

**Coordinates of initial state (IS) and transition state (TS) for proton penetration  
Hexagonal (Path1)**

**IS**

C	0.7424692987	1.7309170883	7.4996704122
C	3.7922614795	3.1630499737	7.4999776004
C	3.7924533660	1.7311253344	7.4998578925
C	0.7425454505	3.1631859007	7.4996657122
C	1.5509584994	0.5756223532	7.4996852647
C	2.9841337773	0.5756042380	7.4997188822
C	5.2777470467	1.7311258861	7.4998576738
C	8.3276580374	3.1631880094	7.4996660639
C	8.3277342031	1.7309144078	7.4996710208
C	5.2779388783	3.1630493201	7.4999768696
C	6.0860666494	0.5756041525	7.4997195234
C	7.5192415887	0.5756221076	7.4996851939
C	9.8126677029	1.7309640751	7.4996943370
C	12.8627345741	3.1632096674	7.4996353778
C	12.8628267359	1.7309673155	7.4996934634
C	9.8127599085	3.1632124265	7.4996365594
C	10.6211040570	0.5756840169	7.4996815550
C	12.0543937826	0.5756841850	7.4996823168
C	0.7425516032	5.4736905106	7.4997207253
C	3.7923889327	6.9056702702	7.4998015474
C	3.7922545832	5.4738311041	7.5000337890
C	0.7425344120	6.9058737331	7.4996134755
C	1.5508763206	4.3183996193	7.4997577741
C	2.9841014890	4.3184013335	7.5000887825
C	5.2779458305	5.4738316609	7.5000335691
C	8.3276690737	6.9058758202	7.4996138597
C	8.3276518800	5.4736878315	7.4997213031
C	5.2778114322	6.9056696298	7.4998008155
C	6.0860989142	4.3184012472	7.5000894040
C	7.5193237654	4.3183993649	7.4997577167
C	9.8127665674	5.4736633401	7.4996913709
C	12.8627620579	6.9058235259	7.4996368097
C	12.8627278603	5.4736665709	7.4996904857
C	9.8127324464	6.9058262634	7.4996379820
C	10.6211008608	4.3183990888	7.4996889055
C	12.0543969655	4.3183992542	7.4996896803
C	0.7423574274	9.2162283817	7.4996902525
C	3.7926156365	10.6486697235	7.4996540795
C	3.7926111162	9.2162345056	7.4997095570
C	0.7423532822	10.6486723644	7.4996346877
C	1.5509575699	8.0612156957	7.4996845966

C	2.9841344041	8.0612369428	7.4997180032
C	5.2775892985	9.2162350711	7.4997093320
C	8.3278501971	10.6486744592	7.4996350847
C	8.3278460492	9.2162256907	7.4996908751
C	5.2775847238	10.6486690764	7.4996533410
C	6.0860660145	8.0612368636	7.4997186451
C	7.5192425160	8.0612154351	7.4996845254
C	9.8126432663	9.2161857780	7.4996931579
C	12.8628557262	10.6487116207	7.4996367629
C	12.8628511806	9.2161890400	7.4996922609
C	9.8126387740	10.6487143694	7.4996379543
C	10.6211031470	8.0611531873	7.4996813426
C	12.0543947035	8.0611533570	7.4996821066
H	4.5350542870	4.3176734630	12.4956356296

# TS

C	0.7583990035	1.7169261554	10.0018369363
C	3.7082413811	3.1559844733	10.0043750260
C	3.8199210097	1.7611329052	10.0033167637
C	0.7180397041	3.1564977267	10.0021574428
C	1.5838405025	0.5833454512	10.0022932450
C	3.0177362606	0.5812902657	10.0028345185
C	5.2993678947	1.7611145183	10.0016149129
C	8.4012415265	3.1565064568	9.9989898215
C	8.3608970012	1.7169189933	9.9988642794
C	5.4110471907	3.1559742107	10.0022601829
C	6.1015506244	0.5812782181	9.9998609194
C	7.5354519105	0.5833424156	9.9986208560
C	9.8491094802	1.7130383412	9.9973349729
C	12.8705270619	3.1538644147	9.9990267269
C	12.8755248778	1.7130212764	9.9988131352
C	9.8540541716	3.1538743901	9.9974683600
C	10.6467454851	0.5686355497	9.9955171773
C	12.0778693631	0.5686179185	9.9961103072
C	0.7180087489	5.4825777613	10.0002914036
C	3.8199077349	6.8777701944	10.0003906146
C	3.7085326908	5.4828587132	10.0024498109
C	0.7583946022	6.9219756361	9.9987190878
C	1.4975595709	4.3195279198	10.0032539475
C	2.9053423454	4.3195311691	10.0043033521
C	5.4107441895	5.4828589618	10.0003407928
C	8.3609041071	6.9220110488	9.9957484576
C	8.4012730717	5.4826095839	9.9971163421
C	5.2993857852	6.8777839299	9.9987078344

C	6.2139380043	4.3195357412	10.0006707767
C	7.6217209092	4.3195445047	9.9990882010
C	9.8541266669	5.4851606134	9.9955936220
C	12.8753906970	6.9258619315	9.9956932827
C	12.8704561029	5.4851454315	9.9971651209
C	9.8492317049	6.9258752172	9.9942108678
C	10.6524961358	4.3194692381	9.9960340737
C	12.0720790602	4.3194560680	9.9966662917
C	0.7814623421	9.2261010876	9.9981320483
C	3.8177845527	10.6571969440	10.0008672409
C	3.8177940083	9.2098047859	9.9997070284
C	0.7814247001	10.6409793965	9.9993906830
C	1.5838211922	8.0556363289	9.9997510240
C	3.0177334507	8.0576343901	10.0003831817
C	5.3015051996	9.2098124070	9.9982679604
C	8.3378862014	10.6409913746	9.9964463232
C	8.3378478701	9.2261139912	9.9951946574
C	5.3015090922	10.6571808223	9.9994053835
C	6.1015578512	8.0576345152	9.9974356202
C	7.5354721955	8.0556519394	9.9961243929
C	9.8351892312	9.2273118023	9.9935276267
C	12.8894545148	10.6398039778	9.9963524053
C	12.8894290159	9.2272930200	9.9950970208
C	9.8351559245	10.6398255255	9.9947880776
C	10.6467365054	8.0704115484	9.9929572589
C	12.0778909817	8.0704027933	9.9935656572
H	4.5597419404	4.3275336773	10.0042867266

### Octagonal (Path1)

IS

C	0.7395173274	1.7276656660	9.8771037043
C	3.7957441545	3.1665997524	9.8820009930
C	3.7956931969	1.7274713874	9.8804327309
C	0.7394743697	3.1663704254	9.8778799406
C	1.5492972261	0.5770193203	9.8769067585
C	2.9857612288	0.5770339616	9.8783133937
C	5.2745991286	1.7274412750	9.8834890364
C	8.3303964668	3.1665680331	9.8881801487
C	8.3303422781	1.7275956972	9.8852317867
C	5.2745762504	3.1666837800	9.8855896574
C	6.0843054290	0.5770573800	9.8839257058
C	7.5207135683	0.5770283475	9.8845844041
C	9.8093871516	1.7275543533	9.8831042845

C	12.8652515477	3.1664347604	9.8789531892
C	12.8652462818	1.7276082554	9.8780475626
C	9.8093388953	3.1665470418	9.8856128543
C	10.6191310794	0.5769585834	9.8807129301
C	12.0555811518	0.5769585743	9.8786506030
C	0.7421369563	5.4747542645	9.8788923473
C	3.7921088274	6.9061616537	9.8831214355
C	3.7930104628	5.4747158173	9.8837341993
C	0.7428664098	6.9060768255	9.8786083235
C	1.5493398351	4.3169333320	9.8787901833
C	2.9857312861	4.3169366925	9.8810199892
C	5.2772906444	5.4747027502	9.8879323402
C	8.3270140538	6.9061890518	9.8906824917
C	8.3277387852	5.4745942126	9.8919859096
C	5.2781385944	6.9061840258	9.8870841708
C	6.0844160598	4.3169439375	9.8893564733
C	7.5206879853	4.3169926323	9.8911858578
C	9.8118691311	5.4746610000	9.8886460340
C	12.8619558079	6.9061051874	9.8798144954
C	12.8626883278	5.4748086157	9.8801193986
C	9.8126593060	6.9062026765	9.8876749691
C	10.6191179756	4.3170446876	9.8850824909
C	12.0554761884	4.3170096978	9.8812594129
C	0.7428951556	9.2158737498	9.8771970541
C	3.7928767697	10.6472081571	9.8796318386
C	3.7920640753	9.2158139138	9.8806193091
C	0.7422439821	10.6471876626	9.8767086776
C	1.5496476478	8.0609759471	9.8780836398
C	2.9852335982	8.0609692970	9.8799964767
C	5.2781806009	9.2157389360	9.8837830720
C	8.3276059534	10.6473171421	9.8838812088
C	8.3269613844	9.2157088206	9.8857399760
C	5.2773751811	10.6472215585	9.8824913050
C	6.0848440583	8.0609506465	9.8872647650
C	7.5203665199	8.0609279791	9.8886681972
C	9.8127683560	9.2157354813	9.8835752008
C	12.8626183958	10.6471396598	9.8776045106
C	12.8619074501	9.2158224436	9.8781980499
C	9.8120660633	10.6472423561	9.8819282848
C	10.6195835986	8.0609203281	9.8836345345
C	12.0550952549	8.0609543144	9.8804089363
H	7.3694005721	6.2011430000	11.9384187629

