
H	-4.09029311	-2.52048151	2.73622341
O	-3.36500455	-3.15582769	2.77749325
H	-3.26717223	-3.49743151	1.88744609
H	-1.86180962	-2.12209772	2.86435704
O	-1.32136663	-1.41655954	2.47479221
H	-0.39086061	-1.65770745	2.43988664
H	-4.23524732	1.76825939	-1.66781008
O	-3.61443549	1.40479813	-1.04180440
H	-3.94018249	0.50246644	-0.80056954
H	-4.83450954	-0.99729408	0.56046749
O	-4.45030785	-0.96267707	-0.32326859
H	-3.71741531	-1.59808988	-0.32168419
H	-2.70337358	3.48501599	1.20344217
O	-3.16727466	2.64752989	1.37308712
H	-3.36836533	2.26456527	0.50611617
H	-0.21422617	0.51172980	-2.69176914
O	0.29096597	-0.24702484	-3.08071223
H	0.03945510	-0.32524827	-3.99656921
H	0.17849131	-1.55075252	-1.90245727
O	0.21553573	-2.15471677	-1.14344172
H	1.06741747	-2.59389005	-1.18759159
H	-1.52908479	-2.67052895	-0.51851731
O	-2.26476649	-2.55929149	0.09265366
H	-1.89712684	-2.03214752	0.81314527
H	2.09135908	-0.07477602	-2.63045617
O	2.97383426	0.02654058	-2.25501781
H	3.11183823	-0.72210823	-1.66592106
H	1.26041709	-0.24221292	1.53692033
H	0.69184276	-1.25357422	0.48995114
O	1.21342281	-1.18035258	1.29999722
C	0.97343272	2.57378598	5.22400736
H	0.01843656	2.24210642	4.85585976
N	-1.44480050	4.76018134	0.67246011
H	-0.57917043	4.37027128	0.29080076
H	-1.36305119	5.77163896	0.63276227
H	1.59450708	1.90387136	5.79151033
H	1.25576255	3.60770260	5.13484720

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ts_ch3_nh2 W18			
H	3.77099113	3.01589653	-1.80247434
O	3.24141308	2.49016555	-1.21131328
H	3.21155187	1.58552147	-1.57627312
H	1.67643612	1.64968226	2.83864391
O	1.08972949	1.27617751	2.18408552
H	0.19232521	1.26588157	2.58604107
H	-1.82899384	1.66776921	-1.51831258
O	-0.93901606	1.78752821	-1.87047835
H	-0.38382985	2.21064080	-1.19600816
H	0.93710572	2.34909497	0.71504959

O	0.80947339	2.91195008	-0.06084502
H	1.66510231	2.90703593	-0.52068825
H	3.73070247	-2.85804951	-0.36376598
O	2.97707470	-2.30959300	-0.56139114
H	2.58696284	-2.01258820	0.27693324
H	-1.95015185	1.55939197	2.43569579
O	-1.39540187	1.07333041	3.06628349
H	-1.49806700	0.12709582	2.87853721
H	-4.13885058	1.80628315	2.83946624
O	-4.37492324	1.14752208	3.50727051
H	-3.56828640	1.02632153	4.00822566
H	-4.96059858	-0.29474359	2.82313007
O	-5.26684233	-1.11492663	2.38235133
H	-6.18193116	-1.23355750	2.62359145
H	-4.13089694	-2.60539762	2.64475858
O	-3.42194648	-3.26019205	2.65183220
H	-3.33507424	-3.55951421	1.74557993
H	-1.89078973	-2.27365136	2.78644732
O	-1.33049021	-1.56610741	2.42992102
H	-0.40709133	-1.83137704	2.38466585
H	-4.20323126	1.89506599	-1.55351651
O	-3.58368240	1.49212843	-0.95086715
H	-3.92410856	0.58579296	-0.74757377
H	-4.84075429	-0.95799413	0.54962335
O	-4.45767512	-0.88938883	-0.33262243
H	-3.73925751	-1.54041784	-0.36400729
H	-2.60716170	3.42866117	1.40243805
O	-3.09176069	2.59446865	1.52273969
H	-3.30745595	2.26869516	0.63619834
H	-0.20875148	0.59312418	-2.65280066
O	0.28208416	-0.15916899	-3.07141639
H	0.03162034	-0.19423931	-3.99024287
H	0.14680185	-1.51398605	-1.95419229
O	0.17457342	-2.15724200	-1.22778675
H	1.01515481	-2.61381711	-1.30186787
H	-1.58130557	-2.65943434	-0.62243659
O	-2.31179669	-2.55868149	-0.00333381
H	-1.92687527	-2.08064338	0.74199189
H	2.08567956	-0.04725961	-2.61449283
O	2.97095527	0.01647344	-2.23737988
H	3.09643402	-0.76568787	-1.69049272
H	1.28700773	-0.42245717	1.54213965
H	0.68249596	-1.36240078	0.45105366
O	1.21106889	-1.34572609	1.25968394
C	0.68915761	3.36280616	4.70052320
H	-0.13964425	2.68710174	4.58489057
N	-1.31344493	4.70041829	0.95727160
H	-0.46466196	4.31142255	0.53859798
H	-1.20171460	5.70937514	0.98655221
H	1.25407365	3.37850989	5.61508860
H	0.88705034	4.10035230	3.94306834

## 2.2.7 HCO + CH2OH

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p_Rc_hco_ch2oh W18			
O	-3.19355990	2.40875635	-1.64983878
O	-1.06275450	0.59268240	-1.43212421
O	1.60395885	0.98518007	-1.39127318
O	2.17882823	-1.67080743	-1.76076569
O	4.73664523	-1.23727141	-2.50266528
O	-2.16818273	1.23223143	1.10896229
O	-4.55757774	0.45845576	-0.20755576
O	-3.86811401	-2.03149675	0.27123664
O	-1.04243968	-0.11734799	3.17001527
O	-2.07591607	-2.38502905	2.44166296
O	-0.51880725	-3.51420380	0.50105084

O	-0.59070468	-2.05899580	-1.88986754
O	-2.61995117	-3.77938299	-1.54387537
O	1.56347576	2.56496953	0.85944602
O	1.60105532	0.82441800	2.99998146
O	3.28182900	-0.79225513	1.84083511
O	2.29540396	-3.03202498	0.66396874
O	3.87104871	2.57245183	-0.79333234
O	5.06807883	0.27388881	-0.16242933
O	-0.84615046	3.42000377	-0.50430560
C	-1.91360595	3.85600131	-0.17003029
H	-5.49521523	0.50433692	-0.04201822
H	-4.30693150	-0.49163194	-0.12564694
H	-3.31155607	-2.12742632	1.05441750
H	-3.54056389	-2.65918838	-0.38500710
H	1.40301681	-3.36904949	0.77783540
H	2.31387369	-2.67488062	-0.23268412
H	0.73985878	2.99458408	0.61263806
H	1.45215549	2.10487958	1.70341155
H	-3.07635981	0.97264057	0.93566021
H	-1.67927081	0.96399018	0.31681158
H	-1.09682932	-4.13332477	0.05331375
H	-1.02503346	-3.16319998	1.25060379
H	-1.63454223	-1.55747390	2.76411592
H	-2.36247224	-2.86875061	3.21166670
H	-1.95891565	-3.18036373	-1.93583997
H	-3.02880427	-4.27746468	-2.24550321
H	-0.87806585	-1.13238511	-1.84020279
H	-0.42652074	-2.33629694	-0.97782650
H	-0.10162793	0.09864214	3.17633325
H	-1.44832495	0.46767603	2.50980765
H	-0.13350542	0.87332370	-1.51347326
H	-1.60478232	1.31488463	-1.76775457
H	3.89299820	-0.47609407	1.16776697
H	2.92361182	-1.64233525	1.52813043
H	3.29214956	2.85617686	-0.07757087
H	3.25146092	2.21882890	-1.43959026
H	4.71042711	1.16900392	-0.34834617
H	5.94437959	0.38394184	0.19784606
H	2.97775039	-1.68261876	-2.30559527
H	1.39626195	-1.93640036	-2.25247803
H	5.14278260	-0.77523804	-3.22964944
H	4.93535952	-0.73682077	-1.69819065
H	2.24295508	0.20273080	2.57338128
H	1.97342972	1.06811258	3.84340840
H	1.88357903	0.05711362	-1.40969549
H	1.62862316	1.30192556	-0.47895963
H	-1.98474096	4.62642975	0.61244931
C	-3.24110231	3.47637873	-0.75882087
H	-3.73198824	1.68502395	-1.30293764
H	-3.62081757	4.37252448	-1.25912443
H	-3.90857042	3.27982495	0.08003363

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p\_dHa2\_hco\_ch2oh W18

C	-2.77205288	3.14181425	1.66432649
O	-2.90155355	4.23765877	1.18508261
C	-0.64802529	5.26556866	1.04699935
O	0.08874589	4.53326403	1.66095172
O	-2.50027565	1.07558923	-0.00824554
O	-4.80319744	-0.21381643	-0.66390669
O	-4.18687306	-2.76936497	-0.14612458
O	-1.08406971	0.84103568	-2.41926507
O	1.39615925	1.30984875	-1.67151638
O	2.03359530	-1.33803711	-1.96121197
O	4.67766344	-1.37507108	-2.45601790
O	1.58872708	2.34432487	0.87281777
O	1.29966231	0.29905243	2.65203385
O	3.18405171	-1.28876800	1.83277553



O	2.13159207	-3.15701688	0.20086079
O	-0.68090785	-1.93369377	-2.31867609
O	-2.50405701	-3.95213861	-2.13424894
O	-1.43661154	-0.18447873	2.14860694
O	-2.31809765	-2.63087202	1.97788242
O	-0.65461568	-3.49659019	-0.00264078
O	5.08455555	-0.11752206	-0.00117668
O	3.95744783	2.22743071	-0.54572894
H	-5.70917686	-0.02373070	-0.44207359
H	-4.65174030	-1.16524763	-0.50351330
H	-3.61632988	-2.76841437	0.63114226
H	-3.70599977	-3.21929551	-0.84867834
H	1.21985462	-3.45692050	0.26888318
H	2.14517659	-2.58719287	-0.57680612
H	1.08123095	3.13015185	1.11712570
H	1.47551708	1.69125693	1.58200354
H	-3.36737302	0.68378971	-0.20398011
H	-2.02365869	1.07801726	-0.84647172
H	-1.17019633	-4.11303025	-0.52638508
H	-1.18883873	-3.27626017	0.77576748
H	-1.99487114	-1.70486498	2.11089971
H	-2.46555485	-3.01638432	2.83678618
H	-1.95565404	-3.23363165	-2.48824686
H	-2.78924009	-4.49805654	-2.86109867
H	-0.95445451	-1.00739783	-2.36578479
H	-0.61556151	-2.17818191	-1.38520825
H	-0.48727275	-0.05156733	2.25956079
H	-1.73030566	0.28293549	1.34762126
H	-0.16211757	1.13121697	-2.23832139
H	-1.40130707	1.30449140	-3.18941969
H	3.85832621	-0.91550801	1.25550619
H	2.81491233	-2.05610288	1.35770132
H	3.28420451	2.42687996	0.12021060
H	3.44455122	2.11532657	-1.34852308
H	4.72898218	0.78227539	-0.16972977
H	5.94984009	-0.01572183	0.38691722
H	2.88059687	-1.45048054	-2.41678804
H	1.30015605	-1.68614424	-2.47774188
H	5.27710795	-1.03249648	-3.11150441
H	4.93190939	-0.99831824	-1.60091364
H	2.01345874	-0.32259980	2.35211416
H	1.43019876	0.43848096	3.58651025
H	1.69618763	0.38569489	-1.67418863
H	1.34459447	1.60685199	-0.74983787
H	-1.79199777	2.75468782	1.95391409
H	-1.15610049	6.09765008	1.53496055
H	-0.80254369	5.15825577	-0.02827162
H	-3.63027721	2.49684602	1.85836094

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C	-3.75404593	1.83143419	3.24444100
O	-4.73045099	1.83756620	2.59047470
C	-0.94543734	4.92620061	0.02355744
O	-0.60959861	3.74514113	0.59345949
O	-1.87675106	1.57966267	-0.26275405
O	-4.41410759	0.86484927	-0.19919068
O	-4.17302206	-1.84590816	-0.13838424
O	-0.68227079	0.88578311	-2.65467614
O	1.76495041	1.09665122	-1.74583223
O	2.19441601	-1.59333607	-1.97781307
O	4.85830640	-1.66077957	-2.30521536
O	1.79059095	2.37711920	0.69140654
O	1.50854419	0.55129533	2.72098872
O	3.15849583	-1.24611969	1.86740005
O	1.99533216	-3.15486522	0.34791995
O	-0.56693404	-1.90806262	-2.45495169
O	-2.79392397	-3.45038665	-2.09594227

O	-1.17253385	0.28518256	2.05044797
O	-2.27982248	-2.10268089	1.96482334
O	-0.81185781	-3.27095610	-0.02609445
O	5.17671742	-0.23664835	0.07486270
O	4.23360443	2.14883897	-0.64371282
H	-4.85790156	1.13232765	0.60512648
H	-4.43184451	-0.10737914	-0.23319754
H	-3.61554769	-2.01757295	0.62691963
H	-3.82088678	-2.37387800	-0.86169807
H	1.06522630	-3.39710811	0.36880198
H	2.11034490	-2.69417219	-0.49159685
H	1.05492123	3.00547061	0.69784209
H	1.70568810	1.83208362	1.48758411
H	-2.83989620	1.37930177	-0.26176267
H	-1.53618519	1.33930475	-1.13625403
H	-1.43647340	-3.81189620	-0.51353414
H	-1.29204962	-2.92498515	0.74082852
H	-1.86001824	-1.21911231	2.06889261
H	-2.42772429	-2.46725514	2.83289573
H	-2.10142435	-2.91384358	-2.51308729
H	-3.21313589	-3.97519789	-2.77184387
H	-0.71725852	-0.95850000	-2.55352522
H	-0.53263139	-2.10521658	-1.50885203
H	-0.23799791	0.35201401	2.29543188
H	-1.29030716	0.70551929	1.18317862
H	0.25659454	1.07511477	-2.42338798
H	-0.90098726	1.36727899	-3.44805942
H	3.86291981	-0.94938505	1.28145393
H	2.72981181	-2.00505190	1.43104037
H	3.56462104	2.46171781	-0.02196831
H	3.72344750	1.96402691	-1.43578848
H	4.89039007	0.67677660	-0.14431596
H	6.02705195	-0.17445228	0.50272505
H	3.06546553	-1.74593110	-2.37314671
H	1.48248309	-1.89663782	-2.54799163
H	5.49837602	-1.38787152	-2.95506598
H	5.07324664	-1.21228696	-1.47445900
H	2.13712106	-0.15680929	2.41724320
H	1.71230307	0.73819888	3.63354925
H	1.98712368	0.15147149	-1.71539107
H	1.68880913	1.42576154	-0.83611489
H	-1.17443744	3.01793509	0.26627632
H	-0.42355237	5.77823268	0.41910985
H	-1.93761330	5.02234518	-0.38526996
H	-2.77513369	1.40934839	2.93743659

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O	-3.76855670	1.50277520	-2.24062647
O	-1.24759866	0.50144827	-1.63476043
O	1.29935513	1.31767304	-1.60150286
O	2.08703022	-1.31242573	-1.73424172
O	4.66827652	-1.18779325	-2.49209732
O	-2.20611725	1.36151499	0.82350090
O	-4.64465475	0.16796132	-0.03191839
O	-3.79850019	-2.23392248	0.56123008
O	-0.91568166	0.12742918	2.89953384
O	-1.86640182	-2.26366654	2.60518475
O	-0.34067713	-3.47495976	0.69268989
O	-0.56751055	-2.14927327	-1.75065169
O	-2.50016995	-3.95577783	-1.24719170
O	1.61211925	2.65714553	0.81504365
O	1.78941094	0.89925020	2.89040721
O	3.56874676	-0.70955096	1.90504685
O	2.43221177	-2.80322325	0.62849386
O	3.81848414	2.57835374	-0.89894212
O	5.16415223	0.37975369	-0.23828153
O	-0.57744491	4.56758120	0.93966706

C	-1.72172485	4.43565627	0.70542890
H	-5.54958092	0.21956548	0.26395891
H	-4.34340055	-0.75847018	0.13333630
H	-3.18999496	-2.24366745	1.31157159
H	-3.45738947	-2.86133367	-0.08827544
H	1.57627322	-3.20342770	0.80187941
H	2.33870328	-2.34815492	-0.21721140
H	0.94828267	3.34027535	0.92995928
H	1.64197059	2.12483092	1.62677982
H	-3.11975865	1.06511355	0.77040817
H	-1.79599538	1.02843939	0.01052042
H	-0.90674001	-4.14562177	0.30824519
H	-0.82710968	-3.10445183	1.44594055
H	-1.47221616	-1.36654773	2.76208478
H	-2.06370318	-2.64099612	3.45816643
H	-1.88913674	-3.34773705	-1.69919016
H	-2.90095502	-4.52096278	-1.90115284
H	-0.89661028	-1.23563872	-1.74922101
H	-0.37472472	-2.37656481	-0.83026022
H	0.02782268	0.33158313	2.90207086
H	-1.33639281	0.66415094	2.20954149
H	-0.39325914	0.94111126	-1.80258985
H	-1.94883132	0.90702038	-2.15506283
H	4.13806099	-0.37237318	1.20521894
H	3.17766608	-1.53599940	1.56914149
H	3.23794311	2.83749313	-0.17279085
H	3.20157104	2.31753790	-1.58768232
H	4.72749340	1.23113240	-0.45962278
H	6.05293782	0.57927722	0.04467156
H	2.90246367	-1.40871010	-2.24810746
H	1.34353402	-1.75524573	-2.15527890
H	5.12164709	-0.82487879	-3.24673865
H	4.95329049	-0.68759179	-1.71350191
H	2.47008689	0.27141947	2.53098043
H	2.08593637	1.16321776	3.75763306
H	1.64878651	0.41182626	-1.58320619
H	1.32895857	1.66270170	-0.69812670
H	-2.18781191	3.52618665	0.27605101
C	-3.89228277	2.82179767	-1.96662713
H	-4.16202872	0.97117099	-1.52848855
H	-3.59525404	3.47292167	-2.76882238
H	-4.65270957	3.12418991	-1.26495186

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O	-3.67532764	1.38302604	-2.30144396
O	-1.20469513	0.55267019	-1.59787344
O	1.38784922	1.35746713	-1.55346710
O	2.06839844	-1.29848125	-1.74680391
O	4.63784119	-1.17455596	-2.55298370
O	-2.03840771	1.42077027	0.90379989
O	-4.52887428	0.28531611	0.11438180
O	-3.80490104	-2.18476108	0.67332819
O	-0.83707971	0.07712398	2.95108255
O	-1.82780124	-2.30089689	2.67291353
O	-0.35434154	-3.48394093	0.69921241
O	-0.58507112	-2.09493088	-1.71458833
O	-2.54635212	-3.87009324	-1.21169720
O	1.63056171	2.55341493	0.97582915
O	1.91157112	0.71865935	2.94681260
O	3.64861058	-0.87071894	1.87732761
O	2.42889967	-2.88120602	0.55595013
O	3.85410831	2.55115086	-0.77997255
O	5.19544113	0.31060584	-0.25029500
O	-0.85029339	4.36278622	1.11792792
C	-1.93707407	4.33695013	0.82335848
H	-5.41540743	0.39423813	0.44746744
H	-4.27852593	-0.65323783	0.27898765

H	-3.18409236	-2.23029771	1.41155100
H	-3.48166121	-2.79301904	-0.00235017
H	1.56513170	-3.25844741	0.74366700
H	2.32611141	-2.39381794	-0.27041190
H	0.92762483	3.17402925	1.15627653
H	1.70966922	1.96732411	1.74856006
H	-2.96764043	1.17593612	0.84428441
H	-1.65775342	1.10070784	0.07239979
H	-0.94722925	-4.12002566	0.29621956
H	-0.82027780	-3.12698366	1.47147584
H	-1.42749595	-1.40606927	2.82550349
H	-2.00966415	-2.68302539	3.52703071
H	-1.93630635	-3.25885985	-1.66099744
H	-2.97291958	-4.40765623	-1.87257542
H	-0.88666886	-1.17020784	-1.70049736
H	-0.38709398	-2.33768061	-0.79980001
H	0.11517193	0.22972685	2.94759121
H	-1.23307431	0.62969431	2.25602928
H	-0.38368979	1.01433672	-1.82620631
H	-1.96860695	0.91864789	-2.07238264
H	4.20272945	-0.50966160	1.17711007
H	3.23256841	-1.67479691	1.51612292
H	3.30958839	2.81066085	-0.02937736
H	3.20094304	2.28751117	-1.43673689
H	4.76376629	1.17640657	-0.41801496
H	6.09536349	0.48598169	0.01268316
H	2.86858386	-1.39795625	-2.28282863
H	1.30593301	-1.72357970	-2.15321559
H	5.06795648	-0.77684205	-3.30374114
H	4.93653380	-0.70063055	-1.76347595
H	2.57747746	0.09374247	2.55239502
H	2.22310999	0.94197652	3.82007858
H	1.68005166	0.43111711	-1.57209536
H	1.35980121	1.62979109	-0.62716561
H	-3.62718591	3.20525151	-1.31167463
C	-3.97214321	2.76041732	-2.24337620
H	-4.08312670	0.94103223	-1.54494536
H	-3.46293281	3.24074054	-3.07148070
H	-5.04102860	2.93761435	-2.34850812

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O	-3.82153372	1.07890860	-2.46278429
O	-1.25051262	0.59904662	-1.60491781
O	1.30955561	1.39892096	-1.59994979
O	2.04995810	-1.25162723	-1.71958477
O	4.62090383	-1.23675218	-2.52311714
O	-2.22750226	1.42921950	0.82696254
O	-4.61675754	0.15826691	-0.01400246
O	-3.83497198	-2.24885951	0.63911740
O	-0.90411968	0.11803121	2.85229656
O	-1.87284491	-2.27981050	2.65255239
O	-0.36536958	-3.46955491	0.70858983
O	-0.60595337	-2.06383274	-1.68764262
O	-2.52753417	-3.89357807	-1.22900881
O	1.74411928	2.67355692	0.85454370
O	1.82102696	0.82601748	2.85545033
O	3.59861690	-0.79220843	1.89007960
O	2.41132604	-2.83468398	0.58637650
O	3.91229501	2.51214781	-0.88977389
O	5.20369327	0.27593984	-0.25460924
O	-0.28983361	4.65930812	1.42821757
C	-1.43887290	4.40348690	1.40389104
H	-5.51624830	0.25309579	0.28796594
H	-4.34089401	-0.76774507	0.19548572
H	-3.22040353	-2.26554561	1.38420436
H	-3.48961133	-2.85772470	-0.02594077
H	1.55184333	-3.22355885	0.76848158

H	2.30697041	-2.34552110	-0.23870529
H	1.17112665	3.41700759	1.05483950
H	1.75961814	2.09584573	1.63561972
H	-3.13858765	1.12663293	0.74536059
H	-1.80997379	1.15200106	-0.00507555
H	-0.93977453	-4.12072260	0.30317084
H	-0.84382787	-3.11995035	1.47619470
H	-1.47705911	-1.37975360	2.77844715
H	-2.04749850	-2.64009682	3.51769540
H	-1.92773408	-3.26318787	-1.66522936
H	-2.92984289	-4.43862635	-1.89897030
H	-0.91254387	-1.14225250	-1.67146206
H	-0.40884420	-2.31187926	-0.77385974
H	0.04268657	0.30660739	2.83384750
H	-1.33492709	0.65215697	2.16749978
H	-0.40537848	1.03989323	-1.80605557
H	-1.95847888	0.90511014	-2.18298783
H	4.17367129	-0.45791628	1.19332005
H	3.19418981	-1.60842394	1.54458333
H	3.34306057	2.77679082	-0.15611217
H	3.28645632	2.29636523	-1.58551909
H	4.78564115	1.13819023	-0.47002811
H	6.10059022	0.45301654	0.01743580
H	2.85335334	-1.37283920	-2.24713452
H	1.29004783	-2.168321540	-2.12304836
H	5.07818450	-0.88189393	-3.27922320
H	4.94077837	-0.76380121	-1.74108967
H	2.49957307	0.19264704	2.49935366
H	2.09999818	1.06086654	3.73693368
H	1.64028935	0.48637074	-1.57572620
H	1.35416309	1.74887258	-0.69996588
H	-1.86924700	3.40564389	1.17704296
C	-4.40077964	2.26604015	-2.75915016
H	-4.17907195	0.71672133	-1.63518142
H	-4.12580214	2.66979165	-3.71617756
H	-5.36041898	2.48533675	-2.32105711

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O	-3.59299915	1.88803920	-2.07937856
O	-1.19178182	0.64141858	-1.48448721
O	1.39655887	1.30526375	-1.46698506
O	2.05701416	-1.34728107	-1.74097950
O	4.64848680	-1.29547143	-2.47108223
O	-2.20285788	1.25396217	1.01717786
O	-4.66135664	0.37490647	-0.05224869
O	-3.90928439	-2.09466924	0.39256516
O	-0.95951584	-0.10328899	3.02870308
O	-2.02198212	-2.40671508	2.47810575
O	-0.51526685	-3.53606260	0.50339976
O	-0.64144659	-2.02135655	-1.83300035
O	-2.66907895	-3.76048273	-1.50292707
O	1.75909994	2.60245102	0.96102380
O	1.72837189	0.75280776	2.97598089
O	3.43943655	-0.89328736	1.92577180
O	2.27778454	-2.92555395	0.57051975
O	3.97268047	2.45251933	-0.74167983
O	5.16322435	0.15049184	-0.13972213
O	-0.39342655	4.51620130	0.52155365
C	-1.53604456	4.23009234	0.55150123
H	-5.57271269	0.44456787	0.21903328
H	-4.40562386	-0.57403297	0.04416001
H	-3.31941747	-2.18528909	1.15179264
H	-3.58733527	-2.69811074	-0.28890726
H	1.41005841	-3.31791861	0.69482486
H	2.22778646	-2.44613650	-0.26563353
H	1.11322105	3.31118334	0.99883603
H	1.69129631	2.06430039	1.76578535

H	-3.13224840	1.03723636	0.89255064
H	-1.77442875	0.99388433	0.18552658
H	-1.09612641	-4.15666791	0.06161015
H	-1.00559865	-3.20080457	1.27064815
H	-1.57385009	-1.56154614	2.73751679
H	-2.26706747	-2.85620822	3.28238768
H	-2.01892583	-3.15153165	-1.89536680
H	-3.08826581	-4.24716955	-2.20659608
H	-0.92707096	-1.09607396	-1.75915025
H	-0.47353895	-2.33121991	-0.93191928
H	-0.01744026	0.10732057	3.02761440
H	-1.38389064	0.47119609	2.37270502
H	-0.30815727	1.03245302	-1.62421640
H	-1.85732310	1.13310466	-1.97809115
H	4.04564437	-0.57032476	1.25069356
H	3.02627741	-1.69765687	1.56430456
H	3.40288573	2.71905181	-0.01001670
H	3.34828619	2.25097488	-1.44315982
H	4.78910973	1.03631708	-0.33876023
H	6.05409997	0.28003944	0.17554546
H	2.86982755	-1.45426247	-2.25652243
H	1.29233720	-1.71554594	-2.19466812
H	5.12543410	-0.91208162	-3.20067563
H	4.93701014	-0.84253476	-1.66539585
H	2.38284121	0.11645506	2.58536600
H	2.03819332	0.95881148	3.85436850
H	1.70789557	0.38600045	-1.48948540
H	1.46441090	1.62182108	-0.55575064
H	-1.94576179	3.29064721	0.96685663
C	-3.62924629	3.19554725	-1.72787788
H	-4.06385621	1.33981497	-1.43129897
H	-3.23859246	3.86732951	-2.46966842
H	-4.39306025	3.51533366	-1.03896856

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ts\_dHa2\_hco\_ch2oh W18

C	-2.66910222	3.01422026	2.24509430
O	-3.44968864	3.85066002	1.98410409
C	-0.86295517	5.18136545	0.83433757
O	-0.44194895	4.09991400	1.47541223
O	-2.33406343	1.27932392	0.24270124
O	-4.67998031	0.09351709	-0.41566740
O	-4.20299124	-2.49160128	0.10737120
O	-0.92696611	1.00286953	-2.16932147
O	1.57996940	1.29801117	-1.42734762
O	2.09373094	-1.37307976	-1.73425394
O	4.73939295	-1.40472453	-2.20656002
O	1.70631659	2.38927450	1.08928112
O	1.37482904	0.39443901	2.93209676
O	3.18747323	-1.24292083	2.06337670
O	2.10302561	-3.12776427	0.47101685
O	-0.66057373	-1.79311814	-2.07928878
O	-2.56461924	-3.73229809	-1.87901194
O	-1.36496023	-0.00713336	2.40748621
O	-2.32930129	-2.43392398	2.23822151
O	-0.69549284	-3.34911607	0.24684745
O	5.12644352	-0.11862806	0.24226515
O	4.09858523	2.26934119	-0.32385080
H	-5.56736790	0.34433529	-0.17912390
H	-4.58603129	-0.86457760	-0.25230716
H	-3.63651026	-2.52042532	0.88652040
H	-3.73934843	-2.95876673	-0.59571199
H	1.17905934	-3.38832369	0.53505526
H	2.15039378	-2.59106288	-0.32882011
H	1.04293638	3.08226183	1.20128139
H	1.59000116	1.76263404	1.82041467
H	-3.21293039	0.92093396	0.03095924
H	-1.85074864	1.29008553	-0.59188038

H	-1.23474956	-3.94182791	-0.28066813
H	-1.22222474	-3.11149012	1.02463457
H	-1.97538997	-1.52214404	2.37661843
H	-2.48061474	-2.82432578	3.09428692
H	-1.99084725	-3.03512404	-2.23583553
H	-2.87150595	-4.26869281	-2.60415901
H	-0.88749492	-0.85446798	-2.12896736
H	-0.59605882	-2.03353175	-1.14501985
H	-0.41532229	0.09024829	2.55514383
H	-1.59697303	0.43722259	1.57251226
H	0.01370596	1.22874295	-1.99239337
H	-1.21272232	1.48513441	-2.94030701
H	3.86774288	-0.88695213	1.48205698
H	2.80219363	-2.00870887	1.59827395
H	3.44296154	2.51392002	0.34214578
H	3.56718254	2.13356197	-1.11173777
H	4.81017116	0.79530628	0.07146219
H	5.99099948	-0.05250197	0.63978477
H	2.93844581	-1.49583062	-2.19111928
H	1.34976480	-1.67689006	-2.26257867
H	5.34257643	-1.06413266	-2.85971949
H	4.97839591	-1.01154063	-1.35454499
H	2.05995193	-0.25067517	2.61328084
H	1.54328627	0.53867397	3.85969730
H	1.83452874	0.36061582	-1.43850684
H	1.52970734	1.58645809	-0.50215089
H	-1.22054883	3.49104338	1.80634793
H	-0.79082590	6.13364548	1.33303767
H	-1.37623227	5.06999632	-0.10695712
H	-2.87170368	2.02203171	2.69919510

## 2.2.8 HCO + CH3

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p_Rc_hco_ch3 W18			
C	-1.28980307	4.38039859	-1.16226435
O	-1.35972318	0.83743719	-2.27751889
O	1.19902991	1.32419042	-1.91614763
O	1.64136721	-1.35622062	-1.88098647
O	3.99622840	-2.62161206	-1.48525979
O	-2.50011023	1.77192167	0.12730918
O	-4.96187713	0.58264854	-0.06606636
O	-4.41501607	-1.98626462	0.52284995
O	-1.31579366	0.48922225	2.25007097
O	-2.33327825	-1.88139642	2.41734766
O	-0.95956941	-3.25332013	0.52234286
O	-1.10109667	-1.92634090	-1.94337917
O	-3.09155719	-3.68662008	-1.37010336
O	1.77363187	2.51570025	0.50136648
O	1.46781294	0.83303625	2.62743506
O	3.13864633	-1.10247973	2.07509780
O	1.81109669	-2.88670765	0.47609980
O	4.03449288	1.89270422	-0.95677085
O	4.97910648	-0.42062180	0.01115094
O	-0.33867795	4.19673557	1.01980356
C	-1.31646382	4.34771030	0.32835581
H	-5.79601308	0.81510086	0.32982581
H	-4.81738464	-0.36669372	0.10750688
H	-3.76444467	-1.98288335	1.23511513
H	-4.08641698	-2.58983045	-0.15085972
H	0.94907028	-3.27074172	0.66844332
H	1.63882295	-2.25701151	-0.23475661
H	1.16880314	3.25738060	0.63620227
H	1.68560322	1.95693131	1.29066272
H	-3.41692983	1.45529525	0.14577153
H	-2.14194093	1.44177045	-0.70486289
H	-1.59830505	-3.84972140	0.12643370

H	-1.40056946	-2.84118978	1.28337327
H	-1.94308829	-0.96911640	2.39108677
H	-2.46725983	-2.11237419	3.33220196
H	-2.50500137	-3.08933846	-1.86140658
H	-3.50961090	-4.27541556	-1.99167171
H	-1.30648988	-0.98546890	-2.03975689
H	-0.96183184	-2.10384969	-1.00333624
H	-0.36493909	0.62487837	2.32711817
H	-1.66192774	1.02561442	1.51789361
H	-0.41450198	1.11094935	-2.22579845
H	-1.71606321	1.15826953	-3.10152823
H	3.84308505	-0.85328966	1.46584841
H	2.66694607	-1.83522844	1.64971322
H	3.39358185	2.28522117	-0.34739817
H	3.55698493	1.81457062	-1.78229901
H	4.66552917	0.42839406	-0.36422987
H	5.91133899	-0.31913460	0.18513135
H	2.45991085	-1.84211947	-2.07191646
H	0.87800724	-1.77836096	-2.28671458
H	3.63105377	-3.18166871	-0.79842460
H	4.46227477	-1.91325277	-1.02417037
H	2.09534285	0.08775340	2.46099756
H	1.64288868	1.16122026	3.50563205
H	1.47992375	0.39548734	-1.88970583
H	1.31926065	1.68557989	-1.02415290
H	-2.28894268	4.51606354	0.80034723
H	-2.12607963	3.81360722	-1.55563289
H	-1.40733579	5.41569478	-1.48195181
H	-0.35200340	3.99428405	-1.54574239

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p\_dHa\_hco\_ch3 W18

C	-1.40433320	4.15619160	-1.79996992
O	-1.62089028	0.45097032	-2.42196809
O	0.85134176	1.37655287	-2.15867839
O	1.69082082	-1.18708154	-1.95551874
O	4.26184504	-1.92435628	-1.59086812
O	-0.90921186	-2.19674976	-1.88577283
O	-2.49160503	-4.26376156	-1.10452983
O	-2.67462096	1.22225839	0.08806440
O	-1.35946788	0.32547368	2.27634467
O	-1.96591050	-2.17444255	2.59404083
O	-0.43058338	-3.30643320	0.65719206
O	-4.95640553	-0.28804307	-0.00867712
O	-4.04003360	-2.71059496	0.75172178
O	1.05345893	2.81166935	0.22432978
O	1.29210378	1.29545049	2.45158136
O	3.24973423	-0.31708178	1.87697976
O	2.22283309	-2.43983295	0.49731064
O	3.39913130	2.56998575	-1.32799477
O	4.84292923	0.54878703	-0.31006770
O	-1.46737339	3.78374078	1.74384646
C	-2.52520806	3.52911925	2.03550853
H	-5.80824326	-0.13229706	0.38711601
H	-4.68451027	-1.19179876	0.23607658
H	-3.38978281	-2.56566095	1.44876678
H	-3.62721833	-3.28830427	0.10228641
H	1.45451481	-2.96185016	0.75216521
H	1.91765832	-1.92825494	-0.26241717
H	0.33379352	3.43275323	0.31586928
H	1.11612029	2.33060442	1.06830363
H	-3.54857548	0.80246657	0.12387677
H	-2.32224249	0.98325643	-0.77619748
H	-0.94874148	-4.03441247	0.30739620
H	-0.91441339	-2.97031696	1.42867249
H	-1.73344312	-1.21293020	2.53000036
H	-2.03466384	-2.39817734	3.51777840
H	-2.05737908	-3.60050231	-1.66430188



H	-2.82104751	-4.96037426	-1.66492071
H	-1.28176450	-1.32176692	-2.06493899
H	-0.72460655	-2.25371251	-0.93913024
H	-0.44207495	0.61720988	2.30608991
H	-1.77633867	0.67943869	1.46956595
H	-0.74598312	0.89156919	-2.46252014
H	-2.13909886	0.74289144	-3.16709734
H	3.87459508	0.00815665	1.21851811
H	2.90422135	-1.15476353	1.52899295
H	2.75930291	2.89737169	-0.68604704
H	2.85581480	2.29992910	-2.07092444
H	4.35164516	1.29736904	-0.70716581
H	5.74770046	0.83294330	-0.20827029
H	2.57641228	-1.52497389	-2.16399429
H	0.99872552	-1.75721502	-2.30509591
H	4.04687838	-2.48725169	-0.84566470
H	4.58816940	-1.09958324	-1.21100327
H	2.04400964	0.67728009	2.26438101
H	1.45169886	1.68329156	3.30815768
H	1.25093275	0.49520133	-2.07172760
H	0.83203742	1.77319646	-1.27694917
H	-1.91337425	3.43587171	-1.16887054
H	-2.09920317	4.54258651	-2.53835241
H	-0.57020922	3.68062228	-2.30473926
H	-1.04170311	4.98373307	-1.19726581

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	r_Rc_dHa_hco_ch3 W18		
C	-4.12413161	1.74290054	-3.27415584
O	-1.33571173	0.83443456	-2.02612521
O	1.28038738	1.24463548	-2.08429084
O	1.58889470	-1.44285428	-1.76921067
O	3.90400454	-2.79917993	-1.43996289
O	-2.17277152	1.96722237	0.36405944
O	-4.68852963	0.92436805	0.07391476
O	-4.27094599	-1.56995564	0.95559392
O	-0.97755779	0.77060070	2.52230462
O	-2.14969170	-1.52602980	2.82289919
O	-0.92195445	-3.06770302	0.94556130
O	-1.16045870	-1.89730006	-1.59702241
O	-3.17267875	-3.52513792	-0.80828276
O	2.03414918	2.62483968	0.22449986
O	1.81980360	1.14623474	2.50946078
O	3.35313057	-0.89501266	1.99351243
O	1.85383310	-2.77414394	0.68971540
O	4.16026706	1.72402488	-1.33670033
O	5.08777180	-0.52655061	-0.22470795
O	0.27778896	4.88455104	0.68559362
C	-0.89276926	4.78637529	0.77079466
H	-5.52389780	1.23121341	0.41388229
H	-4.58616352	-0.00392756	0.36421885
H	-3.61196918	-1.56623072	1.65986073
H	-4.01959708	-2.26822057	0.34185942
H	0.99671769	-3.11427224	0.96687401
H	1.65705277	-2.20902274	-0.06808670
H	1.59981480	3.47440495	0.32908349
H	1.95592063	2.15948826	1.07392214
H	-3.11287494	1.72728699	0.37183210
H	-1.83626986	1.59009608	-0.46154872
H	-1.59765085	-3.66448064	0.61741698
H	-1.31170989	-2.59754687	1.69987015
H	-1.68896827	-0.65136208	2.76147012
H	-2.28347735	-1.71911617	3.74661898
H	-2.58663845	-2.99023264	-1.36873643
H	-3.65020762	-4.13310622	-1.36520293
H	-1.33033508	-0.95374061	-1.73983628
H	-0.96726883	-2.02005268	-0.65829053
H	-0.01759853	0.85867242	2.49245452

H	-1.35617516	1.23757321	1.75967224
H	-0.40590335	1.09086190	-2.20530607
H	-1.90530121	1.17763738	-2.71527843
H	4.02943962	-0.74928583	1.32148199
H	2.82577379	-1.64753312	1.68260491
H	3.59995209	2.20359449	-0.71285333
H	3.60407172	1.60306338	-2.10676854
H	4.78209690	0.29490456	-0.66294205
H	6.03373864	-0.45417327	-0.12700397
H	2.36770300	-1.98220172	-1.98121552
H	0.77982495	-1.85373891	-2.08960194
H	3.56591470	-3.27784014	-0.68158380
H	4.43625056	-2.07979938	-1.07865659
H	2.40423328	0.36414564	2.33959827
H	2.09442842	1.52165301	3.34243319
H	1.50639737	0.30861055	-1.96463390
H	1.44603463	1.68857969	-1.24161797
H	-1.47370870	3.84895056	0.63864447
H	-4.34592931	1.42592856	-2.26867229
H	-4.24919782	1.06046938	-4.09660514
H	-3.93451351	2.78157125	-3.48197380

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ts Rc_hco_ch3 W18			
C	-2.54113585	3.99336611	-2.55224780
O	-1.18420292	1.06333682	-2.07926246
O	1.41365677	1.39720214	-1.73967630
O	1.69271707	-1.30217573	-1.84474558
O	3.99410426	-2.66916315	-1.48455806
O	-2.26755553	1.78741653	0.38170979
O	-4.76780564	0.81389462	-0.00569444
O	-4.39032603	-1.80491392	0.43886726
O	-1.22740951	0.36534929	2.48651265
O	-2.36571040	-1.96934065	2.40467742
O	-1.01438191	-3.19800878	0.38638209
O	-1.07464953	-1.71750667	-2.00894990
O	-3.12927889	-3.43036507	-1.55089045
O	1.95723986	2.49617563	0.75614598
O	1.55448174	0.73637744	2.79782631
O	3.11793015	-1.22896154	2.10788144
O	1.76671796	-2.92383496	0.44096534
O	4.21484613	1.80923845	-0.73389941
O	5.04946162	-0.58433010	0.12705378
O	0.09793295	4.70487106	1.02836140
C	-1.07344766	4.60278799	0.95964059
H	-5.60166265	1.08218690	0.36769702
H	-4.69370494	-0.15259303	0.11466779
H	-3.76613968	-1.89359661	1.16851662
H	-4.07807761	-2.37903924	-0.26813792
H	0.89063113	-3.29335284	0.59299200
H	1.63060767	-2.27295316	-0.25923875
H	1.47940928	3.31874355	0.88470638
H	1.80561012	1.94328837	1.54055648
H	-3.20391231	1.52929726	0.32916925
H	-1.87916634	1.50838283	-0.45924910
H	-1.66220492	-3.74118689	-0.06741223
H	-1.45391258	-2.84612192	1.17673141
H	-1.92603034	-1.08634723	2.49013307
H	-2.53665811	-2.29536084	3.28377337
H	-2.51727020	-2.82747424	-2.00352278
H	-3.56905763	-3.96145177	-2.20848511
H	-1.24122605	-0.76562978	-2.06690241
H	-0.95323117	-1.93836207	-1.07635891
H	-0.27110468	0.46404828	2.56105236
H	-1.54179968	0.91724290	1.75216135
H	-0.22866798	1.29207117	-2.05174214
H	-1.60557108	1.63414824	-2.71983941
H	3.85336162	-1.00149335	1.52698646

H	2.62480332	-1.92970511	1.65257877
H	3.60711428	2.20457780	-0.09591916
H	3.71533938	1.78817850	-1.55070032
H	4.78402399	0.29464876	-0.21491248
H	5.98288657	-0.53870024	0.31758166
H	2.49468892	-1.80545847	-2.05903386
H	0.92285043	-1.65080300	-2.30441268
H	3.59992579	-3.24449067	-0.82713005
H	4.48361988	-2.00236700	-0.98753457
H	2.14859686	-0.02038648	2.56035075
H	1.75288368	0.97291077	3.70043985
H	1.63240811	0.45163509	-1.74680568
H	1.51291692	1.71422249	-0.83135606
H	-1.63033149	3.65552335	0.79748835
H	-3.05642801	3.51908408	-1.73644340
H	-3.07959294	4.27189426	-3.43991087
H	-1.51899820	4.30585782	-2.43138467

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ts\_dHa\_hco\_ch3 W18

C	-3.58248095	3.25261340	-2.23701442
O	-1.23932681	0.94985727	-2.00795361
O	1.33806969	1.50629269	-1.80491512
O	1.85393356	-1.15803231	-1.86774025
O	4.28481600	-2.27051044	-1.48174283
O	-0.86151112	-1.80251630	-1.97167376
O	-2.76477981	-3.67022123	-1.51345326
O	-2.29821720	1.60161263	0.50812252
O	-1.15409497	0.28608513	2.60068522
O	-2.12696004	-2.10667149	2.40790303
O	-0.65816157	-3.25215082	0.42707605
O	-4.73197554	0.51706923	-0.10825949
O	-4.12250910	-2.04463147	0.40129385
O	1.71908210	2.70003647	0.67789473
O	1.57752778	0.97816391	2.79631763
O	3.30663619	-0.83926393	2.08199133
O	2.09072856	-2.68630755	0.46690729
O	4.04079835	2.26507105	-0.82703624
O	5.11873134	-0.02592725	0.05008585
O	-0.70135407	4.27234730	0.39937985
C	-1.69974162	4.10943213	0.99950623
H	-5.59201173	0.69576772	0.26034766
H	-4.56311652	-0.43728865	0.01961477
H	-3.50522426	-2.08202761	1.14157244
H	-3.77840500	-2.63363710	-0.27838131
H	1.25733125	-3.13850564	0.63318087
H	1.89060524	-2.07407435	-0.25268287
H	1.04936153	3.38584253	0.71248573
H	1.63598959	2.16325481	1.48280920
H	-3.21196918	1.29109834	0.41387319
H	-1.87632955	1.37663649	-0.33178390
H	-1.25280133	-3.86081786	-0.01578009
H	-1.13491821	-2.91997018	1.20497410
H	-1.73710427	-1.20315461	2.53215717
H	-2.30677873	-2.46458278	3.27276675
H	-2.19709998	-3.02458776	-1.96580148
H	-3.16284638	-4.23346348	-2.17079188
H	-1.11238405	-0.86782777	-2.01348420
H	-0.71051437	-2.02104028	-1.04248855
H	-0.21160359	0.47838727	2.66533722
H	-1.52424031	0.82408520	1.88061050
H	-0.31253138	1.27180002	-2.05277685
H	-1.76335469	1.44238509	-2.63682694
H	3.99875936	-0.54666743	1.47761704
H	2.86997668	-1.58815182	1.64659249
H	3.40948931	2.60903850	-0.18324695
H	3.52162266	2.16301184	-1.62605884
H	4.76055109	0.81761397	-0.29701591

H	6.04537395	0.11713487	0.22482540
H	2.69592110	-1.58997998	-2.08184533
H	1.11158025	-1.58286843	-2.30804425
H	3.95299363	-2.85697200	-0.80024714
H	4.69673265	-1.53367404	-1.01418784
H	2.23691839	0.28083416	2.55279531
H	1.79240028	1.26925092	3.67888452
H	1.63320632	0.58187221	-1.81049393
H	1.40433519	1.82618934	-0.89437776
H	-2.72051540	4.15201270	0.58240153
H	-4.01760096	2.41029369	-1.72785945
H	-2.63827578	3.65248436	-1.91230163
H	-4.11856558	3.74175728	-3.03018743

## 2.2.9 HCO + CH3O

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p\_Rc\_hco\_ch3o W18

C	-1.71255184	1.61842942	4.21599441
O	-1.41005376	1.78389408	-1.53762871
O	1.21670237	1.79817201	-1.42484985
O	1.44448987	-0.53934564	-2.84314191
O	3.91280303	-0.34489873	-3.89634438
O	-2.29516998	1.31363365	1.08995429
O	-4.80228920	0.36321981	0.57417562
O	-4.39478023	-2.18086274	-0.15804650
O	-0.95957618	-0.81618216	2.16755095
O	-2.10962034	-2.98218746	1.29915817
O	-1.03943936	-3.12590414	-1.20261578
O	-1.35002080	-0.77405986	-2.67851872
O	-3.37237108	-2.58641800	-2.79087641
O	2.05620000	1.96390261	1.18307831
O	1.83856179	-0.57326121	2.19808829
O	3.28124761	-1.78187463	0.40149755
O	1.76591449	-2.98223172	-1.48802186
O	4.01929111	2.35035075	-0.72010888
O	4.89604326	-0.09023972	-1.29791764
C	-0.00704730	3.63436798	1.95472583
O	-0.87253488	3.15282144	2.63409487
H	-5.63335388	0.44170469	1.03144319
H	-4.71592010	-0.56490262	0.28137291
H	-3.67631430	-2.52337008	0.38609889
H	-4.15083462	-2.33819452	-1.07656291
H	0.85774329	-3.26256992	-1.34147268
H	1.69134215	-2.18979519	-2.03305049
H	1.45035864	2.60417670	1.58067741
H	1.97900715	1.13411555	1.67714871
H	-3.21558773	1.02474158	0.98293999
H	-1.99361274	1.53953593	0.20055640
H	-1.73817004	-3.46363129	-1.76599447
H	-1.36628354	-3.17969347	-0.29141234
H	-1.66063847	-2.18402569	1.67497442
H	-2.10271119	-3.66352445	1.96530220
H	-2.80135667	-1.82237224	-2.97524640
H	-3.88369488	-2.77415682	-3.57248663
H	-1.49659161	0.09761010	-2.28476237
H	-1.10216775	-1.38078474	-1.96722089
H	0.00200982	-0.72771712	2.13067293
H	-1.35917003	-0.03102870	1.75511191
H	-0.43485284	1.92077667	-1.51521775
H	-1.80024843	2.53755670	-1.97216990
H	3.84999176	-1.23998476	-0.15542101
H	2.75081421	-2.33195889	-0.20340322
H	3.54861568	2.32987507	0.12458712
H	3.32132811	2.52792646	-1.35398216
H	4.64268680	0.82707416	-1.05333822
H	5.82473250	-0.19146585	-1.10536507

H	2.15778761	-0.46004272	-3.49283858
H	0.58098750	-0.59926457	-3.26190976
H	4.36927852	0.25905668	-4.47378011
H	4.35097852	-0.30902519	-3.03329430
H	2.38306006	-1.05355904	1.52256597
H	2.19862912	-0.79426112	3.05295023
H	1.39645498	0.93919654	-1.83902619
H	1.44493188	1.73963606	-0.48338367
H	-1.90894413	3.48319848	2.59573370
O	-0.62467627	2.19287505	3.49810750
H	-1.65970772	0.54824908	4.07161394
H	-1.60166371	1.87389031	5.26345347
H	-2.65921447	1.98740667	3.83618719

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p\_dHa2\_hco\_ch3o W18

C	-3.97630849	2.43829814	-2.67575444
O	-1.02198752	1.26500729	-1.62818415
O	1.59983393	1.45234630	-1.13997408
O	1.91123612	-1.18804331	-1.86390504
O	4.50559213	-1.33869826	-2.57471583
O	-2.08926816	1.59558534	0.89840765
O	-4.65555495	0.80163046	0.14821711
O	-4.27211477	-1.82657434	0.15394450
O	-1.10790545	-0.22576175	2.70143523
O	-2.36090681	-2.42445035	2.13096016
O	-0.94422074	-3.32155478	-0.02467145
O	-0.86178644	-1.43832865	-2.09153790
O	-3.00441100	-3.07581858	-2.05332994
O	2.02618432	2.10005704	1.52510186
O	1.68561170	-0.14877089	3.03858415
O	3.27231623	-1.77482660	1.78645088
O	1.88978812	-3.27976977	0.02168095
O	4.26495766	1.99408689	-0.11422603
O	5.15392829	-0.50539789	0.00485709
O	0.45154848	4.18152698	2.54995915
C	-0.74754563	4.12199040	2.43902905
H	-5.45552821	0.96762360	0.63886559
H	-4.54910048	-0.17322936	0.11106960
H	-3.67902698	-2.06729185	0.87655952
H	-3.94926627	-2.27456454	-0.63625177
H	0.95883522	-3.50249047	0.11147802
H	1.92385271	-2.61755517	-0.67915736
H	1.54697668	2.85944304	1.87975464
H	1.91484559	1.36748354	2.15099006
H	-3.02411662	1.38616209	0.76800205
H	-1.68601381	1.49547634	0.02257604
H	-1.58800517	-3.76350059	-0.58087501
H	-1.39884467	-3.10102560	0.80264751
H	-1.87762655	-1.60147124	2.39982204
H	-2.56671453	-2.91227571	2.92340343
H	-2.32138297	-2.44017689	-2.33025955
H	-3.39576580	-3.45686607	-2.83379887
H	-1.00627200	-0.48929996	-1.94341572
H	-0.75106683	-1.85370343	-1.22563079
H	-0.14490950	-0.22267030	2.76890760
H	-1.38199611	0.46332628	2.07450015
H	-0.07636812	1.50328121	-1.58013375
H	-1.47524936	1.82880489	-2.26594612
H	3.93215790	-1.38222676	1.20492050
H	2.78028940	-2.42124434	1.24799748
H	3.68723335	2.17458901	0.63934770
H	3.66142147	2.02868106	-0.86060704
H	4.88769233	0.44068560	-0.00386149
H	6.04676264	-0.54825144	0.33760265
H	2.71880055	-1.29269089	-2.38848189
H	1.12207180	-1.36244122	-2.38560079
H	5.04222546	-0.87107381	-3.20727244

H	4.83476723	-1.11298441	-1.69224820
H	2.28407611	-0.78800850	2.56981544
H	1.91902850	-0.17873755	3.96273768
H	1.77874583	0.51225315	-1.30094861
H	1.62198140	1.59983261	-0.18324850
H	-1.24623942	3.29596695	1.92535512
O	-2.89436290	2.64296216	-3.16433325
H	-4.10757740	1.84321072	-1.76797373
H	-1.37661194	4.91448563	2.86067566
H	-4.87884188	2.85388159	-3.13813320

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r_dHa1_hco_ch3o W18			
C	-0.09550423	-0.43724815	5.17055570
O	-1.49736470	1.67321838	-2.15306838
O	1.09366430	1.88426055	-1.78014827
O	1.51738995	-0.66743956	-2.67125777
O	4.07011462	-0.72248173	-3.51287254
O	-2.52796607	1.64496192	0.45068966
O	-5.00591571	0.66251013	-0.04996239
O	-4.51680906	-1.96371237	-0.29365767
O	-1.26169291	-0.16246513	2.07207674
O	-2.37343712	-2.45723361	1.49154133
O	-1.08552104	-3.05864219	-0.84112102
O	-1.26342856	-1.04983422	-2.76859160
O	-3.27272845	-2.88450227	-2.69554946
O	1.71182880	2.42893504	0.85003059
O	1.49036162	0.10251009	2.16129385
O	3.17182040	-1.44229683	0.87986835
O	1.73935403	-2.87802047	-0.92202115
O	3.86387917	2.47136877	-0.90092869
O	4.88410305	0.00917067	-0.95384146
O	-0.21711785	4.21013619	2.10262514
C	-1.38321510	4.04805966	2.09221392
H	-5.84439422	0.80707912	0.37705554
H	-4.89966740	-0.30043788	-0.17234682
H	-3.84652804	-2.18615987	0.36210500
H	-4.20123076	-2.29529451	-1.14106227
H	0.82793212	-3.16019639	-0.80502597
H	1.69651714	-2.16312638	-1.56746148
H	1.20500420	3.12068361	1.28028496
H	1.65119086	1.63198030	1.41055820
H	-3.45665495	1.36919086	0.36506252
H	-2.18856723	1.68448872	-0.45321032
H	-1.73272119	-3.51289070	-1.38406708
H	-1.48807121	-2.94415779	0.03276175
H	-1.95173258	-1.60666055	1.76657481
H	-2.45596595	-3.01029378	2.26302184
H	-2.68667638	-2.16726164	-2.98712451
H	-3.71436451	-3.24095984	-3.46084285
H	-1.46570561	-0.12770322	-2.55846245
H	-1.08525146	-1.50960532	-1.93632740
H	-0.29928272	-0.10355317	1.97523379
H	-1.66837639	0.50647248	1.49478626
H	-0.53662705	1.87738242	-2.07898939
H	-1.88784014	2.29120069	-2.76526761
H	3.78875253	-0.99546371	0.29166274
H	2.67924765	-2.07388745	0.32724832
H	3.31335250	2.59943065	-0.11719226
H	3.24065332	2.54410425	-1.62602634
H	4.57044245	0.93709920	-0.89816796
H	5.79611958	-0.00109954	-0.67472142
H	2.30032023	-0.72343772	-3.23928183
H	0.71078681	-0.86701390	-3.15555472
H	4.59816515	-0.28307437	-4.17203752
H	4.46329622	-0.53302994	-2.64817060
H	2.13626062	-0.50016305	1.71943347
H	1.64783814	0.08827351	3.10981111

H	1.33551152	0.97039126	-2.00484422
H	1.21674789	2.00581258	-0.82635178
H	-1.91850296	3.24735266	1.53921899
O	1.05564873	0.27991322	4.95668020
H	-0.49904715	-0.29625042	6.17065043
H	-0.81550888	-0.09690522	4.41654058
H	0.07746701	-1.49408703	4.95695341

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ts Rc_hco_ch3o W18			
C	-0.42760123	0.20736418	5.12532415
O	-1.52448612	1.74981849	-2.04876839
O	1.08903457	2.03678733	-1.89191838
O	1.49198138	-0.55727445	-2.65985657
O	4.02811965	-0.86042772	-3.50585896
O	-2.53598325	1.58983946	0.56894537
O	-5.00070342	0.62710493	-0.04647611
O	-4.54030474	-1.99578902	-0.40580045
O	-1.29378233	-0.38813762	1.94496014
O	-2.42775951	-2.66155396	1.36152466
O	-1.11278190	-3.10426716	-0.98098769
O	-1.28113557	-0.95409734	-2.74424413
O	-3.28405311	-2.79148740	-2.84698972
O	1.89086441	2.53944515	0.70626308
O	1.39557862	0.25606171	2.01488119
O	3.14327422	-1.39421773	0.96315812
O	1.69781096	-2.75793364	-0.88283807
O	3.99938164	2.39676587	-1.05886652
O	4.89955919	-0.11280708	-0.96467696
O	0.07089002	3.67733294	2.67098152
C	-0.85298487	2.98978487	2.90504180
H	-5.85482175	0.75579368	0.35374525
H	-4.89347741	-0.32983719	-0.20771443
H	-3.89452433	-2.28505456	0.24833300
H	-4.21905911	-2.28933699	-1.26507289
H	0.80095510	-3.10045035	-0.84086619
H	1.65848068	-2.02736014	-1.51051509
H	1.49297854	3.25394746	1.20328032
H	1.73375976	1.72730712	1.22855059
H	-3.46516123	1.33419662	0.44285617
H	-2.18336590	1.71647314	-0.32134900
H	-1.73544328	-3.52872474	-1.57388052
H	-1.53987881	-3.06460031	-0.11190119
H	-1.98451747	-1.82566593	1.64728025
H	-2.49265913	-3.23824524	2.11717116
H	-2.69396986	-2.05418351	-3.07285996
H	-3.72697375	-3.07539371	-3.64130711
H	-1.48306452	-0.04354921	-2.48685913
H	-1.12288646	-1.46493612	-1.93825483
H	-0.33891513	-0.25721546	1.84824548
H	-1.73518365	0.30707047	1.42518189
H	-0.56679034	1.97860249	-2.04497441
H	-1.97082626	2.35788959	-2.63219795
H	3.78391341	-0.98972931	0.36955826
H	2.63466890	-2.01443702	0.41294107
H	3.43508714	2.56939657	-0.29250227
H	3.41626829	2.51936756	-1.80858342
H	4.62652398	0.82875937	-0.97287660
H	5.81498666	-0.14137945	-0.69832108
H	2.26334631	-0.69188328	-3.22984736
H	0.67194117	-0.77123735	-3.11588615
H	4.60053069	-0.49538709	-4.17324663
H	4.43733113	-0.69240716	-2.64451475
H	2.08071865	-0.38071453	1.69960397
H	1.45084503	0.35714722	2.96982380
H	1.33011671	1.11759486	-2.09394186
H	1.27840447	2.19537107	-0.95616785
H	-1.56939186	2.59323140	2.15627763

O	0.66731862	0.91455771	4.68155410
H	-1.08378138	-0.01895060	4.28383937
H	-0.04653376	-0.75272254	5.48993812
H	-0.95512046	0.71762564	5.92769014

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ts_dHa2_hco_ch3o W18			
C	-2.66747785	4.25306971	-1.54942068
O	-1.11300656	1.21196409	-1.60634098
O	1.50035517	1.32862050	-1.00817454
O	1.86193295	-1.23394589	-1.87595241
O	4.45611179	-1.22282411	-2.58977447
O	-2.31934060	1.20534848	0.86754382
O	-4.82777377	0.30715442	0.40706022
O	-4.30537192	-2.31179750	0.25691687
O	-1.20086265	-0.45056981	2.75216833
O	-2.28052824	-2.75532446	2.18831544
O	-0.87251968	-3.40029107	-0.05688239
O	-0.91463552	-1.50675269	-2.12346144
O	-2.94306188	-3.31397061	-2.04448287
O	1.94561610	2.18757732	1.61910389
O	1.58020642	-0.03006911	3.11403796
O	3.17583581	-1.58334118	1.79491201
O	1.93986036	-3.24593573	0.07494364
O	4.13845615	2.11367510	-0.14401038
O	5.08402610	-0.37004167	-0.00104547
O	-0.11362999	4.34999051	1.30517661
C	-1.13778738	3.90991829	0.94944297
H	-5.63484180	0.44578614	0.89287165
H	-4.71088831	-0.65845511	0.30799483
H	-3.67510434	-2.51233703	0.95837809
H	-3.94108862	-2.66808831	-0.56068687
H	1.01797934	-3.51271895	0.14047788
H	1.96124321	-2.62671951	-0.66468760
H	1.42382015	2.95731892	1.84172349
H	1.79854349	1.50058161	2.29162429
H	-3.25513270	0.94953394	0.78740537
H	-1.93919366	1.12524998	-0.02153811
H	-1.48287285	-3.87743578	-0.62229219
H	-1.32570381	-3.26478635	0.78916593
H	-1.86378814	-1.90341211	2.46777016
H	-2.41214320	-3.28688924	2.96818536
H	-2.33448808	-2.61779336	-2.34259632
H	-3.35457845	-3.70015413	-2.81212738
H	-1.11044015	-0.56492097	-2.00748547
H	-0.79669634	-1.89349230	-1.24541937
H	-0.24668293	-0.33555910	2.83151815
H	-1.53692136	0.18378319	2.09932017
H	-0.16047634	1.37627028	-1.46796439
H	-1.45916020	1.94566427	-2.13051338
H	3.84842043	-1.20463939	1.21916203
H	2.72256502	-2.27293564	1.27409149
H	3.61601312	2.30552009	0.64269758
H	3.47630199	2.07122599	-0.83967003
H	4.81740663	0.57433400	-0.01864679
H	5.97875022	-0.41134145	0.32691941
H	2.66450344	-1.28445253	-2.41536798
H	1.06909371	-1.40708037	-2.39333073
H	4.97968863	-0.74104667	-3.22266750
H	4.77712187	-0.98763350	-1.70741849
H	2.18908042	-0.63951050	2.61714812
H	1.80093541	-0.11357980	4.03821031
H	1.70145869	0.39815531	-1.20403287
H	1.54798206	1.46358079	-0.05379828
H	-1.67096355	2.99517567	1.28004238
O	-1.95818447	3.70295369	-2.52321934
H	-3.49673003	3.64024263	-1.18677791
H	-1.96234685	4.29275627	-0.61919226



H	-2.94876947	5.29324071	-1.72173259
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p_dHa1_hco_ch3o W18			
C	-0.23797591	0.44145985	5.60817391
O	-1.47102923	1.78272049	-2.07430901
O	1.15190437	1.97757806	-1.80809111
O	1.49920371	-0.57076750	-2.72348957
O	4.01689317	-0.69729762	-3.66421359
O	-2.45275430	1.56418838	0.57155684
O	-4.95317703	0.62953110	-0.01222446
O	-4.51029687	-2.00607111	-0.34126381
O	-1.15636394	-0.30303880	1.95084849
O	-2.35726694	-2.58342789	1.41796599
O	-1.06792347	-3.04143539	-0.95089348
O	-1.27845123	-0.92497059	-2.75904491
O	-3.25693292	-2.79259588	-2.78927682
O	1.83871351	2.37296526	0.84334057
O	1.58436601	-0.02442230	1.93529588
O	3.33944974	-1.57558511	0.75328717
O	1.76153881	-2.84919068	-1.05854501
O	3.95218438	2.42357923	-0.97102569
O	4.95525344	-0.04941786	-1.12134129
O	-0.48253531	3.43503807	2.54304104
C	-1.29533002	2.94471057	3.14849244
H	-5.78373107	0.77078703	0.43113070
H	-4.86141204	-0.32991971	-0.16240549
H	-3.84891194	-2.26695419	0.30859584
H	-4.18912599	-2.29820491	-1.20083404
H	0.85328414	-3.13782564	-0.93389397
H	1.70264555	-2.09750001	-1.65904987
H	1.32705740	3.00951229	1.33734280
H	1.76429626	1.51783509	1.31785418
H	-3.38230087	1.31011915	0.45746373
H	-2.11893770	1.71448826	-0.32021028
H	-1.70609912	-3.46787467	-1.52631527
H	-1.47501230	-2.99504766	-0.07336288
H	-1.91980368	-1.74353464	1.68921432
H	-2.39328257	-3.15682313	2.17831385
H	-2.68770197	-2.04719899	-3.04030783
H	-3.70063702	-3.10799788	-3.57119150
H	-1.47316000	-0.00888010	-2.51634514
H	-1.10049986	-1.41712566	-1.94581387
H	-0.22176740	-0.29166019	1.69545052
H	-1.61714699	0.39912756	1.44164263
H	-0.51198254	1.99301272	-2.04213151
H	-1.89882378	2.42472142	-2.63453694
H	3.93110830	-1.10775502	0.15587285
H	2.80864540	-2.16790059	0.19358959
H	3.43764420	2.54671329	-0.16393484
H	3.30108370	2.52408733	-1.66845261
H	4.64544782	0.87613693	-1.03003990
H	5.88078583	-0.06355969	-0.89123792
H	2.25791169	-0.64426662	-3.32137619
H	0.67009246	-0.75788302	-3.17470855
H	4.53093420	-0.25393387	-4.33175271
H	4.44935936	-0.54339904	-2.81149229
H	2.27460340	-0.63101231	1.57800216
H	1.57126375	-0.04797665	2.89656738
H	1.36005254	1.06169445	-2.05927548
H	1.28740475	2.06303612	-0.85325769
H	-0.52552049	0.18696931	3.67649079
O	0.19966379	0.40470578	4.27278776
H	-1.01432325	1.19167712	5.75186881
H	-0.61670124	-0.52595714	5.93589758
H	0.61486830	0.70344920	6.22410771

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C	-0.03944063	0.68299601	4.96145179
O	-1.48401077	1.78558178	-2.13953761
O	1.09277577	1.89722323	-1.62709974
O	1.48405498	-0.57402813	-2.72233141
O	4.03147349	-0.54608269	-3.57849017
O	-2.55611495	1.54937141	0.42753970
O	-5.02557900	0.57091522	-0.08655783
O	-4.55442566	-2.04475161	-0.41232478
O	-1.29582965	-0.31562321	1.99257492
O	-2.41765059	-2.60135899	1.36149381
O	-1.11728502	-3.02307396	-1.00947898
O	-1.29850189	-0.92792649	-2.84259790
O	-3.28808131	-2.79168478	-2.86305469
O	1.66697860	2.19926571	1.06136608
O	1.46910088	-0.23992157	2.11902010
O	3.16470027	-1.65509255	0.71736013
O	1.70539955	-2.93644899	-1.17577152
O	3.82844223	2.41875580	-0.68423899
O	4.86424806	-0.02396758	-0.97579265
O	-0.31301217	3.53997303	2.74951682
C	-1.48004017	3.43636572	2.62630937
H	-5.85550782	0.70865067	0.35905508
H	-4.92513424	-0.38989544	-0.23272295
H	-3.89315217	-2.30159149	0.24017962
H	-4.22528862	-2.32424323	-1.27319485
H	0.78790793	-3.18833927	-1.03649482
H	1.66408870	-2.17016346	-1.75883476
H	1.14434937	2.81234991	1.58071594
H	1.62971588	1.33862831	1.52366818
H	-3.48015283	1.26203749	0.32330167
H	-2.22020071	1.68042942	-0.46864756
H	-1.76050450	-3.45283872	-1.57676542
H	-1.51485518	-2.97457690	-0.12718002
H	-2.00707450	-1.75837152	1.66970376
H	-2.45891523	-3.19683621	2.10453907
H	-2.71525214	-2.05092779	-3.11878068
H	-3.72032849	-3.12103445	-3.64565758
H	-1.49255543	-0.01173911	-2.60340282
H	-1.12539375	-1.41784959	-2.02653785
H	-0.33305170	-0.31788369	1.88701009
H	-1.67542246	0.35726523	1.40301052
H	-0.52436132	1.96014954	-2.00814594
H	-1.83026583	2.44459465	-2.73512459
H	3.77408824	-1.15297834	0.16759678
H	2.67316584	-2.24165543	0.11606986
H	3.28798821	2.47776801	0.11360097
H	3.19130816	2.53368369	-1.39230850
H	4.54906890	0.89283852	-0.82798627
H	5.77652379	-0.06093588	-0.69984414
H	2.26404158	-0.58183075	-3.29712281
H	0.67508944	-0.73532249	-3.21689878
H	4.55792681	-0.06452917	-4.20880175
H	4.43226190	-0.42253467	-2.70542028
H	2.11673182	-0.80482380	1.63163393
H	1.58667156	-0.37111263	3.06483738
H	1.31898403	0.99890541	-1.92242113
H	1.18349957	1.93243651	-0.66306980
H	-1.99803890	2.91873312	1.79168357
O	0.96258540	-0.25561188	4.90228878
H	-0.80913964	0.35748852	4.25127304
H	-0.46110873	0.78527842	5.95871125
H	0.32327981	1.64101247	4.58458201

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C	-3.81739596	3.08469832	-2.03999006
O	-0.99155836	1.24225647	-1.59336913
O	1.63147899	1.44090441	-1.12196884

O	1.94546675	-1.18722425	-1.84889415
O	4.54036781	-1.38223197	-2.53750658
O	-2.11020551	1.56504290	0.90412369
O	-4.65086016	0.77051632	0.16595575
O	-4.24348005	-1.85539299	0.09049703
O	-1.11030731	-0.29079925	2.68151733
O	-2.35438632	-2.49424663	2.08467562
O	-0.92540365	-3.37465417	-0.06758269
O	-0.81452442	-1.46509269	-2.10065588
O	-2.96512867	-3.10509103	-2.11300726
O	2.06001415	2.09938122	1.55633050
O	1.68206723	-0.14191141	3.04009454
O	3.26901662	-1.77749598	1.81180787
O	1.90750843	-3.28195116	0.03626649
O	4.30507804	1.96802344	-0.09829138
O	5.18370060	-0.53970943	0.04341850
O	0.21972260	4.12289557	2.53067367
C	-0.94792770	4.03432559	2.40749561
H	-5.45726222	0.91029263	0.65440151
H	-4.54015194	-0.20058992	0.08389201
H	-3.66103413	-2.11148292	0.81583448
H	-3.91729656	-2.29668799	-0.70202907
H	0.97999782	-3.52570828	0.10369502
H	1.94534453	-2.61848465	-0.66301105
H	1.57012101	2.85096363	1.89692024
H	1.93168642	1.36343214	2.17820158
H	-3.04418189	1.34430654	0.76944836
H	-1.69404628	1.45461285	0.03489837
H	-1.56038294	-3.81634771	-0.63415362
H	-1.38956786	-3.16400277	0.75710285
H	-1.87441038	-1.67517839	2.36544044
H	-2.57564424	-2.98550308	2.87085273
H	-2.28399307	-2.46619114	-2.38360971
H	-3.37624642	-3.45620163	-2.89749852
H	-0.97303257	-0.52268711	-1.93374993
H	-0.72600820	-1.90159805	-1.24224671
H	-0.14834335	-0.26660797	2.75609357
H	-1.39582712	0.40677042	2.07125175
H	-0.04555560	1.48126941	-1.55264817
H	-1.45046255	1.79721897	-2.23275333
H	3.94238828	-1.39727646	1.23761360
H	2.78030158	-2.42549873	1.27188108
H	3.73711917	2.16290715	0.65745256
H	3.69816707	2.00220116	-0.84191789
H	4.92557444	0.40747376	0.02509508
H	6.07414690	-0.58740797	0.38198500
H	2.75348658	-1.30641715	-2.36952733
H	1.15542595	-1.36985644	-2.36742928
H	5.10407082	-0.95375405	-3.17414674
H	4.87097609	-1.15582490	-1.65611658
H	2.28370167	-0.78586651	2.57949013
H	1.89570903	-0.17992964	3.96892559
H	1.81280450	0.50152322	-1.29024643
H	1.65598666	1.58244585	-0.16565453
H	-1.48082986	3.20516335	1.89553861
O	-2.96229976	2.64258405	-3.01771215
H	-4.23902358	2.18310750	-1.57427976
H	-3.27710105	3.60387219	-1.24737702
H	-4.62635261	3.69109929	-2.44218687

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ts\_dHa1\_hco\_ch3o W18

C	-0.09642481	-0.03199046	5.84577834
O	-1.13856949	1.51866346	-1.21121926
O	1.48721855	1.80827865	-1.17754726
O	1.86024419	-0.78756496	-1.95367319
O	4.39854287	-1.01017273	-2.81988431
O	-2.02446706	1.32378802	1.47398774

