Supporting Information for

**Gas-phase formation of interstellar nucleobases from dehydrogenated radicals of formamide and vinyl cyanide**

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## 1. Comparison between results obtained using M06 and MP2 methods.

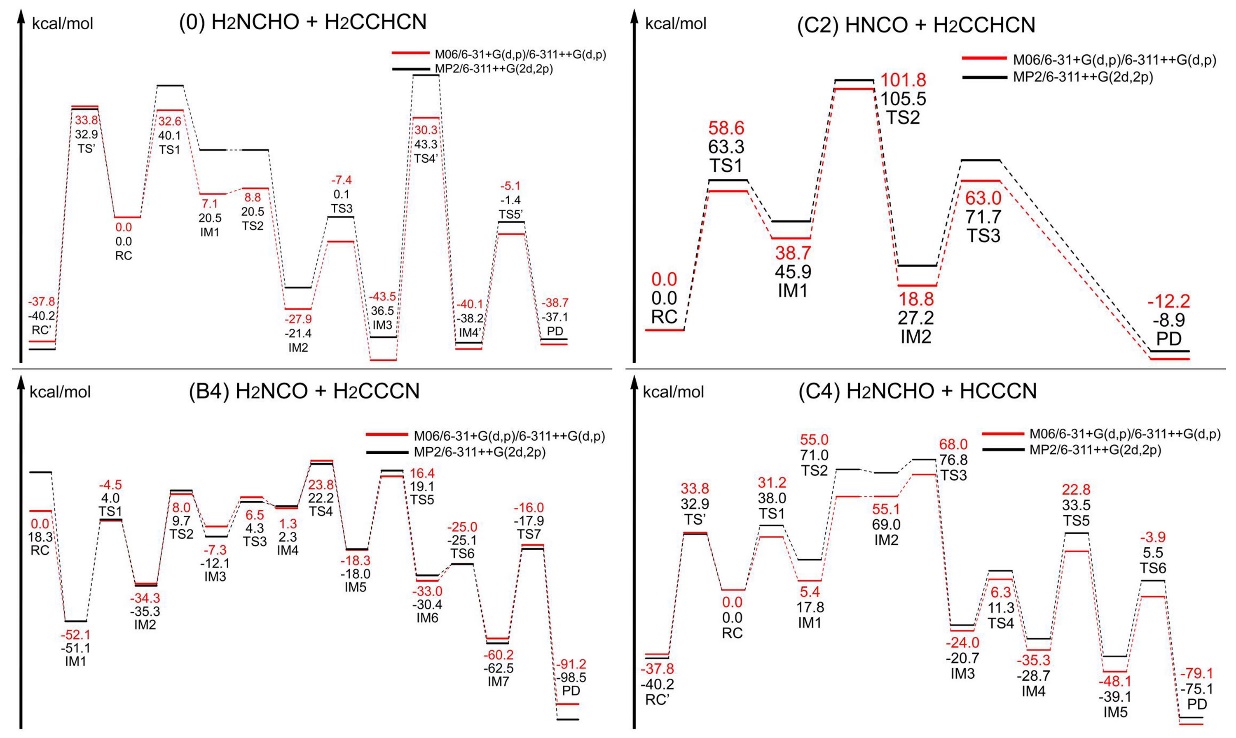


Figure 1. Comparison of the Gibbs free energies computed using M06/6-31+G(d,p)/6-311++G(d,p) and MP2/6-311++G(2d,2p) for the reactant (RC), the intermediate state (IM), the transition state (TS) and the product (PD) in four different reactions of dehydrogenated formamide and vinyl cyanide that leads to the formation of 1H-pyrimidin-2-one, which is a direct precursor of nucleobases.

## 2. Energy diagrams of the reaction for transforming the reactants via H migration.

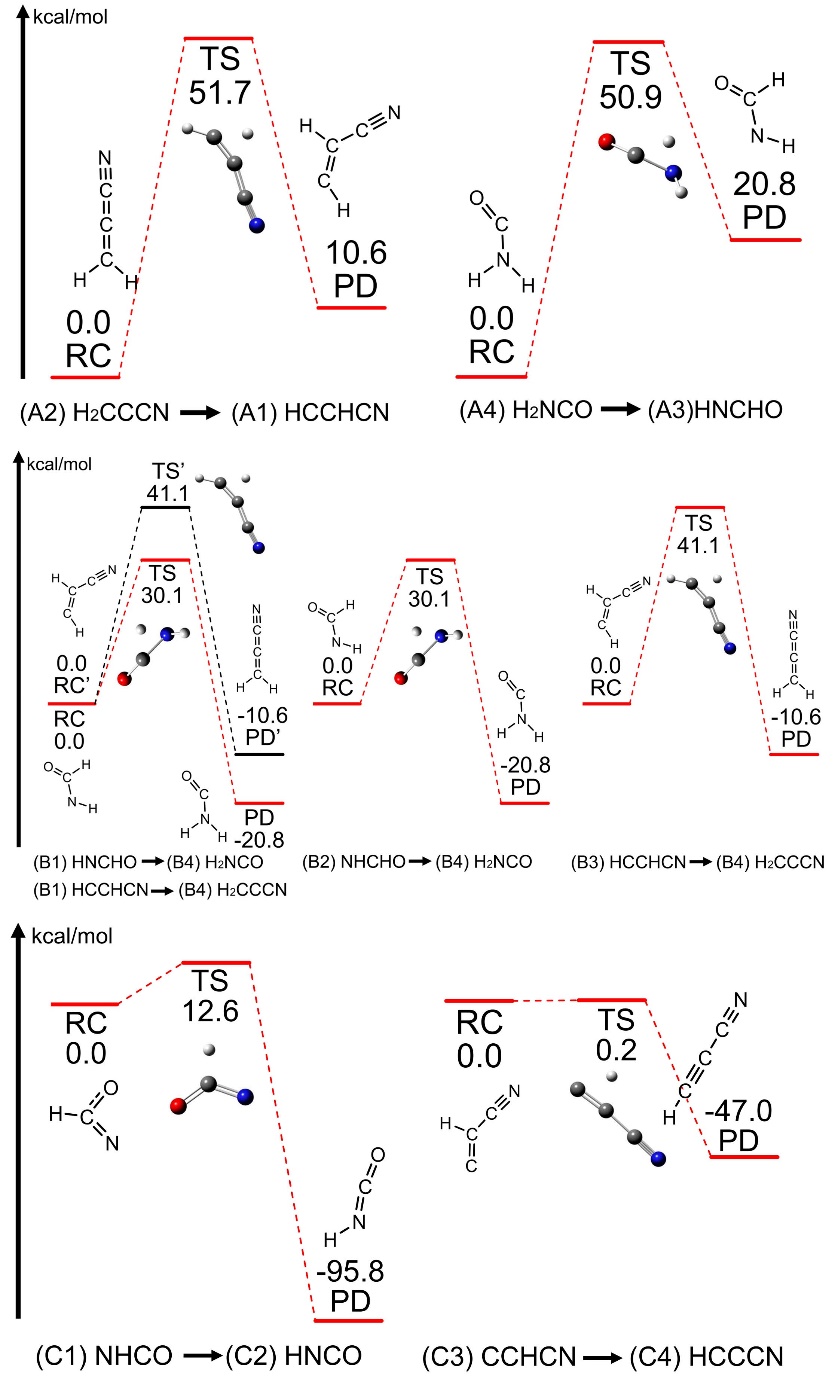


Figure 2. Energy diagram for the transformation of the reactants linking different reactions.

3. Data of atomic coordinates.

The following contain DFT/MP2-optimized atomistic configurations of the reactant (RC), the intermediate (IM), the transition state (TS) and the product (PD) of the reactions between partially dehydrogenated radicals of formamide (H2NCHO) and vinyl cyanide (H2CCHCN) for producing 1H-pyrimidin-2-one (C4H4N2O). The name of these coordinate consists of two parts separated by "\_" including the ID of the reaction (defined in the manuscript), and the molecular state name. For instance, "C4\_TS2a " stands for the 2nd transition state in the reaction C4. These molecular coordinates were optimized at M06/6-31+G(d,p)/6-311++G(d,p) level.

0\_IM1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.30351400 | -0.08315100 | -0.01322600 |
| N |  | -1.81322600 | 1.10655900 | 0.24203600 |
| O |  | -2.15551000 | -1.09064200 | -0.07261100 |
| H |  | -1.61192000 | -1.87286400 | -0.27882400 |
| H |  | -2.79914500 | 1.25495900 | 0.38376000 |
| H |  | -1.09436100 | 1.83768600 | 0.28130100 |
| C |  | 0.77270900 | 0.73763300 | -0.11523900 |
| C |  | 2.18926500 | 0.45634700 | -0.25569400 |
| C |  | 2.78481300 | -0.60568500 | 0.31600500 |
| N |  | -0.01109200 | -0.34888000 | -0.22459800 |
| H |  | 2.18977000 | -1.37399300 | 0.80623600 |
| H |  | 3.86707900 | -0.70185000 | 0.36598500 |
| H |  | 2.80324900 | 1.24657300 | -0.69070700 |

0\_IM2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.76384200 | -0.66956900 | -0.12601600 |
| C |  | 2.21357000 | -0.49617300 | -0.10984500 |
| C |  | 2.81362400 | 0.67276200 | 0.13961100 |
| N |  | -0.04787700 | 0.30864000 | 0.03430300 |
| H |  | 2.22544200 | 1.56461800 | 0.34459100 |
| H |  | 3.89578000 | 0.76457000 | 0.14709200 |
| H |  | 2.80638600 | -1.38763400 | -0.30731300 |
| C |  | -1.42147500 | 0.00200300 | 0.03213400 |
| N |  | -1.90334300 | -1.16161900 | 0.17580500 |
| O |  | -2.17124700 | 1.11493200 | -0.12113500 |
| H |  | 0.37060500 | -1.68493400 | -0.27731700 |
| H |  | -1.56558300 | 1.86829100 | -0.17815500 |
| H |  | -2.92148300 | -1.12764000 | 0.15412600 |