TS

C	0.7409100332	1.7287538368	9.8726879231
C	3.7946010365	3.1644722471	9.8715820304
C	3.7946033931	1.7285256943	9.8719264272
C	0.7409203898	3.1642344448	9.8725440787
C	1.5468400025	0.5752264056	9.8727605266
C	2.9883140894	0.5752382677	9.8724397807
C	5.2757702358	1.7285753077	9.8712315267
C	8.3294351471	3.1644332316	9.8701569240
C	8.3293638847	1.7286819310	9.8708327380
C	5.2757323277	3.1645526944	9.8707647055
C	6.0818364251	0.5752327767	9.8711996866
C	7.5234297526	0.5752225495	9.8710575487
C	9.8108597927	1.7286462133	9.8713175089
C	12.8643672569	3.1642787791	9.8722969374
C	12.8643721012	1.7287658816	9.8724745055
C	9.8108285034	3.1643967791	9.8707375257
C	10.6170120493	0.5752023571	9.8719128283
C	12.0584510856	0.5752029149	9.8723764610
C	0.7409866818	5.4714156134	9.8723006701
C	3.7944443989	6.9070203629	9.8713837198
C	3.7945391810	5.4711701826	9.8711832798
C	0.7410567378	6.9067905726	9.8723869944
C	1.5468613310	4.3177533993	9.8723475414
C	2.9882899064	4.3177500943	9.8718315907
C	5.2757366114	5.4712060503	9.8702731407
C	8.3293848696	6.9069697585	9.8697388106
C	8.3294598700	5.4712364090	9.8692709433
C	5.2758130634	6.9070036454	9.8705307159
C	6.0819020402	4.3178194060	9.8699362345
C	7.5233921284	4.3178414818	9.8695081856
C	9.8107871493	5.4712540397	9.8700430702
C	12.8643205641	6.9067954006	9.8721117597
C	12.8643690434	5.4714657455	9.8720156860
C	9.8108411649	6.9070058879	9.8703583854
C	10.6170333743	4.3178434785	9.8708734117
C	12.0584035262	4.3178171776	9.8717661572
C	0.7410370458	9.2142534783	9.8726718654
C	3.7945028668	10.6498344806	9.8721562431
C	3.7944559333	9.2140510322	9.8719276615
C	0.7410007143	10.6496416469	9.8728086892
C	1.5468061264	8.0605504872	9.8725020520
C	2.9883292162	8.0605378330	9.8720731736
C	5.2758695862	9.2139672135	9.8712761387

C	8.3292718198	10.6496992514	9.8712735507
C	8.3293180741	9.2140468488	9.8708610458
C	5.2758714983	10.6497789936	9.8715682453
C	6.0818547565	8.0604740394	9.8705054870
C	7.5234427595	8.0604576370	9.8702072143
C	9.8109060784	9.2140788522	9.8713014716
C	12.8643042097	10.6495863623	9.8726186611
C	12.8642936244	9.2141961331	9.8724585450
C	9.8109286146	10.6497052429	9.8716714868
C	10.6169996102	8.0604813358	9.8712712549
C	12.0584416109	8.0605105812	9.8719866431
H	7.3775251580	6.2011430000	9.9722982333

### Hexagonal (Path2)

#### IS

C	0.7548915787	1.7385301120	9.3346890465
C	3.8349000959	3.1889059254	9.2664212352
C	3.8349883240	1.7224307108	9.2185224246
C	0.7569740809	3.1722350559	9.3830771170
C	1.5627633532	0.5820490411	9.3042133397
C	3.0034923620	0.5748570734	9.2591720928
C	5.2723911531	1.7107815256	9.2253147418
C	8.3290320262	3.1697300015	9.3649948713
C	8.3297015661	1.7361000492	9.3488892010
C	5.2780596198	3.2016911836	9.2632420343
C	6.0811116834	0.5752129343	9.2981127250
C	7.5208796382	0.5780522758	9.3461988146
C	9.8141659666	1.7359313974	9.3680382676
C	12.8734021351	3.1725154009	9.3945515348
C	12.8717218451	1.7391333183	9.3572583570
C	9.8161015917	3.1694372473	9.3847701561
C	10.6255439126	0.5816302177	9.3721503197
C	12.0563832041	0.5862098731	9.3601330100
C	0.7569815168	5.4856290689	9.4807194292
C	3.7646472109	6.9124287061	10.0929798864
C	3.8301330054	5.4577340686	9.6099032861
C	0.7531853686	6.9152157111	9.4868687765
C	1.5668818683	4.3279312671	9.4342622543
C	3.0104959140	4.3285437016	9.4173138762
C	5.2500365933	5.4971310804	9.5343312557
C	8.3243893133	6.9057423175	9.4766532968
C	8.3265693713	5.4808642184	9.4482769554
C	5.2723043738	6.9026691151	9.7584147659

C	6.0839724813	4.3249784275	9.3653453715
C	7.5179273908	4.3231110028	9.3902891848
C	9.8197650077	5.4810480754	9.4410545485
C	12.8650419933	6.9101201735	9.4554085229
C	12.8704692874	5.4837052815	9.4604085159
C	9.8181650954	6.9079162036	9.4511210559
C	10.6289925844	4.3227516824	9.4178374865
C	12.0610641387	4.3236613265	9.4272777289
C	0.7425408675	9.2265316215	9.3806919076
C	3.8148329775	10.6528814938	9.3071516319
C	3.7867049050	9.1853949763	9.4603357669
C	0.7480844861	10.6546393347	9.3369177494
C	1.5540992785	8.0754903534	9.4754365671
C	2.9809004143	8.0903531439	9.5725358816
C	5.2573321407	9.2027268409	9.5261847272
C	8.3275826109	10.6512959004	9.3882569911
C	8.3222486862	9.2187434339	9.4298215699
C	5.2579015996	10.6404894425	9.3492868913
C	6.0774950171	8.0591994405	9.6181493045
C	7.5157124772	8.0639014870	9.4984192670
C	9.8130632871	9.2200783075	9.4104933070
C	12.8652074514	10.6567815253	9.3518149683
C	12.8609208887	9.2249977461	9.3801999254
C	9.8155177982	10.6499809458	9.3846306590
C	10.6241651623	8.0649399607	9.4258942079
C	12.0547690022	8.0669898147	9.4189698606
H	3.6190529160	6.8936549512	11.1888968886

# TS

C	0.7511698085	1.7500013630	9.9954997813
C	3.7902387854	3.1576295811	9.9947198231
C	3.8067924045	1.7005034906	9.9938480338
C	0.7388699068	3.1803510950	9.9960341746
C	1.5514750164	0.5875790439	9.9950426207
C	2.9899349571	0.5563895259	9.9944408908
C	5.2605347909	1.7000066043	9.9938700291
C	8.3164728416	3.1858272825	9.9955578598
C	8.3190611239	1.7570598713	9.9955668609
C	5.2676325563	3.1584078886	9.9944971913
C	6.0773778796	0.5548013847	9.9947948017
C	7.5166013425	0.5849870557	9.9954725360
C	9.7970190121	1.7643100669	9.9959616802
C	12.8703902927	3.1818561377	9.9962142517
C	12.8648538718	1.7559614553	9.9958639283