O	-4.52722673	0.46592980	0.79877367
O	-4.15018009	-2.16760252	0.36385425
O	-0.87396714	-0.70779730	2.77402368
O	-2.04635048	-2.93563161	2.09987075
O	-0.72659679	-3.33658826	-0.24937290
O	-0.91237132	-1.15838087	-1.97920857
O	-2.92418385	-2.97803829	-2.08969348
O	2.17217074	2.28212535	1.44770337
O	1.81580364	-0.04465814	2.74362360
O	3.59263743	-1.62445256	1.65498974
O	2.09024485	-2.96658812	-0.16341048
O	4.31585389	2.25599310	-0.30571547
O	5.26116680	-0.24063846	-0.27545016
O	-0.01537077	3.56603720	2.86320380
C	-0.73308238	2.88955566	3.49181565
H	-5.38370056	0.60730119	1.18955281
H	-4.44760884	-0.48723712	0.60674085
H	-3.51060112	-2.49108582	1.00774698
H	-3.84514454	-2.46065704	-0.50137234
H	1.19668429	-3.31626049	-0.11248672
H	2.04089551	-2.24141451	-0.79703048
H	1.62163058	2.94107485	1.87342880
H	2.05269384	1.45509839	1.95261886
H	-2.96391774	1.11796166	1.34445729
H	-1.67875546	1.46578914	0.58445892
H	-1.35198072	-3.74733913	-0.84906679
H	-1.15682217	-3.30754617	0.61861061
H	-1.59255709	-2.11564035	2.41480934
H	-2.12073534	-3.53703591	2.83507796
H	-2.33031614	-2.24135612	-2.30863404
H	-3.37779426	-3.24375075	-2.88425467
H	-1.10979387	-0.25226800	-1.70156885
H	-0.74348265	-1.68227410	-1.18399654
H	0.07926400	-0.60238223	2.64351423
H	-1.30225851	0.02049456	2.28080578
H	-0.18788568	1.76096069	-1.27090196
H	-1.63887358	2.14818285	-1.72386339
H	4.20209083	-1.18963635	1.04968163
H	3.07315044	-2.23857975	1.10767175
H	3.76532273	2.41475992	0.47197036
H	3.70668622	2.35651942	-1.03912368
H	4.96773710	0.69496070	-0.25818097
H	6.18270641	-0.25301481	-0.02952367
H	2.62338980	-0.90705167	-2.53749089
H	1.03215310	-0.99340490	-2.39876438
H	4.94435981	-0.60341112	-3.48552725
H	4.79920884	-0.82219482	-1.95878373
H	2.52506654	-0.65240902	2.42136316
H	1.88972985	0.09215003	3.68948414
H	1.70955027	0.88882719	-1.39866650
H	1.65439089	1.93079541	-0.23124575
H	-0.50949580	1.86808584	3.88021206
O	0.70268050	0.89125780	5.20731176
H	-0.69217293	0.41000085	6.64157822
H	-0.74396297	-0.46799773	5.07830299
H	0.52198535	-0.84692149	6.22742655

## 2.2.10 HCO + HCO

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p_Rc_hco_hco W18			
C	-2.92693975	3.50718335	-0.81013713
O	-1.10826943	0.83458938	-1.89326481
O	1.47739046	1.16979120	-1.39968709
O	2.08225247	-1.47938912	-1.72856182
O	4.67474461	-1.23992946	-2.40498889
O	-2.47607592	1.28078447	0.45591081

O	-4.81726918	-0.02287995	0.20962797
O	-4.04624445	-2.53464952	0.64480821
O	-1.24621047	0.21292840	2.69141368
O	-2.02842012	-2.27655802	2.60956086
O	-0.52186625	-3.26469576	0.55537193
O	-0.69837517	-1.92804884	-1.90489700
O	-2.54590960	-3.85387880	-1.38603566
O	1.71214766	2.68245197	0.91099552
O	1.48491617	0.86283885	2.92746045
O	3.24602212	-0.76013832	1.93005432
O	2.27352395	-2.93076882	0.65553022
O	3.94285726	2.53867506	-0.77419368
O	5.08057701	0.24056811	-0.06633811
O	-0.70610317	3.82853880	0.00167154
C	-1.86845930	3.71212332	0.26885215
H	-5.65054486	0.13671684	0.64184201
H	-4.60632890	-0.97136649	0.32696103
H	-3.41125662	-2.50019872	1.36966527
H	-3.62872649	-3.01819951	-0.07658441
H	1.36509975	-3.22215002	0.77904850
H	2.27758564	-2.52822897	-0.22135350
H	0.94621080	3.25073058	0.79506489
H	1.60161146	2.17821335	1.73121685
H	-3.35136253	0.85238340	0.41364500
H	-1.99271269	1.00392912	-0.33944236
H	-1.07929456	-3.91457346	0.12299285
H	-0.99585392	-2.97659794	1.35014033
H	-1.72964323	-1.33838443	2.70048192
H	-2.10440565	-2.64405198	3.48561199
H	-2.00512652	-3.18623093	-1.83980018
H	-2.89653772	-4.45042692	-2.04099755
H	-0.97304222	-1.00600053	-2.00243390
H	-0.54258415	-2.08627422	-0.96402574
H	-0.30293044	0.41432513	2.73708530
H	-1.62296370	0.66537530	1.92201389
H	-0.16347416	1.07194242	-1.77843603
H	-1.50919058	1.52724379	-2.41877080
H	3.88538043	-0.43782379	1.28630276
H	2.89642053	-1.60060436	1.57902049
H	3.36686821	2.83723788	-0.06040210
H	3.32058188	2.25532214	-1.44942212
H	4.73834060	1.13273686	-0.29304775
H	5.95978693	0.35078444	0.28680101
H	2.89857654	-1.53184368	-2.24623402
H	1.32127397	-1.79804638	-2.22168058
H	5.15606885	-0.83857162	-3.12194535
H	4.91535901	-0.76825048	-1.59440767
H	2.15071102	0.22381816	2.56101244
H	1.72458065	1.01990654	3.83706204
H	1.76767507	0.24376762	-1.39478566
H	1.52347184	1.52077101	-0.49981489
H	-2.24510576	3.77351979	1.29407256
O	-2.64805549	3.37501581	-1.96572102
H	-3.96361088	3.50368595	-0.45402601

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p\_dHa2\_hco\_hco W18

C	-4.70541511	1.99687339	-2.44922139
O	-1.06157028	0.75819722	-1.96903339
O	1.50442673	1.22555271	-1.55633622
O	2.07251998	-1.45828473	-1.61563700
O	4.67410061	-1.46698008	-2.30033214
O	-2.30107890	1.45730808	0.42808145
O	-4.66270803	0.17720380	-0.07372059
O	-4.05078631	-2.31393389	0.67901614
O	-1.13055048	0.33669847	2.62074991
O	-2.08136499	-2.09026970	2.70089300
O	-0.55035249	-3.26974119	0.76889308

O	-0.67534394	-1.98720864	-1.71276834
O	-2.56471204	-3.86493265	-1.19296432
O	1.79031536	2.61914771	0.80911034
O	1.63604421	0.81383089	2.85625484
O	3.41550790	-0.87764415	2.02667411
O	2.25948198	-2.95920519	0.75831648
O	4.06125436	2.38622661	-0.78290461
O	5.18285180	0.09069004	-0.04008413
O	-0.52380702	4.16320567	0.80408465
C	-1.50684274	3.78856081	1.39065532
H	-5.54304920	0.39397292	0.21837585
H	-4.49698795	-0.75532647	0.17042424
H	-3.44414904	-2.26922276	1.42723238
H	-3.64380940	-2.88723082	0.02040187
H	1.35132702	-3.23149280	0.92027668
H	2.23694219	-2.51788284	-0.09910797
H	1.07762457	3.26971892	0.85768537
H	1.74252515	2.07421843	1.60946735
H	-3.19031556	1.08098031	0.33192591
H	-1.85363445	1.26556130	-0.40725063
H	-1.12099715	-3.91963801	0.35419989
H	-1.03405922	-2.92473145	1.53476354
H	-1.72175473	-1.16943740	2.73804405
H	-2.21783999	-2.38698932	3.59619580
H	-1.99892918	-3.22441640	-1.65513528
H	-2.91545874	-4.47476305	-1.83541629
H	-0.93143722	-1.06002425	-1.82242683
H	-0.53871608	-2.14221358	-0.76800047
H	-0.17239508	0.45293822	2.64319228
H	-1.48104938	0.74539558	1.81103692
H	-0.12468658	1.05013715	-1.94551524
H	-1.50162519	1.17308191	-2.70675126
H	4.03687051	-0.57601518	1.35552017
H	3.01643424	-1.69939727	1.68582726
H	3.45591523	2.69879767	-0.09824330
H	3.47149920	2.15175572	-1.50338788
H	4.83142391	0.97513409	-0.28314296
H	6.07002747	0.21586916	0.28717416
H	2.88544045	-1.60603758	-2.12039755
H	1.30189917	-1.82825324	-2.05661948
H	5.19121531	-1.15535657	-3.03658835
H	4.95653931	-0.97356963	-1.51642882
H	2.30943915	0.15003115	2.55090441
H	1.85453693	1.03055334	3.75894452
H	1.78466100	0.29848375	-1.48676444
H	1.52524948	1.61419593	-0.66820435
H	-1.44882023	3.10711792	2.24101932
O	-3.74224052	1.71735078	-2.96028238
H	-2.50177999	4.13732716	1.10751330

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r_dHa2_hco_hco W18			
C	-4.41631807	1.29699680	-2.93164148
O	-1.15051869	0.80844023	-1.83522673
O	1.43168824	1.33127827	-1.48657325
O	2.01276589	-1.34592203	-1.64476751
O	4.60189128	-1.42292710	-2.36771161
O	-2.25750770	1.53923870	0.58917295
O	-4.70955805	0.32577371	0.10840278
O	-4.03462163	-2.16912372	0.66470896
O	-1.03303860	0.23953184	2.68960347
O	-2.05372594	-2.14801304	2.66082296
O	-0.57996151	-3.32546913	0.68859868
O	-0.72020350	-1.92464450	-1.72090919
O	-2.68166137	-3.73224082	-1.27195660
O	1.83996879	2.61399072	0.95083801
O	1.73091734	0.73752837	2.90822603
O	3.45841206	-0.96550452	2.00448833

O	2.23054933	-2.95398539	0.65870974
O	4.06057544	2.34547073	-0.71733844
O	5.20273230	0.03209156	-0.06568156
O	-0.18704817	4.60413525	1.53037326
C	-1.34455876	4.39542743	1.47502109
H	-5.53178717	0.51163286	0.55382879
H	-4.49799344	-0.61784035	0.28511215
H	-3.41553741	-2.19481455	1.40494323
H	-3.67859784	-2.74452698	-0.02221588
H	1.33357191	-3.26097062	0.81782924
H	2.18643770	-2.46527475	-0.17178081
H	1.27476517	3.36793189	1.13356426
H	1.80314895	2.02899545	1.72619977
H	-3.16471475	1.20632949	0.53902797
H	-1.85398177	1.30527714	-0.26043416
H	-1.17170666	-3.94926765	0.26458034
H	-1.04621451	-2.98861917	1.46904069
H	-1.65591792	-1.24361109	2.73009824
H	-2.20033259	-2.47041565	3.54569620
H	-2.07617745	-3.10760600	-1.70617798
H	-3.05699079	-4.30068984	-1.93810365
H	-0.96581223	-0.98808334	-1.76718829
H	-0.56498750	-2.14020996	-0.79091774
H	-0.07809361	0.37576906	2.72413758
H	-1.39812186	0.75089461	1.95104362
H	-0.22580365	1.12849524	-1.85713654
H	-1.63966957	1.17178196	-2.57540897
H	4.08048703	-0.65820823	1.33646930
H	3.03167689	-1.76196132	1.63879301
H	3.48307993	2.64493234	-0.00407928
H	3.44773647	2.15868752	-1.43240228
H	4.84521844	0.92101421	-0.28013844
H	6.09913544	0.14965865	0.23843307
H	2.82393096	-1.49247582	-2.15395972
H	1.24222213	-1.71490566	-2.08696343
H	5.11129698	-1.10344797	-3.10601996
H	4.92530035	-0.97391855	-1.57315791
H	2.38926254	0.07006676	2.57691457
H	1.96289337	0.92982267	3.81323336
H	1.71379960	0.40242140	-1.45310967
H	1.46677580	1.68824514	-0.58808120
H	-1.81130213	3.43905787	1.15861120
O	-3.39614697	1.51882787	-3.47352585
H	-4.53576249	0.90778000	-1.89910175

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ts\_dHa1\_hco\_hco W18

C	4.08169666	2.56943547	1.86097843
O	1.10806283	0.79830935	1.84054244
O	-1.45626275	1.29282321	1.38408234
O	-2.12002346	-1.34558886	1.69503037
O	-4.72824764	-1.19555175	2.33594321
O	2.32353493	1.41923435	-0.59161704
O	4.78743029	0.20763418	-0.16229057
O	3.98771220	-2.30246519	-0.44506613
O	1.11170242	0.14685177	-2.71118711
O	2.03521517	-2.26634244	-2.47451636
O	0.50338018	-3.34922890	-0.49627949
O	0.61363146	-1.92966539	1.90561018
O	2.55538555	-3.77648722	1.51093118
O	-1.69647825	2.61304703	-1.04101875
O	-1.62369058	0.74471558	-3.01016431
O	-3.38116988	-0.88208677	-2.01616924
O	-2.29707419	-2.92483268	-0.61881469
O	-3.96034401	2.52387503	0.60060646
O	-5.15577793	0.22946693	-0.02664877
O	0.73308320	4.12083952	-0.64699615
C	1.85664567	4.01241380	-0.97293840

H	5.55099585	0.30963730	-0.72397890
H	4.54376453	-0.74281421	-0.19347435
H	3.36880854	-2.32810160	-1.18529534
H	3.60537881	-2.83373135	0.26260330
H	-1.40127331	-3.25466978	-0.73203855
H	-2.28291816	-2.45517019	0.22384179
H	-0.97528511	3.24401376	-1.07376951
H	-1.64822359	2.05696142	-1.83538805
H	3.20101426	1.01378296	-0.56385102
H	1.88041848	1.16338444	0.23024026
H	1.07237681	-3.98165013	-0.05431614
H	0.99256450	-3.03200265	-1.27142415
H	1.67152434	-1.35434018	-2.61171888
H	2.19127418	-2.64693671	-3.33434226
H	1.95411868	-3.13552012	1.92652978
H	2.91581418	-4.33597564	2.19268916
H	0.89472495	-1.00327058	1.93656164
H	0.47416333	-2.15724285	0.97573114
H	0.16664345	0.32352172	-2.79415019
H	1.46958734	0.69508575	-1.99563871
H	0.17941055	1.10713800	1.78092658
H	1.56935081	1.33832238	2.48191542
H	-4.00556253	-0.53670927	-1.36956814
H	-2.99584237	-1.68870354	-1.62754035
H	-3.36741141	2.79194314	-0.11161140
H	-3.35568769	2.29091810	1.30987934
H	-4.78188511	1.11559848	0.17120620
H	-6.03554061	0.35998114	-0.37140025
H	-2.94951114	-1.41840402	2.18966928
H	-1.37414138	-1.69750682	2.18973316
H	-5.22966176	-0.80637932	3.04576560
H	-4.98462086	-0.74560212	1.51776453
H	-2.29247958	0.10559825	-2.64879522
H	-1.85855431	0.91119355	-3.91929154
H	-1.76528098	0.37218416	1.39280504
H	-1.46936463	1.61261840	0.47058682
H	2.72755308	3.99440685	-0.29277142
O	3.25551900	2.59044069	2.69625454
H	4.51502996	1.66173150	1.39598819

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p\_dHa1\_hco\_hco W18

C	-4.03248693	2.50228171	-2.17956888
O	-1.12455020	0.85880019	-1.69014695
O	1.49232391	1.34898827	-1.31701246
O	2.04220277	-1.29562078	-1.74982864
O	4.62456780	-1.11639334	-2.49373749
O	-1.99874917	1.41744373	0.89638857
O	-4.58965850	0.49845643	0.44251413
O	-3.96918231	-2.09098095	0.61719469
O	-0.91218256	-0.01231883	2.93660890
O	-1.96334439	-2.35324753	2.58234198
O	-0.53944222	-3.37026693	0.48985745
O	-0.69015385	-1.84492386	-1.85081617
O	-2.70547352	-3.59869185	-1.44030324
O	1.64426781	2.47111202	1.22394638
O	1.84900102	0.53601316	3.10193016
O	3.51192970	-1.05776075	1.92493685
O	2.27480181	-2.97860069	0.48522032
O	3.93220366	2.52228009	-0.47579080
O	5.16729702	0.19232704	-0.07908380
O	-0.76745939	4.31105656	0.58359814
C	-1.79979343	4.22209649	0.14319982
H	-5.34640918	0.62918791	1.00684803
H	-4.40718615	-0.46426389	0.44359762
H	-3.33820689	-2.20931303	1.33770580
H	-3.65091823	-2.62052025	-0.12239034
H	1.37968516	-3.29959152	0.62703700



H	2.23189528	-2.46948053	-0.33320723
H	0.90104765	3.05723649	1.35167967
H	1.68559351	1.86608452	1.98436836
H	-2.93597231	1.18331258	0.87738161
H	-1.66172719	1.17300041	0.02302167
H	-1.15014506	-3.95338878	0.03593057
H	-0.99068909	-3.07768896	1.29716337
H	-1.54744392	-1.47289349	2.77223826
H	-2.12241691	-2.78489470	3.41699556
H	-2.08501784	-2.97519088	-1.85545128
H	-3.12744492	-4.10454644	-2.12852955
H	-0.94515638	-0.90822966	-1.83363159
H	-0.52375616	-2.11320677	-0.93681196
H	0.04217351	0.10925371	2.99811052
H	-1.24532011	0.56280179	2.22583795
H	-0.21037167	1.19149479	-1.72560436
H	-1.68471661	1.39619839	-2.26422152
H	4.09761077	-0.68071271	1.26002020
H	3.07775923	-1.82761945	1.51322869
H	3.38597330	2.77007112	0.27671881
H	3.28047126	2.29232164	-1.14661259
H	4.78321619	1.08933415	-0.18530044
H	6.06681077	0.29943350	0.21963506
H	2.84636768	-1.36139779	-2.28487651
H	1.26693302	-1.62221340	-2.21719499
H	5.07743629	-0.67582436	-3.20623039
H	4.91071925	-0.70045264	-1.66779826
H	2.48816914	-0.08985538	2.66808034
H	2.15584946	0.67791864	3.99349353
H	1.75030785	0.41519572	-1.39334938
H	1.45569881	1.57233569	-0.37710758
H	-4.85424283	3.18634563	-2.41778822
O	-3.06145490	2.44859181	-2.89092960
H	-4.13918383	1.87953294	-1.28827682

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r\_Rc-dHa\_hco\_hco W18

C	-4.38948951	1.47082361	-2.98318912
O	-1.12850460	0.95656424	-1.93196392
O	1.46458157	1.40838288	-1.52405477
O	1.98602692	-1.28118887	-1.71679234
O	4.57058142	-1.29916230	-2.45922113
O	-2.19496794	1.55639143	0.56125416
O	-4.69225877	0.43810115	0.03854931
O	-4.07491203	-2.06235403	0.65840177
O	-1.03909324	0.36211268	2.69133419
O	-2.09275550	-2.02761936	2.67144747
O	-0.62146201	-3.16413171	0.65779173
O	-0.76576438	-1.77918280	-1.77256595
O	-2.70608343	-3.59779888	-1.28966685
O	1.77860105	2.63350631	0.95184159
O	1.74440197	0.72653666	2.89138706
O	3.46015335	-0.94432597	1.92032347
O	2.19656402	-2.90571634	0.57146389
O	4.02736992	2.46116353	-0.72089146
O	5.17021059	0.12968642	-0.13658572
O	-0.54706402	4.23348414	1.63260766
C	-1.55628998	3.84311006	2.09108841
H	-5.50870844	0.66164623	0.47708118
H	-4.51015590	-0.50607904	0.23874718
H	-3.45839777	-2.08020512	1.40027539
H	-3.70953997	-2.63282277	-0.02769075
H	1.28886409	-3.16888920	0.74914602
H	2.15763890	-2.41745845	-0.25965291
H	1.11818401	3.30612807	1.13066967
H	1.77867433	2.03049883	1.71326891
H	-3.11000387	1.25671765	0.47613758
H	-1.79933844	1.41723606	-0.31039464

H	-1.21800103	-3.77798634	0.22523413
H	-1.08060443	-2.84294063	1.44796444
H	-1.69076445	-1.12845774	2.75743588
H	-2.23437678	-2.37080254	3.54927195
H	-2.11525185	-2.96563970	-1.73359324
H	-3.07677636	-4.17798260	-1.94825700
H	-0.99173141	-0.83887853	-1.84427571
H	-0.60461313	-1.96979626	-0.83882992
H	-0.07609399	0.43105711	2.71394292
H	-1.36606615	0.77630850	1.87328941
H	-0.20113317	1.26430738	-1.94695268
H	-1.61666637	1.34814842	-2.65806383
H	4.06736874	-0.61453458	1.24922592
H	3.02797257	-1.73268694	1.54246090
H	3.46003856	2.75719329	0.00044433
H	3.40021156	2.26105584	-1.42126333
H	4.81298480	1.02578836	-0.32066096
H	6.07001324	0.23624702	0.16155479
H	2.79221745	-1.41330530	-2.23751890
H	1.20870391	-1.62754890	-2.16473183
H	5.06093983	-0.95098636	-3.19751231
H	4.88735776	-0.85109016	-1.66149776
H	2.39796119	0.06796874	2.53172451
H	2.00278910	0.90747170	3.79148325
H	1.71862819	0.47123463	-1.50701529
H	1.46594619	1.73389837	-0.61255773
H	-1.69103287	2.90083684	2.64972070
O	-3.38087599	1.70170059	-3.54242528
H	-4.48906643	1.06340272	-1.95568145

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ts Rc_hco_hco W18			
C	-3.85188365	2.87939623	-1.75540437
O	-1.11795516	0.79163122	-1.82478187
O	1.47005823	1.23940649	-1.44693590
O	2.06605032	-1.41761207	-1.72630310
O	4.66239856	-1.27613955	-2.41701096
O	-2.20332766	1.39243851	0.66625693
O	-4.73515539	0.38710958	0.23743225
O	-4.01762965	-2.15218183	0.53268979
O	-1.03924574	0.16750943	2.81539682
O	-2.04647989	-2.21536312	2.55929418
O	-0.56947868	-3.32411030	0.54889039
O	-0.68348735	-1.94056814	-1.87738287
O	-2.67125305	-3.71863363	-1.41402421
O	1.68354727	2.60784547	0.94864658
O	1.69638485	0.79744937	2.98077471
O	3.38853706	-0.86993800	1.94811706
O	2.24153086	-2.92984337	0.62678343
O	3.95281149	2.49583069	-0.71383748
O	5.13534256	0.19359505	-0.08715778
O	-0.76628455	4.14029929	0.50626149
C	-1.92473795	3.98270167	0.61771523
H	-5.50817548	0.51550260	0.78016999
H	-4.53208149	-0.57233323	0.26544513
H	-3.39729697	-2.20149463	1.27005398
H	-3.66568997	-2.71005428	-0.17033791
H	1.34330576	-3.24593656	0.75808543
H	2.22610741	-2.48873855	-0.23126648
H	0.95317724	3.22832809	0.96139216
H	1.65198699	2.07876282	1.76177077
H	-3.10990272	1.05548774	0.63075146
H	-1.79278196	1.14402059	-0.17546182
H	-1.15781282	-3.94727639	0.11919296
H	-1.04089704	-2.99514053	1.32987953
H	-1.64459562	-1.32367399	2.71590810
H	-2.21014675	-2.61230206	3.41025815
H	-2.05827086	-3.10410565	-1.85215337

H	-3.06832879	-4.27212550	-2.08016170
H	-0.94699060	-1.00918096	-1.91946052
H	-0.53323513	-2.15374392	-0.94599666
H	-0.08939728	0.32765055	2.87666603
H	-1.38387342	0.67808587	2.06543088
H	-0.18322365	1.08398308	-1.80719828
H	-1.60099563	1.35568753	-2.42979313
H	4.00221575	-0.54653082	1.28017869
H	2.98034686	-1.67789837	1.58644964
H	3.37644283	2.78630968	0.00212976
H	3.33135522	2.24376908	-1.40255349
H	4.76888958	1.08308606	-0.28372277
H	6.02338009	0.31518495	0.23917856
H	2.88475160	-1.50455137	-2.23620252
H	1.30479877	-1.75905418	-2.20467559
H	5.14371798	-0.89431182	-3.14456141
H	4.92985875	-0.80682425	-1.61350862
H	2.34346671	0.14548672	2.60209150
H	1.98346600	0.99035388	3.86946482
H	1.75615706	0.31136680	-1.44784320
H	1.48342347	1.56468492	-0.53559538
H	-2.46598284	3.78222417	1.55814981
O	-3.09398114	2.75758722	-2.64543938
H	-4.29855634	2.04842673	-1.17539445

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ts\_dHa2\_hco\_hco W18

C	-3.81499504	3.26658799	-2.21175480
O	-1.20857318	0.74282580	-1.95965360
O	1.35332813	1.33249567	-1.55565011
O	1.98766156	-1.32342911	-1.69582213
O	4.58836365	-1.33668653	-2.38187096
O	-2.41321464	1.36462991	0.44754604
O	-4.79987855	0.13398921	0.15705559
O	-4.06474655	-2.38946397	0.65329654
O	-1.16561685	0.23463305	2.62821577
O	-2.04935181	-2.21649687	2.63486366
O	-0.55651599	-3.31245414	0.63390380
O	-0.72538619	-1.98856142	-1.82028448
O	-2.61099911	-3.87823317	-1.30221459
O	1.71526730	2.75040612	0.82230559
O	1.56782294	0.93416671	2.82484246
O	3.33551741	-0.74882613	1.96224321
O	2.22857225	-2.83461604	0.66619912
O	3.94644974	2.46050837	-0.83951441
O	5.12122370	0.18783188	-0.10351043
O	-0.45998372	4.71050771	0.68060264
C	-1.53651945	4.26116204	0.53285384
H	-5.64734191	0.30319559	0.55693708
H	-4.59928708	-0.81326980	0.29271811
H	-3.43691149	-2.37051728	1.38478469
H	-3.67106421	-2.92692329	-0.04248698
H	1.34067958	-3.17555019	0.80842126
H	2.18787740	-2.38328698	-0.18533894
H	1.13530067	3.50801791	0.91330798
H	1.64543436	2.21176851	1.62880825
H	-3.31334629	0.99513937	0.42407320
H	-1.99196137	1.08927993	-0.38037565
H	-1.11993336	-3.96703835	0.21701322
H	-1.03152854	-2.99655697	1.41794784
H	-1.70554851	-1.29136158	2.69658325
H	-2.16374666	-2.54530533	3.52200553
H	-2.05015821	-3.23597127	-1.76712463
H	-2.98756474	-4.46932318	-1.94768114
H	-1.01669534	-1.06981522	-1.91032740
H	-0.58746550	-2.16119724	-0.87865305
H	-0.22217423	0.43419877	2.65718438
H	-1.55574373	0.68668431	1.86390015

H	-0.28852843	1.07652189	-1.93677213
H	-1.70451075	1.24390306	-2.60717819
H	3.97195939	-0.45522935	1.30182003
H	2.94229348	-1.57228359	1.61806464
H	3.36725164	2.77170867	-0.13339666
H	3.33312935	2.22745886	-1.54063653
H	4.75779150	1.06536809	-0.35062125
H	6.01086910	0.32377067	0.21251301
H	2.80493720	-1.45914789	-2.19743635
H	1.22794866	-1.71989185	-2.13419940
H	5.10791000	-1.02589618	-3.11677539
H	4.88663791	-0.86340922	-1.59183107
H	2.24260249	0.27680567	2.50616804
H	1.78215544	1.12998375	3.73347902
H	1.65593964	0.40990740	-1.51006233
H	1.38331062	1.70807253	-0.66559924
H	-1.87093274	3.23967386	0.80904452
O	-3.22722885	2.59702318	-2.97289563
H	-3.42840110	3.62314165	-1.23322595

## 2.2.11 HCO + NH2

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p_Rc_hco_nh2	W18		
N	4.41273887	-1.97963358	-0.46492246
O	1.55858106	-1.25717602	-0.86778413
O	-0.84399002	-2.38991365	-0.60411090
O	-1.78826659	-0.42110980	-2.22387752
O	-4.44758860	-0.19626568	-2.55704923
O	-1.03084797	-1.80455809	2.09616300
O	-2.37063424	0.43182166	3.00153296
O	-4.11179769	0.93315158	1.13903358
O	-2.82569876	1.90891627	-1.07884503
O	-3.17883901	-3.30088555	0.71219045
O	-4.99189867	-1.47169953	-0.06973609
O	0.70014159	0.83882548	-2.43144870
O	2.33275029	2.97156366	-2.60455378
O	-0.26406850	3.15689744	-1.16620468
O	0.87551534	3.58997242	1.28079559
O	0.15533919	1.57663844	2.73356873
O	1.60055800	-0.59589022	1.83454559
O	4.15252512	0.42190902	1.21104686
O	3.21588165	2.62634804	0.06839710
O	4.74954208	-4.21128204	-0.18362116
C	4.42666481	-3.13639855	0.25348896
H	4.88723377	0.70240297	1.75038060
H	3.82089674	1.22690391	0.75442214
H	2.46790141	3.02192363	0.53320121
H	3.05223029	2.75795677	-0.87273874
H	-2.16370449	2.60557816	-1.10683932
H	-2.35818063	1.11480028	-1.36767792
H	-0.11048513	-1.68748686	2.34461262
H	-1.51023157	-1.04649653	2.46284017
H	2.51790290	-0.32184105	1.94365209
H	1.52119351	-0.75282351	0.88158783
H	0.32073321	3.60840523	-1.77655638
H	0.06604171	3.37269938	-0.27937954
H	0.56013438	2.86531685	1.87875292
H	0.84662607	4.40654359	1.77173565
H	1.89095299	2.12231777	-2.77735736
H	2.84137551	3.20827827	-3.37468436
H	1.08296093	0.11700668	-1.90892146
H	0.27297318	1.44141876	-1.80852861
H	-0.76340087	1.30314262	2.84605968
H	0.64790183	0.79672394	2.43577983
H	0.82192654	-1.89639925	-0.88301634
H	2.39881505	-1.71534401	-0.95959617

H	-4.50619313	0.13499997	0.76857883
H	-3.69584145	1.40501429	0.40025589
H	-2.67700032	-3.06449336	1.49537259
H	-2.50457920	-3.38093158	0.02981337
H	-4.35443358	-2.15852354	0.21591459
H	-5.86473775	-1.82892988	0.07323112
H	-2.64896451	-0.46633960	-2.66934121
H	-1.09474398	-0.10339622	-2.80783403
H	-4.48531213	0.72993622	-2.31772703
H	-4.72485147	-0.68661834	-1.77340831
H	-3.05697895	0.64808691	2.32053057
H	-2.79100421	0.46949805	3.85644762
H	-1.26282900	-1.73905539	-1.18924359
H	-0.93430234	-2.05480228	0.30044370
H	4.06922857	-3.00506388	1.28052404
H	4.41477372	-1.10424982	0.04390441
H	4.91331944	-2.00607846	-1.33512622

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p_dHa_hco_nh2 W18			
N	-3.64607377	1.91526721	-2.32372049
O	-1.28730184	0.69974954	-1.63706105
O	1.28223880	1.52196998	-1.36246347
O	2.01819795	-1.08245694	-1.87029527
O	4.59413981	-0.55184021	-2.47105356
O	0.96602191	2.25260469	1.28969415
O	1.69220722	0.37793774	3.16547405
O	3.46192377	-1.00020169	1.87510179
O	2.27791133	-2.85786220	0.29286415
O	3.39543258	2.91453015	-0.18587768
O	4.87690925	0.69498670	0.02576141
O	-0.64340887	-1.89389420	-2.03556707
O	-2.77609078	-3.50260378	-1.68306127
O	-0.52500098	-3.50123900	0.25704887
O	-2.03240598	-2.57531503	2.34590528
O	-1.01263571	-0.28061384	2.96899899
O	-1.80000107	1.44661802	0.96808302
O	-4.44643081	0.72340511	0.37018647
O	-3.92340833	-1.90118993	0.37383720
O	-0.57046388	4.36873680	-0.35851865
C	-1.54956639	4.21121877	-0.88469653
H	-5.26231927	0.82392329	0.85233977
H	-4.26922977	-0.23986802	0.32580991
H	-3.34589935	-2.15937016	1.10260679
H	-3.65356789	-2.43126302	-0.38482619
H	1.41250811	-3.25987567	0.40394193
H	2.21075474	-2.30380170	-0.49416553
H	0.01518519	2.37114493	1.35856632
H	1.22209329	1.64891924	2.00320043
H	-2.76431453	1.41130744	0.97699247
H	-1.56969951	1.09469418	0.09209106
H	-1.13097230	-4.06718127	-0.22279335
H	-1.00129093	-3.22255972	1.05486099
H	-1.62229604	-1.72379484	2.64417343
H	-2.24997791	-3.08114867	3.12382749
H	-2.08920463	-2.92922922	-2.06718721
H	-3.22582691	-3.94767070	-2.39518946
H	-0.94127515	-0.97308784	-1.92348983
H	-0.46243210	-2.23300364	-1.14870105
H	-0.06299875	-0.16554765	3.09850520
H	-1.28296026	0.35137690	2.28449924
H	-0.46305509	1.18143649	-1.79944055
H	-2.05243706	1.15488854	-2.05144363
H	3.96240996	-0.49233919	1.22791629
H	3.06278880	-1.75214976	1.40221798
H	2.77351137	3.05556506	0.53264442
H	2.82306300	2.65085602	-0.91635704
H	4.38434389	1.54345643	0.00879738

H	5.75222229	0.88301504	0.35501023
H	2.84655706	-1.05274303	-2.36938892
H	1.29654753	-1.46269837	-2.38038996
H	5.00221060	-0.01596357	-3.14424156
H	4.77499018	-0.12962842	-1.61896374
H	2.37740275	-0.17025974	2.70023071
H	2.03467734	0.59224211	4.02881382
H	1.60493612	0.61820218	-1.50693356
H	1.14559670	1.62088941	-0.40813665
H	-3.57063266	2.91714335	-2.25464419
H	-4.13804243	1.57863974	-1.50473677
H	-4.18796463	1.69311297	-3.14203501

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r\_Rc\_dHa\_hco\_nh2 W18

N	-3.50199689	1.32360434	-3.26537943
O	-1.13004949	0.57929527	-2.01139975
O	1.54922966	0.87944911	-1.88413526
O	1.70264978	-1.82745609	-1.37980807
O	4.26235052	-2.45910958	-1.94207707
O	2.06389957	2.55257415	0.30499177
O	1.64946875	1.17962709	2.62097490
O	3.12205280	-0.90742836	2.18515919
O	1.62188573	-2.93029081	1.21600963
O	4.25335357	1.61506042	-1.15253788
O	5.02002808	-0.63842787	0.03066753
O	-1.06312535	-2.08753257	-1.42908431
O	-3.31971307	-3.40116225	-0.76661637
O	-1.22399459	-2.95888961	1.21901048
O	-2.55773509	-1.14631030	2.76689306
O	-1.16192034	1.02348607	2.48932665
O	-2.09501741	2.03364481	0.11148344
O	-4.69334307	1.16141693	-0.47377458
O	-4.42525125	-1.22006167	0.65492159
O	0.39152421	4.92568739	0.34147199
C	-0.78251423	4.85754806	0.28116104
H	-5.50519702	1.53619677	-0.14356725
H	-4.62713988	0.25744344	-0.09348168
H	-3.84801094	-1.18676040	1.42796750
H	-4.15988696	-1.99163449	0.14067985
H	0.69083138	-3.08932404	1.39356052
H	1.66214145	-2.61618105	0.30467560
H	1.63099055	3.40899768	0.30482536
H	1.91844104	2.15344580	1.17884022
H	-3.04331455	1.87163075	0.01902295
H	-1.68871270	1.52635275	-0.61023412
H	-1.90005558	-3.55500262	0.89292329
H	-1.65739663	-2.37801846	1.86327855
H	-2.00977738	-0.32203242	2.71759577
H	-2.81579044	-1.26717174	3.67647294
H	-2.59325076	-2.98971828	-1.26724365
H	-3.76450521	-4.02156247	-1.33651815
H	-1.16465990	-1.14531930	-1.64706901
H	-0.96344267	-2.14829661	-0.46923569
H	-0.19701862	1.02067456	2.51805600
H	-1.44308514	1.43658595	1.65768677
H	-0.20822392	0.81033184	-2.21570654
H	-1.73990978	0.87339682	-2.70405186
H	3.78749124	-0.84178337	1.49175511
H	2.58276505	-1.69124308	1.97485968
H	3.72019731	2.13961458	-0.54237453
H	3.62169227	1.36807470	-1.83351999
H	4.80108295	0.22338070	-0.38711464
H	5.91877201	-0.58363726	0.34530476
H	2.48757797	-2.20784410	-1.80087725
H	0.88963298	-2.18191620	-1.75389057
H	4.81154605	-2.34514053	-2.71160662
H	4.62663505	-1.89959391	-1.24070599

H	2.20608598	0.37025150	2.46864368
H	1.91482198	1.54103204	3.46293693
H	1.66416687	-0.05234567	-1.63734176
H	1.58942323	1.40161645	-1.07178766
H	-1.36912593	3.91821385	0.19640180
H	-4.11819881	1.30155674	-2.45025107
H	-4.07151047	1.58232655	-4.06556782

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ts Rc_hco_nh2 W18			
N	-3.37577877	2.73962311	-2.00275348
O	-1.22729127	0.98622776	-1.68359041
O	1.41473002	1.50619912	-1.74878682
O	1.74934282	-1.19340355	-1.90749365
O	4.13963197	-2.40704451	-1.55669563
O	1.84102720	2.68205098	0.74418346
O	1.63888975	0.93825610	2.86062175
O	3.23917693	-0.94068468	2.01235569
O	1.93361292	-2.74038554	0.40552350
O	4.12447661	2.14645700	-0.82377884
O	5.08824735	-0.21437265	-0.01258093
O	-0.98831625	-1.71790666	-1.99536570
O	-3.04620777	-3.39680171	-1.57513882
O	-0.83971830	-3.27581049	0.34514799
O	-2.22384688	-2.14920241	2.40605652
O	-1.06965498	0.11713587	2.94383810
O	-2.19305860	1.44047150	0.86731254
O	-4.78866175	0.87496487	0.09938413
O	-4.19312868	-1.70755312	0.39043807
O	-0.32390457	4.57681671	-0.08831416
C	-1.43860810	4.20388270	-0.07014037
H	-5.59118943	1.02711776	0.59069693
H	-4.63615237	-0.09348215	0.11350949
H	-3.57860050	-1.83963649	1.12213485
H	-3.91978032	-2.30676280	-0.31373556
H	1.09645698	-3.18871103	0.55890710
H	1.75064200	-2.12452607	-0.31642803
H	1.25026783	3.43619266	0.73438468
H	1.69869988	2.17420737	1.55873783
H	-3.14078542	1.28936140	0.75075090
H	-1.78259881	1.16825756	0.03103852
H	-1.47372929	-3.82888808	-0.11474969
H	-1.29399122	-2.94261508	1.13563438
H	-1.74084132	-1.32572136	2.66916620
H	-2.46620650	-2.60570971	3.20708959
H	-2.41222806	-2.79381374	-2.00143905
H	-3.50333741	-3.88221777	-2.25570240
H	-1.18171880	-0.76614492	-1.95445172
H	-0.81569772	-2.00658132	-1.08986697
H	-0.12428881	0.30712012	2.95461680
H	-1.45912134	0.67616232	2.25165444
H	-0.32062797	1.31019379	-1.83691388
H	-1.86074281	1.62028834	-2.05292373
H	3.94191397	-0.68458506	1.40341766
H	2.76059851	-1.66597697	1.58169148
H	3.54510580	2.51194630	-0.14548250
H	3.55412914	2.06978993	-1.59154161
H	4.77490325	0.65469392	-0.34091255
H	6.02275300	-0.12701133	0.15674597
H	2.56782952	-1.65399946	-2.14849927
H	0.98485540	-1.55737592	-2.36426736
H	3.78210761	-2.97538062	-0.87287263
H	4.58524550	-1.68870903	-1.09154261
H	2.25415724	0.22562767	2.55391732
H	1.93783569	1.20341889	3.72695571
H	1.64017670	0.56432388	-1.79026224
H	1.50353310	1.78753379	-0.82944710
H	-1.84177745	3.40512402	0.58124575

H	-4.07965148	2.35636147	-1.37115955
H	-3.72820376	3.62513928	-2.35224505

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ts\_dHa\_hco\_nh2 W18

N	-3.41259731	2.20971960	-2.62881047
O	-1.11719648	0.80796210	-1.81943842
O	1.52723017	1.21364457	-1.57001242
O	1.87918456	-1.51032785	-1.63881846
O	4.50123428	-1.71888726	-2.22306405
O	1.78049223	2.56098140	0.84294430
O	1.58646482	0.84528697	2.95035311
O	3.17605659	-1.01688927	2.08772077
O	1.85364574	-2.97135558	0.76683083
O	4.09286740	2.17392379	-0.70474247
O	5.05030555	-0.19264498	0.05145824
O	-0.87314878	-1.91458612	-1.82193348
O	-3.06359428	-3.42904259	-1.39094080
O	-0.98315241	-3.20129057	0.65427180
O	-2.42898712	-1.80765048	2.49968908
O	-1.19993142	0.45095030	2.80152113
O	-2.14200231	1.73668104	0.58737909
O	-4.73211441	0.97796139	-0.19967182
O	-4.26998180	-1.56876404	0.37377319
O	-0.43474881	4.42994776	0.48320863
C	-1.52004985	4.32230575	0.04934543
H	-5.55181045	1.20857346	0.22867889
H	-4.60117470	0.01562416	-0.05157679
H	-3.69553735	-1.64737201	1.14583411
H	-3.96743518	-2.22173713	-0.26800187
H	0.93496238	-3.22671532	0.88661481
H	1.88776011	-2.53538304	-0.09316677
H	1.13441848	3.26889149	0.84860171
H	1.67848513	2.05190934	1.66365259
H	-3.08696998	1.57494962	0.47942745
H	-1.72791049	1.32502323	-0.18532359
H	-1.61835317	-3.78328503	0.23445864
H	-1.45220393	-2.76621287	1.38391710
H	-1.93703875	-0.96148353	2.66488444
H	-2.70145193	-2.14976352	3.34665755
H	-2.35717469	-2.91123826	-1.81518854
H	-3.48706307	-3.96200823	-2.05739312
H	-1.05241809	-0.96115555	-1.87242041
H	-0.77046636	-2.13019519	-0.88455449
H	-0.23996691	0.52574069	2.86360472
H	-1.49443764	1.00572670	2.06074717
H	-0.19617383	1.10886720	-1.91461935
H	-1.71470214	1.34906557	-2.35319525
H	3.82977402	-0.77345259	1.42388269
H	2.69758495	-1.78883385	1.73516052
H	3.51678456	2.53462449	-0.02070424
H	3.47800575	1.96402774	-1.41381387
H	4.76327520	0.71351108	-0.19558615
H	5.93726430	-0.12762541	0.39622828
H	2.70119510	-1.72530121	-2.10310358
H	1.10441332	-1.83979494	-2.10485769
H	5.04308570	-1.41849872	-2.94619406
H	4.78882967	-1.24429867	-1.42951188
H	2.19043359	0.12130093	2.63973173
H	1.86654551	1.08325481	3.83037822
H	1.71558056	0.26202467	-1.52655306
H	1.52060019	1.55339085	-0.66393414
H	-1.80436978	3.78895618	-0.87716875
H	-4.06195287	1.85744581	-1.92180696
H	-3.95083357	2.79324715	-3.26276923



## 3 W33 geometries

### 3.1 Adsorption geometries

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C	-0.12786200	2.00695900	0.15997700
O	0.96765900	1.28905800	-0.19714700
H	-0.31209200	2.86179100	-0.46391600
H	-0.93593100	1.48923100	0.64678400
H	1.06274700	0.47510900	0.31691600
O	5.81613200	-3.90887700	2.71129000
H	5.43484300	-3.37694700	3.41271300
H	4.73749000	-5.27299300	2.02692100
O	0.39808400	-2.54331400	6.36958000
O	0.19250300	0.27826000	3.15124700
H	1.63719400	-3.36473900	5.68508600
H	-0.51009200	-2.71470100	6.08809200
H	0.81662900	0.01648600	2.46642200
H	0.71617700	0.75915000	3.79964100
O	1.86222600	-0.88738600	1.26887100
O	2.40158500	-3.84106300	5.28601100
H	5.83304100	-3.35200500	1.92286400
H	1.35649400	-1.72999600	1.24356600
H	2.52155600	-4.64618500	5.78432300
H	3.77075300	-2.87137200	4.98435100
O	4.53285100	-2.31152300	4.73438900
H	4.08688200	-0.89818100	3.73935400
H	5.07010300	-2.19396500	5.51345000
O	4.11039800	-5.78459300	1.49783500
H	3.24098700	-5.60207500	1.88414300
H	4.31957600	-5.26086500	-0.08358200
O	1.74473600	-4.97899700	2.69731500
H	1.23704300	-4.36831300	2.15009000
H	1.91744100	-4.53151000	3.52896600
O	3.72715000	-0.15109900	3.23363100
H	2.84164900	0.84856700	4.30304200
H	3.09500200	-0.52835700	2.60285300
O	0.36547300	-3.07442400	1.16655800
H	-0.46859700	-2.83797900	1.59861200
H	0.22347500	-3.29228400	0.22989800
O	0.47036300	0.28309800	6.67797600
H	0.59286000	0.60420200	7.56788100
H	0.46792200	-1.59220900	6.50404600
O	-2.56125400	0.80409700	3.15400500
H	-1.61705800	0.89246000	2.98950500
H	-2.77387100	-0.05656700	2.78985600
O	-2.24674300	-2.58631900	5.48946600
H	-2.39735400	-1.63327300	5.67946000
H	-2.95486100	-3.08703300	5.88471100
O	-2.29529700	0.03053100	5.82115100
H	-2.47876700	0.43966100	4.96144500
H	-1.40548400	0.28665400	6.07868300
O	2.18716000	1.36397600	4.82055100
H	1.14840300	0.69876600	6.12383500
H	2.41924700	2.28600600	4.74210300
O	-1.49606500	-1.96525100	2.84858000
H	-1.83322700	-2.42006600	3.62813700
H	-0.87326400	-1.31089100	3.18397000
H	2.58550100	-0.97521300	0.60970300
O	0.40541300	-3.54865800	-1.51584300
H	0.11911100	-4.36363500	-1.91793400
O	4.54290700	-4.76834400	-0.90529700
H	3.50128800	-3.71203000	-1.79129600
H	5.15689400	-5.28767900	-1.44738300
O	5.71276600	0.75606500	-3.77699000
O	5.40686100	1.32599900	1.36283300

H	5.43570300	-0.16729600	-3.75714400
H	6.57245800	0.84392900	-3.34896600
H	4.96547100	0.82981900	2.06204900
H	4.73615300	1.51733900	0.68807400
O	5.73944100	-2.63389500	0.22944800
O	4.97161600	-1.97686600	-3.89278100
H	5.39621400	-3.42562100	-0.22943000
H	6.66285700	-2.51826000	-0.03721300
H	4.86389900	-2.24894200	-4.80109600
H	4.23321700	-2.37146400	-3.39069800
O	3.03312800	-2.97317000	-2.22787000
H	3.18112600	-2.20932600	-1.64834300
H	1.29346800	-3.36045500	-1.86096000
O	6.43270300	-5.65359100	-2.63704800
H	6.89482900	-4.80809300	-2.77934200
H	7.08305000	-6.34837900	-2.62764400
O	7.40100300	-3.15037600	-2.96868900
H	7.77946400	-2.69562900	-2.20942400
H	6.62018800	-2.66075900	-3.24862700
O	3.79277200	-0.99059000	-0.51514600
H	3.94042600	-0.06466800	-0.75411700
H	4.62201700	-1.41516200	-0.21750600
O	8.29818000	-2.02903600	-0.51337600
H	8.20678000	-1.08967400	-0.23256700
H	9.03407400	-2.40796100	-0.04065000
O	4.41420400	2.90053100	-3.00983500
H	3.86827500	3.30788700	-3.67621300
H	4.82844600	2.09717500	-3.40028500
O	6.68071400	3.76262900	1.06301100
H	6.25861400	2.94103700	1.34940900
H	7.57129800	3.74416000	1.40270300
O	7.93906000	1.67759600	-2.34846600
H	7.56058900	2.57003500	-2.16267300
H	8.79158500	1.80042200	-2.75728900
O	6.71750000	3.90255700	-1.71783700
H	6.62211000	3.95772000	-0.75578500
H	5.84261000	3.80593400	-2.10680700
O	3.63174900	1.72652600	-0.68576100
H	3.83603700	2.22293900	-1.49326900
H	2.67514600	1.76592000	-0.55060500
O	7.85138900	0.46927700	0.14744400
H	7.88314400	0.95237600	-0.68976500
H	7.01302500	0.67731100	0.57749800

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C	0.70794541	-3.91239297	0.44983564
H	1.25531142	-3.85467978	-0.47478617
H	0.72736670	-3.07679718	1.12870972
H	0.26640083	-4.84598869	0.75292732
O	0.13146051	2.69224801	3.06015103
H	0.87304371	2.09366100	3.17829719
H	0.57101619	3.99593172	1.81271315
O	6.41614554	0.63554847	1.21449627
O	3.40188914	-2.14162373	-1.17599560
H	5.25778785	1.64941571	1.80909455
H	6.71786912	0.72389841	0.30116508
H	2.58798299	-1.62759492	-1.05768268
H	3.64363395	-2.45180932	-0.29640717
O	1.45838463	-0.33305614	-0.49800100
O	4.59373178	2.28042223	2.16888441
H	-0.58089468	2.2105253	2.62628131
H	1.82685074	0.44004521	-0.96799141
H	5.08091266	3.02340096	2.51662077
H	3.28742748	1.60738671	3.08295553
O	2.53536652	1.17452420	3.52929296
H	2.18768855	-0.37228489	2.64502704
H	2.70837696	1.20224070	4.46647434

O	0.69435937	4.51755633	1.00756160
H	1.54960103	4.24561734	0.63905659
H	-0.63517588	4.16555070	0.09851458
O	3.07936842	3.52804243	0.03764056
H	2.94458601	2.91406363	-0.69620336
H	3.58645167	3.05807268	0.70386279
O	2.03347547	-1.10301519	2.03222880
H	3.18912545	-2.20630429	1.82624664
H	1.82846549	-0.70479993	1.16741841
O	2.58391892	1.64565546	-1.95245743
H	3.35506676	1.19064451	-2.32842044
H	1.99717517	1.92910721	-2.67245252
O	6.45081857	-2.19208931	1.48540665
H	6.97668152	-2.58951694	2.17432745
H	6.43087516	-0.30828902	1.40653469
O	5.36670595	-2.93055073	-3.01287694
H	4.55359536	-2.86887839	-2.49960461
H	5.34757391	-2.15568353	-3.57393966
O	7.24121129	0.40811716	-1.44408964
H	7.42239853	-0.55960722	-1.41895432
H	7.99003657	0.84404770	-1.84081099
O	7.37461554	-2.20588240	-1.22068712
H	6.73418817	-2.60057430	-1.83240904
H	7.07540933	-2.38232911	-0.32346623
O	3.85095503	-2.88329958	1.53164227
H	5.53494846	-2.50412928	1.59382003
H	3.48340929	-3.74229582	1.72278376
O	4.68051680	0.01494732	-2.54549880
H	5.54845588	0.30084959	-2.23809791
H	4.39711439	-0.69054424	-1.95315910
H	0.49148499	-0.24489145	-0.52700113
O	0.69432868	2.41284722	-3.77197928
H	0.70499669	3.31389100	-4.08220372
O	-1.46328554	3.80053999	-0.29460176
H	-1.49727194	2.72880008	-1.60090763
H	-2.13190525	4.50021201	-0.36477349
O	-5.13449955	-0.84497626	-2.50274771
O	-3.45713226	-2.60539170	2.04138291
H	-4.79435928	0.05801785	-2.56461682
H	-5.83287152	-0.87264836	-1.83813875
H	-2.84837612	-2.35104626	2.73062608
H	-2.95546678	-2.62648976	1.20582268
O	-1.97967115	1.74889309	1.39710602
O	-4.21197170	1.76592671	-2.70642273
H	-1.87387744	2.54071009	0.83444664
H	-2.90500786	1.73731107	1.67803055
H	-4.47442228	2.20344039	-3.51265589
H	-3.24279266	1.88936098	-2.61405961
O	-1.58551365	2.01281586	-2.26623339
H	-1.43422206	1.19381447	-1.76875882
H	-0.15502985	2.27894825	-3.32189169
O	-3.67327221	5.33732011	-0.63651922
H	-4.33676470	4.63042014	-0.53394068
H	-3.99676773	6.11399945	-0.19153295
O	-5.24990193	3.15964498	-0.45340632
H	-5.10991058	2.64311846	0.34827652
H	-4.96679938	2.61895386	-1.19886096
O	-1.23895206	-0.03923316	-0.46758188
H	-1.66611426	-0.90337327	-0.43766450
H	-1.54374777	0.49245518	0.29364474
O	-4.71002707	1.71798855	1.92846229
H	-5.07233110	0.80370369	1.89647460
H	-5.05628874	2.13135380	2.71498891
O	-3.83575652	-3.08837383	-2.36083275
H	-3.61724669	-3.42975009	-3.22395543
H	-4.27351785	-2.20907133	-2.48831025
O	-4.96035750	-4.90421531	1.66843438
H	-4.44407486	-4.15832568	1.99890925

H	-5.52409995	-5.20417963	2.37537543
O	-6.93952244	-1.56600044	-0.49198069
H	-6.68446658	-2.51412259	-0.57023175
H	-7.88627726	-1.50919106	-0.58842694
O	-5.98691477	-4.00530101	-0.74183243
H	-5.66766314	-4.41664470	0.07339362
H	-5.23682116	-3.92557107	-1.33947039
O	-2.14589659	-2.66301381	-0.32669766
H	-2.68754039	-2.90107379	-1.10460927
H	-1.33988152	-3.18256617	-0.34402356
O	-5.59988791	-0.75314837	1.81111585
H	-6.13546998	-0.99340150	1.04295745
H	-4.90197546	-1.41204067	1.88903014

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C	0.69981830	-0.29256385	-3.75379451
H	0.42103688	0.28160718	-4.63623657
O	1.32698042	-1.46517762	-4.09390902
H	1.27533713	0.30233864	-3.04815296
H	-0.23354650	-0.59212837	-3.25336047
O	-0.46616044	3.10787234	-2.64325114
H	-1.25836340	2.57655057	-2.75298842
H	-0.84736501	4.23576973	-1.18790048
O	-6.64836335	0.68966578	-0.79638782
O	-3.38770200	-2.42168280	0.71860869
H	-5.60441804	1.88721151	-1.20872589
H	-6.89555221	0.56193718	0.12887669
H	-2.57254263	-1.89906922	0.67415692
H	-3.63117859	-2.60154029	-0.19531641
O	-1.47092810	-0.48935904	0.34698849
O	-4.99454831	2.61847475	-1.46159170
H	0.23215871	2.55527253	-2.27712623
H	-1.82619077	0.16852943	0.97667981
H	-5.53371243	3.39021335	-1.61561770
H	-3.73810175	2.19092774	-2.55536238
O	-3.01370616	1.86049773	-3.12059549
H	-2.54016006	0.21988176	-2.59203996
H	-3.24611122	2.05869234	-4.02385388
O	-0.93386352	4.60664795	-0.30011154
H	-1.75705091	4.24645206	0.06696897
H	0.44248945	4.10811164	0.46012089
O	-3.20620901	3.39672903	0.66631751
H	-3.01247971	2.64412922	1.24087073
H	-3.82753245	3.09001345	0.00182609
O	-2.22358499	-0.62380726	-2.24029732
H	-3.28655790	-1.85093967	-2.23822228
H	-1.95226427	-0.46722883	-1.31602718
O	-2.55700021	1.15759488	2.18788985
H	-3.30332127	0.62051060	2.50139367
H	-1.95051303	1.32605975	2.92744689
O	-6.51105906	-2.01114086	-1.66371662
H	-7.08252391	-2.28228665	-2.37737830
H	-6.59897970	-0.19238517	-1.18078449
O	-5.15522175	-3.63072224	2.51291194
H	-4.39095226	-3.43588706	1.95860954
H	-5.10697849	-2.98316386	3.21537986
O	-7.26822149	-0.13879425	1.79113497
H	-7.40400247	-1.08951189	1.57187254
H	-8.00048476	0.15446485	2.32584653
O	-7.28801147	-2.64827929	1.02099569
H	-6.60252504	-3.12849756	1.51125377
H	-7.02044658	-2.61328239	0.09769104
O	-3.90484096	-2.60689630	-2.07680742
H	-5.60124686	-2.25752289	-1.90523528
H	-3.57357936	-3.36173639	-2.55583699
O	-4.59476545	-0.60520839	2.55290004
H	-5.49751434	-0.30697339	2.39478537

H	-4.35731470	-1.17379458	1.81174218
H	-0.50316883	-0.42652523	0.39527861
O	-0.62472145	1.65696249	4.05700767
H	-0.66572307	2.46673510	4.55770028
O	1.29429317	3.69691270	0.73951199
H	1.43786570	2.45478284	1.88032474
H	1.96260413	4.39250719	0.85393398
O	5.54714938	-0.79726492	2.08150191
O	3.36556750	-2.33795803	-2.36402102
H	5.10066078	0.04277515	2.25211735
H	6.12884261	-0.69759394	1.31788579
H	2.65098571	-2.11080364	-2.97295977
H	2.97148586	-2.48385123	-1.49219383
O	1.72148553	1.89984622	-1.23857334
O	4.29242703	1.62308807	2.59937395
H	1.63123818	2.59681250	-0.55853196
H	2.61238438	1.99819385	-1.60695266
H	4.58767310	2.05252853	3.39868580
H	3.31254099	1.64382122	2.60846453
O	1.60926228	1.66118726	2.43061667
H	1.45583974	0.90863712	1.83831304
H	0.21576989	1.66491637	3.57205985
O	3.46909113	5.27948697	1.08742348
H	4.14960022	4.64577742	0.79391232
H	3.67961862	6.13273982	0.72175521
O	5.09363545	3.24925183	0.40718284
H	4.89053034	2.83586815	-0.43965709
H	4.87996279	2.61484501	1.09989952
O	1.22713906	-0.18092722	0.40845436
H	1.72254736	-1.00390850	0.31941512
H	1.48955932	0.44597432	-0.29116660
O	4.34271941	2.08551969	-2.06532116
H	4.72997509	1.18206735	-2.15767557
H	4.59278682	2.58259677	-2.83966045
O	4.41113729	-3.11516788	1.87668561
H	4.35418446	-3.55606986	2.72027741
H	4.80744002	-2.21974550	2.03284928
O	5.08210003	-4.47584760	-2.40967006
H	4.45572622	-3.75722683	-2.58012161
H	5.52023185	-4.68147848	-3.22994780
O	7.05333016	-1.16280635	-0.23756364
H	6.90100627	-2.13661223	-0.22059389
H	7.99389403	-1.01526850	-0.28686908
O	6.37931611	-3.69783817	-0.10744962
H	5.98469033	-4.06095762	-0.91410724
H	5.71324483	-3.74352848	0.58499188
O	2.36713769	-2.71527985	0.19512075
H	3.07266949	-2.91097109	0.84451062
H	1.68547144	-3.37287824	0.31181054
O	5.31518284	-0.32698321	-2.25334718
H	5.97273988	-0.57979900	-1.59184513
H	4.66492488	-1.03939628	-2.30313759

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C	-0.29978482	1.83005582	3.11614820
H	-0.90284215	0.96268332	2.77501970
O	-0.66169572	2.94600102	3.07590543
O	-1.94713734	-3.37184823	1.92994791
H	-2.65196117	-2.72151541	1.96784577
H	-2.09296711	-4.20651040	0.28138165
O	-6.34251604	0.95338658	-1.01379135
O	-2.15108301	2.90487413	-1.27434294
H	-5.88438181	-0.57536785	-0.60000521
H	-6.30142898	1.22785872	-1.93937851
H	-1.61654067	2.10843099	-1.12435001
H	-2.56654308	3.09039049	-0.42557260
O	-1.14104351	0.42808864	-0.77792512

O	-5.63962951	-1.49815128	-0.35941136
H	-1.10352962	-2.90928690	1.89303978
H	-1.42185357	-0.04571488	-1.58581752
H	-6.40203536	-2.04321255	-0.53734912
H	-4.78808840	-1.64361567	1.12657830
O	-4.22438304	-1.61246802	1.92310364
H	-3.12297384	-0.23245412	1.71842562
H	-4.78895114	-1.73208346	2.68172424
O	-1.98447668	-4.47725028	-0.64056679
H	-2.56063005	-3.89873553	-1.16375116
H	-0.36328463	-4.29370187	-0.85858338
O	-3.56112579	-2.66505579	-2.00694334
H	-3.04527268	-1.98159032	-2.45352439
H	-4.23659055	-2.21692696	-1.49275282
O	-2.49724694	0.48250446	1.53727797
H	-3.04753982	2.05525473	1.48386143
H	-2.07406478	0.30844336	0.67537138
O	-1.97481610	-0.64452208	-3.09373533
H	-2.41307458	0.12545351	-3.49079574
H	-1.22602314	-0.91916515	-3.64700729
O	-5.67610118	3.42038752	0.25911429
H	-6.31899778	3.82387984	0.83643117
H	-6.14356526	1.73954263	-0.49400700
O	-2.86250666	4.75043272	-3.23794107
H	-2.39142325	4.26456641	-2.55091628
H	-2.82424202	4.17548698	-4.00142185
O	-6.03942555	2.10770932	-3.53247373
H	-5.92907204	3.03162558	-3.20775436
H	-6.68595739	2.11089927	-4.23253289
O	-5.50092460	4.42293970	-2.42251303
H	-4.60263946	4.68684930	-2.67630448
H	-5.49962090	4.24552115	-1.47689175
O	-3.24155300	3.00930565	1.34877484
H	-4.84185212	3.34864261	0.75424648
H	-2.68461114	3.48742065	1.96090283
O	-3.24948798	1.70981634	-3.62194938
H	-4.20681871	1.70880412	-3.73191366
H	-3.07707486	2.11463307	-2.76433882
H	-0.22610121	0.16494687	-0.58613285
O	0.29925290	-1.52845887	-4.33057914
H	0.25500197	-2.26866456	-4.92903017
O	0.60139505	-4.09508729	-0.79982248
H	1.35466773	-2.91613943	-1.73480187
H	1.09740812	-4.92896581	-0.76165334
O	5.91472150	-0.76161588	-0.41345110
O	2.90479645	1.40905956	3.26903202
H	5.37552496	-1.47199635	-0.78686117
H	6.16739457	-0.99601139	0.48771586
H	1.99473671	1.48709079	3.55980397
H	2.89765639	1.60763915	2.31805921
O	0.73935327	-2.49778950	1.39858052
O	4.38671580	-2.80925712	-1.47827576
H	0.72913017	-3.14194188	0.66424117
H	1.41054614	-2.80528514	2.02415671
H	4.80624473	-3.32099084	-2.16572163
H	3.48531433	-2.58828056	-1.79384036
O	1.85891372	-2.17501928	-2.13572809
H	1.72424283	-1.43034787	-1.52966157
H	0.91368742	-1.77385390	-3.62056209
O	2.36617368	-6.14783953	-0.57246709
H	3.02893316	-5.69328141	-0.02105512
H	2.24071364	-7.02469654	-0.22383533
O	4.07828277	-4.54938198	0.75390989
H	3.71825637	-4.10376205	1.52902734
H	4.22971698	-3.88255056	0.07561018
O	1.34784613	-0.37054475	-0.10967549
H	1.95386614	0.31617278	0.18908623
H	1.21774066	-1.04778938	0.58310719

O	2.87500263	-3.26814459	2.98005421
H	3.37087803	-2.46315142	3.25440541
H	2.76696894	-3.81330724	3.75485113
O	5.35320032	1.76276197	-0.42605996
H	5.65408800	2.19395424	-1.22162230
H	5.55736801	0.79572896	-0.51176404
O	5.04157587	3.02838965	3.94905207
H	4.22994420	2.50624446	3.90149560
H	5.26218168	3.14507423	4.86825199
O	6.61478069	-0.75033467	2.29062652
H	6.73758641	0.22725284	2.27494471
H	7.42075566	-1.14037092	2.61826547
O	6.70756552	1.86694658	2.08188124
H	6.20483839	2.35315647	2.75089443
H	6.32089247	2.06876009	1.22449988
O	2.87816326	1.88105097	0.56891871
H	3.76595745	1.89616059	0.15523502
H	2.40932487	2.65364479	0.26086316
O	4.19795361	-1.09721114	3.63410636
H	5.06499560	-1.00980443	3.21509851
H	3.74934580	-0.24892064	3.54918989

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N	-0.38315484	2.88535565	2.87987663
H	-1.29551218	2.51402786	2.60818992
H	-0.56282745	3.68407358	3.48166877
O	-0.01062022	-4.06927335	-1.23702955
H	-0.74807056	-4.04383002	-0.62338791
H	-0.58714067	-3.50997976	-2.89959644
O	-6.18704712	-1.79231454	0.45418926
O	-2.89605621	1.45907924	1.88413512
H	-5.16945307	-2.75524441	-0.43466760
H	-6.55411088	-0.97550761	0.09399742
H	-2.31538274	1.03904182	1.21531584
H	-3.08280383	0.76817330	2.53202999
O	-1.46493824	0.11493226	0.07759005
O	-4.59022991	-3.34177124	-0.96994618
H	0.63428112	-3.40508838	-0.97024923
H	-1.90101620	0.24667771	-0.78646137
H	-5.16528863	-3.92264436	-1.46188213
H	-3.20135220	-3.97377488	-0.14008658
O	-2.40334507	-4.21404385	0.36579562
H	-1.95879734	-2.81259845	1.41175588
H	-2.50829426	-5.11407109	0.66153156
O	-0.79126087	-3.01029889	-3.70254350
H	-1.66668082	-2.61871027	-3.56230833
H	0.49693404	-1.97699544	-3.81473927
O	-3.24019098	-1.87241038	-3.07407455
H	-3.14576603	-0.94511470	-2.82250636
H	-3.68448132	-2.31282176	-2.34580045
O	-1.74001272	-1.96425434	1.81799814
H	-2.66819204	-1.33509290	2.93392139
H	-1.61358961	-1.32689534	1.09561380
O	-2.78690845	0.73448144	-2.18858066
H	-3.49090493	1.26876046	-1.79168688
H	-2.25641840	1.29358434	-2.78090869
O	-5.88231783	-1.05030673	3.18328580
H	-6.32008046	-1.57361396	3.84946210
H	-6.07623162	-1.63949930	1.39861896
O	-4.92833122	3.37816333	2.17026612
H	-4.12582142	2.84715236	2.11647233
H	-5.05998568	3.70646073	1.28183462
O	-7.14678650	0.77153251	-0.14304823
H	-7.21495246	1.07967740	0.78957932
H	-7.96278852	0.97851889	-0.58979937
O	-6.95487391	1.46521256	2.38330880
H	-6.29827965	2.17350563	2.45647726

H	-6.59592266	0.68468604	2.81738906
O	-3.22645414	-0.79696136	3.55923389
H	-4.93459051	-1.01841534	3.40656907
H	-2.78686083	-0.79032806	4.40526691
O	-4.61814518	1.91632119	-0.52473745
H	-5.50800060	1.54326713	-0.54725946
H	-4.22286448	1.61920719	0.29779307
H	-0.51297499	0.27480194	-0.06197019
O	-1.08664711	2.15446149	-3.77768494
H	-1.17564972	2.06481358	-4.72227448
O	1.31008927	-1.43581404	-3.68378976
H	1.28164306	0.21295828	-3.32378642
H	1.97367430	-1.67785242	-4.34935432
O	5.10218921	2.80255210	-0.86595089
O	3.27536432	-0.21978179	2.96163933
H	4.69823389	2.39247613	-1.64216020
H	5.76942532	2.20563008	-0.50750636
H	2.64072035	-0.91645811	3.10991081
H	2.78486508	0.54518102	2.59514845
O	1.94239372	-1.99201472	-1.09367021
O	3.97304531	1.65462299	-3.13238404
H	1.79769181	-1.84807075	-2.04813520
H	2.87377092	-2.23069611	-0.98944365
H	4.18761472	2.11455306	-3.94029080
H	3.00204369	1.51754898	-3.12943885
O	1.34455321	1.13219121	-2.98625054
H	1.24829316	1.04647965	-2.02348509
H	-0.18762766	1.86553207	-3.54941109
O	3.49591426	-1.82181155	-5.24854878
H	4.16902560	-1.58583085	-4.58368036
H	3.80112223	-2.59194248	-5.71731783
O	5.09717888	-0.95441701	-3.26505781
H	5.00581308	-1.42133817	-2.42673253
H	4.77672932	-0.05527112	-3.13403522
O	1.15695833	0.46711601	-0.33512266
H	1.57492181	0.94010852	0.39965556
H	1.54415317	-0.42284628	-0.43722057
O	4.67837952	-2.37910473	-0.85109467
H	4.97957725	-1.88433441	-0.05487631
H	5.06702802	-3.24869758	-0.80922270
O	3.84831794	3.79511423	1.19138849
H	3.64634077	4.71931310	1.07395674
H	4.26824772	3.47385304	0.35623663
O	4.95528492	1.08875679	4.72965279
H	4.35756176	0.50576463	4.24298034
H	5.55835608	0.53700061	5.21904874
O	6.83152516	1.33916206	0.78003219
H	6.60483085	1.89126060	1.56493857
H	7.77951174	1.34859533	0.68018744
O	5.95819080	2.79151838	2.78550806
H	5.63405284	2.27434249	3.53632475
H	5.21106471	3.27884931	2.42201172
O	2.03329090	1.86623029	1.85526047
H	2.62583769	2.60734069	1.64479670
H	1.22350994	2.23599713	2.25242318
O	5.41102592	-1.00633953	1.26354573
H	5.95944966	-0.22960421	1.08775993
H	4.69248259	-0.72756584	1.84217533

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O	-0.27580700	2.70198000	-2.96735100
H	-1.04422600	2.14622400	-3.11963400
H	-0.68985700	3.92406600	-1.63888000
O	-6.55485400	0.59017600	-1.14547100
O	-3.44855300	-2.45091500	0.82445800
H	-5.42077300	1.66459600	-1.66764600
H	-6.81921000	0.58321800	-0.21642700



H	-2.60895800	-1.97371600	0.74439800
H	-3.69120100	-2.70498800	-0.07246000
O	-1.44131700	-0.63948500	0.30816900
O	-4.76567000	2.32896700	-1.98203000
H	0.41852200	2.16205500	-2.57560400
H	-1.80230400	0.08970400	0.84807500
H	-5.25961100	3.10304800	-2.24070000
H	-3.48652400	1.73945500	-2.98790400
O	-2.75154300	1.34227100	-3.49164800
H	-2.36764200	-0.27469900	-2.76959100
H	-2.95594200	1.44105700	-4.41757900
O	-0.79721500	4.39483600	-0.80061900
H	-1.63568600	4.08559400	-0.42240300
H	0.55442700	3.97831600	0.03344200
O	-3.12798800	3.31154100	0.18808900
H	-2.95585000	2.61323100	0.83363400
H	-3.68588000	2.93019300	-0.49408900
O	-2.17814500	-1.08322900	-2.27668100
H	-3.30159000	-2.20412600	-2.16040900
H	-1.88832700	-0.81682800	-1.38718000
O	-2.54017800	1.22537900	1.93662100
H	-3.30722300	0.74487300	2.28866000
H	-1.94943000	1.46531600	2.66869700
O	-6.54530700	-2.19589800	-1.68331600
H	-7.10056100	-2.52392000	-2.38562400
H	-6.55029700	-0.33225400	-1.42377400
O	-5.33163000	-3.37487700	2.68205000
H	-4.54506900	-3.29730500	2.13073100
H	-5.27081600	-2.62638200	3.27558000
O	-7.25666100	0.08627400	1.50876900
H	-7.43872500	-0.87506600	1.39490100
H	-7.98256300	0.47517200	1.98826700
O	-7.39535400	-2.49280900	1.03202200
H	-6.73824400	-2.94215600	1.58603200
H	-7.11404000	-2.57372400	0.11546400
O	-3.96116300	-2.91304500	-1.93309800
H	-5.63548100	-2.49488600	-1.86160100
H	-3.64958200	-3.73059900	-2.31143500
O	-4.64375600	-0.42831700	2.42625700
H	-5.52067300	-0.10441000	2.19070500
H	-4.39247800	-1.06686600	1.74867000
H	-0.47567400	-0.56486700	0.35910900
O	-0.65326000	1.91879500	3.79622900
H	-0.70506700	2.79242200	4.17351600
O	1.39886100	3.59740600	0.37523900
H	1.48647100	2.46227000	1.61596200
H	2.06346700	4.30091600	0.44918600
O	5.48610400	-0.82231400	2.23993700
O	3.45052100	-2.69062700	-2.13353800
H	5.05760600	0.03987600	2.33349900
H	6.11432900	-0.78731500	1.50883900
H	2.76696700	-2.46915800	-2.76153000
H	3.02736100	-2.76955300	-1.26119100
O	1.86371000	1.60917700	-1.41317000
O	4.28579400	1.65193800	2.52508200
H	1.76845600	2.37495000	-0.81403600
H	2.76373700	1.65165600	-1.76441800
H	4.55364600	2.13721300	3.30176400
H	3.30578000	1.68931400	2.48745800
O	1.62363100	1.71821700	2.24167900
H	1.47029800	0.91801600	1.71526600
H	0.19828700	1.86007200	3.33485900
O	3.57863600	5.19595400	0.66204800
H	4.25960400	4.52879500	0.45920000
H	3.81532000	6.00541100	0.22064900
O	5.19969700	3.08655100	0.24339100
H	5.01995500	2.60339900	-0.57101300
H	4.94424000	2.52014300	0.97956200