0\_IM3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.97147800 | 1.28959100 | -0.03055700 |
| C |  | -1.78038100 | 0.22041600 | -0.03323900 |
| C |  | -1.22548000 | -1.16606200 | 0.09803500 |
| N |  | 0.42164600 | 1.23521400 | 0.06362700 |
| H |  | -1.67180200 | -1.84302700 | -0.64416400 |
| H |  | -1.44827000 | -1.59750200 | 1.09125500 |
| H |  | -2.85740000 | 0.33824700 | -0.10660600 |
| C |  | 0.90898100 | 0.04476300 | -0.00209000 |
| N |  | 0.21806700 | -1.11101500 | -0.12579900 |
| O |  | 2.23786800 | -0.14603700 | 0.01333300 |
| H |  | -1.38061900 | 2.29442000 | -0.11113300 |
| H |  | 2.63022400 | 0.73953200 | 0.04323500 |
| H |  | 0.75708400 | -1.96501000 | -0.13692800 |

0\_IM4

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.99636900 | 1.26362400 | -0.04162900 |
| C |  | -1.77303400 | 0.17841400 | -0.05719600 |
| C |  | -1.18045100 | -1.18535200 | 0.10250700 |
| N |  | 0.38501300 | 1.17120700 | 0.10047700 |
| H |  | -1.61312900 | -1.88017200 | -0.63094700 |
| H |  | -1.41833700 | -1.59624600 | 1.09986500 |
| H |  | -2.84793600 | 0.27559500 | -0.16280100 |
| C |  | 1.06557800 | -0.03246400 | 0.00172700 |
| N |  | 0.26283400 | -1.13376400 | -0.10202900 |
| O |  | 2.28515800 | -0.08358500 | -0.01613100 |
| H |  | -1.39118800 | 2.27075900 | -0.13420300 |
| H |  | 0.97440600 | 1.98926200 | 0.06324000 |
| H |  | 0.78563600 | -1.99794600 | -0.12769200 |

0\_IM4a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.06951600 | -1.31668600 | -0.00042800 |
| C |  | -1.79908700 | -0.13506500 | 0.00010400 |
| C |  | -1.05238100 | 1.03896100 | 0.00053200 |
| N |  | 0.26293300 | -1.33585900 | -0.00035000 |
| H |  | -1.53908100 | 2.01560500 | 0.00085400 |
| H |  | -2.88350900 | -0.12783400 | 0.00012400 |
| C |  | 0.85951600 | -0.14269100 | 0.00010400 |
| N |  | 0.27781900 | 1.05257400 | 0.00050900 |
| O |  | 2.19541100 | -0.13489200 | 0.00018300 |
| H |  | -1.56461000 | -2.28753300 | -0.00076500 |
| H |  | 2.48388000 | -1.05921200 | -0.00034400 |
| H |  | 0.40881200 | 3.58393800 | -0.00184000 |
| H |  | 0.11476200 | 4.27004900 | -0.00247900 |

0\_PD

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.21416500 | -1.19634700 | -0.00004800 |
| C |  | 1.79023600 | 0.03744400 | -0.00031900 |
| C |  | 0.89479900 | 1.14128100 | 0.00007800 |
| N |  | -0.13352200 | -1.29288900 | 0.00042000 |
| H |  | -0.46908600 | 4.25764300 | -0.00000800 |
| H |  | 1.30920300 | 2.15411500 | 0.00042600 |
| H |  | 2.86523900 | 0.16808800 | -0.00074000 |
| C |  | -1.01338000 | -0.17946400 | 0.00003700 |
| N |  | -0.40720400 | 1.06293400 | 0.00021600 |
| O |  | -2.21008700 | -0.37810000 | -0.00037500 |
| H |  | 1.77485200 | -2.12734000 | -0.00010500 |
| H |  | -0.59673300 | -2.19432600 | 0.00042000 |
| H |  | -0.73262400 | 3.55881500 | 0.00006800 |

0\_RC

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.50508000 | -0.49043800 | -0.31260200 |
| N |  | 1.75207800 | -0.74635800 | 0.96845900 |
| O |  | 2.33377700 | 0.49468400 | -0.69096100 |
| H |  | 2.13076000 | 0.71743000 | -1.60568500 |
| H |  | 2.42793700 | -0.21354400 | 1.51539200 |
| H |  | 1.21105100 | -1.45207500 | 1.44199400 |
| C |  | -1.49049900 | 0.93121900 | 0.15465000 |
| C |  | -2.26162300 | -0.26771000 | 0.04486000 |
| C |  | -1.75901200 | -1.39754300 | -0.46313900 |
| N |  | -0.89681000 | 1.92691600 | 0.25689000 |
| H |  | -0.72125400 | -1.43936800 | -0.80134400 |
| H |  | -2.37890700 | -2.28672200 | -0.53734800 |
| H |  | -3.29035600 | -0.20027600 | 0.39463200 |

0\_RCa

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.16116800 | 0.38886800 | -0.00026900 |
| N |  | -1.08179600 | -0.15821300 | -0.00000500 |
| O |  | 1.19435600 | -0.24652600 | 0.00009900 |
| H |  | 0.13639300 | 1.49759900 | 0.00043700 |
| H |  | -1.17417800 | -1.16450100 | 0.00000500 |
| H |  | -1.91149600 | 0.41339300 | 0.00040700 |

0\_TS1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.11263300 | 0.14819700 | 0.21584900 |
| N |  | 1.39995800 | 1.20528800 | -0.54823300 |
| O |  | 2.24073000 | -0.43408100 | 0.63843300 |
| H |  | 1.99667800 | -1.27067400 | 1.05774500 |
| H |  | 2.34451600 | 1.39304800 | -0.87432800 |
| H |  | 0.64529400 | 1.76934000 | -0.90596400 |
| C |  | -1.10226800 | -0.88382500 | -0.68949700 |
| C |  | -2.11086300 | 0.06842800 | -0.33877700 |
| C |  | -2.21220200 | 0.48933900 | 0.93465000 |
| N |  | 0.06976500 | -1.07049200 | -0.44499900 |
| H |  | -1.53509800 | 0.11422300 | 1.69922900 |
| H |  | -2.98731500 | 1.18517400 | 1.24442200 |
| H |  | -2.80177200 | 0.40513000 | -1.10928600 |

0\_TS2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.35150700 | -0.06548200 | 0.00022400 |
| N |  | -1.63747600 | 1.17747500 | 0.22740500 |
| O |  | -2.26217400 | -1.01563900 | -0.04853600 |
| H |  | -1.77518300 | -1.83780100 | -0.24149400 |
| H |  | -2.57710300 | 1.51573000 | 0.36884100 |
| C |  | 0.72025900 | 0.63937300 | -0.12124700 |
| C |  | 2.15594900 | 0.44976500 | -0.23052300 |
| C |  | 2.79611600 | -0.61372100 | 0.27972700 |
| N |  | -0.04440600 | -0.43523200 | -0.20931200 |
| H |  | 2.23587300 | -1.43285100 | 0.72645300 |
| H |  | 3.88168800 | -0.67320700 | 0.30439700 |
| H |  | 2.73149100 | 1.28638500 | -0.62833500 |
| H |  | -0.55109900 | 1.61155900 | 0.16268500 |

0\_TS3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.89377600 | -1.27724700 | 0.00601600 |
| C |  | -1.82222500 | -0.27109100 | -0.31076800 |
| C |  | -1.63168500 | 0.98685200 | 0.22816300 |
| N |  | 0.36969600 | -1.07678600 | 0.34088200 |
| H |  | -1.31038800 | 1.08598800 | 1.25825900 |
| H |  | -2.15285400 | 1.85397600 | -0.17358900 |
| H |  | -2.56466600 | -0.45318300 | -1.08514700 |
| C |  | 0.96683700 | 0.12359600 | 0.06356200 |
| N |  | 0.43451500 | 1.29908200 | -0.03212000 |
| O |  | 2.28936500 | -0.01215600 | -0.17276600 |
| H |  | -1.17087000 | -2.32881000 | -0.12004600 |
| H |  | 2.47681700 | -0.96134100 | -0.10772100 |
| H |  | 1.06265900 | 1.97188600 | -0.47280300 |

0\_TS4

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.83984300 | 1.35677700 | -0.03421000 |
| C |  | -1.72771500 | 0.34963000 | -0.07296600 |
| C |  | -1.30592000 | -1.08362700 | 0.09985100 |
| N |  | 0.51620300 | 1.10875300 | 0.11901400 |
| H |  | -1.80223500 | -1.72690400 | -0.63888700 |
| H |  | -1.59131400 | -1.46580600 | 1.09503300 |
| H |  | -2.78598700 | 0.55193100 | -0.20232400 |
| C |  | 0.94556500 | -0.14842100 | 0.01376600 |
| N |  | 0.14887800 | -1.21337800 | -0.08094900 |
| O |  | 2.22678100 | -0.11022900 | -0.03563300 |
| H |  | -1.13571900 | 2.39722800 | -0.13022400 |
| H |  | 0.57947400 | -2.12274200 | -0.16546600 |
| H |  | 1.83344400 | 1.13435100 | 0.02183300 |

0\_TS4a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.95346800 | -1.32174800 | 0.06884600 |
| C |  | 1.78498800 | -0.22356200 | -0.04710300 |
| C |  | 1.18967800 | 1.03619900 | -0.11509700 |
| N |  | -0.39540200 | -1.25525100 | 0.07941800 |
| H |  | 1.65855300 | 2.01662900 | -0.13600800 |
| H |  | 2.86262000 | -0.33356300 | -0.07754100 |
| C |  | -0.90402700 | -0.04313600 | -0.02686400 |
| N |  | -0.17378700 | 1.06708900 | -0.12732100 |
| O |  | -2.21605300 | 0.13370500 | -0.02421600 |
| H |  | 1.36943600 | -2.32503600 | 0.14596600 |
| H |  | -2.62507300 | -0.73886800 | 0.08561900 |
| H |  | -0.53401300 | 2.01379700 | 0.09955600 |
| H |  | 0.83658800 | 2.92801800 | 1.13276400 |