C	9.8020788024	3.1880923675	9.9959566059
C	10.6188567691	0.6165596064	9.9960339796
C	12.0460486833	0.6174230970	9.9958752089
C	0.7364749565	5.4868757533	9.9968878124
C	3.4927027087	6.8212284859	10.0051089986
C	3.7865707200	5.4801514339	9.9994849432
C	0.6966456443	6.9360520359	9.9969463506
C	1.5536830020	4.3343757180	9.9966575385
C	2.9859704218	4.2910755099	9.9968122158
C	5.2686814007	5.4809405666	9.9983623908
C	8.3647664884	6.9297309623	9.9966213834
C	8.3149323580	5.4886616664	9.9961840552
C	5.5652432460	6.8227110297	10.0024398489
C	6.0682294643	4.2921923495	9.9958204707
C	7.5024214841	4.3360566652	9.9957703528
C	9.8113292131	5.4835825074	9.9960654428
C	12.8445768232	6.9251079315	9.9961979431
C	12.8612910726	5.4819844623	9.9964628343
C	9.8207043885	6.9154697831	9.9960690938
C	10.6196246372	4.3370868815	9.9962137490
C	12.0546352369	4.3363662621	9.9964207602
C	0.6797448834	9.2601455396	9.9957731346
C	3.7984414112	10.6182667554	9.9954190170
C	3.7665578716	9.1788840268	9.9982359553
C	0.7173701994	10.6842694675	9.9952701991
C	1.4638680978	8.1059899391	9.9976623612
C	2.8761799381	8.0929382262	10.0007850438
C	5.2938380705	9.1795075264	9.9984193896
C	8.3588960192	10.6925461477	9.9958349049
C	8.3919869717	9.2511342629	9.9961803861
C	5.2667840714	10.6169215824	9.9956922406
C	6.1852773626	8.0954083243	10.0003084401
C	7.5986217441	8.1100357357	9.9976992453
C	9.8361295133	9.2428502642	9.9957429233
C	12.8344164384	10.6882961323	9.9953833708
C	12.8286147927	9.2558211438	9.9954724249
C	9.8268832536	10.6986358215	9.9957957674
C	10.6247507030	8.0794332556	9.9958990395
C	12.0435576079	8.0789149662	9.9958500771
H	4.5300994027	7.3916781812	9.9936210434

**Octagonal (Path2)****IS**

C	0.7429754474	1.7478953427	9.4142546244
C	3.8126094889	3.1972371299	9.5800267115
C	3.8125933974	1.7600265960	9.4016031998
C	0.7478328911	3.1810911961	9.4572958705
C	1.5499791108	0.5938596312	9.3783480014
C	2.9898168247	0.5975651876	9.3425277739
C	5.2555837394	1.7474623655	9.3611676800
C	8.3280877493	3.1736350903	9.4150000442
C	8.3221950866	1.7447701435	9.3666131160
C	5.2839039421	3.2143420102	9.5168220788
C	6.0668363733	0.5978964169	9.3053737756
C	7.5077585270	0.5902443041	9.3387466951
C	9.8103159738	1.7428147558	9.3687285394
C	12.8632958624	3.1797093800	9.4273139648
C	12.8604376556	1.7493853296	9.3991147893
C	9.8136621134	3.1751129847	9.4008795357
C	10.6194178726	0.5859954657	9.3685177842
C	12.0504873270	0.5903234290	9.3798860692
C	0.7453662574	5.4938601378	9.5030330507
C	3.8205031420	6.9033474542	9.5791804228
C	3.7973465306	5.4976847129	9.8050171932
C	0.7440736379	6.9195044813	9.4717597047
C	1.5542028597	4.3359492878	9.5331981194
C	2.9916136961	4.3411603948	9.6639880508
C	5.3055451636	5.4886995186	10.1415874330
C	8.3139128949	6.9150814548	9.5115787825
C	8.3182378837	5.4847864163	9.5220177294
C	5.2401008739	6.9427666416	9.6563776606
C	6.0900755382	4.3096207902	9.6244341411
C	7.5166026695	4.3244076098	9.5184842209
C	9.8101972559	5.4896871555	9.4771375944
C	12.8563149790	6.9190243658	9.4548996350
C	12.8582178561	5.4917880838	9.4668447947
C	9.8054272042	6.9168149508	9.4785759414
C	10.6208518923	4.3330331559	9.4358127516
C	12.0513342794	4.3348682106	9.4401116455
C	0.7423446480	9.2307733889	9.3858398700
C	3.7986223882	10.6900394173	9.2708268295
C	3.7925528769	9.1987961377	9.3070910652
C	0.7416868885	10.6628481620	9.3705902940
C	1.5530949017	8.0765160312	9.4203003000
C	2.9870160615	8.0752814957	9.4062358671

C	5.2356440484	9.2113472478	9.3108792840
C	8.3150735834	10.6606281716	9.3581557859
C	8.3131383880	9.2282888144	9.4061319989
C	5.2355095068	10.6779978829	9.2649020737
C	6.0597943032	8.0711283715	9.4603014745
C	7.5036510675	8.0716811816	9.4679887746
C	9.8029619966	9.2279645697	9.4059847854
C	12.8611030671	10.6631336372	9.3779879785
C	12.8592295955	9.2307560604	9.3940754041
C	9.8048087374	10.6600710703	9.3679473415
C	10.6149321136	8.0755337548	9.4368268379
C	12.0470063070	8.0764961541	9.4255080066
H	5.4495265411	5.5110003266	11.2375907561

# TS

C	0.7362280986	1.7328515405	10.0000968021
C	3.8139495839	3.1751769617	10.0000729087
C	3.7985142657	1.6984067086	10.0001408771
C	0.7496572080	3.1722348063	10.0000905527
C	1.5391913229	0.5786272606	10.0001077694
C	2.9714205813	0.5785765841	10.0001338738
C	5.2231057477	1.6808808738	10.0001419928
C	8.3546112610	3.1585688373	10.0000901525
C	8.3484989514	1.7254600167	10.0001096369
C	5.2432184811	3.1266185092	10.0000635710
C	6.0785289351	0.5785837458	10.0001414039
C	7.5222785513	0.5786218135	10.0001201967
C	9.8235040341	1.7281047766	10.0001104220
C	12.8742588432	3.1741317104	10.0000966453
C	12.8706179714	1.7352976038	10.0000975593
C	9.8321048458	3.1671304221	10.0001085152
C	10.6368042857	0.5786218012	10.0001031262
C	12.0615980532	0.5786520514	10.0000980114
C	0.7566908826	5.4758841945	10.0000759158
C	3.8588909262	6.9271913369	10.0000779381
C	3.8589304496	5.4581197108	9.9999300859
C	0.7566069363	6.9095788041	10.0000826383
C	1.5690643815	4.3210231518	10.0000661755
C	3.0066732304	4.3122271247	10.0000226292
C	5.2197994182	5.2630554152	9.9997729383
C	8.3140073360	6.9094955332	10.0000546124
C	8.3139769652	5.4759076670	10.0000475337
C	5.2197598826	7.1223040155	10.0000421916
C	6.1075461020	4.2038552041	9.9999368516

C	7.5356900836	4.2879086841	10.0000205937
C	9.8104447203	5.4817866255	10.0000871670
C	12.8797963500	6.9092265400	10.0000886278
C	12.8798895485	5.4761845511	10.0000874248
C	9.8104416842	6.9036347242	10.0000860664
C	10.6286471199	4.3222881965	10.0000996229
C	12.0631531511	4.3247730128	10.0000957488
C	0.7495976976	9.2131987532	10.0001009048
C	3.7984731214	10.6868578093	10.0001482574
C	3.8139315523	9.2100860624	10.0001183460
C	0.7361808911	10.6525403611	10.0001034365
C	1.5689803538	8.0644189840	10.0000968581
C	3.0066060237	8.0730934369	10.0001061949
C	5.2432063584	9.2587135994	10.0000937519
C	8.3485300173	10.6599496328	10.0001070448
C	8.3545400466	9.2268400836	10.0000851816
C	5.2230551273	10.7044172595	10.0001442623
C	6.1075596253	8.1814903019	10.0000249618
C	7.5356903369	8.0974718417	10.0000525165
C	9.8320174805	9.2182575580	10.0000930790
C	12.8705831611	10.6501053014	10.0000979920
C	12.8741869472	9.2112877474	10.0000971921
C	9.8235137863	10.6572616332	10.0001044103
C	10.6285909526	8.0631682762	10.0000933502
C	12.0630690399	8.0606619946	10.0000960052
H	6.0022504557	6.1926753837	10.0002064030