O	1.26513400	-0.29408900	0.38668800
H	1.76106300	-1.11926600	0.37335500
H	1.54307900	0.27035100	-0.36126500
O	4.54078800	1.71641800	-2.15095500
H	4.93254800	0.81427600	-2.16374900
H	4.80837700	2.15471800	-2.95443800
O	4.33017700	-3.13264400	-2.18099600
H	4.22029400	-3.49478000	3.05637200
H	4.73004700	-2.22933700	2.27792900
O	5.19088500	-4.84715000	-1.95104800
H	4.57832100	-4.15198500	-2.22075300
H	5.69417300	-5.10590300	-2.71739600
O	7.12596400	-1.39990800	0.05245100
H	6.95573900	-2.36516900	0.14798700
H	8.07004800	-1.26707400	0.05089800
O	6.38226900	-3.90354300	0.36311700
H	6.01733600	-4.32690400	-0.42641700
H	5.68595400	-3.87964300	1.02665000
O	2.38779600	-2.86983600	0.37073600
H	3.05623500	-3.01429200	1.07247900
H	1.66922200	-3.47692200	0.53265000
O	5.51582100	-0.72522000	-2.11586800
H	6.13527600	-0.92207400	-1.40001800
H	4.84497100	-1.41547400	-2.11334400

## 3.2 PES geometries

### 3.2.1 CH2OH + CH2OH

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i1_dHa1_ch2oh_ch2oh W33			
C	-2.62654349	4.13448340	0.39746540
O	-2.06710621	2.91180901	0.25545781
H	-2.59092678	4.80873109	-0.44257680
H	-3.44363203	4.16739722	1.09588239
H	-1.44907094	2.88637959	-0.49168848
C	-0.20821815	3.85057840	-2.59483467
O	-0.37589462	2.68072828	-1.91137746
H	-1.10764022	4.23673713	-3.03798507
H	0.61313360	4.48307473	-2.30635184
H	0.48183764	2.36793028	-1.54216961
O	3.34817397	-1.65513951	-2.03986364
H	3.57708658	-0.75100999	-1.81708058
H	3.77612064	-2.82611918	-0.67286519
O	3.85989288	2.86942843	2.62274918
O	1.00677935	2.57909224	2.62031471
H	4.72877622	1.64220834	1.79091835
H	3.86168803	2.97523838	3.58496590
H	0.78464533	1.79472049	2.09022241
H	1.96419594	2.68080231	2.53086456
O	0.98229104	0.31149137	1.20824899
O	5.18464392	0.97227427	1.24461032
H	2.38692069	-1.71846445	-2.08921128
H	1.36581833	-0.21081459	1.93830889
H	6.09219971	0.93876905	1.53662784
H	4.71921477	0.96412728	-0.45437709
O	4.29765469	0.98084208	-1.33118455
H	2.67637771	1.70785627	-1.08286496
H	4.95574778	1.24129189	-1.96989661
O	3.76126995	-3.42218619	0.08892813
H	3.96628692	-2.87566403	0.86163848
H	2.24199874	-4.09695450	-0.00267277
O	4.25696864	-1.63686208	2.16921017
H	3.47713437	-1.45967868	2.71097088
H	4.52804377	-0.78692996	1.81726181
O	1.84361130	1.99656409	-0.68252857

H	1.95183399	3.77500622	-0.19801049
H	1.62966938	1.33501780	0.00528052
O	1.87980127	-0.94612291	3.44000478
H	1.81521225	-0.28616616	4.14792086
H	1.30329770	-1.69651238	3.66231815
O	3.89273172	5.40317716	1.55887987
H	4.56492731	5.98172111	1.21039372
H	4.02866378	3.75086462	2.25698183
O	0.05358478	4.95706616	1.96783948
H	0.23186273	4.03206798	2.23023506
H	-0.87499815	5.01222822	1.73962610
O	3.22661691	3.61286529	5.19911059
H	2.73799707	4.36902545	4.81629987
H	3.71405255	3.94277682	5.94882232
O	2.14599492	5.65123191	3.80091704
H	1.28074413	5.60622550	3.38215080
H	2.77171475	5.78248479	3.08095791
O	1.93936591	4.73016263	-0.04815598
H	3.23043320	5.22749818	0.84999749
H	1.18888157	4.90461471	0.53924506
O	1.49849812	1.26005919	5.05873767
H	2.15096815	1.86854903	5.41004714
H	1.08220491	1.76037931	4.34860772
H	0.27418819	-0.22568357	0.80706544
O	0.23537094	-3.09669322	3.80073203
H	0.59597084	-3.89819520	4.16877883
O	1.30644221	-4.32886228	-0.20225368
H	0.01692647	-3.92106607	0.81930149
H	1.25729325	-5.22672176	-0.56670374
O	-4.89571751	-3.12456964	-0.90579076
O	-2.38279229	0.89673279	-2.93545193
H	-4.14650289	-3.66468925	-0.62212498
H	-4.89216052	-3.06167904	-1.86827803
H	-1.58526183	1.41734750	-2.80002856
H	-2.68967797	0.66765731	-2.04140573
O	0.60520078	-2.33002321	-1.90801325
O	-2.78707853	-4.75280955	-0.08463898
H	0.84305498	-3.11416218	-1.37755625
H	0.19871792	-2.65594657	-2.72362076
H	-3.08526490	-5.54991433	0.34678072
H	-2.07979302	-4.37155573	0.47668378
O	-0.78140721	-3.58877075	1.28119554
H	-0.89909789	-2.68588925	0.94286346
H	-0.18259010	-3.33390042	2.95709699
O	0.62962313	-6.68574360	-1.36182158
H	-0.13418871	-6.35464183	-1.86945895
H	1.10921848	-7.29496948	-1.91383273
O	-1.51299790	-5.52446616	-2.51218588
H	-1.33045049	-4.77075895	-3.08466435
H	-2.00865113	-5.20209949	-1.75164908
O	-0.88018436	-1.17212110	0.00342188
H	-1.70710149	-0.70264317	-0.17522441
H	-0.47142158	-1.48458225	-0.82588311
O	-0.78209484	-3.29099953	-4.09152104
H	-1.48293495	-2.61901099	-4.26258483
H	-0.35040482	-3.47155911	-4.92213659
O	-5.51610314	-0.75196537	-0.02718864
H	-6.07538368	-0.77066941	0.74436807
H	-5.29896097	-1.68631822	-0.26629912
O	-4.76422802	2.00014606	-3.73121090
H	-3.85423499	1.70523786	-3.57650670
H	-4.85628470	2.16458454	-4.66524851
O	-5.15503685	-2.32389687	-3.57869773
H	-5.62546406	-1.49826924	-3.31683993
H	-5.72138791	-2.80008992	-4.18004750
O	-6.24486951	-0.10156599	-2.69264202
H	-5.81728644	0.70214181	-3.02169722
H	-6.14083635	-0.12689531	-1.73611115

O	-3.09568148	0.39748923	-0.35755977
H	-3.97964583	0.06187311	-0.13062468
H	-2.94750481	1.24035152	0.08424446
O	-2.63747856	-1.47664807	-4.43747171
H	-3.52200871	-1.77940643	-4.19133274
H	-2.48014721	-0.64612337	-3.97214375

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C	-3.02327394	3.22316661	-0.40199023
O	-2.08978431	2.43046254	-0.96975307
H	-3.18173245	4.14896037	-0.92808559
H	-3.83699755	2.75471455	0.12679324
H	-2.04107092	1.53976703	-0.57805721
C	-0.02121224	4.46697535	1.22492739
O	-1.19886736	4.24752402	1.87591267
H	0.76006388	4.86798047	1.84159779
H	-0.05158994	4.65940006	0.16745621
H	-1.88520213	3.98994948	1.24687220
O	2.53823206	-3.19548171	1.48795494
H	2.18894144	-2.66939613	2.21046572
H	1.39513252	-4.48852511	0.78049034
O	-2.82404340	-1.57839710	5.22521760
O	-2.90711778	0.90514383	2.16440907
H	-1.64172979	-2.43329807	4.47796258
H	-3.74434276	-1.71757387	4.96654047
H	-2.30098808	0.65878856	1.45784634
H	-2.35212657	1.31805136	2.83872772
O	-1.39588229	0.01775236	0.05936646
O	-0.91852848	-2.94875505	4.05179917
H	2.56817552	-2.61593238	0.71677535
H	-1.94972292	-0.79127291	-0.02172107
H	-0.84934073	-3.77403792	4.52638996
H	0.52708757	-2.08218454	3.77623092
O	1.33151820	-1.58054946	3.53705801
H	0.96125803	-0.13594050	2.54129456
H	1.85279710	-1.47913374	4.32912715
O	0.73820597	-4.95439646	0.24499423
H	-0.11831762	-4.71994487	0.63163562
H	0.97479635	-4.42097915	-1.32806657
O	-1.58188199	-4.01461033	1.43711360
H	-2.08104612	-3.39988935	0.88754602
H	-1.41388043	-3.57443840	2.27375018
O	0.62634960	0.62971266	2.04810432
H	-0.28877803	1.66106642	3.23611342
H	-0.02407977	0.28284343	1.42607634
O	-2.96644791	-2.10848628	-0.10292463
H	-3.79920636	-1.92443669	0.35493853
H	-3.11523266	-2.33000411	-1.03731439
O	-2.67215755	1.24095481	5.60870476
H	-2.5359167	1.57421248	6.49189628
H	-2.72355737	-0.63535283	5.39463182
O	-5.51935524	1.78989689	2.02871680
H	-4.57108171	1.62141713	1.97433063
H	-5.91156711	1.00185391	1.65207039
O	-5.50223539	-1.58193167	4.42041709
H	-5.60349055	-0.61881665	4.58666643
H	-6.19030965	-2.03803467	4.89682221
O	-5.43172232	1.04649905	4.73413343
H	-5.57446169	1.46352411	3.87249094
H	-4.54157443	1.27452559	5.01850443
O	-0.98225415	2.16212396	3.69649963
H	-1.99245202	1.63965436	5.03974953
H	-1.03711852	3.01366162	3.24188183
O	-4.77359359	-1.13942293	1.72587109
H	-5.16471282	-1.57530686	2.48915272
H	-4.09119385	-0.56801139	2.09476259
H	-0.64963838	-0.08998857	-0.57176034

O	-2.89099651	-2.58651077	-2.78341070
H	-3.17483035	-3.39878624	-3.19278522
O	1.21705307	-3.92557852	-2.14290591
H	0.21282926	-2.82409086	-3.01097103
H	1.81290689	-4.45816225	-2.69234977
O	2.56986276	1.63427499	-4.92927700
O	2.33055146	2.07775154	0.20723733
H	2.28139726	0.71437523	-4.90734570
H	3.41574476	1.72184633	-4.47450447
H	1.86380862	1.61143324	0.91231674
H	1.66778930	2.28717592	-0.46740464
O	2.48043983	-1.85213561	-0.96279205
O	1.73817992	-1.07369660	-5.06852640
H	2.11680929	-2.62448233	-1.43816558
H	3.40492317	-1.75052308	-1.23294811
H	1.61994724	-1.32154906	-5.98250037
H	0.98988949	-1.45856695	-4.57366643
O	-0.23194222	-2.06004963	-3.42915493
H	-0.06459064	-1.31910247	-2.82599286
H	-1.98964456	-2.41218260	-3.10029500
O	3.07098700	-4.84750570	-3.89309647
H	3.55902867	-4.01445510	-4.02250980
H	3.69999043	-5.56175528	-3.89367029
O	4.12007287	-2.37243854	-4.18410312
H	4.51611224	-1.94624468	-3.41681666
H	3.35881681	-1.84703913	-4.45214138
O	0.57846146	-0.14570416	-1.65884057
H	0.76231361	0.77363712	-1.89559292
H	1.39295078	-0.60545789	-1.36874809
O	5.04856437	-1.31297970	-1.72195996
H	4.99967438	-0.36951519	-1.43991356
H	5.77445093	-1.72079751	-1.25779106
O	1.23003788	3.75099432	-4.17699986
H	0.68503611	4.15201574	-4.84783313
H	1.66972459	2.96031553	-4.56772897
O	3.15827837	4.68796102	0.04542743
H	2.93696407	3.77795765	0.29429157
H	3.95783381	4.92103353	0.50864050
O	4.75126150	2.57099907	-3.43326928
H	4.34045403	3.43498359	-3.19511018
H	5.59422278	2.75341549	-3.83980899
O	3.45013049	4.73832807	-2.72848219
H	3.29024332	4.80074957	-1.77561052
H	2.60259211	4.65284899	-3.17515476
O	0.53186416	2.57650616	-1.83477328
H	0.70008429	3.05515591	-2.66148079
H	-0.39715644	2.69700256	-1.60616892
O	4.72507455	1.18698439	-1.02892634
H	4.76038764	1.71910359	-1.83519724
H	3.91296738	1.41970064	-0.56138291

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C	-0.02480238	4.20831681	-1.41065129
O	0.46755336	2.99712374	-1.05966666
H	0.69193248	5.00505190	-1.32894992
H	-0.81350466	4.23905755	-2.14428083
H	-0.16451967	2.27619888	-1.18499290
C	0.66774751	0.91022512	4.00964363
O	0.79710404	1.77420383	2.97135749
H	1.52961496	0.85853758	4.64964575
H	0.02174853	0.05785005	3.88581521
H	0.01681584	1.73042270	2.39491143
O	-1.17583519	-2.29793829	3.27617888
H	-1.76549820	-1.54625945	3.18507648
H	-1.81120775	-3.65994527	2.15722293
O	-6.39090224	1.18986038	0.58258649
O	-2.78656796	2.49399068	-2.26560356

H	-5.67271740	-0.06756622	1.34413532
H	-6.69372654	1.07858076	-0.32864286
H	-2.09312336	1.83335847	-2.22619934
H	-2.85671371	2.84441372	-1.36588482
O	-0.97809038	0.62103320	-0.99733487
O	-5.23430854	-0.81633692	1.81103996
H	-0.35763832	-2.09036659	2.80749378
H	-1.60904743	-0.03722577	-1.36854284
H	-5.92196525	-1.34383595	2.20972201
H	-3.85503133	-0.37212816	2.70474363
O	-3.01195526	-0.08593372	3.10842270
H	-2.07498279	0.95204222	2.06260108
H	-3.20000351	0.21320271	3.99460251
O	-1.99873555	-4.21443469	1.38787162
H	-2.67424633	-3.73584201	0.88446297
H	-0.52276734	-4.35701268	0.61648678
O	-3.80042035	-2.60643213	0.04257603
H	-3.42199016	-2.11506205	-0.69676838
H	-4.29818081	-1.98160151	0.57462850
O	-1.51012444	1.51312565	1.50460179
H	-2.27666066	2.88590590	0.86102348
H	-1.35492948	1.04420448	0.66447742
O	-2.66746138	-1.13169994	-2.05972774
H	-3.39773836	-0.70677071	-2.54367758
H	-2.17020144	-1.71336657	-2.66037977
O	-5.37790486	3.85841846	0.51201588
H	-5.67822681	4.50695337	1.14346052
H	-6.05897102	2.09097725	0.65204512
O	-4.20667498	4.27594212	-3.80641272
H	-3.56319944	3.63946129	-3.47307372
H	-4.24788001	4.17556938	-4.75311464
O	-7.08289311	1.22264954	-2.11744046
H	-6.91494635	2.18504734	-2.22791832
H	-7.95663845	1.03533366	-2.44899428
O	-6.38486124	3.76322552	-2.16048678
H	-5.69714567	4.02585366	-2.78810200
H	-6.05825584	3.96451252	-1.27817590
O	-2.68093576	3.58884794	0.30975422
H	-4.40641526	3.86473062	0.52275637
H	-2.00391462	4.25377246	0.17657172
O	-4.56490834	0.45944863	-3.13870480
H	-5.48742028	0.50352032	-2.86656565
H	-4.16652166	1.28649476	-2.85416659
H	-0.13775241	0.13606692	-0.85012342
O	-0.99510591	-2.72096128	-3.50689112
H	-1.26514540	-3.58503062	-3.80450113
O	0.40235085	-4.26422282	0.29423916
H	0.87187387	-3.48332525	-1.14809136
H	0.89330741	-5.08405338	0.46593637
O	5.57707804	-1.10295745	-1.68424787
O	3.37598982	1.90831511	1.92182837
H	4.96858567	-1.85210744	-1.68575493
H	6.02476789	-1.06321004	-0.83013878
H	2.49841597	1.95450655	2.32522681
H	3.22505677	1.81881410	0.96715010
O	1.15640772	-2.09014725	1.72939370
O	3.89657501	-3.34990162	-1.72131923
H	0.96318002	-2.92932717	1.26876165
H	1.97723648	-2.22777630	2.22680059
H	4.19763973	-4.01558055	-2.33500485
H	2.93348878	-3.24916184	-1.85887519
O	1.22494034	-2.92772708	-1.87361303
H	1.27413995	-2.03385490	-1.49823182
H	-0.17090242	-2.83870989	-3.00617238
O	2.21338920	-6.24270788	0.67352468
H	2.98745637	-5.67059149	0.83142608
H	2.25221384	-6.96907760	1.28737515
O	4.17786000	-4.42014449	0.90673503

H	4.04976506	-3.75493699	1.59305646
H	4.15115603	-3.97251434	0.05443761
O	1.32147688	-0.57850067	-0.47073587
H	2.00951080	0.10135036	-0.53394139
H	1.34402688	-0.99690839	0.41307487
O	3.59607308	-2.51526444	2.91356979
H	4.11477658	-1.67580622	2.85094470
H	3.65498860	-2.81951217	3.81522712
O	5.05897054	1.37977716	-2.31291765
H	5.19563678	1.57275453	-3.23608538
H	5.23189884	0.41758721	-2.17547748
O	5.40969218	3.70820795	1.67406295
H	4.64292782	3.17119050	1.92738864
H	5.82945827	4.00693864	2.47510288
O	6.87001361	-0.33499539	0.67439845
H	6.91331219	0.61035302	0.39597508
H	7.75844960	-0.61782752	0.87353111
O	6.75561490	2.14968409	-0.16376009
H	6.33734548	2.77036837	0.45172209
H	6.22020039	2.11951842	-0.96267419
O	2.86939358	1.64281841	-0.74568159
H	3.59221133	1.65854223	-1.39418436
H	2.19234887	2.28088035	-0.99497948
O	4.91979668	-0.28790849	2.67480097
H	5.63893848	-0.32502079	2.03043058
H	4.38059212	0.48562429	2.45711107

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C	-2.15155024	3.45132522	-0.20510950
O	-2.09015504	2.48164105	-1.15285620
H	-2.14636496	4.44883777	-0.60627572
H	-2.67110103	3.22665722	0.70999763
H	-2.12345726	1.59473222	-0.76259453
C	0.89938231	5.17417104	2.50718307
O	-0.09732510	4.31220861	2.15954838
H	0.68574193	5.74163726	3.39354079
H	1.53810881	5.54269806	1.72421451
H	0.06254294	3.93281263	1.29401518
O	2.53868881	-3.19839122	1.48678597
H	2.18401759	-2.67043418	2.20541351
H	1.41703086	-4.53246945	0.79966280
O	-2.81575120	-1.67095394	5.18446278
O	-3.19068353	1.08630161	1.93034301
H	-1.62037493	-2.49958471	4.45104709
H	-3.72809864	-1.84330493	4.91611618
H	-2.59282906	0.78522870	1.23965376
H	-2.61881403	1.49714353	2.59197002
O	-1.54435617	0.00088421	-0.04072863
O	-0.88416611	-2.99253740	4.01815626
H	2.52051941	-2.63049316	0.70688462
H	-2.08377983	-0.82105964	-0.08238466
H	-0.77431944	-3.81071434	4.49716691
H	0.50522263	-2.06399412	3.71045829
O	1.27830756	-1.52695441	3.44390871
H	0.79564495	-0.16678368	2.37766395
H	1.77734945	-1.33020555	4.23234925
O	0.77126726	-5.01053836	0.26194519
H	-0.09311678	-4.76462722	0.62387418
H	1.03086455	-4.50607256	-1.31659048
O	-1.56151038	-4.04853409	1.40682293
H	-2.09065694	-3.44329634	0.87470071
H	-1.39738489	-3.61844496	2.24943681
O	0.39954354	0.57463543	1.89263683
H	-0.51512886	1.54004910	3.07070941
H	-0.26539746	0.20205860	1.29609172
O	-3.03253309	-2.18460011	-0.10608080
H	-3.86644566	-1.98947982	0.34721649

H	-3.17900134	-2.44524176	-1.02979626
O	-2.75254134	1.15357625	5.49293632
H	-2.59135633	1.50608641	6.36436973
H	-2.74461485	-0.72077608	5.32837996
O	-5.93281861	1.66100759	2.12045658
H	-5.00479304	1.69741398	1.86826666
H	-6.25258386	0.85611574	1.71296248
O	-5.47347886	-1.76531288	4.35390534
H	-5.62053511	-0.81434959	4.56044305
H	-6.15127791	-2.27331157	4.79085295
O	-5.53265706	0.83899446	4.74415353
H	-5.74997451	1.26059707	3.89844333
H	-4.64080414	1.10917955	4.98149798
O	-1.15772209	2.11618790	3.52075812
H	-2.11457427	1.56895578	4.88799533
H	-0.90460421	3.00963014	3.25856827
O	-4.87685842	-1.17141399	1.65549284
H	-5.17230007	-1.62387206	2.45262865
H	-4.27703970	-0.48411630	1.96508297
H	-0.81288578	-0.12293209	-0.68367061
O	-2.91969048	-2.78769447	-2.77134187
H	-3.21534630	-3.60687915	-3.15775735
O	1.27007729	-4.01656635	-2.13609370
H	0.20727659	-2.98782218	-3.04156643
H	1.91525771	-4.52422672	-2.65157397
O	2.57010843	1.48976785	-5.08075899
H	1.85086003	2.30427161	0.15546386
O	2.26294740	0.57851469	-5.01092368
H	3.36896143	1.60250408	-4.55289123
H	1.44056380	1.69133461	0.78199344
H	1.31306095	2.32685471	-0.65191252
O	2.38149746	-1.86329666	-0.96415414
O	1.73313043	-1.22423651	-5.07071725
H	2.07878975	-2.66161540	-1.44086278
H	3.30663918	-1.70452785	-1.20030858
H	1.67830501	-1.53505245	-5.97147356
H	0.97858940	-1.61814780	-4.59283095
O	-0.26366251	-2.25013095	-3.47608961
H	-0.13708724	-1.49370273	-2.88210981
H	-2.02437114	-2.62475472	-3.10839098
O	3.26800344	-4.84339083	-3.77708020
H	3.71429513	-3.98537323	-3.88569934
H	3.93448680	-5.52208590	-3.74570605
O	4.16656243	-2.30079092	-4.04366487
H	4.50907346	-1.82163328	-3.28304506
H	3.37462367	-1.84564944	-4.34922607
O	0.43965712	-0.25113841	-1.75650484
H	0.63321471	0.63791636	-2.08559604
H	1.25257266	-0.69032507	-1.43178917
O	4.93598328	-1.11378574	-1.56538571
H	4.79638229	-0.18540151	-1.27479290
H	5.65357917	-1.47672495	-1.05330101
O	1.18293892	3.62878254	-4.48830305
H	0.62672125	3.98086442	-5.17732351
H	1.64794648	2.83455829	-4.83950880
O	2.97390574	4.77587833	-0.18621329
H	2.66089734	3.90564591	0.09872334
H	3.83370059	4.90139556	0.20700458
O	4.60118011	2.51661002	-3.43083152
H	4.19203152	3.40421457	-3.30407377
H	5.48260126	2.64805361	-3.77027827
O	3.28762875	4.74185118	-2.97756883
H	3.08233822	4.84376871	-2.03825290
H	2.46529333	4.61864022	-3.46185237
O	0.42323651	2.41809490	-2.17797461
H	0.62903368	2.90454510	-2.99122752
H	-0.51678452	2.53978297	-1.98401058
O	4.39175707	1.38220565	-0.91345576



H	4.45535337	1.84646447	-1.75971390
H	3.54902754	1.61626321	-0.50939255

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C	-0.90987058	-3.75806475	0.51631337
O	0.21325233	-4.02053099	-0.20840734
H	-1.85668370	-4.03367626	0.08933543
H	-0.75305072	-3.73653126	1.57808768
H	0.01394042	-4.02306749	-1.14965142
C	-0.52531137	-3.58837132	-3.23937435
O	-1.67069236	-3.23893132	-2.62495370
H	-0.51526926	-4.58963115	-3.63411265
H	0.05046111	-2.81056770	-3.71643781
H	-1.71339375	-2.27825076	-2.44253603
O	-0.09885675	2.89803195	-3.04354946
H	-0.87885348	2.34291899	-3.10755524
H	-0.46420081	4.21898491	-1.77706073
O	-6.48990381	1.12269444	-0.96637060
O	-3.54475729	-1.83775550	1.28404764
H	-5.30585571	2.06360169	-1.62397080
H	-6.73058349	1.24042347	-0.03774119
H	-2.66821162	-1.45663781	1.12860802
H	-3.84633548	-2.15964905	0.42893246
O	-1.44078894	-0.19623502	0.49441747
O	-4.62539656	2.66578143	-2.00240897
H	0.60402042	2.38842269	-2.62500354
H	-1.73634015	0.59343177	0.98890634
H	-5.08596611	3.44132610	-2.31344540
H	-3.35418052	1.98423630	-2.93442165
O	-2.62106459	1.52531053	-3.38905513
H	-2.34475576	0.01964996	-2.52737056
H	-2.80392271	1.55531414	-4.32451179
O	-0.55955784	4.72665014	-0.95996733
H	-1.41492027	4.47109607	-0.58040565
H	0.76336434	4.28317041	-0.07538755
O	-2.93241867	3.78181591	0.07241063
H	-2.77118802	3.14286185	0.77986882
H	-3.50932043	3.35566560	-0.56509667
O	-2.24794306	-0.75809383	-1.95572942
H	-3.65403808	-1.73820771	-1.68188243
H	-1.92936760	-0.45494858	-1.07564079
O	-2.39100155	1.84354334	1.98869956
H	-3.18114098	1.44752343	2.39253611
H	-1.77431507	2.10168875	2.69395946
O	-6.82566117	-1.69617850	-1.18662963
H	-7.42954190	-2.08083981	-1.81639575
H	-6.62791709	0.18901883	-1.15719745
O	-5.46319010	-2.43780987	3.25497007
H	-4.68094916	-2.48540628	2.69559552
H	-5.33501941	-1.63507373	3.76071218
O	-7.16302444	0.99718006	1.73219017
H	-7.42591684	0.04778097	1.74546889
H	-7.83914808	1.50334600	2.17365900
O	-7.52843835	-1.59747577	1.58721951
H	-6.87817407	-2.03263324	2.16029766
H	-7.31493202	-1.81614992	0.67525564
O	-4.24830198	-2.46486132	-1.41337811
H	-5.94274765	-2.06622286	-1.35663091
H	-3.86193161	-3.25253204	-1.79552438
O	-4.58124571	0.39891135	2.67994493
H	-5.43730390	0.75358055	2.41378055
H	-4.37712488	-0.32329206	2.07415737
H	-0.46877441	-0.19222163	0.50634668
O	-0.45283648	2.50642501	3.78759873
H	-0.41015983	3.40402317	4.10500020
O	1.58475802	3.88116866	0.29321193
H	1.63760998	2.75352940	1.54887608

H	2.26844559	4.56566468	0.37714525
O	5.47439525	-0.66507826	2.43980251
O	3.80472679	-2.48809785	-2.12023623
H	5.07890538	0.21481768	2.49794625
H	6.14971965	-0.65677497	1.75118301
H	3.18295161	-2.29594038	-2.81708715
H	3.30417616	-2.49028360	-1.27794285
O	2.00287190	1.83984610	-1.44229221
O	4.38203555	1.87940335	2.62352795
H	1.92922595	2.62068511	-0.85994127
H	2.92281405	1.81891436	-1.74069581
H	4.62035515	2.34449509	3.42175349
H	3.40788593	1.94736252	2.53080295
O	1.74336890	2.02622485	2.19883602
H	1.56255902	1.21312129	1.70090940
H	0.37646981	2.33346774	3.31360921
O	3.78767727	5.42395504	0.64712780
H	4.45949491	4.73199633	0.50137391
H	4.07579625	6.21561923	0.20412129
O	5.37138972	3.27287919	0.35526394
H	5.18656561	2.77049111	-0.44652020
H	5.10783266	2.72752966	1.10470681
O	1.27664176	-0.01632645	0.39815337
H	1.75773876	-0.85536910	0.36355343
H	1.56468511	0.53507121	-0.35305617
O	4.72853956	1.86123876	-2.01903505
H	5.16282861	0.97746822	-1.99481367
H	5.03927505	2.30493801	-2.80397049
O	4.22438567	-2.93943299	2.22449086
H	4.01316028	-3.31634989	3.07439368
H	4.63989002	-2.05626681	2.38340657
O	5.44593985	-4.69857002	-1.80206417
H	4.86561098	-3.98160189	-2.08866709
H	6.03245852	-4.90338386	-2.52422241
O	7.23902997	-1.27222025	0.35354405
H	7.02785172	-2.23181597	0.43217878
H	8.18393488	-1.17434922	0.43370107
O	6.41127581	-3.75287166	0.61365531
H	6.12049379	-4.18621608	-0.20082862
H	5.65112451	-3.70453425	1.20291712
O	2.47194857	-2.50236340	0.20187510
H	3.03538181	-2.73101018	0.96229748
H	1.72611785	-3.11800239	0.16894870
O	5.82414793	-0.52169981	-1.92712348
H	6.38391710	-0.72675652	-1.16577397
H	5.17067536	-1.22646609	-1.99620413

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C	-0.93794040	-3.90541786	0.72658898
O	0.23749423	-4.01258902	0.05755120
H	-1.81520319	-3.61458771	0.17739641
H	-1.00627986	-4.50239162	1.61601357
H	0.19261951	-3.54610255	-0.78806534
C	-0.14213440	-3.24520205	-3.45233634
O	0.12299683	-2.55983144	-2.30867383
H	0.39967298	-4.16370285	-3.57374067
H	-1.06600456	-3.04079246	-3.96367704
H	-0.52479513	-1.82972013	-2.19248498
O	-0.02488315	2.76001822	-2.93468004
H	-0.80495806	2.21813464	-3.06713928
H	-0.40754829	4.14369643	-1.74083841
O	-6.42563552	1.10130206	-1.26793165
O	-3.64877255	-1.81007423	1.27529302
H	-5.20681026	2.03479181	-1.83494866
H	-6.73001083	1.19638656	-0.35519140
H	-2.76743257	-1.41009886	1.22243267
H	-3.84921937	-2.10745994	0.38337366

O	-1.49024312	-0.22508403	0.61472778
O	-4.47971632	2.59835534	-2.18873766
H	0.61091683	2.24323367	-2.42466997
H	-1.81891152	0.59381559	1.04189599
H	-4.88649384	3.37178608	-2.57185758
H	-3.21818208	1.80174737	-3.00744483
O	-2.47668840	1.30330399	-3.40685969
H	-2.04720295	-0.11197759	-2.48044088
H	-2.61559601	1.28961898	-4.35016931
O	-0.52400208	4.68471386	-0.94828191
H	-1.40273187	4.46397513	-0.60212121
H	0.74552252	4.23491588	0.02450274
O	-2.96457824	3.80208910	-0.02226930
H	-2.82633800	3.17403287	0.69980435
H	-3.48238812	3.34796300	-0.69028726
O	-1.85681131	-0.86562092	-1.89580995
H	-3.15498063	-1.94478740	-1.75148636
H	-1.73518338	-0.51052437	-0.98078358
O	-2.50190246	1.87971928	1.92721471
H	-3.32735955	1.50712139	2.28432630
H	-1.92347996	2.13749809	2.66398926
O	-6.47950034	-1.72397713	-1.59308869
H	-6.98508124	-2.11007260	-2.30352397
H	-6.45994038	0.15930777	-1.46329876
O	-5.65783758	-2.95616870	2.75475565
H	-4.81072961	-2.63399012	2.42078279
H	-5.69881145	-2.71978213	3.67744317
O	-7.28435935	0.89975432	1.37376934
H	-7.47678664	-0.06436405	1.34420234
H	-8.03862473	1.34346539	1.75118251
O	-7.49638647	-1.70885336	1.09256962
H	-6.92843949	-2.21361969	1.69416771
H	-7.19983446	-1.88768421	0.19591926
O	-3.87831979	-2.55636079	-1.49617527
H	-5.57282191	-2.06356710	-1.65592136
H	-3.60579020	-3.44291598	-1.71925096
O	-4.74060099	0.50329508	2.53622147
H	-5.60643534	0.79693264	2.23451161
H	-4.54315128	-0.30533070	2.05312983
H	-0.52468356	-0.24060313	0.74262417
O	-0.64716309	2.53169549	3.82990701
H	-0.62768510	3.41600744	4.18446744
O	1.53888155	3.82753785	0.44270186
H	1.57799810	2.74817396	1.75484601
H	2.25293322	4.48496840	0.47550927
O	5.62827314	-0.67988645	2.25897470
O	3.00976127	-2.36858516	-1.78669713
H	5.16262142	0.16168666	2.34554885
H	6.11182133	-0.68737515	1.42424420
H	2.13153556	-2.26492637	-2.16030181
H	2.87917272	-2.40433536	-0.82244087
O	1.89364328	1.67760362	-1.17538298
O	4.37289527	1.79770220	2.55302650
H	1.84096394	2.48133765	-0.62299362
H	2.77447840	1.69068501	-1.57803760
H	4.71722306	2.29270232	3.29258576
H	3.39882357	1.89555216	2.57569525
O	1.68440076	2.04100209	2.42450358
H	1.47677062	1.21545156	1.95811924
H	0.22527522	2.36433706	3.43938041
O	3.80989471	5.30579611	0.62386754
H	4.45173134	4.60033878	0.41960843
H	4.07121449	6.09016750	0.15212606
O	5.30921037	3.11461223	0.20864677
H	5.08779307	2.63697933	-0.59915293
H	5.03122655	2.57232328	0.95466822
O	1.20204618	-0.09489258	0.75005482
H	1.70030519	-0.91987051	0.84387850

H	1.52454351	0.39186039	-0.03108912
O	4.47498422	1.79544772	-2.14684448
H	4.80311778	0.86989075	-2.24300237
H	4.62817469	2.24475696	-2.97374680
O	4.53442234	-3.03657544	2.47268116
H	4.54187457	-3.38226042	3.36081412
H	4.93397165	-2.13315494	2.49405449
O	4.65657502	-4.57483525	-1.94362454
H	4.02451497	-3.85013487	-2.05069210
H	5.14441614	-4.64703094	-2.75903694
O	6.88961486	-1.37204579	-0.14736958
H	6.70040792	-2.32966883	-0.00723971
H	7.83356079	-1.27379531	-0.23957327
O	6.14253882	-3.85187652	0.28354186
H	5.62970022	-4.21714751	-0.45181006
H	5.57407449	-3.82091750	1.05971138
O	2.42412848	-2.54892224	0.85411928
H	3.10209272	-2.80089223	1.50322606
H	1.73049169	-3.21921042	0.83157249
O	5.21969992	-0.70209897	-2.27887445
H	5.84545989	-0.92963178	-1.57742533
H	4.44491810	-1.26590482	-2.16360954

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C	0.05733705	3.86902019	0.07694993
O	0.18477857	2.88890128	-0.93121657
H	0.29843169	4.82648567	-0.37735494
H	-0.97636411	3.91620785	0.41416234
H	-0.23963592	2.04970167	-0.66005409
C	0.96441824	3.66044365	1.26969001
O	0.77346968	2.42055878	1.90951130
H	2.00370854	3.68751235	0.95920908
H	0.80620082	4.48674572	1.96591968
H	-0.15444345	2.26440805	2.12143435
O	-1.21672889	-2.47540472	3.22899242
H	-1.71070017	-1.65704484	3.15463513
H	-1.83340540	-3.73056761	2.00461666
O	-6.49384156	0.60857358	0.19448918
O	-2.57043770	3.32350663	-1.90817699
H	-5.65653293	-0.48492275	1.09209684
H	-6.49421762	0.59195197	-0.77150555
H	-1.61335976	3.22457522	-1.87682694
H	-2.87628533	3.37955315	-0.99437920
O	-0.95663426	0.56031174	-0.25701479
O	-5.15943287	-1.14956123	1.62158609
H	-0.30928492	-2.31506475	2.94474721
H	-1.48446107	0.07576053	-0.92927314
H	-5.78521042	-1.81864086	1.88829167
H	-3.91261763	-0.63719455	2.70827002
O	-3.17040783	-0.31663630	3.2523835
H	-2.39083178	1.08673927	2.49116497
H	-3.44457914	-0.37038445	4.16702174
O	-1.98492808	-4.29511172	1.23426219
H	-2.54816836	-3.78017211	0.63662936
H	-0.44326821	-4.56667100	0.66061611
O	-3.57383056	-2.61896310	-0.29140881
H	-3.17051409	-2.02232493	-0.93537237
H	-4.09041693	-2.07421013	0.30663183
O	-1.97447932	1.71309479	1.87840772
H	-2.97333109	2.87677305	1.27874096
H	-1.67745709	1.17666109	1.11015488
O	-2.30877626	-0.85555373	-2.05446819
H	-2.84876730	-0.25230702	-2.59780624
H	-1.75427009	-1.40097911	-2.63753532
O	-6.18858947	3.38057683	0.66546191
H	-6.62206748	3.83643574	1.38182559
H	-6.47875118	1.53915980	0.44018397

O	-4.39913712	4.99294436	-3.12046533
H	-3.63070956	4.48022620	-2.83624740
H	-4.31071407	5.14513462	-4.05692959
O	-6.47276742	1.10474183	-2.56567566
H	-6.61526076	2.07542683	-2.49697478
H	-7.12497923	0.75319497	-3.16556011
O	-6.64186466	3.69640568	-2.12788294
H	-5.91743868	4.21437493	-2.50740361
H	-6.58039642	3.77839179	-1.17188343
O	-3.46907316	3.58837873	0.80487404
H	-5.22880594	3.47264234	0.78669277
H	-3.17702912	4.42232399	1.16572948
O	-3.74226053	1.06559869	-3.25166512
H	-4.68911544	1.02919009	-3.07211712
H	-3.40328523	1.86330873	-2.83473405
H	-0.17389437	-0.00153297	-0.09359948
O	-0.69257620	-2.54303084	-3.47215013
H	-1.11105638	-3.35031039	-3.75750807
O	0.51025553	-4.51115059	0.42446551
H	0.96394909	-3.67412721	-0.98602671
H	0.94615736	-5.36841462	0.54631195
O	5.50727447	-1.22653069	-1.82871204
O	3.33683962	1.45667594	1.83594793
H	4.94955230	-2.01427080	-1.77891336
H	6.01189707	-1.15163960	-1.01020097
H	2.45617649	1.62017600	2.19435172
H	3.18845986	1.44451804	0.87585486
O	1.35228736	-2.47840773	2.02959422
O	3.94155179	-3.52657635	-1.71546741
H	1.11783933	-3.27423754	1.51544458
H	2.19282199	-2.66708343	2.46929915
H	4.16617810	-4.15605777	-2.39638827
H	2.97222044	-3.38299843	-1.76610708
O	1.30766225	-3.05089167	-1.65967927
H	1.30531858	-2.19210187	-1.20352128
H	0.04746535	-2.79579269	-2.89561874
O	2.26587034	-6.56581726	0.64634788
H	3.05612292	-6.00623138	0.76297649
H	2.35049430	-7.31784975	1.22339787
O	4.28772756	-4.79017564	0.81616715
H	4.22457091	-4.15434192	1.53809992
H	4.24850391	-4.29719733	-0.01070167
O	1.29856688	-0.83600108	-0.07547833
H	1.94537527	-0.14054828	-0.25075141
H	1.47008521	-1.28372867	0.77445967
O	3.92087978	-2.95529346	2.94297057
H	4.38207528	-2.09304297	2.81442847
O	4.13314230	-3.26272123	3.81997616
O	4.77160914	1.19877325	-2.46430079
H	4.86026900	1.37795712	-3.39613904
H	5.01512686	0.25347752	-2.31491486
O	5.15380746	3.47903733	1.61824106
H	4.50475215	2.80929700	1.88452590
H	5.65157369	3.72134064	2.39363525
O	6.89033545	-0.37137337	0.45170512
H	6.82031697	0.57169962	0.17501110
H	7.81497827	-0.56617855	0.57799329
O	6.48727791	2.09190885	-0.38504222
H	6.05541247	2.67651752	0.25374737
O	5.91808037	2.01711447	-1.15801484
H	2.65247185	1.45578442	-0.80034088
H	3.31225599	1.45062581	-1.51195603
H	1.92221831	2.04286111	-1.03145456
O	5.05331933	-0.62994494	2.54649090
H	5.73681140	-0.57853867	1.86563739
H	4.42443767	0.08088065	2.36590244

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C	-1.95706453	3.93377894	-0.08369338
O	-1.71557646	2.81051915	0.64434148
H	-1.11096747	4.46927564	-0.47851585
H	-2.88634243	3.90347624	-0.62296730
H	-0.84028693	2.81164691	1.04580272
C	0.05357485	3.65184131	-3.02143873
O	-0.01156141	2.34365421	-2.67776268
H	-0.72191342	3.98395360	-3.68594512
H	0.57777804	4.32727329	-2.36785216
H	0.63238238	2.14177658	-1.97704653
O	3.38071358	-1.58038752	-2.02848610
H	3.54680814	-0.66173032	-1.81137580
H	3.80385401	-2.76288775	-0.67803418
O	3.43997041	2.88127532	2.50817986
O	0.60073489	2.51099294	2.29703724
H	4.45805576	1.67529921	1.77754710
H	3.46629105	2.94913366	3.47356896
H	0.58973157	1.59389645	1.94063908
H	1.54209975	2.73967301	2.27383411
O	0.99489079	0.19461998	1.18188226
O	5.02072909	1.03573258	1.30123400
H	2.43075030	-1.69673931	-2.14951005
H	1.38112235	-0.31985611	1.91649221
H	5.89634877	1.09292191	1.67542615
H	4.68049795	1.04319229	-0.43401540
O	4.25954252	1.09370481	-1.30834497
H	2.65796229	1.83931604	-1.02212358
H	4.92445910	1.33203977	-1.94862359
O	3.79755198	-3.38639726	0.06195431
H	3.98339025	-2.86390753	0.85471850
H	2.30660178	-4.13164180	-0.08300085
O	4.25248061	-1.63396058	2.19669814
H	3.47416351	-1.48400725	2.74683652
H	4.48071723	-0.77553966	1.83506250
O	1.78068143	2.05313957	-0.67152351
H	1.61067045	3.79645682	-0.08725023
H	1.58109146	1.34340981	-0.03711160
O	1.84037273	-0.99931569	3.45249780
H	1.68465343	-0.30757583	4.11178328
H	1.27289203	-1.76226865	3.65837365
O	3.66559706	5.45519271	1.53143658
H	4.34832939	5.98055042	1.12376219
H	3.68421191	3.75655223	2.17418826
O	-0.14693546	5.11673541	2.41949094
H	-0.17492728	4.16970884	2.60334734
H	-1.04741340	5.41508316	2.30877486
O	3.02861699	3.53234589	5.15852459
H	2.66388329	4.38904266	4.85484953
H	3.58190431	3.70230608	5.91594052
O	2.16438139	5.74645188	3.93354950
H	1.27127758	5.72574474	3.57589601
H	2.74247603	5.86590759	3.17250061
O	1.56802883	4.74402862	0.11136009
H	2.95537661	5.29526068	0.87154871
H	0.88994632	4.88317058	0.78019238
O	1.22230316	1.30618487	4.87768444
H	1.84365250	1.96329228	5.20178831
H	0.74796903	1.74943921	4.17093967
H	0.33672401	-0.37597169	0.73499501
O	0.23345737	-3.17348402	3.74890397
H	0.58550087	-3.97165517	4.13211187
O	1.38161130	-4.38330511	-0.30147205
H	0.09188501	-4.01342155	0.73981453
H	1.35106059	-5.28008089	-0.66962570
O	-4.83918812	-3.01694722	-0.70299974
O	-2.36576407	0.91501022	-2.98362902
H	-4.10393070	-3.60918356	-0.49953415

H	-4.92150641	-2.93810892	-1.66110049
H	-1.51330035	1.37208885	-2.97965728
H	-2.56403159	0.72873073	-2.05145572
O	0.68050242	-2.40015995	-2.03239321
O	-2.77188750	-4.79835099	-0.08895432
H	0.92008220	-3.18765470	-1.50891095
H	0.22751204	-2.71229988	-2.82900513
H	-3.09284931	-5.58270458	0.34923826
H	-2.03484988	-4.44769616	0.45281096
O	-0.69949284	-3.67774835	1.21122541
H	-0.82339741	-2.78226875	0.85444538
H	-0.14547404	-3.41421956	2.88668193
O	0.69170889	-6.72568288	-1.47260858
H	-0.09659812	-6.38472195	-1.93489974
H	1.13558415	-7.33181931	-2.05687201
O	-1.50150128	-5.56273332	-2.52297952
H	-1.35428724	-4.80392198	-3.09948303
H	-2.00523571	-5.25710631	-1.76094502
O	-0.77794552	-1.28874410	-0.09272841
H	-1.56867156	-0.75503958	-0.26428967
H	-0.36801337	-1.58640137	-0.92821743
O	-0.87656437	-3.31226744	-4.11719843
H	-1.59160390	-2.63912191	-4.21992998
H	-0.52457452	-3.48351293	-4.98648534
O	-5.25322183	-0.61274538	0.23221851
H	-5.74841652	-0.60894543	1.04647506
H	-5.09841631	-1.55415864	-0.02277705
O	-4.72194995	2.21125375	-3.39276331
H	-3.82270464	1.84418126	-3.38279524
H	-4.90359859	2.50314593	-4.28116947
O	-5.27892069	-2.17919669	-3.33717964
H	-5.66943175	-1.32357974	-3.04215125
H	-5.91820287	-2.60694643	-3.90042053
O	-6.17308534	0.09382658	-2.35874100
H	-5.74863891	0.89426396	-2.70101013
H	-5.99298514	0.04491474	-1.41450147
O	-2.83331813	0.46332194	-0.33343306
H	-3.70629490	0.17564279	-0.01958855
H	-2.56015158	1.25621241	0.14272445
O	-2.74901177	-1.50324585	-4.32775055
H	-3.63409184	-1.76502652	-4.04300748
H	-2.56182240	-0.64725796	-3.91863845

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C	-1.03018410	-3.80630552	0.92546020
O	0.15214802	-3.92969753	0.27400890
H	-1.91440878	-3.60679607	0.34614217
H	-1.08459084	-4.33518590	1.85840003
H	0.10474399	-3.52328084	-0.60266048
C	-0.25120445	-3.38187541	-3.26981001
O	0.04126274	-2.63268302	-2.17277819
H	0.29906035	-4.30000366	-3.35367565
H	-1.21040779	-3.23956106	-3.73585173
H	-0.60140376	-1.89369670	-2.08242549
O	-0.06138922	2.74469706	-2.93217039
H	-0.84257817	2.19715383	-3.03027671
H	-0.41069352	4.15278843	-1.75815312
O	-6.49582645	1.23948920	-1.16338914
O	-3.63673438	-1.62429474	1.43015756
H	-5.23255136	2.12191224	-1.72164711
H	-6.71544594	1.18651603	-0.22392023
H	-2.72544605	-1.29955249	1.36881850
H	-3.97141367	-1.58178827	0.52889333
O	-1.45359266	-0.13760805	0.69080059
O	-4.48178607	2.64532944	-2.08664516
H	0.59167934	2.24067198	-2.43120933
H	-1.78511044	0.67925692	1.11903138

H	-4.85306704	3.43981167	-2.46290238
H	-3.24843989	1.79641054	-2.90964247
O	-2.52406070	1.28114017	-3.31805671
H	-2.06895303	-0.13706621	-2.39092273
H	-2.67955147	1.26535337	-4.25874280
O	-0.50278642	4.71333691	-0.97598685
H	-1.36745927	4.49651969	-0.59373061
H	0.80403016	4.29498427	-0.03962612
O	-2.91547033	3.84914659	0.03810502
H	-2.78126001	3.23799493	0.77541487
H	-3.44915302	3.38647956	-0.61124275
O	-1.88903249	-0.87961473	-1.78963401
H	-3.32317737	-1.81793226	-1.60577944
H	-1.73586160	-0.49560441	-0.89240885
O	-2.46139994	1.96501724	2.02278170
H	-3.27433797	1.61143019	2.42625803
H	-1.85372798	2.24188138	2.72837299
O	-6.67316445	-1.47261780	-1.93607971
H	-7.04246772	-1.80935958	-2.74760381
H	-6.63228803	0.35570385	-1.52039048
O	-5.27667323	-3.75385044	1.52043884
H	-4.56381219	-3.14503070	1.76013288
H	-5.37437054	-4.38478663	2.22768597
O	-7.15720824	0.60707840	1.48635583
H	-7.25895906	-0.35662754	1.33884592
H	-7.96032490	0.91971019	1.89415191
O	-7.32113010	-1.95922251	0.78990095
H	-6.69774166	-2.62922943	1.09861567
H	-7.26084347	-1.94326619	-0.16966023
O	-4.16313860	-2.23428621	-1.32900256
H	-5.75120025	-1.77322587	-1.87043042
H	-4.01067986	-3.16228694	-1.16378748
O	-4.65787622	0.61234125	2.83488066
H	-5.53230566	0.78897222	2.47437590
H	-4.39995169	-0.23990739	2.46740359
H	-0.48526910	-0.13969460	0.79785743
O	-0.53363206	2.67594891	3.83242381
H	-0.51464433	3.56611719	4.17192354
O	1.60946539	3.89550419	0.36282673
H	1.66401490	2.85751067	1.70744510
H	2.32842037	4.54802258	0.35476055
O	5.65175932	-0.62791385	2.23462341
O	2.92692783	-2.42931465	-1.70228476
H	5.20706983	0.22665720	2.30325838
H	6.11679167	-0.67369279	1.39068582
H	2.04185260	-2.34152931	-2.06446167
H	2.81311578	-2.42322360	-0.73542939
O	1.90752325	1.70218495	-1.20700804
O	4.45823523	1.88492664	2.47231468
H	1.87751742	2.52113073	-0.67565783
H	2.77953823	1.68889170	-1.62818188
H	4.82699841	2.39606972	3.18873587
H	3.48637623	1.99975838	2.51317236
O	1.77368187	2.16540041	2.39215897
H	1.54858499	1.33189022	1.94829394
H	0.33091387	2.50950896	3.42461247
O	3.90523309	5.34523512	0.43268338
H	4.52895592	4.62031891	0.24122324
H	4.17235368	6.10703240	-0.07162781
O	5.35895382	3.11318010	0.06655840
H	5.11950721	2.60941855	-0.71986895
H	5.08998648	2.60004551	0.83617414
O	1.23741730	-0.00253900	0.78220048
H	1.72077191	-0.83446255	0.89072536
H	1.55070332	0.45542658	-0.01991203
O	4.47088647	1.72436656	-2.22974626
H	4.76780518	0.78588889	-2.29711799
H	4.62504808	2.13815799	-3.07477109



O	4.52042253	-2.95434547	2.55461927
H	4.54017379	-3.26722836	3.45463147
H	4.93568970	-2.05791133	2.53500655
O	4.53716241	-4.66356913	-1.79914734
H	3.91648811	-3.93132694	-1.92244306
H	5.00670109	-4.77744248	-2.62050842
O	6.84807720	-1.42888624	-0.17113690
H	6.64797352	-2.37752208	0.00915866
H	7.79093853	-1.34912394	-0.28871229
O	6.07524984	-3.87914394	0.37019292
H	5.54358595	-4.26443103	-0.34124126
H	5.52131289	-3.80851554	1.15424016
O	2.38993575	-2.48417967	0.95626335
H	3.07380983	-2.72783199	1.60219855
H	1.67403937	-3.13046880	0.98059750
O	5.14234653	-0.79763933	-2.28633238
H	5.77746945	-1.01676242	-1.59068378
H	4.36147474	-1.34641648	-2.14314558

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C	-0.82190004	-3.71911818	0.34825773
O	0.24953122	-4.07921161	-0.35612067
H	-1.62103239	-4.42755942	0.48422980
H	-0.87477040	-2.71332506	0.72723395
H	0.07629292	-4.13475579	-1.37814451
C	-0.56275257	-3.86367390	-2.84736679
O	-1.74408646	-3.38245729	-2.42307205
H	-0.62847348	-4.85604563	-3.26644066
H	0.11163128	-3.15959120	-3.31693783
H	-1.73100548	-2.41493291	-2.27874206
O	-0.06883539	2.84659483	-3.02521411
H	-0.83278403	2.26927087	-3.08730693
H	-0.45350433	4.17091573	-1.76555396
O	-6.47598433	1.07407307	-0.99986596
O	-3.61637382	-1.78884461	1.41724402
H	-5.27062742	1.98309384	-1.66247103
H	-6.73780877	1.23023698	-0.08261838
H	-2.74160253	-1.40617874	1.27133077
H	-3.89910254	-2.13439119	0.56361016
O	-1.43723867	-0.22853778	0.58989660
O	-4.57756206	2.57026011	-2.04170647
H	0.64694377	2.35881913	-2.60262960
H	-1.75131717	0.56823274	1.06383848
H	-5.02557397	3.34128750	-2.38117053
H	-3.29229923	1.86404728	-2.93481060
O	-2.55058539	1.39588883	-3.36570020
H	-2.30452392	-0.09351371	-2.46350147
H	-2.72147993	1.39769413	-4.30396597
O	-0.55888611	4.68010517	-0.95069483
H	-1.41993853	4.42670953	-0.58272527
H	0.74975025	4.24876805	-0.03922798
O	-2.94254785	3.73582327	0.05170618
H	-2.78576013	3.11149012	0.77283953
H	-3.50009387	3.29080055	-0.59018461
O	-2.22938700	-0.85287533	-1.86437235
H	-3.66926991	-1.80333939	-1.55463688
H	-1.92437991	-0.52313198	-0.99144818
O	-2.42127720	1.83450064	2.01314708
H	-3.23024413	1.47692863	2.41658374
H	-1.80847060	2.09975093	2.71950128
O	-6.84521014	-1.74713687	-1.12655822
H	-7.43435697	-2.15527600	-1.75547949
H	-6.62595883	0.13670127	-1.16119978
O	-5.58098603	-2.33825699	3.36315508
H	-4.78254213	-2.40193613	2.82925379
H	-5.46022725	-1.53297069	3.86619946
O	-7.21621569	1.07055707	1.68425114

H	-7.48504824	0.12366466	1.72702790
H	-7.90451584	1.59721625	2.08065955
O	-7.59880577	-1.52480506	1.62573742
H	-6.96567424	-1.94804294	2.22608300
H	-7.37431690	-1.78238987	0.72662623
O	-4.26230037	-2.51331879	-1.24675568
H	-5.96023754	-2.12807091	-1.25687055
H	-3.84292344	-3.32250389	-1.54085338
O	-4.66594969	0.49054815	2.72238701
H	-5.51125098	0.84987056	2.42955201
H	-4.47027367	-0.26028545	2.14996805
O	-0.46545489	-0.18021295	0.56480440
H	-0.48240351	2.49290626	3.80820383
H	-0.42314253	3.39065136	4.12256998
O	1.56720575	3.85299362	0.34465191
H	1.61867064	2.70982677	1.58773098
H	2.24017640	4.54464127	0.45408260
O	5.41267784	-0.75616965	2.44838851
O	3.83459503	-2.33224042	-2.21156954
H	5.02816782	0.12676644	2.52600152
H	6.11655512	-0.73141696	1.78945487
H	3.25177841	-2.03048965	-2.90312124
H	3.30691967	-2.39016481	-1.38736157
O	2.03930145	1.84006884	-1.40356971
O	4.35115998	1.80235635	2.70233405
H	1.94575576	2.61497680	-0.81570199
H	2.96679124	1.83052657	-1.67875112
H	4.57763120	2.22303056	3.52817941
H	3.37998544	1.88358737	2.59485243
O	1.71901355	1.97767821	2.23304833
H	1.54698423	1.16836412	1.72715963
H	0.34608521	2.30121326	3.34039971
O	3.74065352	5.41116823	0.78393498
H	4.42438089	4.72834886	0.65015788
H	4.03813866	6.21470596	0.36944768
O	5.35862901	3.28550237	0.50013721
H	5.19491343	2.79823465	-0.31546854
H	5.09555865	2.71715758	1.23246019
O	1.26401626	-0.03821515	0.39084276
H	1.73109477	-0.88425984	0.32275196
H	1.56260550	0.53151151	-0.34283598
O	4.77672258	1.91891553	-1.91534316
H	5.23100515	1.04467290	-1.90392857
H	5.09345478	2.38969838	-2.68193234
O	4.15906953	-3.01656143	2.09813379
H	3.91428561	-3.42752426	2.92293907
H	4.57090751	-2.14334120	2.30824084
O	5.44961899	-4.57268639	-1.99082407
H	4.87998141	-3.83937104	-2.25573210
H	6.05293797	-4.74465506	-2.70769716
O	7.25338261	-1.30527275	0.41214599
H	7.02218261	-2.26341690	0.42987538
H	8.19658193	-1.23061809	0.52863586
O	6.36991737	-3.77798765	0.49961001
H	6.09100684	-4.15745719	-0.34525109
H	5.59704704	-3.74926796	1.07355932
O	2.44037572	-2.50957231	0.06225860
H	2.99626022	-2.76446335	0.81995664
H	1.71255401	-3.14686135	-0.01630192
O	5.90519970	-0.44737530	-1.86839595
H	6.44841179	-0.68124282	-1.10343733
H	5.24363199	-1.14088688	-1.96896186

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C	-0.93385432	-3.96800535	0.76412535
O	0.16914932	-4.01643851	-0.02518600
H	-1.89770740	-3.92293616	0.28788994

H	-0.81378292	-4.42087482	1.73027386
H	-0.02536113	-3.65796157	-0.90311792
C	0.47039628	-2.65053392	-3.42872671
O	-0.41205081	-2.78874332	-2.41591459
H	0.87606011	-3.57750436	-3.79591516
H	0.35021942	-1.80343680	-4.08447617
H	-0.93243373	-1.96943473	-2.26307183
O	-0.10861976	2.79950904	-3.00647755
H	-0.89374268	2.25405550	-3.08276257
H	-0.46589307	4.16575551	-1.77920350
O	-6.46864299	1.10020080	-1.04958112
O	-3.59858833	-1.80266077	1.31611303
H	-5.28457258	2.04989716	-1.66783518
H	-6.75561777	1.22367481	-0.13480643
H	-2.71045609	-1.42841308	1.22120030
H	-3.82076088	-2.16423693	0.45405359
O	-1.46193502	-0.19134041	0.59645149
O	-4.58350141	2.63349041	-2.04039396
H	0.56674364	2.29214748	-2.54019089
H	-1.77774922	0.60794406	1.06427218
H	-5.01984921	3.40710295	-2.38900190
H	-3.33808188	1.88018108	-2.92646448
O	-2.61127814	1.39156691	-3.36259735
H	-2.22547846	-0.04780626	-2.45679292
H	-2.79121407	1.38998106	-4.29907117
O	-0.55991801	4.69604198	-0.97664845
H	-1.41978080	4.45910760	-0.59574962
H	0.75150551	4.25748355	-0.05954967
O	-2.94976962	3.79138917	0.05684285
H	-2.79912475	3.16517562	0.77762047
H	-3.51036310	3.35072205	-0.58520957
O	-2.04276383	-0.80602719	-1.87689883
H	-3.31338824	-1.90846251	-1.69411863
H	-1.83630177	-0.45945660	-0.97454863
O	-2.44770882	1.87643858	2.01071005
H	-3.25169187	1.49751629	2.40249130
H	-1.83954137	2.13875879	2.72225324
O	-6.57390809	-1.73339547	-1.26123101
H	-7.15210569	-2.12592076	-1.91025220
H	-6.51194415	0.15258770	-1.21500753
O	-5.52307006	-2.41823244	3.25585218
H	-4.72630672	-2.43595256	2.71451985
H	-5.42882023	-1.62574562	3.78386789
O	-7.25028574	0.98275806	1.61753956
H	-7.47340327	0.02381223	1.62412048
H	-7.96758283	1.46198957	2.02262050
O	-7.49215819	-1.62922595	1.46296301
H	-6.87690197	-2.03726340	2.09261616
H	-7.19203808	-1.84636473	0.57593293
O	-3.98364491	-2.57171044	-1.42475900
H	-5.68233064	-2.08835862	-1.40744357
H	-3.69891850	-3.41757301	-1.76188035
O	-4.67711642	0.45818142	2.64836544
H	-5.53218378	0.80355700	2.36878524
H	-4.46789890	-0.27341507	2.05676640
H	-0.48982709	-0.19185035	0.65782788
O	-0.52270955	2.54465385	3.82063149
H	-0.48417330	3.43438303	4.15979316
O	1.56170490	3.85304988	0.32820151
H	1.61484905	2.76844613	1.63096830
H	2.26442127	4.52214705	0.36987813
O	5.54684893	-0.66831599	2.33589851
O	3.35281482	-2.48179578	-1.96045662
H	5.12277801	0.19718593	2.40018153
H	6.11846998	-0.67848540	1.55888930
H	2.57092686	-2.37847081	-2.50768998
H	3.03907590	-2.48343471	-1.03553068
O	1.91444496	1.74143362	-1.34021178

O	4.39489528	1.85814061	2.54856100
H	1.86439905	2.53732979	-0.77627949
H	2.81256880	1.73009607	-1.70175171
H	4.70055950	2.34660218	3.30903976
H	3.41920049	1.94591504	2.52561017
O	1.72398979	2.05849923	2.29804304
H	1.52970289	1.23404585	1.82358749
H	0.32320172	2.37416951	3.37558576
O	3.80834794	5.35787017	0.55099922
H	4.46032018	4.65280632	0.37927398
H	4.08393617	6.13800107	0.08041105
O	5.33602358	3.17507402	0.21062267
H	5.12188373	2.67554621	-0.58586143
H	5.07270878	2.64174283	0.96855376
O	1.23598084	-0.04329040	0.58518938
H	1.71167672	-0.88685214	0.61664862
H	1.53153524	0.45950175	-0.19620282
O	4.56687431	1.79219142	-2.13529441
H	4.94568762	0.88180741	-2.16800732
H	4.80458212	2.22910795	-2.94883495
O	4.35009054	-2.98442932	2.38382836
H	4.25159248	-3.33404949	3.26512463
H	4.76496989	-2.09068125	2.45822070
O	5.01897514	-4.68006028	-1.86134158
H	4.40266376	-3.95998533	-2.05493347
H	5.55881033	-4.81078951	-2.63541794
O	7.03385763	-1.34481854	0.06016992
H	6.83446902	-2.30202670	0.18893763
H	7.98201181	-1.24610845	0.04298912
O	6.25720758	-3.82128613	0.46014428
H	5.84822586	-4.23122506	-0.31547080
H	5.59116058	-3.77334044	1.15378012
O	2.39880860	-2.52833729	0.55823322
H	3.02136575	-2.76997326	1.26490198
H	1.67092293	-3.16485639	0.53833171
O	5.47970727	-0.65618206	-2.15238086
H	6.07442424	-0.86921444	-1.42015050
H	4.75342206	-1.29083246	-2.12323982

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C	-0.84784908	-3.65149226	0.46286953
O	0.22085324	-4.20934452	0.40783722
H	-1.78132669	-4.21399943	0.49117241
H	-0.92658850	-2.56584464	0.51987412
H	0.43059424	-3.62523816	-2.41120595
C	-0.56121972	-3.89695085	-2.76925711
O	-1.56910742	-3.23281185	-2.04254336
H	-0.69270107	-4.96128791	-2.61633860
H	-0.63266403	-3.68280182	-3.83381796
H	-1.53066279	-2.27840155	-2.18916414
O	-0.05501648	3.01545638	-3.01478155
H	-0.85192697	2.49568064	-3.14131730
H	-0.42302938	4.29675802	-1.71759555
O	-6.44460646	1.13836157	-1.04146017
O	-3.50927294	-1.78127751	1.27435051
H	-5.27178230	2.12655099	-1.65392942
H	-6.69293840	1.20585066	-0.10983633
H	-2.69356728	-1.27486769	1.14657821
H	-3.82525535	-1.99500627	0.38741735
O	-1.44201308	-0.09372105	0.55408305
O	-4.60302467	2.75640789	-2.00669767
H	0.60694444	2.45792024	-2.59113583
H	-1.74224211	0.69395589	1.05458032
H	-5.07883606	3.53608033	-2.28250476
H	-3.32624187	2.13601435	-2.98184081
O	-2.58544786	1.70791131	-3.45270200
H	-2.25447288	0.19953153	-2.57156207

H	-2.78736232	1.73174090	-4.38421475
O	-0.52263560	4.78105951	-0.88666887
H	-1.38776315	4.52910547	-0.52754157
H	0.78120722	4.28923664	-0.00571406
O	-2.92229728	3.84648112	0.09160436
H	-2.77844174	3.21367166	0.80785197
H	-3.49236515	3.41988277	-0.55187392
O	-2.16149215	-0.56437198	-1.98429985
H	-3.57661476	-1.54177801	-1.71441099
H	-1.88686286	-0.24168188	-1.10426578
O	-2.41763871	1.91386342	2.02739039
H	-3.21766474	1.50897465	2.40676732
H	-1.80930735	2.15292333	2.74583832
O	-6.74731675	-1.67035400	-1.42119310
H	-7.28314410	-2.06110856	-2.10606160
H	-6.58208176	0.21762835	-1.28734491
O	-5.47532823	-2.94057744	2.82782839
H	-4.64719473	-2.61727768	2.45248305
H	-5.47491669	-2.68947733	3.74772725
O	-7.16527245	0.89262220	1.64436258
H	-7.38265650	-0.06703236	1.60438094
H	-7.89370503	1.34585013	2.05937974
O	-7.46945527	-1.69712793	1.33489376
H	-6.83944464	-2.21428382	1.85798720
H	-7.28452809	-1.86181108	0.40498735
O	-4.13729550	-2.28778632	-1.42730879
H	-5.83864828	-2.00437031	-1.52359456
H	-3.62381733	-3.05965740	-1.67886058
O	-4.59179684	0.46373009	2.70037862
H	-5.47036400	0.75656334	2.43427557
H	-4.40336253	-0.32754599	2.18657812
H	-0.46863715	-0.08789862	0.56462633
O	-0.45737902	2.49651681	3.83713100
H	-0.39182296	3.37730687	4.19500420
O	1.59647398	3.86863729	0.35693115
H	1.64471813	2.73931415	1.60658655
H	2.29455468	4.53992199	0.43110362
O	5.55074729	-0.65628497	2.36492654
O	3.58120094	-2.49249479	-2.10940733
H	5.14596734	0.21833283	2.43348356
H	6.18850813	-0.65001221	1.64135002
H	2.93554919	-2.26374115	-2.77269125
H	3.11795530	-2.52146844	-1.24627464
O	1.96686208	1.82843778	-1.39313816
O	4.41487074	1.86892192	2.58582127
H	1.90857217	2.60581857	-0.80439439
H	2.87700094	1.81270807	-1.72159062
H	4.68253373	2.34934884	3.36547743
H	3.43828788	1.93213808	2.53085078
O	1.75354826	2.00970445	2.25397572
H	1.56973168	1.19876286	1.75526934
H	0.37223461	2.31978023	3.36574276
O	3.82435192	5.38897182	0.65719547
H	4.48760309	4.69783163	0.47392355
H	4.08968415	6.18302008	0.20422154
O	5.38043897	3.23029647	0.28669641
H	5.17510899	2.73609472	-0.51516673
H	5.11579413	2.68723861	1.03727664
O	1.26126446	-0.02999480	0.44175184
H	1.71768942	-0.88357514	0.40769855
H	1.55570304	0.51692167	-0.31136231
O	4.65970952	1.84010797	-2.07615686
H	5.06319110	0.94126692	-2.07392164
H	4.94190161	2.27478915	-2.87669985
O	4.28287712	-2.92368794	2.19038237
H	4.10065309	-3.30529980	3.04492451
H	4.71191539	-2.04535191	2.33819858
O	5.28848189	-4.66892297	-1.90861023

H	4.67159522	-3.96835316	-2.15584731
H	5.84031056	-4.84835974	-2.66408395
O	7.19750616	-1.28787351	0.19077613
H	6.98925997	-2.24760050	0.27968609
H	8.14563535	-1.19131477	0.21433896
O	6.37240490	-3.76380335	0.47357696
H	6.03730859	-4.18146035	-0.33213860
H	5.64117858	-3.71021083	1.09801694
O	2.38751194	-2.54857775	0.28346437
H	3.02489779	-2.72415501	0.99886142
H	1.67566877	-3.20538746	0.35716777
O	5.66567336	-0.57990284	-2.02261240
H	6.26115476	-0.78196723	-1.28779220
H	4.98834598	-1.26507332	-2.03963560

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C	-3.48315118	2.68708534	-1.18183642
O	-2.37142397	1.97024653	-1.49446028
H	-3.66509983	3.51907185	-1.83606208
H	-4.28969734	2.18144902	-0.68117613
H	-2.28067772	1.17245555	-0.95587824
C	1.05682914	5.34492746	2.41955074
O	0.51545294	4.11190339	2.23674223
H	0.45369453	6.00306142	3.01688851
H	1.72839502	5.71159173	1.66278507
H	1.02011179	3.59595396	1.59401424
O	2.60132278	-3.23054803	1.49016837
H	2.23081572	-2.75366995	2.23626261
H	1.47451355	-4.54297701	0.78483751
O	-2.82147589	-1.53135410	5.14514804
O	-2.98251749	1.16922047	1.89275744
H	-1.65633859	-2.46574593	4.48140202
H	-3.74274166	-1.66813811	4.88854661
H	-2.38346885	0.85947407	1.20618235
H	-2.41828711	1.63425985	2.52322083
O	-1.43352693	-0.15748063	0.02629498
O	-0.94152876	-3.03179779	4.10651097
H	2.57823636	-2.62364807	0.74100869
H	-1.94793433	-0.99458873	0.00607217
H	-0.90643857	-3.82338417	4.63845677
H	0.51498947	-2.20550961	3.80125642
O	1.31454264	-1.70573796	3.54084677
H	0.87273861	-0.34415211	2.47049265
H	1.81154150	-1.52505051	4.33438959
O	0.81772568	-5.00847838	0.24920917
H	-0.03758768	-4.80213332	0.65485652
H	1.03668035	-4.43969718	-1.30765358
O	-1.51150685	-4.15936647	1.49125513
H	-2.06065930	-3.57429126	0.95658219
H	-1.37324690	-3.72294396	2.33520725
O	0.50626204	0.39814310	1.96444338
H	-0.36317248	1.48040035	3.10773356
H	-0.16864793	0.03729703	1.37078979
O	-2.97383515	-2.30713801	-0.02673835
H	-3.78309788	-2.01006149	0.41581219
H	-3.13753865	-2.51332660	-0.96123491
O	-2.67993424	1.29137548	5.41345091
H	-2.54188827	1.65216861	6.28546717
H	-2.71101812	-0.58219075	5.27270466
O	-5.70761618	1.78940906	1.88239389
H	-4.75963813	1.85352665	1.72491303
H	-5.93093984	0.91517657	1.55939927
O	-5.48382440	-1.50830331	4.31677314
H	-5.59470843	-0.54329846	4.47908698
H	-6.20140370	-1.96807287	4.74331860
O	-5.44258603	1.10900148	4.57903738
H	-5.61820230	1.49849059	3.70894321

H	-4.54143487	1.34035614	4.82401997
O	-0.94737321	2.13805660	3.51938586
H	-1.99981910	1.67205966	4.83060654
H	-0.57377006	2.99049675	3.26056079
O	-4.72869676	-1.02728322	1.65045344
H	-5.08018154	-1.43072718	2.45185737
H	-4.08114590	-0.38010278	1.95435081
H	-0.71507231	-0.23348241	-0.63534296
O	-2.92189222	-2.72663271	-2.72456733
H	-3.23495661	-3.50661803	-3.17318142
O	1.26787758	-3.92439891	-2.11430470
H	0.19805509	-2.89229243	-2.99756281
H	1.89884045	-4.42214139	-2.65654401
O	2.29969754	1.62609529	-4.84901359
O	1.80183961	2.34271304	0.44054931
H	2.03865345	0.69814182	-4.88299571
H	3.15725908	1.70238130	-4.41604232
H	1.48364552	1.58389600	0.95691349
H	1.21659974	2.43604134	-0.33478866
O	2.44101140	-1.81272890	-0.92799866
O	1.66261465	-1.11825351	-5.06406426
H	2.10679766	-2.59900333	-1.40451098
H	3.36437807	-1.68041264	-1.18234798
H	1.59497124	-1.39916929	-5.97357631
H	0.92334550	-1.53660675	-4.58290853
O	-0.27951602	-2.15818882	-3.43205686
H	-0.12559660	-1.39140312	-2.85945721
H	-2.03014154	-2.54521613	-3.06195254
O	3.22043006	-4.72067366	-3.82359348
H	3.66757675	-3.86361521	-3.93406023
H	3.88360534	-5.40334394	-3.82321171
O	4.12235044	-2.17649065	-4.08342920
H	4.47955148	-1.70892634	-3.32290034
H	3.32461309	-1.71892839	-4.37005178
O	0.52680352	-0.17347027	-1.73780880
H	0.66580363	0.76211977	-1.93569257
H	1.34715539	-0.60377446	-1.42377390
O	4.98393673	-1.05439348	-1.59300888
H	4.82272578	-0.14660315	-1.26145036
H	5.73330105	-1.41169106	-1.12440102
O	1.02274640	3.78378449	-4.08469280
H	0.44510546	4.18381741	-4.72863594
H	1.42054582	2.97760465	-4.48520982
O	3.33842650	4.63531521	-0.04656536
H	2.98167423	3.78901512	0.24180397
H	4.23733628	4.67382191	0.27030885
O	4.51186756	2.52369418	-3.37844990
H	4.16031311	3.43547935	-3.24578189
H	5.38445111	2.59600338	-3.75625281
O	3.33321202	4.79916786	-2.84918332
H	3.23399727	4.86523463	-1.89060996
H	2.45874575	4.69872134	-3.24003784
O	0.27833207	2.55231808	-1.77452654
H	0.48446679	3.07836185	-2.56265253
H	-0.68704656	2.52065292	-1.69323867
O	4.34081654	1.41317765	-0.85598980
H	4.36953104	1.87336713	-1.70745064
H	3.49925116	1.60939560	-0.43636128