0\_TS5

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.98671700 | -1.31303200 | 0.04343100 |
| C |  | 1.77797300 | -0.19965800 | -0.01576800 |
| C |  | 1.14136500 | 1.04723200 | -0.10672900 |
| N |  | -0.36880500 | -1.20113200 | 0.03998000 |
| H |  | 1.54028000 | 2.09582300 | -0.01521100 |
| H |  | 2.85794900 | -0.28139800 | -0.02592300 |
| C |  | -1.06238200 | 0.02108200 | -0.01672900 |
| N |  | -0.20339100 | 1.09299100 | -0.08162000 |
| O |  | -2.26911200 | 0.07768200 | -0.00461000 |
| H |  | 1.38136800 | -2.32520200 | 0.06832700 |
| H |  | -0.96484300 | -2.01591400 | 0.12519000 |
| H |  | -0.54977700 | 2.06708300 | 0.04450800 |
| H |  | 0.83125100 | 3.26139300 | 0.70623600 |

0\_TS5a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.91618200 | 1.26317500 | 0.00001100 |
| C |  | 1.74775200 | 0.15361400 | 0.00001300 |
| C |  | 1.13219700 | -1.10766100 | 0.00000400 |
| N |  | -0.39647800 | 1.05787800 | -0.00003700 |
| H |  | 1.75767700 | -2.00162500 | -0.00000500 |
| H |  | 2.82666500 | 0.25361200 | 0.00000500 |
| C |  | -0.91932700 | -0.21482500 | -0.00001900 |
| N |  | -0.17905400 | -1.32869200 | -0.00000600 |
| O |  | -2.18127300 | -0.05347100 | 0.00002100 |
| H |  | 1.27839700 | 2.28850000 | 0.00002000 |
| H |  | -1.64466300 | 1.21716100 | 0.00006500 |

0\_TSa

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.08414800 | -0.47317400 | -0.00012000 |
| N |  | 1.11014800 | 0.10832500 | 0.00002700 |
| O |  | -1.14761400 | 0.29038600 | -0.00002700 |
| H |  | 1.16023800 | 1.12664900 | 0.00019900 |
| H |  | 1.95958900 | -0.43339900 | -0.00003000 |
| H |  | -1.20506700 | -0.93556100 | 0.00057400 |

A1\_IM1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 2.03711600 | -0.11604700 | -0.14690800 |
| C |  | 1.27242000 | 1.05456000 | -0.25301300 |
| C |  | -0.02373600 | 1.07378200 | 0.23069400 |
| N |  | 2.56439500 | -1.15718200 | -0.01632500 |
| H |  | -0.69920800 | 1.91846500 | 0.21962000 |
| H |  | 1.69301800 | 1.93506100 | -0.72546300 |
| C |  | -1.62444700 | -0.46668800 | -0.42753200 |
| N |  | -0.62148800 | -0.16451800 | 0.68843600 |
| O |  | -2.80158200 | -0.28666100 | -0.20012200 |
| H |  | -1.09146600 | -0.60928000 | -1.37492900 |
| H |  | -1.15709800 | -0.07954100 | 1.55752000 |
| H |  | 0.09893700 | -0.89315300 | 0.80000200 |

A1\_IM2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.62042800 | -0.54668300 | -0.22385800 |
| C |  | -1.29991200 | 0.83161300 | 0.14705600 |
| C |  | -0.08606200 | 1.40047600 | 0.05092700 |
| N |  | -2.71848400 | -1.10846600 | 0.02822500 |
| H |  | 0.02106700 | 2.46797200 | 0.23646100 |
| H |  | -2.12962500 | 1.44512900 | 0.48773200 |
| C |  | 1.51014200 | -0.47656900 | 0.25691100 |
| N |  | 1.10506600 | 0.74111000 | -0.25078200 |
| O |  | 2.58118200 | -0.97614000 | 0.00547200 |
| H |  | 0.75855800 | -0.92921700 | 0.93267600 |
| H |  | 1.83912300 | 1.25556000 | -0.72668200 |
| H |  | -0.86708800 | -1.11186100 | -0.80227900 |

A1\_IM3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.90344400 | -0.57265600 | 0.11484700 |
| C |  | 1.49830100 | 0.82570600 | -0.06754500 |
| C |  | 0.30210400 | 1.44124500 | -0.05505700 |
| N |  | 1.27521100 | -1.67106600 | -0.04517300 |
| H |  | 0.28991600 | 2.52531000 | -0.13929200 |
| H |  | 2.33582100 | 1.51501700 | -0.16585300 |
| C |  | -1.39705300 | -0.34938500 | -0.08300700 |
| N |  | -0.98911100 | 0.93057500 | 0.08430000 |
| O |  | -2.50073300 | -0.79361700 | 0.02882900 |
| H |  | 0.31528500 | -1.51778500 | -0.38041800 |
| H |  | -1.72658600 | 1.60565000 | 0.28411500 |
| H |  | 2.94795000 | -0.66527700 | 0.44150200 |

A1\_IM3a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.03247000 | -1.19909600 | -0.07528600 |
| C |  | 1.78918000 | 0.00405000 | 0.13317600 |
| C |  | 1.09457100 | 1.16673900 | -0.01635600 |
| N |  | -0.25666600 | -1.27955200 | -0.12861100 |
| H |  | 1.57226600 | 2.14061600 | -0.09448000 |
| H |  | 2.86893400 | -0.00612900 | 0.21627800 |
| C |  | -0.98721000 | -0.07937900 | 0.21003700 |
| N |  | -0.24969100 | 1.12939800 | -0.14495200 |
| O |  | -2.27203100 | -0.02062300 | -0.06014200 |
| H |  | -1.07405800 | -0.11269700 | 1.35327800 |
| H |  | -0.79748800 | 1.96463900 | -0.30329900 |
| H |  | 1.57702800 | -2.12425600 | -0.28512700 |

A1\_IM4

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.10832300 | 1.19550800 | 0.00000200 |
| C |  | 1.80022800 | 0.00000300 | 0.00020800 |
| C |  | 1.10832100 | -1.19550900 | 0.00009100 |
| N |  | -0.29186000 | 1.15705500 | -0.00039300 |
| H |  | 1.56674800 | -2.17584100 | -0.00058700 |
| H |  | 2.88448600 | -0.00000600 | 0.00038300 |
| C |  | -1.04340300 | 0.00000500 | -0.00006900 |
| N |  | -0.29184600 | -1.15705600 | -0.00034800 |
| O |  | -2.26179600 | -0.00000800 | 0.00030800 |
| H |  | -0.83921900 | 2.00565500 | -0.00010800 |
| H |  | -0.83923300 | -2.00564200 | 0.00086800 |
| H |  | 1.56672100 | 2.17585800 | 0.00077600 |

A1\_PD

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.23810900 | -1.04550500 | 0.26024000 |
| C |  | 1.79913800 | 0.17547600 | 0.04135800 |
| C |  | 0.89579200 | 1.22797300 | -0.27153100 |
| N |  | -0.10360800 | -1.17751000 | 0.17022100 |
| H |  | 1.30138500 | 2.22619900 | -0.45670200 |
| H |  | 2.86875900 | 0.33361700 | 0.10177900 |
| C |  | -0.99086300 | -0.11428600 | -0.14232700 |
| N |  | -0.40035800 | 1.11604700 | -0.36232500 |
| O |  | -2.18122500 | -0.34277200 | -0.19631200 |
| H |  | -0.55660600 | -2.07059700 | 0.32615500 |
| H |  | 1.80593200 | -1.93874200 | 0.50720700 |
| H |  | -2.66756763 | 5.44976892 | -1.40528719 |

A1\_RC

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.85615600 | -0.36637200 | -0.10452700 |
| C |  | 1.75431100 | 1.04955000 | 0.07729200 |
| C |  | 0.57744600 | 1.62656300 | 0.23275200 |
| N |  | 1.91558700 | -1.51882800 | -0.25236300 |
| H |  | 0.18297300 | 2.62263500 | 0.37445800 |
| H |  | 2.69232900 | 1.61352500 | 0.07672800 |
| C |  | -1.63937100 | -0.25800300 | -0.40176400 |
| N |  | -1.26801400 | -1.12971900 | 0.56593200 |
| O |  | -2.42120700 | 0.66168900 | -0.24941600 |
| H |  | -1.14455500 | -0.47082400 | -1.37312400 |
| H |  | -1.64263100 | -1.01494200 | 1.49760500 |
| H |  | -0.54273100 | -1.81450800 | 0.40216200 |

A1\_TS1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 2.11519300 | -0.09329400 | -0.14925900 |
| C |  | 1.30504400 | 1.06140400 | -0.28101300 |
| C |  | 0.17487700 | 1.16340200 | 0.46656300 |
| N |  | 2.66202000 | -1.12061500 | -0.03852600 |
| H |  | -0.59261200 | 1.92413100 | 0.33936700 |
| H |  | 1.60133800 | 1.82312100 | -1.00212400 |
| C |  | -1.73415200 | -0.45138000 | -0.41504000 |
| N |  | -0.75843400 | -0.41571600 | 0.61182500 |
| O |  | -2.87582400 | -0.10535400 | -0.21977200 |
| H |  | -1.30614800 | -0.72176700 | -1.39548100 |
| H |  | -1.18010600 | -0.40428600 | 1.53941100 |
| H |  | -0.00674900 | -1.10484400 | 0.53641000 |

A1\_TS2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.71314500 | -0.38861900 | 0.11689000 |
| C |  | 1.37781600 | 0.95374500 | -0.30345100 |
| C |  | 0.11822200 | 1.35563300 | -0.01056200 |
| N |  | 2.35485400 | -1.39790700 | 0.00610200 |
| H |  | -0.33109200 | 2.33390700 | -0.11336000 |
| H |  | 2.14113700 | 1.62402200 | -0.68780000 |
| C |  | -1.55668300 | -0.36874000 | -0.37505000 |
| N |  | -0.66913400 | 0.28370300 | 0.56404100 |
| O |  | -2.69840700 | -0.62868900 | -0.08337400 |
| H |  | -1.05003600 | -0.57239600 | -1.33221000 |
| H |  | -1.21807500 | 0.54527300 | 1.38935500 |
| H |  | 0.33028900 | -0.41397700 | 0.85304600 |