#### Hexagonal (Dissociation-penetration)

##### IS

C	0.7921827099	1.7286477224	9.8727583318
C	3.8459518994	3.1644861504	9.8728649040
C	3.8459766305	1.7284522227	9.8728157877
C	0.7922558616	3.1643393193	9.8727777031
C	1.5982016972	0.5752584459	9.8728369616
C	3.0396963403	0.5752447081	9.8727909940
C	5.3269976793	1.7285350221	9.8727856799
C	8.3806988763	3.1643005929	9.8728765061
C	8.3806868317	1.7287756815	9.8728154550
C	5.3269750979	3.1645806490	9.8727917572
C	6.1332678207	0.5753010405	9.8728617637
C	7.5747304957	0.5752517025	9.8728010279
C	9.8624149789	1.7287095893	9.8728033812
C	12.9159212968	3.1643178183	9.8728736604

C	12.9159750337	1.7286173534	9.8728110519
C	9.8624612874	3.1642617852	9.8728176234
C	10.6684547665	0.5752261594	9.8728469316
C	12.1097830033	0.5751822174	9.8727844464
C	0.7923781435	5.4714911481	9.8727895660
C	3.8457642579	6.9070519769	9.8728689187
C	3.8457954107	5.4712931205	9.8728047687
C	0.7924153337	6.9068815289	9.8727888121
C	1.5981982472	4.3177628222	9.8728478135
C	3.0397119791	4.3177270759	9.8728135062
C	5.3270466381	5.4712894907	9.8727756605
C	8.3805547690	6.9067636016	9.8728847079
C	8.3806040306	5.4714956005	9.8728394667
C	5.3271592257	6.9070099014	9.8728043878
C	6.1332616886	4.3178052665	9.8728924052
C	7.5746966581	4.3177733470	9.8728292860
C	9.8625507936	5.4715595204	9.8727940314
C	12.9157912614	6.9068770743	9.8728661423
C	12.9157894698	5.4715189922	9.8728124012
C	9.8625749487	6.9068664615	9.8728113114
C	10.6684346048	4.3177969367	9.8728648467
C	12.1097914899	4.3177500590	9.8727944848
C	0.7923354927	9.2141645663	9.8727709771
C	3.8458849873	10.6498749783	9.8728570314
C	3.8458017648	9.2140597485	9.8728068520
C	0.7922587122	10.6498102241	9.8727957188
C	1.5981719626	8.0606699696	9.8728362186
C	3.0397321621	8.0606121025	9.8727596196
C	5.3271650691	9.2140239634	9.8727825576
C	8.3806045640	10.6496587617	9.8728887817
C	8.3805478693	9.2142213610	9.8728203565
C	5.3271195198	10.6498809888	9.8727916558
C	6.1332437838	8.0605808492	9.8728220295
C	7.5747505138	8.0605601101	9.8727894129
C	9.8625011233	9.2142753708	9.8727830253
C	12.9159568252	10.6497427892	9.8728608659
C	12.9158837862	9.2141419873	9.8728036598
C	9.8624633138	10.6496598590	9.8727952729
C	10.6684220608	8.0606667188	9.8728500626
C	12.1098009969	8.0606525504	9.8727904383
H	1.1369387599	2.3477694544	17.7006942333
H	1.7191925558	3.7783873649	17.6142122241
O	1.6284951439	2.9429781424	17.1127552023
H	4.9554024483	2.2346041855	17.0464601400

H	3.4159836449	2.0486407293	17.0725191616
O	4.2550071781	1.5468801316	17.1065184694
H	1.2114347835	6.2158423212	17.3778576308
H	2.3287995545	5.5550744790	16.5584103603
O	2.0624850874	5.7550935074	17.4748720687
H	3.6651966280	6.9777564879	17.4382791218
H	4.4425882586	8.2796370506	17.1053838901
O	4.3983356617	7.3323690837	16.8926813803
H	7.4981987825	6.5347594771	16.8934652841
H	6.0006319375	6.5481209693	17.2976479243
O	6.8616748468	6.0964623839	17.4783327131
H	6.6316038953	4.3222552806	17.1254026993
H	7.2119978758	2.9092972653	17.3842701359
O	6.5197492581	3.3679017673	16.8839112809
H	0.9767531316	2.4117929199	2.1247094833
H	1.5708718808	3.7947772251	2.4975917111
O	1.4795131845	2.8707681147	2.8152955334
H	4.6522862786	2.1846027312	2.8935005495
H	3.1309418387	1.9629075893	2.9985359230
O	3.9861240734	1.4822463087	3.0367431418
H	0.9147279903	6.1135664438	2.6259930903
H	2.1802235090	5.7323152911	3.4121729380
O	1.7820711295	5.6860425087	2.5234433148
H	3.5207547394	6.8939089730	2.1830949934
H	4.3385968600	8.1784989026	2.4463789092
O	4.2493524432	7.2516435221	2.7284375787
H	7.3437114290	6.5921431371	2.8619913140
H	5.8886911912	6.5440029207	2.3433420556
O	6.8002842900	6.2131690404	2.1533055971
H	6.5757244391	4.4151102864	2.6100619815
H	6.9922783672	2.9207973877	2.6301184383
O	6.3699292771	3.5443957711	3.0330903551
H	5.2419783721	3.7981085700	13.7185952471

# TS

C	0.7921339303	1.7286125640	9.8727043302
C	3.8460145622	3.1645295030	9.8727832876
C	3.8460421327	1.7284055135	9.8727231611
C	0.7922088944	3.1643711938	9.8727125311
C	1.5982113349	0.5752623482	9.8728264589
C	3.0396886002	0.5752491431	9.8727570856
C	5.3269333137	1.7284883880	9.8727063777
C	8.3807512721	3.1643369553	9.8727940373
C	8.3807415278	1.7287353239	9.8727396695

C	5.3269145567	3.1646233276	9.8727207919
C	6.1332738886	0.5753064141	9.8728149344
C	7.5747219763	0.5752566048	9.8727647777
C	9.8623583663	1.7286702835	9.8726999351
C	12.9159689530	3.1643519512	9.8727963428
C	12.9160236206	1.7285832206	9.8727398900
C	9.8624054161	3.1643012846	9.8727162761
C	10.6684639342	0.5752291825	9.8728199738
C	12.1097730612	0.5751848173	9.8727702732
C	0.7923382120	5.4714605405	9.8727148991
C	3.8458148340	6.9070855874	9.8727648490
C	3.8458487631	5.4712570439	9.8727165870
C	0.7923770395	6.9069092328	9.8727221708
C	1.5982060043	4.3177571526	9.8728216834
C	3.0397053558	4.3177198184	9.8727415790
C	5.3269961889	5.4712521560	9.8726959133
C	8.3805961242	6.9067945832	9.8727994354
C	8.3806478282	5.4714599848	9.8727480393
C	5.3271121952	6.9070430595	9.8727123929
C	6.1332668990	4.3177970503	9.8728011137
C	7.5746900924	4.3177661543	9.8727605213
C	9.8624992964	5.4715275187	9.8726926300
C	12.9158337522	6.9069045142	9.8727884946
C	12.9158330086	5.4714907244	9.8727318955
C	9.8625250452	6.9068978344	9.8727049923
C	10.6684428625	4.3177939997	9.8728184030
C	12.1097820909	4.3177473241	9.8727706723
C	0.7922933760	9.2141384221	9.8727032091
C	3.8459457782	10.6499196415	9.8727787970
C	3.8458567689	9.2140246588	9.8727233320
C	0.7922132699	10.6498466438	9.8727308118
C	1.5981778968	8.0606740355	9.8728244746
C	3.0397263843	8.0606168426	9.8727282423
C	5.3271129310	9.2139899779	9.8726928941
C	8.3806549941	10.6497004948	9.8727987792
C	8.3805934427	9.2141920445	9.8727298646
C	5.3270603568	10.6499271004	9.8727055321
C	6.1332476225	8.0605859512	9.8727811592
C	7.5747460545	8.0605643686	9.8727555562
C	9.8624495953	9.2142424103	9.8726969041
C	12.9160031849	10.6497761144	9.8727939333
C	12.9159280609	9.2141131702	9.8727331882
C	9.8624095952	10.6496973085	9.8727118873
C	10.6684296556	8.0606689087	9.8728229968