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C	-2.83769460	3.33100811	-0.04503521
O	-1.89050845	2.60887575	-0.68887726
H	-3.07694254	4.25021515	-0.55954876
H	-3.65309002	2.77912993	0.39853044
H	-1.85427750	1.67951448	-0.39543220
C	-0.02764867	4.19742738	1.30947668
O	-1.24240812	4.16477190	1.84357634

H	0.65223460	3.39109394	1.52424221
H	0.23057571	4.97886946	0.61437626
H	-2.00882005	3.91497406	1.15788945
O	2.53951816	-3.14045202	1.50046788
H	2.18858624	-2.59971486	2.21119357
H	1.40257695	-4.45096516	0.81098016
O	-2.82698427	-1.63221831	5.26948374
O	-2.95322366	0.75980039	2.21011779
H	-1.62817505	-2.42891354	4.49133287
H	-3.74095823	-1.79631978	5.00202444
H	-2.33652989	0.55201295	1.50253558
H	-2.41845197	1.20688258	2.87958761
O	-1.35176052	0.05737363	0.06934776
O	-0.89619489	-2.91327903	4.04309679
H	2.57557337	-2.57761676	0.71726468
H	-1.93718129	-0.72599956	-0.03818412
H	-0.80197774	-3.75049063	4.49193499
H	0.53000047	-2.01913723	3.77352271
O	1.32987470	-1.50719100	3.53940454
H	0.97114146	-0.06340696	2.54638060
H	1.85325900	-1.41480813	4.33124123
O	0.74903095	-4.92827610	0.28164574
H	-0.11025955	-4.67902113	0.65290093
H	0.98886857	-4.42427401	-1.29914937
O	-1.57361347	-3.94634635	1.42408022
H	-2.05947649	-3.32778866	0.86708486
H	-1.40984200	-3.50752407	2.26229570
O	0.64895608	0.70045425	2.04135969
H	-0.36326656	1.66823411	3.27825571
H	-0.00530801	0.35077610	1.42381160
O	-2.95413484	-2.04712041	-0.13547431
H	-3.79562935	-1.92572688	0.32733805
H	-3.09299145	-2.29186064	-1.06582374
O	-2.74470227	1.19312179	5.65113819
H	-2.61684990	1.54009323	6.53033464
H	-2.75394126	-0.68732884	5.44210968
O	-5.56671334	1.66192232	2.06377322
H	-4.62285529	1.47335373	2.00322668
H	-5.97785023	0.89362668	1.66773274
O	-5.49755548	-1.72250744	4.44610850
H	-5.62274387	-0.76151755	4.60676770
H	-6.16705202	-2.19195669	4.93588442
O	-5.49329289	0.90954556	4.76111897
H	-5.63514375	1.32504809	3.89844164
H	-4.61464481	1.16360208	5.05845997
O	-1.09843289	2.13365693	3.70570684
H	-2.08073984	1.60780570	5.07582909
H	-1.19171217	2.97081930	3.22545616
O	-4.80590705	-1.26769217	1.73544877
H	-5.19017482	-1.73066538	2.48534478
H	-4.13288210	-0.69728578	2.12247714
H	-0.61479921	-0.06895320	-0.57009228
O	-2.87065158	-2.60107658	-2.79989423
H	-3.14656941	-3.43057266	-3.17910509
O	1.23073043	-3.94295025	-2.12260435
H	0.23188375	-2.84739064	-3.00161211
H	1.81819781	-4.48923684	-2.66785362
O	2.61185221	1.55716194	-4.93425174
O	2.47189733	2.00939565	0.18255031
H	2.32228751	0.63741835	-4.91784519
H	3.46772763	1.63853121	-4.49739437
H	1.99395446	1.52188626	0.86489358
H	1.82867854	2.20903147	-0.51517044
O	2.50329194	-1.85426023	-0.98185166
O	1.77012450	-1.14292175	-5.08007105
H	2.13399515	-2.63387003	-1.44104546
H	3.42981665	-1.77042400	-1.25182470
H	1.64315355	-1.39125206	-5.99272872



H	1.01839348	-1.51437469	-4.57983786
O	-0.20854252	-2.08784462	-3.43260356
H	-0.04795231	-1.33996104	-2.83633578
H	-1.96769627	-2.43389891	-3.11597061
O	3.05860669	-4.91755887	-3.87030692
H	3.55864730	-4.09420605	-4.01580260
H	3.67579588	-5.64202417	-3.86669087
O	4.14144397	-2.46361181	-4.20082406
H	4.54388991	-2.03772818	-3.43663323
H	3.38468650	-1.93182369	-4.46905184
O	0.59179149	-0.15587956	-1.67342007
H	0.77292500	0.76432801	-1.91054323
H	1.40998056	-0.61454421	-1.39203559
O	5.08794331	-1.40302788	-1.74714177
H	5.08061341	-0.45479190	-1.47683805
H	5.79623725	-1.83601491	-1.27850718
O	1.29797623	3.69167645	-4.18956656
H	0.73314393	4.08095361	-4.85085739
H	1.72325818	2.89173690	-4.57722111
O	3.18411806	4.66103705	-0.05036884
H	3.03726143	3.74961979	0.23829627
H	3.86842641	5.02984534	0.50045898
O	4.83531863	2.47768207	-3.48907753
H	4.43516294	3.34864822	-3.25793776
H	5.67126543	2.64791132	-3.91502850
O	3.56165367	4.66925350	-2.80927403
H	3.40042912	4.74490635	-1.85790772
H	2.71104830	4.58986690	-3.25146135
O	0.65587313	2.56180301	-1.81217347
H	0.80399370	3.03659458	-2.64540872
H	-0.21472099	2.80667630	-1.47929994
O	4.86195330	1.11183790	-1.07492244
H	4.88418926	1.63893463	-1.88517053
H	4.06363327	1.35645640	-0.59105198

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C	-0.01810850	4.17709268	-1.29961484
O	0.47443299	2.95783228	-0.97897931
H	0.69584524	4.97288839	-1.18950928
H	-0.80043110	4.22655798	-2.03916922
H	-0.15698736	2.23961901	-1.12241485
C	0.35865569	2.52552668	4.09844973
O	0.75977724	2.10720893	2.87663288
H	1.15628324	2.69498081	4.79834521
H	-0.61803618	2.22119657	4.43748943
H	-0.00743070	1.86053330	2.33301666
O	-1.14905288	-2.39988060	3.21125516
H	-1.70709009	-1.62050853	3.18046256
H	-1.79022012	-3.70802046	2.06012222
O	-6.37567659	1.11258264	0.59135765
O	-2.77918551	2.48713251	-2.21752839
H	-5.63912640	-0.14961684	1.33069063
H	-6.67815267	1.01157321	-0.32122411
H	-2.08820942	1.82404002	-2.18151426
H	-2.85690094	2.82665949	-1.31426105
O	-0.97418124	0.58815127	-0.94922142
O	-5.19392367	-0.90384029	1.78182948
H	-0.30768986	-2.17641724	2.79495465
H	-1.59878173	-0.05914275	-1.34914244
H	-5.87766402	-1.45082197	2.16063829
H	-3.82727342	-0.47240120	2.70244672
O	-3.00308927	-0.17960875	3.13948564
H	-2.06466680	0.88323379	2.11369590
H	-3.22438341	0.05890337	4.03592706
O	-1.98180109	-4.26413970	1.29210662
H	-2.65860759	-3.78724783	0.78920513
H	-0.50826440	-4.41282316	0.52642402

O	-3.79673924	-2.66142330	-0.04640903
H	-3.40877491	-2.15446521	-0.77008966
H	-4.27483074	-2.04104420	0.50839226
O	-1.53298775	1.46527091	1.54521865
H	-2.31352569	2.83532295	0.91462133
H	-1.36799554	0.99963159	0.70420096
O	-2.64344846	-1.13044564	-2.09640621
H	-3.37322572	-0.69835597	-2.57469437
H	-2.14014426	-1.69610988	-2.70750588
O	-5.40784110	3.79968620	0.55852425
H	-5.71833770	4.43974849	1.19364468
H	-6.06054591	2.01839380	0.67560882
O	-4.21308992	4.26922083	-3.74885907
H	-3.56211269	3.63928244	-3.41796334
H	-4.25058193	4.17349038	-4.69622268
O	-7.07203769	1.17882290	-2.10725933
H	-6.91432961	2.14425001	-2.20582282
H	-7.94361081	0.98602263	-2.44136448
O	-6.39732997	3.72574795	-2.12045137
H	-5.70702153	3.99838532	-2.74096691
H	-6.07729085	3.91956371	-1.23407703
O	-2.70913437	3.54863471	0.37125060
H	-4.43656309	3.81591903	0.57426065
H	-2.02831058	4.21382962	0.26021080
O	-4.54742773	0.46966708	-3.14967690
H	-5.46979963	0.49607069	-2.87472005
H	-4.15696022	1.29189670	-2.84146164
H	-0.13530522	0.09923170	-0.80465582
O	-0.96674769	-2.68663228	-3.57040105
H	-1.23989429	-3.54536436	-3.88041573
O	0.41842899	-4.32393923	0.20640359
H	0.88353420	-3.50633007	-1.21125152
H	0.89958421	-5.15409154	0.35295626
O	5.57762807	-1.12469613	-1.72900247
O	3.39108971	1.77673171	1.97593786
H	4.97102208	-1.87532065	-1.74714575
H	6.02956619	-1.10700260	-0.87640726
H	2.51620846	1.90124702	2.36661654
H	3.24365863	1.72143622	1.01791865
O	1.21746280	-2.20170354	1.70111662
O	3.90148273	-3.37033368	-1.81396942
H	1.00167097	-3.02502459	1.22303669
H	2.04361634	-2.36628692	2.18041083
H	4.19052384	-4.01493371	-2.45528322
H	2.93702422	-3.25917767	-1.93484961
O	1.23405317	-2.93035870	-1.92267997
H	1.28197238	-2.04729316	-1.52226845
H	-0.14842866	-2.81608169	-3.06251515
O	2.21476984	-6.32993174	0.51620413
H	2.99624196	-5.76880982	0.67714029
H	2.25537228	-7.07071930	1.11244262
O	4.20419073	-4.53571724	0.77167326
H	4.09452404	-3.89128256	1.48070588
H	4.17139236	-4.06003321	-0.06506182
O	1.32676953	-0.62199512	-0.45137933
H	2.01664722	0.05630631	-0.50870653
H	1.36904475	-1.07037855	0.41751185
O	3.66947312	-2.69022009	2.84379531
H	4.17650266	-1.84254399	2.80588708
H	3.72981960	-3.01809250	3.73703746
O	5.05509617	1.37302932	-2.28984138
H	5.18336644	1.58881344	-3.20915281
H	5.22819227	0.40745616	-2.17818120
O	5.45717513	3.55386082	1.78475258
H	4.68508379	3.01214325	2.01134057
H	5.89598891	3.78309710	2.59844561
O	6.88177284	-0.41853297	0.64194571
H	6.93066750	0.53171861	0.38165242

H	7.76891391	-0.71175252	0.83160871
O	6.77775378	2.08403182	-0.14124382
H	6.36286550	2.68045568	0.50000654
H	6.23258341	2.07563459	-0.93410692
O	2.87944266	1.60135960	-0.69683380
H	3.59590546	1.63140164	-1.35172186
H	2.19986505	2.24464196	-0.92535587
O	4.95336943	-0.43209091	2.66641093
H	5.66005926	-0.43789547	2.00741875
H	4.39376545	0.33494515	2.48141732

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C	-0.89879591	-3.74943392	0.52200972
O	0.23021123	-4.05305986	-0.17681417
H	-1.83996878	-4.08144137	0.12272632
H	-0.74460338	-3.62550511	1.57710900
H	0.03362161	-4.13017158	-1.11894287
C	-0.63914642	-3.78603962	-3.09921661
O	-1.81109726	-3.31219369	-2.64463758
H	-0.68064795	-4.79398013	-3.47538273
H	0.06016137	-3.08163819	-3.52375762
H	-1.78401075	-2.35064634	-2.46664595
O	-0.07659205	2.87989656	-3.04214553
H	-0.85227658	2.31861828	-3.10591324
H	-0.45037840	4.20435348	-1.78077013
O	-6.48512963	1.13606467	-0.98049550
O	-3.54929535	-1.84106646	1.28724236
H	-5.28909633	2.05548234	-1.64793005
H	-6.71989121	1.25994304	-0.05118482
H	-2.67307160	-1.46266922	1.12426556
H	-3.86318971	-2.15446268	0.43307918
O	-1.44107223	-0.21029754	0.47939596
O	-4.60255246	2.64791784	-2.03060062
H	0.62945372	2.37727217	-2.62072715
H	-1.73890902	0.58189653	0.96823479
H	-5.05630271	3.42375251	-2.35084377
H	-3.32554105	1.95503599	-2.94982715
O	-2.59057039	1.49458219	-3.39964356
H	-2.33326692	-0.02225014	-2.54478140
H	-2.76541881	1.52927312	-4.33649312
O	-0.54984465	4.71448084	-0.96574052
H	-1.40790433	4.46115658	-0.59057287
H	0.76772084	4.27647636	-0.07109505
O	-2.92892461	3.77479888	0.05401152
H	-2.76815477	3.13572579	0.76156351
H	-3.49838275	3.34538282	-0.58802338
O	-2.24944116	-0.79992232	-1.97124763
H	-3.69325420	-1.73649996	-1.67501127
H	-1.92674873	-0.49607780	-1.09367590
O	-2.38788934	1.83711826	1.96949776
H	-3.17830071	1.44411980	2.37607164
H	-1.77082503	2.09593391	2.67415552
O	-6.86770651	-1.67603360	-1.18858179
H	-7.46947375	-2.06125142	-1.81996943
H	-6.64388630	0.20525572	-1.16932213
O	-5.48679599	-2.42410058	3.24861523
H	-4.70182613	-2.48090396	2.69413098
H	-5.35302032	-1.62202809	3.75399428
O	-7.15091800	1.02424606	1.72115891
H	-7.42648240	0.07847851	1.73830546
H	-7.81867431	1.54078922	2.16335163
O	-7.55169032	-1.56562356	1.58734431
H	-6.90189207	-2.00759059	2.15554285
H	-7.34969925	-1.78891192	0.67381416
O	-4.29504708	-2.45253392	-1.39706223
H	-5.98466253	-2.04938563	-1.35206591
H	-3.91277705	-3.24729636	-1.76959806

O	-4.57836182	0.40302153	2.67605984
H	-5.43114712	0.76145032	2.40416858
H	-4.37511171	-0.32366720	2.07526420
H	-0.46929608	-0.20104195	0.49274083
O	-0.45798928	2.50267817	3.77785748
H	-0.41843918	3.40158803	4.09196823
O	1.58858737	3.87836928	0.30303227
H	1.64367935	2.74722954	1.55668088
H	2.26680997	4.56712140	0.39602391
O	5.48607177	-0.67963520	2.43806475
O	3.79734765	-2.37734540	-2.13615966
H	5.08791501	0.19884927	2.49949012
H	6.17135120	-0.66370324	1.75953021
H	3.19097767	-2.09825395	-2.81693996
H	3.29521097	-2.41776399	-1.29586950
O	2.03068125	1.84309167	-1.43178021
O	4.38511343	1.86160646	2.64104201
H	1.94639585	2.62270992	-0.84897321
H	2.95299843	1.83175992	-1.72310189
H	4.61732788	2.31212037	3.44939148
H	3.41162789	1.93175503	2.54258888
O	1.74864855	2.01824283	2.20477185
H	1.56460527	1.20701995	1.70500285
H	0.37525937	2.32827816	3.31156623
O	3.77648083	5.43414275	0.68979996
H	4.45517125	4.74787939	0.54907554
H	4.06561968	6.23103541	0.25696112
O	5.37935220	3.29684418	0.40095570
H	5.20273149	2.80188323	-0.40724401
H	5.11568896	2.74087338	1.14253312
O	1.27794312	-0.01602873	0.39682089
H	1.75626243	-0.85672627	0.36262997
H	1.57538242	0.53721419	-0.34919934
O	4.76110353	1.90214516	-1.98968831
H	5.20678548	1.02405174	-1.96773600
H	5.07094907	2.35531931	-2.76954672
O	4.24265608	-2.95379659	2.18492678
H	4.03800211	-3.34708917	3.02900986
H	4.65630942	-2.07233675	2.35745555
O	5.42815071	-4.60523828	-1.90234013
H	4.84988039	-3.88045713	-2.17188927
H	6.01271127	-4.79568052	-2.63002499
O	7.27594357	-1.26411692	0.36674829
H	7.05318393	-2.22301392	0.41452131
H	8.22111749	-1.17915801	0.45743276
O	6.41232295	-3.74038177	0.53983252
H	6.11312052	-4.14298836	-0.28718256
H	5.65519973	-3.70149368	1.13370686
O	2.47051673	-2.49813660	0.18524819
H	3.04390307	-2.73175544	0.93675375
H	1.73104368	-3.12189724	0.15243948
O	5.87048907	-0.47407489	-1.90428604
H	6.43175448	-0.68572385	-1.14594071
H	5.20615510	-1.16915549	-1.96773464

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C	-2.96712969	3.31162733	-0.68667461
O	-1.68769229	2.71834101	-0.56322483
H	-2.81684957	4.35462504	-0.93909070
H	-3.54607927	2.83690592	-1.47490440
H	-1.76708517	1.77905606	-0.35712376
C	-0.17111696	4.26546593	1.20658425
O	-0.78390240	4.50721094	2.21614503
H	0.38536155	3.33778890	1.08228881
H	-0.13142616	4.97363935	0.37789180
H	-3.51164898	3.25036551	0.25048806
O	2.53872501	-3.15516517	1.43106110

H	2.20204651	-2.62057743	2.15343151
H	1.38952507	-4.46424547	0.75357312
O	-2.75227444	-1.61512348	5.23126989
O	-3.05987773	1.12010767	2.04000328
H	-1.56151375	-2.45076441	4.49076390
H	-3.66837796	-1.77285831	4.96770423
H	-2.45688945	0.83182314	1.34977089
H	-2.48772399	1.52380540	2.70687319
O	-1.32528580	0.02508382	0.13552126
O	-0.83274306	-2.95589473	4.05979739
H	2.55313016	-2.58766958	0.65077092
H	-1.90174993	-0.76870641	0.07980702
H	-0.74207587	-3.77670057	4.53838264
H	0.58387687	-2.05963151	3.75889935
O	1.37330240	-1.53994907	3.50660286
H	0.96039177	-0.09633430	2.53084080
H	1.91238144	-1.44074817	4.28693696
O	0.73014577	-4.94050436	0.23073918
H	-0.12354403	-4.71143150	0.62752984
H	0.94519840	-4.43158254	-1.35323636
O	-1.57237791	-4.01720633	1.46352802
H	-2.07558523	-3.38858013	0.93317460
H	-1.37440792	-3.58605260	2.29840051
O	0.61859182	0.65748210	2.02395440
H	-0.36571621	1.64835588	3.20291517
H	-0.05972829	0.29819547	1.43138075
O	-2.95226656	-2.06968967	-0.02131623
H	-3.78092778	-1.85971804	0.43550646
H	-3.10904979	-2.27549929	-0.95720426
O	-2.67399845	1.20030752	5.58780475
H	-2.51777210	1.55247079	6.46027701
H	-2.67202283	-0.66896917	5.39647367
O	-5.77315443	1.77964391	2.15634817
H	-4.83081767	1.77557939	1.95844583
H	-6.09112554	0.96414487	1.76816478
O	-5.42213250	-1.66170106	4.42006457
H	-5.55552709	-0.70798736	4.62193134
H	-6.10421503	-2.15811133	4.86355140
O	-5.44441584	0.94708330	4.80189971
H	-5.64361837	1.38016220	3.95836796
H	-4.55047280	1.19878969	5.05274817
O	-1.05821174	2.16610474	3.64445864
H	-2.02616365	1.61008784	4.98887127
H	-0.96476193	3.07650096	3.32457754
O	-4.80107350	-1.06258428	1.73383504
H	-5.11374769	-1.52505999	2.51846610
H	-4.17388789	-0.40812319	2.06165843
H	-0.64467660	-0.08843076	-0.56167206
O	-2.93247936	-2.53607377	-2.72039202
H	-3.26670974	-3.33585300	-3.11616586
O	1.17874626	-3.94901304	-2.17835657
H	0.16113939	-2.85437331	-3.05483084
H	1.76571990	-4.49177802	-2.72696396
O	2.62187753	1.60712141	-4.90734978
O	2.39353807	1.95373632	0.19126104
H	2.31896796	0.69192361	-4.88397114
H	3.44595695	1.69434151	-4.41522833
H	1.89762165	1.44657646	0.84942393
H	1.79707566	2.10891108	-0.55687007
O	2.45993183	-1.86315712	-1.04834234
O	1.71710142	-1.08236985	-5.07519491
H	2.08884592	-2.64374952	-1.50504826
H	3.38648265	-1.77950131	-1.31690811
H	1.59907331	-1.30801398	-5.99499448
H	0.96310475	-1.47174264	-4.59268682
O	-0.28121844	-2.08834008	-3.47056567
H	-0.11192923	-1.34956053	-2.86457708
H	-2.03859629	-2.40047572	-3.07417571

O	3.01507428	-4.89574593	-3.93636881
H	3.51184474	-4.06922675	-4.07221436
H	3.63373016	-5.61880495	-3.95083039
O	4.08970542	-2.43054540	-4.23915985
H	4.50365744	-2.01351529	-3.47652223
H	3.32910187	-1.89523352	-4.48882739
O	0.53718536	-0.17322289	-1.72223902
H	0.72440643	0.74103420	-1.97744321
H	1.35687881	-0.63447504	-1.44960136
O	5.05632879	-1.39923654	-1.77864655
H	5.05008005	-0.46318763	-1.47140132
H	5.75050676	-1.85561928	-1.31095121
O	1.27118031	3.74291122	-4.23122546
H	0.72022801	4.12739791	-4.90669924
H	1.71888902	2.95061320	-4.60805107
O	2.76666720	4.65691521	0.14584649
H	2.77387471	3.70944376	0.34998430
H	3.42899793	5.07331126	0.69046415
O	4.74511556	2.59091862	-3.33191884
H	4.30241505	3.42907512	-3.06736612
H	5.57230639	2.82305402	-3.74584363
O	3.36286803	4.72036723	-2.61049336
H	3.10813739	4.77360909	-1.67963492
H	2.56175165	4.64160753	-3.13728362
O	0.65069617	2.52966609	-1.87437986
H	0.78964251	3.01724885	-2.69952723
H	-0.23623568	2.73932994	-1.54223345
O	4.82952484	1.09214625	-1.00248561
H	4.84734876	1.65726784	-1.78670927
H	4.02659592	1.31128791	-0.51456793

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C	-2.05463948	3.97072393	-0.02270753
O	-1.72475815	2.76956317	0.52847203
H	-1.31019377	4.47285926	-0.61573282
H	-3.10051951	4.05887000	-0.25289917
H	-0.77686530	2.65968403	0.58932912
C	0.00386627	3.67138212	-2.96743954
O	-0.12333116	2.37912653	-2.58155975
H	-0.77262758	4.02653967	-3.61855793
H	0.58864086	4.33381784	-2.35247697
H	0.54817781	2.15238033	-1.91504213
O	3.33539623	-1.53056894	-2.03291410
H	3.50665584	-0.61631822	-1.80154343
H	3.77860327	-2.73015278	-0.69856866
O	3.69443213	2.87438082	2.60487372
O	0.85514854	2.56310921	2.62103015
H	4.64164832	1.67707962	1.80906795
H	3.74243661	2.97457258	3.56707174
H	0.65811781	1.72902931	2.15951275
H	1.81178342	2.68048722	2.52744217
O	0.83361030	0.29863729	1.24414325
O	5.12908037	1.02352546	1.27100633
H	2.38223031	-1.64463288	-2.12896556
H	1.25431015	-0.22500365	1.95426231
H	6.03482961	1.02262513	1.57023582
H	4.64753390	1.07883090	-0.42037575
O	4.18165884	1.14211071	-1.27179243
H	2.57256756	1.82872834	-0.95221696
H	4.80514872	1.43363217	-1.93159554
O	3.77785785	-3.35242952	0.04223420
H	3.96858888	-2.82695477	0.83244936
H	2.27985551	-4.08019088	-0.06996720
O	4.23225479	-1.60483094	2.16734529
H	3.44392238	-1.43430589	2.69812050
H	4.50503490	-0.75236775	1.82311953
O	1.69221234	2.04694538	-0.60914772

H	1.65477328	3.81307308	-0.08111155
H	1.48623602	1.34767644	0.03983552
O	1.83447688	-0.94110842	3.42690529
H	1.77707202	-0.29253745	4.14487376
H	1.27781433	-1.70691110	3.65083812
O	3.72704974	5.41563009	1.54535977
H	4.39052894	5.97385503	1.14975072
H	3.86207001	3.75386556	2.23427748
O	-0.05070468	5.03541952	2.32973571
H	0.06654139	4.08780338	2.52336258
H	-0.98473654	5.19922862	2.21853671
O	3.24897361	3.56589263	5.22997063
H	2.79236871	4.36662545	4.90099260
H	3.79439583	3.82953465	5.96594921
O	2.19955247	5.67851271	3.94330957
H	1.30494807	5.64995013	3.58946540
H	2.77075105	5.80711381	3.17896374
O	1.63365409	4.76539697	0.09030616
H	3.01460716	5.26018556	0.88490091
H	0.95393923	4.93083568	0.75637910
O	1.47620061	1.25910868	5.07641946
H	2.13789040	1.87313744	5.40151627
H	1.00846586	1.75962427	4.40175390
H	0.18504045	-0.28060639	0.79578999
O	0.23955384	-3.12055930	3.76107681
H	0.59927342	-3.91857910	4.13746472
O	1.35019018	-4.32965229	-0.27300890
H	0.05959830	-3.95435592	0.76407934
H	1.31476503	-5.22788951	-0.63791691
O	-4.87210254	-3.05937957	-0.77491058
H	-2.43496328	0.89774982	-3.04788201
H	-4.13032681	-3.62974649	-0.53572379
H	-4.92828661	-3.00615025	-1.73670165
H	-1.59483006	1.37363389	-3.00794359
H	-2.66802639	0.71177090	-2.12405595
O	0.63369004	-2.34087891	-1.98483027
O	-2.78319522	-4.78307533	-0.08057107
H	0.88023502	-3.12742451	-1.46239979
H	0.19873832	-2.65987909	-2.78904781
H	-3.09316812	-5.57352081	0.35462701
H	-2.05652401	-4.42019458	0.46682184
O	-0.73625955	-3.62948712	1.23553849
H	-0.87678157	-2.73621170	0.88081591
H	-0.15778086	-3.36204020	2.90785711
O	0.67548639	-6.68602032	-1.42664249
H	-0.10766725	-6.35608559	-1.90535430
H	1.13513631	-7.29338869	-1.99730401
O	-1.50740976	-5.54156033	-2.51433804
H	-1.34802561	-4.78349411	-3.08855530
H	-2.01134801	-5.23229254	-1.75395785
O	-0.87179088	-1.23660698	-0.07290429
H	-1.68188440	-0.74565766	-0.27520172
H	-0.43431240	-1.53507526	-0.89438483
O	-0.84747627	-3.29678191	-4.10331907
H	-1.57066777	-2.63928480	-4.24374670
H	-0.45812536	-3.47466417	-4.95520048
O	-5.39307934	-0.65573900	0.10128204
H	-5.91834602	-0.65334881	0.89652145
H	-5.20244718	-1.59654216	-0.13189372
O	-4.83143557	2.06581635	-3.62087360
H	-3.91609654	1.75108524	-3.54784166
H	-4.98317935	2.29794105	-4.53224813
O	-5.26115338	-2.29902108	-3.43914542
H	-5.69378107	-1.45453869	-3.17169079
H	-5.86723263	-2.76458821	-4.00912438
O	-6.25818750	-0.03976866	-2.53652541
H	-5.84234755	0.75827803	-2.89493896
H	-6.10183619	-0.05547006	-1.58710066

O	-2.98027109	0.44558140	-0.41044082
H	-3.85717937	0.15298544	-0.11094971
H	-2.71674147	1.23876876	0.06684081
O	-2.74740785	-1.53051381	-4.39933892
H	-3.62705793	-1.81836496	-4.12234368
H	-2.58527961	-0.67202758	-3.98545233

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C	-0.90565943	-3.95929594	0.82272738
O	0.23269482	-4.05635858	0.09100157
H	-1.82678737	-3.74767537	0.30914960
H	-0.89495611	-4.50702385	1.74597540
H	0.12668501	-3.61946178	-0.76610847
C	0.20490176	-2.97622150	-3.50984484
O	-0.01563046	-2.61257886	-2.22345306
H	0.68812440	-3.92762594	-3.63678575
H	-0.42660851	-2.55287034	-4.27162405
H	-0.65107177	-1.86736306	-2.15711490
O	-0.06701622	2.80286910	-2.94428604
H	-0.84250588	2.25043288	-3.05856486
H	-0.44174779	4.16677364	-1.72580359
O	-6.42146500	1.09664332	-1.12467540
O	-3.60270174	-1.78016692	1.30674100
H	-5.22258536	2.03736828	-1.72557988
H	-6.72493514	1.22447142	-0.21580598
H	-2.71730257	-1.39547341	1.22519633
H	-3.81202119	-2.13212640	0.43757916
O	-1.46005160	-0.18099369	0.61164668
O	-4.50950258	2.61196821	-2.08928611
H	0.59532816	2.29157406	-2.46348255
H	-1.78335528	0.62142495	1.06942992
H	-4.93230244	3.38702445	-2.45125617
H	-3.26277175	1.84064062	-2.95598577
O	-2.53028008	1.35041596	-3.38094397
H	-2.11891607	-0.08171676	-2.46908493
H	-2.69043906	1.35546906	-4.32094284
O	-0.54472919	4.70058281	-0.92650745
H	-1.41260231	4.47053769	-0.56012349
H	0.75337639	4.25953142	0.01074419
O	-2.95898275	3.80122630	0.05685022
H	-2.81013390	3.17683276	0.77950569
H	-3.48600049	3.34541411	-0.60283900
O	-1.93255695	-0.83185332	-1.87958548
H	-3.20408088	-1.93560590	-1.70812523
H	-1.77626802	-0.46891373	-0.97365326
O	-2.45971044	1.88744451	2.01258867
H	-3.26884631	1.51194648	2.39695850
H	-1.85626491	2.14620246	2.72945566
O	-6.49757161	-1.73764961	-1.33529618
H	-7.06007371	-2.13276982	-1.99643785
H	-6.45556587	0.14784581	-1.28496130
O	-5.55651617	-2.41721227	3.20634248
H	-4.74784046	-2.42056946	2.68256257
H	-5.47942675	-1.63570623	3.75287591
O	-7.25412674	0.98992402	1.52761306
H	-7.47272836	0.03016839	1.53045949
H	-7.98470651	1.46652346	1.91154212
O	-7.48119579	-1.62451826	1.36876192
H	-6.88177313	-2.03138154	2.01426330
H	-7.15936119	-1.84400008	0.49010656
O	-3.89895753	-2.57352470	-1.43837568
H	-5.60115817	-2.08583920	-1.46445820
H	-3.62096154	-3.44218686	-1.71746802
O	-4.70399052	0.47867956	2.62440451
H	-5.55326093	0.82369116	2.32754632
H	-4.48699510	-0.25670430	2.04057573
H	-0.49020643	-0.18896358	0.70527861



O	-0.55246714	2.54377666	3.84872533
H	-0.51983486	3.42938197	4.19911484
O	1.55964580	3.85656247	0.40784427
H	1.61931751	2.77040745	1.71123862
H	2.26460341	4.52369884	0.44303579
O	5.63516704	-0.64640861	2.28105835
O	3.16500825	-2.37227269	-1.89041976
H	5.18676973	0.20551095	2.35856574
H	6.16154448	-0.65175503	1.47269712
H	2.35106362	-2.23109614	-2.37256118
H	2.92149411	-2.40715191	-0.94605377
O	1.91644918	1.73385115	-1.24620595
O	4.41615217	1.84822853	2.54863666
H	1.86366402	2.53088569	-0.68422208
H	2.80487207	1.74070332	-1.63145898
H	4.74259487	2.33605999	3.30091459
H	3.44054684	1.93562886	2.55467962
O	1.73274919	2.05993834	2.37664432
H	1.53014053	1.23620744	1.90447524
H	0.30575572	2.37417625	3.42788240
O	3.81048030	5.36069300	0.60202581
H	4.46097151	4.65984836	0.40913309
H	4.07196900	6.14582634	0.13167964
O	5.33573091	3.18403855	0.21075549
H	5.11772422	2.69684393	-0.59225766
H	5.07196837	2.64144518	0.96182862
O	1.23418995	-0.04962777	0.67751843
H	1.71367085	-0.88955886	0.73301655
H	1.54191643	0.44441330	-0.10472184
O	4.53131301	1.83364108	-2.13962791
H	4.88709978	0.91590865	-2.20599102
H	4.72233439	2.27644026	-2.96218864
O	4.48291888	-2.98159305	2.39693485
H	4.43684154	-3.33527196	3.28085993
H	4.89296734	-2.08410077	2.45033792
O	4.83777513	-4.56889770	-1.95405311
H	4.20586813	-3.85024454	-2.09330666
H	5.34648271	-4.65868118	-2.75474414
O	6.99966731	-1.32662478	-0.07065224
H	6.80232880	-2.28461027	0.05560066
H	7.94622052	-1.23130852	-0.13411600
O	6.22621821	-3.80464979	0.32120334
H	5.75543926	-4.18091439	-0.43619346
H	5.61333998	-3.76650610	1.06271796
O	2.42291074	-2.52316051	0.69976446
H	3.09388719	-2.75660467	1.36352022
H	1.72114491	-3.18744302	0.70728629
O	5.36120120	-0.64118029	-2.21904229
H	5.98065198	-0.86258386	-1.51006098
H	4.60794646	-1.23848881	-2.13787274

### 3.2.2 CH3O + CH3O

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p_Rc_ch3o_ch3o W33			
C	0.73830158	-1.27929820	-3.03244025
H	1.10326568	-1.22352445	-4.05241799
O	0.96888337	-2.62595034	-2.64202393
H	1.29460104	-0.59817052	-2.39915139
H	-0.32024231	-1.04758019	-2.99453338
C	-0.72614107	-3.47492945	-1.37876211
O	0.49501360	-2.77405450	-1.31212978
H	-1.06673101	-3.54852978	-0.35172238
H	-1.45261714	-2.91691134	-1.96037026
H	-0.57584430	-4.46564036	-1.79867423
O	-0.58520972	3.00687599	-2.66837225
H	-1.42309921	2.54230946	-2.73163242

H	-0.79830911	4.25555847	-1.30446427
O	-6.80103671	1.05557916	-0.41446430
O	-3.53635996	-2.36711724	0.88514519
H	-5.69683889	2.16846638	-0.91500166
H	-6.96986695	0.91650744	0.52647177
H	-2.71078834	-1.86364413	0.80079928
H	-3.87895518	-2.47194980	-0.00875558
O	-1.52213980	-0.56387502	0.41177033
O	-5.05596944	2.84580888	-1.23162004
H	0.07016327	2.40692515	-2.29590590
H	-1.81240576	0.13866824	1.02745114
H	-5.54837743	3.65070630	-1.37140884
H	-3.89465388	2.30100923	-2.38332562
O	-3.22348677	1.91462780	-2.97731797
H	-2.77877058	0.26571326	-2.44852998
H	-3.49211438	2.10367002	-3.87235656
O	-0.82196215	4.69861948	-0.44511229
H	-1.61118724	4.35648009	0.00468730
H	0.57641374	4.19969066	0.25430491
O	-3.02626380	3.51941992	0.71533488
H	-2.84336909	2.74853893	1.26991326
H	-3.72951327	3.26621664	0.11308634
O	-2.53175663	-0.60353800	-2.10398972
H	-3.70501504	-1.69150601	-2.02966229
H	-2.13776321	-0.47136433	-1.22149036
O	-2.46642458	1.23034531	2.19757005
H	-3.23971863	0.74170170	2.52866197
H	-1.86867235	1.40029183	2.94464388
O	-6.91281433	-1.62386836	-1.34787808
H	-7.51621107	-1.84521505	-2.05221247
H	-6.85210154	0.18392168	-0.82121712
O	-5.35288023	-3.66025247	2.51869059
H	-4.57294903	-3.34016814	2.04783096
H	-5.25263383	-3.36634849	3.42095442
O	-7.25107775	0.16535347	2.19279444
H	-7.45748296	-0.76982957	1.96457972
H	-7.91192682	0.47870052	2.80362026
O	-7.49633232	-2.31352480	1.36046434
H	-6.80964740	-2.87998164	1.74378851
H	-7.33488599	-2.25539058	0.41383920
O	-4.37202426	-2.40141284	-1.83785282
H	-6.02501999	-1.92285473	-1.61245578
H	-4.16028724	-3.15642327	-2.38002668
O	-4.54691696	-0.41087383	2.73661751
H	-5.45710657	-0.10860521	2.64532325
H	-4.39772186	-1.06747104	2.04930704
H	-0.55114041	-0.55864866	0.44619059
O	-0.59420683	1.71444919	4.12415020
H	-0.65090787	2.48029677	4.68773702
O	1.39514319	3.72852314	0.54217852
H	1.35715799	2.55714995	1.81507404
H	2.11623496	4.35629530	0.67100046
O	5.93181045	0.12053097	2.20844613
O	3.58381807	-2.85071043	-1.67827084
H	5.41225556	0.93413000	2.26297799
H	6.37198019	0.09240438	1.35030779
H	2.76127414	-2.89672267	-2.17885451
H	3.31248834	-2.71571992	-0.75664380
O	1.56590256	1.72310386	-1.30486923
O	4.23109080	2.28504421	2.16775207
H	1.60870881	2.48438231	-0.69733053
H	2.37446447	1.73711492	-1.83718625
H	4.27723577	3.24076052	2.23840008
H	3.30828511	2.04868236	2.36145152
O	1.53387510	1.81662366	2.42599718
H	1.39656554	1.01829522	1.89078039
H	0.23217816	1.78798049	3.61684979
O	3.86987467	4.93885607	0.98937908

H	4.35091663	4.43797616	0.30382268
H	4.17090476	5.84232701	0.96769478
O	5.02815586	3.03196783	-0.45474309
H	4.71590695	2.63921301	-1.27802848
H	4.78229622	2.43519818	0.25807398
O	1.17800507	-0.18399859	0.58440706
H	1.78327142	-0.93476933	0.61758416
H	1.39995737	0.37691768	-0.17948533
O	3.96784524	1.65641303	-2.65455001
H	4.41930343	0.78188556	-2.56079054
H	4.08421547	1.95191984	-3.55319426
O	4.89592824	-2.22747483	2.57298194
H	4.91308202	-2.46402551	3.49654248
H	5.25338306	-1.30413172	2.49986185
O	5.66697298	-4.58332901	-1.34164853
H	4.87726096	-4.08992120	-1.60763364
H	5.52345303	-5.50518029	-1.52912216
O	7.08198038	-0.64068553	-0.23401388
H	7.08968757	-1.58141100	0.05740290
H	7.97817520	-0.39972722	-0.45337343
O	6.83232102	-3.10556834	0.66073654
H	6.48812871	-3.73245509	0.00949208
H	6.18938454	-3.03904317	1.37307745
O	2.78639081	-2.44502749	0.92085127
H	3.49884320	-2.38999593	1.58729151
H	2.18525684	-3.13565231	1.18943515
O	5.17145560	-0.61516382	-2.27729315
H	5.87134099	-0.59697654	-1.60998135
H	4.64605647	-1.41053131	-2.12240048

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C	0.74246853	-0.52606945	-3.02629094
H	-0.26998479	-0.29963940	-2.69172106
O	1.22392907	-1.61914886	-2.83915227
H	1.30572319	0.25364558	-3.54146269
H	0.62389980	-3.03907985	-1.68866237
C	-0.74732567	-3.77377164	-0.49537701
O	0.57788840	-3.67269848	-0.96656015
H	-1.39702530	-4.21092557	-1.25256395
H	-0.73965291	-4.42947830	0.36706146
H	-1.14007001	-2.80714221	-0.19670782
O	-0.52680655	2.89237812	-2.78029108
H	-1.35867089	2.41417317	-2.73598753
H	-0.84856914	4.21306146	-1.42664716
O	-6.81300692	0.91305663	-0.48286246
O	-3.54013994	-2.19315065	1.32422929
H	-5.74916947	2.03872238	-1.00447949
H	-7.01549620	0.84280644	0.45973293
H	-2.69981510	-1.71647793	1.25503997
H	-3.80843358	-2.37843244	0.41754351
O	-1.49924489	-0.43094636	0.72832160
O	-5.11871143	2.72304013	-1.33105357
H	0.15622945	2.37790114	-2.33897307
H	-1.81134882	0.31651078	1.27880959
H	-5.63124138	3.49882354	-1.54378981
H	-3.87153408	2.15959101	-2.36475723
O	-3.16156910	1.75293998	-2.89846723
H	-2.67704460	0.18459716	-2.19893373
H	-3.42385154	1.82213181	-3.81271984
O	-0.90914887	4.63707853	-0.56264197
H	-1.73452082	4.32423341	-0.15683407
H	0.43551995	4.10101676	0.23314978
O	-3.14867181	3.56873091	0.58392838
H	-2.95477432	2.86875111	1.22270253
H	-3.85407467	3.24958312	0.01668125
O	-2.33564978	-0.63757812	-1.82005374
H	-3.44535017	-1.82073602	-1.69027788

H	-2.03816770	-0.44482507	-0.90986139
O	-2.52923855	1.48081272	2.30516905
H	-3.31040378	1.02145445	2.66224759
H	-1.93524224	1.71256371	3.03782361
O	-6.70501205	-1.83136001	-1.20554065
H	-7.25105467	-2.14964779	-1.91951118
H	-6.78580309	0.00971578	-0.81629379
O	-5.35649645	-3.64239801	2.77980204
H	-4.56142036	-3.22309740	2.42520440
H	-5.30646415	-3.57524402	3.72927331
O	-7.32675241	0.25457714	2.17486758
H	-7.46607743	-0.70736194	2.01850248
H	-8.04596848	0.57700323	2.71047243
O	-7.42835327	-2.28848154	1.52476532
H	-6.77036827	-2.83612476	1.97873907
H	-7.22276580	-2.30670281	0.58532835
O	-4.09698803	-2.52485115	-1.44778947
H	-5.79081539	-2.11160319	-1.38444446
H	-3.79607881	-3.34436941	-1.83105695
O	-4.62726958	-0.09188206	2.92198110
H	-5.54457410	0.15912989	2.77143240
H	-4.44481913	-0.83782058	2.34166616
H	-0.52771602	-0.41657830	0.74708978
O	-0.59938503	2.09237304	4.13631246
H	-0.58508077	2.95324603	4.54457147
O	1.26884187	3.67295048	0.53961297
H	1.40231121	2.55252662	1.82020601
H	1.95029293	4.36040018	0.63259069
O	5.51059897	-0.68991195	2.46088110
O	3.87357318	-2.31439001	-2.10298525
H	5.03546157	0.14376721	2.56636670
H	6.12737012	-0.59684243	1.72445799
H	3.10751418	-2.13650823	-2.65439259
H	3.51562515	-2.36537076	-1.19781803
O	1.63883723	1.71508991	-1.28486636
O	4.23852928	1.77618353	2.75715149
H	1.54888350	2.45937341	-0.65407153
H	2.54982688	1.77642136	-1.61221626
H	4.50370932	2.24310264	3.54576962
H	3.26035947	1.81231162	2.71724256
O	1.56918119	1.82612539	2.45567592
H	1.43055464	1.01205318	1.94541969
H	0.22346081	2.00312208	3.62945980
O	3.41007414	5.28900038	0.91262034
H	4.11708542	4.64491555	0.71875827
H	3.63709952	6.11621661	0.50006467
O	5.07237240	3.23753484	0.47197562
H	4.83825684	2.77063652	-0.33823736
H	4.86561951	2.65773685	1.21352739
O	1.21419080	-0.20037567	0.62328800
H	1.77729689	-0.99036198	0.57620090
H	1.43187757	0.37127190	-0.13211069
O	4.31009516	1.96734028	-1.95246565
H	4.85597341	1.14236232	-1.98618137
H	4.56899834	2.50476201	-2.69670607
O	4.48037013	-3.08774224	2.23797260
H	4.38796701	-3.52925387	3.07756755
H	4.81599117	-2.17668596	2.41313601
O	5.55318366	-4.48060639	-2.00725248
H	4.92822316	-3.77512980	-2.22856863
H	6.08422869	-4.65125953	-2.77914037
O	7.17529093	-1.00540026	0.23271443
H	7.03715856	-1.98189561	0.25343481
H	8.11306690	-0.84644415	0.29831907
O	6.57866678	-3.55919884	0.38054081
H	6.27841948	-3.98025040	-0.43802743
H	5.86625364	-3.63034994	1.02439605
O	2.64455627	-2.50271783	0.31750223

H	3.18159874	-2.85029905	1.04659794
H	1.94427297	-3.12743765	0.07259760
O	5.69657821	-0.23176547	-2.00973831
H	6.27819870	-0.41665622	-1.25997112
H	5.10479144	-0.99213244	-2.09356017

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C	0.72537177	-0.69200074	-3.43097621
H	0.38527278	-0.44268878	-4.43727403
O	1.03329076	-2.02899650	-3.36101375
H	1.53716597	-0.04679469	-3.10728126
H	-0.14950363	-0.54821166	-2.78276159
C	-0.41951105	-3.51022063	-0.67368676
O	0.48830290	-4.26117874	0.03421500
H	-0.01058024	-3.43811077	-1.69009003
H	-1.39464913	-3.98981551	-0.72164764
H	-0.49135767	-2.49621290	-0.28724026
O	-0.49316769	3.16673619	-2.54357771
H	-1.32466008	2.69546512	-2.63611479
H	-0.73212437	4.35415352	-1.11177119
O	-6.69490181	0.99800128	-0.56114705
O	-3.50702816	-2.28084781	0.99145473
H	-5.60802355	2.16506425	-0.94459899
H	-6.94684360	0.84153103	0.35856637
H	-2.69233444	-1.75598505	0.98598240
H	-3.74166677	-2.40817130	0.06632567
O	-1.53564882	-0.39591587	0.64471582
O	-4.96848049	2.86738488	-1.20708485
H	0.15871839	2.56441683	-2.16823665
H	-1.86604746	0.29202857	1.25976903
H	-5.47317858	3.66262699	-1.35823441
H	-3.77592786	2.35509790	-2.32609790
O	-3.08390685	1.98185932	-2.90605449
H	-2.54496083	0.38297999	-2.31428462
H	-3.36105862	2.12504773	-3.80698612
O	-0.76882282	4.74507432	-0.22851549
H	-1.58379134	4.40781388	0.17715656
H	0.58955073	4.18473447	0.50360687
O	-3.03616743	3.58743069	0.82061271
H	-2.89191204	2.84509628	1.42279155
H	-3.70963223	3.31048114	0.19522933
O	-2.22709327	-0.45523767	-1.94967470
H	-3.32127399	-1.64920838	-1.97094783
H	-1.99174139	-0.29911592	-1.01489339
O	-2.58075301	1.33752841	2.39556416
H	-3.36955460	0.83693425	2.66897185
H	-1.99312711	1.44430737	3.16153624
O	-6.57517649	-1.66697359	-1.54418194
H	-7.11187496	-1.90109892	-2.29679614
H	-6.65326019	0.12952313	-0.97554043
O	-5.35781833	-3.82547441	2.30264800
H	-4.55522288	-3.38365010	1.99607173
H	-5.32930057	-3.82252629	3.25541080
O	-7.35096642	0.08164219	1.98916282
H	-7.48083396	-0.86065851	1.73577960
H	-8.08965338	0.35180708	2.52707099
O	-7.40354764	-2.38862547	1.09764097
H	-6.75513966	-2.96707897	1.52665513
H	-7.15566141	-2.31319612	0.17135802
O	-3.97095264	-2.38166701	-1.82131921
H	-5.66246145	-1.94395332	-1.73441383
H	-3.68695178	-3.13590372	-2.33059103
O	-4.67058353	-0.33089305	2.75746714
H	-5.58754188	-0.07440184	2.61374392
H	-4.46887850	-1.01356503	2.11040600
H	-0.56494089	-0.36426854	0.66961845
O	-0.63831824	1.57408235	4.29077124

H	-0.58546525	2.26847220	4.94047657
O	1.38849446	3.68367436	0.79666402
H	1.30817476	2.42567708	1.97459233
H	2.10999412	4.28983815	1.00539379
O	5.77432224	-0.21150757	2.21740510
O	3.51605706	-2.53049956	-2.04881835
H	5.29461787	0.61526291	2.35632989
H	6.26003489	-0.15026653	1.38604649
H	2.71080308	-2.43810321	-2.56867914
H	3.24089016	-2.51591749	-1.11626699
O	1.61564987	1.82880185	-1.18451740
O	4.18260044	2.04946080	2.38266450
H	1.63902552	2.53916845	-0.51637608
H	2.43629473	1.89363025	-1.69472375
H	4.26288940	2.98892892	2.55784434
H	3.24766768	1.83359254	2.53475756
O	1.46167653	1.64387590	2.53937945
H	1.34390399	0.88483350	1.94863837
H	0.17345117	1.61197317	3.75768053
O	3.84837292	4.82292100	1.44184294
H	4.34854169	4.37733426	0.73210880
H	4.15172337	5.72393285	1.50156846
O	5.04035389	3.04707083	-0.13500536
H	4.74649586	2.74175938	-1.00087484
H	4.77836250	2.38226846	0.50845507
O	1.15831924	-0.22045648	0.52025502
H	1.75370817	-0.98440570	0.51809261
H	1.40936369	0.39857838	-0.18901209
O	4.03160256	1.91977758	-2.49768983
H	4.50716136	1.05144199	-2.49454222
H	4.16837860	2.32860002	-3.34780246
O	4.71047832	-2.58944527	2.26062986
H	4.70471185	-2.94921339	3.14357347
H	5.06761588	-1.66800951	2.31970466
O	5.49786946	-4.41929897	-1.91603408
H	4.74087268	-3.85539540	-2.12853960
H	5.25964735	-5.32036063	-2.10964732
O	7.04546779	-0.69294290	-0.23889555
H	7.00095424	-1.66484569	-0.08212508
H	7.96203267	-0.46451758	-0.36958702
O	6.66066533	-3.24202776	0.28495489
H	6.31125592	-3.76224926	-0.45216911
H	6.00412625	-3.25106291	0.98836888
O	2.64040967	-2.52145658	0.52761024
H	3.32236300	-2.61403063	1.21747339
H	2.01101369	-3.24771073	0.59406383
O	5.25701639	-0.35835323	-2.35711105
H	5.92531459	-0.42974535	-1.66122679
H	4.69515581	-1.14146786	-2.29570280

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C	0.80492225	-1.24665157	-2.91741321
H	1.00605954	-1.05157578	-3.97544296
O	1.04411053	-2.60751385	-2.77420427
H	1.48546220	-0.64608864	-2.32254172
H	-0.23173810	-0.99739696	-2.71208634
C	-0.77582436	-3.58563392	-1.02529578
O	0.45721418	-2.99101676	-0.84391577
H	-1.20200612	-3.65511286	-0.02010392
H	-1.43450748	-2.96255386	-1.62372327
H	-0.68873808	-4.58825382	-1.43806630
O	-0.57522708	3.01332786	-2.55649039
H	-1.40935308	2.54231185	-2.62218523
H	-0.79187268	4.25630848	-1.18531593
O	-6.78298887	1.02777991	-0.31600579
O	-3.51454809	-2.38077392	1.03898189
H	-5.67866737	2.14152240	-0.81283943

H	-6.95947120	0.89038265	0.62376459
H	-2.70092836	-1.85597354	0.96333908
H	-3.85227679	-2.48143446	0.14264595
O	-1.52197184	-0.55958765	0.57973015
O	-5.03665065	2.81776707	-1.12964055
H	0.08344761	2.41700555	-2.18371393
H	-1.81337624	0.14858404	1.18898256
H	-5.52895086	3.62137332	-1.27711151
H	-3.87078437	2.26748459	-2.27277385
O	-3.19588198	1.88003328	-2.86198291
H	-2.72926181	0.24348736	-2.30741262
H	-3.46970766	2.04996338	-3.75927068
O	-0.81654595	4.69486587	-0.32373115
H	-1.60744952	4.35225878	0.12266870
H	0.57913968	4.19294378	0.38139219
O	-3.02542049	3.51514850	0.82849290
H	-2.84698204	2.75270271	1.39588374
H	-3.72207621	3.25225054	0.22276294
O	-2.47788699	-0.61912456	-1.94950422
H	-3.64970843	-1.71141937	-1.88580010
H	-2.11124911	-0.47452846	-1.05698676
O	-2.47770098	1.24361423	2.34256847
H	-3.25143632	0.75253860	2.66893819
H	-1.88186462	1.41222727	3.09157119
O	-6.87001770	-1.65206080	-1.25007188
H	-7.46102646	-1.87715118	-1.96365221
H	-6.82652430	0.15507903	-0.72136424
O	-5.35359668	-3.71621213	2.60457805
H	-4.56468808	-3.36508503	2.17223831
H	-5.26938494	-3.49933173	3.52966331
O	-7.25477041	0.14154860	2.28931018
H	-7.45228947	-0.79502557	2.05954166
H	-7.92587217	0.45134393	2.89070119
O	-7.48000652	-2.33819658	1.45279133
H	-6.79917298	-2.90938239	1.83906575
H	-7.31257921	-2.28031162	0.50720864
O	-4.31771070	-2.42105225	-1.69666330
H	-5.97665975	-1.94713608	-1.49983665
H	-4.09868456	-3.17847333	-2.23264887
O	-4.55349947	-0.40710960	2.87016974
H	-5.46602829	-0.11533081	2.76891126
H	-4.39697915	-1.07827168	2.19924054
H	-0.55014099	-0.55055001	0.60488419
O	-0.59589880	1.71174876	4.26064985
H	-0.63619478	2.47550410	4.82842945
O	1.39490889	3.71815164	0.67136820
H	1.34898097	2.54191402	1.93871826
H	2.11649978	4.34287887	0.81227605
O	5.88481278	0.04007026	2.33214189
O	3.61014650	-2.81968303	-1.65280635
H	5.37736385	0.86004445	2.39930563
H	6.33243640	0.02448739	1.47751309
H	2.78292608	-2.88347860	-2.14489862
H	3.34610117	-2.67855051	-0.72985684
O	1.56976615	1.72938460	-1.19205472
O	4.22265392	2.23978318	2.31367511
H	1.61163191	2.48498216	-0.57729867
H	2.38214740	1.74570894	-1.71840741
H	4.28158743	3.19332550	2.39995319
H	3.29489713	2.01441692	2.49691687
O	1.52045622	1.79784994	2.54698514
H	1.38624276	1.00289920	2.00607992
H	0.22644070	1.77614194	3.74540234
O	3.86893917	4.91364352	1.15435587
H	4.35260329	4.41347743	0.47001918
H	4.17395446	5.81588103	1.13781347
O	5.02991658	3.01382545	-0.29692933
H	4.71953547	2.63143979	-1.12578159

H	4.78075266	2.40990153	0.40872982
O	1.17418573	-0.18718450	0.68748720
H	1.78086333	-0.93812927	0.70996116
H	1.39069339	0.37885875	-0.07421554
O	3.98075334	1.67822622	-2.52775439
H	4.44301479	0.80681506	-2.45407895
H	4.10556690	2.00211030	-3.41544582
O	4.84662708	-2.31748993	2.65379228
H	4.84960402	-2.56982816	3.57323823
H	5.20253954	-1.39295044	2.60124699
O	5.65512885	-4.59262042	-1.30256826
H	4.87904933	-4.07979688	-1.57321942
H	5.49365884	-5.50945067	-1.49977920
O	7.06115163	-0.67253728	-0.11379182
H	7.06020994	-1.61854406	0.16055373
H	7.96312074	-0.43063592	-0.30703289
O	6.79860425	-3.15182748	0.73725343
H	6.46106353	-3.76896506	0.07322924
H	6.15139375	-3.10031457	1.44695314
O	2.78279764	-2.44352070	0.93423410
H	3.46576462	-2.44446882	1.63182088
H	2.17610591	-3.16206346	1.09801160
O	5.20578309	-0.58851617	-2.20785562
H	5.88837037	-0.58689197	-1.52255342
H	4.67579585	-1.38630586	-2.08158644

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C	0.50152479	-1.99948890	-2.63610890
H	-0.52420481	-1.91047680	-2.98742815
O	1.39617550	-2.34214386	-3.55528596
H	0.80412047	-1.18778141	-1.97451786
H	0.48647060	-2.93853223	-1.93315593
C	-0.76895355	-3.68105822	-0.06186508
O	0.38131480	-3.94163954	-0.79897786
H	-1.66691096	-3.76173340	-0.66735578
H	-0.79787542	-4.46659289	0.69756571
H	-0.72391142	-2.72210927	0.44397910
O	-0.48956491	3.04158084	-2.56356343
H	-1.25435530	2.47822258	-2.70081973
H	-0.85592007	4.21320393	-1.17386408
O	-6.71711818	0.94601017	-0.56399458
O	-3.56112116	-2.21484708	1.13231403
H	-5.59709597	2.01775975	-1.12130924
H	-6.94221718	0.91491489	0.37480160
H	-2.74836463	-1.69890006	1.02999692
H	-3.85635880	-2.43234404	0.24213195
O	-1.53250621	-0.39939322	0.59483959
O	-4.94150656	2.67548862	-1.44749617
H	0.23750041	2.50053784	-2.23771059
H	-1.85831160	0.30984967	1.18600894
H	-5.42640516	3.46952617	-1.65881201
H	-3.71027119	2.10204676	-2.51562068
O	-2.99886543	1.70341092	-3.05190674
H	-2.63083026	0.07937632	-2.40938347
H	-3.20850706	1.86341063	-3.96825050
O	-0.93201320	4.64855226	-0.31367444
H	-1.76351280	4.33689616	0.07689282
H	0.43129809	4.16404880	0.46521304
O	-3.23615415	3.54937605	0.71503519
H	-3.03040417	2.82172594	1.31637205
H	-3.81708128	3.19830814	0.03606259
O	-2.42618829	-0.74548006	-1.94630599
H	-3.57201965	-1.86099274	-1.84115748
H	-2.10053287	-0.50197883	-1.06147155
O	-2.55868347	1.37929007	2.32916933
H	-3.32427609	0.90356560	2.69161850
H	-1.94171161	1.58229189	3.05240551



O	-6.79518023	-1.81711116	-1.20801103
H	-7.38982821	-2.10996623	-1.89362283
H	-6.75637120	0.03530758	-0.87491995
O	-5.38381106	-3.20498961	3.03053233
H	-4.61565778	-3.08606317	2.46214164
H	-5.29461548	-2.52061613	3.69314154
O	-7.31791096	0.36210021	2.10007421
H	-7.52125346	-0.59111228	1.96196732
H	-8.01627019	0.74694150	2.62205234
O	-7.51223903	-2.19769181	1.53567008
H	-6.83916989	-2.68538610	2.03440141
H	-7.28540695	-2.25183736	0.60251248
O	-4.22421119	-2.57337665	-1.61271752
H	-5.90078132	-2.11934205	-1.44221697
H	-3.99771491	-3.35145026	-2.11491105
O	-4.67942684	-0.23151859	2.86593308
H	-5.56232924	0.11760892	2.69728583
H	-4.49138528	-0.85902363	2.16033477
H	-0.56257064	-0.33928762	0.58926601
O	-0.61172751	1.91762245	4.15540544
H	-0.60866829	2.76240020	4.59652532
O	1.28097810	3.76038243	0.76369609
H	1.40483268	2.53179250	1.90088104
H	1.93828387	4.46370486	0.89510026
O	5.55462659	-0.62631818	2.33438525
O	3.93247636	-2.24794167	-2.29099985
H	5.08256021	0.20282692	2.48636287
H	6.17319647	-0.50210947	1.60384028
H	3.19774096	-2.22530531	-2.91378942
H	3.52505287	-2.30693356	-1.41155731
O	1.72463321	1.89825627	-1.16017108
O	4.23596896	1.77490577	2.76882952
H	1.63712936	2.62593896	-0.51426537
H	2.62220696	1.96846220	-1.51782304
H	4.48260172	2.22766064	3.57164687
H	3.25713220	1.77074499	2.73030165
O	1.56437468	1.75331679	2.47832262
H	1.41712750	0.98138530	1.91117751
H	0.21421357	1.85833641	3.64853026
O	3.40792099	5.38866447	1.18914497
H	4.10763870	4.76297643	0.92324805
H	3.60956578	6.23844169	0.81049373
O	5.07526645	3.37916617	0.57302229
H	4.87863555	2.95626975	-0.27125159
H	4.85810671	2.75095154	1.27006256
O	1.18210794	-0.15309898	0.48499918
H	1.76226030	-0.92401921	0.41084495
H	1.44063779	0.50176628	-0.19408324
O	4.38010892	2.18076208	-1.89420201
H	4.88348490	1.33602554	-1.98373429
H	4.59176634	2.71406777	-2.65606241
O	4.48891645	-2.97791085	2.03349305
H	4.37412584	-3.42919024	2.86535297
H	4.84620266	-2.07578753	2.22907136
O	5.67021771	-4.36597398	-2.13619395
H	5.05122286	-3.65514066	-2.36020063
H	6.19539902	-4.54962250	-2.90919901
O	7.21409970	-0.88853177	0.10494206
H	7.10511656	-1.86789420	0.12831534
H	8.14790501	-0.70045469	0.14571832
O	6.67095177	-3.45683074	0.25799622
H	6.39089417	-3.87509998	-0.56941224
H	5.94016721	-3.53004496	0.87964676
O	2.63643599	-2.48544874	0.13093876
H	3.23131209	-2.75277755	0.85477689
O	1.98840643	-3.18058811	-0.01860453
H	5.67695756	-0.07705646	-2.09153737
H	6.26671044	-0.30535456	-1.36088069

H 5.09732531 -0.83623850 -2.23396674

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C	0.81632393	-0.30741464	-3.64793541
H	1.21824739	0.28303051	-4.46566573
O	1.28580269	-1.65241849	-3.70225532
H	1.16437139	0.11326098	-2.71473284
H	-0.26886385	-0.27982980	-3.66396357
C	-0.10455070	-2.88706083	-1.55856399
O	0.40597896	-3.82411397	-1.00076967
H	1.11110031	-2.02656779	-4.56157956
H	-0.84133874	-3.02099631	-2.35218289
H	0.12959958	-1.85697320	-1.28972438
O	-0.44670758	2.88130331	-2.70091501
H	-1.22415505	2.31846544	-2.72247827
H	-0.84279411	4.15256020	-1.34664576
O	-6.72137790	0.75541293	-0.62319123
O	-3.55537116	-2.23988501	1.28697865
H	-5.61383751	1.82640318	-1.18782714
H	-6.96054311	0.76401633	0.31316079
H	-2.70136064	-1.79885608	1.17581450
H	-3.82655090	-2.51154668	0.40432148
O	-1.52958336	-0.46617892	0.61473608
O	-4.97157939	2.49428601	-1.52295441
H	0.26831265	2.40784233	-2.26173337
H	-1.87098013	0.25751511	1.17703016
H	-5.47648161	3.26671788	-1.76502733
H	-3.70185661	1.92807621	-2.53556584
O	-2.97492638	1.53606385	-3.05711690
H	-2.62944466	-0.09041660	-2.38071332
H	-3.17184064	1.69798846	-3.97601083
O	-0.94031070	4.59098909	-0.49216230
H	-1.77193711	4.26533938	-0.11123687
H	0.40612627	4.14581586	0.36373117
O	-3.21723232	3.47119727	0.54910193
H	-3.01561619	2.77920098	1.19359908
H	-3.82704095	3.09321803	-0.08860058
O	-2.39093655	-0.89717372	-1.90451532
H	-3.52058481	-2.05088625	-1.72242948
H	-2.09120752	-0.62269920	-1.01697865
O	-2.57080538	1.39122111	2.27594199
H	-3.34349754	0.93453831	2.64940842
H	-1.96084199	1.61572867	2.99826747
O	-6.74629959	-2.04123413	-1.11787085
H	-7.33214948	-2.39025560	-1.78441152
H	-6.73647626	-0.16997863	-0.89012518
O	-5.37287395	-3.15110660	3.21855725
H	-4.59868781	-3.08115033	2.64940549
H	-5.28479995	-2.41538147	3.82395394
O	-7.34046692	0.30968560	2.05439072
H	-7.52385823	-0.65459532	1.97144596
H	-8.04631538	0.70864374	2.55517097
O	-7.48879498	-2.27829855	1.64099309
H	-6.81215720	-2.71955940	2.17826685
H	-7.24546066	-2.38204550	0.71638924
O	-4.15734536	-2.75650775	-1.44762534
H	-5.84684313	-2.34777266	-1.32452301
H	-3.84925343	-3.58862252	-1.79623196
O	-4.69014212	-0.18816824	2.87512877
H	-5.57651942	0.13115181	2.67223649
H	-4.47387270	-0.85434844	2.21239305
H	-0.56124535	-0.40219294	0.63890458
O	-0.64933017	1.98606751	4.11935211
H	-0.65331050	2.83959705	4.54312015
O	1.24408635	3.75526060	0.70477565
H	1.38936934	2.54572646	1.89053738
H	1.90081295	4.46170778	0.82301058

O	5.52270969	-0.70764847	2.27033664
O	3.61553580	-2.20919289	-2.26272437
H	5.05798995	0.12643997	2.41405388
H	6.12904995	-0.60371701	1.52666523
H	2.86606791	-2.03847359	-2.84633168
H	3.25365263	-2.30212137	-1.36561368
O	1.73571812	1.87216142	-1.16347725
O	4.23777411	1.72414861	2.73208518
H	1.62472706	2.60031798	-0.51955167
H	2.63617846	1.96457114	-1.51172482
H	4.50868612	2.13218418	3.55092376
H	3.25911659	1.75359077	2.70789836
O	1.55809012	1.78147930	2.48029294
H	1.40131223	0.99752851	1.93142381
H	0.18843098	1.91245570	3.63527624
O	3.37644214	5.37337449	1.10923809
H	4.07889406	4.73859569	0.87297168
H	3.60330399	6.22012887	0.73841283
O	5.05722074	3.35749035	0.55668731
H	4.87304484	2.92285098	-0.28415883
H	4.85249385	2.72982719	1.25842083
O	1.18181027	-0.16116056	0.53908046
H	1.73649548	-0.95450646	0.48984771
H	1.45812923	0.46476402	-0.15484568
O	4.37092194	2.14816006	-1.90885959
H	4.82999586	1.27598105	-1.99604405
H	4.61454334	2.67209923	-2.66743328
O	4.44684249	-3.07114952	2.03605029
H	4.36180762	-3.51647650	2.87462886
H	4.81010622	-2.16881041	2.21119396
O	5.36164651	-4.32118952	-2.26683765
H	4.69894857	-3.63126688	-2.42024925
H	4.96812749	-5.15826378	-2.49279178
O	7.12809376	-1.03192529	0.00547647
H	6.98881480	-2.00796221	0.01724470
H	8.06855047	-0.87543472	0.00039228
O	6.50008741	-3.58153676	0.12933493
H	6.15510372	-3.94990704	-0.69679478
H	5.79675157	-3.63109118	0.78452214
O	2.51457905	-2.53252910	0.22279021
H	3.12370698	-2.82958542	0.92040018
H	1.84149759	-3.20576724	0.06481836
O	5.51880293	-0.17245957	-2.11003486
H	6.13826090	-0.42798566	-1.41337088
H	4.89431232	-0.90193682	-2.21776342

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C	0.76836430	-0.60007424	-3.57350399
H	0.69483323	-0.22934162	-4.59609427
O	0.95613460	-1.95962252	-3.56154395
H	1.52038680	-0.06148032	-3.00177977
H	-0.21585063	-0.43529399	-3.11230385
C	-0.73762723	-2.46104089	3.14175456
O	0.45458121	-3.08290752	2.86317398
H	-1.31304495	-2.26181815	2.24180468
H	-1.31601626	-3.01040168	3.88303220
H	-0.46894811	-1.48813077	3.57876226
O	-0.60291512	3.46701900	-2.35922556
H	-1.42840790	3.00846256	-2.53333488
H	-0.82409299	4.45498744	-0.80759595
O	-6.58212294	0.78013897	-0.50194399
O	-3.33214404	-2.39357416	0.33926532
H	-5.58189462	2.06353912	-0.77121218
H	-6.81984670	0.51163302	0.39455308
H	-2.54469326	-1.82646588	0.30888120
H	-3.60887687	-2.49316223	-0.57760095
O	-1.47587788	-0.41279675	0.23070048

O	-5.00584379	2.84145970	-0.94912571
H	0.06079578	2.81709861	-2.10389622
H	-1.79487889	0.16194345	0.95174675
H	-5.57081720	3.61018510	-0.95125254
H	-3.86922059	2.59438629	-2.22232816
O	-3.19592447	2.35216973	-2.88586289
H	-2.62663882	0.67907587	-2.58933931
H	-3.50722412	2.65257361	-3.73538670
O	-0.83718718	4.75514329	0.11210374
H	-1.61731526	4.34183991	0.51294343
H	0.58621018	4.18396945	0.70159214
O	-3.03409932	3.38352359	1.09858079
H	-2.85590103	2.58018117	1.60244477
H	-3.70467849	3.15930314	0.44897055
O	-2.28948782	-0.19175165	-2.33871888
H	-3.31220534	-1.44861368	-2.49595646
H	-2.00609689	-0.13872391	-1.40816924
O	-2.48026850	0.93691605	2.35535257
H	-3.22697685	0.35195122	2.56612209
H	-1.85061912	0.90750715	3.09100160
O	-6.48616663	-1.75363088	-1.78863932
H	-7.10214285	-1.91201080	-2.49931439
H	-6.54423460	-0.03061112	-1.02100818
O	-4.92720064	-3.90169578	2.07537755
H	-4.20963158	-3.62795602	1.49360644
H	-4.86736819	-3.29893366	2.81617361
O	-7.16503233	-0.44222455	1.94184577
H	-7.28838407	-1.34998161	1.57910531
H	-7.89530541	-0.24732282	2.52225939
O	-7.14868101	-2.80135924	0.79419110
H	-6.43881225	-3.33047246	1.18929812
H	-6.90960430	-2.62256489	-0.12059785
O	-3.90626605	-2.23722855	-2.43446879
H	-5.59419220	-1.95080265	-2.12394766
H	-3.56442902	-2.90628509	-3.02165472
O	-4.45573037	-0.92569755	2.48274725
H	-5.37492984	-0.63744833	2.43521037
H	-4.25778118	-1.34998391	1.63906936
O	-0.50341969	-0.38780455	0.26241177
O	-0.42079240	0.72294159	4.16441660
H	-0.38756723	1.11349078	5.03295852
O	1.40911515	3.67791361	0.90497377
H	1.35201394	2.36385245	2.02894671
H	2.14005182	4.27781638	1.09528344
O	5.89951932	-0.26058231	2.16156091
O	2.99770985	-2.73913983	-1.77261557
H	5.40646687	0.56221822	2.27334161
H	6.31280110	-0.25235587	1.28999364
H	2.23496565	-2.59856327	-2.34573841
H	2.68740834	-2.76225577	-0.85399502
O	1.56783824	1.98786241	-1.24708933
O	4.24660751	1.95973236	2.27549477
H	1.62305202	2.64646774	-0.53108348
H	2.37203186	2.06293344	-1.77996085
H	4.30753028	2.90351000	2.43914128
H	3.32201667	1.72168651	2.44596531
O	1.51603020	1.51565724	2.48492996
H	1.39671712	0.84746563	1.78925311
H	0.33060020	1.07985892	3.65193331
O	3.93354523	4.73628175	1.42574879
H	4.38546513	4.30858894	0.67405482
H	4.28334016	5.61708091	1.52236431
O	5.03373508	2.99401924	-0.25697416
H	4.73743289	2.69466080	-1.12384355
H	4.80190975	2.30979009	0.37723653
O	1.19183179	-0.14373258	0.34498865
H	1.78918409	-0.90306313	0.40120839
H	1.46390553	0.48789031	-0.34435178

O	3.95843051	1.86713786	-2.59151901
H	4.25521160	0.93072275	-2.48729135
H	4.16683627	2.14854764	-3.47771532
O	4.73895546	-2.59321099	2.28286301
H	4.76671397	-2.95843383	3.16325522
H	5.14547735	-1.69229245	2.32138157
O	5.04333588	-4.55894198	-1.85351909
H	4.25423852	-4.00742063	-1.95669112
H	4.78408974	-5.46633227	-1.97983793
O	6.88085812	-0.89174013	-0.39062356
H	6.83512118	-1.86156941	-0.21361023
H	7.76613858	-0.69132081	-0.68235791
O	6.47699379	-3.41441508	0.19686223
H	6.03081782	-3.91579106	-0.50084988
H	5.87765052	-3.36547614	0.94896190
O	2.40703630	-2.51315119	0.88181558
H	3.22551749	-2.55388836	1.40770787
H	1.69554253	-2.82464387	1.45284371
O	4.74529684	-0.56506833	-2.14538358
H	5.51742206	-0.66579259	-1.57141540
H	4.17472664	-1.33409169	-2.02106587