A1\_TS3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.76422800 | -0.74988900 | 0.00002300 |
| C |  | 1.60321100 | 0.69937000 | -0.00001100 |
| C |  | 0.46669200 | 1.42723500 | -0.00001000 |
| N |  | 0.88845800 | -1.67550200 | -0.00001300 |
| H |  | 0.55000100 | 2.51125000 | -0.00002900 |
| H |  | 2.52450600 | 1.27597700 | -0.00003200 |
| C |  | -1.29234600 | -0.30108600 | -0.00002700 |
| N |  | -0.84871500 | 1.00012500 | 0.00001700 |
| O |  | -2.45190900 | -0.61831300 | 0.00001200 |
| H |  | -0.22323300 | -1.18984100 | -0.00006700 |
| H |  | -1.57709200 | 1.71030100 | 0.00006300 |
| H |  | 2.81218000 | -1.08731900 | 0.00009500 |

A1\_TS3a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.15910900 | -1.15243300 | -0.10141300 |
| C |  | 1.76868200 | 0.11755900 | 0.19410800 |
| C |  | 0.99365800 | 1.22143200 | -0.01832900 |
| N |  | -0.09911200 | -1.38311700 | -0.17675400 |
| H |  | 1.42687100 | 2.21483600 | -0.11923400 |
| H |  | 2.83537600 | 0.19901000 | 0.36311900 |
| C |  | -1.09017800 | -0.04493400 | 0.27994500 |
| N |  | -0.33867900 | 1.10888700 | -0.18759600 |
| O |  | -2.28921200 | -0.11884500 | -0.01929900 |
| H |  | -0.79257800 | -0.24292800 | 1.34496900 |
| H |  | -0.88712000 | 1.84081500 | -0.62450900 |
| H |  | 1.80806500 | -1.99110600 | -0.38537300 |

A1\_TS4

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.38584600 | 1.02910200 | -0.02815900 |
| C |  | 1.73870600 | -0.34239900 | 0.17187300 |
| C |  | 0.81179000 | -1.32847700 | -0.02502300 |
| N |  | 0.15588600 | 1.40451700 | -0.10872200 |
| H |  | 1.12362600 | -2.36769800 | -0.11400100 |
| H |  | 2.78190700 | -0.61204700 | 0.29000700 |
| C |  | -1.21310800 | 0.03905000 | 0.33165200 |
| N |  | -0.51181900 | -1.09989400 | -0.18006200 |
| O |  | -2.35250400 | 0.27506300 | 0.02183700 |
| H |  | -0.02874700 | 2.37482100 | -0.35219600 |
| H |  | -1.11104200 | -1.85407800 | -0.50369600 |
| H |  | 2.20641900 | 1.74248500 | -0.17537400 |

A1\_TS4a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.03255700 | -1.19491600 | -0.05876100 |
| C |  | 1.78607700 | 0.00525600 | 0.09300200 |
| C |  | 1.08468600 | 1.17038700 | -0.00341200 |
| N |  | -0.26571000 | -1.26929000 | -0.11620400 |
| H |  | 1.55030800 | 2.15261900 | -0.01509900 |
| H |  | 2.86516100 | -0.00279400 | 0.18505500 |
| C |  | -1.01168000 | -0.08656200 | 0.05533400 |
| N |  | -0.25728600 | 1.12317000 | -0.13830200 |
| O |  | -2.24233000 | -0.01964800 | -0.01939800 |
| H |  | -0.81574500 | 1.96632000 | -0.19915900 |
| H |  | 1.56951000 | -2.14037300 | -0.17065300 |
| H |  | -0.91945800 | -0.16073600 | 1.61960100 |

A1\_TS5

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.15451800 | -1.14508500 | 0.05750000 |
| C |  | 1.79668600 | 0.05636200 | 0.01919000 |
| C |  | 0.97589400 | 1.20616100 | -0.08224000 |
| N |  | -0.19971400 | -1.16664600 | 0.01811100 |
| H |  | 1.44259900 | 2.19089900 | -0.14991300 |
| H |  | 2.87755600 | 0.12537800 | 0.03544000 |
| C |  | -1.01533800 | -0.01690200 | -0.04388200 |
| N |  | -0.33761300 | 1.19602500 | -0.10034300 |
| O |  | -2.22116500 | -0.13673800 | -0.04530300 |
| H |  | -0.71210900 | -2.04090600 | 0.03361700 |
| H |  | 1.66054900 | -2.10455000 | 0.11162000 |
| H |  | -1.20853400 | 2.11421500 | 1.20387500 |

A3\_IM1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 2.16929300 | -0.04410800 | -0.00124400 |
| C |  | 1.32170800 | 1.05166100 | -0.00045800 |
| C |  | -0.15752100 | 0.92080300 | 0.00217900 |
| N |  | 2.84179000 | -1.00848700 | -0.00172200 |
| H |  | -0.57431600 | 1.45206800 | 0.87466100 |
| H |  | -0.57730100 | 1.45052700 | -0.86972300 |
| H |  | 1.75697500 | 2.04752000 | -0.00135900 |
| C |  | -1.94276200 | -0.72283000 | 0.00029800 |
| N |  | -0.61175100 | -0.45058800 | 0.00329900 |
| O |  | -2.80719900 | 0.13145800 | -0.00353900 |
| H |  | -2.15811400 | -1.80911900 | 0.00163300 |
| H |  | 0.05576900 | -1.21229300 | 0.00741400 |

A3\_IM2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -2.10881500 | -0.34757500 | 0.00871900 |
| C |  | -1.54437600 | 0.98481500 | 0.21647500 |
| C |  | -0.12667900 | 1.07347400 | -0.23690700 |
| N |  | -2.50433700 | -1.42870600 | -0.13973100 |
| H |  | 2.46343200 | 1.15591800 | -0.27750200 |
| H |  | 0.31342600 | 2.03489200 | -0.47976900 |
| H |  | -2.15535700 | 1.71554100 | -0.32666000 |
| C |  | 2.11837000 | 0.12586700 | -0.05604300 |
| N |  | 0.74908300 | 0.04047900 | 0.02758900 |
| O |  | 2.86338200 | -0.81730600 | 0.09806100 |
| H |  | -1.65917900 | 1.22575000 | 1.28970700 |
| H |  | 0.38640200 | -0.89555400 | 0.20126300 |

A3\_IM3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.62042800 | -0.54668300 | -0.22385800 |
| C |  | -1.29991200 | 0.83161300 | 0.14705600 |
| C |  | -0.08606200 | 1.40047600 | 0.05092700 |
| N |  | -2.71848400 | -1.10846600 | 0.02822500 |
| H |  | 0.02106700 | 2.46797200 | 0.23646100 |
| H |  | -2.12962500 | 1.44512900 | 0.48773200 |
| C |  | 1.51014200 | -0.47656900 | 0.25691100 |
| N |  | 1.10506600 | 0.74111000 | -0.25078200 |
| O |  | 2.58118200 | -0.97614000 | 0.00547200 |
| H |  | 0.75855800 | -0.92921700 | 0.93267600 |
| H |  | 1.83912300 | 1.25556000 | -0.72668200 |
| H |  | -0.86708800 | -1.11186100 | -0.80227900 |

A3\_IM3a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.74983800 | 0.61206700 | 0.05659500 |
| C |  | 1.55022500 | -0.82310700 | 0.21665300 |
| C |  | 0.22118500 | -1.28918000 | -0.38311700 |
| N |  | 1.89417500 | 1.75508400 | -0.08350300 |
| H |  | 0.16937300 | -1.01574200 | -1.44303300 |
| H |  | 0.16359700 | -2.38208700 | -0.31818000 |
| H |  | 2.38138800 | -1.35381800 | -0.26421700 |
| C |  | -1.66935400 | 0.26486300 | -0.31410600 |
| N |  | -0.92844300 | -0.69639200 | 0.26346500 |
| O |  | -2.62604700 | 0.85050500 | 0.10153700 |
| H |  | 1.59419800 | -1.06768400 | 1.28609900 |
| H |  | -1.17167000 | -0.98340000 | 1.21114600 |

A3\_IM4

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.90344400 | -0.57265600 | 0.11484700 |
| C |  | 1.49830100 | 0.82570600 | -0.06754500 |
| C |  | 0.30210400 | 1.44124500 | -0.05505700 |
| N |  | 1.27521100 | -1.67106600 | -0.04517300 |
| H |  | 0.28991600 | 2.52531000 | -0.13929200 |
| H |  | 2.33582100 | 1.51501700 | -0.16585300 |
| C |  | -1.39705300 | -0.34938500 | -0.08300700 |
| N |  | -0.98911100 | 0.93057500 | 0.08430000 |
| O |  | -2.50073300 | -0.79361700 | 0.02882900 |
| H |  | 0.31528500 | -1.51778500 | -0.38041800 |
| H |  | -1.72658600 | 1.60565000 | 0.28411500 |
| H |  | 2.94795000 | -0.66527700 | 0.44150200 |

A3\_IM4a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.81407700 | -1.34787900 | -0.06055100 |
| C |  | -1.76954400 | -0.25826900 | 0.28959600 |
| C |  | -1.16683900 | 1.03178900 | -0.25779700 |
| N |  | 0.41228300 | -1.26820900 | -0.22489100 |
| H |  | -1.31444300 | 1.07466300 | -1.34844600 |
| H |  | -1.66076800 | 1.90620600 | 0.17862200 |
| H |  | -1.85354100 | -0.22831000 | 1.38546000 |
| C |  | 1.08618200 | -0.00496500 | -0.00387100 |
| N |  | 0.24355900 | 1.07466800 | 0.08301900 |
| O |  | 2.28395000 | 0.06946000 | 0.12031100 |
| H |  | -2.76999500 | -0.44241700 | -0.11254900 |
| H |  | 0.72192200 | 1.96490200 | 0.12327300 |

A3\_IM5

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.10832300 | 1.19550800 | 0.00000200 |
| C |  | 1.80022800 | 0.00000300 | 0.00020800 |
| C |  | 1.10832100 | -1.19550900 | 0.00009100 |
| N |  | -0.29186000 | 1.15705500 | -0.00039300 |
| H |  | 1.56674800 | -2.17584100 | -0.00058700 |
| H |  | 2.88448600 | -0.00000600 | 0.00038300 |
| C |  | -1.04340300 | 0.00000500 | -0.00006900 |
| N |  | -0.29184600 | -1.15705600 | -0.00034800 |
| O |  | -2.26179600 | -0.00000800 | 0.00030800 |
| H |  | -0.83921900 | 2.00565500 | -0.00010800 |
| H |  | -0.83923300 | -2.00564200 | 0.00086800 |
| H |  | 1.56672100 | 2.17585800 | 0.00077600 |