C	12.1097925516	8.0606546004	9.8727753807
H	1.1047666773	2.3690629991	17.6942121252
H	1.7129341981	3.7887098108	17.5971853624
O	1.6293591270	2.9420512752	17.1129682232
H	4.9512228994	2.2340874633	17.0983196922
H	3.4107862213	2.0417867710	17.1119093542
O	4.2512343278	1.5452451450	17.1843718306
H	1.2096630201	6.2149821526	17.3772803412
H	2.3359520884	5.5665263222	16.5591163327
O	2.0609052490	5.7547261492	17.4755415201
H	3.6656579935	6.9752946650	17.4445760979
H	4.4603680924	8.2634662761	17.1050411540
O	4.4006819117	7.3163369704	16.8936170269
H	7.5050633934	6.4667371691	16.9146147331
H	6.0003909725	6.5080603524	17.2966449965
O	6.8478950644	6.0336605725	17.4802456197
H	6.5923968290	4.3063733958	17.1377130581
H	7.1682066303	2.8793129999	17.3318021083
O	6.4521918867	3.3571141365	16.8854418504
H	0.9045835666	2.4389083594	2.1823004673
H	1.5443458017	3.8118677182	2.5338299787
O	1.4949102070	2.8719920666	2.8174657597
H	4.3847633574	1.5193186601	2.1510590455
H	3.2727420893	2.1302251149	3.0178120173
O	4.1850725149	1.7648837915	3.0675280480
H	0.9002368453	6.1049629177	2.6382141095
H	2.2080988126	5.7935599085	3.3851149365
O	1.7680547489	5.6816015893	2.5221276135
H	3.4548801118	6.9335999955	2.1580498124
H	4.4210008446	8.0975250154	2.4764954884
O	4.1115712513	7.2390207800	2.8127982782
H	7.3310976961	6.5372041748	2.9188863629
H	5.8363820859	6.5651165209	2.5221966667
O	6.7428462630	6.5058526548	2.1482706745
H	6.8305333758	4.4243232022	2.4163248677
H	6.1705188901	3.1351202665	2.9699419596
O	7.0093861547	3.6322283821	2.9617333260
H	4.5901546917	4.4541234746	9.8744479380

#### Octagonal (Dissociation-penetration)

IS

C	3.4938223096	5.6717211546	9.4914931231
C	6.5473591587	7.1074450844	9.4914931231

C	6.5473591587	5.6715306889	9.4914931231
C	3.4938223096	7.1072542816	9.4914931231
C	4.2998625731	4.5181846202	9.4914932266
C	5.7411283091	4.5181846202	9.4914932266
C	8.0286530545	5.6715307914	9.4914931231
C	11.0821897832	7.1074450844	9.4914931231
C	11.0821896807	5.6717210517	9.4914931231
C	8.0286530545	7.1076364472	9.4914931231
C	8.8346107866	4.5181846202	9.4914932266
C	10.2764228713	4.5181846202	9.4914932266
C	12.5638659823	5.6717210517	9.4914931231
C	15.6172119088	7.1072542816	9.4914931231
C	15.6172119088	5.6717211546	9.4914931231
C	12.5638659823	7.1074450844	9.4914931231
C	13.3699060122	4.5181846202	9.4914932266
C	14.8114445389	4.5181846202	9.4914932266
C	3.4940135693	9.4145195923	9.4914931231
C	6.5471682355	10.8500516000	9.4914931231
C	6.5473590557	9.4143281271	9.4914931231
C	3.4940136729	10.8498602367	9.4914931231
C	4.2998625731	8.2607906957	9.4914932266
C	5.7411283091	8.2607906957	9.4914932266
C	8.0286530545	9.4143281271	9.4914931231
C	11.0827663594	10.9379642701	9.4880308534
C	11.0826842676	9.3530926034	9.4887727997
C	8.0288437543	10.8500516000	9.4914931231
C	8.8348842406	8.2607906957	9.4914931231
C	10.2762321715	8.2519721712	9.4910808330
C	12.5636747226	9.4143282301	9.4914931231
C	15.6172119088	10.8498602367	9.4914931231
C	15.6172119088	9.4145195923	9.4914931231
C	12.5638659823	10.8500516000	9.4916829439
C	13.3699060122	8.2607906957	9.4914931231
C	14.8112542786	8.2607906957	9.4914932266
C	3.4940136729	13.1573170316	9.4914931231
C	6.5473590557	14.5928490382	9.4914931231
C	6.5471682355	13.1571261079	9.4914931231
C	3.4940135693	14.5926576750	9.4914931231
C	4.2995885759	12.0035891339	9.4914932266
C	5.7411283091	12.0035891339	9.4914932266
C	8.0288438573	13.1571261079	9.4914931231
C	11.0819995408	14.5926577785	9.4914931231
C	11.0819995408	13.1571261079	9.4914931231
C	8.0288437543	14.5928490382	9.4914931231

C	8.8348842406	12.0035891339	9.4914931231
C	10.2763402375	12.0124076584	9.4919871679
C	12.5638660859	13.1571261079	9.4914931231
C	15.6172119088	14.5926576750	9.4914931231
C	15.6170205286	13.1573170316	9.4914931231
C	12.5638660859	14.5926577785	9.4914931231
C	13.3699059087	12.0035891339	9.4914931231
C	14.8114445389	12.0035891339	9.4914932266
H	6.1429058418	8.3251591636	17.0146146620
H	6.6796445529	9.7505850139	16.7331812375
O	6.6559103864	8.8401026509	16.3722505839
H	9.9702835645	8.2837518455	16.3373166959
H	8.4312625764	8.0495937967	16.3741280997
O	9.2879747564	7.5769859649	16.3664450842
H	6.1303880147	12.1363248747	16.3752390757
H	7.3158034580	11.5156126042	15.6148902945
O	6.9649325178	11.6560478440	16.5132071888
H	8.6235103822	12.8057429620	16.8260800328
H	9.4086512990	14.1406315018	16.7054546439
O	9.4302386275	13.2054114815	16.4429171428
H	12.5083635650	12.5759548333	16.0563569493
H	11.0661955303	12.4639951804	16.6274279090
O	11.9662164719	12.0572335836	16.6685972887
H	11.7380939589	10.2866611993	16.4011904225
H	12.1806973700	8.8438697337	16.7717151680
O	11.5544629875	9.3316927653	16.2153319484
H	6.1090100666	8.3805874109	1.8348363735
H	6.6878270475	9.7444603683	2.2758286426
O	6.5210601473	8.8309378067	2.5889603247
H	9.8816133660	8.2187255846	2.6873467755
H	8.3460589357	7.9635358911	2.7187279857
O	9.2104340454	7.5134951275	2.8062038230
H	6.0597865151	12.0128347962	2.5610681117
H	7.2836345111	11.5537112878	3.3689789020
O	6.9549915973	11.6472736942	2.4559670843
H	8.6390369488	12.7558541818	2.2546789444
H	9.6581979669	13.9171333796	2.2938106026
O	9.4314511418	13.0784517196	2.7309287627
H	12.4873146681	12.3656167543	3.0266110749
H	11.0408493327	12.2595753499	2.4764918002
O	11.9739530355	11.9864010062	2.2968701819
H	11.8432132955	10.1575317704	2.5116205912
H	12.2486119646	8.6557235937	2.3826634013
O	11.6158174852	9.2459743281	2.8182077084