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C	0.67564271	-0.24785246	-3.80437618
H	0.54471010	0.28707832	-4.74387078
O	1.20007701	-1.49976013	-4.00269064
H	1.24439760	0.33521432	-3.08222382
H	-0.32467182	-0.41932435	-3.37759841
C	-0.71853293	-1.95941321	3.01487803
O	-0.58412484	-2.59816350	1.80092363
H	-1.73733794	-1.99153925	3.39156742
H	-0.00008526	-2.35881555	3.73075782
H	-0.44152833	-0.91340852	2.85513483
O	-0.54733542	3.29857818	-2.69191011
H	-1.32588698	2.73958407	-2.74747660
H	-0.86793408	4.40187700	-1.21325397
O	-6.50848432	0.71366091	-0.47646085
O	-3.24750667	-2.78405018	0.74437469
H	-5.56644439	1.97661025	-0.94250476
H	-6.62237605	0.45664342	0.44731458
H	-2.30100610	-2.66572412	0.87750550
H	-3.42720902	-2.62741109	-0.19246331
O	-1.30579646	-0.35385563	0.07745483
O	-5.02051542	2.73876355	-1.24399982
H	0.20136605	2.76740253	-2.40256433
H	-1.73928319	0.21525166	0.73537617
H	-5.61156161	3.47987637	-1.34921467
H	-3.81191380	2.35836885	-2.42728298
O	-3.12088906	2.05632669	-3.04558521
H	-2.61978085	0.37110366	-2.66299592
H	-3.38177059	2.33430991	-3.91951554
O	-0.91207720	4.77936687	-0.32478386
H	-1.68623761	4.37868820	0.10123854
H	0.54955188	4.36448980	0.32521548
O	-3.08786653	3.47258003	0.76203117
H	-2.89258351	2.67990406	1.27807196
H	-3.75742978	3.22129671	0.12122862
O	-2.26390971	-0.48069421	-2.37696582
H	-3.27728455	-1.69401710	-2.22229796
H	-1.90586126	-0.35623165	-1.47071903
O	-2.43728002	1.10804864	2.09174952
H	-3.10604886	0.46786338	2.39614756
H	-1.78101134	1.21803952	2.79361487
O	-6.47943259	-1.81829403	-1.74763238
H	-6.97100650	-1.97263585	-2.54975481
H	-6.52193784	-0.10418596	-0.98560134
O	-5.19046720	-4.57636104	1.43511345

H	-4.38493004	-4.05787946	1.29218432
H	-5.10809194	-5.01295923	2.27749092
O	-6.86096761	-0.50039721	2.03384703
H	-7.07091357	-1.38818537	1.66188665
H	-7.55893627	-0.26263464	2.63771716
O	-7.21636019	-2.80058516	0.81654478
H	-6.58803753	-3.49375018	1.06702338
H	-7.06399078	-2.60960819	-0.11440750
O	-3.86466508	-2.45878573	-1.97811036
H	-5.55451977	-2.07827239	-1.91131353
H	-3.56927693	-3.21961845	-2.47210060
O	-4.14706972	-0.89848719	2.63956393
H	-5.08913922	-0.70499958	2.56823149
H	-3.94807594	-1.53856604	1.94516937
H	-0.36280150	-0.13772814	0.11974510
O	-0.32809045	1.26800759	3.88088158
H	-0.39940263	1.75436474	4.69715396
O	1.42510758	3.97119190	0.55012456
H	1.57061032	2.79347548	1.76594753
H	2.09602156	4.66935055	0.61213266
O	5.44495767	-0.71139807	2.23301632
O	2.95058151	-2.43767744	-2.02341485
H	5.07839183	0.17839406	2.31723093
H	6.00726059	-0.73850820	1.44896165
H	2.28371605	-2.20674461	-2.68258755
H	2.51231222	-2.51968066	-1.16292944
O	1.79186649	2.17349077	-1.45983950
O	4.42292234	1.86794751	2.47418631
H	1.73179692	2.87676804	-0.78402848
H	2.68196836	2.22225086	-1.83680637
H	4.74805025	2.36003212	3.22415548
H	3.44575647	1.93842695	2.48440929
O	1.74492249	1.98120235	2.28771476
H	1.61756375	1.26068761	1.64514972
H	0.44153131	1.62054393	3.39795117
O	3.67150724	5.48082365	0.74939603
H	4.30604543	4.79038785	0.48248085
H	3.93433068	6.29825552	0.33867673
O	5.19565538	3.33965447	0.16077714
H	4.99099991	2.87647515	-0.65941745
H	4.99678090	2.74309214	0.89041103
O	1.36071619	0.19273363	0.29105527
H	1.81649171	-0.65861364	0.27806091
H	1.63420274	0.76178226	-0.45161426
O	4.43252763	2.02396214	-2.23123911
H	4.65536092	1.06458074	-2.17973553
H	4.80276383	2.35810329	-3.04366713
O	4.11767242	-2.95689713	2.20713055
H	4.10999752	-3.37108900	3.06558213
H	4.57656391	-2.08636288	2.29925256
O	4.58664323	-4.63604324	-2.02327180
H	3.97269827	-3.90308703	-2.18165619
H	4.99687202	-4.85500699	-2.85435762
O	6.81526116	-1.37578398	-0.10331868
H	6.59038589	-2.33287589	-0.01646237
H	7.75879663	-1.30624725	-0.21933189
O	5.96061682	-3.83094441	0.21879300
H	5.52834295	-4.21166687	-0.56045914
H	5.29638978	-3.75899429	0.91172088
O	2.01325848	-2.45286786	0.55364933
H	2.70436237	-2.70288806	1.18927794
H	1.16020407	-2.67796686	0.93805255
O	4.99508440	-0.52040122	-2.03804692
H	5.67184272	-0.78842382	-1.40277770
H	4.29879257	-1.19017204	-2.02619953

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C	0.75103989	-0.87560524	-3.20975501
H	0.97784448	-0.51441209	-4.21621070
O	1.03599399	-2.24105135	-3.25346937
H	1.36941352	-0.34358826	-2.49437671
H	-0.30579564	-0.70410276	-3.02207526
C	-0.19322143	-3.23062800	-1.11758847
O	0.58917765	-4.09898791	-0.49535268
H	0.42726054	-2.92210621	-2.06827706
H	-1.10313692	-3.65580560	-1.54101338
H	-0.34451861	-2.28648462	-0.59845099
O	-0.50207771	3.09353217	-2.54389926
H	-1.32954856	2.61306693	-2.62536170
H	-0.73936778	4.30554107	-1.13301166
O	-6.74066832	1.03022581	-0.52086132
O	-3.56489649	-2.28104663	1.02765607
H	-5.63115539	2.16201546	-0.94743314
H	-6.97702144	0.89567489	0.40637351
H	-2.73142784	-1.78938637	0.99280159
H	-3.82644529	-2.42308909	0.11172096
O	-1.55126829	-0.43288112	0.59910654
O	-4.98368127	2.84893443	-1.23028635
H	0.15939275	2.50349399	-2.16665028
H	-1.88484944	0.25892505	1.20808722
H	-5.47957566	3.64681430	-1.39606048
H	-3.79124375	2.30718608	-2.34010230
O	-3.10171438	1.92175902	-2.91479506
H	-2.64643378	0.28841594	-2.34661296
H	-3.35762486	2.09164438	-3.81745481
O	-0.77687949	4.71196834	-0.25682205
H	-1.59569399	4.38590878	0.15079326
H	0.57686526	4.16324636	0.48961902
O	-3.05264828	3.5805793	0.79592088
H	-2.90122446	2.83150310	1.38833534
H	-3.72418453	3.30475748	0.16787894
O	-2.36341271	-0.55872249	-1.97409568
H	-3.49116413	-1.71476269	-1.93966405
H	-2.07229722	-0.38838137	-1.05852956
O	-2.58034690	1.32090527	2.34708556
H	-3.37417727	0.83542681	2.63485415
H	-1.99274950	1.43625393	3.11196394
O	-6.73079202	-1.65503743	-1.45002839
H	-7.28566259	-1.89191185	-2.18842620
H	-6.73932717	0.15457961	-0.92215669
O	-5.42996951	-3.74538318	2.42001322
H	-4.62240088	-3.34142852	2.07687789
H	-5.38509321	-3.68427882	3.37032280
O	-7.36618800	0.16747787	2.05633749
H	-7.52425786	-0.77653964	1.82595949
H	-8.08227222	0.46520094	2.61000567
O	-7.49155797	-2.31971707	1.22382467
H	-6.83470082	-2.89429210	1.64524500
H	-7.27267813	-2.26575951	0.28872904
O	-4.15215329	-2.42932523	-1.75552869
H	-5.82765986	-1.95679649	-1.64934282
H	-3.89597322	-3.20480539	-2.24725290
O	-4.68375792	-0.30291166	2.77745523
H	-5.59707985	-0.03009949	2.64029735
H	-4.49758851	-0.99294700	2.13320442
H	-0.58225032	-0.39834367	0.63834893
O	-0.66677803	1.58273256	4.27077211
H	-0.63309331	2.29201176	4.90553469
O	1.37648451	3.66791109	0.79134121
H	1.29637236	2.41198347	1.97073896
H	2.09131987	4.27890991	1.00936235
O	5.74881578	-0.22159496	2.23017925
H	3.65596953	-2.56525192	-2.11618358
O	5.27219950	0.60508789	2.37942302
H	6.24536696	-0.14691016	1.40637306

H	2.85318082	-2.55571034	-2.64579087
H	3.36413298	-2.52429167	-1.18944573
O	1.64060086	1.80891087	-1.17471818
O	4.16838989	2.04579032	2.41473807
H	1.64915924	2.52648680	-0.51341027
H	2.46341353	1.88114030	-1.68107215
H	4.24775670	2.98325784	2.59986632
H	3.23136870	1.82978937	2.55462627
O	1.45059389	1.63556331	2.54289576
H	1.33244145	0.87004696	1.96104234
H	0.15398427	1.61685458	3.75177246
O	3.81765896	4.82486446	1.47078451
H	4.33245737	4.38180040	0.76998355
H	4.11129004	5.72904881	1.53129321
O	5.04836205	3.05827658	-0.08759943
H	4.76459579	2.75310327	-0.95695426
H	4.78212935	2.39157398	0.55215613
O	1.16144082	-0.23772041	0.52641521
H	1.77334211	-0.98830800	0.51458795
H	1.41725197	0.39902709	-0.16531378
O	4.06735477	1.93949681	-2.46378954
H	4.55086752	1.07628121	-2.47837014
H	4.19654773	2.36329503	-3.30777664
O	4.70371032	-2.60822211	2.24044558
H	4.67457151	-2.97147683	3.12150292
H	5.05118336	-1.68410655	2.31324082
O	5.64761548	-4.44293110	-1.89565993
H	4.89510564	-3.88335613	-2.13340196
H	5.41408988	-5.34707633	-2.08079326
O	7.06389728	-0.66516623	-0.21063525
H	7.03542879	-1.63722235	-0.05155308
H	7.97874055	-0.41894254	-0.31970744
O	6.72492387	-3.21959830	0.32146610
H	6.41044109	-3.75743867	-0.41869409
H	6.05115383	-3.24262108	1.00795784
O	2.69787162	-2.50723660	0.43947480
H	3.35145084	-2.62592383	1.15268232
H	2.06946057	-3.23603090	0.44465353
O	5.32790196	-0.32609287	-2.37171945
H	5.97755571	-0.40248201	-1.65869019
H	4.78774425	-1.12574788	-2.35160732

### 3.2.3 CH3 + CH2OH

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C	-0.50186044	-3.53451256	-3.01975494
O	0.16152339	-2.51471098	-2.43280867
H	0.10596785	-4.39108563	-3.24901321
H	-1.35743031	-3.29040800	-3.62949627
H	-0.44060862	-1.75763147	-2.29101502
C	-0.59989457	-4.12460892	0.61225463
H	-1.33846181	-3.67845094	1.25494515
H	-0.26696054	-5.13163327	0.79208632
H	-0.27124015	-3.60833776	-0.27226822
O	-0.16538407	2.65903544	-3.16944183
H	-0.95465382	2.12519462	-3.27886767
H	-0.55186933	4.06831834	-2.02424093
O	-6.29461270	0.51783991	-1.08088182
O	-3.15736765	-1.86554697	1.45029215
H	-5.27313035	1.62918202	-1.73935532
H	-6.60427706	0.61993314	-0.17099188
H	-2.41090387	-1.26786232	1.27559738
H	-3.36912961	-2.25357991	0.59481078
O	-1.39398804	0.00964401	0.58001099
O	-4.68177731	2.30178976	-2.14835962
H	0.47778894	2.14596792	-2.66648377



H	-1.76250387	0.81233937	1.00382717
H	-5.24286820	2.99101277	-2.49531411
H	-3.40497542	1.66598133	-3.08873375
O	-2.64834107	1.22876433	-3.52700912
H	-2.08131885	-0.09542504	-2.53520069
H	-2.85450158	1.15274457	-4.45469122
O	-0.66051995	4.64193826	-1.25337550
H	-1.52012026	4.41235636	-0.86878497
H	0.68729784	4.29651499	-0.34609788
O	-3.06418056	3.74821908	-0.20818408
H	-2.91611184	3.20698169	0.57835192
H	-3.60436812	3.22671786	-0.80569175
O	-1.78525540	-0.77925481	-1.91291396
H	-2.86365528	-2.05411119	-1.57746480
H	-1.65369640	-0.35582233	-1.03571095
O	-2.51073584	2.04059114	1.91616027
H	-3.25879494	1.57640332	2.32868249
H	-1.91155953	2.36837175	2.60663090
O	-6.07864377	-2.32562492	-1.24175451
H	-6.57855762	-2.80666056	-1.89599794
H	-6.22288674	-0.42994487	-1.23395403
O	-4.96436239	-3.00209136	3.19415717
H	-4.18167600	-2.65698248	2.74630704
H	-5.01579420	-2.54842436	4.03165513
O	-7.11306259	0.37579595	1.58065099
H	-7.18832960	-0.60533670	1.60976895
H	-7.91440986	0.74790499	1.93777845
O	-7.00643983	-2.24724460	1.46801034
H	-6.35379998	-2.60919794	2.08641095
H	-6.70546787	-2.44602357	0.57640293
O	-3.40896810	-2.79126911	-1.23434911
H	-5.14757253	-2.58874689	-1.32929323
H	-2.89491856	-3.58854892	-1.35245376
O	-4.50838614	0.36542521	2.66462515
H	-5.41532758	0.53236023	2.38681926
H	-4.22455562	-0.42472818	2.19468166
H	-0.42631148	0.04362999	0.69234511
O	-0.57981478	2.90283480	3.65284527
H	-0.58265297	3.80922267	3.94695546
O	1.51568775	3.93188542	0.04269687
H	1.60473722	3.02775221	1.47307884
H	2.22603498	4.58899196	-0.03552475
O	5.41640066	-0.49353594	2.34939539
O	2.79881181	-2.69666587	-1.48184949
H	5.03851787	0.39551645	2.33157858
H	5.92440271	-0.63759203	1.54185369
H	1.95574409	-2.59334683	-1.93918873
H	2.59318457	-2.61884824	-0.53762224
O	1.82880285	1.65859457	-1.41632090
O	4.40156572	2.10225402	2.32762729
H	1.79453674	2.50886722	-0.93734719
H	2.70536797	1.60904603	-1.82492403
H	4.78634302	2.66276460	2.99710767
H	3.43275212	2.24457542	2.35810854
O	1.72409393	2.38969112	2.20804453
H	1.53526141	1.52295432	1.81465128
H	0.28005124	2.74484428	3.23111176
O	3.81396357	5.37257198	-0.05154820
H	4.43210002	4.62763267	-0.16905370
H	4.08762192	6.07796741	-0.62908529
O	5.26694182	3.11088357	-0.19421822
H	5.04009819	2.52478402	-0.92541433
H	5.01630273	2.66959564	0.62436061
O	1.27302974	0.13039573	0.71756539
H	1.67813377	-0.73433123	0.86073492
H	1.56943314	0.51506645	-0.12996696
O	4.41935147	1.48366817	-2.34658539
H	4.66855190	0.53166481	-2.27654351

H	4.64542663	1.77561141	-3.22558583
O	4.18046345	-2.72312622	2.85471771
H	4.16913430	-2.93893969	3.78314844
H	4.62739385	-1.84597418	2.75299566
O	4.31390567	-4.96532257	-1.21808326
H	3.74229454	-4.22859692	-1.48124685
H	4.77601498	-5.26181304	-1.99671043
O	6.68655622	-1.56002553	0.09865102
H	6.45198028	-2.48115680	0.35910544
H	7.63278193	-1.52171379	-0.01189752
O	5.81817888	-3.92163629	0.85720347
H	5.30620765	-4.38412518	0.17756348
H	5.23636918	-3.75206376	1.60440203
O	2.11011545	-2.46380655	1.16931091
H	2.78546323	-2.62006715	1.85560970
H	1.35253407	-3.02052060	1.35435220
O	4.99744047	-1.04884615	-2.06708439
H	5.62735689	-1.22470678	-1.35556729
H	4.22530694	-1.60791043	-1.91220343

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C	0.42569543	-1.29111989	-3.13705441
O	0.90188286	-2.39198227	-3.00945843
H	0.69226812	-0.46530648	-2.47642130
H	-0.27552655	-1.07407311	-3.94411563
H	-0.65224790	-3.75396988	-1.28154955
C	-0.52722383	-3.79456517	-0.20555129
H	-1.39901010	-4.23352762	0.26746200
H	0.34660841	-4.39900871	0.01609928
H	-0.39512735	-2.78363627	0.16448871
O	-0.29797717	2.45134311	-3.27960399
H	-1.13629759	1.98274059	-3.26631258
H	-0.62864393	3.94693704	-2.16921747
O	-6.54597622	0.70530392	-0.99487787
O	-3.36334796	-1.94244397	1.37463254
H	-5.49663543	1.78692094	-1.63167508
H	-6.80685392	0.77494405	-0.06681042
H	-2.54291947	-1.44044944	1.25035597
H	-3.57407888	-2.29984695	0.50510584
O	-1.40668411	-0.19066471	0.61406647
O	-4.87734566	2.43778897	-2.03782573
H	0.33442489	1.96891109	-2.73762375
H	-1.76240597	0.62244441	1.02680455
H	-5.40798287	3.15049103	-2.38475074
H	-3.62335520	1.73355969	-2.96571907
O	-2.90204695	1.25757465	-3.42163755
H	-2.36450446	-0.14732086	-2.44754498
H	-3.15333559	1.17538005	-4.33772384
O	-0.70359592	4.52132846	-1.39688645
H	-1.54589258	4.29538652	-0.97036601
H	0.64136381	4.13866769	-0.51562943
O	-3.02814318	3.67573172	-0.20036547
H	-2.87365021	3.10139191	0.56174893
H	-3.68010303	3.23891030	-0.75312152
O	-2.00573500	-0.87548442	-1.92206075
H	-3.07467234	-2.08283619	-1.64326490
H	-1.78368584	-0.51996813	-1.04053445
O	-2.49584329	1.91093005	1.87919884
H	-3.26726562	1.47921318	2.28602968
H	-1.90798268	2.24885833	2.57351732
O	-6.33972689	-2.11642196	-1.27983681
H	-6.85685796	-2.54924557	-1.95400456
H	-6.47194364	-0.23707001	-1.18078758
O	-5.17224248	-3.13619268	3.05370247
H	-4.38478084	-2.77931336	2.62140329
H	-5.17619406	-2.79030231	3.94217739
O	-7.22002487	0.45878114	1.69803884

H	-7.32397425	-0.52028093	1.68258247
H	-7.98742356	0.83351651	2.12081594
O	-7.21231945	-2.15577832	1.44699464
H	-6.56372191	-2.58491672	2.02545963
H	-6.94066495	-2.31387591	0.53777965
O	-3.71450325	-2.76623732	-1.32669866
H	-5.41657946	-2.40503680	-1.38590219
H	-3.33564608	-3.62127834	-1.51319104
O	-4.55726077	0.33193256	2.62964700
H	-5.47191043	0.53030947	2.40336787
H	-4.32440611	-0.46810156	2.14712611
H	-0.44100168	-0.15343143	0.71026280
O	-0.57271621	2.82600417	3.60649835
H	-0.59562891	3.73318430	3.89714236
O	1.46860628	3.76161928	-0.13416806
H	1.56565956	2.93530262	1.34890350
H	2.18357127	4.41262451	-0.23091600
O	5.55930208	-0.34723349	2.42254295
O	3.01641407	-2.91124739	-1.29020124
H	5.13884632	0.51928703	2.34674844
H	6.08634881	-0.51409427	1.63134352
H	2.25673892	-2.79248063	-1.87855321
H	2.70568408	-2.79144752	-0.38248254
O	1.74199005	1.44745614	-1.51184044
O	4.39884380	2.17572549	2.22811985
H	1.70233760	2.31098118	-1.05273074
H	2.62292861	1.39964911	-1.91468605
H	4.75607224	2.81025743	2.84481299
H	3.42412898	2.26817231	2.25646665
O	1.70856038	2.33671425	2.11171538
H	1.53086100	1.44874044	1.76433242
H	0.28045664	2.69054213	3.16497444
O	3.73459867	5.24476367	-0.27835551
H	4.37514028	4.51728568	-0.38528339
H	3.97218464	5.94202132	-0.88126735
O	5.22921788	3.01504489	-0.36277259
H	4.97669467	2.39376631	-1.05540341
H	4.99342173	2.62216371	0.48447698
O	1.28779835	-0.00435246	0.72660876
H	1.74284404	-0.83506039	0.91320817
H	1.56596342	0.35458040	-0.13503811
O	4.33410731	1.26600047	-2.40202999
H	4.65189063	0.34457027	-2.23729115
H	4.59182186	1.50366372	-3.28871950
O	4.36564656	-2.57595771	2.99956756
H	4.35456372	-2.74999538	3.93686388
H	4.79508100	-1.69390413	2.86133002
O	4.58119565	-5.09997607	-0.80567343
H	3.99067260	-4.41331223	-1.15028131
H	4.95357422	-5.56315725	-1.54992443
O	6.88545893	-1.47350067	0.24095589
H	6.68476447	-2.39148942	0.53966549
H	7.82792778	-1.40860235	0.11268069
O	6.09873074	-3.82336913	1.10841196
H	5.61323747	-4.35698191	0.46161366
H	5.49940853	-3.63240331	1.83604126
O	2.25731479	-2.51938276	1.34900645
H	2.97513417	-2.58458760	2.00885053
H	1.53530463	-3.06725166	1.64771362
O	5.10976623	-1.16242472	-1.88876174
H	5.77669043	-1.25396564	-1.19552307
H	4.39984891	-1.78902483	-1.69370022
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C	1.00047670	-1.03136884	-3.83902688
O	0.62592437	-1.77130287	-2.76314115
H	1.97332588	-1.27623721	-4.22506876

H	0.60091906	-0.03594238	-3.93329808
H	-0.22341474	-1.45506243	-2.40668904
C	-0.58221146	-3.96990069	0.26322489
H	-1.29123963	-3.60569346	0.98571570
H	-0.22480871	-4.98305241	0.31305895
H	-0.26791234	-3.33894699	-0.54930041
O	-0.22945791	2.42230356	-3.21484388
H	-1.04793021	1.92164934	-3.23151448
H	-0.58808675	3.93177558	-2.14789121
O	-6.41523559	0.51484575	-1.05293002
O	-3.23321955	-1.90676530	1.52191301
H	-5.38014343	1.59270862	-1.72600002
H	-6.70513437	0.61647307	-0.13654871
H	-2.47583778	-1.31907621	1.36043288
H	-3.45674666	-2.26759792	0.65747800
O	-1.43143238	-0.07078068	0.66611048
O	-4.76612043	2.23353214	-2.15413600
H	0.39356330	1.97081264	-2.63204836
H	-1.80512869	0.75030887	1.04887324
H	-5.30373582	2.91633796	-2.54764734
H	-3.49535813	1.50898485	-3.02909739
O	-2.74090292	1.03567138	-3.43257634
H	-2.14236848	-0.25962005	-2.42331368
H	-2.93882789	0.90612564	-4.35635583
O	-0.69152475	4.53103513	-1.39725176
H	-1.54716682	4.31199263	-0.99679523
H	0.65260248	4.22901398	-0.45936916
O	-3.07377081	3.67672561	-0.28946950
H	-2.93495014	3.15364710	0.51096208
H	-3.65482607	3.16682255	-0.85810840
O	-1.77079636	-0.92388998	-1.81952106
H	-2.86767984	-2.17492350	-1.50717637
H	-1.66033959	-0.49266490	-0.94386605
O	-2.55551271	2.02376719	1.88772401
H	-3.30909089	1.57584303	2.30879379
H	-1.96151362	2.37390538	2.57141177
O	-6.15517275	-2.31523400	-1.23793140
H	-6.63741372	-2.78712311	-1.91184324
H	-6.33253296	-0.43256461	-1.20444500
O	-5.05887655	-3.14853808	3.15198419
H	-4.27130628	-2.74712956	2.76263204
H	-5.10688925	-2.84499075	4.05441275
O	-7.17496820	0.35927314	1.62504802
H	-7.25018488	-0.62186315	1.64410102
H	-7.97086341	0.72660210	1.99897566
O	-7.08576080	-2.26367286	1.47239737
H	-6.44135506	-2.65793333	2.07903984
H	-6.79666475	-2.45504948	0.57529092
O	-3.49536702	-2.84552710	-1.16203604
H	-5.22118748	-2.57366508	-1.30798895
H	-3.06341410	-3.69457561	-1.22428732
O	-4.55825462	0.37874284	2.68013588
H	-5.47003172	0.52910565	2.40881407
H	-4.28152019	-0.43833793	2.25444565
H	-0.46453337	-0.02512844	0.78094954
O	-0.62739397	2.94624547	3.60063314
H	-0.63806505	3.85709047	3.88037635
O	1.47515390	3.88119254	-0.04520762
H	1.56516765	3.02403302	1.42249873
H	2.18808569	4.53218533	-0.14873632
O	5.41869481	-0.46942798	2.36690968
O	2.80517237	-2.75336196	-1.37024701
H	5.03059134	0.41374239	2.31560631
H	5.93064532	-0.63889588	1.56667556
H	2.01959040	-2.48095120	-1.86540047
H	2.59212080	-2.64173042	-0.43248399
O	1.74309501	1.54736321	-1.40347383
O	4.37257899	2.11618398	2.26403416

H	1.73743763	2.41619021	-0.95743258
H	2.60699492	1.46502598	-1.83417142
H	4.76968064	2.70105686	2.90493062
H	3.40513532	2.26231375	2.30627140
O	1.68954967	2.41169358	2.17725046
H	1.49827767	1.53117113	1.81681935
H	0.23595937	2.78726917	3.18691228
O	3.77456772	5.31193559	-0.20298524
H	4.38603510	4.55982172	-0.30967950
H	4.04493384	6.00081438	-0.80162539
O	5.20303981	3.03467714	-0.30378555
H	4.95708948	2.42903634	-1.01262165
H	4.96189880	2.62139332	0.53204922
O	1.23125970	0.09258232	0.78629736
H	1.65032103	-0.76140878	0.95122154
H	1.50676679	0.44889042	-0.08065810
O	4.30972944	1.33554127	-2.38075909
H	4.60028007	0.39815108	-2.27308992
H	4.51791650	1.59972232	-3.27284033
O	4.19347126	-2.68379464	2.95394628
H	4.19484441	-2.87074987	3.88866251
H	4.63862069	-1.81002843	2.81874447
O	4.17290365	-5.08313167	-0.98183912
H	3.63741251	-4.34614188	-1.31139350
H	4.54688622	-5.52878784	-1.73606294
O	6.70372165	-1.60614254	0.15866999
H	6.44710834	-2.51890530	0.42683542
H	7.65188666	-1.58906353	0.06035310
O	5.78677898	-3.93988829	0.95337473
H	5.25479557	-4.42485248	0.30539476
H	5.22526599	-3.74791660	1.71038179
O	2.11318159	-2.47300940	1.28183572
H	2.79424708	-2.61449900	1.96636631
H	1.37351219	-3.05253680	1.46075233
O	5.00220477	-1.15207375	-2.00937014
H	5.65616660	-1.28773450	-1.31122344
H	4.25078583	-1.72643208	-1.80829010

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C	-0.43322359	-3.48873198	-2.96504241
O	0.23005367	-2.40769332	-2.50109920
H	0.18710428	-4.34524858	-3.15793155
H	-1.32461348	-3.31683408	-3.54756571
H	-0.38998504	-1.66443964	-2.36446925
C	-0.62496231	-4.02569638	0.41722234
H	-0.20194280	-5.01313236	0.36359470
H	-0.28149775	-3.26648922	-0.26085854
H	-1.42261127	-3.81276838	1.10650474
O	-0.11948144	2.72713986	-3.13093821
H	-0.91035702	2.20001643	-3.25987278
H	-0.51917061	4.11950187	-1.96979181
O	-6.28517270	0.56161903	-1.16301467
O	-3.20078143	-1.85419361	1.38681394
H	-5.25510275	1.68540249	-1.78591126
H	-6.60523107	0.64769594	-0.25500025
H	-2.43430321	-1.27520473	1.24117442
H	-3.40592778	-2.21125325	0.51622895
O	-1.38960283	0.00237432	0.56237492
O	-4.65847995	2.36602819	-2.17344826
H	0.51328973	2.20262974	-2.62674223
H	-1.76369808	0.79978768	0.99138210
H	-5.21491982	3.06168944	-2.51495446
H	-3.36794452	1.74756021	-3.10616644
O	-2.60544090	1.31701328	-3.54077438
H	-2.05017626	-0.02303745	-2.56483430
H	-2.80142925	1.25015083	-4.47137228
O	-0.63850839	4.68041495	-1.19120633

H	-1.50331634	4.44444551	-0.82234524
H	0.69538994	4.31695260	-0.27170934
O	-3.05365107	3.76922728	-0.19154618
H	-2.91239620	3.21120988	0.58456270
H	-3.59192795	3.26242263	-0.80323357
O	-1.75538298	-0.72092562	-1.95767099
H	-2.84777643	-1.99323017	-1.64407567
H	-1.63036556	-0.31966516	-1.06934641
O	-2.52304328	2.02127300	1.90468853
H	-3.28284681	1.56076998	2.30017584
H	-1.93461071	2.33965109	2.60855862
O	-6.06986804	-2.28049883	-1.37160839
H	-6.55571200	-2.75134546	-2.04359974
H	-6.21279306	-0.38324352	-1.33268945
O	-5.02125279	-3.07438911	3.04840492
H	-4.23491508	-2.69491578	2.63562536
H	-5.08420929	-2.68799377	3.91801500
O	-7.13593129	0.37855991	1.48527979
H	-7.21109019	-0.60283050	1.49745863
H	-7.94336219	0.74411732	1.83541155
O	-7.03590124	-2.24310764	1.32551450
H	-6.39521870	-2.62679692	1.94313512
H	-6.72726951	-2.42748517	0.43341514
O	-3.39952979	-2.73162200	-1.31465718
H	-5.13698404	-2.54144265	-1.44413109
H	-2.86398984	-3.52076842	-1.38448177
O	-4.54728947	0.36358128	2.61049968
H	-5.45018302	0.53318012	2.32182053
H	-4.25923549	-0.42595473	2.14164864
H	-0.42400936	0.03560672	0.68894491
O	-0.61857611	2.85973758	3.68362899
H	-0.62765710	3.76174614	3.99079981
O	1.51895866	3.94596378	0.12149939
H	1.59403373	3.01968562	1.53770064
H	2.22958800	4.60482933	0.06237298
O	5.42416273	-0.49433518	2.39631591
O	2.83198817	-2.63063696	-1.48021595
H	5.03834262	0.39147837	2.38809564
H	5.94007640	-0.62254461	1.59109593
H	1.99741514	-2.50390875	-1.94792850
H	2.61495929	-2.58013125	-0.53712718
O	1.84931181	1.69275159	-1.36530520
O	4.38543850	2.09182490	2.40379591
H	1.80787746	2.53602229	-0.87463545
H	2.72916028	1.65368581	-1.76801002
H	4.76099747	2.64640146	3.08339838
H	3.41565372	2.22875749	2.42726747
O	1.70746119	2.37097256	2.26428933
H	1.52368289	1.50979012	1.85675760
H	0.24790307	2.70939530	3.27298273
O	3.81332582	5.39587811	0.07722690
H	4.43579838	4.65591660	-0.04851362
H	4.08758824	6.11226127	-0.48634656
O	5.27509383	3.14214399	-0.09293358
H	5.05495048	2.56965740	-0.83688507
H	5.01577402	2.68637901	0.71491346
O	1.27769493	0.12943562	0.73849098
H	1.69056719	-0.73181980	0.87826110
H	1.58255133	0.52768033	-0.09980819
O	4.44791639	1.55035919	-2.27874834
H	4.70372877	0.59933538	-2.22004194
H	4.67658569	1.85611683	-3.15236581
O	4.19976753	-2.73844137	2.85751566
H	4.18866602	-2.97107875	3.78188782
H	4.64263931	-1.85726524	2.77207953
O	4.35134733	-4.90044123	-1.26017291
H	3.77931073	-4.16003084	-1.51158526
H	4.81892766	-5.17937942	-2.04204088

O	6.71821584	-1.51885901	0.14032359
H	6.48372705	-2.44552422	0.38005366
H	7.66506720	-1.47621949	0.03700877
O	5.84638521	-3.89680833	0.84296166
H	5.33759172	-4.34517427	0.15159240
H	5.26120323	-3.74258579	1.59079172
O	2.12938019	-2.46684114	1.17721299
H	2.80768487	-2.62666802	1.86010990
H	1.37312796	-3.02342335	1.36360056
O	5.03869771	-0.98152902	-2.02637386
H	5.66642333	-1.16373038	-1.31458446
H	4.26596046	-1.54183076	-1.87889085

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C	-0.17612284	-3.81627056	-2.33879233
O	0.41400152	-2.54210048	-2.47805766
H	0.49583553	-4.52336277	-2.81549942
H	-1.11552478	-3.84366112	-2.89239777
H	-0.25773483	-1.86697001	-2.30874674
C	-0.39284188	-4.19702837	-0.88666475
H	0.55940098	-4.24314619	-0.36583415
H	-1.02585348	-3.47196089	-0.38082072
H	-0.86175370	-5.17615989	-0.81029805
O	-0.14625010	2.61063421	-3.08039501
H	-0.90843107	2.04070078	-3.20098380
H	-0.55364043	4.02002905	-1.94923188
O	-6.39737732	0.75944809	-1.14699587
O	-3.36316702	-1.94338523	1.33396076
H	-5.25855311	1.74808589	-1.80062737
H	-6.69141247	0.88340674	-0.23500962
H	-2.53840289	-1.44813799	1.21146553
H	-3.57724582	-2.30671289	0.46938865
O	-1.39112933	-0.19307417	0.60091400
O	-4.58472827	2.34446308	-2.20041830
H	0.51779331	2.12091291	-2.58118988
H	-1.76814489	0.60698436	1.02016181
H	-5.05619667	3.07770037	-2.58828072
H	-3.31807806	1.58387182	-3.07097028
O	-2.57275276	1.10461336	-3.48274897
H	-2.06812648	-0.28078390	-2.51495077
H	-2.74921116	1.04410052	-4.4177989
O	-0.66452233	4.60605802	-1.18767862
H	-1.51538213	4.36694116	-0.78939618
H	0.68294451	4.29016941	-0.27547919
O	-3.04582935	3.67788760	-0.13182690
H	-2.89333328	3.08902161	0.61866996
H	-3.56249681	3.18456416	-0.77284983
O	-1.82036948	-0.99126100	-1.90197951
H	-3.02785507	-2.11974716	-1.67689654
H	-1.67515981	-0.57913913	-1.02391830
O	-2.50265129	1.87035965	1.91931704
H	-3.27371035	1.44728789	2.33083693
H	-1.91031507	2.20607949	2.61258515
O	-6.33375481	-2.07558963	-1.32026938
H	-6.86297869	-2.50437766	-1.98774983
H	-6.38612700	-0.19208117	-1.29478453
O	-5.30120783	-2.66483032	3.21492411
H	-4.49018026	-2.60760796	2.69736414
H	-5.28078719	-1.89029180	3.77565951
O	-7.19092732	0.63000162	1.52336165
H	-7.36034537	-0.33965701	1.53307459
H	-7.94320016	1.07082252	1.90812542
O	-7.28765934	-1.99340627	1.38714699
H	-6.65650508	-2.36346323	2.02381427
O	-6.97250979	-2.20269009	0.50320154
H	-3.70660704	-2.76873676	-1.38066565
H	-5.41620158	-2.37309710	-1.43449174

H	-3.37887718	-3.64177755	-1.57937495
O	-4.61198493	0.29325385	2.60980679
H	-5.48602077	0.56777970	2.31009397
H	-4.35074039	-0.44662370	2.05111191
H	-0.42479844	-0.12324537	0.69993608
O	-0.62238053	2.78393762	3.68090387
H	-0.66842617	3.69029160	3.97171250
O	1.51238026	3.94014790	0.12523136
H	1.58958718	3.01015918	1.53551249
H	2.21089838	4.61138390	0.06238119
O	5.54041320	-0.39064936	2.40830630
O	2.89216014	-2.56899907	-1.35452389
H	5.12218261	0.48031211	2.38643134
H	6.05155502	-0.51915388	1.59985375
H	2.05519407	-2.47086131	-1.83925129
H	2.66041673	-2.54020959	-0.41723170
O	1.87278709	1.67222738	-1.33232833
O	4.39464095	2.14549441	2.38817835
H	1.82382926	2.52122031	-0.85280507
H	2.74916988	1.64014319	-1.74345786
H	4.75220462	2.72439139	3.05719816
H	3.42077804	2.24969929	2.41269065
O	1.70894124	2.35875412	2.25905355
H	1.52237850	1.49831012	1.85080028
H	0.24873779	2.66256078	3.26989260
O	3.77962127	5.43309370	0.06726254
H	4.41226831	4.70295719	-0.06515145
H	4.03541992	6.15264579	-0.50095938
O	5.27184931	3.20070694	-0.11328750
H	5.05974696	2.62497966	-0.85724909
H	5.01506316	2.74228959	0.69373127
O	1.27572042	0.10025689	0.75329988
H	1.74252654	-0.72551225	0.92462466
H	1.58368933	0.50360018	-0.08215258
O	4.45975910	1.57588220	-2.27683322
H	4.73069495	0.62963812	-2.20200591
H	4.66204160	1.86457554	-3.16264622
O	4.36381060	-2.64242686	2.91637234
H	4.39629191	-2.87023169	3.84152323
H	4.79460065	-1.75646806	2.80738112
O	4.44949871	-4.80617267	-1.19990821
H	3.86309685	-4.06543142	-1.41961900
H	4.90475742	-5.05593919	-1.99879546
O	6.82511986	-1.42366689	0.15646028
H	6.60588443	-2.35232651	0.40218813
H	7.76872526	-1.37014247	0.03125393
O	5.98265857	-3.80795108	0.87558097
H	5.46377481	-4.25531628	0.19051893
H	5.40725969	-3.65294571	1.63047741
O	2.21021056	-2.44849039	1.34601991
H	2.93815411	-2.56420527	1.98776179
H	1.46223292	-2.94858654	1.66308096
O	5.07948150	-0.93895898	-1.97364158
H	5.72845868	-1.10153965	-1.27685820
H	4.30939398	-1.49238543	-1.78670350

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C	0.94164623	-1.16279601	-3.80801956
O	0.57814418	-1.87293315	-2.70854875
H	1.90723904	-1.42374133	-4.20168404
H	0.54736508	-0.16721945	-3.92125263
H	-0.26454572	-1.54291665	-2.34888737
C	-0.61043579	-3.99965186	0.37355794
H	-1.30721382	-3.60888675	1.09411268
H	-0.26175448	-5.01437120	0.44748259
H	-0.30010195	-3.39464554	-0.45994791
O	-0.25341625	2.31387248	-3.24558886



H	-1.07539752	1.81875129	-3.24200324
H	-0.59050777	3.84896767	-2.20843646
O	-6.42784763	0.49639917	-0.97442248
O	-3.23389581	-1.88807809	1.61935140
H	-5.39350714	1.55212914	-1.68279898
H	-6.70731041	0.62039813	-0.05755892
H	-2.47489675	-1.30873930	1.43661300
H	-3.46915225	-2.26662911	0.76568760
O	-1.43059611	-0.08283578	0.70418715
O	-4.78014700	2.17914145	-2.13181588
H	0.37303352	1.87107724	-2.65981670
H	-1.79464353	0.74902574	1.07271281
H	-5.31762804	2.85678025	-2.53433503
H	-3.52356863	1.42725096	-3.00407662
O	-2.77646573	0.94015691	-3.40482268
H	-2.17566462	-0.33567539	-2.37260874
H	-2.98528765	0.79091335	-4.32321427
O	-0.68203350	4.46529023	-1.47017480
H	-1.53471858	4.26084135	-1.05594009
H	0.67005906	4.17507483	-0.54007388
O	-3.05770919	3.65172808	-0.31850504
H	-2.91418823	3.14637114	0.49240906
H	-3.64830613	3.13307684	-0.86911915
O	-1.80211053	-0.98869315	-1.75785356
H	-2.90330668	-2.22550205	-1.40656999
H	-1.67976933	-0.53874357	-0.89326223
O	-2.52787753	2.04570250	1.89083665
H	-3.27965496	1.61206301	2.32970063
H	-1.92425535	2.40685459	2.56022324
O	-6.18840202	-2.33878756	-1.09873950
H	-6.68091087	-2.82229870	-1.75680061
H	-6.35299734	-0.45469594	-1.10557864
O	-5.04983034	-3.07961505	3.29725525
H	-4.26393672	-2.69291809	2.89004152
H	-5.08620086	-2.75403069	4.19252267
O	-7.16016410	0.40562775	1.71419686
H	-7.24151362	-0.57431406	1.75603707
H	-7.94961107	0.78655555	2.08818708
O	-7.08936574	-2.22061414	1.61956406
H	-6.44080267	-2.60516023	2.22801257
H	-6.81120930	-2.43394987	0.72395446
O	-3.53132045	-2.88435432	-1.04007045
H	-5.25687100	-2.60478409	-1.17309824
H	-3.10529700	-3.73730953	-1.08822903
O	-4.53207855	0.43124768	2.74042982
H	-5.44580923	0.58145769	2.47566279
H	-4.26499331	-0.39667896	2.32979859
H	-0.46216355	-0.04127615	0.80719796
O	-0.57473887	2.99230360	3.56173676
H	-0.57594696	3.90905526	3.82168182
O	1.49472519	3.83098430	-0.12700429
H	1.59446107	3.00636467	1.35859113
H	2.21065926	4.47482487	-0.25225436
O	5.43405185	-0.49190553	2.34050958
O	2.76784883	-2.83728369	-1.31966818
H	5.05155058	0.39267171	2.27369707
H	5.93689357	-0.68236473	1.53921481
H	1.97877360	-2.57011169	-1.81219428
H	2.56548732	-2.70399943	-0.38232795
O	1.73288381	1.46592428	-1.43602920
O	4.40457036	2.09823542	2.19103920
H	1.73771857	2.34444918	-1.00940229
H	2.59172299	1.36807014	-1.87354092
H	4.81236863	2.69447806	2.81450484
H	3.43862985	2.25196722	2.24012423
O	1.72274014	2.41016811	2.12552631
H	1.52187426	1.52319223	1.78681082
H	0.28285818	2.81815485	3.14216568

O	3.80147341	5.24266841	-0.33984407
H	4.40683719	4.48423321	-0.43612452
H	4.07009796	5.91628451	-0.95637020
O	5.21371658	2.95404580	-0.40500508
H	4.95636715	2.33470912	-1.09778499
H	4.97864102	2.56083100	0.44216060
O	1.23416444	0.06427779	0.79097031
H	1.64880546	-0.78903431	0.97001596
H	1.50271357	0.39940959	-0.08657734
O	4.28790663	1.21588690	-2.43471213
H	4.57430454	0.27938202	-2.30956124
H	4.48815231	1.45928280	-3.33449190
O	4.19955532	-2.68421934	2.98797553
H	4.20920135	-2.85062703	3.92651947
H	4.64920459	-1.81676174	2.82913287
O	4.12234100	-5.16827927	-0.89401758
H	3.58887308	-4.43474002	-1.23438105
H	4.48537427	-5.63322118	-1.64192214
O	6.68918185	-1.68538409	0.14503914
H	6.42879406	-2.59021131	0.43552022
H	7.63643465	-1.67734193	0.03722753
O	5.76381708	-3.99465432	0.99937503
H	5.22194433	-4.48979599	0.36748615
H	5.21139222	-3.78236107	1.75764619
O	2.10403252	-2.49608776	1.33244570
H	2.79088551	-2.62722703	2.01323851
H	1.36294000	-3.06756241	1.53034827
O	4.96978243	-1.26711102	-2.01621328
H	5.62964744	-1.39176064	-1.32158165
H	4.21652303	-1.83160179	-1.79506319

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C	0.28782811	-2.34915930	-3.96654163
O	0.34304632	-2.26970196	-2.61486454
H	1.10920643	-2.87546004	-4.41765457
H	-0.21774786	-1.55778017	-4.49492606
H	-0.38212417	-1.70826781	-2.28016610
C	-0.59807586	-4.10257948	0.35904668
H	-1.25859890	-3.54705695	1.00197441
H	-0.35208945	-5.12257584	0.59608543
H	-0.23841176	-3.67162378	-0.55955539
O	-0.21974179	2.43047709	-3.21502099
H	-1.01689158	1.90120615	-3.27870759
H	-0.58194124	3.90320108	-2.13309910
O	-6.37178807	0.51761267	-0.98676766
O	-3.18535151	-1.86592454	1.58673959
H	-5.33633860	1.58286847	-1.68464885
H	-6.65636569	0.63621384	-0.07073539
H	-2.43938618	-1.27113322	1.40010798
H	-3.42501093	-2.24255000	0.73349351
O	-1.41578750	-0.02185458	0.67685384
O	-4.72693118	2.22086619	-2.12300386
H	0.42727391	1.94406406	-2.69063571
H	-1.78001637	0.79926160	1.06873467
H	-5.26842371	2.90798021	-2.50363992
H	-3.47232222	1.50308405	-3.02740676
O	-2.73424337	1.02429576	-3.45462523
H	-2.14871341	-0.24865919	-2.40933974
H	-2.96947105	0.89098196	-4.36888454
O	-0.67668918	4.51529189	-1.39081420
H	-1.53089187	4.31027229	-0.98068509
H	0.67575294	4.21300954	-0.47548929
O	-3.06434521	3.70003615	-0.25757194
H	-2.91673863	3.18708544	0.54775971
H	-3.62727069	3.16941203	-0.82540131
O	-1.81124355	-0.90775193	-1.78096358
H	-2.89724591	-2.16187252	-1.44008507

H	-1.67991477	-0.45718552	-0.91737978
O	-2.51699938	2.06687457	1.92688243
H	-3.26272062	1.61800262	2.36054408
H	-1.91227530	2.41833922	2.60059561
O	-6.16012220	-2.32061449	-1.12321409
H	-6.65516039	-2.80388065	-1.77952108
H	-6.30744684	-0.43304691	-1.12600932
O	-5.00086229	-3.05054974	3.27739738
H	-4.21425852	-2.67398131	2.86255778
H	-5.04034150	-2.69733370	4.16213178
O	-7.12326663	0.41182381	1.69666460
H	-7.20530572	-0.56830006	1.73511132
H	-7.91470336	0.79219168	2.06700681
O	-7.04934694	-2.21354524	1.59813936
H	-6.39548849	-2.59327034	2.20408005
H	-6.77315191	-2.42397261	0.70122164
O	-3.50084711	-2.84338181	-1.07579641
H	-5.22884576	-2.58677697	-1.20052274
H	-3.05251009	-3.68364878	-1.14355991
O	-4.50681346	0.42093645	2.75051725
H	-5.41754732	0.57534429	2.47772633
H	-4.23209306	-0.39529280	2.32197205
H	-0.44651856	0.01779080	0.77371375
O	-0.56426183	2.98944858	3.60758138
H	-0.56158276	3.90596549	3.86839931
O	1.50450240	3.86503430	-0.07263854
H	1.59892074	3.02232527	1.39590975
H	2.21362438	4.52006549	-0.17596990
O	5.39182023	-0.48744056	2.38569921
O	2.80245340	-2.71606934	-1.37460442
H	5.02118896	0.40342644	2.33567503
H	5.91168046	-0.65941741	1.59117332
H	1.97692670	-2.54186481	-1.84605233
H	2.59518618	-2.62534544	-0.43267844
O	1.79772016	1.53142867	-1.43726425
O	4.39794474	2.11571416	2.27701402
H	1.76954804	2.40156904	-0.99493523
H	2.67193051	1.46426399	-1.84858417
H	4.78754794	2.69186287	2.93023487
H	3.43030297	2.26608291	2.30453745
O	1.72129849	2.41489062	2.15584726
H	1.52740931	1.53339818	1.79966047
H	0.28945189	2.81429866	3.18016835
O	3.79593879	5.31217390	-0.21442212
H	4.41681303	4.56532326	-0.30284669
H	4.06920359	5.99700989	-0.81636193
O	5.25298141	3.05105400	-0.27755792
H	5.01742127	2.44390604	-0.98875387
H	5.00742474	2.63538879	0.55580016
O	1.24998649	0.09923154	0.76171985
H	1.64788038	-0.76370845	0.93160717
H	1.53905672	0.44761937	-0.10424907
O	4.38996045	1.35645335	-2.36856240
H	4.66802697	0.41490585	-2.26640906
H	4.60685032	1.62481621	-3.25734285
O	4.14695206	-2.69421526	2.96311351
H	4.13855432	-2.87919875	3.89819397
H	4.59624820	-1.82221231	2.83088035
O	4.19437514	-5.04525828	-1.01003314
H	3.65893901	-4.30094392	-1.32287437
H	4.60134262	-5.44831599	-1.77117692
O	6.69203567	-1.62549055	0.18827017
H	6.43396110	-2.53654008	0.46090237
H	7.64085014	-1.60832549	0.09638911
O	5.76740188	-3.95435030	0.98659710
H	5.24125161	-4.42699598	0.32495841
H	5.19508838	-3.76015487	1.73497188
O	2.08462034	-2.48393613	1.26826782

H	2.75472680	-2.62778342	1.96286545
H	1.34742814	-3.07404964	1.42406901
O	5.02986598	-1.14767127	-2.00756006
H	5.66200043	-1.30051642	-1.29300752
H	4.25516912	-1.69552684	-1.82392615

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C	0.65680471	-1.29682152	-3.20967330
O	0.97905426	-2.47805357	-2.68714010
H	1.23275951	-0.43663755	-2.91520444
H	-0.27713366	-1.20489644	-3.73536040
H	0.30267928	-2.87359221	-2.01699672
C	-0.41076894	-3.59689691	-0.71482941
H	-1.30460477	-3.93417988	-1.21185304
H	0.34021704	-4.33944212	-0.49609122
H	-0.51163514	-2.75483274	-0.05096168
O	-0.30358777	2.32226379	-3.19582985
H	-1.08408251	1.76301895	-3.20119426
H	-0.66657031	3.78389118	-2.09689220
O	-6.62249587	0.79831045	-0.95292001
O	-3.57948964	-2.06435294	1.39368751
H	-5.46014633	1.70800371	-1.67686585
H	-6.85630534	0.95365106	-0.02858126
H	-2.71571291	-1.66359152	1.22420369
H	-3.86167431	-2.45043413	0.55782060
O	-1.47629024	-0.46524251	0.52686064
O	-4.78269928	2.27551354	-2.11159024
H	0.39796740	1.86694390	-2.71941853
H	-1.82040757	0.34238148	0.95747005
H	-5.24599585	3.01848187	-2.49048019
H	-3.54357894	1.47648004	-3.00810766
O	-2.83335598	0.96950478	-3.44590852
H	-2.55109057	-0.53803621	-2.50911969
H	-3.02111784	0.97110655	-4.38086391
O	-0.74476770	4.38508633	-1.34405903
H	-1.57692931	4.15470737	-0.90114307
H	0.61977312	4.06512008	-0.47878580
O	-3.05970486	3.50468573	-0.14563018
H	-2.88603783	2.89405859	0.58313735
H	-3.65313986	3.05518935	-0.75192079
O	-2.36852613	-1.27645084	-1.91286138
H	-3.55645683	-2.30322861	-1.59187262
H	-2.02748375	-0.89129709	-1.08594844
O	-2.48540173	1.65937241	1.85916272
H	-3.26626786	1.28685853	2.30128708
H	-1.87302590	1.99931797	2.53244323
O	-6.78468993	-2.03116350	-1.04250782
H	-7.37705144	-2.43849033	-1.66898828
H	-6.68559666	-0.15417026	-1.08297217
O	-5.46262443	-2.58703385	3.41520454
H	-4.68600079	-2.64655518	2.84876748
H	-5.34403346	-1.76032750	3.88292864
O	-7.25928179	0.75341746	1.76302217
H	-7.49544008	-0.20152887	1.81094271
H	-7.94264880	1.25509354	2.19836019
O	-7.54285948	-1.85717325	1.71090862
H	-6.88770571	-2.25215213	2.30683915
H	-7.30558475	-2.09695232	0.81004309
O	-4.24296116	-2.92476596	-1.23438459
H	-5.89662505	-2.40103153	-1.19065919
H	-4.01772478	-3.80726001	-1.51538815
O	-4.64793910	0.23729761	2.67394318
H	-5.51580721	0.56718717	2.41382526
H	-4.45189225	-0.51440965	2.10304603
O	-0.50882303	-0.38256104	0.54767103
H	-0.57105797	2.59776766	3.56943242
H	-0.61383744	3.51328952	3.83057808

O	1.46035590	3.71856707	-0.09587704
H	1.54311138	2.78927267	1.30746949
H	2.14302780	4.40786295	-0.14312358
O	5.63046865	-0.32747281	2.48705903
O	3.38361457	-2.87801927	-1.37233200
H	5.18190061	0.52470751	2.40278889
H	6.20526119	-0.46018147	1.72316849
H	2.61691852	-2.76154017	-1.95054948
H	3.04973713	-2.78539987	-0.46903743
O	1.87699455	1.45927450	-1.53584890
O	4.35556760	2.12506409	2.28221848
H	1.79594416	2.31016506	-1.06186772
H	2.77642435	1.43679326	-1.89594626
H	4.62836922	2.76012658	2.94016478
H	3.37593808	2.14501859	2.25582712
O	1.67743944	2.14746190	2.03771291
H	1.49101122	1.28028289	1.64544281
H	0.27735308	2.47092157	3.11545636
O	3.66668467	5.29740869	-0.10430870
H	4.33482526	4.59654137	-0.21989222
H	3.90011515	6.02653586	-0.66999173
O	5.24894754	3.12895144	-0.22728516
H	5.05449707	2.52236896	-0.95106785
H	5.00144969	2.69027111	0.59373704
O	1.22606839	-0.13988963	0.54254895
H	1.74156643	-0.93259192	0.73163646
H	1.54166767	0.28010595	-0.27942258
O	4.51525126	1.38241783	-2.32953145
H	4.88099286	0.47880578	-2.17320571
H	4.77035290	1.64393892	-3.21030779
O	4.43204537	-2.57403981	2.94321165
H	4.37687011	-2.76408183	3.87594903
H	4.86120730	-1.68522024	2.84230662
O	4.96890017	-5.05137231	-0.88764338
H	4.38686324	-4.36527416	-1.24669609
H	5.41940720	-5.46261444	-1.61922813
O	7.10044824	-1.36167884	0.35390670
H	6.90209839	-2.28867053	0.62234289
H	8.04712659	-1.27569528	0.28102561
O	6.31184778	-3.74430043	1.13964443
H	5.88879603	-4.29074548	0.46103693
H	5.66302479	-3.58210833	1.83083492
O	2.39888746	-2.58322532	1.20788394
H	3.09102889	-2.60228496	1.89931091
H	1.71282074	-3.18896765	1.47783075
O	5.41809696	-1.01727636	-1.85008802
H	6.05877159	-1.10565330	-1.13244546
H	4.73096629	-1.68091859	-1.70551501

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C	-0.04955053	-3.13378355	1.80429963
H	0.70183684	-3.73203093	2.31309099
H	0.42893722	-2.66865339	0.94740822
H	-0.81211479	-3.82024885	1.44030708
C	-0.62937175	-2.08160058	2.73764436
H	-1.33641651	-1.43414592	2.22452013
H	-1.13011179	-2.53815249	3.59137595
H	0.15976450	-1.44418010	3.12030709
O	0.28069019	2.70017443	3.02084791
H	1.09711252	2.20718359	3.13050283
H	0.63349644	3.99728789	1.74810073
O	6.65179672	0.93018317	1.03701310
O	3.56600063	-2.19483299	-0.88626322
H	5.52708143	2.00211755	1.58811036

H	6.89553552	0.92952803	0.10226995
H	2.71493589	-1.74329036	-0.78334032
H	3.83508517	-2.45096427	0.00256145
O	1.50946995	-0.45416035	-0.30867437
O	4.87737010	2.66537389	1.91553707
H	-0.38108770	2.12382033	2.62588352
H	1.83572770	0.28950642	-0.85169281
H	5.37233196	3.44625743	2.15024139
H	3.62596925	2.06199303	2.94877123
O	2.91605257	1.62629914	3.45606177
H	2.61818948	0.02436513	2.71120486
H	3.12116021	1.72983216	4.38126252
O	0.71977834	4.50802466	0.93131008
H	1.56148147	4.23984309	0.52972055
H	-0.62621181	4.06462228	0.10817002
O	3.06414436	3.55001216	-0.14824370
H	2.91543350	2.84743549	-0.79505667
H	3.69266098	3.21235375	0.49428676
O	2.42501370	-0.79386179	2.23575704
H	3.52411203	-1.93276360	2.09197066
H	2.06584668	-0.55444555	1.36405720
O	2.53789641	1.46371782	-1.91697400
H	3.31474094	1.01236262	-2.28640348
H	1.94476401	1.72168718	-2.64134810
O	6.72743691	-1.86404530	1.55165351
H	7.31003388	-2.18367429	2.23546653
H	6.67127205	0.00745004	1.31337790
O	5.43467034	-3.04866294	-2.78966587
H	4.65783663	-2.99666236	-2.22169264
H	5.33979554	-2.30046521	-3.37890148
O	7.30042508	0.45306574	-1.63483123
H	7.50895997	-0.50453653	-1.53407027
H	8.00137608	0.86262236	-2.13384636
O	7.51517468	-2.12412145	-1.18470693
H	6.85565535	-2.58666173	-1.72480413
H	7.25961321	-2.21720063	-0.26172766
O	4.16856905	-2.64927519	1.84882082
H	5.83279160	-2.19641465	1.74644391
H	3.86270406	-3.46190260	2.24190317
O	4.67436190	-0.11853772	-2.47852125
H	5.55034760	0.22155786	-2.26337608
H	4.45767597	-0.77628214	-1.80734182
H	0.54165272	-0.43299169	-0.37254845
O	0.65375817	2.21075178	-3.75200836
H	0.69441839	3.10641882	-4.07514503
O	-1.46114905	3.66468492	-0.23544838
H	-1.49304983	2.59598466	-1.52893023
H	-2.14719470	4.35003006	-0.28262841
O	-5.46034140	-0.59760732	-2.60965106
O	-3.74694311	-2.96210409	1.73143264
H	-5.03587433	0.27164691	-2.60325532
H	-6.11333941	-0.63372895	-1.90041473
H	-3.10553595	-2.83767257	2.42775800
H	-3.26044006	-2.89279179	0.89170685
O	-1.84592298	1.56205404	1.44638847
O	-4.25015613	1.88065621	-2.58369246
H	-1.78114151	2.36576211	0.89534088
H	-2.75415613	1.53608730	1.77729559
H	-4.47989431	2.46223512	-3.30441369
H	-3.27182101	1.89129322	-2.50656623
O	-1.60249784	1.88674525	-2.19977873
H	-1.44087688	1.05988735	-1.71898323
H	-0.19305358	2.11503227	-3.28754008
O	-3.66960329	5.23432063	-0.46355040
H	-4.33718304	4.54225124	-0.30350833
H	-3.91776767	6.00730847	0.03349825
O	-5.23421132	3.06393509	-0.19319033
H	-5.03519104	2.52290513	0.57935107

H	-4.95653110	2.57041550	-0.97259277
O	-1.20901260	-0.22388354	-0.45446883
H	-1.72369908	-1.03702447	-0.50137965
H	-1.49837280	0.30232247	0.31686596
O	-4.55789515	1.50806945	2.08231092
H	-4.97792996	0.62433816	1.97986625
H	-4.87126525	1.87398498	2.90535224
O	-4.22393212	-2.86630184	-2.65228624
H	-4.03255073	-3.14640098	-3.54357669
H	-4.64985672	-1.97104560	-2.70447449
O	-5.37242547	-5.11558074	1.13287920
H	-4.81100568	-4.44115468	1.53632901
H	-5.90643394	-5.50266285	1.82013286
O	-7.16377052	-1.36067802	-0.53090393
H	-6.98229621	-2.31122766	-0.71269967
H	-8.10807698	-1.23276210	-0.56075247
O	-6.40204219	-3.81992657	-1.08124209
H	-6.10419096	-4.36419047	-0.33904965
H	-5.66039335	-3.72792539	-1.68723566
O	-2.44478874	-2.74214945	-0.66095256
H	-3.04392961	-2.82151706	-1.43173330
H	-1.72574645	-3.35614620	-0.79380942
O	-5.65153280	-0.86283602	1.75932005
H	-6.24118930	-0.98170106	1.00257795
H	-5.04159069	-1.60816480	1.76317778

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C	0.67343004	-3.91062769	0.43111273
H	1.26950559	-3.88298122	-0.46416981
H	0.66258545	-3.05682208	1.08625134
H	0.19292982	-4.82570670	0.73065383
C	-1.10608318	-0.89508954	3.53321601
H	-1.60054107	-0.03961236	3.10699457
H	-1.39850553	-1.24473755	4.50860578
H	-0.18870344	-1.24447363	3.09075337
O	0.13820662	2.72486668	3.05339384
H	0.87354302	2.12039467	3.18074548
H	0.58394703	4.01725314	1.79897361
O	6.39518258	0.61762178	1.22589186
O	3.37503333	-2.15321829	-1.14937889
H	5.25651916	1.65653638	1.81369447
H	6.70153112	0.69639981	0.31315579
H	2.56638677	-1.63044103	-1.03355338
H	3.61201301	-2.46263761	-0.26828899
O	1.45101450	-0.32313992	-0.47248597
O	4.60167464	2.29982949	2.16871164
H	-0.57956005	2.24165999	2.63238180
H	1.82420953	0.44464304	-0.94811753
H	5.09889310	3.03938517	2.50943272
H	3.29486140	1.64215777	3.08838222
O	2.54132778	1.20703789	3.53048260
H	2.19876531	-0.33086830	2.65377029
H	2.71015004	1.22977032	4.46861549
O	0.70267126	4.53226033	0.98910192
H	1.55755385	4.25975131	0.62029212
H	-0.63687597	4.16283792	0.10162438
O	3.08903793	3.53714147	0.02784923
H	2.95253584	2.91594907	-0.69957447
H	3.59615503	3.07331981	0.69828049
O	2.01298026	-1.07032428	2.05903155
H	3.15006430	-2.20422485	1.85665012
H	1.81827102	-0.68348106	1.18556755
O	2.58152250	1.63762529	-1.94215119
H	3.34860238	1.17587722	-2.31832116
H	1.99303794	1.92019499	-2.66121245
O	6.40708173	-2.21001592	1.51837872
H	6.93230556	-2.60603014	2.20865064

H	6.39991716	-0.32470460	1.42541175
O	5.33363363	-2.97090917	-2.97859515
H	4.52006474	-2.89417276	-2.46805599
H	5.32260756	-2.20604941	-3.55324446
O	7.22888935	0.36807775	-1.42715323
H	7.40183259	-0.60095537	-1.39533824
H	7.98330353	0.79539209	-1.82268233
O	7.33976735	-2.24507113	-1.18567280
H	6.69936516	-2.63967412	-1.79747325
H	7.03595408	-2.41412938	-0.28862338
O	3.80167777	-2.89010381	1.56390502
H	5.49106373	-2.52034625	1.62781782
H	3.42197950	-3.74381472	1.75535237
O	4.66638333	-0.00941266	-2.53046083
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H	4.38080138	-0.71221082	-1.93617703
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O	-1.46967861	3.79162458	-0.27526995
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H	-4.84294816	0.05680124	-2.56421529
H	-5.86670878	-0.88431631	-1.82944969
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ts_Rc_ch3_ch3 W33
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### 3.2.5 CH3 + CH3O

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p_Rc_ch3_ch3o W33			
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p\_dHa\_ch3\_ch3o W33

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H	3.17810308	-2.42256921	-2.44883064
O	1.46510640	-2.26540730	-2.34748792
H	1.39908545	-1.41595283	-1.88399814
H	0.04378108	-2.26693636	-3.46668643
O	2.97955654	-5.72497019	-0.34508126
H	3.70931207	-5.11650642	-0.12561783
H	3.09598887	-6.52403384	0.15896028
O	4.76167875	-3.76059447	0.07681070
H	4.57109895	-3.20877280	0.84404699
H	4.61439994	-3.22795560	-0.71211428
O	1.32067019	-0.09552049	-0.66031230
H	1.89286042	0.67957513	-0.72177722
H	1.51337283	-0.60236470	0.14877731
O	4.03963847	-2.19277325	2.32164158
H	4.48769855	-1.31210884	2.29222703
H	4.22782952	-2.58173661	3.17158713
O	4.80855282	2.29472727	-2.49766742
H	4.85716392	2.59294054	-3.40190363
H	5.10613952	1.35004378	-2.47489184
O	5.22374634	4.22939867	1.62247804
H	4.53151079	3.59362564	1.85822435
H	5.62706996	4.53255440	2.43027531
O	7.04234373	0.48431976	0.13014624
H	6.98226711	1.45324487	-0.04253664
H	7.96118464	0.26931511	0.26588751
O	6.62348930	3.01722407	-0.41908585
H	6.19182925	3.52318416	0.28551509
H	6.03238804	3.01314726	-1.17782201
O	2.65139127	2.31662441	-0.91046120
H	3.39584298	2.36751598	-1.54140814
H	2.02358066	2.99638126	-1.14384620
O	5.16249464	0.14734482	2.16420466
H	5.86113308	0.23483469	1.50237348
H	4.55400354	0.88896371	2.04418360
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r_Rc_ch3_ch3o W33			
C	-0.57258311	-3.82139767	-0.33112115
H	-0.07067361	-4.71938317	-0.64615124
H	-0.54900824	-2.94607997	-0.95623250

H	-1.18842373	-3.82522164	0.55098936
C	0.90199207	-0.79174226	-3.50705155
O	1.47185267	-2.02582751	-3.69966597
H	1.52069059	-0.13319047	-2.90173070
H	0.62052215	-0.32786607	-4.45112503
H	-0.02656830	-0.98347212	-2.94861375
O	-0.28083462	2.66827241	-3.07597897
H	-1.05983107	2.10757322	-3.10010667
H	-0.71475164	4.04773736	-1.86525496
O	-6.51054658	0.51556025	-1.03667406
O	-3.29917594	-2.16187026	1.30088997
H	-5.45639731	1.62684360	-1.63033512
H	-6.78791407	0.54898368	-0.11160468
H	-2.52216972	-1.59252380	1.18235493
H	-3.53830502	-2.45710276	0.41512413
O	-1.46230171	-0.26810916	0.58497998
O	-4.84528694	2.30472840	-2.00114295
H	0.41379572	2.21578005	-2.58577841
H	-1.84347250	0.50626230	1.04662127
H	-5.38781496	3.01696047	-2.33042239
H	-3.53500652	1.69305240	-2.93025601
O	-2.78090908	1.26958201	-3.38403834
H	-2.33015656	-0.21665005	-2.50042112
H	-2.97334152	1.27528618	-4.31794404
O	-0.83747624	4.57248205	-1.06370150
H	-1.68080089	4.28580449	-0.67809833
H	0.50413975	4.24034963	-0.15463153
O	-3.16773211	3.55894884	-0.00780178
H	-3.01469612	2.95444633	0.73080427
H	-3.75017808	3.10639777	-0.62212675
O	-2.02817789	-0.95231407	-1.94918335
H	-3.09796707	-2.16566696	-1.72355393
H	-1.83757565	-0.58645119	-1.06386776
O	-2.62378233	1.70318150	1.98858967
H	-3.37873684	1.21706889	2.36358265
H	-2.04923415	2.00832514	2.70923089
O	-6.35211533	-2.29801852	-1.42526766
H	-6.84743426	-2.71005291	-2.12813886
H	-6.46086067	-0.41877099	-1.26535469
O	-5.15577748	-3.43194634	2.88777194
H	-4.35915449	-3.05445666	2.49317116
H	-5.19552852	-3.10460291	3.78259114
O	-7.24375819	0.15174531	1.63154770
H	-7.34470264	-0.82623310	1.57832591
H	-8.01972719	0.50972565	2.05325805
O	-7.21409355	-2.45279018	1.29413217
H	-6.55239766	-2.88701178	1.85317219
H	-6.95006482	-2.57667904	0.37732990
O	-3.71679418	-2.87456809	-1.42165007
H	-5.42211076	-2.56839569	-1.51971928
H	-3.30355173	-3.71313206	-1.61189504
O	-4.62017037	0.00574532	2.65185014
H	-5.52924705	0.19333555	2.39425102
H	-4.34361705	-0.76154127	2.14102274
H	-0.49552653	-0.17846920	0.63158730
O	-0.74969943	2.53023369	3.80254057
H	-0.78413954	3.42392475	4.13147488
O	1.33687469	3.88746172	0.23765303
H	1.41181047	2.87081513	1.59621341
H	2.00809171	4.58877270	0.26222048
O	5.24254198	-0.53697049	2.57492389
O	3.44716916	-2.65581120	-1.79248718
H	4.85809227	0.34943778	2.58679832
H	5.89040342	-0.58826388	1.86157704
H	2.77603794	-2.52234978	-2.47364493
H	2.99633504	-2.61562680	-0.93511778
O	1.84352771	1.78493945	-1.38142605
O	4.19219459	2.03932116	2.63689220

H	1.73172431	2.59029001	-0.83766434
H	2.76173203	1.79260308	-1.69098078
H	4.47476384	2.54627506	3.39418935
H	3.21748998	2.12664906	2.57988411
O	1.53473204	2.18484067	2.28577952
H	1.39970859	1.34253561	1.82398868
H	0.10301797	2.42650477	3.35118494
O	3.53828573	5.45431797	0.43699283
H	4.20986519	4.75576863	0.32722360
H	3.82477608	6.22075847	-0.04924645
O	5.13637376	3.29737011	0.26740371
H	4.98037807	2.74230664	-0.50512984
H	4.88391735	2.78992704	1.04647287
O	1.22364760	0.04314547	0.58230350
H	1.68229303	-0.80656016	0.61289212
H	1.51334723	0.54373539	-0.20325957
O	4.52456743	1.74415742	-2.02405117
H	4.88878246	0.82938990	-1.95024666
H	4.84996364	2.11205770	-2.84141950
O	4.01043917	-2.82455189	2.63714835
H	3.85277983	-3.12450562	3.52830516
H	4.42972549	-1.92946116	2.69147058
O	4.98268844	-4.87275310	-1.32077585
H	4.43525953	-4.15122185	-1.66483790
H	5.49491685	-5.22023995	-2.04467624
O	6.92131767	-1.31963487	0.48578391
H	6.70876779	-2.27067929	0.63465976
H	7.86964465	-1.22620341	0.51440369
O	6.10164951	-3.77337817	0.94555775
H	5.76018041	-4.25190092	0.17577815
H	5.37983578	-3.68548419	1.57549298
O	2.21401329	-2.53194788	0.66537399
H	2.79250501	-2.71892098	1.42955116
H	1.44335850	-3.09799098	0.71975696
O	5.43830357	-0.68944901	-1.79436896
H	6.01521996	-0.87261367	-1.04107654
H	4.77287684	-1.38931405	-1.82226311

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C	-0.15580817	3.85687319	0.47703510
H	0.42504109	4.68408449	0.84563775
H	-0.25950349	2.96663640	1.07220921
H	-0.72253742	3.95452555	-0.43218608
C	0.81472475	0.57799221	3.60086267
H	-0.05765783	0.89037227	3.00739394
O	1.50663901	1.73369846	3.86627805
H	0.43653543	0.11822988	4.51259996
H	1.38692072	-0.12570463	3.00063395
O	-0.71762931	-2.70977407	2.98715862
H	-1.43079310	-2.06698933	2.99348568
H	-1.23784845	-3.99472024	1.70780675
O	-6.56195426	0.19099541	0.73660240
O	-2.96197571	2.56340905	-1.34314933
H	-5.66915693	-1.05026075	1.33825479
H	-6.79558020	0.21807749	-0.20063015
H	-2.26004162	1.90664406	-1.20916808
H	-3.21123007	2.85651216	-0.45950475
O	-1.38523047	0.45352967	-0.61326454
O	-5.15656558	-1.80357453	1.71268973
H	0.04655484	-2.32309505	2.54665536
H	-1.82578966	-0.25804695	-1.12081337
H	-5.79069752	-2.46024436	1.98962470
H	-3.83475124	-1.37296196	2.72378531
O	-3.06219339	-1.05205032	3.22779603
H	-2.40686693	0.40343791	2.42417657
H	-3.30056919	-1.06737444	4.15093825
O	-1.37699160	-4.47648633	0.88231814