A3\_IM5a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.92411300 | 1.29475900 | -0.00098100 |
| C |  | 1.74225200 | 0.16788900 | 0.00228500 |
| C |  | 1.14981700 | -1.18256000 | 0.00318500 |
| N |  | -0.39613100 | 1.28381900 | -0.00220600 |
| H |  | 1.52057800 | -1.74998000 | -0.86982900 |
| H |  | 1.50679000 | -1.74292000 | 0.88679200 |
| H |  | 2.82459100 | 0.26664000 | 0.00475500 |
| C |  | -1.05756800 | 0.03555400 | -0.00063000 |
| N |  | -0.28885900 | -1.10753300 | -0.00961800 |
| O |  | -2.27160000 | -0.02755700 | 0.00519800 |
| H |  | 1.39275200 | 2.28138200 | -0.00250700 |
| H |  | -0.82865800 | -1.96251800 | -0.00118500 |

A3\_PD

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.79064700 | -1.22497200 | -0.09306000 |
| C |  | 0.54615100 | -1.70166000 | -0.00662000 |
| C |  | 1.51440500 | -0.74801500 | 0.07431700 |
| N |  | -1.15259600 | 0.02804900 | -0.09996700 |
| H |  | 2.57677400 | -0.96637600 | 0.14439600 |
| H |  | 0.78161000 | -2.75872100 | -0.00558500 |
| C |  | -0.18557900 | 1.01242900 | -0.01744100 |
| N |  | 1.15546200 | 0.55458900 | 0.06818400 |
| O |  | -0.39674800 | 2.20716300 | -0.01380000 |
| H |  | -1.60164200 | -1.95494100 | -0.16067600 |
| H |  | 1.84813800 | 1.29211600 | 0.12644700 |
| H |  | -6.95694000 | -1.37453500 | 0.48513500 |

A3\_RC

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.24944700 | 1.00063900 | 0.07899500 |
| C |  | 2.31257100 | 0.04987200 | 0.03423500 |
| C |  | 2.07326100 | -1.25389400 | -0.13706200 |
| N |  | 0.39100300 | 1.78500300 | 0.11491800 |
| H |  | 1.05773600 | -1.62838300 | -0.24387200 |
| H |  | 2.89537000 | -1.96260500 | -0.17100400 |
| H |  | 3.31912400 | 0.44775200 | 0.14410200 |
| C |  | -2.16885000 | -0.54459700 | 0.24252600 |
| N |  | -2.38891100 | 0.66104100 | -0.36340000 |
| O |  | -1.18860000 | -1.23633900 | 0.01213600 |
| H |  | -3.00268100 | -0.89422200 | 0.88309300 |
| H |  | -1.57397200 | 1.29374400 | -0.28219300 |

A3\_TS1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.95522900 | -0.19132700 | -0.25654700 |
| C |  | 1.13902300 | 0.97187000 | -0.38546500 |
| C |  | 0.47844400 | 1.48581000 | 0.66000800 |
| N |  | 2.56990700 | -1.17559600 | -0.16173300 |
| H |  | 0.57906900 | 1.06915800 | 1.65874300 |
| H |  | -0.19068100 | 2.33043000 | 0.52962200 |
| H |  | 1.03554000 | 1.38682600 | -1.38574500 |
| C |  | -2.01554100 | -0.65255900 | -0.13473700 |
| N |  | -1.00744100 | -0.93431500 | 0.75739700 |
| O |  | -2.34799500 | 0.43842400 | -0.53579700 |
| H |  | -2.58615500 | -1.58000800 | -0.39363900 |
| H |  | -0.33399600 | -1.62719800 | 0.40819400 |

A3\_TS2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -2.18719300 | -0.05100700 | 0.02502600 |
| C |  | -1.31923600 | 1.05413900 | -0.03334100 |
| C |  | 0.14696300 | 0.84713600 | -0.08974600 |
| N |  | -2.85068800 | -1.01312900 | 0.09605100 |
| H |  | 0.80260100 | 1.66725500 | -0.36121000 |
| H |  | -1.70267600 | 2.02733700 | -0.32214500 |
| C |  | 2.00351300 | -0.69385500 | -0.02702000 |
| N |  | 0.65807800 | -0.44075600 | -0.15519700 |
| O |  | 2.83317900 | 0.16905500 | 0.16264100 |
| H |  | 2.23941300 | -1.76889800 | -0.12985800 |
| H |  | 0.02546500 | -1.21762000 | -0.32267300 |
| H |  | -0.54625300 | 1.17820300 | 0.99925600 |

A3\_TS3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.74255400 | -0.49234300 | 0.06474100 |
| C |  | 1.42436400 | 0.89075200 | -0.15798700 |
| C |  | 0.17487900 | 1.47600600 | -0.07030200 |
| N |  | 1.91668300 | -1.67026700 | 0.03283000 |
| H |  | -0.59233600 | -1.03833400 | -0.69542600 |
| H |  | 0.10953300 | 2.55891400 | -0.09960900 |
| C |  | -1.38873300 | -0.46667400 | -0.18901500 |
| N |  | -1.02205000 | 0.82148400 | 0.16398500 |
| O |  | -2.49552300 | -0.89861800 | 0.03879700 |
| H |  | 2.26817600 | 1.51357200 | -0.44459600 |
| H |  | -1.79357900 | 1.36577900 | 0.53709300 |
| H |  | 1.99157600 | 0.28404400 | 1.12982700 |

A3\_TS3a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.76570600 | 0.54078000 | 0.00166100 |
| C |  | 1.52587500 | -0.89670400 | -0.08576900 |
| C |  | 0.07139000 | -1.23419200 | -0.28308100 |
| N |  | 1.94378200 | 1.68498400 | 0.07686800 |
| H |  | -0.68014700 | -0.32509800 | -1.18192700 |
| H |  | 2.11257900 | -1.30626200 | -0.91759200 |
| C |  | -1.58289400 | 0.17572600 | -0.21917500 |
| N |  | -0.88631300 | -0.62665200 | 0.61229800 |
| O |  | -2.53100500 | 0.89536400 | -0.13451400 |
| H |  | 1.92431400 | -1.36410000 | 0.83026900 |
| H |  | -1.06484500 | -0.81541500 | 1.59331900 |
| H |  | -0.12661300 | -2.27403100 | -0.55393300 |

A3\_TS4

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.76422800 | -0.74988900 | 0.00002300 |
| C |  | 1.60321100 | 0.69937000 | -0.00001100 |
| C |  | 0.46669200 | 1.42723500 | -0.00001000 |
| N |  | 0.88845800 | -1.67550200 | -0.00001300 |
| H |  | 0.55000100 | 2.51125000 | -0.00002900 |
| H |  | 2.52450600 | 1.27597700 | -0.00003200 |
| C |  | -1.29234600 | -0.30108600 | -0.00002700 |
| N |  | -0.84871500 | 1.00012500 | 0.00001700 |
| O |  | -2.45190900 | -0.61831300 | 0.00001200 |
| H |  | -0.22323300 | -1.18984100 | -0.00006700 |
| H |  | -1.57709200 | 1.71030100 | 0.00006300 |
| H |  | 2.81218000 | -1.08731900 | 0.00009500 |

A3\_TS4a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.05380700 | 1.24848600 | -0.05136400 |
| C |  | -1.81450300 | 0.01134300 | -0.29277000 |
| C |  | -0.98996200 | -1.11560600 | 0.33511600 |
| N |  | 0.04856100 | 1.62074000 | 0.21071500 |
| H |  | -1.03372700 | -1.02492000 | 1.42892900 |
| H |  | -1.40222100 | -2.09261000 | 0.06758200 |
| H |  | -2.81876800 | 0.05041100 | 0.14182300 |
| C |  | 1.21844100 | -0.03096400 | 0.08858900 |
| N |  | 0.39370600 | -1.07692400 | -0.11974600 |
| O |  | 2.38677600 | 0.08061500 | -0.11612100 |
| H |  | -1.92635400 | -0.12935800 | -1.37556600 |
| H |  | 0.82997800 | -1.93471100 | -0.44800000 |

A3\_TS5

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.38584600 | 1.02910200 | -0.02815900 |
| C |  | 1.73870600 | -0.34239900 | 0.17187300 |
| C |  | 0.81179000 | -1.32847700 | -0.02502300 |
| N |  | 0.15588600 | 1.40451700 | -0.10872200 |
| H |  | 1.12362600 | -2.36769800 | -0.11400100 |
| H |  | 2.78190700 | -0.61204700 | 0.29000700 |
| C |  | -1.21310800 | 0.03905000 | 0.33165200 |
| N |  | -0.51181900 | -1.09989400 | -0.18006200 |
| O |  | -2.35250400 | 0.27506300 | 0.02183700 |
| H |  | -0.02874700 | 2.37482100 | -0.35219600 |
| H |  | -1.11104200 | -1.85407800 | -0.50369600 |
| H |  | 2.20641900 | 1.74248500 | -0.17537400 |

A3\_TS5a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.82974600 | -1.27369500 | -0.15430400 |
| C |  | 1.73350900 | -0.21088600 | -0.24883800 |
| C |  | 1.15778700 | 1.09625700 | 0.22911700 |
| N |  | -0.37232900 | -1.23867300 | 0.27728700 |
| H |  | 1.33806400 | 1.23319800 | 1.30953700 |
| H |  | 1.63923100 | 1.93466700 | -0.28811500 |
| H |  | 2.67850600 | -0.30587000 | -0.77596600 |
| C |  | -1.07816200 | -0.04033500 | 0.00976200 |
| N |  | -0.25535900 | 1.07404600 | -0.10200600 |
| O |  | -2.27957600 | 0.03409900 | -0.10900300 |
| H |  | -0.76107000 | 1.94661900 | -0.17252600 |
| H |  | 1.87841500 | -1.35706800 | 0.55769800 |