H	10.3484210262	10.0797649538	13.1823523395
<b>TS</b>			
C	3.3142145962	5.4920954614	9.3973162634
C	6.3677431915	6.9278287343	9.3973162634
C	6.3677431915	5.4919123848	9.3973162634
C	3.3142145962	6.9276407443	9.3973162634
C	4.1203025235	4.3385584652	9.3973123073
C	5.5614731633	4.3385584652	9.3973123073
C	7.8490480952	5.4919084692	9.3973162634
C	10.9025776660	6.9278287343	9.3973162634
C	10.9025815815	5.4920993972	9.3973162634
C	7.8490480952	6.9280167467	9.3973162634
C	8.6549444961	4.3385584652	9.3973123073
C	10.0968722154	4.3385584652	9.3973123073
C	12.3842605568	5.4920993972	9.3973162634
C	15.4376021173	6.9276407443	9.3973162634
C	15.4376021173	5.4920954614	9.3973162634
C	12.3842605568	6.9278287343	9.3973162634
C	13.1903396145	4.3385584652	9.3973123073
C	14.6318927491	4.3385584652	9.3973123073
C	3.3144065445	9.2349047449	9.3973162634
C	6.3675561770	10.6704499628	9.3973162634
C	6.3677471274	9.2347206480	9.3973162634
C	3.3144025884	10.6702619706	9.3973162634
C	4.1203025235	8.0811787160	9.3973123073
C	5.5614731633	8.0811787160	9.3973123073
C	7.8490480952	9.2347206480	9.3973162634
C	10.9038908654	10.8702880439	9.3894555708
C	10.9037003370	9.0956881328	9.3911400762
C	7.8492400210	10.6704499628	9.3973162634
C	8.6553230572	8.0811787160	9.3973162634
C	10.0966802895	8.0611572514	9.3963802053
C	12.3840686086	9.2347167122	9.3973162634
C	15.4376021173	10.6702619706	9.3973162634
C	15.4376021173	9.2349047449	9.3973162634
C	12.3842605568	10.6704499628	9.3975061934
C	13.1903396145	8.0811787160	9.3973162634
C	14.6317018212	8.0811787160	9.3973123073
C	3.3144025884	12.9777129675	9.3973162634
C	6.3677471274	14.4132582260	9.3973162634
C	6.3675561770	12.9775259733	9.3973162634
C	3.3144065445	14.4130702339	9.3973162634
C	4.1199269205	11.8239879792	9.3973123073

C	5.5614731633	11.8239879792	9.3973123073
C	7.8492360852	12.9775259733	9.3973162634
C	10.9023896780	14.4130662778	9.3973162634
C	10.9023896780	12.9775259733	9.3973162634
C	7.8492400210	14.4132582260	9.3973162634
C	8.6553230572	11.8239879792	9.3973162634
C	10.0966846046	11.8440094439	9.3984379365
C	12.3842566007	12.9775259733	9.3973162634
C	15.4376021173	14.4130702339	9.3973162634
C	15.4374111446	12.9777129675	9.3973162634
C	12.3842566007	14.4130662778	9.3973162634
C	13.1903435706	11.8239879792	9.3973162634
C	14.6318927491	11.8239879792	9.3973123073
H	5.9251242380	8.1342284945	17.0021821369
H	6.4549439689	9.5422105170	16.6299382732
O	6.3770524507	8.6241369047	16.2972944327
H	9.7512842384	8.0757017043	16.3006714340
H	8.2104003258	7.8369216641	16.2821908748
O	9.0692088575	7.3675461851	16.2939517325
H	5.9658906352	11.9117426987	16.2865840207
H	7.1483886820	11.3167500985	15.4994743433
O	6.8075134756	11.4389158119	16.4037492755
H	8.4463969759	12.6047609609	16.6690757490
H	9.2312740080	13.9314982290	16.4878505219
O	9.2192919582	12.9986222820	16.2159442012
H	12.3340778471	12.3105072763	16.1140231935
H	10.8590760390	12.2581753494	16.5910762994
O	11.7506802525	11.8581899211	16.7419396397
H	11.5194329654	10.1058726182	16.4484939729
H	12.0089344215	8.6521634314	16.6983056841
O	11.3389378491	9.1595557539	16.2160617866
H	5.9901156269	8.1763747229	1.7826461158
H	6.5533409541	9.5504637727	2.2204707255
O	6.4411787767	8.6223250765	2.5169758964
H	9.6869481968	8.0063794721	2.4682138945
H	8.1520199121	7.7717245273	2.5594400693
O	9.0094406937	7.2980273639	2.5205069565
H	5.8485623617	11.8098057193	2.4788135226
H	7.0906135930	11.4019361256	3.2881026600
O	6.7417215471	11.4380867866	2.3787751531
H	8.4538015783	12.5326011177	2.0927326779
H	9.4366910809	13.7234827518	2.1482155049
O	9.2275257342	12.8790720883	2.5821226768
H	12.3080214476	12.2042144605	2.9715094486

H	10.8862277020	12.0986716411	2.3681015736
O	11.8200717561	11.7999075291	2.2363819611
H	11.6199759463	10.0173280761	2.3589073827
H	12.0528329680	8.5167591781	2.3147821607
O	11.3338656138	9.1005360154	2.5969837563
H	10.0912406057	9.9669636295	9.3917425866

#### Hexagonal (Adsorption-penetration)

##### IS

C	3.8355900000	6.0112810000	9.1776090000
C	6.9154930000	7.4617400000	9.1093790000
C	6.9156920000	5.9952610000	9.0615180000
C	3.8375680000	7.4449290000	9.2258660000
C	4.6434890000	4.8549070000	9.1471530000
C	6.0840600000	4.8475900000	9.1020610000
C	8.3530990000	5.9835920000	9.0682420000
C	11.4096650000	7.4425560000	9.2078690000
C	11.4102580000	6.0089070000	9.1918500000
C	8.3586360000	7.4743970000	9.1062150000
C	9.1617880000	4.8479850000	9.1410220000
C	10.6015690000	4.8507540000	9.1890810000
C	12.8947350000	6.0087090000	9.2110340000
C	15.9540690000	7.4453250000	9.2375350000
C	15.9522900000	6.0118730000	9.2001560000
C	12.8967130000	7.4421610000	9.2276470000
C	13.7061930000	4.8543140000	9.2149890000
C	15.1370740000	4.8590600000	9.2029250000
C	3.8375680000	9.7584670000	9.3235650000
C	6.8452850000	11.1851930000	9.9358680000
C	6.9107470000	9.7305800000	9.4529090000
C	3.8338100000	11.1879630000	9.3296970000
C	4.6474440000	8.6007090000	9.2770890000
C	6.0911800000	8.6013020000	9.2602790000
C	8.3307500000	9.7699370000	9.3771620000
C	11.4051160000	11.1784700000	9.3196110000
C	11.4070940000	9.7537200000	9.2911310000
C	8.3529010000	11.1755020000	9.6012370000
C	9.1645570000	8.5977420000	9.2082650000
C	10.5986010000	8.5959630000	9.2331840000
C	12.9004700000	9.7539180000	9.2840110000
C	15.9457640000	11.1828200000	9.2982510000
C	15.9511040000	9.7564890000	9.3033920000
C	12.8988880000	11.1806450000	9.2940980000

C	13.7095560000	8.5955670000	9.2606740000
C	15.1416230000	8.5963570000	9.2701670000
C	3.8231310000	13.4993240000	9.2236910000
C	6.8955190000	14.9256550000	9.1501200000
C	6.8672370000	13.4581880000	9.3031950000
C	3.8286680000	14.9274360000	9.1797860000
C	4.6347870000	12.3482900000	9.3184240000
C	6.0615140000	12.3631230000	9.4155290000
C	8.3378700000	13.4755920000	9.3690530000
C	11.4082800000	14.9240730000	9.2312060000
C	11.4029400000	13.4916110000	9.2727380000
C	8.3384640000	14.9131960000	9.1922450000
C	9.1582290000	12.3320730000	9.4610180000
C	10.5964270000	12.3366220000	9.3413650000
C	12.8937460000	13.4927980000	9.2533570000
C	15.9457640000	14.9296110000	9.1948170000
C	15.9416100000	13.4977420000	9.2230980000
C	12.8961190000	14.9226890000	9.2274480000
C	13.7048090000	12.3378090000	9.2687830000
C	15.1354910000	12.3397870000	9.2618610000
H	4.1688360000	8.8999390000	17.7994800000
H	4.6041330000	10.3591000000	17.5455420000
O	4.4963460000	9.4924630000	17.1047080000
H	7.9395580000	8.9084420000	17.1952860000
H	6.4093950000	8.6887180000	17.0764260000
O	7.2445860000	8.2168340000	17.2500690000
H	4.1652760000	12.8011890000	17.2263370000
H	5.4157890000	12.1714830000	16.6017720000
O	4.9994790000	12.3613430000	17.4636630000
H	6.6599720000	13.5936610000	17.5287300000
H	7.4544230000	14.8188580000	17.0074040000
O	7.4126930000	13.8489860000	16.9585530000
H	10.4910140000	13.0209130000	16.7597920000
H	9.0601340000	13.0729280000	17.3438130000
O	9.9453610000	12.6530570000	17.4721680000
H	9.6769850000	10.9134540000	17.2449280000
H	10.2186820000	9.4550840000	17.3418370000
O	9.4649720000	9.9722590000	17.0224340000
H	4.1644850000	8.9928910000	1.9777200000
H	4.6591130000	10.3191500000	2.5933840000
O	4.4921930000	9.3763700000	2.8055930000
H	7.7471250000	8.7193720000	2.7294510000
H	6.2523640000	8.4294390000	2.9560980000
O	7.1186060000	7.9834630000	2.8787690000