H	-2.16327330	-4.08519544	0.46914177
H	0.03670223	-4.26732961	0.04867174
O	-3.52562687	-3.17554289	-0.24168430
H	-3.27064804	-2.56942099	-0.95019560
H	-4.08576939	-2.68025837	0.36028754
O	-1.99832561	1.11788719	1.91535881
H	-2.91482677	2.45046948	1.68534158
H	-1.80521160	0.76111929	1.02688432
O	-2.68464941	-1.32990346	-2.14185498
H	-3.36207614	-0.75064687	-2.53227460
H	-2.11178950	-1.67305184	-2.84655897
O	-6.11425711	2.95539319	1.23598079
H	-6.59724377	3.39714094	1.92932708
H	-6.42028721	1.10617216	1.00143569
O	-4.58233080	4.07982069	-2.97219031
H	-3.85368146	3.60461202	-2.55262640
H	-4.61284059	3.78275211	-3.87788444
O	-7.11830059	0.71990044	-1.94708326
H	-7.11263439	1.70084903	-1.86270260
H	-7.90669290	0.46491616	-2.41775015
O	-6.81532909	3.29252443	-1.51300267
H	-6.08170828	3.66588348	-2.02419113
H	-6.58552579	3.35639607	-0.58095008
O	-3.43516731	3.23363325	1.38124495
H	-5.16639441	3.11749990	1.38505987
H	-2.94191727	4.01398507	1.62186653
O	-4.44520325	0.60111071	-2.83275825
H	-5.38174809	0.50935305	-2.62680523
H	-4.11212309	1.31581040	-2.28102532
O	-0.43313922	0.25755915	-0.61796915
H	-0.82345846	-2.29935791	-3.89766785
H	-0.93880883	-3.17130830	-4.26434617
O	0.92153990	-3.99698680	-0.29163754
H	1.17408631	-2.95224564	-1.60710157
H	1.51227347	-4.76744987	-0.31125749
O	5.39923564	0.03879240	-2.28320991
O	3.63255362	2.20146227	2.07767442
H	4.92096845	-0.79854066	-2.34481501
H	6.01347335	-0.00496289	-1.54021239
H	2.91790747	2.12108109	2.72188915
H	3.22303346	2.23883612	1.19969389
O	1.57374102	-2.01673172	1.42627264
O	4.07691922	-2.40158733	-2.48748119
H	1.40167238	-2.78693273	0.84837748
H	2.46912336	-2.13613547	1.77701804
H	4.33928412	-2.91231543	-3.24949742
H	3.09690392	-2.38171377	-2.47828912
O	1.40531105	-2.26221478	-2.26400388
H	1.34040794	-1.42555247	-1.77742973
H	0.01140463	-2.30738084	-3.40313375
O	2.94521882	-5.79199428	-0.44732185
H	3.68310513	-5.17628715	-0.28162847
H	3.12154019	-6.60033384	0.02324631
O	4.75948453	-3.83218004	-0.12592416
H	4.62664536	-3.28826773	0.65876812
H	4.60280794	-3.27527106	-0.89630228
O	1.24626736	-0.15534302	-0.49741159
H	1.79630573	0.63854511	-0.47481364
H	1.43979060	-0.71007939	0.28134650
O	4.20795725	-2.29513615	2.19172689
H	4.67409846	-1.42504088	2.16854456
H	4.45035373	-2.72321968	3.00861776
O	4.42751341	2.44917203	-2.31315853
H	4.34728655	2.79367443	-3.19852500
H	4.74896813	1.51545276	-2.38239389
O	5.42140479	4.24911117	1.75866424
H	4.78242690	3.58199034	2.05077222
H	5.93222491	4.51488411	2.51733542



O	7.04773026	0.56285828	-0.09187013
H	6.94766198	1.53598422	-0.21369146
H	7.98049631	0.36621165	-0.07960136
O	6.52364052	3.10601399	-0.49417189
H	6.19902921	3.59415309	0.27686471
H	5.82822497	3.11875761	-1.15884657
O	2.51616211	2.29421551	-0.43666338
H	3.14839568	2.44031714	-1.16642413
H	1.81601686	2.94423023	-0.50426948
O	5.39452510	0.02707633	2.09330661
H	6.02337378	0.16935287	1.37347616
H	4.80955474	0.79552709	2.11872986

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C	-0.12791648	-3.43484168	-0.76781795
H	0.62428364	-4.13099938	-1.09000887
H	0.11459140	-2.39980816	-0.61714457
H	-1.13951276	-3.76419634	-0.61758470
C	0.79324828	-1.11676526	-3.43515958
O	1.20582835	-2.41488766	-3.23505610
H	1.46205124	-0.38391121	-2.99000427
H	0.64708940	-0.93318102	-4.50014321
H	-0.19526200	-1.03094046	-2.96778879
O	-0.35502528	2.68548313	-3.01178105
H	-1.17378852	2.18849320	-3.07434012
H	-0.75411813	4.03258664	-1.77145899
O	-6.60456218	0.61777930	-0.98482375
O	-3.36552630	-2.23763738	1.01043395
H	-5.58293722	1.78878042	-1.51839363
H	-6.88052132	0.60132181	-0.05904137
H	-2.56544520	-1.69566380	0.92701733
H	-3.57146013	-2.53871450	0.11988061
O	-1.48455131	-0.31967878	0.48364384
O	-4.98552728	2.49927299	-1.84784373
H	0.30044655	2.15355491	-2.54891643
H	-1.85558580	0.41728854	1.00842729
H	-5.53794962	3.23517066	-2.09905056
H	-3.70792812	1.95412521	-2.86477328
O	-2.97475088	1.54541031	-3.36282129
H	-2.49593545	0.03105531	-2.56052406
H	-3.19440871	1.59753564	-4.28903689
O	-0.86050220	4.54689896	-0.96049105
H	-1.69439204	4.25587786	-0.55867235
H	0.49678752	4.15770133	-0.11157554
O	-3.17152417	3.53303293	0.14200794
H	-3.02188734	2.88032454	0.83843992
H	-3.80801245	3.15327464	-0.46812024
O	-2.17501198	-0.74836773	-2.08637854
H	-3.17285139	-2.01434857	-1.98139194
H	-1.93017144	-0.46964303	-1.18429128
O	-2.62787051	1.55868297	2.03296831
H	-3.37418624	1.05305992	2.39437907
H	-2.04633658	1.84273131	2.75702040
O	-6.38927967	-2.17147979	-1.49438429
H	-6.93880549	-2.54181701	-2.18018050
H	-6.52139974	-0.30397028	-1.25235450
O	-5.16658779	-3.22936987	2.89340336
H	-4.38998964	-3.08341597	2.34067678
H	-5.14816819	-2.50963544	3.52289223
O	-7.29928626	0.11207958	1.66704031
H	-7.41216783	-0.86140994	1.56544126
H	-8.05514055	0.45536152	2.13496893
O	-7.25498088	-2.47322872	1.22108889
H	-6.58309628	-2.87603242	1.79319728
H	-6.95168267	-2.55023876	0.31141328
O	-3.76508021	-2.77680316	-1.76054012
H	-5.47108548	-2.43631458	-1.67826053

H	-3.40374622	-3.55441759	-2.17734380
O	-4.64227195	-0.19489653	2.55681318
H	-5.54647617	0.05881096	2.34013898
H	-4.37888764	-0.85582220	1.90707781
H	-0.51943432	-0.27323610	0.57778385
O	-0.74182436	2.36405984	3.83890004
H	-0.79368820	3.24504255	4.19839931
O	1.33576876	3.78220144	0.24603820
H	1.40176404	2.77984993	1.60344298
H	2.01783015	4.47364395	0.25188588
O	5.49601613	-0.38678534	2.60239191
O	3.37730290	-2.76805591	-1.49612362
H	5.03830771	0.46408505	2.58093921
H	6.07151350	-0.45395234	1.83056662
H	2.62905594	-2.69592156	-2.10337625
H	3.02212515	-2.70182698	-0.59714867
O	1.75897778	1.64080793	-1.36852133
O	4.21186661	2.07344045	2.55378763
H	1.67215745	2.45301838	-0.83166533
H	2.65701845	1.65403373	-1.73130746
H	4.48729083	2.67296181	3.24319765
H	3.23252788	2.09709858	2.52920536
O	1.53298923	2.09510498	2.29390527
H	1.38890344	1.25242035	1.83579410
H	0.10880397	2.29529292	3.37651064
O	3.53914371	5.36281279	0.36141033
H	4.20773853	4.67127313	0.20190070
H	3.77486874	6.12867058	-0.15239752
O	5.11714977	3.20287431	0.10379240
H	4.92359897	2.64393199	-0.65736387
H	4.86275357	2.71739177	0.89594270
O	1.21175361	-0.08358274	0.62384069
H	1.74133791	-0.87868559	0.76097568
H	1.51157214	0.39714807	-0.17091112
O	4.40834522	1.61612798	-2.13633277
H	4.77973210	0.70678018	-2.03753109
H	4.70244870	1.95377205	-2.97814682
O	4.35077185	-2.69549354	2.88676603
H	4.26930661	-2.95308370	3.80111307
H	4.75494042	-1.79112779	2.86220265
O	5.02082528	-4.91561279	-1.05978570
H	4.42481593	-4.22865309	-1.39290700
H	5.48259443	-5.28765436	-1.80512052
O	6.99073511	-1.23077893	0.39918757
H	6.82442207	-2.17811901	0.61525205
H	7.93449327	-1.10710398	0.34402344
O	6.29629022	-3.67993735	1.04936018
H	5.90148676	-4.20422113	0.33714692
H	5.63481591	-3.58396265	1.74119674
O	2.38795754	-2.55664515	1.06921045
H	3.04185656	-2.65808169	1.78832235
H	1.66648406	-3.16043970	1.23653677
O	5.34070767	-0.79901447	-1.81101952
H	5.96849686	-0.91789987	-1.08578626
H	4.67746374	-1.49708735	-1.73320259

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C	-0.04777957	3.49757369	0.84250100
H	0.79082628	4.11754469	1.10851207
H	0.05738951	2.72951055	0.09871963
H	-1.03768071	3.81172829	1.11724055
C	0.64079605	1.47647739	3.09077543
H	0.32780419	2.26108891	2.33700486
O	1.77265041	1.95540622	3.64404733
H	-0.18647547	1.38115129	3.78865417
H	0.79444405	0.57383342	2.49880509
O	-0.77831889	-2.64674323	2.91091229

H	-1.52617307	-2.05094826	2.99690842
H	-1.25954524	-3.87716499	1.60302692
O	-6.78043536	-0.07677787	0.69630398
O	-3.24515853	2.63329510	-1.07063313
H	-5.81736252	-1.27046369	1.28610844
H	-6.99073992	-0.04455840	-0.24604289
H	-2.46408714	2.07179521	-0.95810986
H	-3.48500046	2.93544516	-0.18916041
O	-1.43369148	0.63085267	-0.49034200
O	-5.25488566	-1.99812210	1.63859346
H	-0.03645317	-2.16156557	2.53645497
H	-1.84108372	-0.06219093	-1.04737948
H	-5.83877312	-2.71857092	1.86237553
H	-3.97960858	-1.53818554	2.70574659
O	-3.23825211	-1.19659584	3.24080981
H	-2.63481676	0.31396232	2.50197290
H	-3.49669813	-1.2555326	4.15662146
O	-1.37522011	-4.35603053	0.77130875
H	-2.16466620	-3.98457945	0.34628661
H	0.03583075	-4.04264029	-0.00030710
O	-3.53450723	-3.11380612	-0.38834092
H	-3.26365501	-2.44385910	-1.02990240
H	-4.12708235	-2.68671313	0.23473365
O	-2.29197539	1.09404421	2.04562563
H	-3.26675342	2.35306845	1.91215619
H	-1.98281476	0.81028688	1.16718471
O	-2.65403668	-1.12426655	-2.12961811
H	-3.35434874	-0.57451237	-2.51823256
H	-2.06780926	-1.44313135	-2.83555010
O	-6.45957339	2.68889896	1.23886137
H	-7.01875873	3.08532836	1.90184835
H	-6.68007642	0.84008726	0.97458017
O	-4.90201968	3.73215253	-3.04678144
H	-4.16186172	3.57309293	-2.45076140
H	-4.88075628	2.98753387	-3.64750308
O	-7.26497829	0.49142759	-1.99159806
H	-7.34343187	1.46775232	-1.88763714
H	-7.99826339	0.18469915	-2.51732600
O	-7.13207488	3.07085439	-1.51803641
H	-6.40480120	3.44652916	-2.03831046
H	-6.88740735	3.12319694	-0.58922770
O	-3.82571285	3.13968648	1.67613773
H	-5.53612257	2.88432113	1.47617843
H	-3.51041164	3.88686885	2.17693173
O	-4.55683393	0.72011574	-2.72655454
H	-5.47799504	0.49209953	-2.55659996
H	-4.29311076	1.34130007	-2.03850115
H	-0.47474041	0.48923453	-0.52933473
O	-0.78441328	-2.03833321	-3.89775176
H	-0.89840183	-2.90552486	-4.27612625
O	0.92717112	-3.74532737	-0.30359496
H	1.17845220	-2.69514655	-1.58908380
H	1.51481173	-4.51852306	-0.34090085
O	5.73409107	-0.19268155	-2.29781138
O	3.96643671	2.15414498	1.94356023
H	5.15720043	-0.96710580	-2.34222732
H	6.32559577	-0.28224256	-1.54015785
H	3.25527993	2.06299123	2.59326385
H	3.55494335	2.23864764	1.07251456
O	1.51634171	-1.72728039	1.42087938
O	4.08450034	-2.41088504	-2.43234283
H	1.35720679	-2.50403873	0.84919198
H	2.39150405	-1.86831920	1.81237539
H	4.27568482	-3.01831472	-3.14300050
H	3.11490856	-2.26923602	-2.43102748
O	1.42991065	-2.01362668	-2.25028586
H	1.36465843	-1.17006272	-1.77769879
H	0.05006846	-2.05169963	-3.40237537

O	2.85739716	-5.64673359	-0.48873958
H	3.62323060	-5.08895150	-0.25713010
H	2.92770135	-6.46455054	-0.00653488
O	4.73132208	-3.78598934	-0.02434815
H	4.55494440	-3.25480934	0.76107495
H	4.57942202	-3.22645411	-0.79337260
O	1.25100259	0.13765303	-0.50216490
H	1.87868903	0.86939551	-0.53692178
H	1.44720893	-0.42714666	0.27017447
O	4.10751547	-2.22641594	2.25253413
H	4.69483343	-1.43374219	2.21332656
H	4.26230342	-2.65147319	3.09209736
O	4.91152854	2.25669413	-2.35108347
H	4.88677402	2.59313347	-3.24304065
H	5.18667591	1.304006342	-2.39920935
O	5.91383596	4.05831037	1.69222978
H	5.21653973	3.44466359	1.96702192
H	6.40495862	4.30777949	2.46926569
O	7.35924382	0.21885905	-0.07292691
H	7.33660339	1.19558479	-0.19846781
H	8.27315313	-0.04890485	-0.02912000
O	7.01794403	2.79386722	-0.49549040
H	6.70923624	3.31376028	0.26111466
H	6.33931928	2.84576304	-1.17505890
O	2.88273125	2.40618760	-0.61466015
H	3.59243864	2.38226005	-1.28910405
H	2.37857812	3.20137953	-0.77080090
O	5.60551923	-0.09834285	2.08241880
H	6.26453798	-0.05686672	1.37757816
H	5.08274855	0.71263076	2.03534549

### 3.2.6 CH3 + NH2

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p_Rc_ch3_nh2 W33			
N	-0.26240272	2.83940921	3.09700998
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C	-0.06198438	1.98892162	4.26587763
H	0.01453243	0.95636974	3.93951700
H	0.88114249	2.23125040	4.74313942
H	-0.85837164	2.06958651	5.00704773
H	-0.28151708	3.81078794	3.36173041
O	0.34449958	-3.91181668	-1.46930785
H	-0.27249415	-3.96282679	-0.73648908
H	-0.39739912	-3.43802433	-3.11240569
O	-5.62844447	-2.08743780	0.84293907
O	-2.72712613	1.57585942	1.70899900
H	-4.54319134	-2.93755810	-0.05872344
H	-6.11145431	-1.33279914	0.48245050
H	-2.14693243	1.22980683	1.00080244
H	-2.76630618	0.87253301	2.36647102
O	-1.31367908	0.30067177	-0.16248072
O	-3.89647032	-3.46703984	-0.57785199
H	0.89250414	-3.13000361	-1.32616705
H	-1.86171626	0.31689286	-0.97209676
H	-4.38739540	-4.16992478	-0.99700180
H	-2.43404234	-3.84535799	0.23762808
O	-1.57149282	-3.98060712	0.67669209
H	-0.92676149	-2.46244781	1.41007891
H	-1.60253451	-4.82221592	1.12326654
O	-0.68857844	-2.95510731	-3.89782827
H	-1.57493451	-2.62603626	-3.68668258
H	0.51921435	-1.81621024	-4.16700032
O	-3.14546885	-2.01787680	-2.99622906
H	-3.11640441	-1.06588452	-2.83926507
H	-3.36430660	-2.42715920	-2.15609080
O	-0.73045041	-1.55400822	1.68447846

H	-1.76839353	-1.05191939	2.89064261
H	-0.96584961	-0.98953357	0.92140087
O	-2.84952435	0.67308310	-2.33068357
H	-3.56178022	1.17108709	-1.90145092
H	-2.37145631	1.24991277	-2.94862271
O	-5.05245461	-1.22751655	3.48852887
H	-5.33380221	-1.76940773	4.22104811
H	-5.44004099	-1.87197604	1.76225766
O	-4.80206939	3.27016914	2.42297652
H	-3.99150802	2.84223184	2.12179545
H	-5.09597054	3.81906247	1.69968171
O	-6.92511744	0.31607293	0.23803743
H	-6.91090235	0.65155106	1.16252788
H	-7.81575372	0.38837219	-0.09352918
O	-6.52607937	1.10448292	2.71798451
H	-5.97189580	1.89874851	2.73193512
H	-6.03174308	0.39482739	3.13867301
O	-2.40665074	-0.61810735	3.50350825
H	-4.09445102	-1.08884214	3.57324871
H	-1.92681561	-0.37675464	4.29175363
O	-4.64169854	1.75480185	-0.56078991
H	-5.47889115	1.28940049	-0.45064634
H	-4.15429689	1.61590454	0.25413545
H	-0.41093543	0.55121932	-0.44401626
O	-1.26812803	2.16018212	-4.01739687
H	-1.43017461	2.11454034	-4.95537632
O	1.29349808	-1.21287334	-4.11054115
H	1.28542028	0.48622541	-3.79549562
H	1.98288116	-1.50668721	-4.72615838
O	5.10185325	2.31498771	-0.53729850
O	1.93436831	-0.60906308	2.29459371
H	4.69382474	2.03905142	-1.36691195
H	5.49569297	1.55291516	-0.09790505
H	1.09081963	-1.02956244	2.08397136
H	1.89279372	0.30753316	1.97260915
O	1.97296033	-1.63654789	-1.52574657
O	4.05031323	1.63646232	-3.07338307
H	1.81471346	-1.51537135	-2.48184326
H	2.86360459	-2.00172360	-1.42628957
H	4.46954863	2.16679532	-3.74682920
H	3.09619748	1.61544010	-3.28501015
O	1.35435308	1.40083469	-3.45848459
H	1.23283527	1.32326708	-2.49755528
H	-0.32260555	1.98433280	-3.88814057
O	3.59221532	-1.75405773	-5.45250733
H	4.22084117	-1.56246609	-4.73326163
H	3.91160866	-2.51347079	-5.92902880
O	5.09391833	-1.00101428	-3.33446543
H	5.01073530	-1.51307494	-2.52335711
H	4.76825032	-0.11219076	-3.15541725
O	1.19273685	0.82300994	-0.82102417
H	1.52954061	1.30953134	-0.05110484
H	1.61126198	-0.05572121	-0.88561657
O	4.50412305	-2.59222877	-1.06065238
H	4.51594642	-2.32244075	-0.11324555
H	4.63091376	-3.53632335	-1.09780033
O	3.98593215	3.65952587	1.40949425
H	4.01404815	4.60642437	1.30837487
H	4.41016901	3.25472563	0.61735626
O	3.12125176	0.30089607	4.59612527
H	2.64910712	-0.16626429	3.89063916
H	3.54355435	-0.36218256	5.13511644
O	6.08107529	0.50286345	1.38478508
H	5.77709871	1.02566008	2.16245566
H	7.01907372	0.36125345	1.48079497
O	5.04110368	1.91550765	3.34669164
H	4.34551069	1.44052225	3.82249388
H	4.63796965	2.65849768	2.88583266

O	1.79405303	2.00700374	1.51149077
H	2.52136421	2.64517167	1.51385098
H	1.04326976	2.40404559	2.01482635
O	4.40012757	-1.70676956	1.40424645
H	5.00439949	-0.95375917	1.45511383
H	3.52822699	-1.39413801	1.67684595

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N	-0.37593965	2.80601157	2.94370575
H	-1.28139653	2.43808257	2.64382004
C	0.24163967	-0.73182988	4.07160211
H	-0.11709305	-1.35170757	3.26756938
H	0.30329717	0.33477319	3.94356165
H	0.50109877	-1.16487536	5.02208747
H	-0.57208951	3.59352432	3.55521004
O	-0.04368691	-4.10196697	-1.30554083
H	-0.79367548	-4.10141148	-0.70709176
H	-0.61082130	-3.50890083	-2.95705388
O	-6.18221981	-1.78021887	0.47006484
O	-2.86271580	1.41594261	1.87178062
H	-5.20392582	-2.73709952	-0.47078791
H	-6.54658309	-0.95278747	0.13164677
H	-2.29367250	1.00562853	1.18639498
H	-3.05530554	0.70646860	2.49834418
O	-1.46423918	0.09641652	0.03102768
O	-4.65022065	-3.31649142	-1.03955557
H	0.58860121	-3.43881793	-1.00761824
H	-1.89432836	0.25482872	-0.83184528
H	-5.24876142	-3.86050307	-1.54539024
H	-3.27102283	-4.01545818	-0.25324460
O	-2.47234510	-4.27802012	0.24043553
H	-1.99746108	-2.88171154	1.26219428
H	-2.59822694	-5.17292525	0.54322003
O	-0.81069655	-2.99244253	-3.75045093
H	-1.68214545	-2.59520576	-3.60290282
H	0.48913568	-1.97094113	-3.82973743
O	-3.25042159	-1.83745435	-3.10632940
H	-3.15457440	-0.91109475	-2.85240771
H	-3.71163398	-2.27657779	-2.38798194
O	-1.75996952	-2.04234151	1.67699524
H	-2.66562336	-1.40773026	2.83335125
H	-1.63918737	-1.38914809	0.96693013
O	-2.78903575	0.76764065	-2.21278390
H	-3.48733774	1.29927155	-1.80253826
H	-2.25617063	1.33211949	-2.79782470
O	-5.84226727	-1.08651232	3.21487964
H	-6.27513964	-1.61042149	3.88376150
H	-6.06016294	-1.65004056	1.41636261
O	-4.85932620	3.34841461	2.24259526
H	-4.06829563	2.80583811	2.14677247
H	-5.00804836	3.71749957	1.37331634
O	-7.12856465	0.79696345	-0.08289404
H	-7.17828546	1.09154259	0.85538546
H	-7.95377554	1.00958314	-0.50966751
O	-6.89703658	1.44802199	2.45080354
H	-6.23388679	2.14973432	2.52714924
H	-6.54187209	0.65890322	2.87241130
O	-3.17475678	-0.86847019	3.49320773
H	-4.89114997	-1.06671118	3.42323689
H	-2.64527097	-0.83186179	4.28639209
O	-4.60009799	1.93080910	-0.51072743
H	-5.49370842	1.56662271	-0.52085470
H	-4.19563310	1.62412118	0.30374652
H	-0.51009695	0.26020953	-0.09033839
O	-1.06423566	2.18961612	-3.77065535
H	-1.14427600	2.12044385	-4.71773886
O	1.30565152	-1.43956070	-3.68126192

H	1.27780545	0.20391928	-3.31434994
H	1.97779946	-1.68562446	-4.33675250
O	5.10883181	2.78874174	-0.89463410
O	3.32369235	-0.10831884	3.07426659
H	4.70561876	2.37384396	-1.66869734
H	5.75236539	2.17963087	-0.51373444
H	2.63813005	-0.70702424	3.36807028
H	2.85915373	0.63860006	2.64520308
O	1.89703150	-2.01724179	-1.08212642
O	3.97867036	1.61187949	-3.14037900
H	1.77019425	-1.86646984	-2.03769897
H	2.82477619	-2.26229219	-0.96092826
H	4.19946353	2.03918002	-3.96433330
H	3.00603057	1.48836693	-3.13178479
O	1.34519876	1.12235263	-2.97459078
H	1.25464085	1.03470445	-2.01154467
H	-0.17243333	1.88151852	-3.53847510
O	3.51179492	-1.85254404	-5.21116186
H	4.17638187	-1.63009808	-4.53315315
H	3.80860091	-2.63122745	-5.67116931
O	5.08830027	-1.00626930	-3.19977998
H	4.98099591	-1.46457567	-2.35849362
H	4.77082065	-0.10409593	-3.08377370
O	1.16102949	0.45464157	-0.32075782
H	1.58575750	0.92746778	0.40998561
H	1.53485140	-0.44155720	-0.41917529
O	4.62530653	-2.40858858	-0.78129725
H	4.91572992	-1.90980250	0.01672255
H	5.01202976	-3.27838271	-0.72739009
O	3.83970821	3.84544091	1.11967455
H	3.63698182	4.76536070	0.97363085
H	4.26696999	3.50039160	0.29756395
O	4.98500441	1.29295072	4.77269685
H	4.40058975	0.68868229	4.29327776
H	5.59676687	0.76265706	5.27486085
O	6.77937848	1.31106535	0.79779169
H	6.56869410	1.90370351	1.55710880
H	7.72686125	1.29883124	0.69292938
O	5.96152090	2.88809126	2.73312575
H	5.64733324	2.41856710	3.51888196
H	5.21425440	3.36737188	2.35967733
O	2.06117150	1.90316118	1.83499751
H	2.62967779	2.65602117	1.60123786
H	1.25328573	2.25205431	2.25128015
O	5.35503737	-1.02855034	1.32955058
H	5.89773785	-0.25024392	1.14376151
H	4.65486839	-0.75336150	1.93251428

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N	-0.36114636	2.55133440	3.11830889
H	-1.27158785	2.30190666	2.72720791
C	0.20581843	-0.52648398	4.18818156
H	-0.14892253	-0.98633600	3.28156019
H	0.72125711	0.41551964	4.16021306
H	0.04695099	-1.01185908	5.13556471
H	-0.54614051	3.09100120	3.95923074
O	-0.01450614	-4.10429418	-1.26758659
H	-0.75245939	-4.08043369	-0.65462213
H	-0.59172077	-3.53232488	-2.92568614
O	-6.18342418	-1.78517811	0.45861422
O	-2.90716448	1.48655696	1.80268503
H	-5.16912517	-2.74734011	-0.43476925
H	-6.53876504	-0.96173056	0.10110078
H	-2.32606644	1.07667755	1.12784205
H	-3.12480599	0.77396569	2.41732803
O	-1.47303366	0.13832323	0.00676420
O	-4.59422721	-3.33324014	-0.97549992

H	0.63118442	-3.44264570	-0.99604552
H	-1.90220164	0.27135693	-0.86134570
H	-5.17361993	-3.90527121	-1.47271467
H	-3.20697984	-3.97971337	-0.16010780
O	-2.40540438	-4.22121887	0.33999657
H	-1.94662682	-2.79637719	1.33698824
H	-2.52199654	-5.11035922	0.66295806
O	-0.79552030	-3.02595892	-3.72451616
H	-1.66955274	-2.63264760	-3.58049197
H	0.49370840	-1.99430160	-3.82902614
O	-3.23946529	-1.88040951	-3.09095395
H	-3.14870231	-0.94764910	-2.85866173
H	-3.68398990	-2.30775522	-2.35520481
O	-1.73579868	-1.93821482	1.72726958
H	-2.68771487	-1.30561448	2.84296744
H	-1.63321163	-1.30570907	0.99535102
O	-2.79530490	0.74251929	-2.25252904
H	-3.49935041	1.27515220	-1.85127873
H	-2.26507061	1.30323269	-2.84306222
O	-5.89061770	-1.06376915	3.20006813
H	-6.31078869	-1.58812752	3.87653735
H	-6.08470269	-1.64340969	1.40591158
O	-4.89813901	3.37349717	2.29798600
H	-4.10345873	2.85937288	2.11220672
H	-5.05399613	3.89783810	1.51533195
O	-7.12713997	0.78373147	-0.14095705
H	-7.18386321	1.08999898	0.79289211
H	-7.95237598	0.98408461	-0.57355903
O	-6.92973941	1.46063171	2.38985184
H	-6.26726546	2.16025557	2.48648624
H	-6.59316668	0.67277021	2.82851420
O	-3.23196017	-0.76343285	3.47251096
H	-4.94002476	-1.01775751	3.40621756
H	-2.71634702	-0.66184327	4.26887750
O	-4.61499838	1.94657359	-0.60413996
H	-5.50624067	1.57753673	-0.59414110
H	-4.21767081	1.71000365	0.23663122
H	-0.51657211	0.28302396	-0.11905054
O	-1.06832356	2.15752590	-3.81903035
H	-1.13821486	2.07092295	-4.76548431
O	1.30708179	-1.45425385	-3.69416191
H	1.27708959	0.19050425	-3.32659321
H	1.97179359	-1.69342858	-4.35964700
O	5.05271515	2.79867013	-0.87456165
O	3.38987833	-0.21993018	3.03699714
H	4.66349635	2.38874708	-1.65840899
H	5.72168970	2.20619733	-0.51190360
H	2.74032450	-0.86045497	3.32062329
H	2.89037541	0.51712332	2.63006862
O	1.93158667	-2.02531764	-1.10514283
O	3.96441451	1.64142796	-3.15255079
H	1.79254174	-1.87664566	-2.05959032
H	2.86458964	-2.25510218	-0.99474998
H	4.17648789	2.09845400	-3.96271111
H	2.99399025	1.50009378	-3.14711523
O	1.34115864	1.11006294	-2.98952883
H	1.25243583	1.02527360	-2.02624409
H	-0.17782550	1.85779531	-3.57243030
O	3.49586377	-1.83425805	-5.25616597
H	4.16701500	-1.59873186	-4.58908112
H	3.80217640	-2.60455996	-5.72394442
O	5.09180043	-0.96676853	-3.26888064
H	4.99775542	-1.43077779	-2.42913216
H	4.77208552	-0.06679422	-3.14205672
O	1.16284268	0.43539478	-0.33619557
H	1.57808201	0.88783332	0.41275221
H	1.53511106	-0.46057971	-0.44341121
O	4.67065789	-2.38990358	-0.85493873



H	4.97920080	-1.90016261	-0.05820601
H	5.06135523	-3.25897712	-0.82119335
O	3.77492917	3.78583061	1.17052269
H	3.54159829	4.70084211	1.03991942
H	4.20037433	3.46508746	0.33788749
O	4.99559170	1.21582618	4.76369363
H	4.43956820	0.59488208	4.27256235
H	5.61580966	0.70417883	5.27477336
O	6.79287040	1.34996705	0.77373439
H	6.56807289	1.91904696	1.54669397
H	7.73940736	1.37208038	0.66224891
O	5.93713947	2.86199616	2.74579541
H	5.63750068	2.37225070	3.52461778
H	5.17615978	3.32857346	2.38391633
O	2.05273966	1.79313821	1.88001869
H	2.60205850	2.56340981	1.65671045
H	1.24451664	2.11291655	2.32027504
O	5.43813602	-1.03911938	1.26171901
H	5.96150859	-0.24545594	1.08572580
H	4.73856250	-0.79046888	1.87646596

### 3.2.7 HCO + CH2OH

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C	4.00541901	0.84980205	-1.14869404
O	3.66361769	1.24011393	0.11278561
H	3.49057962	1.29255326	-1.98239614
H	5.00876137	0.47568031	-1.22431801
H	2.81033897	1.67888505	0.13005297
O	1.11305728	2.67873057	2.48796835
C	1.00511402	2.56790693	1.32512713
H	0.11338511	2.80377813	0.70951121
O	-3.90279424	1.33526663	1.02569324
H	-3.65061857	1.97296580	0.35494473
H	-4.60801842	-0.10765791	0.09064397
O	-2.62971013	3.17446338	-5.52063816
O	1.59549091	1.76015597	-3.49689417
H	-3.61846493	2.67912189	-4.30410913
H	-2.25497961	2.53793687	-6.14359618
H	1.21546805	1.25218353	-2.76130854
H	1.33964083	2.67669834	-3.34696699
O	0.10917048	0.55973356	-1.53878486
O	-4.22210629	2.38207353	-3.58497402
H	-3.10717897	1.00202015	1.45393354
H	-0.39233611	-0.08609344	-2.08083444
H	-5.10937946	2.41184293	-3.93406948
H	-3.87201224	2.94295078	-1.99517425
O	-3.55376996	3.23881961	-1.12080718
H	-1.79751394	3.15280616	-1.09021215
H	-4.04709634	4.01991979	-0.88511580
O	-4.73221854	-0.94541591	-0.37535549
H	-4.47312768	-0.78816227	-1.29687712
H	-3.71856893	-1.93544054	0.45528846
O	-3.82882176	-0.39775060	-2.91684205
H	-2.91277521	-0.66882872	-3.06314618
H	-3.90122528	0.51911131	-3.19123744
O	-0.83634702	3.02781203	-1.08752652
H	0.03415875	3.94729381	-2.12374751
H	-0.65050053	2.08809556	-1.28029520
O	-1.14997311	-1.10659554	-3.20011810
H	-0.73124980	-0.86014218	-4.04324694
H	-0.97752225	-2.04592975	-3.01939920
O	-0.43062475	4.94881341	-5.20912429
H	-0.54295038	5.88324529	-5.36236667
H	-1.95211564	3.84582631	-5.38867835
O	2.97046302	1.90482296	-5.88999591

H	2.65807222	1.71647346	-4.99659359
H	3.15747603	1.06220353	-6.29561659
O	-1.13419084	1.57962711	-7.25784355
H	-0.37138419	2.19630155	-7.34043836
H	-1.39379415	1.30558667	-8.13291998
O	0.87477709	3.26512628	-7.11211434
H	1.67064911	2.85736153	-6.73942968
H	0.57775886	3.94284387	-6.49761244
O	0.64166579	4.34923533	-2.79061573
H	-0.05292845	4.83645418	-4.32036329
H	1.25466306	4.91416059	-2.32756014
O	0.13535184	0.01546200	-5.29195416
H	-0.36587000	0.41978141	-6.00886907
H	0.59177836	0.72908996	-4.83741528
H	0.33132414	0.11738771	-0.70247935
O	-0.69464248	-3.65949591	-2.37253785
H	-1.35165290	-4.32560700	-2.55358031
O	-3.05648163	-2.36399378	1.04814974
H	-1.55694327	-2.88355764	0.51434693
H	-3.51227793	-3.01134554	1.61135969
O	2.34243716	-4.32562472	3.76888401
O	2.57771812	0.91467076	4.31976344
H	1.49279739	-4.44043356	3.32347630
H	2.18010264	-3.97669540	4.65399732
H	2.16465101	1.71087025	3.98636522
H	2.74942356	0.36559320	3.53222257
O	-1.80705123	-0.24089158	2.20958500
O	-0.10257154	-4.63381611	2.50680165
H	-2.30088853	-1.01721652	1.88292105
H	-1.75526253	-0.34363672	3.17102685
H	-0.37875510	-5.53254836	2.34386786
H	-0.25866112	-4.13303470	1.67995074
O	-0.62708787	-3.14082977	0.32909910
H	-0.11214494	-2.32686650	0.43510280
H	-0.63611271	-3.57161025	-1.40733954
O	-3.97205549	-4.20552621	2.82215330
H	-3.32620325	-4.03224198	3.53251852
H	-4.83698748	-4.26675681	3.21512287
O	-1.92114908	-3.63800697	4.45047765
H	-1.79507452	-2.70022761	4.63662269
H	-1.20583065	-3.91725227	3.86886488
O	0.49903677	-0.63665854	0.87317592
H	1.32276125	-0.68062241	1.38063979
H	-0.24611882	-0.42098164	1.46664082
O	-1.56532888	-0.86514852	4.90445559
H	-0.65713811	-0.77345173	5.27913682
H	-2.16793273	-0.48896968	5.54074479
O	4.25594310	-2.87217947	2.77368015
H	4.84641431	-3.37511520	2.21944999
H	3.53581648	-3.48028448	3.07514156
O	4.95440449	0.62985210	5.66433444
H	4.12042979	0.90401005	5.25645090
H	5.03627431	1.08817941	6.49516971
O	2.40154251	-2.96727568	6.21146297
H	3.31771761	-2.65209251	6.02894418
H	2.41626099	-3.43373666	7.04282285
O	4.77296555	-2.11432943	5.46511350
H	4.94445666	-1.16760319	5.57267035
H	4.83189329	-2.31614061	4.52571901
O	2.98292705	-0.57450263	2.09101599
H	3.47945515	-1.39645903	2.24989267
H	3.45042559	-0.05588286	1.42472364
O	0.85611349	-0.65977859	5.87454170
H	1.33502744	-1.48011804	6.05319399
H	1.45641751	-0.08357129	5.38502360

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C	-0.68036758	3.25873616	2.79736692
O	-0.18028646	1.98046259	2.45714892
H	-0.20955940	3.55267884	3.72814248
H	-0.44088253	3.99485580	2.03258012
H	-0.60085619	1.66265614	1.64977533
O	0.26665420	-1.01720093	3.80519255
C	-0.78819795	-0.68739150	4.01171571
H	-1.75714373	3.22847330	2.93821806
O	-0.35021089	-4.03489465	-1.70901311
H	-1.09835368	-3.89863035	-1.12292531
H	-0.69746850	-3.23360657	-3.33625378
O	-6.52004621	-1.22626303	-0.48879793
O	-3.53894577	1.65304634	1.48799438
H	-5.38035952	-2.13347630	-1.25907240
H	-6.78213657	-0.37902953	-0.87173830
H	-2.68088336	1.38669214	1.14621215
H	-3.79865481	0.94828159	2.09575711
O	-1.20528404	0.62936468	0.20820559
O	-4.71235235	-2.67336033	-1.73946554
H	0.39726622	-3.53411493	-1.36402029
H	-1.58611937	0.89356331	-0.65730225
H	-5.18375834	-3.18773669	-2.39016963
H	-3.49106501	-3.41966841	-0.77692564
O	-2.77454379	-3.73551466	-0.19476871
H	-2.36502649	-2.40202943	0.93122685
H	-3.03520613	-4.58878767	0.14163284
O	-0.76198822	-2.62514193	-4.08609299
H	-1.53485946	-2.06743788	-3.91080812
H	0.68289227	-1.82533941	-4.03537547
O	-2.93091917	-1.07383512	-3.35041174
H	-2.73274882	-0.22132609	-2.94424839
H	-3.54361641	-1.53204571	-2.77020161
O	-2.19218482	-1.63253039	1.49089426
H	-3.34515407	-1.09019488	2.48641880
H	-1.83871230	-0.92815935	0.92845484
O	-2.31562138	1.36976192	-2.10421182
H	-3.12304323	1.87325886	-1.91415841
H	-1.70905794	1.90257293	-2.64642341
O	-6.57530265	-0.59332783	2.28765851
H	-7.16969235	-1.08261909	2.85046605
H	-6.53790375	-1.10581871	0.46669918
O	-5.30234281	3.84755672	1.52721783
H	-4.55222635	3.27237249	1.70656118
H	-5.21532157	4.05334039	0.59601061
O	-7.21038311	1.38645801	-1.18914763
H	-7.40296530	1.67693577	-0.26843965
H	-7.94614050	1.63390916	-1.74207731
O	-7.38596771	1.99724627	1.36278795
H	-6.73927360	2.69087385	1.56219023
H	-7.12004467	1.20132292	1.83340418
O	-3.98753964	-0.60073994	3.05841595
H	-5.68284584	-0.66732458	2.66745601
H	-3.57785423	-0.52029996	3.91669696
O	-4.59366782	2.40830607	-1.02691429
H	-5.45940170	2.08695540	-1.30363509
H	-4.41376701	1.99374651	-0.17575961
H	-0.27486979	0.38272665	0.02693971
O	-0.34948162	2.60391020	-3.51455778
H	-0.40777728	2.66041159	-4.46407074
O	1.54848348	-1.41749517	-3.79780546
H	1.65450602	0.17570486	-3.25499046
H	2.22552830	-1.67410710	-4.44388034
O	5.61051528	2.10563045	-0.41314377
O	3.32936688	-0.93810379	3.27790668
H	5.20593649	1.80520583	-1.23740579
H	6.15467826	1.39307735	-0.05700790
H	2.57654978	-1.47371102	3.51720951
H	2.96337788	-0.13110201	2.86190243

O	1.87999063	-2.33362441	-1.25876770
O	4.47319059	1.24675811	-2.79736875
H	1.85166579	-2.07340574	-2.19915424
H	2.76899300	-2.67569230	-1.08802718
H	4.78225130	1.70888383	-3.57277116
H	3.49453073	1.23243536	-2.84174657
O	1.79311437	1.03323134	-2.79772333
H	1.63487670	0.83724766	-1.86016254
H	0.45584522	2.09959410	-3.30946546
O	3.79523335	-1.92706277	-5.23167238
H	4.42401385	-1.85162676	-4.49026012
H	4.05238772	-2.67418574	-5.76240356
O	5.29092268	-1.46672439	-3.04100395
H	5.08070046	-1.98246286	-2.25425261
H	5.06900505	-0.54773782	-2.85593985
O	1.36524840	0.08888417	-0.24586439
H	1.89274630	0.40697602	0.50150797
H	1.60084201	-0.83610196	-0.45857677
O	4.52035776	-3.01121211	-0.79055782
H	4.80989885	-2.61282935	0.06279566
H	4.82032847	-3.91628577	-0.79411599
O	4.33615158	3.10036123	1.63091804
H	4.23042682	4.04593325	1.57380546
H	4.77725081	2.79688300	0.80011593
O	5.04254605	0.18953405	5.12282322
H	4.42197181	-0.32111141	4.58359446
H	5.55374699	-0.42817281	5.63717221
O	6.98577440	0.28628283	1.20929064
H	6.80816663	0.83584942	2.00890597
H	7.92899292	0.16258267	1.14612358
O	6.26912504	1.79077939	3.23695341
H	5.87796973	1.30583273	3.97774760
H	5.59290843	2.37675583	2.88100509
O	2.38980440	1.23020189	2.03169364
H	3.01628334	1.96375355	1.91903499
H	1.52801031	1.59488290	2.29582644
O	5.27914050	-1.90620043	1.46450223
H	5.91185421	-1.18029819	1.37644076
H	4.60536754	-1.62725765	2.09518484

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C	-1.15776681	1.73109365	3.66288373
O	-0.36268852	1.18974411	2.70781420
H	-0.68282415	1.81916606	4.62290126
H	-1.92076677	2.42445116	3.34922600
H	-0.79012843	1.16822630	1.83997406
O	1.09908779	-1.97827942	3.75629814
C	0.59635862	-1.71942860	2.72386791
H	-0.47679683	-1.79472021	2.46716464
O	-0.43614476	-4.07334271	-1.45037027
H	-1.21254919	-3.85684202	-0.92994724
H	-0.72188698	-3.40462091	-3.15679878
O	-6.57658915	-1.02178411	-0.53212875
O	-3.44144528	2.27702650	1.14560524
H	-5.51514190	-2.03212416	-1.28039577
H	-6.80470264	-0.17811570	-0.94453213
H	-2.59186213	2.07349164	0.74963234
H	-3.67916563	1.49957652	1.67204845
O	-1.20089723	0.71501348	0.11171324
O	-4.88691454	-2.63684383	-1.73737833
H	0.30752149	-3.55547116	-1.12278813
H	-1.61663518	0.91143115	-0.75971872
H	-5.39727247	-3.16814965	-2.34331680
H	-3.67361431	-3.34362501	-0.74277459
O	-2.96801703	-3.61918752	-0.12712772
H	-2.52773712	-2.23415165	0.87163327
H	-3.23599830	-4.44751654	0.26201815

O	-0.77166923	-2.84643326	-3.94517801
H	-1.54730255	-2.27944821	-3.81919376
H	0.67741052	-2.04474274	-3.91762251
O	-2.94211655	-1.24295326	-3.34919970
H	-2.75215667	-0.37208171	-2.97883628
H	-3.62431234	-1.64250769	-2.80473057
O	-2.25787694	-1.45536400	1.38150935
H	-3.33239851	-0.61572181	2.27367360
H	-1.88669485	-0.79887819	0.76923995
O	-2.34069188	1.25402982	-2.21998207
H	-3.15249364	1.78180034	-2.11230420
H	-1.72410877	1.72335684	-2.80889721
O	-6.53850684	-0.25267906	2.21737508
H	-7.03824257	-0.73225597	2.87274453
H	-6.57711148	-0.86596692	0.41798043
O	-5.36529542	4.10421679	1.89089755
H	-4.54524727	3.67401655	1.62183743
H	-5.36455398	4.98014651	1.51548125
O	-7.18860396	1.58177000	-1.33705831
H	-7.34420012	1.92404680	-0.42793267
H	-7.93752725	1.82077573	-1.87592397
O	-7.34692244	2.27999451	1.19402754
H	-6.73516307	2.97085844	1.48486687
H	-7.14043752	1.48316186	1.69250317
O	-3.90073530	0.04077266	2.74380201
H	-5.61780474	-0.19991210	2.52596511
H	-3.45509613	0.25075982	3.56354724
O	-4.55912341	2.57822885	-1.46403782
H	-5.45460064	2.25928383	-1.62067295
H	-4.40833950	2.50389383	-0.51773405
H	-0.26107445	0.51085991	-0.07842534
O	-0.37780302	2.34764621	-3.74185778
H	-0.44265782	2.30115633	-4.69152997
O	1.54039412	-1.62846877	-3.68786121
H	1.65920121	0.00026010	-3.26705620
H	2.22567381	-1.92064117	-4.31028139
O	5.38737894	2.28510340	-0.50264791
O	3.71713847	-0.74909695	3.46953003
H	5.04484295	1.92688790	-1.33176189
H	6.01630988	1.65279117	-0.13379436
H	3.03020378	-1.35492435	3.75421327
H	3.24936173	-0.04544735	2.98543282
O	1.81061374	-2.36449362	-1.08321272
O	4.45109939	1.22580199	-2.89603303
H	1.80112349	-2.17690634	-2.04107537
H	2.71019114	-2.65018024	-0.86786324
H	4.75940211	1.66780326	-3.68319968
H	3.47546197	1.16236064	-2.96148637
O	1.79168818	0.89537981	-2.88630076
H	1.65627062	0.77874699	-1.93226654
H	0.43764623	1.88268290	-3.48946555
O	3.79472968	-2.18366257	-5.08534827
H	4.42204832	-2.01661687	-4.35716009
H	4.08124830	-2.96386707	-5.54918500
O	5.27619753	-1.49756995	-2.94951821
H	5.04634115	-1.94778246	-2.12829649
H	5.06774895	-0.56363359	-2.83884467
O	1.37397581	0.15128988	-0.27181259
H	1.87378026	0.44547047	0.50371084
H	1.55127524	-0.79910014	-0.42237213
O	4.49524417	-2.87881632	-0.59875069
H	4.86109720	-2.41997170	0.19379448
H	4.82343219	-3.77392117	-0.57263291
O	4.05574657	3.24076027	1.52803116
H	3.86575204	4.16960519	1.42922100
H	4.49927984	2.93708828	0.69877474
O	5.25470038	0.73645726	5.17966595
H	4.70704802	0.09811733	4.69781740

H	5.81442348	0.24789010	5.77554603
O	7.00032897	0.67711653	1.11271783
H	6.79712384	1.24314394	1.89402178
H	7.94841576	0.64504701	1.01811665
O	6.22177340	2.23279181	3.08278563
H	5.93454104	1.78507518	3.89208669
H	5.46729520	2.72019823	2.73694468
O	2.38104181	1.17958177	2.07979901
H	2.87404148	2.00647513	1.94332672
H	1.51547380	1.37807304	2.45228959
O	5.49376956	-1.65348674	1.49313246
H	6.07019805	-0.89435807	1.33492383
H	4.89696702	-1.40852021	2.21135336

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C	3.73961230	1.88905068	-0.92770224
O	2.70735196	1.38619734	-0.20339878
H	3.62329464	1.99269011	-1.99098778
H	4.46599939	2.43306459	-0.35570593
H	2.02279086	1.00047123	-0.76662206
O	1.36376553	3.18644559	2.70502595
C	0.77983637	2.57807946	1.88403141
H	0.36444488	2.96819922	0.93609280
O	-3.94918352	1.30999200	1.05719506
H	-3.57564963	1.92560158	0.42325472
H	-4.65452734	-0.11434584	0.09822119
O	-2.46986644	3.23142967	-5.41221432
O	1.73200432	1.45554942	-3.72152162
H	-3.43007322	2.73131184	-4.17683814
H	-2.16157449	2.59694245	-6.07262676
H	1.47823293	0.89882331	-2.98257000
H	1.49498657	2.35907335	-3.46984879
O	0.40431838	0.35190119	-1.35113754
O	-4.00814916	2.43067062	-3.43849003
H	-3.22885261	0.91294328	1.55952785
H	-0.09465436	-0.19037041	-2.00589524
H	-4.91051976	2.49947690	-3.74017626
H	-3.56364283	2.94984048	-1.86030651
O	-3.20259482	3.21111965	-0.99158281
H	-1.44694077	3.04747040	-1.00342479
H	-3.62420651	4.02960199	-0.74289254
O	-4.78740164	-0.94431380	-0.38030117
H	-4.43365524	-0.79674552	-1.27040591
H	-3.91631664	-2.02822923	0.51953394
O	-3.63208931	-0.35884797	-2.82009581
H	-2.71089012	-0.61849745	-2.94561075
H	-3.70735994	0.56107722	-3.08395275
O	-0.48799444	2.90399434	-1.01265885
H	0.41771028	3.68405502	-2.10140500
H	-0.32533896	1.95238703	-1.13248680
O	-0.93806429	-1.08091727	-3.12839425
H	-0.63685869	-0.88491602	-4.03380320
H	-0.85707190	-2.03576504	-2.95770099
O	-0.14751843	4.85086526	-5.09991125
H	-0.20721652	5.79855004	-5.18740199
H	-1.74369942	3.84822378	-5.27330090
O	3.12915221	1.87176307	-6.06421955
H	2.82450933	1.54037328	-5.21172776
H	3.52780711	1.14048534	-6.52746610
O	-1.17502564	1.59195718	-7.26707276
H	-0.37796597	2.16157021	-7.35481156
H	-1.49606253	1.39266374	-8.14204357
O	0.92236359	3.17569153	-7.14583751
H	1.74506532	2.76143630	-6.84926704
H	0.69200359	3.85276852	-6.50239637
O	1.03558392	4.00053454	-2.80689447
H	0.28372620	4.65755149	-4.25047730

H	1.76706505	4.43467674	-2.37408528
O	0.07737361	-0.13568005	-5.43351832
H	-0.45527542	0.29676281	-6.10993349
H	0.63505866	0.54672333	-5.05069384
H	0.29783221	-0.11193424	-0.49315532
O	-0.76830373	-3.66569778	-2.32196430
H	-1.43963358	-4.28163218	-2.60157263
O	-3.29717014	-2.49097743	1.13041090
H	-1.80916068	-3.07969220	0.59581531
H	-3.78824725	-3.11033202	1.69400219
O	2.36423525	-4.14765538	3.49313232
O	2.49222282	1.06538836	4.35260984
H	1.49020519	-4.36608385	3.14472379
H	2.26271377	-3.84365836	4.40342980
H	2.13087433	1.91548433	4.09491595
H	2.59153678	0.56860693	3.52027108
O	-2.06419359	-0.38928073	2.33819187
O	-0.16346567	-4.78751235	2.53375963
H	-2.55930135	-1.16369007	2.00957731
H	-1.95672849	-0.51547303	3.29207576
H	-0.31886007	-5.71858852	2.39574263
H	-0.42292734	-4.32495364	1.70983095
O	-0.87990424	-3.32890260	0.40118644
H	-0.36909361	-2.51988261	0.56525869
H	-0.79885043	-3.63305120	-1.35091695
O	-4.19629332	-4.27129376	2.96530408
H	-3.47862954	-4.13563013	3.61207749
H	-5.01724354	-4.33229604	3.44308213
O	-2.01220733	-3.80784715	4.46139789
H	-1.84166605	-2.88222074	4.67121725
H	-1.30202121	-4.11233282	3.88609121
O	0.21020912	-0.87438947	1.00611994
H	1.03269537	-0.74757365	1.50245007
H	-0.54314259	-0.58593169	1.55946277
O	-1.60837981	-1.05122383	4.99339740
H	-0.68110717	-0.90378213	5.29576603
H	-2.17736853	-0.72026240	5.68353219
O	4.15217304	-2.57915638	2.41853805
H	4.72075495	-3.03852660	1.80671320
H	3.46956169	-3.22070642	2.73283893
O	4.98111597	0.75762383	5.45301447
H	4.10039766	1.01131259	5.13733478
H	5.11584328	1.17041470	6.30065861
O	2.56001324	-2.89876983	5.98479789
H	3.45316048	-2.55306626	5.74960758
H	2.64624968	-3.39282193	6.79556403
O	4.85641967	-1.96960816	5.10931050
H	5.01585306	-1.02592898	5.25740749
H	4.84214799	-2.11602440	4.15801063
O	2.70806857	-0.31545668	2.01775017
H	3.30123571	-1.08522302	2.05051169
H	2.95102833	0.24409227	1.27114273
O	0.85370132	-0.68484291	5.81238682
H	1.40496536	-1.46940976	5.93235537
H	1.39587353	-0.02591714	5.36074253

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C	0.27637425	-0.60553420	-0.17914309
O	0.19249760	-0.42882988	1.12917992
H	0.51820831	0.23476907	-0.80995721
H	-0.01763871	-1.55310161	-0.60041566
H	-0.70200469	-0.00243061	1.50071798
O	-2.17264659	0.61415702	3.31363242
C	-2.04474268	0.51232804	2.14853098
H	-2.80875544	0.75031755	1.37898164
O	-6.92657568	-0.64432287	1.75944368
H	-6.62000522	-0.01817249	1.10033977

H	-7.70092772	-2.05847798	0.83347421
O	-5.77052060	1.18927473	-4.80138205
O	-1.56891322	-0.46377242	-3.05104817
H	-6.69819446	0.73377684	-3.52549975
H	-5.46820189	0.53479021	-5.44497087
H	-1.86203343	-0.94171098	-2.26115261
H	-1.73487991	0.46736076	-2.86951834
O	-2.95470145	-1.57429799	-0.93167117
O	-7.26691753	0.46266623	-2.76826181
H	-6.16148171	-1.02769649	2.20156842
H	-3.52075548	-2.18752246	-1.44665710
H	-8.17296377	0.54666315	-3.05485481
H	-6.78493870	0.99268852	-1.20559419
O	-6.40815462	1.26671853	-0.34709191
H	-4.65253165	1.11260498	-0.39886798
H	-6.84776596	2.07199006	-0.08717891
O	-7.86667889	-2.88992492	0.36888523
H	-7.63237230	-2.73588860	-0.56002701
H	-6.87380888	-3.93654062	1.15215775
O	-7.01907034	-2.35583264	-2.19096137
H	-6.11897925	-2.67080856	-2.34901157
H	-7.04060885	-1.42765922	-2.43446049
O	-3.69762857	0.94849270	-0.43917604
H	-2.84915366	1.81501588	-1.54108253
H	-3.56608326	0.00152041	-0.64687512
O	-4.38003875	-3.17260220	-2.53034368
H	-4.01002314	-2.94125789	-3.40105894
H	-4.21900889	-4.11473463	-2.35653256
O	-3.46198915	2.83606146	-4.60240995
H	-3.53371634	3.77532863	-4.75029978
H	-5.04734950	1.81745961	-4.70301142
O	-0.24697167	-0.33244015	-5.46324163
H	-0.53932751	-0.53923016	-4.56668383
H	-0.05357138	-1.16382196	-5.88798265
O	-4.47238042	-0.48442822	-6.61866917
H	-3.67753719	0.08342976	-6.73816147
H	-4.79358232	-0.73442706	-7.48036656
O	-2.36408864	1.08460199	-6.57682285
H	-1.56592233	0.64267451	-6.25095022
H	-2.59051228	1.77697438	-5.94884569
O	-2.27047577	2.18079811	-2.25261999
H	-3.03751256	2.70282261	-3.73815820
H	-1.59256709	2.70761887	-1.83783288
O	-3.20199074	-2.12647969	-4.71419260
H	-3.72005706	-1.70187212	-5.40646729
H	-2.68426297	-1.43376479	-4.29243533
H	-2.77565551	-1.99410660	-0.07490564
O	-3.91047082	-5.72763601	-1.70473288
H	-4.56856819	-6.39869458	-1.86203769
O	-6.21521207	-4.40206440	1.72107949
H	-4.71711558	-4.92032178	1.18305649
H	-6.67657488	-5.06371135	2.26266768
O	-0.73497945	-6.31864362	4.36642699
O	-0.71438793	-1.15992607	5.13952673
H	-1.58209168	-6.44990102	3.92086721
H	-0.90623989	-6.02269149	5.26906150
H	-1.16585979	-0.37704151	4.82319712
H	-0.51807489	-1.68360473	4.34145817
O	-4.93156591	-2.33396746	2.93134304
O	-3.18227545	-6.70329566	3.12046738
H	-5.43985103	-3.09377537	2.58804705
H	-4.87531924	-2.46492290	3.88908777
H	-3.39844243	-7.61343960	2.93233742
H	-3.37664837	-6.18989796	2.30947006
O	-3.78858164	-5.17732280	0.98986177
H	-3.27084797	-4.36605544	1.10017570
H	-3.83200768	-5.62526548	-0.74260723
O	-7.12569289	-6.30475791	3.42917323



H	-6.46678506	-6.16923323	4.13586476
H	-7.98339610	-6.38589821	3.83412250
O	-5.05887193	-5.81466615	5.06411563
H	-4.94086314	-4.88194858	5.27929085
H	-4.33301818	-6.07234672	4.48567616
O	-2.64788068	-2.67785063	1.54987646
H	-1.83301731	-2.71661031	2.07154291
H	-3.39941701	-2.47510507	2.14118220
O	-4.73645581	-3.05499744	5.60737755
H	-3.84499035	-2.96611959	6.02094466
H	-5.36802908	-2.70404126	6.22992571
O	1.16590126	-4.79126495	3.45690124
H	1.78613082	-5.26414404	2.90879568
H	0.45327999	-5.42448940	3.72135856
O	1.67316502	-1.37366016	6.48108557
H	0.82796129	-1.12353197	6.08151797
H	1.73415783	-0.94094429	7.32733783
O	-0.72021916	-5.10155936	6.88221113
H	0.18173067	-4.73928344	6.71802025
H	-0.68446071	-5.61369219	7.68558720
O	1.61453014	-4.11490601	6.18402793
H	1.74392417	-3.16632219	6.32770765
H	1.69077005	-4.27920853	5.23863986
O	-0.21264104	-2.54022022	2.84884404
H	0.34784902	-3.32630328	2.97116954
H	0.21833302	-1.92935861	2.23885779
O	-2.35366342	-2.83942845	6.66603354
H	-1.84930181	-3.65174375	6.80662296
H	-1.77508460	-2.22833041	6.19301908

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C	-1.04509924	1.67881575	3.67265313
O	-0.16470585	1.67664719	2.64593290
H	-0.60019176	1.88458325	4.62938765
H	-2.05972530	1.97263581	3.46022768
H	-0.60496730	1.51192825	1.79583204
O	1.04878528	-1.50324694	4.00778863
C	0.29877009	-1.14733661	3.17691110
H	-0.74773512	-0.81574784	3.33264076
O	-0.43156501	-3.98292259	-1.40015768
H	-1.17058540	-3.75037181	-0.83404658
H	-0.73996086	-3.31116994	-3.09638656
O	-6.66074763	-1.08549175	-0.79734770
O	-3.66500089	2.09632830	1.34101262
H	-5.46722061	-2.05568797	-1.37381242
H	-6.83033561	-0.23071035	-1.21463107
H	-2.79300361	1.86228019	1.01963691
H	-3.97349817	1.34420657	1.86543974
O	-1.20349294	0.73437643	0.30832606
O	-4.75216288	-2.63052220	-1.73141930
H	0.34710275	-3.50297288	-1.09655294
H	-1.58824293	0.98616243	-0.56341036
H	-5.14910323	-3.19973807	-2.38614801
H	-3.58412863	-3.26006787	-0.62937078
O	-2.90332439	-3.51908762	0.02030634
H	-2.58240299	-2.15024573	1.10372297
H	-3.14915614	-4.37394346	0.36422772
O	-0.78556499	-2.76547470	-3.89407782
H	-1.53003504	-2.15962048	-3.75920020
H	0.67971518	-2.00133429	-3.89773195
O	-2.88159102	-1.08156458	-3.27387554
H	-2.67541048	-0.23535193	-2.85795358
H	-3.53631624	-1.51906841	-2.72446619
O	-2.43163299	-1.34910364	1.62708403
H	-3.65961669	-0.70040589	2.40970319
H	-1.98795307	-0.70229760	1.05529695
O	-2.26592736	1.36576313	-2.03536157

H	-3.08894344	1.87842154	-1.94137934
H	-1.64933242	1.84293848	-2.61786651
O	-6.90990395	-0.40991644	1.95101531
H	-7.47654151	-0.91738995	2.52596651
H	-6.77398295	-0.94819622	0.14900847
O	-5.63912051	3.95934221	1.87427776
H	-4.79438069	3.52711435	1.70609580
H	-5.59598862	4.82557571	1.47890056
O	-7.15892917	1.55631637	-1.56998409
H	-7.41346462	1.86731613	-0.67244250
H	-7.83961688	1.82338557	-2.18132395
O	-7.57298214	2.17687765	0.95475025
H	-6.97606751	2.84492227	1.32034647
H	-7.42930406	1.36110840	1.44404973
O	-4.36202181	-0.14709815	2.84174321
H	-6.02275004	-0.38894614	2.34879574
H	-4.13955712	-0.07412646	3.76665514
O	-4.55382941	2.59116559	-1.33286757
H	-5.41920859	2.26652568	-1.60540303
H	-4.48790662	2.42465598	-0.38880081
H	-0.28856065	0.44357896	0.10541357
O	-0.32316633	2.45539926	-3.58670323
H	-0.42741931	2.41723686	-4.53326203
O	1.55094905	-1.59285192	-3.68440175
H	1.66018320	0.02013340	-3.21422073
H	2.21833011	-1.87623818	-4.32967564
O	5.61690658	2.20387435	-0.62055525
O	3.77272617	-0.74121960	3.33505385
H	5.20998721	1.84733670	-1.42110618
H	6.21468427	1.53891299	-0.25756341
H	3.05542919	-1.28546657	3.66341715
H	3.33797893	-0.00129419	2.87407243
O	1.87608641	-2.35745124	-1.09385269
O	4.46677089	1.16893505	-2.92065498
H	1.84910859	-2.15666613	-2.04847806
H	2.77408449	-2.66336829	-0.90157789
H	4.73193398	1.59397142	-3.73259966
H	3.48744878	1.13067259	-2.92124642
O	1.80069043	0.90198330	-2.80604947
H	1.64426163	0.76268544	-1.85818290
H	0.47903190	1.95156392	-3.36857699
O	3.76158433	-2.15104776	-5.15338145
H	4.40707757	-2.02218800	-4.43339746
H	4.01540352	-2.92716075	-5.64246789
O	5.29553203	-1.55001109	-3.02974676
H	5.08384925	-2.01761685	-2.21341396
H	5.08072763	-0.62039594	-2.89658398
O	1.34356040	0.11229768	-0.20113097
H	1.89514609	0.44221678	0.52304456
H	1.56359310	-0.82486749	-0.37469992
O	4.55301877	-2.95056535	-0.67957009
H	4.93079468	-2.50242247	0.11362873
H	4.85412089	-3.85510329	-0.65550225
O	4.34473354	3.21343734	1.41598275
H	4.18119990	4.14707374	1.31437731
H	4.77609306	2.89288742	0.58583628
O	5.43444634	0.62638205	5.03889448
H	4.84116963	0.03374169	4.55327433
H	5.97669048	0.09016747	5.60949555
O	7.15572748	0.52173382	0.99438009
H	6.98649186	1.10237610	1.77323224
H	8.10032960	0.44335427	0.89205874
O	6.46470627	2.11539124	2.96580524
H	6.15627518	1.67075083	3.76884462
H	5.73234805	2.63792685	2.62339832
O	2.53154747	1.28211710	2.00326424
H	3.09935888	2.05188060	1.82506518
H	1.70618493	1.58720981	2.39480519

O	5.56031524	-1.74064821	1.41422867
H	6.16196312	-1.00225441	1.25078899
H	4.94943732	-1.46124401	2.10736920

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C	-0.47062791	0.72525967	3.54635205
O	-0.16983149	1.74461951	2.62410487
H	-0.19031116	1.06788780	4.53561906
H	-1.53306877	0.48749922	3.54309570
H	-0.62221830	1.58128465	1.78509198
O	0.83547675	-1.20804614	4.06238163
C	0.30104332	-0.53001462	3.22392237
H	0.38530427	-0.77680082	2.16009582
O	-0.40760132	-3.93910100	-1.34517320
H	-1.13709424	-3.71738890	-0.76224789
H	-0.73705930	-3.29699808	-3.05064219
O	-6.64896549	-1.15951340	-0.77827869
O	-3.75015899	2.23506167	1.32570203
H	-5.42745302	-2.11573341	-1.30687664
H	-6.83021085	-0.31674487	-1.21492621
H	-2.82515840	2.13583139	1.10011976
H	-3.98354839	1.47531537	1.87607903
O	-1.23425654	0.81969572	0.25634746
O	-4.69107202	-2.68385333	-1.63168822
H	0.36731188	-3.44126395	-1.06203399
H	-1.66113855	1.04950660	-0.60151939
H	-5.06226213	-3.28978229	-2.26842323
H	-3.51864963	-3.24212367	-0.50016902
O	-2.82793985	-3.46737584	0.15223784
H	-2.49454811	-2.05764544	1.18693498
H	-3.06174421	-4.30880845	0.53552747
O	-0.78820478	-2.76415251	-3.85652111
H	-1.54144383	-2.16655985	-3.73174593
H	0.66441049	-1.98314738	-3.88027579
O	-2.90904246	-1.11133590	-3.25489588
H	-2.71943207	-0.24808614	-2.86649797
H	-3.53290971	-1.55545830	-2.67571478
O	-2.34953075	-1.22966315	1.66876884
H	-3.61471676	-0.60065472	2.42498260
H	-1.98103756	-0.58613866	1.04041535
O	-2.33730815	1.37516395	-2.08463620
H	-3.16560097	1.87991758	-1.98717996
H	-1.72623355	1.85565701	-2.66895049
O	-6.88306513	-0.42831689	1.95191794
H	-7.41380095	-0.94542091	2.55203671
H	-6.76258799	-1.00061958	0.16464689
O	-5.83822727	3.96618458	1.86046612
H	-4.96919669	3.57928758	1.70220094
H	-5.82440782	4.84993442	1.50409444
O	-7.19505467	1.45868984	-1.59432828
H	-7.47369305	1.77650212	-0.70615310
H	-7.86998268	1.70160874	-2.22193913
O	-7.67280993	2.10692337	0.91096441
H	-7.11188625	2.80677866	1.27485525
H	-7.49563391	1.30671743	1.41433110
O	-4.33363215	-0.05190032	2.83424411
H	-5.98935557	-0.35936918	2.32801008
H	-4.17250470	-0.00956585	3.77355499
O	-4.62327467	2.57827230	-1.37231864
H	-5.48241562	2.22030221	-1.62223681
H	-4.53758363	2.44709519	-0.42385884
H	-0.32162877	0.55808782	0.02580362
O	-0.38568494	2.47509902	-3.63080892
H	-0.48145586	2.45540923	-4.57876673
O	1.53287812	-1.56162682	-3.67895709
H	1.63236542	0.06467664	-3.24279373
H	2.20099486	-1.85420344	-4.31947361

O	5.64530684	2.14289386	-0.59072443
O	3.62429828	-0.72092349	3.34520293
H	5.22003832	1.80418960	-1.38914377
H	6.21592307	1.45475797	-0.22728325
H	2.88450631	-1.22532032	3.68970646
H	3.23186728	0.04595944	2.89452487
O	1.87963920	-2.27617102	-1.08520176
O	4.45206492	1.16581990	-2.90058804
H	1.84354516	-2.09363519	-2.04406811
H	2.76916075	-2.61109432	-0.89869380
H	4.74633616	1.58590325	-3.70513540
H	3.47308492	1.14968737	-2.92607557
O	1.77104685	0.95225769	-2.84699586
H	1.61002124	0.82681001	-1.89892619
H	0.42475623	1.98425307	-3.41659830
O	3.74677907	-2.14813851	-5.13034506
H	4.39091456	-2.02710551	-4.40815035
H	3.99624566	-2.92347564	-5.62289133
O	5.27516565	-1.55689371	-2.99814722
H	5.06793660	-2.02723867	-2.18247019
H	5.05395632	-0.62893532	-2.86454122
O	1.34242736	0.18800892	-0.21831926
H	1.91769371	0.54945856	0.47103191
H	1.58928803	-0.74151301	-0.40323138
O	4.51750318	-2.96443120	-0.65604377
H	4.87291704	-2.53302437	0.15681279
H	4.78948920	-3.87802663	-0.62898265
O	4.44015472	3.22126168	1.45094614
H	4.31986919	4.16208047	1.35497346
H	4.85328327	2.88377110	0.61862814
O	5.36095590	0.56479910	5.05352461
H	4.73941370	0.00043491	4.57116538
H	5.85559739	0.00986649	5.64891832
O	7.11909702	0.41603596	1.03918615
H	6.97555396	1.00470716	1.81761437
H	8.05932290	0.29635581	0.93612057
O	6.49154574	2.02624278	3.01425597
H	6.15288567	1.58552367	3.80714024
H	5.78686710	2.58360086	2.66862109
O	2.50609790	1.39365435	1.97753286
H	3.13427612	2.12137605	1.82558303
H	1.66365499	1.76628270	2.27055675
O	5.45234021	-1.78168599	1.48144561
H	6.07456145	-1.05810748	1.32690413
H	4.82409329	-1.48374081	2.15012934

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C	3.89175558	0.46508738	-1.99648468
O	4.04542580	0.83474826	-0.86074952
H	4.29963905	1.02502023	-2.83957996
H	3.35711989	-0.45866022	-2.23293378
H	-0.81428533	1.75367634	2.00840241
O	0.55095001	3.15824318	2.46741348
C	-0.54504310	2.80625395	2.10816206
H	-1.32698392	3.53702427	1.89382313
O	-3.94769662	1.26026235	1.11946149
H	-3.70749702	1.91198121	0.45706702
H	-4.69890189	-0.15629262	0.13667669
O	-2.06079842	3.40405283	-5.04071121
O	1.55140253	1.41519115	-3.04446828
H	-3.25787819	2.84232420	-4.04963469
H	-1.73772001	2.86896110	-5.77669372
H	0.97897413	0.91334210	-2.43001172
H	1.51669061	2.32694309	-2.73085426
O	-0.24184473	0.23573107	-1.47161825
O	-3.98310458	2.52813327	-3.46405686
H	-3.14462993	0.85303287	1.46063478

H	-0.76076954	-0.34394772	-2.06277080
H	-4.80306656	2.68974189	-3.92404688
H	-3.78155573	3.01553429	-1.82666428
O	-3.52702138	3.25761908	-0.91599166
H	-1.76888085	2.99201037	-0.73574119
H	-3.99357459	4.05736502	-0.68907722
O	-4.82061956	-0.97607802	-0.35922410
H	-4.60297861	-0.77318481	-1.28198046
H	-3.80643283	-2.03390204	0.42264001
O	-4.01084922	-0.31646303	-2.91926790
H	-3.15467499	-0.71057368	-3.12782542
H	-3.94768870	0.61735389	-3.13224497
O	-0.85317818	2.71708533	-0.59372856
H	0.32725946	3.56605054	-1.34407337
H	-0.77566037	1.79575771	-0.89968635
O	-1.43401648	-1.31174442	-3.31676814
H	-0.93884303	-1.02360894	-4.09814256
H	-1.25005726	-2.24979926	-3.14276866
O	0.32487334	4.80158362	-4.33455096
H	0.31852151	5.75014114	-4.43454765
H	-1.31109105	3.92824369	-4.73938793
O	3.01414528	1.16546286	-5.36378849
H	2.55630837	1.16429840	-4.51367110
H	2.66560985	0.40697133	-5.82937653
O	-0.71762968	1.96824599	-7.02514680
H	0.12760946	2.46672587	-6.95315353
H	-0.95833431	1.91466463	-7.94569793
O	1.49848827	3.26456683	-6.44486244
H	2.16349745	2.63857050	-6.12474553
H	1.26213986	3.84112243	-5.71115715
O	1.07062052	3.93368926	-1.88087223
H	0.61365374	4.60609818	-3.42631499
H	1.72355920	4.27542101	-1.27481830
O	0.10048445	0.03699328	-5.15239797
H	-0.29690746	0.53442887	-5.87592993
H	0.43831834	0.69253504	-4.53627289
H	0.01240869	-0.28417582	-0.68656773
O	-0.89293906	-3.85189580	-2.48928622
H	-1.46948466	-4.57825622	-2.70816196
O	-3.14583647	-2.48665720	0.99567205
H	-1.69999500	-3.18990883	0.44016898
H	-3.61303372	-3.07696790	1.61034179
O	2.48677884	-3.98082057	3.51512099
O	2.27071817	1.19977508	3.44646284
H	1.62147014	-4.21207830	3.15523299
H	2.36535615	-3.58194359	4.38564720
H	1.74747337	1.93633322	3.10155462
O	2.54059962	0.65812708	2.68699539
O	-1.83594731	-0.40323708	2.14159605
O	-0.02142119	-4.71849791	2.52191980
H	-2.34185368	-1.16673160	1.79871958
H	-1.80980366	-0.50858466	3.10525938
H	-0.14799044	-5.66336958	2.48345806
H	-0.30391756	-4.35560867	1.65811150
O	-0.78987038	-3.49434176	0.24053295
H	-0.23975736	-2.70221824	0.35181685
H	-0.83409168	-3.81686300	-1.51996546
O	-4.02578360	-4.17817102	2.91900042
H	-3.31873934	-4.02594308	3.57377426
H	-4.85698399	-4.21131554	3.38167518
O	-1.86095155	-3.67146917	4.42354655
H	-1.70846403	-2.73732579	4.60748565
H	-1.15041971	-3.97800248	3.84983492
O	0.3959405	-1.08356906	0.75781611
H	1.29884401	-0.89150676	1.05822321
H	-0.25752774	-0.76568129	1.40508128
O	-1.53458614	-0.88892972	4.82721770
H	-0.60005686	-0.66329337	5.06095202

H	-2.09547875	-0.51001291	5.49866360
O	4.34986308	-2.56083840	2.35885640
H	4.97957401	-3.10470559	1.89386191
H	3.64789039	-3.15563257	2.71723439
O	4.63524000	1.29336477	4.81751978
H	3.78510648	1.42952993	4.37136871
H	4.64701957	1.84852430	5.59121083
O	2.65042499	-2.46494315	5.85332501
H	3.52630784	-2.08830905	5.59670332
H	2.74141776	-2.84691411	6.72195134
O	4.87570812	-1.44529280	4.92204945
H	4.89416155	-0.47621899	4.91577372
H	4.91448055	-1.74270701	4.00741935
O	2.96429965	-0.43676858	1.36575981
H	3.52907397	-1.17638137	1.64596896
H	3.39077115	0.00221676	0.61661516
O	0.94000111	-0.31381367	5.36753600
H	1.50981800	-1.05948748	5.59818226
H	1.41035105	0.22092740	4.71236976