A3\_TS6

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.15451800 | -1.14508500 | 0.05750000 |
| C |  | 1.79668600 | 0.05636200 | 0.01919000 |
| C |  | 0.97589400 | 1.20616100 | -0.08224000 |
| N |  | -0.19971400 | -1.16664600 | 0.01811100 |
| H |  | 1.44259900 | 2.19089900 | -0.14991300 |
| H |  | 2.87755600 | 0.12537800 | 0.03544000 |
| C |  | -1.01533800 | -0.01690200 | -0.04388200 |
| N |  | -0.33761300 | 1.19602500 | -0.10034300 |
| O |  | -2.22116500 | -0.13673800 | -0.04530300 |
| H |  | -0.71210900 | -2.04090600 | 0.03361700 |
| H |  | 1.66054900 | -2.10455000 | 0.11162000 |
| H |  | -1.20853400 | 2.11421500 | 1.20387500 |

A3\_TS6a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.91739400 | 1.27527900 | -0.00599800 |
| C |  | -1.74149400 | 0.12463200 | -0.07881200 |
| C |  | -1.09264200 | -1.09116400 | -0.09150500 |
| N |  | 0.38813200 | 1.27306500 | 0.03725100 |
| H |  | -1.59555800 | -2.03778700 | -0.26925100 |
| H |  | -2.82277500 | 0.18741800 | -0.09253500 |
| C |  | 1.06543700 | 0.06559600 | 0.00056300 |
| N |  | 0.26228300 | -1.09562800 | -0.12292000 |
| O |  | 2.27063600 | -0.05750500 | 0.04810700 |
| H |  | -1.39452000 | 2.25818800 | 0.01307600 |
| H |  | 0.78179800 | -1.96524400 | -0.14498600 |
| H |  | -1.57038400 | -1.47065700 | 1.76303300 |

B4\_IM1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.81989300 | -0.44528000 | 0.00000200 |
| C |  | 2.06007900 | -0.16309500 | 0.00000100 |
| C |  | 3.32987600 | 0.17919600 | -0.00000400 |
| N |  | -0.36263000 | -0.83054700 | -0.00002200 |
| H |  | 3.64042400 | 1.22489100 | -0.00035400 |
| H |  | 4.12633800 | -0.56620000 | 0.00036000 |
| C |  | -1.39742300 | 0.17289400 | -0.00004200 |
| N |  | -2.61191800 | -0.42685300 | 0.00000600 |
| O |  | -1.21211600 | 1.37038500 | 0.00004700 |
| H |  | -3.43835100 | 0.14966400 | 0.00002600 |
| H |  | -2.68420000 | -1.43191800 | -0.00004300 |

B4\_IM2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.82611100 | -0.41658900 | -0.00276800 |
| C |  | 2.06866300 | -0.15383500 | 0.00033700 |
| C |  | 3.33991900 | 0.18572800 | 0.00215300 |
| N |  | -0.35787400 | -0.80173900 | -0.00314500 |
| H |  | 4.13451100 | -0.56112000 | 0.00021900 |
| H |  | 3.65095800 | 1.23107700 | 0.00609300 |
| C |  | -1.41203100 | 0.14137100 | -0.00047200 |
| N |  | -1.24514000 | 1.39477700 | -0.00173200 |
| O |  | -2.61110500 | -0.47452100 | 0.00363500 |
| H |  | -2.46178100 | -1.43104500 | 0.00272000 |
| H |  | -2.14970900 | 1.86595000 | 0.00051600 |

B4\_IM3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.79768300 | 1.21178400 | -0.00045400 |
| C |  | 1.86615800 | 0.58843800 | 0.00126300 |
| C |  | 1.52053200 | -0.87978900 | -0.00026300 |
| N |  | -0.52931900 | 1.27228600 | -0.00042800 |
| H |  | 1.91402900 | -1.39291000 | -0.88742200 |
| H |  | 1.91394000 | -1.39431600 | 0.88613800 |
| C |  | -0.85832600 | -0.00047000 | -0.00004200 |
| N |  | 0.01545600 | -1.03119300 | -0.00053300 |
| O |  | -2.14150200 | -0.36402400 | 0.00027500 |
| H |  | -2.66689800 | 0.45028100 | 0.00130600 |
| H |  | -0.38830400 | -1.95828700 | 0.00148300 |

B4\_IM4

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.19928900 | -0.39420900 | 0.02726600 |
| C |  | -2.43752000 | -0.84598000 | -0.10366300 |
| C |  | -0.95919500 | 1.12649500 | 0.09813800 |
| N |  | 0.02818000 | -1.07640000 | 0.07532500 |
| H |  | -1.52065100 | 1.69508100 | -0.64824900 |
| H |  | -1.18831800 | 1.51995300 | 1.09812200 |
| C |  | 0.91521300 | -0.14250000 | -0.01656200 |
| N |  | 0.47851700 | 1.14216900 | -0.16637400 |
| O |  | 2.22668900 | -0.34365600 | -0.00695400 |
| H |  | 2.37150000 | -1.29822900 | 0.07345100 |
| H |  | 1.06182500 | 1.90922500 | 0.13857100 |

B4\_IM5

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.00740900 | -0.74129200 | -0.23462000 |
| C |  | 2.01010400 | -0.26255200 | 0.46344300 |
| C |  | 1.20325600 | 0.71795700 | -0.34221300 |
| N |  | -0.30101200 | -1.17452300 | -0.27042900 |
| H |  | 2.58127100 | -0.38529400 | 1.37413200 |
| H |  | 1.56866200 | 1.26636100 | -1.21212200 |
| C |  | -0.90906700 | -0.03725900 | -0.02270300 |
| N |  | -0.14821900 | 1.08585000 | 0.09959800 |
| O |  | -2.21700000 | 0.06273300 | 0.19569200 |
| H |  | -2.58316800 | -0.83274500 | 0.15161500 |
| H |  | -0.55636300 | 2.00939600 | 0.13321500 |

B4\_IM5a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.20309100 | -0.34426500 | 0.02494400 |
| C |  | -2.45109000 | -0.72600200 | -0.19774600 |
| C |  | -0.87637100 | 1.14833100 | 0.13555600 |
| N |  | 0.00942000 | -1.00592200 | 0.17999500 |
| H |  | -1.44587700 | 1.75610500 | -0.57341800 |
| H |  | -1.07845300 | 1.49943800 | 1.15758000 |
| C |  | 1.08943100 | -0.13586500 | -0.01483900 |
| N |  | 0.54127500 | 1.11857100 | -0.16344300 |
| O |  | 2.25537900 | -0.45284700 | -0.04761700 |
| H |  | 0.13442000 | -1.99550300 | 0.02485700 |
| H |  | 1.13873400 | 1.92099600 | -0.03143700 |

B4\_IM6

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.01278000 | -0.73092300 | 0.16616800 |
| C |  | -2.00419300 | -0.15928900 | -0.47418200 |
| C |  | -1.13387300 | 0.71980100 | 0.36610600 |
| N |  | 0.28141500 | -1.13353000 | 0.29968300 |
| H |  | -2.75817000 | -0.23198500 | -1.24415000 |
| H |  | -1.45236500 | 1.16248900 | 1.31296700 |
| C |  | 1.07104400 | 0.03830800 | -0.00799300 |
| N |  | 0.20423000 | 1.10326500 | -0.06512400 |
| O |  | 2.26006400 | 0.00616400 | -0.22347600 |
| H |  | 0.63636900 | -2.01238900 | -0.05642000 |
| H |  | 0.57295100 | 2.03705200 | -0.16709500 |

B4\_IM7

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.07540500 | -1.36632300 | 0.00045900 |
| C |  | 1.79370300 | -0.12017400 | -0.00065000 |
| C |  | 1.16035600 | 1.08048300 | 0.00001900 |
| N |  | -0.26711600 | -1.16458800 | 0.00028100 |
| H |  | 2.87938100 | -0.13980100 | -0.00099400 |
| H |  | 1.67234000 | 2.04101900 | 0.00032800 |
| C |  | -1.01155300 | 0.01931400 | -0.00068600 |
| N |  | -0.20398200 | 1.14271500 | 0.00057000 |
| O |  | -2.22368200 | 0.06579300 | -0.00028300 |
| H |  | -0.87434200 | -1.98078500 | 0.00099300 |
| H |  | -0.69770200 | 2.02653200 | 0.00112800 |

B4\_PD

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.06909900 | 1.16483500 | 0.00007300 |
| C |  | 1.77639400 | 0.00156700 | -0.00078000 |
| C |  | 1.00701600 | -1.19415000 | -0.00001800 |
| N |  | -0.28108700 | 1.11259700 | 0.00053300 |
| H |  | 1.53240800 | -2.15290600 | 0.00077000 |
| H |  | 2.85926200 | -0.01050500 | -0.00146800 |
| C |  | -1.03308000 | -0.09150400 | 0.00004600 |
| N |  | -0.29543000 | -1.26055800 | 0.00080800 |
| O |  | -2.24451200 | -0.02432400 | -0.00081800 |
| H |  | -0.84084900 | 1.95745900 | 0.00154300 |
| H |  | 1.52431200 | 2.15178400 | 0.00038900 |

B4\_RC

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -3.11415100 | -0.18550200 | 0.07641200 |
| N |  | -3.20105900 | 1.15137100 | 0.03615100 |
| O |  | -3.96279100 | -1.01544600 | -0.07988800 |
| H |  | -4.08754700 | 1.61369900 | -0.14979700 |
| H |  | -2.38317900 | 1.71762000 | 0.19077900 |
| C |  | 2.84390800 | -0.89038900 | 0.00812600 |
| C |  | 2.99351800 | 0.43893800 | -0.01176100 |
| C |  | 3.14352000 | 1.73297600 | -0.03115300 |
| N |  | 2.70852700 | -2.06506800 | 0.02496900 |
| H |  | 4.13189400 | 2.19894100 | -0.04551000 |
| H |  | 2.28810700 | 2.41304600 | -0.03395000 |

B4\_TS1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.83885100 | -0.46083300 | -0.00009000 |
| C |  | 2.06782900 | -0.14320400 | 0.00000700 |
| C |  | 3.32194800 | 0.25536500 | 0.00012900 |
| N |  | -0.32556400 | -0.91209800 | -0.00020100 |
| H |  | 3.58508100 | 1.31379700 | 0.00041700 |
| H |  | 4.14908400 | -0.45531000 | -0.00004800 |
| C |  | -1.38553100 | -0.00883400 | -0.00003300 |
| N |  | -2.65350100 | -0.32102900 | 0.00023500 |
| O |  | -1.29490900 | 1.27475800 | -0.00014300 |
| H |  | -3.00940700 | -1.26956100 | 0.00034200 |
| H |  | -2.57060600 | 0.98993900 | 0.00012400 |