H	3.8834510000	12.5472490000	2.6370920000
H	5.1507740000	12.3508620000	3.4857320000
O	4.7918180000	12.2039180000	2.5908130000
H	6.5053140000	13.3956920000	2.1472110000
H	7.3130150000	14.6901090000	2.4179600000
O	7.2647600000	13.7471320000	2.6511340000
H	10.3547490000	13.0519640000	2.7802790000
H	8.9027070000	13.0149800000	2.2607320000
O	9.8110740000	12.6765920000	2.0700800000
H	9.5440820000	10.8924900000	2.4157850000
H	10.0426650000	9.4620070000	2.7939250000
O	9.2446550000	10.0066700000	2.7343960000
H	6.6997240000	11.1664060000	11.0317220000

# TS

C	3.8637448465	6.0237714299	9.7481132910
C	6.9032010696	7.4123707714	9.7378000270
C	6.9087525381	5.9698821388	9.7301412308
C	3.8611623709	7.4500849741	9.7554401214
C	4.6613461207	4.8509420229	9.7433423847
C	6.0993274177	4.8200296494	9.7364442918
C	8.3836318303	5.9701090727	9.7310354332
C	11.4326638724	7.4498924609	9.7523146970
C	11.4294903948	6.0231819202	9.7502161037
C	8.3899628282	7.4123388420	9.7371991602
C	9.1935118272	4.8206241514	9.7421696013
C	10.6315073343	4.8507407802	9.7496689912
C	12.9169408770	6.0289328897	9.7533116245
C	15.9782598719	7.4502814721	9.7571531622
C	15.9814353389	6.0295194039	9.7516616180
C	12.9203063684	7.4500919568	9.7554881050
C	13.7361323368	4.8812656323	9.7540282712
C	15.1618583653	4.8816638785	9.7522360391
C	3.8607653719	9.7596559919	9.7696272254
C	6.6103470082	11.0878420342	9.8633273174
C	6.9044020341	9.7416839410	9.7907238637
C	3.8179490889	11.1897464878	9.7704437360
C	4.6750033480	8.6011059990	9.7631423765
C	6.1064464151	8.5582777373	9.7611242973
C	8.3900463950	9.7415846565	9.7790411443
C	11.4759123325	11.1901684370	9.7687263658
C	11.4332527036	9.7602624629	9.7642011836
C	8.6830216881	11.0880649808	9.8151383921
C	9.1877543719	8.5578897191	9.7527635762

C	10.6194203882	8.6011179715	9.7560282314
C	12.9339783175	9.7529265051	9.7630577375
C	15.9552799451	11.1800440147	9.7651339797
C	15.9649829238	9.7521260214	9.7663756954
C	12.9441069718	11.1808424970	9.7643791755
C	13.7329508689	8.6003249726	9.7601979050
C	15.1654158704	8.6001254827	9.7618253018
C	3.7957691489	13.5167709019	9.7545596079
C	6.9028544583	14.8808472495	9.7445250246
C	6.8811037065	13.4526350270	9.7693375241
C	3.8260905142	14.9545993516	9.7480278083
C	4.5824432867	12.3732738673	9.7701436272
C	5.9931108761	12.3577695290	9.7880073047
C	8.4128165893	13.4529891240	9.7783758444
C	11.4661756839	14.9540133394	9.7557823121
C	11.4975159831	13.5163953653	9.7618047239
C	8.3906082113	14.8812605203	9.7504530658
C	9.3004019386	12.3578478577	9.7932123108
C	10.7108288713	12.3731048023	9.7731755828
C	12.9516406813	13.5138148851	9.7584726104
C	15.9552799451	14.9571713506	9.7501823096
C	15.9473604700	13.5139999100	9.7539006425
C	12.9425147464	14.9567908109	9.7552768209
C	13.7404988068	12.3473249451	9.7606788609
C	15.1592848729	12.3469249614	9.7597587852
H	4.1970758560	8.8597435915	17.7923248021
H	4.6347783277	10.3247364409	17.5664359254
O	4.5383133959	9.4635812146	17.1130252519
H	7.9906938608	8.8834366361	17.2033068576
H	6.4473794280	8.6727591839	17.1015337101
O	7.2859640906	8.1962289834	17.2567073731
H	4.1956875484	12.7740435742	17.2770476292
H	5.4189795825	12.1404782482	16.5977624538
O	5.0397229520	12.3340441768	17.4750932271
H	6.7021977951	13.5353923556	17.5288095811
H	7.4752509487	14.7923041783	17.0518159907
O	7.4474123736	13.8251174096	16.9641447675
H	10.5337682814	12.9747755758	16.7792120960
H	9.0914570838	13.0595426589	17.3421558325
O	9.9666652841	12.6239189683	17.4827012065
H	9.6762470574	10.8635161642	17.2540412574
H	10.2342367241	9.4236557181	17.4378808901
O	9.5027214306	9.9122802344	17.0317507996
H	4.6219136836	9.0013047886	1.9854807583

H	5.1036500748	10.3307352306	2.6029648075
O	4.9583734351	9.3839171798	2.8117295031
H	8.2318484543	8.7881564828	2.8092663141
H	6.7106282332	8.5123057775	2.9581931474
O	7.5832411987	8.0658247574	2.9639076455
H	4.3483117912	12.6329311046	2.6039050743
H	5.5825747788	12.4161430102	3.5006622236
O	5.2523278780	12.2757504993	2.5952331928
H	6.9838600157	13.4264144606	2.1659768924
H	7.7124546678	14.7676991045	2.4288581118
O	7.7248372269	13.8246884582	2.6641871246
H	10.8017669769	13.0819443991	2.7367724816
H	9.3421277000	13.0973801118	2.2376631540
O	10.2143356828	12.6563792274	2.0911652387
H	9.9170107701	10.9341735695	2.4809387487
H	10.5198187874	9.5215074946	2.7036117197
O	9.7145845654	10.0379396617	2.8561926446
H	7.6553876823	11.4239901754	9.1675271758

#### Octagonal (Adsorption-penetration)

IS

C	0.7429754474	1.7478953427	9.4142546244
C	3.8126094889	3.1972371299	9.5800267115
C	3.8125933974	1.7600265960	9.4016031998
C	0.7478328911	3.1810911961	9.4572958705
C	1.5499791108	0.5938596312	9.3783480014
C	2.9898168247	0.5975651876	9.3425277739
C	5.2555837394	1.7474623655	9.3611676800
C	8.3280877493	3.1736350903	9.4150000442
C	8.3221950866	1.7447701435	9.3666131160
C	5.2839039421	3.2143420102	9.5168220788
C	6.0668363733	0.5978964169	9.3053737756
C	7.5077585270	0.5902443041	9.3387466951
C	9.8103159738	1.7428147558	9.3687285394
C	12.8632958624	3.1797093800	9.4273139648
C	12.8604376556	1.7493853296	9.3991147893
C	9.8136621134	3.1751129847	9.4008795357
C	10.6194178726	0.5859954657	9.3685177842
C	12.0504873270	0.5903234290	9.3798860692
C	0.7453662574	5.4938601378	9.5030330507
C	3.8205031420	6.9033474542	9.5791804228
C	3.7973465306	5.4976847129	9.8050171932
C	0.7440736379	6.9195044813	9.4717597047