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C	-1.15792302	1.72913312	3.66086402
O	-0.36314044	1.18788692	2.70548555
H	-0.68290365	1.81647180	4.62090942
H	-1.92058367	2.42303230	3.34757855
H	-0.79059956	1.16716112	1.83760748
O	1.09470405	-1.98235619	3.75281751
C	0.59256452	-1.72236814	2.72039761
H	-0.48065649	-1.79607120	2.46342090
O	-0.44123900	-4.07254077	-1.45600601
H	-1.21754448	-3.85550012	-0.93565367
H	-0.72574949	-3.40245148	-3.16211075
O	-6.57897468	-1.01546717	-0.53796467
O	-3.44092317	2.27893562	1.14339117
H	-5.51827063	-2.02643291	-1.28643229
H	-6.80602780	-0.17127574	-0.94985845
H	-2.59141894	2.07479399	0.74755583
H	-3.67962837	1.50137796	1.66924197
O	-1.20148369	0.71567872	0.10887771
O	-4.89044220	-2.63151193	-1.74349806
H	0.30292136	-3.55566948	-1.12790982
H	-1.61679149	0.91305244	-0.76254782
H	-5.40106097	-3.16200585	-2.34992769
H	-3.67812535	-3.33995723	-0.74885876
O	-2.97300212	-3.61653708	-0.13314113
H	-2.53152647	-2.23258062	0.86656425
H	-3.24189941	-4.44482689	0.25545611
O	-0.77472645	-2.84370956	-3.95014913
H	-1.54983495	-2.27602554	-3.82402956
H	0.67515197	-2.04349942	-3.92168510
O	-2.94375615	-1.23846837	-3.35373800
H	-2.75306229	-0.36801793	-2.98275715
H	-3.62652808	-1.63771172	-2.80976636
O	-2.26099297	-1.45443134	1.37702465
H	-3.33511568	-0.61458985	2.26937024
H	-1.88896982	-0.79788764	0.76529889
O	-2.34012149	1.25719095	-2.22279380
H	-3.15136130	1.78578330	-2.11497657
H	-1.72288722	1.72618983	-2.81130322
O	-6.54102295	-0.24839247	2.21209789
H	-7.04148006	-0.72794296	2.86693669
H	-6.57970694	-0.86031161	0.41225345
O	-5.36318885	4.10753181	1.88929406
H	-4.54347085	3.67671824	1.62021146
H	-5.36140012	4.98378845	1.51464654
O	-7.18791993	1.58931109	-1.34119466
H	-7.34349526	1.93108358	-0.43187679

H	-7.93639099	1.82950062	-1.88016248
O	-7.34644668	2.28588180	1.19034355
H	-6.73408569	2.97590585	1.48189763
H	-7.14095070	1.48849079	1.68832742
O	-3.90312571	0.04198235	2.73979485
H	-5.62036105	-0.19682948	2.52102785
H	-3.45775856	0.25084792	3.55996962
O	-4.55736745	2.58313231	-1.46649295
H	-5.45311880	2.26523755	-1.62366300
H	-4.40696721	2.50797390	-0.52018231
H	-0.26180795	0.51079345	-0.08117711
O	-0.37570438	2.34950342	-3.74366959
H	-0.44035823	2.30339750	-4.69337474
O	1.53849570	-1.62824944	-3.69144196
H	1.65892154	0.00006794	-3.26949864
H	2.22364925	-1.92074653	-4.31385313
O	5.38866381	2.27916015	-0.50250488
O	3.71427066	-0.75599137	3.46733502
H	5.04600361	1.92185404	-1.33195689
H	6.01683993	1.64596863	-0.13389926
H	3.02670068	-1.36136027	3.75139165
H	3.24733177	-0.05160654	2.98350119
O	1.80716685	-2.36618869	-1.08719564
O	4.45198013	1.22249119	-2.89690257
H	1.79816525	-2.17800625	-2.04494573
H	2.70639716	-2.65292261	-0.87174804
H	4.76099493	1.66473997	-3.68365081
H	3.47630056	1.16011885	-2.96270132
O	1.79222145	0.89482171	-2.88816698
H	1.65642859	0.77776196	-1.93425541
H	0.43925218	1.88369982	-3.49123441
O	3.79265434	-2.18491612	-5.08862892
H	4.41994012	-2.01898610	-4.36015220
H	4.07850324	-2.96511115	-5.55289438
O	5.27421939	-1.50170873	-2.95194084
H	5.04366334	-1.95219414	-2.13105959
H	5.06672142	-0.56762761	-2.84074463
O	1.37294466	0.14954642	-0.27428294
H	1.87290116	0.44256983	0.50155164
H	1.54920899	-0.80093559	-0.42547532
O	4.49113642	-2.88363814	-0.60227151
H	4.85729693	-2.42574066	0.19070537
H	4.81832866	-3.77912308	-0.57669198
O	4.05742575	3.23480315	1.52843549
H	3.86833485	4.16389009	1.43016929
H	4.50088932	2.93124457	0.69911245
O	5.25275460	0.72704229	5.17880960
H	4.70461719	0.08953742	4.69641119
H	5.81180885	0.23756634	5.77457167
O	6.99950841	0.66848878	1.11226630
H	6.79666011	1.23421420	1.89389444
H	7.94758825	0.63550176	1.01791338
O	6.22198925	2.22367721	3.08315107
H	5.93405108	1.77574395	3.89207686
H	5.46811129	2.71207796	2.73739839
O	2.38056659	1.17485545	2.07836748
H	2.87442451	2.00134983	1.94258933
H	1.51504932	1.37401274	2.45059751
O	5.49049188	-1.66083714	1.49074440
H	6.06771446	-0.90217473	1.33318828
H	4.89377548	-1.41575834	2.20900176

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C	4.05134474	0.81430410	-1.21488537
O	3.56402121	1.18230740	0.00516232
H	3.57821519	1.21179112	-2.09465448
H	5.08619824	0.52961514	-1.19320173

H	2.68152689	1.54949841	-0.06118602
O	1.06051345	2.68559999	2.53400668
C	0.92669852	2.55351646	1.37576316
H	0.03336278	2.81313709	0.77304875
O	-3.92709392	1.33061297	1.01685632
H	-3.67318486	1.96457464	0.34323677
H	-4.62296732	-0.11662744	0.08163510
O	-2.60528784	3.16964519	-5.52055624
O	1.61335582	1.77556532	-3.45593334
H	-3.61076868	2.66600373	-4.32055411
H	-2.22254293	2.53701831	-6.14254498
H	1.22787614	1.26570476	-2.72495183
H	1.35618232	2.69187669	-3.30510531
O	0.12461717	0.56586413	-1.50279273
O	-4.22287234	2.36411918	-3.61077054
H	-3.13315517	1.00173079	1.45136245
H	-0.36967451	-0.07472429	-2.05820702
H	-5.10553059	2.39100199	-3.97152635
H	-3.89140573	2.92549581	-2.01647293
O	-3.57975473	3.22293721	-1.14041510
H	-1.82360317	3.14644529	-1.09906862
H	-4.07664923	4.00296320	-0.90866745
O	-4.74179596	-0.95517641	-0.38433043
H	-4.47078073	-0.79914351	-1.30250674
H	-3.73897504	-1.94326992	0.46408510
O	-3.80813231	-0.40525846	-2.91587832
H	-2.88804018	-0.66542829	-3.05581897
H	-3.89190308	0.50758382	-3.20029108
O	-0.86151130	3.03117178	-1.07994623
H	0.02377758	3.95113614	-2.09865711
H	-0.66192281	2.09244785	-1.25960149
O	-1.12025710	-1.09140785	-3.18285731
H	-0.69892782	-0.84745671	-4.02523488
H	-0.95498102	-2.03220438	-3.00195963
O	-0.41320878	4.94952273	-5.18272323
H	-0.52869030	5.88343842	-5.33688383
H	-1.93064522	3.84173977	-5.37768822
O	2.99213903	1.90322517	-5.85254705
H	2.67718422	1.72571822	-4.95806429
H	3.15574470	1.05410492	-6.25498126
O	-1.08898584	1.58476327	-7.24907343
H	-0.32917052	2.20594716	-7.32539035
H	-1.34082157	1.31021584	-8.12626286
O	0.91075996	3.27902263	-7.08356238
H	1.70397230	2.87008845	-6.70666207
H	0.60705865	3.95221113	-6.46727004
O	0.64166662	4.35494206	-2.75530748
H	-0.04121638	4.83921900	-4.29123602
H	1.24299364	4.92399258	-2.28203196
O	0.17280406	0.03100366	-5.27060289
H	-0.32536724	0.43120565	-5.99203497
H	0.61792744	0.74842911	-4.81112433
H	0.32127918	0.11487763	-0.66388444
O	-0.69854016	-3.65047069	-2.36070398
H	-1.35904119	-4.30852576	-2.55784629
O	-3.08149904	-2.36758822	1.06478772
H	-1.58525301	-2.90142909	0.53200457
H	-3.54115994	-3.00822861	1.63251586
O	2.34570090	-4.31684357	3.75098234
O	2.59026316	0.92781186	4.29961971
H	1.49071356	-4.43740277	3.31753237
H	2.19330556	-3.96677269	4.63742102
H	2.16722154	1.72104554	3.97078205
H	2.75560608	0.38023948	3.50984635
O	-1.83420309	-0.23914787	2.21868638
O	-0.11589606	-4.64463830	2.52432969
H	-2.32876709	-1.01640734	1.89509202
H	-1.77677035	-0.34060643	3.18000379



H	-0.38581243	-5.54644941	2.36814581
H	-0.28071109	-4.14955149	1.69566365
O	-0.65599992	-3.15991168	0.34576440
H	-0.14052677	-2.34654262	0.45548495
H	-0.65276100	-3.57314270	-1.39378820
O	-3.99928044	-4.19086872	2.85502668
H	-3.34422517	-4.02063092	3.55769514
H	-4.85998468	-4.24590069	3.25802635
O	-1.93034953	-3.63343268	4.46454597
H	-1.79683077	-2.69607415	4.64757309
H	-1.21729611	-3.92065479	3.88400938
O	0.46902426	-0.66220430	0.89217499
H	1.29431111	-0.69483030	1.39832003
H	-0.27609754	-0.43710040	1.48250915
O	-1.56036952	-0.86046804	4.91064764
H	-0.64669319	-0.76809469	5.27167099
H	-2.15304893	-0.48450175	5.55632411
O	4.24891100	-2.86309479	2.73449012
H	4.83394699	-3.36635868	2.17483186
H	3.53168621	-3.47089855	3.04298494
O	4.98061510	0.64348528	5.61468724
H	4.14163449	0.91846292	5.21733798
H	5.07444029	1.10324752	6.44344674
O	2.42838702	-2.95431952	6.18993320
H	3.34219375	-2.63765423	5.99822240
H	2.45142189	-3.41703309	7.02318049
O	4.79177698	-2.10025576	5.41998939
H	4.96531030	-1.15355143	5.52490703
H	4.84156563	-2.30330324	4.48035111
O	2.96486048	-0.56653511	2.06983723
H	3.46758767	-1.38630179	2.21983400
H	3.40486326	-0.05594495	1.37920176
O	0.87283296	-0.65354832	5.85073070
H	1.35511806	-1.47161682	6.03033633
H	1.47149520	-0.07453125	5.36224850

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C	-0.87309148	1.77747677	3.60597864
O	-0.12054506	1.97720168	2.49749558
H	-0.38359825	2.05749009	4.52110244
H	-1.94186207	1.87229775	3.50382734
H	-0.59150855	1.70814153	1.69483464
O	1.11138134	-1.91216812	3.79616653
C	0.48953783	-1.44149461	2.91527152
H	-0.57237560	-1.63451942	2.67082412
O	-0.46758451	-4.01891892	-1.43459743
H	-1.22982191	-3.77632130	-0.90477962
H	-0.74871913	-3.33819953	-3.13845817
O	-6.68453089	-1.05798478	-0.79558059
O	-3.65952974	2.01839484	1.37377113
H	-5.52212278	-2.01598201	-1.44043462
H	-6.86366112	-0.19094265	-1.18302531
H	-2.78379494	1.79290746	1.05424719
H	-3.95100685	1.26954878	1.91037497
O	-1.22852177	0.76582843	0.27579502
O	-4.82069513	-2.58906416	-1.82788788
H	0.29608697	-3.52748233	-1.11199858
H	-1.60160126	1.00607100	-0.60477075
H	-5.23712753	-3.14387787	-2.48277992
H	-3.65158255	-3.23395689	-0.74880227
O	-2.97351494	-3.50258754	-0.09917406
H	-2.57172996	-2.15281508	0.95978356
H	-3.24521559	-4.34173897	0.26364423
O	-0.78278030	-2.77916282	-3.92697908
H	-1.52633707	-2.17234571	-3.79153896
H	0.68488193	-2.01835869	-3.88582348
O	-2.87243613	-1.08457289	-3.31517738

H	-2.67704516	-0.23402645	-2.90257695
H	-3.56363963	-1.50333140	-2.79708269
O	-2.35948006	-1.39489157	1.52693619
H	-3.57651654	-0.78941981	2.40839396
H	-1.97804607	-0.69573405	0.96863638
O	-2.27905700	1.36516897	-2.07836874
H	-3.09795462	1.87912080	-1.96047279
H	-1.66518753	1.84905588	-2.65791327
O	-6.83827614	-0.46984713	1.98200125
H	-7.40922186	-0.98382814	2.54695616
H	-6.75869020	-0.94622813	0.15794864
O	-5.57915643	3.89437611	2.01293874
H	-4.74469004	3.45809589	1.80637160
H	-5.52716892	4.78242952	1.67095568
O	-7.18639899	1.60179563	-1.48373511
H	-7.41126589	1.88987077	-0.57065982
H	-7.88097185	1.89432871	-2.06714751
O	-7.52666835	2.14832665	1.06838756
H	-6.92632097	2.81065852	1.43937276
H	-7.36531009	1.32088486	1.53145000
O	-4.27544449	-0.26468676	2.87237854
H	-5.94972247	-0.47327165	2.37536960
H	-4.03915707	-0.22210121	3.79570489
O	-4.54949799	2.57046608	-1.28678374
H	-5.42845434	2.27656511	-1.54949357
H	-4.47178730	2.38187376	-0.34751760
O	-0.30639623	0.48351689	0.09277218
H	-0.32140495	2.45232499	-3.61225805
H	-0.41082595	2.42523858	-4.56066375
O	1.55260852	-1.61601884	-3.64873046
H	1.65790186	0.00937587	-3.20689722
H	2.23420821	-1.90983190	-4.27461850
O	5.65466572	2.20757034	-0.64432343
O	3.71371590	-0.62986407	3.41893378
H	5.23937135	1.83345652	-1.43213475
H	6.23435171	1.54055981	-0.25657050
H	3.01112022	-1.20922928	3.71910827
H	3.27268072	0.08595580	2.92536608
O	1.81123163	-2.36269368	-1.04656184
O	4.47260887	1.12570652	-2.90998800
H	1.80628695	-2.16709220	-2.00314956
H	2.70547311	-2.66602723	-0.83195476
H	4.74859909	1.51633728	-3.73551594
H	3.49323466	1.10377541	-2.91474102
O	1.79757037	0.89614550	-2.81014214
H	1.63476572	0.76890305	-1.86174967
H	0.47793822	1.94716424	-3.38737786
O	3.78530744	-2.21326073	-5.06676489
H	4.41898649	-2.08525108	-4.33615872
H	4.03523437	-2.99977260	-5.54104605
O	5.28104512	-1.59953620	-2.92206529
H	5.04658175	-2.04669680	-2.10061151
H	5.07035773	-0.66545914	-2.81584970
O	1.31989647	0.13374790	-0.19982207
H	1.88098073	0.46700903	0.51703110
H	1.52743407	-0.80769300	-0.36290940
O	4.47552378	-2.94041463	-0.55586058
H	4.84671879	-2.46839448	0.22704910
H	4.78095072	-3.84235914	-0.50387731
O	4.36090659	3.24901936	1.36516556
H	4.18572125	4.17865217	1.24765357
H	4.80241007	2.92034724	0.54417256
O	5.36920760	0.78069352	5.08504879
H	4.76958846	0.17913139	4.61813824
H	5.89558894	0.25893566	5.68317281
O	7.13339036	0.53456340	1.03724361
H	6.96422109	1.13253521	1.80324819
H	8.07756810	0.43345712	0.95262653

O	6.44580026	2.17568597	2.96891815
H	6.12357939	1.76025684	3.78215161
H	5.72332069	2.69693800	2.60385365
O	2.52504059	1.33101293	1.96508991
H	3.10965070	2.08439138	1.77417142
H	1.68474158	1.67179423	2.29659313
O	5.48072119	-1.67446191	1.50305050
H	6.10132149	-0.95601953	1.32203260
H	4.88404353	-1.36725772	2.19723866

### 3.2.8 HCO + CH3O

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C	-0.18841610	3.24221918	1.34426783
H	-0.09605323	2.98391948	0.29705559
O	0.91207750	2.68924280	2.06570864
C	0.70720639	1.57800624	2.76318516
H	-0.31542287	1.19785197	2.73590883
O	1.58905903	1.05087204	3.37943728
O	-0.94298887	-3.60676107	1.66099262
H	-1.64530341	-3.04757785	2.00044737
H	-1.35940727	-4.27784156	-0.00705650
O	-6.84202963	-0.36910527	0.54650453
O	-3.39846240	2.86901429	-0.21831730
H	-5.81391852	-1.64874175	0.70604843
H	-7.07724058	-0.03028612	-0.32690195
H	-2.64353008	2.26891610	-0.31003008
H	-3.66563099	2.82918986	0.70532444
O	-1.60169585	0.77428453	-0.32749718
O	-5.21669179	-2.42508733	0.80110870
H	-0.17119701	-3.05319827	1.49614091
H	-1.97233937	0.31010718	-1.10622469
H	-5.76691119	-3.20380694	0.76490782
H	-3.98192919	-2.31051956	1.99994577
O	-3.24630597	-2.16430165	2.62503057
H	-2.66141080	-0.48308888	2.46517528
H	-3.49727718	-2.55014182	3.46007023
O	-1.44992247	-4.42787404	-0.95897880
H	-2.22315602	-3.91161095	-1.23614775
H	-0.03941423	-3.86579557	-1.56427086
O	-3.58335792	-2.78875545	-1.56679884
H	-3.32029902	-1.94283649	-1.95219813
H	-4.12346101	-2.59011036	-0.79839015
O	-2.38290068	0.41321756	2.22643689
H	-3.43312031	1.60889581	2.51389292
H	-2.14776363	0.39590640	1.28020459
O	-2.77144552	-0.28528975	-2.49774496
H	-3.50158428	0.33901862	-2.64434861
H	-2.17326855	-0.24642972	-3.26299669
O	-6.65018862	2.05707911	2.01041665
H	-7.20810925	2.17813067	2.77429741
H	-6.79409523	0.40061840	1.12323569
O	-5.13564364	4.54975916	-1.64463781
H	-4.37486468	4.18716769	-1.17811935
H	-5.11801323	4.11991605	-2.49885616
O	-7.41810272	1.06208777	-1.77939993
H	-7.52161354	1.94225069	-1.35085678
H	-8.15243647	0.92603332	-2.37138567
O	-7.34298265	3.33177940	-0.45720973
H	-6.62576035	3.88162765	-0.80818150
H	-7.10624565	3.07437013	0.43869484
O	-4.01034224	2.41355740	2.53055403
H	-5.72916839	2.19036456	2.29184322
H	-3.70249054	2.98322154	3.23033589
O	-4.73148599	1.59238772	-2.41361748
H	-5.64706964	1.30356166	-2.32493421

H	-4.47610641	1.97107347	-1.56628580
H	-0.64169838	0.63451489	-0.32939513
O	-0.82616869	-0.15856442	-4.38663567
H	-0.81234815	-0.64985200	-5.20251051
O	0.82228621	-3.41763139	-1.74736927
H	0.91059954	-1.84958678	-2.40692903
H	1.42682877	-4.01879815	-2.19918805
O	5.75134201	0.02922665	-2.32760870
O	4.27033264	1.08181677	2.62576032
H	5.12260557	-0.62920954	-2.65223273
H	6.24469129	-0.35704172	-1.59359906
H	3.44813400	1.06069184	3.12924308
H	3.98246589	1.32978632	1.73472817
O	1.37110960	-2.28668852	0.68397556
O	3.77527216	-1.78178299	-2.96983263
H	1.29070304	-2.77049383	-0.15700754
H	2.18994479	-2.58754274	1.10475729
H	3.66767488	-2.61918047	-3.42570802
H	2.88919302	-1.38650855	-2.93061475
O	1.16191019	-0.95126567	-2.70236562
H	1.13424337	-0.40537312	-1.90345001
H	-0.04625066	-0.42683087	-3.87145612
O	3.03371702	-4.61396165	-2.95057346
H	3.62412941	-4.51433825	-2.17865322
H	3.18161980	-5.47408464	-3.33228262
O	4.55241763	-3.68085608	-0.98909007
H	4.31811279	-3.64244888	-0.05374597
H	4.39669383	-2.80597542	-1.35550233
O	1.07548646	0.24650125	-0.18048562
H	1.83866846	0.82425122	-0.04119506
H	1.24842028	-0.61032977	0.25662627
O	3.79282133	-3.21488378	1.65391537
H	4.45766182	-2.52439626	1.89574809
H	3.79653811	-3.87462398	2.34212044
O	5.06683260	2.42069332	-1.57395193
H	5.06590525	3.02946186	-2.30764856
H	5.28111415	1.52209171	-1.93419742
O	6.28608239	2.90420568	2.83208999
H	5.56364694	2.27031559	2.96027131
H	6.83071262	2.88759918	3.61325415
O	7.16910206	-0.49740947	0.03662029
H	7.25750095	0.46980627	0.19658344
H	8.04948412	-0.85752698	-0.03201707
O	7.16824723	2.12354341	0.34017915
H	6.94452194	2.47691154	1.21349087
H	6.52026971	2.46027316	-0.28585708
O	3.15452097	2.01351101	0.27253980
H	3.78069136	2.26515228	-0.43214313
H	2.77149005	2.80192512	0.65346580
O	5.53690445	-1.34748646	2.16470627
H	6.14043592	-1.14365235	1.43811216
H	5.11910979	-0.51292652	2.41691599
H	-1.12846014	2.86165492	1.72437784
H	-0.14647913	4.31538924	1.47360546

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C	0.63941772	4.12622361	-0.91474868
H	0.25456129	3.25840933	-1.45292976
O	1.70479764	4.10219053	-0.34661025
C	-0.47231832	2.25393483	1.53143228
H	-0.97250254	1.33560150	1.84194795
O	-1.08346704	3.17454790	1.04682165
O	-1.90100104	-3.09264738	2.77269684
H	-2.72052223	-2.59309927	2.76611486
H	-1.94187269	-4.07088840	1.21651301
O	-6.76550949	-0.04899697	-1.02419777
O	-2.76704964	2.55167640	-2.19759788

H	-5.96213453	-1.33777616	-0.43222442
H	-6.70568800	0.11416035	-1.97596353
H	-1.89284679	2.14729616	-2.05710158
H	-3.21377604	2.48374815	-1.34297513
O	-0.48832238	1.14249230	-1.90600582
O	-5.45402714	-2.11404503	-0.09333186
H	-1.17221321	-2.48393429	2.61093324
H	-0.84109224	0.37571883	-2.38533114
H	-5.93380744	-2.89949225	-0.34368239
H	-4.89860934	-1.97736771	1.58278044
O	-4.45134457	-1.77010055	2.42204738
H	-3.31203714	-0.44000263	1.78891442
H	-5.11099832	-1.75430322	3.10935935
O	-1.83906755	-4.30947010	0.28314772
H	-2.17053828	-3.53842018	-0.19649323
H	-0.18522790	-4.20800852	0.09821234
O	-2.74526807	-1.88572852	-0.79036802
H	-2.43846514	-1.61331694	-1.67459500
H	-3.70478752	-1.97594714	-0.80653157
O	-2.73773052	0.03563832	1.17988409
H	-3.43625077	1.47260763	0.67286824
H	-2.58062671	-0.58974013	0.45192730
O	-1.78749268	-0.95388885	-3.13169964
H	-2.46357315	-0.50600225	-3.67010579
H	-1.15641571	-1.43853672	-3.68387117
O	-6.32147933	2.59092401	-0.07911288
H	-6.83710992	3.02685488	0.59367935
H	-6.68875639	0.81467942	-0.60256694
O	-4.08303352	4.51157821	-3.53645121
H	-3.45194858	3.89690249	-3.13138327
H	-3.86477390	4.56772764	-4.46232939
O	-6.48512556	0.77148100	-3.67237118
H	-6.51177526	1.73357495	-3.45702240
H	-7.14906952	0.60736242	-4.33632538
O	-6.45043496	3.26093154	-2.84417498
H	-5.68219346	3.78741148	-3.11315804
H	-6.44495004	3.21126403	-1.88284463
O	-3.70943976	2.37863625	0.41328303
H	-5.38682493	2.61014926	0.20155797
H	-2.99412807	2.93849293	0.73143917
O	-3.67337375	0.68823591	-4.10564198
H	-4.62771244	0.56920339	-4.07226561
H	-3.46764062	1.38677098	-3.47119269
H	-0.03996415	0.78796305	-1.12919260
O	0.42890297	-2.16046178	-4.11517860
H	0.59448185	-3.01111116	-4.50951052
O	0.74614494	-3.89347607	0.08871851
H	1.19616480	-2.72475823	-1.08811012
H	1.35810702	-4.63796110	0.14146263
O	6.08956093	-1.21938127	-0.34582749
O	3.68984575	2.38793316	3.01985372
H	5.46419035	-1.93120940	-0.53496532
H	6.33582166	-1.26831969	0.58548350
H	2.92052552	2.74524602	3.45506511
H	3.46067728	2.24096440	2.07850504
O	0.59961290	-1.88709825	1.97076009
O	4.04833161	-3.01449580	-0.73840878
H	0.72923012	-2.65678976	1.39077954
H	1.26515578	-1.95327206	2.66988288
H	3.91526213	-3.96195939	-0.81116794
H	3.26840149	-2.59810136	-1.13994540
O	1.62973737	-2.04051332	-1.63315010
H	1.46118021	-1.20780730	-1.17137072
H	0.93266567	-2.12242658	-3.28611398
O	2.98058168	-5.52600967	0.28422069
H	3.34325792	-5.08339388	1.07579744
H	3.12144678	-6.46399043	0.37177144
O	4.00359526	-3.77729447	1.99392333

H	3.54317156	-3.29990321	2.69375148
H	4.07133173	-3.18186432	1.24168914
O	1.05673041	0.08484404	0.14274623
H	1.86295284	0.58962495	0.31699484
H	0.89613129	-0.53745967	0.87554167
O	2.66487086	-2.11547731	3.81634346
H	3.32205257	-1.38085689	3.84815997
H	2.50387208	-2.39618514	4.71315575
O	5.48333699	1.27264024	-0.77853023
H	5.66430271	1.52027119	-1.68154806
H	5.67773815	0.30485073	-0.69485409
O	6.15774303	3.65020926	3.03699942
H	5.25073391	3.32641427	3.11477660
H	6.12154942	4.59209723	2.90096386
O	6.78973998	-0.66193582	2.31550171
H	7.06341927	0.24305305	2.03801839
H	7.53960705	-1.07500996	2.73543522
O	7.27088535	1.75033040	1.38390301
H	6.99482604	2.48652086	1.94699944
H	6.74353204	1.79286825	0.57954715
O	3.13462971	1.90133978	0.44516762
H	3.95167338	1.69091034	-0.04294912
H	2.72673664	2.67527021	0.02772265
O	4.47398002	-0.22858963	3.80784101
H	5.29537851	-0.42621694	3.33537860
H	4.24063042	0.68409710	3.60952891
H	0.61182594	2.31680084	1.65577819
H	0.03012178	5.03278108	-0.91518362

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C	-0.46032136	2.74599165	-2.60786502
O	0.19754137	2.76525821	-1.40418395
O	2.71466838	2.10578448	-0.35082176
O	3.19276375	2.00931174	2.30545051
O	4.97891321	2.12603310	-1.85524449
O	5.81223478	-0.34293968	-1.91627404
O	1.20200507	-0.17431285	-0.15806706
O	1.27062649	-2.48312387	1.18704861
O	-1.44397288	0.36620575	-0.12286785
O	-2.62993042	-0.58287547	-2.37477149
O	-2.21282635	0.06835586	2.42358387
O	-3.41026558	2.40795694	2.63772380
O	-6.05287804	2.44298622	2.14624568
O	-4.30999768	1.55842252	-2.29511881
O	1.32331396	-1.59493886	-2.47511519
O	0.93033753	-3.88625629	-1.14771617
O	-1.44747452	-4.73269107	-0.47006344
O	-0.45775551	-0.34112283	-4.04274133
O	-2.91713551	2.67262866	-0.13533631
O	3.64900268	-2.79827816	2.54023598
O	4.68166167	-0.39607416	2.57073217
O	5.38086546	3.68753548	2.47396895
O	6.70052387	2.48059768	0.37217467
O	6.74941126	-0.11629764	0.72459885
O	3.97514953	-2.36678441	-2.33609642
O	-3.42901335	-2.36434049	2.88440170
O	-5.27645736	-2.31513365	0.92318741
O	-6.50794214	0.01049555	0.72724160
O	-3.47986664	-3.00884472	-1.25354239
O	-1.06783388	-3.81064023	2.13227786
O	3.33278303	-5.16363160	-1.77756723
O	4.60687925	-3.73911648	0.07999700
O	-7.03021642	1.43694947	-1.61660954
O	-6.65366363	3.70273284	-0.35081473
O	-4.33824924	4.51742856	-1.68130661
O	-0.54261956	2.90784768	3.53891403
C	0.07008010	1.95064418	3.24802348

H	-0.39365292	1.71166358	-2.97247705
H	-0.37757715	0.95996321	3.02701545
H	-1.81640809	-3.27780414	2.41109557
H	-1.40451520	-4.54654767	0.47900451
H	-5.71143644	-1.43621881	0.84575885
H	-6.74568368	0.36853102	-0.13747326
H	-2.19472819	2.02675852	-0.17853083
H	-3.16058490	2.70876309	0.79658180
H	-0.32465396	-3.22144506	1.96353226
H	-1.83637923	-0.07882081	-0.89519412
H	-5.96629778	-2.97020666	0.85051331
H	-4.13379687	-2.41711876	2.21154704
H	-2.62792728	-0.76776151	2.67377281
H	-3.79509922	-2.66383545	3.71201271
H	-2.17372812	-4.18875994	-0.81108364
H	0.04438663	-4.29682333	-0.99843629
H	-3.20967608	-2.21231532	-1.72583690
H	-4.06661491	-2.72476305	-0.54853473
H	-3.03000277	1.50094309	2.64584811
H	-1.99069897	0.01864932	1.47494616
H	-3.28443236	0.12153847	-2.51442317
H	-1.97497605	-0.53575716	-3.08593909
H	-6.60555575	2.65188105	2.89480994
H	-6.35285235	0.77189882	1.29671059
H	-3.65540894	4.11712214	-1.13169406
H	-4.40821134	3.92239389	-2.42809298
H	-7.01177731	2.33059283	-1.20107170
H	-7.81040998	1.37363771	-2.16013900
H	-5.88829410	4.14592236	-0.74748100
H	-6.41382980	3.44425791	0.54480953
H	-5.12686753	2.49030425	2.44308438
H	-2.80793041	2.95747224	3.13723772
H	-5.25708412	1.39802214	-2.20842994
H	-4.00443189	1.87035482	-1.43309192
H	-0.48305340	0.23484200	-0.16392975
H	-0.40950956	-0.57024174	-4.96633439
H	1.04902493	-2.46293129	-2.11970454
H	1.57900220	-4.55157733	-1.40434929
H	5.24806840	-1.09215154	-2.14827503
H	6.16735714	-0.49308237	-1.03209326
H	2.35819663	2.08009436	2.77190424
H	2.99278100	2.13317770	1.35976945
H	1.26342817	-3.06614794	0.40711103
H	2.05316718	-2.69579913	1.71418270
H	3.93961798	-3.29084073	-2.59320050
H	3.07991057	-2.01939739	-2.47581309
H	1.29385272	-1.00586818	-1.70220992
H	0.22408469	-0.86134349	-3.57464634
H	3.81744364	-4.87040659	-0.98346337
H	3.58643325	-6.06247797	-1.96541135
H	4.34257842	-3.50204605	0.97626104
H	4.45376509	-2.97225644	-0.47884994
H	1.89479565	0.49561730	-0.09903915
H	1.35445110	-0.91187766	0.46243038
H	4.02411013	-1.88998012	2.61575958
H	3.76387165	-3.23546774	3.37923482
H	5.10260276	2.57074783	-2.68930076
H	5.26317718	1.18550266	-1.97182241
H	4.57740145	3.16219471	2.58925735
H	5.77388163	3.81061763	3.33273870
H	6.82754743	0.86319408	0.63635220
H	7.60984763	-0.45613873	0.95593872
H	6.30435428	2.98724909	1.09563939
H	6.14998742	2.60242874	-0.40811226
H	3.48746907	2.16332721	-0.93884456
H	1.97296184	2.54596395	-0.77981426
H	5.42313033	-0.30925066	1.95503202
H	4.15713773	0.41088491	2.51460352

H	-1.51263204	2.99772894	-2.49816498
H	0.03431845	3.37588799	-3.34692245

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C	-0.01895506	3.87055523	-0.27639895
H	0.02070065	2.92586305	-0.81347636
O	1.01144101	4.01686654	0.62459077
C	0.48833091	1.10427838	2.91107526
H	-0.47345855	0.55934698	2.83364752
O	1.41036583	0.78691096	3.56773732
O	-1.04726948	-3.84522602	1.56574405
H	-1.77933305	-3.32306624	1.90125607
H	-1.42516737	-4.39970979	-0.15392647
O	-6.83758391	-0.34820747	0.53084073
O	-3.27528593	2.77820056	0.14496805
H	-5.88996489	-1.69847366	0.56691749
H	-7.05019198	0.08087701	-0.30791308
H	-2.55294528	2.14010278	0.02869256
H	-3.56315699	2.68611557	1.05941380
O	-1.57834470	0.65483736	-0.14161195
O	-5.34274225	-2.51603820	0.58742116
H	-0.28227376	-3.26793210	1.46579493
H	-1.92662679	0.26680144	-0.96992652
H	-5.93651439	-3.25106435	0.45514891
H	-4.14796956	-2.58609268	1.82667666
O	-3.43225475	-2.51881515	2.48725561
H	-2.79355400	-0.85850184	2.46196403
H	-3.73260086	-2.95019508	3.28271974
O	-1.49147074	-4.48060863	-1.11600504
H	-2.24026334	-3.92328801	-1.37953415
H	-0.04472087	-3.91165604	-1.62250108
O	-3.56190654	-2.74355891	-1.68647322
H	-3.28484323	-1.87615293	-2.00824072
H	-4.15736331	-2.59236830	-0.94881973
O	-2.45676482	0.03905485	2.32490001
H	-3.42142795	1.28907746	2.73057836
H	-2.20151783	0.11806635	1.38684812
O	-2.70570875	-0.18708111	-2.42899010
H	-3.41084549	0.47271810	-2.53116564
H	-2.09210260	-0.10537148	-3.17841592
O	-6.58729595	1.93054109	2.21311895
H	-7.16696091	2.00751409	2.96649759
H	-6.76573081	0.36042830	1.17912162
O	-4.89135547	4.62471380	-1.22109243
H	-4.17351665	4.19858702	-0.74080262
H	-4.88073731	4.20175420	-2.07944858
O	-7.32151559	1.30425099	-1.66460597
H	-7.39771271	2.14660017	-1.16044454
H	-8.05044534	1.25102643	-2.27620583
O	-7.17905590	3.44222456	-0.14533347
H	-6.43425556	3.98695759	-0.44206822
H	-6.96487562	3.09823979	0.72712418
O	-3.95453426	2.11646423	2.82168931
H	-5.67277891	2.00455424	2.53536907
H	-3.58175864	2.62852292	3.53440280
O	-4.59798670	1.75498831	-2.18344187
H	-5.52707881	1.49955788	-2.14462750
H	-4.34679008	2.02365204	-1.29347679
H	-0.61583521	0.52176850	-0.13341253
O	-0.71969518	0.02521627	-4.26682215
H	-0.71601036	-0.38009674	-5.12876269
O	0.83056824	-3.46911644	-1.74284312
H	0.94167742	-1.88776148	-2.38004317
H	1.45194928	-4.06710024	-2.17604309
O	5.77586296	-0.01265897	-2.27505665
O	4.12792145	1.31223628	2.72109995
H	5.16276342	-0.69106521	-2.58734962



H	6.28849328	-0.37809781	-1.54360686
H	3.38297604	1.16529013	3.30529497
H	3.73795385	1.59517249	1.87530255
O	1.29116562	-2.43188794	0.75001946
O	3.81462396	-1.84740874	-2.88877147
H	1.23824926	-2.88639504	-0.10976826
H	2.11525279	-2.71560886	1.17295522
H	3.70005433	-2.68834536	-3.33658027
H	2.93392088	-1.44034121	-2.85668018
O	1.20694690	-0.98208580	-2.63759854
H	1.17596945	-0.47085040	-1.81529476
H	0.03626878	-0.33530125	-3.77120808
O	3.08044523	-4.67168154	-2.85885276
H	3.64999762	-4.56636138	-2.07236532
H	3.24021740	-5.53341433	-3.23206903
O	4.55538818	-3.71784705	-0.87215645
H	4.31394010	-3.65461958	0.05957527
H	4.41634713	-2.84882944	-1.25916101
O	1.08071775	0.11336327	-0.08643057
H	1.81978411	0.71245629	0.09688530
H	1.24436747	-0.75315628	0.33414305
O	3.75616285	-3.17179703	1.75128422
H	4.35429230	-2.40674504	1.93395134
H	3.84508348	-3.78622038	2.47470257
O	4.97509583	2.32958571	-1.47726280
H	4.97994373	2.94681111	-2.20393067
H	5.22741322	1.44433351	-1.84481788
O	6.39406741	2.83178457	2.90811552
H	5.56245583	2.35007842	3.02390172
H	6.31166723	3.67260035	3.34673721
O	7.18052960	-0.46057854	0.10600700
H	7.28011175	0.51019769	0.24063516
H	8.05265157	-0.84557227	0.12425967
O	7.16052997	2.15996813	0.35450396
H	6.96950220	2.49622552	1.24159339
H	6.44662375	2.44226954	-0.22557062
O	2.99175689	2.04007467	0.35718904
H	3.65002942	2.19408274	-0.34382409
H	2.43763173	2.82610681	0.43632486
O	5.35133460	-1.14658326	2.11234142
H	6.01766494	-0.97644603	1.43296039
H	4.97582059	-0.29499633	2.36781494
H	-0.98484712	4.01608168	0.20284189
H	0.10643392	4.68998006	-0.99409836

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C	0.93123487	3.75238444	-1.05974068
H	0.95105034	2.89351756	-1.73046304
O	2.12833353	4.10121534	-0.57164357
C	-1.08254150	2.72859391	0.97697697
H	-1.21537873	1.63364336	0.99384598
O	-1.83131595	3.53975525	1.36865612
O	-1.90710610	-2.91768975	2.76141979
H	-2.71705217	-2.40286373	2.74359400
H	-2.00779328	-3.94123705	1.23250291
O	-7.08596722	-0.41011901	-1.15427059
O	-3.13792752	2.67840827	-2.18102507
H	-6.18618746	-1.54556879	-0.40454124
H	-6.95501413	-0.26150286	-2.10103005
H	-2.26155115	2.31519675	-1.98740536
H	-3.63506291	2.59937956	-1.35688362
O	-0.96671091	1.14239374	-1.55176525
O	-5.60225771	-2.21785034	0.02191364
H	-1.17012026	-2.33523551	2.54654708
H	-1.25890579	0.39474929	-2.09668950
H	-5.98631181	-3.07570127	-0.14086267
H	-4.94788765	-1.88986847	1.64320994

O	-4.46745139	-1.60712165	2.44079951
H	-3.44014855	-0.22101801	1.72811476
H	-5.07997112	-1.62363242	3.17059120
O	-1.95565313	-4.18535788	0.29656660
H	-2.31002158	-3.41414982	-0.16623558
H	-0.31017279	-4.09700096	0.01187992
O	-2.95411333	-1.79119775	-0.75207528
H	-2.67171185	-1.56041603	-1.65596232
H	-3.90355715	-1.95670266	-0.74578905
O	-2.98123096	0.28357855	1.04757117
H	-3.90704912	1.58476809	0.60332693
H	-2.82603527	-0.36283335	0.33613908
O	-2.01066132	-0.89056977	-3.08774832
H	-2.65757848	-0.41446893	-3.63913916
H	-1.30840112	-1.27960081	-3.63085884
O	-6.98055670	2.26418909	-0.24845213
H	-7.55615477	2.65130020	0.40536458
H	-7.15002340	0.46662974	-0.75855690
O	-4.70627559	4.44197460	-3.55055687
H	-3.97955159	3.93659710	-3.15972006
H	-4.46639537	4.63167789	-4.45289083
O	-6.66656390	0.43483446	-3.78424768
H	-6.82237166	1.38934735	-3.59192785
H	-7.24496362	0.18732593	-4.50048198
O	-6.95749637	2.92578134	-3.01766859
H	-6.22636644	3.52497391	-3.23156858
H	-7.03310319	2.88864477	-2.05923336
O	-4.36330634	2.41663020	0.33768743
H	-6.06168952	2.36859894	0.06034618
H	-3.94256375	3.11353806	0.84011643
O	-3.86575460	0.73670626	-4.12591652
H	-4.80392208	0.52087460	-4.09792701
H	-3.73042592	1.45551612	-3.49715203
H	-0.22539855	0.82754013	-1.01977222
O	0.29717182	-1.85754103	-4.14523272
H	0.48342093	-2.63285477	-4.66555371
O	0.62717746	-3.80726225	-0.03973703
H	1.13397105	-2.64125303	-1.20725520
H	1.21582575	-4.57079076	0.00911426
O	6.13985464	-1.46110129	-0.31616434
O	3.69597716	2.15700883	2.99352500
H	5.46037122	-2.11274748	-0.53368523
H	6.34624974	-1.53333485	0.62342447
H	2.88512231	2.45981463	3.39358066
H	3.53231605	2.05252788	2.03356995
O	0.57746735	-1.79084749	1.84579049
O	3.96740865	-3.07396386	-0.80980161
H	0.67155761	-2.55835162	1.25655746
H	1.22485531	-1.91130902	2.55538302
H	3.78239218	-4.01169609	-0.89681964
H	3.22041887	-2.61027415	-1.22058824
O	1.60424885	-1.96608321	-1.73186262
H	1.47859097	-1.13722854	-1.24693248
H	0.83898939	-1.90971296	-3.34052875
O	2.78339653	-5.54652861	0.14269674
H	3.15975654	-5.14727211	0.95110216
H	2.87283988	-6.49297979	0.20191843
O	3.86378276	-3.89891095	1.91028987
H	3.40636360	-3.42682809	2.61607287
H	3.96232087	-3.28381576	1.17788667
O	1.12003301	0.17030387	0.01230520
H	1.92677209	0.67387240	0.19161667
H	0.94282230	-0.42581096	0.76186485
O	2.55545613	-2.23126005	3.73917933
H	3.25371202	-1.53801081	3.81770105
H	2.32773346	-2.51572147	4.62018484
O	5.70765172	1.06706519	-0.73532602
H	5.95971074	1.32018038	-1.61949116

H	5.84669175	0.08906551	-0.65743113
O	6.18782437	3.34908767	3.17740688
H	5.26631403	3.06078824	3.20939052
H	6.19487395	4.29603825	3.07674553
O	6.77530401	-0.96713596	2.37537934
H	7.08613728	-0.06316951	2.13647152
H	7.49676952	-1.41628353	2.80785210
O	7.35685297	1.46017581	1.54518455
H	7.05775654	2.18630798	2.10968874
H	6.88175230	1.53172796	0.71085140
O	3.33170388	1.82629662	0.35843771
H	4.15971104	1.55113224	-0.07541002
H	3.04853126	2.65879646	-0.05174348
O	4.45309406	-0.44511632	3.82993576
H	5.27376503	-0.67703383	3.37234735
H	4.24080708	0.46519742	3.59774909
H	0.33670600	3.36826461	-0.16212524
H	0.35491199	4.58666721	-1.45852831

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C	-0.07944627	2.48746113	-2.27102478
H	0.61702237	1.71809084	-2.57714195
O	0.51525457	3.20078838	-1.19742014
C	-1.29323545	5.21337343	0.47962077
H	-0.10569333	3.82168859	-0.81885906
O	-1.90358765	5.70863934	1.28071483
H	-1.08843258	-3.85773101	2.11236291
H	-1.82552851	-3.29942215	2.37059413
H	-1.41426554	-4.58689241	0.45612627
O	-6.60514755	-0.12006045	0.61127638
O	-2.85668269	2.64290589	0.23505625
H	-5.78257956	-1.56021084	0.76759727
H	-6.78256156	0.27888843	-0.24914859
H	-2.22057561	1.90508408	0.19107933
H	-3.19231263	2.64241518	1.13939247
O	-1.45064089	0.34754834	0.15709167
O	-5.33771110	-2.43019310	0.86996754
H	-0.31608226	-3.29880772	1.97401747
H	-1.81971740	-0.09312609	-0.63059217
H	-6.01575969	-3.09552672	0.78213554
H	-4.18882990	-2.52261256	2.17532788
O	-3.50185837	-2.47742671	2.86508912
H	-2.79848172	-0.80876238	2.86948347
H	-3.84265968	-2.91411384	3.64090777
O	-1.45770923	-4.77664403	-0.49232890
H	-2.18096330	-4.22958129	-0.83521359
H	0.03933421	-4.34292350	-1.01551898
O	-3.47950951	-3.04407299	-1.27748070
H	-3.16900525	-2.21475875	-1.66202389
H	-4.09028477	-2.80524026	-0.57616954
O	-2.41049578	0.05790505	2.69497115
H	-3.24168020	1.38760040	2.91246989
H	-2.04502834	0.02931862	1.79527994
O	-2.53593651	-0.56475189	-2.16073806
H	-3.18239238	0.14432996	-2.30686434
H	-1.88875747	-0.53438922	-2.88387452
O	-6.29048969	2.23285999	2.17843927
H	-6.89888670	2.37757329	2.89834110
H	-6.50817181	0.61486914	1.22637173
O	-4.17620856	4.55142593	-1.28044267
H	-3.58429089	3.97773330	-0.77912893
H	-4.20837816	4.15553454	-2.15021018
O	-6.96246662	1.47710819	-1.66552120
H	-6.96589642	2.34808516	-1.20708710
H	-7.68675577	1.45792955	-2.28444553
O	-6.64116089	3.67334880	-0.25579816
H	-5.83498144	4.12623994	-0.54270815

H	-6.49710266	3.35111053	0.63989589
O	-3.70139982	2.27086105	2.90076373
H	-5.38764626	2.26368596	2.54364484
H	-3.31723940	2.80943955	3.58719759
O	-4.19712708	1.58704368	-2.08511020
H	-5.15203029	1.45157937	-2.08408118
H	-3.95883546	1.87111447	-1.19693518
H	-0.48742621	0.21268544	0.11923472
O	-0.50540185	-0.45475897	-3.98496249
H	-0.56065008	-0.83837283	-4.85514257
O	0.92852335	-3.93705002	-1.15529168
H	1.06010876	-2.46879699	-2.04132866
H	1.56417124	-4.59411789	-1.46161128
O	5.76882455	-0.32306203	-1.94563341
O	3.43031223	1.82497050	2.53546311
H	5.22002729	-1.08250220	-2.18130966
H	6.22139043	-0.52065084	-1.11721714
H	2.68004028	1.75351494	3.11976820
H	3.08775730	1.97611085	1.63103555
O	1.31507277	-2.60820825	1.21612843
O	3.96952214	-2.37477756	-2.36903869
H	1.29185915	-3.16656141	0.41910248
H	2.11730457	-2.82744465	1.70917633
H	3.92155228	-3.27495712	-2.69698555
H	3.06860070	-2.01800269	-2.44333877
O	1.33532354	-1.59288460	-2.37689725
H	1.28282015	-1.01384473	-1.59792134
H	0.21029488	-0.91401302	-3.50808963
O	3.28832453	-5.20710928	-1.92908745
H	3.80348946	-4.94618845	-1.14254711
H	3.51955269	-6.10433676	-2.15031698
O	4.64449202	-3.87949711	-0.05925470
H	4.39544561	-3.66927127	0.84792816
H	4.49356065	-3.09053943	-0.58811448
O	1.16600730	-0.23464535	-0.02017942
H	1.83652874	0.45479502	0.08315395
H	1.34004733	-0.99727268	0.56284076
O	3.76368787	-2.97637598	2.44471291
H	4.18665062	-2.08918740	2.50616992
H	3.91353961	-3.42897931	3.26992318
O	4.84489793	2.09639151	-1.63305007
H	4.86778648	2.58443197	-2.45182244
H	5.14340169	1.17405679	-1.83086251
O	5.69014111	3.41153099	2.67583914
H	4.85376490	2.93830219	2.77583727
H	5.54207710	4.32200138	2.91170775
O	6.95166747	-0.23153253	0.60079425
H	7.01463243	0.75124854	0.56010043
H	7.82344083	-0.57130078	0.78420181
O	6.82256881	2.38273820	0.37847091
H	6.49906607	2.83643386	1.16879950
H	6.16874844	2.50890547	-0.31741462
O	2.65409617	2.05280436	-0.00289245
H	3.40446096	2.10717904	-0.61897726
H	1.91683832	2.55984321	-0.38424137
O	4.91516810	-0.62558580	2.45961105
H	5.65204135	-0.51511430	1.84240265
H	4.44051188	0.21047905	2.50627649
H	-1.00435056	2.01132901	-1.96583531
H	-0.26853990	3.14508572	-3.11533616

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C	-0.17115466	3.25923229	-1.84197754
H	-0.01365727	2.51379578	-2.63448613
O	1.08011407	3.68887011	-1.47434568
C	0.38578740	0.78544421	3.17163704
H	-0.51226151	0.13781972	3.16120601

O	1.42615099	0.53677248	3.65982278
O	-1.14675699	-3.95215159	1.45966798
H	-1.89556975	-3.45366391	1.79413634
H	-1.47626941	-4.39552832	-0.29813872
O	-6.84538846	-0.30597276	0.43617663
O	-3.28404117	2.73238014	0.56513789
H	-5.92267501	-1.66999023	0.37775661
H	-7.00699516	0.21429730	-0.36122954
H	-2.51940970	2.14742291	0.45699926
H	-3.60646591	2.57376907	1.45854319
O	-1.53596979	0.65024211	0.17156015
O	-5.38816964	-2.49566292	0.34119488
H	-0.37908042	-3.37095977	1.42993038
H	-1.87459179	0.35005587	-0.69393062
H	-5.98420387	-3.20236797	0.10526658
H	-4.26913328	-2.71257629	1.63581372
O	-3.59540057	-2.72577821	2.34191020
H	-2.91987416	-1.09132393	2.53778473
H	-3.94564833	-3.23842524	3.06546384
O	-1.50956457	-4.42114223	-1.26505417
H	-2.21372534	-3.80730392	-1.52475469
H	-0.02108309	-3.88023942	-1.67018044
O	-3.46302127	-2.54106861	-1.81257221
H	-3.16019527	-1.65427008	-2.04228044
H	-4.11064206	-2.44413561	-1.11026365
O	-2.54238888	-0.19995940	2.52991289
H	-3.51680575	1.02321743	3.00332425
H	-2.23064162	-0.02075502	1.62381836
O	-2.56682532	0.08313696	-2.26176763
H	-3.26955784	0.75281430	-2.31764676
H	-1.90923995	0.27143960	-2.94813883
O	-6.64779967	1.76627521	2.36977384
H	-7.27095951	1.77283903	3.09169108
H	-6.79265781	0.32776302	1.15974405
O	-4.74670759	4.77628610	-0.68076947
H	-4.06028127	4.30507349	-0.19651399
H	-4.69264667	4.41928224	-1.56694976
O	-7.18874599	1.57907278	-1.59462833
H	-7.27798514	2.36086836	-1.00194041
H	-7.89214165	1.60562111	-2.23710754
O	-7.09621959	3.53037869	0.15809148
H	-6.33149868	4.09123271	-0.04321044
H	-6.92882249	3.09201654	0.99787966
O	-4.05559692	1.83927802	3.14634304
H	-5.75367595	1.78710802	2.75185293
H	-3.70780293	2.29001674	3.91116283
O	-4.43567197	2.01527395	-1.91672735
H	-5.37068133	1.78282938	-1.96193322
H	-4.23476621	2.17700753	-0.98717682
H	-0.57448454	0.50641666	0.16078509
O	-0.42002802	0.61198099	-3.89679822
H	-0.39735509	0.50358487	-4.84324855
O	0.86727557	-3.45236010	-1.73246164
H	0.99513786	-1.85493135	-2.34631949
H	1.50148168	-4.05768474	-2.13531196
O	5.96648240	-0.13493460	-2.26290501
O	3.85705370	1.60587404	2.51598963
H	5.31091149	-0.79833320	-2.51585486
H	6.43346003	-0.45513793	-1.48158716
H	3.12733066	1.37676277	3.09422430
H	3.46745101	1.89224770	1.67338102
O	1.23856848	-2.50809945	0.82413440
O	3.88707779	-1.87986480	-2.72193711
H	1.21771286	-2.93164039	-0.05233089
H	2.05110988	-2.79367032	1.26724384
H	3.74249330	-2.72685155	-3.15069537
H	3.02489995	-1.43721449	-2.70271995
O	1.28017472	-0.93575642	-2.52053679

H	1.22524644	-0.49870915	-1.65577053
H	0.24014986	0.00174586	-3.51430208
O	3.16113147	-4.67960907	-2.71805628
H	3.69913981	-4.58712096	-1.90826992
H	3.34326049	-5.53064829	-3.10530404
O	4.57399163	-3.74551107	-0.67577804
H	4.31755872	-3.67116908	0.25064404
H	4.46229577	-2.87459038	-1.06732861
O	1.09870208	0.05159766	0.04906240
H	1.85684658	0.64559894	0.14463367
H	1.27255595	-0.81615495	0.46168105
O	3.70001776	-3.10834971	1.90716271
H	4.20905917	-2.26934700	2.00709738
H	3.83380847	-3.62437039	2.69723037
O	5.12875451	2.22803259	-1.56573057
H	5.14465753	2.83472991	-2.30131327
H	5.41076636	1.34156482	-1.90632584
O	6.19741071	2.98809205	2.83892265
H	5.32857966	2.56453389	2.88710769
H	6.11533601	3.86596186	3.19805205
O	7.18792293	-0.43373409	0.24219313
H	7.30091689	0.54028543	0.34472275
H	8.03633647	-0.84290083	0.38917406
O	7.18313302	2.18763545	0.39582255
H	6.91909629	2.55418182	1.25174195
H	6.50611686	2.43004405	-0.24444248
O	2.91004585	2.10987375	0.01110988
H	3.68508149	2.12916693	-0.57879363
H	2.28038911	2.74303456	-0.35367911
O	5.07732188	-0.89897959	2.00759424
H	5.83624039	-0.78957507	1.41888663
H	4.71288239	-0.02564152	2.19302912
H	-0.68199040	2.74952291	-1.02820053
H	-0.76994013	4.06732324	-2.25787687

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r_dHa2_hco_ch3o W33			
C	0.68897681	3.94113570	-1.55583009
H	0.43834394	3.06196468	-2.16374066
O	2.05804166	3.93853399	-1.45246294
C	-0.15244252	1.68156382	2.03200761
H	-0.65392478	0.70773104	1.87988961
O	-0.57803142	2.72707223	1.70009166
O	-1.81356306	-3.09124183	2.73174789
H	-2.64297441	-2.60870167	2.74793026
H	-1.87145759	-4.11854095	1.19204122
O	-6.67112748	0.08203368	-0.83391194
O	-2.62893963	2.57730220	-2.10746640
H	-5.92968826	-1.26719649	-0.31146013
H	-6.66340942	0.26420505	-1.78424163
H	-1.78676031	2.08632788	-2.05696435
H	-2.98364140	2.55892537	-1.21029392
O	-0.47621886	1.00908260	-2.04090511
O	-5.45361256	-2.07372119	0.00362161
H	-1.11150446	-2.47154216	2.50566741
H	-0.87068137	0.22904407	-2.46158262
H	-5.98831462	-2.82985407	-0.22452254
H	-4.83815092	-1.93218925	1.64965598
O	-4.34923247	-1.71856657	2.46426352
H	-3.16767005	-0.47122336	1.78142054
H	-4.97785044	-1.66104750	3.17801795
O	-1.78498133	-4.35821184	0.25802863
H	-2.14844873	-3.59737134	-0.21385667
H	-0.12811545	-4.22519657	0.02161388
O	-2.76270764	-1.94010326	-0.78067413
H	-2.48612749	-1.69112890	-1.68212955
H	-3.72336945	-2.01670252	-0.75976610
O	-2.56392821	-0.03549742	1.16898386

H	-3.09554621	1.48546688	0.78529940
H	-2.48801877	-0.65506250	0.42037187
O	-1.88132708	-1.06664369	-3.16076461
H	-2.54682136	-0.56304582	-3.66017894
H	-1.26868156	-1.53938123	-3.74299579
O	-6.00583965	2.65966874	0.16380100
H	-6.49464970	3.09462218	0.85723224
H	-6.50106892	0.92600159	-0.40049935
O	-3.92648153	4.58537604	-3.38239601
H	-3.30130580	3.93913800	-3.01904540
H	-3.73591654	4.67162811	-4.31194458
O	-6.50836169	0.95461825	-3.47045576
H	-6.47543972	1.91108994	-3.23316798
H	-7.20674680	0.83915316	-4.10877273
O	-6.29355936	3.41400144	-2.58140785
H	-5.52370434	3.91350384	-2.89473385
H	-6.21483117	3.33432151	-1.62590088
O	-3.35623535	2.41409757	0.59062630
H	-5.06670037	2.65475008	0.42126216
H	-2.69339738	2.95940513	1.01317304
O	-3.71547965	0.72833261	-3.96514706
H	-4.67429220	0.66233655	-3.91963888
H	-3.46310067	1.41436428	-3.33498116
H	0.03013756	0.69109045	-1.28301936
O	0.32309463	-2.23326191	-4.21542937
H	0.51405357	-3.05209555	-4.66195884
O	0.79532111	-3.89297072	-0.00967243
H	1.26940864	-2.78697247	-1.25628641
H	1.42047080	-4.62341909	0.07820246
O	6.16904351	-1.19174166	-0.14828315
O	3.06418421	2.19248053	2.74668768
H	5.53130565	-1.87786719	-0.38412931
H	6.30358185	-1.20876958	0.80686705
H	2.13096724	2.23394970	2.95126459
H	3.12484483	2.11291460	1.77514975
O	0.62373498	-1.83871289	1.81903000
O	4.11338801	-2.96025550	-0.71102693
H	0.74961078	-2.61752922	1.24946150
H	1.23494221	-1.94335926	2.56373700
H	4.01706603	-3.91352232	-0.76588821
H	3.35916888	-2.58940552	-1.19533808
O	1.70492599	-2.12178041	-1.82109641
H	1.55018759	-1.27848434	-1.37254187
H	0.88685761	-2.19554134	-3.42564757
O	3.04863250	-5.48896339	0.27725731
H	3.37796984	-5.04316344	1.08186785
H	3.20197022	-6.42487552	0.36595127
O	3.97481983	-3.73351511	2.02790220
H	3.47410333	-3.29231653	2.72439401
H	4.04204595	-3.11780162	1.29286247
O	1.19921405	0.02406326	-0.08744077
H	1.98327055	0.57697985	0.03990100
H	1.06732746	-0.55828054	0.68075300
O	2.49472748	-2.17357556	3.81251721
H	3.10530052	-1.39960665	3.89104461
H	2.25157228	-2.44943687	4.69196445
O	5.73068212	1.30922388	-0.71853012
H	6.07266939	1.54787085	-1.57597697
H	5.89258206	0.34091844	-0.59079804
O	5.35399520	3.63883782	3.25091962
H	4.45816018	3.28067455	3.20495269
H	5.29178590	4.58872592	3.23294552
O	6.57135366	-0.54151234	2.55785936
H	6.80115338	0.38948600	2.33025352
H	7.30249791	-0.90789657	3.04825563
O	6.94657516	1.93646355	1.76510601
H	6.47273708	2.60977031	2.27250705
H	6.59844849	1.94595538	0.86759949

O	3.20765761	1.89835880	0.07879282
H	4.09835466	1.69770116	-0.26170681
H	2.86016714	2.63861808	-0.43736150
O	4.13975096	-0.16858084	3.86584200
H	5.00317082	-0.33863657	3.46334261
H	3.81660580	0.67004164	3.51620376
H	0.21907319	3.77726254	-0.58603379
H	0.31247334	4.83641212	-2.04437260

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ts_dHal_hco_ch3o W33			
C	-0.55068362	2.81314687	-2.39099815
H	-0.41517307	1.96871199	-3.08179893
O	0.33709256	2.58248213	-1.36712543
C	0.03153961	2.98671352	1.56623235
H	0.02409328	2.90312697	0.44406453
O	-0.78200383	3.47479049	2.24419421
O	-1.08226701	-3.80351727	2.09460921
H	-1.81648288	-3.26702653	2.40405976
H	-1.40922799	-4.51677043	0.43850593
O	-6.58350622	-0.09097818	0.74095600
O	-3.03544173	2.53834880	0.00677134
H	-5.72299861	-1.50623263	0.85754393
H	-6.82337229	0.26602304	-0.12308858
H	-2.35131302	1.84745768	0.00991793
H	-3.31985146	2.60735708	0.92688958
O	-1.42530087	0.36347085	0.04987424
O	-5.25596802	-2.36820290	0.93041208
H	-0.32709642	-3.22450020	1.94552914
H	-1.79469902	-0.07707378	-0.73613843
H	-5.92243534	-3.04659796	0.85310230
H	-4.12347724	-2.44505317	2.24603727
O	-3.43432261	-2.39323183	2.93345009
H	-2.71091639	-0.71819856	2.85559049
H	-3.79403837	-2.76722386	3.73304520
O	-1.44955931	-4.70159133	-0.51151138
H	-2.18298623	-4.16592859	-0.85066957
H	0.02816979	-4.24416958	-1.04897776
O	-3.48984990	-2.99086953	-1.28793497
H	-3.17999018	-2.18035847	-1.70893866
H	-4.05909018	-2.72316707	-0.56195468
O	-2.32947783	0.13711684	2.62474964
H	-3.15476536	1.51467840	2.79937433
H	-1.99323852	0.06188018	1.71887255
O	-2.56311822	-0.52646889	-2.26202204
H	-3.25909111	0.13556836	-2.40575864
H	-1.91094096	-0.43446489	-2.97156734
O	-6.22358415	2.33719987	2.18987733
H	-6.79882451	2.51146174	2.93018902
H	-6.45606385	0.66995865	1.31804109
O	-4.40592127	4.42748562	-1.56403195
H	-3.74396352	4.01901183	-0.99700104
H	-4.46766441	3.82629428	-2.30720846
O	-7.11069716	1.33946626	-1.60593881
H	-7.10676387	2.22958029	-1.18400765
H	-7.88693782	1.26912897	-2.15419395
O	-6.77227374	3.59908496	-0.30970145
H	-5.99731145	4.05028576	-0.67549688
H	-6.56168449	3.33468220	0.59198875
O	-3.60504465	2.39508604	2.74775612
H	-5.30551210	2.40655059	2.50925077
H	-3.02852217	3.02988315	3.16710298
O	-4.37916082	1.50472128	-2.20623664
H	-5.32368157	1.31432413	-2.16366815
H	-4.11729669	1.78958603	-1.32094318
H	-0.46003791	0.27635948	-0.00201396
O	-0.42847816	-0.16632666	-3.97242977
H	-0.41126258	-0.43684920	-4.88606107



O	0.91254863	-3.83089652	-1.20422854
H	1.03707496	-2.35613702	-2.09768764
H	1.55458565	-4.49281009	-1.48409974
O	5.94416304	-0.44465279	-1.85841438
O	3.27340403	1.97945722	2.29973368
H	5.31878559	-1.14491643	-2.08898065
H	6.28934125	-0.62374503	-0.97548063
H	2.42167954	2.03603728	2.72852856
H	3.10890373	2.09872483	1.34736035
O	1.28798858	-2.51867000	1.18033579
O	3.96100053	-2.31345368	-2.29197115
H	1.27078553	-3.07446331	0.38168968
H	2.05940549	-2.76869704	1.70706075
H	3.89137360	-3.22867199	-2.57454182
H	3.07895953	-1.92987753	-2.41633468
O	1.31849672	-1.47330607	-2.40848155
H	1.28401592	-0.91998929	-1.60988545
H	0.24994136	-0.68921393	-3.50137124
O	3.30634521	-5.11095091	-1.87263054
H	3.79150268	-4.87139079	-1.06089622
H	3.55400310	-5.99786650	-2.11673205
O	4.59327735	-3.80485457	0.05921218
H	4.33595768	-3.61063596	0.96775523
H	4.44563071	-3.00738481	-0.45622763
O	1.23764884	-0.14316707	-0.03018326
H	1.98303611	0.46562316	-0.00273395
H	1.38450065	-0.91590776	0.54876149
O	3.64755870	-2.92144207	2.54080790
H	4.02038790	-2.01305361	2.60819090
H	3.73997913	-3.34343020	3.39022472
O	5.21819611	2.04622432	-1.77557812
H	5.37798520	2.49226722	-2.60283070
H	5.47301134	1.09517958	-1.89425299
O	5.59695731	3.44290696	2.61663861
H	4.72708188	3.02605767	2.66786277
H	5.51509008	4.33937226	2.92629957
O	6.85411235	-0.28501295	0.79347970
H	6.98766833	0.68904216	0.72606415
H	7.67890759	-0.67238795	1.07456198
O	6.92567052	2.32184624	0.47735979
H	6.53263758	2.81497913	1.21045424
H	6.37660689	2.46326907	-0.30045727
O	2.90499387	2.06589470	-0.37082530
H	3.70597030	2.09858433	-0.92387365
H	2.18652792	2.48171654	-0.85391190
O	4.67949457	-0.51786318	2.52008914
H	5.45485614	-0.43206509	1.94803620
H	4.20123429	0.31705535	2.50486794
H	-1.57688886	2.75493237	-2.03519871
H	-0.35715866	3.74774997	-2.91281625

### 3.2.9 HCO + HCO

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M1\_dHa2\_hco\_hco W33

C	-0.64394666	2.88086926	2.62966007
H	-0.01360332	2.91584004	1.73410703
O	-1.39228013	3.76403741	2.94046539
C	-0.46038874	1.66593202	3.50746068
H	-1.28982073	1.42959539	4.17825860
O	0.57045413	1.05126522	3.50266637
H	-1.56081186	-2.90923033	2.20194826
O	-2.21367393	-2.20770469	2.24534065
H	-1.91832381	-3.91934973	0.68706564
O	-6.57430775	0.82259172	-0.69523865
O	-2.45470900	3.09147278	-1.56123267
H	-5.88891032	-0.52684092	-0.06164201

H	-6.58301116	0.95241565	-1.65278287
H	-1.79070415	2.41711509	-1.35731222
H	-2.86391916	3.31939319	-0.71916793
O	-1.09191659	0.80453583	-0.82130270
O	-5.49871132	-1.35355462	0.30590930
H	-0.70081756	-2.51578441	2.01557902
H	-1.47219563	0.23551167	-1.52107320
H	-6.19915516	-2.00057243	0.33818242
H	-4.41413052	-1.19473481	1.62332731
O	-3.74976730	-1.03703930	2.32249457
H	-2.76742555	0.36539382	1.87862726
H	-4.19026647	-1.14040258	3.16172841
O	-1.93438333	-4.29428122	-0.20422771
H	-2.55778003	-3.75323847	-0.71333253
H	-0.35570274	-4.17930511	-0.66945465
O	-3.62545200	-2.56865696	-1.53481797
H	-3.14385904	-1.90096610	-2.04073907
H	-4.24001979	-2.10125844	-0.96462376
O	-2.25089916	1.12346127	1.56602778
H	-3.18830481	2.52926359	1.29231228
H	-1.85818491	0.87752247	0.70376143
O	-2.15844790	-0.60134609	-2.85423314
H	-2.68824987	0.06912077	-3.31678368
H	-1.48162279	-0.94853437	-3.45865358
O	-6.10011365	3.48365663	0.16603075
H	-6.70491843	3.92042566	0.75993540
H	-6.46491545	1.69929599	-0.31090358
O	-3.58263830	4.60191198	-3.63834378
H	-2.98646621	4.28260613	-2.95223232
H	-3.53871534	3.93000661	-4.31812527
O	-6.44886574	1.63342837	-3.35907986
H	-6.43452619	2.60128293	-3.17494994
H	-7.10636543	1.46460002	-4.02800140
O	-6.13157368	4.13139919	-2.62174352
H	-5.27495294	4.44672282	-2.94898210
H	-6.08776098	4.09503261	-1.66140276
O	-3.54995038	3.40203154	1.03457627
H	-5.21552937	3.51046545	0.57145425
H	-3.10616006	4.03613759	1.59762298
O	-3.64689378	1.53534987	-3.62366212
H	-4.60535941	1.43102065	-3.62792170
H	-3.42914143	2.06154701	-2.84577392
H	-0.17590195	0.50369678	-0.69601940
O	-0.10284566	-1.64788189	-4.32009397
H	-0.26180077	-2.43945165	-4.82639243
O	0.60916721	-4.00146094	-0.76872926
H	1.26382429	-2.86622944	-1.82334941
H	1.09261062	-4.84350899	-0.75394954
O	6.07276980	-0.82531639	-1.08264585
O	3.26741732	1.35062706	2.60558497
H	5.44641471	-1.51020304	-1.35363671
H	6.41209730	-1.03388801	-0.20359883
H	2.36678444	1.23302631	2.92178366
H	3.21244818	1.59359414	1.67048723
O	1.04150381	-2.24042477	1.26186737
O	4.30350509	-2.80148390	-1.88627594
H	0.93942184	-2.93751014	0.58619632
H	1.76262737	-2.52909557	1.83977946
H	4.62631882	-3.34862167	-2.59838243
H	3.37880024	-2.56352042	-2.10730874
O	1.72566542	-2.15130066	-2.31260729
H	1.63059490	-1.36419717	-1.75406455
O	0.60895044	-1.85076582	-3.69220621
H	2.34169775	-6.09203564	-0.68320402
H	3.07123708	-5.63758753	-0.22273605
H	2.23566666	-6.95375520	-0.29286288
O	4.21351455	-4.49793202	0.40327356
H	3.93391539	-4.03330009	1.20066592

H	4.29724042	-3.84500559	-0.29965351
O	1.39454091	-0.17279328	-0.40687327
H	2.09523056	0.47187409	-0.26060088
H	1.35814656	-0.81389281	0.33076172
O	3.25740573	-3.10759935	2.67208959
H	3.83599190	-2.33477977	2.87121618
H	3.14623615	-3.59856062	3.48185538
O	5.60607488	1.71519033	-1.14489304
H	5.89908937	2.10766331	-1.96305893
H	5.77379766	0.73848431	-1.20293005
O	5.38794346	2.96637889	3.27755477
H	4.57647689	2.44192747	3.23792800
H	5.67021809	2.99346492	4.18704309
O	7.04214275	-0.73422516	1.53097655
H	7.13664383	0.24584738	1.50545099
H	7.87989653	-1.10306498	1.79740730
O	7.02535212	1.88736767	1.32421994
H	6.51709935	2.34323675	2.01072303
H	6.60310473	2.06780767	0.47907790
O	3.16902857	1.96729248	-0.08819271
H	4.04394882	1.91864163	-0.52560692
H	2.75168506	2.77137385	-0.38738576
O	4.74419692	-0.99789349	3.09376628
H	5.57327394	-0.96011559	2.59917769
H	4.26763487	-0.17655324	2.92292621

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C	0.14563197	4.38826505	-0.06156432
H	-0.27810147	5.25686629	-0.57120457
O	1.17817767	3.87184163	-0.39436415
C	-0.60856446	3.89237812	1.14939265
H	-0.37568741	2.87124678	1.47219664
O	-1.38237809	4.60146953	1.72883290
O	-1.87581460	-3.41226478	1.96048868
H	-2.53541681	-2.71825770	2.03040426
H	-2.05430065	-4.23949226	0.31868734
O	-6.35574647	0.79190746	-1.13221913
O	-1.99841813	2.94374547	-0.96896993
H	-5.82200187	-0.66082059	-0.53496678
H	-6.19055816	1.07309068	-2.04051462
H	-1.60540521	2.04742354	-0.90835808
H	-2.70950639	2.96916483	-0.31289459
O	-1.18387653	0.43085305	-0.65564639
O	-5.54300816	-1.54131601	-0.19820777
H	-1.00331120	-3.00551676	1.93535541
H	-1.46180075	-0.05834135	-1.45653013
H	-6.27989730	-2.13157390	-0.33585201
H	-4.64813413	-1.60382254	1.29452338
O	-4.08355677	-1.57136561	2.08872542
H	-3.07034920	-0.07559454	1.96685153
H	-4.62966596	-1.79020418	2.83878754
O	-1.96112953	-4.52759387	-0.60015184
H	-2.53296161	-3.94698789	-1.12533602
H	-0.33544499	-4.39849326	-0.84500282
O	-3.54785803	-2.70317556	-1.94725014
H	-3.03298269	-2.00934885	-2.37833054
H	-4.18518905	-2.26369481	-1.37935788
O	-2.54407232	0.68982657	1.70241487
H	-3.36897325	2.08909693	1.52058759
H	-2.09461452	0.44620223	0.87723307
O	-1.94000168	-0.67194758	-2.98064846
H	-2.31307614	0.12449680	-3.39060640
H	-1.19208074	-0.98588489	-3.51614848
O	-6.15484539	3.27594419	0.21177229
H	-6.82015545	3.60568505	0.80960945
H	-6.37920010	1.59853352	-0.60587225
O	-2.83913810	5.02785347	-2.58421715