B4\_TS2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.81840600 | -1.10211600 | 0.03662000 |
| C |  | -1.94575300 | -0.60990400 | -0.26081500 |
| C |  | -1.88984900 | 0.74940100 | 0.06578000 |
| N |  | 0.45116400 | -1.16950700 | 0.15683200 |
| H |  | -2.11805800 | 1.49085100 | -0.70075000 |
| H |  | -1.98827900 | 1.11099300 | 1.08972200 |
| C |  | 0.95374100 | 0.09281300 | 0.02083700 |
| N |  | 0.21590300 | 1.15772600 | 0.04722900 |
| O |  | 2.28583600 | 0.17554100 | -0.09381500 |
| H |  | 2.63370700 | -0.72842600 | -0.12202400 |
| H |  | 0.71807500 | 2.02355200 | -0.11938900 |

B4\_TS3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.04626500 | -0.82698600 | 0.01469800 |
| C |  | -2.26565800 | -0.54781200 | -0.25143400 |
| C |  | -1.18177900 | 0.92410600 | 0.21284500 |
| N |  | 0.25525000 | -1.17516200 | 0.13955300 |
| H |  | -1.80759600 | 1.58049000 | -0.38942100 |
| H |  | -1.32535200 | 1.12992400 | 1.28165000 |
| C |  | 0.92178700 | -0.07221700 | -0.00702600 |
| N |  | 0.22250700 | 1.07745200 | -0.17896300 |
| O |  | 2.24330900 | 0.00409300 | -0.03707300 |
| H |  | 2.59259400 | -0.89892500 | 0.00171600 |
| H |  | 0.68107300 | 1.97719100 | -0.13599000 |

B4\_TS4

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.04808700 | -0.69677200 | 0.21575600 |
| C |  | -2.07219100 | -0.50115500 | -0.61232200 |
| C |  | -1.14586200 | 0.76817700 | 0.31976100 |
| N |  | 0.26398900 | -1.15370500 | 0.29611900 |
| H |  | -1.51146100 | 1.22091100 | 1.24487300 |
| C |  | 0.90984100 | -0.05805800 | 0.02441200 |
| N |  | 0.16835800 | 1.09518300 | -0.12104800 |
| O |  | 2.21800700 | 0.02684800 | -0.17890000 |
| H |  | 2.57762900 | -0.87158400 | -0.13459500 |
| H |  | 0.58116100 | 2.01443500 | -0.18821100 |
| H |  | -2.28001200 | 0.75796000 | -0.40201500 |

B4\_TS4a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.16442200 | -0.41919700 | 0.01712900 |
| C |  | -2.38041600 | -0.93540600 | -0.10557200 |
| C |  | -0.97166400 | 1.11657400 | 0.08677800 |
| N |  | 0.11300400 | -0.97669600 | 0.08538700 |
| H |  | -1.53581200 | 1.65031600 | -0.68332300 |
| H |  | -1.25699200 | 1.50128600 | 1.07425200 |
| C |  | 1.00848300 | -0.00060600 | -0.01108200 |
| N |  | 0.47763600 | 1.22923000 | -0.12493100 |
| O |  | 2.17590600 | -0.50418900 | -0.01513900 |
| H |  | 0.99943000 | 2.07791000 | 0.03038200 |
| H |  | 1.29976900 | -1.53193800 | 0.05309000 |

B4\_TS5

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.91921500 | -0.79731800 | -0.19969300 |
| C |  | 1.93646500 | -0.36118300 | 0.50633700 |
| C |  | 1.23964900 | 0.64880200 | -0.33239800 |
| N |  | -0.41252000 | -1.04459000 | -0.37084800 |
| H |  | 2.60186400 | -0.52675000 | 1.34143800 |
| H |  | 1.65453100 | 1.12208900 | -1.22338200 |
| C |  | -0.96328200 | 0.16130300 | -0.04366000 |
| N |  | -0.10209500 | 1.18395000 | 0.04126100 |
| O |  | -2.17960400 | -0.04429500 | 0.27851500 |
| H |  | -0.36536200 | 2.11811400 | 0.31887700 |
| H |  | -1.64417700 | -1.24423500 | 0.05853300 |

B4\_TS5a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.05526800 | -0.66106200 | 0.18096700 |
| C |  | 2.07583100 | -0.42164200 | -0.64285400 |
| C |  | 1.07825200 | 0.78447700 | 0.33954300 |
| N |  | -0.24158700 | -1.10272000 | 0.34303400 |
| H |  | 1.46237900 | 1.21173900 | 1.26936100 |
| C |  | -1.06798200 | -0.00005400 | -0.00753200 |
| N |  | -0.23141200 | 1.11380300 | -0.07705100 |
| O |  | -2.25346900 | -0.04500000 | -0.22292300 |
| H |  | -0.55576600 | -2.01855000 | 0.05143900 |
| H |  | -0.62089300 | 2.03544400 | -0.20945900 |
| H |  | 2.20481400 | 0.84347400 | -0.41058600 |

B4\_TS6

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.03215200 | 0.97317500 | 0.03712700 |
| C |  | 1.94340500 | 0.10056500 | -0.41500500 |
| C |  | 1.16296300 | -0.82815100 | 0.30212400 |
| N |  | -0.28210000 | 1.11480600 | 0.24023400 |
| H |  | 2.97464300 | 0.19791300 | -0.73323200 |
| H |  | 1.46634700 | -1.29015300 | 1.24899100 |
| C |  | -1.07642400 | -0.04060400 | -0.01497200 |
| N |  | -0.19140900 | -1.08841900 | -0.06676400 |
| O |  | -2.27252500 | -0.03827000 | -0.18543500 |
| H |  | -0.74459700 | 2.00661000 | 0.35983300 |
| H |  | -0.57420400 | -2.02283900 | -0.06204900 |

B4\_TS7

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.07859800 | 1.26657800 | -0.00958400 |
| C |  | 1.81819900 | 0.05170400 | 0.04906800 |
| C |  | 1.11548800 | -1.11357900 | -0.00043900 |
| N |  | -0.28032400 | 1.19831100 | -0.08754500 |
| H |  | 1.58379000 | -2.09653300 | 0.00203200 |
| H |  | 2.90025500 | 0.04621500 | 0.11345200 |
| C |  | -1.04928400 | 0.03749600 | -0.00770600 |
| N |  | -0.24448600 | -1.11297400 | -0.04690400 |
| O |  | -2.25402200 | -0.03280400 | 0.06471000 |
| H |  | -0.76074100 | -1.98522000 | -0.04058400 |
| H |  | 0.20453700 | 2.24742200 | 0.16052600 |

C2\_IM1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.75858200 | -1.17780600 | -0.02619800 |
| C |  | -1.78450800 | -0.40696400 | -0.31737700 |
| C |  | -1.29000700 | 0.93534900 | 0.23545200 |
| N |  | 0.40054500 | -1.23741500 | 0.38032900 |
| H |  | -1.78038700 | 1.72432400 | -0.34417400 |
| H |  | -1.52744500 | 1.08645900 | 1.29837300 |
| H |  | -2.54118500 | -0.52757700 | -1.07750300 |
| C |  | 1.06504000 | 0.01059200 | -0.00898100 |
| N |  | 0.16182800 | 1.05115300 | 0.01193000 |
| O |  | 2.24359300 | 0.11135100 | -0.22336700 |
| H |  | 0.57200200 | 1.96279100 | -0.13295700 |

C2\_IM2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.07548800 | -1.36631700 | 0.00010200 |
| C |  | 1.79383300 | -0.12010200 | -0.00033300 |
| C |  | 1.16029300 | 1.08058500 | -0.00013600 |
| N |  | -0.26699200 | -1.16453900 | 0.00037900 |
| H |  | 1.67205500 | 2.04125200 | -0.00017000 |
| H |  | -0.87415700 | -1.98086400 | 0.00104000 |
| H |  | 2.87946400 | -0.13959500 | -0.00120800 |
| C |  | -1.01159400 | 0.01925500 | 0.00000100 |
| N |  | -0.20405100 | 1.14261600 | 0.00044900 |
| O |  | -2.22377900 | 0.06573000 | -0.00062500 |
| H |  | -0.69795100 | 2.02629700 | 0.00174300 |

C2\_IM2a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.66012300 | 1.33089800 | -0.06265900 |
| C |  | 1.32955700 | 0.16336000 | -0.54129300 |
| C |  | 1.48994300 | -0.86451200 | 0.49308400 |
| N |  | -0.63314500 | 1.26005200 | 0.18498100 |
| H |  | 2.09506400 | -1.75494000 | 0.31928400 |
| H |  | 1.29849800 | -0.64942800 | 1.54832800 |
| H |  | 1.19074500 | 2.26396900 | 0.11825300 |
| C |  | -1.01891700 | -0.04227400 | 0.03980100 |
| N |  | 0.23676700 | -0.83954400 | -0.33175700 |
| O |  | -2.08359500 | -0.59078300 | 0.05729300 |
| H |  | 0.09487400 | -1.60172400 | -0.99037700 |

C2\_IM3a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.74872700 | 1.26657500 | -0.07496700 |
| C |  | 1.32888200 | -0.04055200 | -0.43830500 |
| C |  | 1.42492400 | -1.05757900 | 0.67057100 |
| N |  | -0.50663100 | 1.27876600 | 0.23492600 |
| H |  | 1.93723300 | -0.14742900 | -1.33734600 |
| H |  | 1.09162600 | -0.57213100 | 1.60387600 |
| H |  | 1.35204400 | 2.16915500 | 0.01846500 |
| C |  | -0.99360400 | -0.01663500 | 0.00266200 |
| N |  | 0.15408000 | -0.89954600 | -0.28264600 |
| O |  | -2.11844200 | -0.41459000 | -0.00297000 |
| H |  | -0.01908700 | -1.69827400 | -0.88695700 |