C	1.5542028597	4.3359492878	9.5331981194
C	2.9916136961	4.3411603948	9.6639880508
C	5.3055451636	5.4886995186	10.1415874330
C	8.3139128949	6.9150814548	9.5115787825
C	8.3182378837	5.4847864163	9.5220177294
C	5.2401008739	6.9427666416	9.6563776606
C	6.0900755382	4.3096207902	9.6244341411
C	7.5166026695	4.3244076098	9.5184842209
C	9.8101972559	5.4896871555	9.4771375944
C	12.8563149790	6.9190243658	9.4548996350
C	12.8582178561	5.4917880838	9.4668447947
C	9.8054272042	6.9168149508	9.4785759414
C	10.6208518923	4.3330331559	9.4358127516
C	12.0513342794	4.3348682106	9.4401116455
C	0.7423446480	9.2307733889	9.3858398700
C	3.7986223882	10.6900394173	9.2708268295
C	3.7925528769	9.1987961377	9.3070910652
C	0.7416868885	10.6628481620	9.3705902940
C	1.5530949017	8.0765160312	9.4203003000
C	2.9870160615	8.0752814957	9.4062358671
C	5.2356440484	9.2113472478	9.3108792840
C	8.3150735834	10.6606281716	9.3581557859
C	8.3131383880	9.2282888144	9.4061319989
C	5.2355095068	10.6779978829	9.2649020737
C	6.0597943032	8.0711283715	9.4603014745
C	7.5036510675	8.0716811816	9.4679887746
C	9.8029619966	9.2279645697	9.4059847854
C	12.8611030671	10.6631336372	9.3779879785
C	12.8592295955	9.2307560604	9.3940754041
C	9.8048087374	10.6600710703	9.3679473415
C	10.6149321136	8.0755337548	9.4368268379
C	12.0470063070	8.0764961541	9.4255080066
H	3.3091429056	4.0640369964	16.6954876596
H	3.3267551568	4.2116410818	18.2368709107
O	3.6197689867	4.6385664541	17.4143087280
H	7.0461683837	3.8994875899	16.8933861136
H	5.5593492242	3.7891718107	17.2300162944
O	6.3170557456	3.2422044181	16.9613232235
H	3.4865914921	7.7940622851	16.8779665812
H	4.2061947676	6.5384716003	17.3991580735
O	4.2500068205	7.5176376960	17.4091606325
H	5.7451628250	8.5275759183	17.0850793455
H	6.3101094281	9.9684246256	17.3061476097
O	6.5133398187	9.1177060479	16.8875482674

H	9.4766534206	8.2255680543	16.5913994790
H	8.0600984079	8.3965547825	17.2051686268
O	8.9261746160	7.9226964133	17.3297242371
H	8.6048274463	6.1607078866	17.1605371856
H	8.8737378644	4.8649179536	17.9557953513
O	8.5032871749	5.1739536693	17.1148338529
H	4.6786054996	4.0325778081	2.8804797807
H	4.1305358474	5.3791796034	2.4195905554
O	3.8313381066	4.4867860072	2.6648793258
H	7.0974761834	4.1872843471	3.1441306475
H	6.5704485906	3.1648075119	4.1786263589
O	6.4507551100	3.4452287457	3.2585008009
H	3.6200655494	7.7152888564	1.8262396057
H	3.7248274913	7.3849791733	3.3328006850
O	4.2490025115	7.4410447895	2.5148345330
H	5.7993651119	8.4201646897	2.6346164676
H	6.3321970701	9.8578260381	2.3799791935
O	6.5911397795	8.9959673565	2.7414362043
H	9.6544409512	8.3371801536	2.6612448356
H	8.1479809806	8.3778980168	2.2693657349
O	9.0051804447	7.9144091371	2.0778779695
H	8.6693591527	6.2560408112	2.6371163019
H	9.2143141494	4.8099790099	2.4924833350
O	8.5418220990	5.3239683462	2.9646106280
H	5.4495265411	5.5110003266	11.2375907561

# TS

C	0.7379662270	1.7384092319	10.0009719598
C	3.7941584750	3.1677648615	10.0006987158
C	3.7789108985	1.7170078799	10.0009954710
C	0.7505033653	3.1695652715	10.0009016357
C	1.5380345346	0.5769466637	10.0010308670
C	2.9651907890	0.5783824245	10.0010926992
C	5.2408098330	1.7034852270	10.0010640479
C	8.3451079966	3.1585948404	10.0009725194
C	8.3407510857	1.7297137223	10.0010530522
C	5.2619857554	3.1185337322	10.0008043860
C	6.0854813516	0.5784288688	10.0011569362
C	7.5207746900	0.5791440679	10.0010995872
C	9.8212632411	1.7326544609	10.0010484848
C	12.8646317762	3.1721697117	10.0009497559
C	12.8655909927	1.7388351951	10.0009953190
C	9.8321876714	3.1663975302	10.0009957677
C	10.6318447732	0.5773538953	10.0010480579

C	12.0596881608	0.5765005261	10.0010282862
C	0.7578982977	5.4798021907	10.0008246774
C	3.8346597340	6.9053683470	10.0006938590
C	3.8297799745	5.4784401205	10.0003154061
C	0.7579146456	6.9021424484	10.0008770069
C	1.5642906563	4.3212464241	10.0007758877
C	2.9999572159	4.3161573471	10.0005586189
C	5.2489085033	5.3062910625	9.9997229927
C	8.3118711825	6.9012036846	10.0008091855
C	8.3105530261	5.4840328320	10.0007913375
C	5.2468365949	7.0746256210	10.0005375769
C	6.1089639044	4.2258970081	10.0006081762
C	7.5343905997	4.2901918791	10.0007951558
C	9.8206092812	5.4864806618	10.0008691752
C	12.8714172374	6.9026254473	10.0009038943
C	12.8681111302	5.4797611929	10.0008842676
C	9.8214151452	6.8984713475	10.0008664225
C	10.6260573445	4.3209922926	10.0009371292
C	12.0597201933	4.3226536535	10.0009290061
C	0.7492722861	9.2120891683	10.0010186301
C	3.7854022375	10.6768702479	10.0012165348
C	3.8047796144	9.2158345638	10.0011564472
C	0.7370082645	10.6528222617	10.0010427897
C	1.5669680822	8.0654556743	10.0009638777
C	3.0027518354	8.0710162269	10.0009892450
C	5.2574085694	9.2620461359	10.0011476634
C	8.3435311724	10.6566410328	10.0010662780
C	8.3496637014	9.2251504551	10.0009858261
C	5.2394457222	10.6932360139	10.0012257532
C	6.1080416330	8.1628867430	10.0008830406
C	7.5341186263	8.0958793970	10.0008791826
C	9.8325569816	9.2169854019	10.0009873603
C	12.8688140371	10.6500740934	10.0010326791
C	12.8719270883	9.2095213740	10.0010063769
C	9.8203324388	10.6554749234	10.0010502909
C	10.6289037102	8.0643484091	10.0009349122
C	12.0618086498	8.0624836590	10.0009534078
H	3.2963356924	4.0544559214	16.7087938285
H	3.3155606744	4.2287553490	18.2447572633
O	3.6201532764	4.6359386283	17.4154321908
H	7.0482761750	3.9130310139	16.9139626229
H	5.5593586158	3.7902982588	17.2538142033
O	6.3163355270	3.2553535030	16.9573082198
H	3.4773706690	7.7958923432	16.9018061056

H	4.1917086272	6.5298595617	17.4064939837
O	4.2536389970	7.5088610307	17.4068996597
H	5.7505828593	8.5264060808	17.1007784649
H	6.3251348799	9.9600587979	17.3346068727
O	6.5112802142	9.1205036684	16.8852961343
H	9.4856031112	8.2389490491	16.6084220261
H	8.0595951490	8.3994402655	17.2097727746
O	8.9232738679	7.9202302969	17.3300700865
H	8.6007753092	6.1677596112	17.1676417280
H	8.8755743146	4.8672199454	17.9516539834
O	8.5026247405	5.1802263157	17.1126865007
H	4.6826449069	4.0320344465	2.8641899305
H	4.1281153202	5.3752628743	2.4000766942
O	3.8316118321	4.4881229707	2.6684343103
H	7.1122018287	4.1796257819	3.1255267486
H	6.5825569593	3.1758473351	4.1771366394
O	6.4525268996	3.4501709852	3.2575663630
H	3.6258246648	7.7192842583	1.8184519951
H	3.7142665712	7.3765300487	3.3212638779
O	4.2490094983	7.4417601004	2.5118265990
H	5.7986437926	8.4324873967	2.6231337793
H	6.3421761147	9.8633565226	2.3564970727
O	6.5885066131	9.0089011154	2.7443030921
H	9.6466166058	8.3350806350	2.6331997214
H	8.1377607910	8.3580944572	2.2609002170
O	8.9909379519	7.8794366136	2.0818728771
H	8.6727776165	6.2498767083	2.6329982302
H	9.2182073228	4.8069538511	2.4646830945
O	8.5645293208	5.3159381966	2.9678632626
H	6.0742188643	6.1919781132	10.0041533429