H	-2.39212492	4.30943213	-2.12140667
H	-2.59265361	4.95159982	-3.50290650
O	-5.78267269	2.07544881	-3.56745843
H	-5.77565033	2.98899379	-3.20118186
H	-6.34951402	2.06542740	-4.33365649
O	-5.56339473	4.38369445	-2.33020859
H	-4.66174153	4.73080604	-2.36991029
H	-5.77278988	4.19405042	-1.40958174
O	-3.72353687	2.97255456	1.25689105
H	-5.31822239	3.19379944	0.70701292
H	-3.27589665	3.62616418	1.79481120
O	-3.00458694	1.76741888	-3.56494124
H	-3.96196104	1.80016141	-3.68465365
H	-2.82306469	2.21361407	-2.73625273
O	-0.27553900	0.13882226	-0.45763507
H	0.26344882	-1.64756616	-4.25755165
H	0.15372117	-2.41995040	-4.80492219
O	0.63358810	-4.21974948	-0.80311199
H	1.38198599	-3.01430834	-1.70811053
H	1.11989887	-5.05980213	-0.79388190
O	5.93605424	-0.75181345	-0.48869138
O	2.83669240	1.13105668	3.26612625
H	5.40135526	-1.47391491	-0.84510435
H	6.24017753	-0.99124420	0.39463745
H	1.95340136	1.00964196	3.60532787
H	2.75899446	1.39297075	2.32859351
O	0.83283032	-2.66092168	1.41573833
O	4.42700250	-2.83018959	-1.53807256
H	0.80487508	-3.29548215	0.67391362
H	1.53622172	-2.96209011	2.00742261
H	4.84229639	-3.27769059	-2.27134982
H	3.50866542	-2.62199006	-1.81223337
O	1.86703193	-2.25590498	-2.09979786
H	1.70129255	-1.51813720	-1.49164898
H	0.90281787	-1.87920433	-3.56450607
O	2.40604726	-6.27104317	-0.66674957
H	3.09191425	-5.81181185	-0.14794254
H	2.31570625	-7.15385000	-0.32248104
O	4.17018711	-4.68311363	0.60440084
H	3.83710481	-4.25414957	1.40062412
H	4.31640703	-3.99704363	-0.05602115
O	1.27575829	-0.47695086	-0.08027876
H	1.88678564	0.21261669	0.21142238
H	1.18993568	-1.17146460	0.60166916
O	3.04774309	-3.44005587	2.89360738
H	3.55250840	-2.63874578	3.16112749
H	2.97044145	-3.99702293	3.66366447
O	5.24189075	1.74898672	-0.37126416
H	5.47767305	2.23009088	-1.16006741
H	5.48944648	0.80098244	-0.51088325
O	4.90268935	2.80856470	4.05010384
H	4.11375258	2.25921151	3.96223690
H	5.14521995	2.82329379	4.97121085
O	6.74290790	-0.76067146	2.19172832
H	6.79186985	0.22361154	2.21319691
H	7.58257580	-1.10181868	2.48736623
O	6.62562881	1.86129361	2.09735056
H	6.09311453	2.27607621	2.79019309
H	6.20672009	2.05756219	1.25288862
O	2.74368183	1.74417411	0.64635790
H	3.63167614	1.79449294	0.24477771
H	2.23089795	2.48166572	0.29780043
O	4.36281899	-1.25938509	3.54149261
H	5.22308560	-1.13624541	3.11714161
H	3.87456112	-0.43464905	3.44843996

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C	-0.08823988	4.47893408	-0.30268992
H	-0.60198574	5.07432864	-1.07893692
O	0.95898027	3.95632667	-0.41495019
C	-0.32338633	1.77986281	3.09818158
H	-0.86597932	0.89169782	2.71370359
O	-0.72768889	2.88070878	3.04671165
O	-1.99086215	-3.42145421	1.95754810
H	-2.70054939	-2.77627921	1.97630819
H	-2.12011974	-4.26981784	0.31571525
O	-6.25302161	1.02843313	-1.07462558
O	-2.05446524	2.73283984	-1.27037715
H	-5.85692281	-0.53280985	-0.65879222
H	-6.18241130	1.33839875	-1.98643577
H	-1.60260904	1.87481651	-1.15081378
H	-2.52483926	2.88729063	-0.44130520
O	-1.20601383	0.24251780	-0.82887580
O	-5.66465785	-1.46540650	-0.41493337
H	-1.14941583	-2.95378240	1.93097514
H	-1.46802512	-0.24411574	-1.63577961
H	-6.44718358	-1.97069988	-0.62089204
H	-4.84969053	-1.68088283	1.09486581
O	-4.29908656	-1.68522654	1.90011373
H	-3.15814617	-0.33580664	1.72041207
H	-4.87565960	-1.82357160	2.64631811
O	-2.00783744	-4.54693879	-0.60382710
H	-2.59541623	-3.98516068	-1.13169044
H	-0.38078055	-4.34831263	-0.81310882
O	-3.61411697	-2.77476236	-2.00258087
H	-3.08960485	-2.12376877	-2.48597761
H	-4.27072772	-2.28591639	-1.50164162
O	-2.51557405	0.35746318	1.51658826
H	-3.03324499	1.93168161	1.44681184
H	-2.11218768	0.15145237	0.65314494
O	-1.99981347	-0.82082541	-3.15726364
H	-2.41184028	-0.03426275	-3.54916063
H	-1.24036882	-1.09647237	-3.69583325
O	-5.62439259	3.44911489	0.30882324
H	-6.24850330	3.83612027	0.91703781
H	-6.09102731	1.79835123	-0.51957513
O	-2.47475034	4.96097640	-2.73231321
H	-2.21661066	4.09862051	-2.37635405
H	-2.27970603	4.94352228	-3.66596988
O	-5.87997622	2.30761427	-3.53993238
H	-5.69812243	3.20117631	-3.17364434
H	-6.54026172	2.39504737	-4.22151339
O	-5.23302189	4.54356705	-2.28990904
H	-4.32018913	4.82870868	-2.42856912
H	-5.33658316	4.33224006	-1.35614042
O	-3.19331889	2.89034768	1.29292924
H	-4.78609857	3.31802886	0.78667320
H	-2.59007288	3.35573986	1.87184585
O	-3.15772914	1.59520247	-3.67196408
H	-4.10405765	1.70992848	-3.80674161
H	-2.96083607	2.01178685	-2.82801286
H	-0.28087427	0.01700757	-0.62579873
O	0.30261627	-1.68637170	-4.34300327
H	0.28577758	-2.45097418	-4.91140408
O	0.58059063	-4.14086671	-0.74615221
H	1.33606072	-2.97194551	-1.69436915
H	1.08376771	-4.96976170	-0.69393203
O	5.83607938	-0.66220719	-0.49998947
O	2.88102584	1.47104138	3.28146984
H	5.32047501	-1.40387152	-0.84328266
H	6.11912892	-0.86872255	0.39883864
H	1.98815727	1.53771416	3.62136481
H	2.81288320	1.64979551	2.32513765
O	0.69367403	-2.52637748	1.44642331
O	4.38016568	-2.81169770	-1.48056692

H	0.69415604	-3.17560970	0.71709466
H	1.38596598	-2.80484244	2.06236928
H	4.80944280	-3.30989006	-2.17177149
H	3.47001271	-2.61708693	-1.78779192
O	1.83366936	-2.23414034	-2.10899018
H	1.69846269	-1.48194845	-1.51162112
H	0.90892775	-1.88957870	-3.61228961
O	2.36878309	-6.16717291	-0.48782893
H	3.03543522	-5.68670992	0.03702635
H	2.26089202	-7.03342455	-0.10825364
O	4.08475924	-4.52273450	0.77197795
H	3.72919793	-4.05874818	1.53848737
H	4.24207834	-3.87009243	0.08105462
O	1.28708091	-0.41965091	-0.11107259
H	1.84042036	0.31302444	0.19171879
H	1.16386139	-1.07944937	0.59793770
O	2.89715453	-3.20403326	2.98416317
H	3.38967906	-2.38638780	3.22738227
H	2.83019184	-3.73707639	3.77192285
O	5.14063962	1.84387591	-0.48624347
H	5.37627771	2.28998174	-1.29528701
H	5.38335864	0.89011032	-0.58750150
O	4.99792873	3.13281006	3.89956984
H	4.19533998	2.59557129	3.85072156
H	5.25580534	3.18863368	4.81474381
O	6.59317419	-0.59225298	2.19091375
H	6.68044992	0.38945557	2.15877482
H	7.42087548	-0.94773372	2.50305641
O	6.59945390	2.02158458	1.94676724
H	6.11540749	2.49821660	2.63626002
H	6.15923963	2.19608726	1.10868689
O	2.67406921	1.86658446	0.61079472
H	3.53910169	1.92380067	0.16349714
H	2.14482280	2.61122953	0.31372076
O	4.21130843	-1.01205010	3.57943056
H	5.06665962	-0.90504392	3.14143377
H	3.74800392	-0.16910364	3.51515491

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C	0.06650300	3.29147300	0.84141000
H	-0.33321500	2.46737300	0.22434100
O	-0.56395600	4.02001600	1.50902800
C	0.36128100	0.70345700	2.86675000
H	-0.67665000	0.38052100	2.66314600
O	0.99032200	0.55551500	3.84653000
O	-1.80386000	-2.97904800	2.32208900
H	-2.51283700	-2.33202700	2.31915800
H	-2.06845400	-3.97903400	0.77201100
O	-6.63466100	0.84260000	-0.75641900
O	-2.45627300	2.92291400	-1.62607700
H	-6.08419000	-0.60704100	-0.21746900
H	-6.62645400	1.03733300	-1.70312700
H	-1.86691100	2.16955300	-1.47727600
H	-2.88076100	3.08595900	-0.77473200
O	-1.19139800	0.59629700	-0.89032600
O	-5.76839500	-1.48246800	0.10585300
H	-0.96675500	-2.52333300	2.19237000
H	-1.55378200	0.02674200	-1.60384800
H	-6.51065000	-2.08033400	0.06662600
H	-4.75778600	-1.41718900	1.49344000
O	-4.12171200	-1.26784600	2.21917900
H	-3.06999300	0.08123700	1.76537600
H	-4.61230400	-1.27439700	3.03667600
O	-2.02538000	-4.32426000	-0.12942600
H	-2.66438600	-3.81411500	-0.65158500
H	-0.44534100	-4.08170500	-0.50252900
O	-3.73851300	-2.70382800	-1.54344200

H	-3.26444500	-2.04704700	-2.06989200
H	-4.41953200	-2.23916000	-1.05176100
O	-2.44302800	0.77224300	1.50693800
H	-3.10432900	2.29635900	1.30155600
H	-2.07186300	0.53757800	0.63822900
O	-2.26737600	-0.76745700	-2.90453200
H	-2.79417000	-0.08397200	-3.35561300
H	-1.58395600	-1.10398100	-3.50703200
O	-5.98533600	3.40894900	0.30068400
H	-6.55326900	3.83440900	0.93759600
H	-6.45418300	1.67644400	-0.30936200
O	-3.43535000	4.96058300	-3.18828000
H	-2.88259400	4.29868400	-2.75417500
H	-3.23123800	4.92769800	-4.11886100
O	-6.46109700	1.78624500	-3.37592200
H	-6.36004200	2.73306800	-3.12461800
H	-7.15724900	1.72406000	-4.02385600
O	-6.00024100	4.19830600	-2.44616600
H	-5.14558100	4.56512200	-2.71687600
H	-5.98814300	4.10500400	-1.48858200
O	-3.39612300	3.19280500	1.02388900
H	-5.08411000	3.40092200	0.66736300
H	-2.79190100	3.81430100	1.42853400
O	-3.69106300	1.38446600	-3.69751300
H	-4.65380000	1.38664600	-3.72840000
H	-3.44377400	2.00066900	-3.00109000
H	-0.26650000	0.33262600	-0.74597600
O	-0.12636600	-1.75530200	-4.27955400
H	-0.20608400	-2.56640300	-4.77336000
O	0.51562100	-3.85958500	-0.53988400
H	1.18405400	-2.79234600	-1.65702300
H	1.02192800	-4.68944400	-0.51596900
O	5.87354900	-0.59062100	-1.13257700
O	3.65536200	1.44906800	3.08876400
H	5.29453600	-1.32031900	-1.38945800
H	6.32373600	-0.82541900	-0.31159000
H	2.84525800	1.25967700	3.56634400
H	3.40020200	1.62879700	2.17041800
O	0.83521700	-2.08674700	1.49567500
O	4.24511600	-2.72229800	-1.85219700
H	0.74683400	-2.78686500	0.81831000
H	1.60176700	-2.34211000	2.03113800
H	4.57500500	-3.25655200	-2.57058700
H	3.30725600	-2.52073700	-2.05078400
O	1.64874900	-2.10953300	-2.18856700
H	1.60052700	-1.30518800	-1.65053400
H	0.56188100	-1.89652900	-3.61003100
O	2.24987300	-5.94193800	-0.48704600
H	3.00820300	-5.48823400	-0.07386600
H	2.14883000	-6.79277700	-0.07218000
O	4.16705400	-4.34386400	0.48865900
H	3.86325600	-3.84535900	1.25632500
H	4.26792000	-3.72300400	-0.24072300
O	1.33856200	-0.12736500	-0.28396500
H	1.96566200	0.56151000	-0.02715800
H	1.23708200	-0.75424500	0.45820700
O	3.18830800	-2.89817300	2.71953300
H	3.86292000	-2.19609600	2.87750400
H	3.13642200	-3.41744400	3.51798900
O	5.26935500	1.92914000	-0.97487900
H	5.43289900	2.37799100	-1.80009700
H	5.45994700	0.96715000	-1.11590100
O	5.76822100	3.17393300	3.35186400
H	4.98196000	2.62251000	3.46602100
H	6.13164800	3.35009900	4.21432300
O	7.12351700	-0.63586800	1.35769000
H	7.20326400	0.34591000	1.36751400
H	7.99078500	-1.00081700	1.51084400

O	7.08010500	1.99180600	1.23409900
H	6.71247900	2.46825000	1.99241700
H	6.52849800	2.19696000	0.47309000
O	3.00001200	1.98115100	0.45615000
H	3.79475100	2.05800300	-0.10772700
H	2.51330900	2.80319900	0.40853200
O	4.96876900	-1.01901700	3.09403000
H	5.75277600	-0.98495800	2.53093800
H	4.59188600	-0.13085900	3.11143100

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C	0.25785197	4.27530099	-0.70285410
H	-0.46399337	5.02713238	-1.06166187
O	1.24520401	3.94262755	-1.24610878
C	0.02159195	2.70073089	2.26484988
H	0.01546143	2.67810892	1.15165834
O	-0.69482687	3.34185526	2.93133892
O	-1.40787538	-3.23774756	1.81075740
H	-2.07680778	-2.55982324	1.93021148
H	-1.72484892	-4.14505447	0.23464709
O	-6.15104923	0.87711713	-0.90139581
O	-1.93550232	2.91092726	-1.48612587
H	-5.56565063	-0.57857149	-0.36378786
H	-6.13197206	1.12829524	-1.83329570
H	-1.47140631	2.05472224	-1.39326184
H	-2.40256348	3.05444960	-0.65340370
O	-0.95126393	0.46408490	-1.09857940
O	-5.25184686	-1.45293004	-0.04191450
H	-0.56060444	-2.80406404	1.66100679
H	-1.31085386	-0.06636468	-1.83877563
H	-5.99937139	-2.04449113	-0.08179934
H	-4.22553530	-1.44900353	1.35619343
O	-3.57853934	-1.37503399	2.08237433
H	-2.52012716	0.03926536	1.72940299
H	-4.04723331	-1.50185130	2.90263370
O	-1.71389714	-4.47165387	-0.67605376
H	-2.34416950	-3.92205669	-1.16625581
H	-0.11899422	-4.32748585	-1.08451609
O	-3.45000963	-2.71767237	-1.93384026
H	-2.98104497	-2.05719427	-2.45946582
H	-4.01880750	-2.23778652	-1.32744221
O	-2.00521482	0.77314083	1.36885534
H	-2.77045180	2.19699205	1.27511316
H	-1.67558109	0.49406479	0.49732408
O	-1.97243276	-0.75359722	-3.25160223
H	-2.42639724	0.00938019	-3.64435493
H	-1.27612674	-1.06486200	-3.85297046
O	-5.64282159	3.38707070	0.32606399
H	-6.22896027	3.73975439	0.99020610
H	-6.03866204	1.69439475	-0.40436737
O	-2.80676268	5.07220942	-2.89908234
H	-2.37370033	4.27030399	-2.57940326
H	-2.64042057	5.12237067	-3.83686249
O	-5.96006749	2.05820441	-3.44128725
H	-5.85420297	2.98090612	-3.11908511
H	-6.64742089	2.05085128	-4.10143286
O	-5.47676392	4.39800562	-2.32293440
H	-4.59550622	4.74957587	-2.50820051
H	-5.53349832	4.22945506	-1.37667009
O	-3.08778342	3.11751150	1.09760199
H	-4.75091845	3.32646715	0.71479535
H	-2.64467739	3.67311314	1.73716479
O	-3.20848417	1.61472410	-3.78088140
H	-4.17090188	1.65861544	-3.80932281
H	-2.94462048	2.09962940	-2.99515668
H	-0.01972179	0.20202564	-0.98671153
O	0.15213777	-1.71995807	-4.67526306



H	0.03005001	-2.49981007	-5.20914936
O	0.84587835	-4.13322731	-1.14345357
H	1.50896284	-2.97974616	-2.18160873
H	1.34695118	-4.96347845	-1.10272215
O	6.13052433	-0.66636168	-1.24107036
O	3.13484505	1.56952141	2.43272165
H	5.56692845	-1.39193787	-1.54099233
H	6.42100686	-0.84263198	-0.33831793
H	2.23780284	1.63244182	2.75990019
H	3.09351463	1.73283606	1.47335504
O	1.18726978	-2.43331703	0.95253434
O	4.54923127	-2.77072603	-2.12892421
H	1.11941073	-3.11245776	0.25440847
H	1.90735395	-2.70645035	1.53837178
H	4.94348515	-3.28507105	-2.82925991
H	3.62324062	-2.58920151	-2.39382817
O	1.96088285	-2.24497568	-2.64937181
H	1.84816614	-1.47663408	-2.06753010
H	0.85321154	-1.92245787	-4.03499528
O	2.65720582	-6.14814231	-0.94031496
H	3.35150906	-5.64950506	-0.47190569
H	2.58420238	-7.00597830	-0.53426096
O	4.44277266	-4.45806884	0.16174376
H	4.15584364	-3.99102957	0.95451453
H	4.52686478	-3.81004801	-0.54594743
O	1.56741193	-0.35335901	-0.69083042
H	2.19747581	0.35106308	-0.49315542
H	1.52560867	-0.99907039	0.04180038
O	3.41845429	-3.10918409	2.43397337
H	3.87387247	-2.26328093	2.64924309
H	3.34968013	-3.61082056	3.24183080
O	5.53858793	1.85846542	-1.33236423
H	5.78012891	2.26528477	-2.16012020
H	5.75489221	0.89424216	-1.39443532
O	5.25533142	3.24748445	3.02406293
H	4.45613238	2.70520981	2.98920856
H	5.52004086	3.31401381	3.93677711
O	6.94045547	-0.46976619	1.43071364
H	7.02952683	0.50996572	1.36721596
H	7.77070042	-0.81824077	1.74418337
O	6.93103152	2.13774771	1.12222739
H	6.41098860	2.61389883	1.78508077
H	6.51500158	2.28124646	0.26617708
O	3.07153575	1.92940493	-0.25634689
H	3.94708263	1.95723044	-0.68662564
H	2.54177195	2.63306890	-0.63865073
O	4.61103411	-0.82172391	2.91479683
H	5.44782171	-0.71390681	2.44218599
H	4.09445757	-0.02009598	2.77905779

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M2\_dHa2\_hco\_hco W33

C	0.46911479	3.53722852	0.86543953
H	0.02687981	-0.34975800	2.59803952
O	-0.41879430	3.92534660	1.43161692
C	-0.19499333	0.45054404	3.30591481
H	-1.11555552	0.36302564	3.88398374
O	0.55391275	1.38199358	3.47137782
O	-1.72205197	-3.03685793	2.28278500
H	-2.40147242	-2.36072199	2.22266702
H	-2.02606065	-4.07455057	0.73463471
O	-6.57783474	0.82976060	-0.74977865
O	-2.33553894	3.02263015	-1.44762417
H	-5.99178861	-0.60423915	-0.22137285
H	-6.54933785	1.04990861	-1.69041637
H	-1.72229946	2.28520434	-1.30086557
H	-2.76002708	3.17558717	-0.59581305
O	-1.09698968	0.67085147	-0.82969742

O	-5.65673623	-1.47047407	0.10919732
H	-0.87002402	-2.63824963	2.07948010
H	-1.47489054	0.10400578	-1.53330897
H	-6.39286195	-2.07703777	0.10133729
H	-4.59720062	-1.37520265	1.45288240
O	-3.95258423	-1.23512667	2.17347084
H	-2.89183686	0.15198782	1.78370740
H	-4.43221607	-1.29195454	2.99557285
O	-1.99550520	-4.41171271	-0.16957953
H	-2.60534660	-3.86127135	-0.68655312
H	-0.40238674	-4.23352784	-0.56805970
O	-3.63261825	-2.68586963	-1.54750004
H	-3.15822023	-2.01256484	-2.05354461
H	-4.32056120	-2.23418073	-1.05348583
O	-2.27564321	0.86832973	1.57742927
H	-3.00238460	2.33555312	1.43033246
H	-1.88341325	0.67939289	0.70364128
O	-2.18707703	-0.70432709	-2.85576725
H	-2.69717591	0.00586054	-3.28309545
H	-1.51617513	-1.03911060	-3.47249064
O	-5.95569655	3.35228176	0.39977389
H	-6.54183274	3.73937882	1.04455204
H	-6.40392848	1.65197546	-0.27868290
O	-3.35451961	5.03764978	-3.00733690
H	-2.79778997	4.38701591	-2.55961830
H	-3.15861597	4.97257571	-3.93808576
O	-6.34168363	1.87527017	-3.32448019
H	-6.26280080	2.81506156	-3.04103652
H	-7.00261624	1.82514137	-4.00916485
O	-5.92861893	4.26180258	-2.31009734
H	-5.06692502	4.63174572	-2.55425711
H	-5.92975879	4.12766176	-1.35738696
O	-3.38152287	3.21502030	1.19148754
H	-5.06084327	3.34022561	0.78278128
H	-2.88835588	3.87329018	1.67479557
O	-3.55421193	1.51509309	-3.56647581
H	-4.51639992	1.52600819	-3.60877040
H	-3.30589799	2.09511980	-2.83950890
H	-0.17692424	0.38351952	-0.70498740
O	-0.11563369	-1.74559810	-4.31135034
H	-0.26214433	-2.53199496	-4.82915554
O	0.55913660	-4.02339594	-0.62587646
H	1.22385053	-2.94616427	-1.75979407
H	1.06565745	-4.85146485	-0.58159918
O	5.94137455	-0.68136095	-1.10297062
O	3.22698939	1.49101968	2.69345035
H	5.34839667	-1.40059643	-1.35693187
H	6.27326243	-0.84875659	-0.21223787
H	2.31196737	1.48551733	3.00492738
H	3.18791632	1.62927418	1.73527820
O	0.91000949	-2.25492467	1.39733134
O	4.28484096	-2.79433707	-1.83776060
H	0.81992948	-2.94593812	0.71002808
H	1.65234392	-2.53282160	1.95584392
H	4.64471130	-3.33888217	-2.53379197
H	3.35081013	-2.61247305	-2.07129993
O	1.68424190	-2.24930885	-2.27301175
H	1.60587588	-1.45208720	-1.72555607
H	0.58083348	-1.95399604	-3.66849358
O	2.33974500	-6.06322673	-0.48276109
H	3.07244414	-5.57853500	-0.05916565
H	2.26916975	-6.91766570	-0.06921955
O	4.20004227	-4.40148694	0.51029142
H	3.90577094	-3.90785628	1.28442066
H	4.29140577	-3.77815343	-0.21845081
O	1.39276424	-0.27216060	-0.38428360
H	2.06347276	0.40488372	-0.22417425
H	1.33464751	-0.88075073	0.37382050

O	3.18922680	-2.99715896	2.75393255
H	3.75132314	-2.20399751	2.93257641
H	3.16040951	-3.51148311	3.55637047
O	5.42129310	1.86097015	-1.23728599
H	5.67347400	2.24519478	-2.07244989
H	5.60897599	0.88999916	-1.28174934
O	5.24143099	3.28427813	3.13202755
H	4.46650077	2.70354307	3.16540324
H	5.52625021	3.44121541	4.02722825
O	6.87714433	-0.51044241	1.52350220
H	6.94642238	0.47129785	1.46729425
H	7.73175484	-0.84646746	1.77991841
O	6.84373008	2.10035247	1.22404407
H	6.35139068	2.59420393	1.89635561
H	6.42014789	2.25881634	0.37506584
O	3.03664461	1.89826806	-0.01604967
H	3.86085609	1.98331101	-0.53123161
H	2.49108677	2.66833695	-0.16617333
O	4.63562077	-0.86952994	3.15290368
H	5.44892351	-0.79987464	2.63566114
H	4.15460216	-0.03841456	3.03999443

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p_dHa1_hco_hco W33			
C	0.43870858	4.23721499	-1.19458041
H	0.54791627	3.72896005	-2.15507368
O	1.08287445	3.91539054	-0.22836386
C	0.30832708	2.66645090	2.76030109
H	-0.26616518	5.06872682	-1.15695258
O	-0.51415737	3.43053662	2.72280688
H	-1.44379578	-3.23164677	1.82292938
O	-2.09189459	-2.53139777	1.92662885
H	-1.75161325	-4.12394734	0.23618315
O	-6.16484992	0.89648122	-0.88221911
O	-1.92190827	2.95410197	-1.39639332
H	-5.60049811	-0.57115998	-0.34941911
H	-6.16801351	1.12646814	-1.81959612
H	-1.47574396	2.09326167	-1.26351170
H	-2.36937810	3.14492871	-0.56183648
O	-0.98535590	0.49730182	-0.95140202
O	-5.29782360	-1.45295931	-0.03843367
H	-0.57599349	-2.83027467	1.70330994
H	-1.33472367	-0.03085291	-1.69525619
H	-6.05362291	-2.03363255	-0.08067692
H	-4.27244990	-1.45665304	1.36359041
O	-3.63432780	-1.37855823	2.09658088
H	-2.64320153	0.10417496	1.82284534
H	-4.09737856	-1.57997233	2.90506466
O	-1.73987071	-4.44635285	-0.67604762
H	-2.37346486	-3.89829037	-1.16350385
H	-0.14519123	-4.29935609	-1.09170058
O	-3.48184523	-2.69399642	-1.93025428
H	-2.99902184	-2.01932893	-2.42427563
H	-4.05929990	-2.22993838	-1.31960497
O	-2.10849315	0.84576704	1.51118149
H	-2.78626498	2.29214318	1.36485926
H	-1.72641931	0.57860654	0.65873685
O	-1.97494067	-0.69396448	-3.15932284
H	-2.42837742	0.06690894	-3.55345081
H	-1.27038227	-0.99096605	-3.75918815
O	-5.62271682	3.44193351	0.26313943
H	-6.23200645	3.81060662	0.89722012
H	-6.02388231	1.72226497	-0.40690864
O	-2.88695479	4.76665954	-3.26445318
H	-2.42481923	4.17248181	-2.66127413
H	-2.88419438	4.31154919	-4.10497170
O	-6.00690172	2.00505202	-3.45249354
H	-5.93328215	2.94135237	-3.15897624

H	-6.67954873	1.95246707	-4.12557759
O	-5.53777101	4.38075514	-2.42315565
H	-4.64975752	4.67164467	-2.67503231
H	-5.54285936	4.23471679	-1.47152214
O	-3.09775610	3.20805193	1.14228485
H	-4.74413349	3.40236249	0.68308917
H	-2.62822830	3.80346711	1.72132949
O	-3.23123174	1.67922433	-3.68462412
H	-4.19471693	1.67242927	-3.73096608
H	-3.00545445	2.08906645	-2.84548517
H	-0.05811056	0.22523152	-0.82194921
O	0.15432239	-1.58339201	-4.61299497
H	0.04233281	-2.35174646	-5.16550437
O	0.81921102	-4.10484247	-1.15255762
H	1.47570641	-2.90637643	-2.13979767
H	1.31987627	-4.93612592	-1.16672514
O	6.03613598	-0.50428389	-1.29895343
O	3.29266868	1.35752156	2.67026385
H	5.49491796	-1.24079315	-1.61282860
H	6.38748751	-0.72548051	-0.42816539
H	2.41006320	1.43602036	3.02844558
H	3.20499826	1.56757870	1.72051141
O	1.19019129	-2.50224378	1.01794146
O	4.52772575	-2.65519178	-2.20394988
H	1.11054478	-3.14989030	0.29229076
H	1.93656628	-2.78926302	1.56242996
H	4.90548425	-3.11244101	-2.95126393
H	3.58622628	-2.48392422	-2.41732306
O	1.91948373	-2.15106109	-2.58248567
H	1.81349187	-1.40792391	-1.96617791
H	0.84420906	-1.79923838	-3.96362383
O	2.64407725	-6.11559566	-1.12100170
H	3.35734931	-5.63060510	-0.66607298
H	2.60289863	-6.99289954	-0.75403932
O	4.46985278	-4.47459187	-0.01548921
H	4.19609790	-4.04551157	0.80332576
H	4.55165482	-3.79163251	-0.68992236
O	1.52489768	-0.34911998	-0.55357035
H	2.12852273	0.36626167	-0.30830429
H	1.48838878	-1.02191083	0.15345209
O	3.50403297	-3.24865214	2.34744251
H	3.99646298	-2.43031749	2.58941617
H	3.47844178	-3.80382556	3.12215824
O	5.38007794	2.01438772	-1.20681917
H	5.60932091	2.47613885	-2.00858460
H	5.60416354	1.06600730	-1.33646742
O	5.39327613	3.03439848	3.29608196
H	4.60581539	2.47554463	3.23588977
H	5.73253976	2.95875425	4.18308504
O	7.00440278	-0.48704939	1.32539884
H	7.06255986	0.49719032	1.31890527
H	7.86577206	-0.82763901	1.55116544
O	6.92127377	2.13374794	1.17685242
H	6.44780902	2.55094645	1.91091100
H	6.43656489	2.32526203	0.36738581
O	2.97992329	1.89893532	0.05279731
H	3.79654142	2.03980195	-0.45590074
H	2.38024487	2.64111001	-0.10286164
O	4.78040337	-1.03153398	2.92335809
H	5.58402149	-0.87689749	2.40863015
H	4.24893474	-0.22850049	2.87309468

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r_dHa1_hco_hco W33			
C	0.06551084	4.55522180	-0.79710209
H	-0.51908762	5.12098553	-1.54486163
O	1.10603546	4.03975489	-0.98145482
C	0.15740599	1.96608520	2.68816708

H	-0.40438125	1.06114219	2.37738876
O	-0.26415152	3.06058183	2.63970104
O	-1.53305180	-3.29109364	1.85150977
H	-2.24601447	-2.65221379	1.91300792
H	-1.79256019	-4.19080131	0.25297028
O	-6.09812062	1.02040647	-0.93138250
O	-1.95126258	2.76027511	-1.54130968
H	-5.64687787	-0.52216588	-0.50188209
H	-6.10801949	1.30156690	-1.85513415
H	-1.47958404	1.91125529	-1.43489044
H	-2.35194870	2.93544981	-0.68037047
O	-1.03661248	0.29337894	-1.09913176
O	-5.42159350	-1.44429954	-0.24677642
H	-0.70259844	-2.81666313	1.73866868
H	-1.36104444	-0.22062257	-1.86537535
H	-6.21165531	-1.96471931	-0.36947611
H	-4.47621790	-1.60446886	1.19177475
O	-3.85748850	-1.57873284	1.94552077
H	-2.75448404	-0.22381101	1.62596087
H	-4.36499220	-1.69982165	2.74312574
O	-1.75647003	-4.49502327	-0.66416488
H	-2.39474911	-3.95588069	-1.15544122
H	-0.15569852	-4.28718452	-1.01910841
O	-3.50076243	-2.78096179	-1.96827027
H	-3.02766847	-2.14034665	-2.51449880
H	-4.11603626	-2.28286384	-1.42572185
O	-2.14215426	0.46999533	1.34529373
H	-2.68580800	2.03524077	1.27225198
H	-1.81178934	0.24070500	0.45701678
O	-2.01448840	-0.84994550	-3.31688043
H	-2.46787924	-0.08010938	-3.69613472
H	-1.30134855	-1.13627696	-3.91040287
O	-5.38500036	3.49046637	0.31745576
H	-5.95872938	3.89074024	0.96539432
H	-5.90048561	1.80947682	-0.41620143
O	-2.52536026	4.93731116	-3.02780577
H	-2.22593338	4.08929159	-2.66977880
H	-2.41115993	4.89298192	-3.97387992
O	-5.95110684	2.22410527	-3.45799575
H	-5.75070683	3.13073622	-3.13617814
H	-6.66861282	2.28277353	-4.08243485
O	-5.23012140	4.50560445	-2.33758702
H	-4.33616755	4.79564260	-2.56235725
H	-5.25134451	4.32318552	-1.39229417
O	-2.87112739	2.98682617	1.10352026
H	-4.50696575	3.38238298	0.72444832
H	-2.22706560	3.47663918	1.61433354
O	-3.24124940	1.53734150	-3.80445027
H	-4.19710681	1.63806182	-3.86002128
H	-2.97769113	1.98195285	-2.99364667
H	-0.09487585	0.08275313	-0.96970760
O	0.18597076	-1.73282461	-4.67117877
H	0.12843737	-2.51697511	-5.20949803
O	0.80520042	-4.06843779	-1.04150096
H	1.46219810	-2.92135873	-2.08534015
H	1.32142494	-4.89025340	-1.00855744
O	6.01680636	-0.52703826	-1.35192015
O	3.36846570	1.68801430	2.60655311
H	5.48381553	-1.28424971	-1.62815092
H	6.37781311	-0.70323455	-0.47483192
H	2.50714713	1.75757577	3.01945458
H	3.21696802	1.83650135	1.65461517
O	1.08616908	-2.38676021	1.08430752
O	4.51109840	-2.72125430	-2.14006225
H	1.03225700	-3.05813206	0.37735961
H	1.83199830	-2.63926570	1.64659475
H	4.88609939	-3.23627024	-2.85025140
H	3.57537481	-2.54627930	-2.37338492

O	1.91257072	-2.19151126	-2.56315370
H	1.81946322	-1.42276190	-1.97896390
H	0.85647092	-1.90501762	-3.99028903
O	2.63662883	-6.06580781	-0.87983796
H	3.33929651	-5.56232945	-0.42870703
H	2.57502884	-6.92208470	-0.46861988
O	4.43207731	-4.36546791	0.17920039
H	4.13759644	-3.88259464	0.95981520
H	4.52073510	-3.73222986	-0.54136050
O	1.51706354	-0.32264776	-0.58000180
H	2.08474061	0.42457323	-0.34750847
H	1.46360564	-0.96182792	0.15607573
O	3.42123894	-2.99455832	2.44689041
H	3.92150100	-2.16460057	2.62341448
H	3.42891918	-3.50466569	3.25244052
O	5.29328295	1.97123702	-1.35174611
H	5.45238849	2.39511929	-2.19084826
H	5.53858702	1.01741829	-1.44576646
O	5.50839165	3.39021237	2.99094703
H	4.71186540	2.84303679	3.02721125
H	5.84322928	3.47640223	3.87842453
O	6.99914116	-0.36790661	1.26133442
H	7.07064766	0.61324354	1.19319254
H	7.85514900	-0.70514033	1.51117168
O	6.95147018	2.23729635	0.94149456
H	6.52154529	2.72943297	1.65553723
H	6.43980798	2.38221396	0.13912368
O	2.92993419	1.99977946	-0.04708436
H	3.75260307	2.05308430	-0.56860880
H	2.36726275	2.72937366	-0.31897697
O	4.75152810	-0.77102429	2.86278919
H	5.56440818	-0.66814928	2.34941524
H	4.27303455	0.06443176	2.81386287

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C	-0.57162530	-3.76833096	0.18455058
H	-1.45759327	-4.38046839	-0.05409356
O	0.08780397	-3.84317906	1.15168486
C	-0.25319625	-2.66627191	-2.57768701
H	-0.47501983	-1.58436103	-2.48517672
O	-0.99942137	-3.46930111	-3.00007519
O	-0.45687721	3.38788314	-2.73460449
H	-1.26456510	2.90941226	-2.93330585
H	-0.83211855	4.50675233	-1.31089555
O	-6.45072078	0.70356653	-0.79823035
O	-2.90037399	-2.26078035	0.63926465
H	-5.50034902	1.97829372	-1.24252077
H	-6.63721659	0.51124934	0.12975183
H	-2.27027416	-1.51453160	0.63251588
H	-3.25614794	-2.31094887	-0.25625827
O	-1.38759817	-0.05726729	0.40304629
O	-4.95694989	2.75213534	-1.51502313
H	0.18924017	2.76420996	-2.38598833
H	-1.74836569	0.59338724	1.04023688
H	-5.55509394	3.48806152	-1.61865151
H	-3.73077755	2.44171467	-2.68767868
O	-3.00061569	2.16471512	-3.27312359
H	-2.35347311	0.63230422	-2.63860432
H	-3.28437049	2.29609733	-4.17353120
O	-0.91224492	4.90909566	-0.43501293
H	-1.71717982	4.53958583	-0.04103047
H	0.51702771	4.45590599	0.25719576
O	-3.17045819	3.66472227	0.57669874
H	-2.98685748	2.95549371	1.20585389
H	-3.77096874	3.30737041	-0.08130917
O	-2.05433892	-0.17432284	-2.19636637
H	-3.10485046	-1.44166441	-2.22876900

H	-1.83214357	0.04914717	-1.27360861
O	-2.48849738	1.53356183	2.24330153
H	-3.15406033	0.90380586	2.56523875
H	-1.87417977	1.75969030	2.96075719
O	-6.28100424	-1.93429324	-1.84692049
H	-6.80031900	-2.20795863	-2.59821810
H	-6.42520122	-0.14849744	-1.24649926
O	-4.60696835	-4.00712984	1.89201557
H	-3.87738110	-3.43264406	1.62746562
H	-4.57970800	-4.07343178	2.84264623
O	-6.93111020	-0.31155220	1.76694809
H	-7.00381398	-1.25313986	1.48903469
H	-7.68727125	-0.10175472	2.30781331
O	-6.85620700	-2.75996519	0.81657893
H	-6.13098299	-3.28613164	1.18289837
H	-6.69488010	-2.65468976	-0.12637807
O	-3.62550286	-2.26983894	-2.10671343
H	-5.34448726	-2.10474075	-2.05284472
H	-3.16052003	-2.94959933	-2.59293336
O	-4.25789500	-0.49900870	2.60821495
H	-5.19299895	-0.33774249	2.43721434
H	-3.96898784	-1.12848862	1.94350885
H	-0.41872452	-0.03108651	0.49583103
O	-0.53060248	2.23082012	4.01959646
H	-0.60240986	3.06389132	4.47657779
O	1.38286229	4.05460815	0.50475838
H	1.52885912	2.94816224	1.76932385
H	2.07320400	4.73637455	0.48013948
O	5.75101551	-0.20362986	2.16592011
O	2.99495556	-2.70121950	-1.67367172
H	5.27325452	0.63372545	2.23311414
H	6.16819348	-0.25882988	1.29793775
H	2.13985303	-2.80044003	-2.09300762
H	2.81804409	-2.57790198	-0.72231514
O	1.63770286	2.04501437	-1.31734370
O	4.39483210	2.20668709	2.36617590
H	1.62614393	2.81175744	-0.71311470
H	2.48991445	2.05874975	-1.77499889
H	4.73315670	2.81041957	3.02316055
H	3.41873260	2.20957481	2.45147753
O	1.69994129	2.20436173	2.38599394
H	1.52795075	1.40666134	1.86051078
H	0.30603038	2.24798329	3.52734438
O	3.63734326	5.57351631	0.43564664
H	4.25125501	4.87383749	0.14720320
H	3.82594165	6.35903112	-0.06791211
O	5.09851088	3.38192398	-0.12622351
H	4.84566074	2.85638997	-0.89330006
H	4.89124624	2.87042694	0.66324633
O	1.28184820	0.17334291	0.57293267
H	1.82949095	-0.61898325	0.64441380
H	1.52577242	0.70586530	-0.20829919
O	4.18579074	1.90604852	-2.37166553
H	4.44298700	0.95623069	-2.35748180
H	4.41407092	2.25050975	-3.23083540
O	4.63512574	-2.51365786	2.55381872
H	4.62026901	-2.78246392	3.46834613
H	5.04651870	-1.61429452	2.50674795
O	4.82491323	-4.76243154	-1.45245959
H	4.15341018	-4.10785870	-1.68853469
H	5.22204690	-5.07544088	-2.25974131
O	6.81053123	-1.04818742	-0.28826689
H	6.71558523	-1.99468754	-0.02791773
H	7.72695130	-0.89814019	-0.50486906
O	6.31868125	-3.50263877	0.49947522
H	5.84255271	-4.04177412	-0.14805296
H	5.75536682	-3.40888336	1.27433256
O	2.48207678	-2.29044437	0.94534200

H	3.21550670	-2.40212805	1.57825786
H	1.75003727	-2.83635641	1.24155560
O	4.87551387	-0.62664781	-2.24544287
H	5.57641573	-0.78554908	-1.59772144
H	4.21215553	-1.31531039	-2.13130413

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C	0.37789848	3.34230217	0.60068025
H	0.13549321	2.27428577	0.43118035
O	-0.31691442	4.12944615	1.11858370
C	0.56807358	0.60370351	2.57280973
H	-0.42819624	0.14806185	2.45491266
O	1.25039181	0.61739096	3.52913987
O	-1.54648517	-2.91801779	2.01100170
H	-2.25396330	-2.26926244	1.98622363
H	-1.81482041	-3.92762613	0.45715238
O	-6.37840128	0.90402146	-1.07523681
O	-2.18488478	2.98640423	-1.92207325
H	-5.82469954	-0.54239592	-0.53842059
H	-6.36666016	1.09936730	-2.02186828
H	-1.57939931	2.24803393	-1.75810063
H	-2.61077721	3.15736878	-1.07342922
O	-0.93814970	0.65481295	-1.20130536
O	-5.50935388	-1.41864859	-0.21565457
H	-0.70749150	-2.47175597	1.86394661
H	-1.29959422	0.08495753	-1.91366559
H	-6.25290405	-2.01499416	-0.25336511
H	-4.49556869	-1.35493259	1.16664439
O	-3.85893516	-1.20817701	1.89274699
H	-2.82177624	0.16229786	1.44433330
H	-4.34887027	-1.22520899	2.71049706
O	-1.76697400	-4.26463927	-0.44669096
H	-2.40622901	-3.75248951	-0.96731332
H	-0.18814776	-4.01452794	-0.81645349
O	-3.47690523	-2.64425434	-1.85738271
H	-3.00371689	-1.98889695	-2.38690843
H	-4.16043741	-2.17868254	-1.37003661
O	-2.19039639	0.85121194	1.19355581
H	-2.85203737	2.37225597	0.99425321
H	-1.81646837	0.61775487	0.32565964
O	-2.01017820	-0.71314184	-3.22233116
H	-2.53224430	-0.02179842	-3.66739701
H	-1.32608832	-1.04509943	-3.82594929
O	-5.73606815	3.47014125	-0.01926428
H	-6.30689725	3.89573006	0.61492590
H	-6.19875200	1.73787199	-0.62757084
O	-3.16764070	5.00951528	-3.50141664
H	-2.61415608	4.35869757	-3.05089614
H	-2.96668690	4.94685779	-4.43114355
O	-6.19171997	1.85019595	-3.69127539
H	-6.09350682	2.79780683	-3.44076318
H	-6.87803879	1.78668320	-4.34939520
O	-5.73770057	4.26326556	-2.76473091
H	-4.87860744	4.62346116	-3.03128995
H	-5.73002107	4.16857687	-1.80721352
O	-3.15418544	3.26690466	0.72081883
H	-4.83571468	3.46523067	0.35035175
H	-2.55185499	3.89406204	1.11857298
O	-3.41625037	1.45338103	-3.99659778
H	-4.37894870	1.46077849	-4.02520611
H	-3.16192347	2.05829995	-3.29206819
H	-0.00901975	0.40586332	-1.07098342
O	0.13500616	-1.69553388	-4.60193494
H	0.05566968	-2.50671344	-5.09564121
O	0.77260126	-3.79057894	-0.85245039
H	1.44198432	-2.72536388	-1.97342675
H	1.27986195	-4.61993553	-0.82882545



O	6.13843496	-0.53731313	-1.44824853
O	3.89344045	1.53905947	2.73878302
H	5.55777428	-1.26551111	-1.70596964
H	6.58658361	-0.77214177	-0.62618789
H	3.07833339	1.35257134	3.20906710
H	3.64700644	1.73514377	1.82155387
O	1.09975995	-2.02160061	1.18060294
O	4.50372261	-2.66168302	-2.16943685
H	1.00613783	-2.71624121	0.49753853
H	1.86694108	-2.28593345	1.71122742
H	4.83191542	-3.19661354	-2.88813343
H	3.56597226	-2.45828314	-2.36734339
O	1.90924647	-2.04536314	-2.50586276
H	1.86038056	-1.23860283	-1.97182754
H	0.82296486	-1.83602746	-3.93243834
O	2.50606131	-5.87404732	-0.80246612
H	3.26611865	-5.42372743	-0.38903321
H	2.40385450	-6.72658128	-0.39139539
O	4.42819546	-4.28053161	0.17211637
H	4.12650462	-3.78058184	0.93949003
H	4.52816522	-3.66098509	-0.55857411
O	1.61013941	-0.05402638	-0.60581615
H	2.24254267	0.63421233	-0.36218683
H	1.51216655	-0.67548914	0.13991073
O	3.44986228	-2.83205929	2.40413010
H	4.11807276	-2.12321639	2.55917724
H	3.40471566	-3.35081621	3.20332901
O	5.54386655	1.98254086	-1.30024984
H	5.71243534	2.42920611	-2.12573290
H	5.73320256	1.01950140	-1.43797500
O	6.02955850	3.23538005	3.03356431
H	5.23514823	2.69450264	3.13910963
H	6.38955114	3.40130778	3.89948689
O	7.38078227	-0.57537216	1.04548202
H	7.46467694	0.40612042	1.05247180
H	8.24479618	-0.94396167	1.20796343
O	7.34360143	2.05135421	0.91720233
H	6.97459629	2.52919374	1.67390285
H	6.79581501	2.25681354	0.15359593
O	3.26222549	2.07940451	0.09926508
H	4.06874553	2.12421321	-0.45271395
H	2.78500943	2.90146556	-0.00869319
O	5.21246337	-0.93420857	2.76789576
H	6.00085293	-0.90479159	2.21045364
H	4.83287701	-0.04716696	2.77208955

### 3.2.10 HCO + NH2

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O	-0.61345423	2.88397336	-3.11175881
H	-1.35856263	2.29272555	-3.23818848
H	-1.03597525	4.12095982	-1.81275535
O	-6.59999883	0.49139084	-0.88316465
O	-2.48415186	-2.86103486	0.74671601
H	-5.60897093	1.64780171	-1.52578625
H	-6.81926803	0.50830309	0.05728930
H	-2.14803420	-1.94022111	0.71190885
H	-3.00354643	-2.98267048	-0.05847465
O	-1.56676502	-0.36955766	0.42484671
O	-5.02330474	2.34192288	-1.90341434
H	0.11986066	2.37684236	-2.74656402
H	-1.97155020	0.30461530	1.01264801
H	-5.57656714	3.08743080	-2.12272205
H	-3.78817251	1.80499496	-2.99075661
O	-3.06018685	1.41635243	-3.51074244
H	-2.54044504	-0.08335635	-2.69183324

H	-3.30195387	1.46796244	-4.43140199
O	-1.12957391	4.62472849	-0.99179813
H	-1.90470304	4.25984114	-0.53817427
H	0.31590471	4.34353334	-0.25367876
O	-3.31393201	3.39642258	0.17808229
H	-3.13468146	2.73227004	0.85629819
H	-3.88903473	2.98838325	-0.47313461
O	-2.29285858	-0.83015167	-2.12952603
H	-3.22299940	-2.10661978	-2.02753530
H	-2.06585837	-0.48157897	-1.24966196
O	-2.67535989	1.41928781	2.05171495
H	-3.40389250	0.98316040	2.52972004
H	-2.04661786	1.77675257	2.70086869
O	-6.32972495	-2.31437886	-1.33690181
H	-6.92406202	-2.70398007	-1.97283060
H	-6.49733938	-0.43660259	-1.11786699
O	-4.34281739	-2.78830255	2.70422348
H	-3.61755803	-2.87878130	2.05613950
H	-4.15330865	-3.36943558	3.43587080
O	-7.19872293	0.07186413	1.82639964
H	-7.20278477	-0.90640091	1.75201469
H	-8.01331597	0.34241747	2.24089727
O	-6.84349163	-2.52368365	1.43969043
H	-6.02194053	-2.75850414	1.88768317
H	-6.68380631	-2.60463718	0.49313999
O	-3.73593390	-2.92829123	-1.79848063
H	-5.42392664	-2.58060701	-1.57652470
H	-3.45550218	-3.61809213	-2.39461789
O	-4.69891699	0.03403788	3.17298774
H	-5.56366701	0.20460041	2.78513798
H	-4.55825667	-0.91533198	3.11055975
H	-0.60636539	-0.20560872	0.42286298
O	-0.72996124	2.43987669	3.67546996
H	-0.84432510	3.33750902	3.97455582
O	1.19326532	4.01159997	0.05096572
H	1.31744196	2.97472689	1.36063547
H	1.84460805	4.73066248	0.02977676
O	5.40121133	-0.08060262	2.42593136
O	3.70151065	-2.80219610	-1.73141905
H	4.95647970	0.77707384	2.38905466
H	5.98303464	-0.16143403	1.66011253
H	2.93039943	-3.02108857	-2.26573113
H	3.32759607	-2.58873319	-0.86263463
O	1.59929685	1.89299087	-1.61294948
O	4.13119280	2.37078915	2.31295850
H	1.54374023	2.70416720	-1.07381641
H	2.49786403	1.85731229	-1.97072436
H	4.37248579	2.99613226	2.99192484
H	3.15132125	2.34624274	2.27874472
O	1.46942266	2.27388003	2.03210674
H	1.32695285	1.44003693	1.55622975
H	0.09602427	2.41360427	3.16516267
O	3.36841978	5.63773345	0.07243619
H	4.03064835	4.93972495	-0.08698633
H	3.58860734	6.38419744	-0.47562771
O	4.95693961	3.48125890	-0.17387123
H	4.76970634	2.89311659	-0.91486475
H	4.73811098	3.00808176	0.63607850
O	1.08630996	0.12452476	0.33730141
H	1.66997770	-0.64154816	0.41346032
H	1.32225480	0.64065734	-0.45939908
O	4.27319867	1.80226102	-2.34961525
H	4.67651649	0.90854274	-2.24636260
H	4.54238070	2.12944306	-3.20398445
O	4.19999108	-2.36273323	2.70481198
H	4.04946502	-2.57962874	3.62077518
H	4.61489333	-1.46315004	2.67469907
O	5.31439142	-4.86881079	-0.96901587

H	4.74867130	-4.20087989	-1.38858719
H	5.85387130	-5.26080679	-1.64908187
O	6.92822298	-0.94692836	0.25302955
H	6.79315876	-1.88211218	0.53195578
H	7.86811716	-0.79166384	0.21324342
O	6.33509873	-3.37017525	1.09659194
H	6.03691072	-3.99225852	0.41660023
H	5.61427023	-3.25730845	1.72363394
O	2.43288034	-2.27175851	0.67305208
H	2.98202374	-2.36252233	1.47356019
H	1.69892611	-2.88502592	0.72626060
O	5.36239207	-0.56427364	-2.04630476
H	5.95074489	-0.67001800	-1.28740261
H	4.78680765	-1.33899810	-2.06543426
N	0.00530323	-3.83927703	-0.44747494
H	-0.82766098	-3.65731330	0.09799753
H	0.43746901	-4.74306742	-0.38481026
H	-0.43455526	-2.26791466	-1.69794565
C	0.21273833	-3.13887589	-1.58256277
O	1.06053999	-3.42109237	-2.40665664

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O	-0.28282569	2.97996010	-2.99497998
H	-1.07376622	2.45063098	-3.11721671
H	-0.61539871	4.24349850	-1.68855889
O	-6.36631923	0.80696570	-0.74153383
O	-2.87672516	-2.12916878	0.96942457
H	-5.34980013	1.94760649	-1.39218847
H	-6.56348347	0.77896569	0.20292881
H	-2.27362390	-1.37701577	0.80010897
H	-3.27402616	-2.33921026	0.11529745
O	-1.42423656	0.02316487	0.33012492
O	-4.77814485	2.64766649	-1.77832151
H	0.40957347	2.42077848	-2.62613852
H	-1.74468087	0.74996597	0.89883896
H	-5.34940915	3.38161209	-1.99081079
H	-3.56060950	2.12556444	-2.90585888
O	-2.85328554	1.74799527	-3.46040578
H	-2.40121130	0.15309492	-2.75745084
H	-3.07937382	1.91607138	-4.37101624
O	-0.67755399	4.74800508	-0.86547056
H	-1.51316401	4.48693219	-0.44950381
H	0.72256610	4.32830383	-0.08938266
O	-3.03621058	3.79481560	0.23589052
H	-2.87200157	3.15044151	0.93596440
H	-3.60873140	3.36678482	-0.40494426
O	-2.15948866	-0.60324075	-2.20729574
H	-3.22552898	-1.77931163	-1.97317040
H	-1.87857595	-0.24439808	-1.34776502
O	-2.40026802	1.81448506	2.09308225
H	-3.06834020	1.24550392	2.50487499
H	-1.74700777	2.07310489	2.76492932
O	-6.40753066	-1.97070486	-1.33877641
H	-6.97916507	-2.30729774	-2.02360872
H	-6.40501068	-0.10596234	-1.04600987
O	-4.70026152	-3.17591432	2.83751750
H	-3.95058438	-2.94073587	2.27937527
H	-4.67795302	-2.54166170	3.55270028
O	-6.88914559	0.21966942	1.94961542
H	-7.04697833	-0.74420213	1.82420301
H	-7.60045862	0.57576372	2.47454748
O	-6.96980933	-2.35198138	1.42521395
H	-6.23476362	-2.78369797	1.88501188
H	-6.80192138	-2.40604699	0.47898909
O	-3.80522256	-2.52864935	-1.67740426
H	-5.49379915	-2.22815351	-1.55852978
H	-3.43988572	-3.32547958	-2.05306424

O	-4.22223161	-0.12478169	2.73027944
H	-5.13980959	0.10854545	2.54217066
H	-3.95750917	-0.75264398	2.05392085
H	-0.45002343	0.03595204	0.38466026
O	-0.39505354	2.53204613	3.79309203
H	-0.39080950	3.42721226	4.12004987
O	1.57170562	3.93153805	0.21500975
H	1.67391154	2.86558914	1.51516603
H	2.26788515	4.60779441	0.21374874
O	5.39163017	-0.69048966	2.29125470
O	3.04896604	-2.56981353	-1.86762756
H	5.05302781	0.21441041	2.31539503
H	5.98068023	-0.78304275	1.53330954
H	2.32619191	-2.37413166	-2.46042490
H	2.66094899	-2.57885135	-0.96823558
O	1.88285866	1.84737927	-1.51338975
O	4.45152349	1.92110776	2.39484693
H	1.84844359	2.63885229	-0.94351780
H	2.77608773	1.81618671	-1.88268798
H	4.77655066	2.41650509	3.14263094
H	3.47620498	2.02574855	2.38254061
O	1.79184051	2.14647457	2.17275665
H	1.58395572	1.33264106	1.68485507
H	0.43239180	2.40669573	3.29949956
O	3.84400064	5.41385170	0.30863941
H	4.47279480	4.68614076	0.14644570
H	4.12436514	6.16581422	-0.20314604
O	5.33069702	3.19097125	0.00701363
H	5.11215832	2.66087635	-0.76805884
H	5.09198084	2.67737003	0.78649832
O	1.24407196	0.10053747	0.43343759
H	1.61053822	-0.79629565	0.47036058
H	1.55757727	0.57020816	-0.36212819
O	4.55229924	1.70121017	-2.27259745
H	4.84270132	0.76178267	-2.21403569
H	4.86069373	2.04109315	-3.10831116
O	3.99748269	-2.89071382	2.41434774
H	3.90342864	-3.19228298	3.31371435
H	4.47678832	-2.02684412	2.44167959
O	4.55553494	-4.87132259	-1.70995184
H	4.00412357	-4.10969856	-1.93719649
H	5.08211813	-5.08255348	-2.47535775
O	6.85302209	-1.59004673	0.07982033
H	6.57231184	-2.52121166	0.23969808
H	7.80553555	-1.57462703	0.04550288
O	5.85427640	-3.97240284	0.57055954
H	5.42312779	-4.39165703	-0.18737580
H	5.18267410	-3.82264647	1.24469458
O	1.98843597	-2.52334634	0.58597601
H	2.63376305	-2.70114379	1.28907943
H	1.17229984	-3.03470396	0.78313384
O	5.24955444	-0.82014758	-2.07001934
H	5.86671908	-1.05066959	-1.36280524
H	4.50011720	-1.42353120	-2.00194001
N	-0.34112691	-3.95544769	1.12857844
H	-1.18340098	-3.39298563	1.10035341
H	-0.28320775	-4.35353899	2.05304527
H	-0.46711942	-4.72213393	0.48656813
C	-0.09363936	-2.92411609	-2.37778899
O	-0.98071905	-3.57501581	-2.14646402

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O	-0.37476822	3.13000339	-2.99229441
H	-1.18117871	2.63125689	-3.13855756
H	-0.71708994	4.34569893	-1.63928978
O	-6.34394732	0.61933613	-0.82059179
O	-2.84427392	-2.13189189	1.03131494

H	-5.41215059	1.87100244	-1.37390219
H	-6.57270125	0.54788589	0.11505652
H	-2.26628249	-1.35025784	0.91327700
H	-3.18943761	-2.32290792	0.14934330
O	-1.44317641	0.07263533	0.47357670
O	-4.88252819	2.63071153	-1.70473090
H	0.29041536	2.53769635	-2.62505770
H	-1.76994978	0.78824339	1.05589501
H	-5.49382343	3.34465692	-1.86814429
H	-3.66605833	2.22845003	-2.86005097
O	-2.94220796	1.88802531	-3.41904692
H	-2.36375007	0.40044281	-2.63706094
H	-3.21837179	1.96067515	-4.32842740
O	-0.78340137	4.80847570	-0.79264482
H	-1.61103176	4.51233972	-0.38459021
H	0.62353702	4.35807667	-0.04898981
O	-3.11071697	3.76471194	0.29451151
H	-2.94993298	3.13818574	1.01118335
H	-3.69992867	3.33314561	-0.32820889
O	-2.06038509	-0.34735478	-2.10350884
H	-3.03496849	-1.67056891	-1.93329608
H	-1.86346546	-0.01754672	-1.20710358
O	-2.48382731	1.82562775	2.20212610
H	-3.15666460	1.23855482	2.58158400
H	-1.84378621	2.07508209	2.88926672
O	-6.16516182	-2.14767996	-1.50214314
H	-6.68289125	-2.51424549	-2.21402196
H	-6.30096456	-0.28248473	-1.15525620
O	-4.63624300	-3.52039750	2.63165709
H	-3.89081011	-3.06917796	2.21745350
H	-4.65817734	-3.22631847	3.53899639
O	-6.93437533	-0.03103470	1.83594551
H	-7.01738794	-0.99999821	1.68093506
H	-7.70401174	0.26232268	2.31547722
O	-6.85251637	-2.58268076	1.22724376
H	-6.13394097	-3.02446430	1.70259955
H	-6.64476913	-2.61037225	0.28780814
O	-3.50463417	-2.50029701	-1.68564244
H	-5.23083282	-2.36057793	-1.67363385
H	-2.97031986	-3.21645253	-2.02752026
O	-4.28353500	-0.15207044	2.75498183
H	-5.21137265	0.00575964	2.54408687
H	-3.98357742	-0.83011914	2.14619105
H	-0.46848964	0.07816943	0.51686629
O	-0.44723197	2.50433704	3.88188952
H	-0.42633898	3.37613485	4.26602196
O	1.47491342	3.94955446	0.23309944
H	1.58410016	2.89693502	1.54428708
H	2.17845699	4.61817864	0.21129968
O	5.41379301	-0.54943804	2.29351032
O	3.13505743	-2.86075744	-1.86573425
H	5.04938230	0.34504280	2.31667966
H	5.96143545	-0.64140912	1.50482873
H	2.37111421	-2.87607704	-2.44162895
H	2.78171365	-2.73568815	-0.96113021
O	1.73101977	1.87698219	-1.51543734
O	4.39347036	2.03208189	2.36683424
H	1.71933288	2.66535556	-0.93971610
H	2.61645723	1.83004615	-1.90275694
H	4.73235307	2.57727686	3.07261612
H	3.41675339	2.11251125	2.38354491
O	1.71779282	2.18339774	2.20496912
H	1.53779190	1.36306393	1.71826377
H	0.36710413	2.40349687	3.36199014
O	3.75873996	5.41603977	0.23687446
H	4.37602138	4.68542491	0.04699323
H	4.01530542	6.16510501	-0.29144677
O	5.21302603	3.17795970	-0.10174150

H	4.97179688	2.62658891	-0.85472798
H	4.98854020	2.69330305	0.70010310
O	1.22702008	0.11760628	0.45657783
H	1.64934777	-0.75489498	0.47762222
H	1.49113858	0.60862382	-0.34458174
O	4.36855293	1.64535794	-2.33409464
H	4.65556441	0.70479052	-2.27458835
H	4.67194492	1.97844123	-3.17445814
O	4.06300662	-2.77123141	2.48513409
H	3.92643425	-3.03906912	3.38973538
H	4.52887119	-1.89984029	2.49811826
O	4.74524910	-5.05601134	-1.42857249
H	4.16235313	-4.34702632	-1.73541995
H	5.24233049	-5.36740995	-2.17910250
O	6.78697847	-1.45392664	0.02644374
H	6.57901141	-2.38961859	0.25850840
H	7.73420001	-1.37885938	-0.05159148
O	5.99681577	-3.85961913	0.72329872
H	5.59985102	-4.38114532	0.01122305
H	5.31890560	-3.71514791	1.39190824
O	2.12960893	-2.46277291	0.58551162
H	2.75035077	-2.62496577	1.31577437
H	1.32064185	-2.98358376	0.74340111
O	5.12155143	-0.86103812	-2.13238082
H	5.74563184	-1.05000628	-1.41826118
H	4.43909260	-1.54135904	-2.10293243
N	-0.30267454	-3.83286573	0.82336850
H	-1.20383299	-3.39735256	1.02653422
H	-0.48781017	-4.81391290	0.63499411
H	-0.40299420	-1.60364527	-2.46800029
C	-0.07666315	-2.66270588	-2.52653610
O	-0.79571352	-3.58768685	-2.44265067

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O	-0.33302317	3.12729811	-3.03384830
H	-1.13466072	2.61927819	-3.17531376
H	-0.66558999	4.34608184	-1.68452117
O	-6.37276887	0.77986784	-0.78450456
O	-2.85097673	-2.17585006	0.94806406
H	-5.38065719	1.96094363	-1.38641679
H	-6.56071171	0.71192695	0.16023611
H	-2.27602039	-1.39077345	0.84322440
H	-3.26216060	-2.31273595	0.08442530
O	-1.43208950	0.03506436	0.43603444
O	-4.81700203	2.68437858	-1.74150562
H	0.34249285	2.54111672	-2.67595747
H	-1.74651940	0.75273707	1.02295146
H	-5.39380971	3.42477084	-1.91274835
H	-3.60867859	2.22906347	-2.89318914
O	-2.89304619	1.87315502	-3.45278210
H	-2.36607449	0.35456084	-2.67623937
H	-3.16673666	1.95732386	-4.36195682
O	-0.72348362	4.81601331	-0.84101027
H	-1.54352081	4.51786892	-0.41920397
H	0.68989194	4.37500340	-0.10908715
O	-3.03623903	3.76970654	0.27275429
H	-2.88177797	3.13289966	0.98165731
H	-3.62779807	3.35108767	-0.35668110
O	-2.12493374	-0.39920662	-2.12039487
H	-3.21242535	-1.63099329	-1.97031507
H	-1.90524460	-0.05689051	-1.23488141
O	-2.42698049	1.81015331	2.16751532
H	-3.09637829	1.22699616	2.55894443
H	-1.78162571	2.06650950	2.84735872
O	-6.37519613	-1.97550933	-1.49342871
H	-6.91302428	-2.31785060	-2.20233088
H	-6.40810925	-0.11911106	-1.12819278

O	-4.70944961	-3.48673842	2.54738483
H	-3.94077336	-3.08016595	2.12953540
H	-4.69086897	-3.22120680	3.46351124
O	-6.87961100	0.10922590	1.88931548
H	-7.01690796	-0.85215668	1.72440853
H	-7.61294716	0.43195631	2.40553188
O	-6.94412288	-2.43439408	1.25317764
H	-6.21906127	-2.91094386	1.68267567
H	-6.79185553	-2.45817616	0.30297556
O	-3.74059100	-2.42550822	-1.72324807
H	-5.44821805	-2.20961644	-1.68085117
H	-3.28502021	-3.17437993	-2.10687797
O	-4.22752371	-0.15254279	2.75310776
H	-5.15229244	0.03615775	2.55158169
H	-3.95478320	-0.83843756	2.14135862
H	-0.45680390	0.04845362	0.45916623
O	-0.39107516	2.51982968	3.83218312
H	-0.37861948	3.40056323	4.19581922
O	1.54112387	3.96528956	0.17264649
H	1.63139633	2.90732256	1.47756018
H	2.24698172	4.63126364	0.15253398
O	5.42483756	-0.53691426	2.32271099
O	3.23460480	-2.95188849	-1.86252468
H	5.06991543	0.36181091	2.33167483
H	5.98273507	-0.64158159	1.54295658
H	2.49621140	-3.03846089	-2.46080210
H	2.84968260	-2.77916294	-0.97676740
O	1.78753150	1.88772446	-1.56950866
O	4.42328901	2.04751144	2.34453819
H	1.78351543	2.67889697	-0.99769253
H	2.67672329	1.81949530	-1.94417525
H	4.74697002	2.60468489	3.04808372
H	3.44566351	2.12247139	2.34275920
O	1.75457994	2.19101985	2.13761545
H	1.56573534	1.37316974	1.64991731
H	0.41819963	2.41875448	3.30434381
O	3.83639797	5.41438570	0.18185086
H	4.44687015	4.67602633	0.00053604
H	4.10541270	6.15772634	-0.34835034
O	5.27095525	3.15849075	-0.12903317
H	5.03082203	2.59834475	-0.87575124
H	5.03831722	2.68606662	0.67783777
O	1.24034192	0.12671868	0.38895040
H	1.68293716	-0.73538401	0.41215790
H	1.50613379	0.62460012	-0.40776287
O	4.43575209	1.59760237	-2.34795316
H	4.71929510	0.65789710	-2.27199315
H	4.75531895	1.91864511	-3.18705024
O	4.04177055	-2.73795395	2.51013501
H	3.86753640	-2.98625699	3.41386152
H	4.51710871	-1.87149397	2.52402937
O	4.84717731	-5.12588606	-1.30618457
H	4.27604632	-4.42126446	-1.64289850
H	5.36968434	-5.44831719	-2.03453072
O	6.82372010	-1.47625836	0.08470172
H	6.61668301	-2.40578503	0.34081008
H	7.77165852	-1.39888120	0.01814808
O	6.03571659	-3.86455470	0.84374984
H	5.66113471	-4.41168429	0.13909392
H	5.33866815	-3.70396111	1.48869867
O	2.18637800	-2.43791523	0.53229427
H	2.77611643	-2.59736383	1.28842694
H	1.36600595	-2.94938569	0.65860646
O	5.19360476	-0.90932311	-2.10795117
H	5.80322319	-1.09152160	-1.37952308
H	4.52231811	-1.60021436	-2.09804006
N	-0.25276218	-3.79604493	0.62515258
H	-1.17480953	-3.40739078	0.83251798

H	-0.39681504	-4.77196195	0.38181418
H	-0.55988654	-1.91428152	-2.07476540
C	-0.38469106	-3.00808858	-2.08413065
O	-1.19331519	-3.81606946	-2.35566823

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O	-0.20854439	2.95158852	-3.07797205
H	-0.98793463	2.41615910	-3.24254551
H	-0.57971846	4.23062478	-1.79920691
O	-6.29172290	0.72482538	-0.97809467
O	-2.94246496	-2.05937771	1.12902049
H	-5.25655069	1.85501897	-1.60579852
H	-6.54292486	0.73658739	-0.04590691
H	-2.34099577	-1.30211426	0.97531527
H	-3.27867038	-2.30346010	0.25632466
O	-1.43767355	0.05581333	0.49461610
O	-4.66622450	2.54622412	-1.98061352
H	0.46137489	2.39492076	-2.66608308
H	-1.76774738	0.81365252	1.01882912
H	-5.22461135	3.27644283	-2.23615614
H	-3.42804475	1.98699290	-3.05459774
O	-2.69679495	1.58982236	-3.56369099
H	-2.20903988	0.09854297	-2.68399785
H	-2.93472565	1.62134408	-4.48618340
O	-0.66031173	4.74341075	-0.98267752
H	-1.50515574	4.48613444	-0.58343907
H	0.71469396	4.33815493	-0.16167532
O	-3.03942326	3.79330648	0.07347742
H	-2.89938019	3.19907776	0.82114837
H	-3.57187320	3.31638893	-0.56737860
O	-1.99654305	-0.60843259	-2.06036564
H	-3.06964093	-1.81330214	-1.84987562
H	-1.81219505	-0.19058092	-1.20175977
O	-2.47455090	1.93887328	2.08518009
H	-3.17598809	1.40083453	2.48449795
H	-1.84259575	2.20989133	2.77170771
O	-6.24853983	-2.07884369	-1.46214654
H	-6.76191647	-2.46271523	-2.16799977
H	-6.29785239	-0.20057562	-1.24481521
O	-4.85649566	-3.19701444	2.80788265
H	-4.07766127	-2.84564169	2.36085894
H	-4.89185866	-2.76172907	3.65658839
O	-6.97396772	0.28520821	1.70438337
H	-7.10738349	-0.68573510	1.60915221
H	-7.73711953	0.65121907	2.14257389
O	-7.00744280	-2.30368734	1.26927505
H	-6.31538083	-2.73715383	1.78919455
H	-6.78411085	-2.40440156	0.33830142
O	-3.61270770	-2.58764221	-1.56199374
H	-5.31821081	-2.33619916	-1.59573174
H	-3.17477560	-3.35743609	-1.92248689
O	-4.36436583	0.06713724	2.70515153
H	-5.27512916	0.26549924	2.45560766
H	-4.07878786	-0.64278212	2.12695901
H	-0.46386101	0.07106199	0.54207088
O	-0.46614265	2.65501696	3.78541209
H	-0.43938349	3.54473244	4.12574202
O	1.55432770	3.94597495	0.17501678
H	1.63064634	2.91962337	1.50859223
H	2.25817710	4.61409164	0.15501548
O	5.38955487	-0.60967853	2.30862740
O	3.06345392	-2.77225613	-1.84357934
H	5.03776205	0.29014276	2.32451828
H	5.96051186	-0.71024713	1.53777326
H	2.32548672	-2.68393076	-2.44472491
H	2.69698619	-2.68959399	-0.94122803
O	1.86374836	1.81599423	-1.48695621



O	4.41125525	1.99061421	2.38545450
H	1.83633815	2.62488489	-0.94096884
H	2.75509224	1.76369857	-1.85990502
H	4.75328675	2.51336808	3.10659551
H	3.43733308	2.10119533	2.38671922
O	1.74156634	2.21989968	2.18814762
H	1.54769476	1.39147199	1.72150564
H	0.36208448	2.51300087	3.29846525
O	3.84429543	5.40234317	0.21140304
H	4.46375413	4.66611559	0.05346268
H	4.12367383	6.14255840	-0.31780550
O	5.30177569	3.15393321	-0.05307673
H	5.08348234	2.60133662	-0.81217117
H	5.05200173	2.66985218	0.74147771
O	1.23710494	0.11323236	0.48892029
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H	1.53218199	0.58697393	-0.31336685
O	4.50530617	1.60958093	-2.29138088
H	4.78183354	0.66593761	-2.23507026
H	4.79252540	1.93839498	-3.13906365
O	4.02909246	-2.82056268	2.50071546
H	3.90173422	-3.08991373	3.40627033
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O	4.60574108	-5.03237923	-1.45937050
H	4.04729701	-4.30428247	-1.76404381
H	5.08222072	-5.36694688	-2.21336423
O	6.81422379	-1.55109198	0.09042713
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H	7.76453454	-1.50297362	0.03115156
O	5.92238968	-3.94188266	0.71557820
H	5.50028655	-4.42305623	-0.01011008
H	5.25295835	-3.78607265	1.38994610
O	2.07158279	-2.49766767	0.64339811
H	2.71422976	-2.66455492	1.35466934
H	1.25402057	-2.98294847	0.84835294
O	5.19435310	-0.91384374	-2.08629177
H	5.80711339	-1.11973523	-1.36721113
H	4.47177920	-1.54975820	-2.03921850
N	-0.43068164	-3.75287588	0.99147443
H	-1.30714946	-3.30115589	1.25970735
H	-0.64906576	-4.73452083	0.84285177
H	-0.30209431	-2.41028407	-1.10034499
C	-0.23214954	-2.93469566	-2.07341970
O	-1.00273802	-3.70471509	-2.50338731