C2\_PD

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.00699500 | -1.19407100 | 0.00015000 |
| C |  | -1.77638300 | 0.00153100 | -0.00040300 |
| C |  | -1.06904000 | 1.16482200 | 0.00008200 |
| N |  | 0.29562500 | -1.26066200 | 0.00059200 |
| H |  | -1.52430800 | 2.15167800 | -0.00026200 |
| H |  | -1.53230800 | -2.15265100 | -0.00076100 |
| H |  | -2.85931500 | -0.01050700 | -0.00146100 |
| C |  | 1.03296700 | -0.09150400 | 0.00020900 |
| N |  | 0.28108400 | 1.11256600 | 0.00043800 |
| O |  | 2.24432200 | -0.02422600 | -0.00069700 |
| H |  | 0.84109800 | 1.95729100 | 0.00061900 |

C2\_RC

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.86389300 | 0.81879100 | -0.00122400 |
| C |  | 2.53923500 | -0.43849500 | -0.00229000 |
| C |  | 1.85121800 | -1.58439900 | 0.00100100 |
| N |  | 1.28359900 | 1.82762800 | -0.00027500 |
| H |  | 2.36809900 | -2.53924400 | 0.00009400 |
| H |  | 0.76243800 | -1.58809700 | 0.00459900 |
| H |  | 3.62643300 | -0.41104800 | -0.00586600 |
| C |  | -2.46933400 | -0.03572200 | 0.00052900 |
| N |  | -1.26253100 | 0.07570900 | 0.00628400 |
| O |  | -3.61355600 | -0.28395300 | -0.00431700 |
| H |  | -0.70606200 | 0.92560900 | 0.00554600 |

C2\_TS1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.89089800 | 1.17979100 | -0.05101200 |
| C |  | 1.84113900 | 0.24129500 | -0.36440300 |
| C |  | 1.37735100 | -0.93533900 | 0.30911700 |
| N |  | -0.16054600 | 1.57277000 | 0.33805200 |
| H |  | 1.78410500 | -1.88838500 | -0.03568700 |
| H |  | 1.31022200 | -0.89379300 | 1.39739400 |
| H |  | 2.28050900 | 0.20039100 | -1.35490000 |
| C |  | -1.23108500 | -0.27877000 | -0.04796200 |
| N |  | -0.30820100 | -1.15351600 | -0.00110200 |
| O |  | -2.34532000 | 0.06431900 | -0.15938400 |
| H |  | -0.60086400 | -2.10940500 | -0.16482700 |

C2\_TS2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.78989500 | -1.17923000 | -0.32878500 |
| C |  | -1.79400300 | -0.27186000 | -0.34313200 |
| C |  | -1.11394100 | 0.90212900 | 0.26922400 |
| N |  | 0.08822200 | -0.96737400 | 0.60517700 |
| H |  | -1.66207400 | 1.84800200 | 0.28769500 |
| H |  | -2.77603000 | -0.23789300 | -0.79746500 |
| C |  | 1.06050400 | -0.00753700 | 0.03812400 |
| N |  | 0.28373300 | 1.13625000 | -0.01565800 |
| O |  | 2.20740000 | -0.16328400 | -0.26433000 |
| H |  | 0.60268400 | 1.92002100 | -0.57356300 |
| H |  | -0.60345400 | -0.06701100 | 1.25875900 |

C2\_TS2a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.78227300 | -1.10526300 | -0.08000400 |
| C |  | -1.76646600 | -0.32679100 | -0.56233600 |
| C |  | -1.30756200 | 0.94663000 | 0.22869400 |
| N |  | 0.39545500 | -1.26052800 | 0.31195300 |
| H |  | -1.78693800 | 1.81217200 | -0.23798200 |
| H |  | -1.59521400 | 0.92923200 | 1.29049700 |
| C |  | 1.04465600 | -0.00024100 | 0.00968700 |
| N |  | 0.14126700 | 1.05956900 | 0.03643500 |
| O |  | 2.22706500 | 0.12813700 | -0.16340800 |
| H |  | 0.53851500 | 1.95405200 | -0.21302700 |
| H |  | -1.86006600 | -1.39984500 | 0.45280700 |

C2\_TS3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.07860800 | 1.26657300 | -0.00956800 |
| C |  | -1.81821500 | 0.05169600 | 0.04897600 |
| C |  | -1.11548600 | -1.11358200 | -0.00043800 |
| N |  | 0.28031400 | 1.19830700 | -0.08741200 |
| H |  | -1.58377900 | -2.09654000 | 0.00203900 |
| H |  | -2.90027700 | 0.04619800 | 0.11324400 |
| C |  | 1.04929300 | 0.03749900 | -0.00769100 |
| N |  | 0.24449200 | -1.11297100 | -0.04681500 |
| O |  | 2.25404000 | -0.03279800 | 0.06459400 |
| H |  | 0.76074900 | -1.98521500 | -0.04049100 |
| H |  | -0.20456100 | 2.24746700 | 0.16037300 |

C2\_TS3a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.74801800 | 1.28222900 | -0.07158100 |
| C |  | 1.30571300 | 0.05972400 | -0.58251200 |
| C |  | 1.31281600 | -1.08722800 | 0.65105800 |
| N |  | -0.52692800 | 1.28570600 | 0.22843900 |
| H |  | 1.06028100 | -0.56513700 | 1.58114300 |
| H |  | 1.34687700 | 2.17949500 | 0.07097200 |
| C |  | -0.99128400 | 0.00719500 | 0.02247000 |
| N |  | 0.21467800 | -0.87539700 | -0.32694400 |
| O |  | -2.08784500 | -0.46201800 | 0.00865800 |
| H |  | 0.00042200 | -1.63942100 | -0.96769800 |
| H |  | 2.22935500 | -0.72248200 | -0.18075700 |

C2\_TS4a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.75504900 | 1.23209200 | -0.07438500 |
| C |  | 1.51076400 | 0.02702700 | -0.44291700 |
| C |  | 1.35441900 | -1.05127100 | 0.49471500 |
| N |  | -0.48173600 | 1.22992300 | 0.31578400 |
| H |  | 2.30306500 | 0.08616900 | -1.20260900 |
| H |  | 1.38364700 | -0.99774800 | 1.58011000 |
| H |  | 1.33209900 | 2.15830200 | 0.01699300 |
| C |  | -1.03275000 | -0.01274100 | 0.06308800 |
| N |  | 0.05127300 | -0.99791300 | -0.12349800 |
| O |  | -2.17994800 | -0.30413500 | -0.13236400 |
| H |  | -0.09087700 | -1.60835800 | -0.92458400 |

C4\_IM1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.05560300 | -0.04280500 | 0.74781400 |
| C |  | -2.27715500 | -0.01592300 | 0.05567200 |
| C |  | -3.42279000 | -0.01442000 | -0.36479600 |
| N |  | 0.04022300 | 0.05789700 | 0.07963800 |
| H |  | -4.41722400 | -0.01134300 | -0.75269300 |
| C |  | 1.30639400 | 0.01538200 | -0.01620100 |
| N |  | 2.05139500 | -1.12650700 | -0.06853600 |
| O |  | 2.06371400 | 1.12579000 | -0.13795300 |
| H |  | 1.49282300 | 1.89931300 | -0.04005000 |
| H |  | 1.54105900 | -1.99241700 | -0.14666200 |
| H |  | 2.92722000 | -1.07500900 | -0.56962700 |

C4\_IM2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | C | 1.04283100 | -1.17577800 | 0.38662600 |
|  | C | 1.80895500 | -0.31583900 | -0.29892700 |
|  | C | 1.35417400 | 0.93570300 | -0.31531800 |
|  | N | -0.25825500 | -1.27019100 | -0.04807700 |
|  | H | 1.62486400 | 1.87104900 | -0.78688100 |
|  | C | -0.81522200 | -0.13154100 | 0.00048700 |
|  | N | -0.04061700 | 1.05224900 | 0.42093100 |
|  | O | -2.10903200 | 0.18275500 | -0.19346600 |
|  | H | -2.55162200 | -0.60354100 | -0.54531600 |
|  | H | 0.10458700 | 1.01818800 | 1.44350500 |
|  | H | -0.55790300 | 1.90258500 | 0.18922500 |

C4\_IM3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.09910400 | -1.18397500 | -0.00345600 |
| C |  | -1.95494600 | -0.06084900 | 0.00099200 |
| C |  | -1.21442400 | 1.09995200 | 0.00260300 |
| N |  | 0.25849200 | -1.20284100 | 0.00422400 |
| H |  | -1.63614200 | 2.10697300 | 0.01058100 |
| C |  | 0.84783100 | -0.03771800 | 0.00079400 |
| N |  | 0.17238800 | 1.11933900 | -0.00407700 |
| O |  | 2.17804800 | 0.07566700 | 0.00018500 |
| H |  | 2.53604300 | -0.82592800 | 0.00193900 |
| H |  | -1.52107900 | -2.19254800 | -0.01112800 |
| H |  | 0.70449200 | 1.98621400 | -0.00950100 |

C4\_IM4

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.14112100 | 1.14720200 | -0.10553700 |
| C |  | -1.87963300 | 0.00003200 | -0.00018100 |
| C |  | -1.14122700 | -1.14719700 | 0.10544600 |
| N |  | 0.21593000 | 1.14626300 | 0.13679400 |
| H |  | -1.54430900 | -2.11486800 | 0.40726300 |
| C |  | 0.98542300 | 0.00001300 | 0.00012300 |
| N |  | 0.21578300 | -1.14618800 | -0.13649200 |
| O |  | 2.20142700 | -0.00012400 | -0.00023300 |
| H |  | 0.75728100 | 1.99772000 | 0.24601400 |
| H |  | -1.54420500 | 2.11490900 | -0.40714000 |
| H |  | 0.75717400 | -1.99759100 | -0.24549900 |

C4\_IM4a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.05970400 | -1.41021400 | 0.00001900 |
| C |  | -1.80238900 | -0.16153800 | -0.00002300 |
| C |  | -1.21065900 | 1.05976000 | -0.00000400 |
| N |  | 0.31617500 | -1.22496900 | 0.00000900 |
| H |  | -1.72414200 | 2.01821300 | 0.00001300 |
| C |  | 0.85157700 | -0.03923100 | 0.00000400 |
| N |  | 0.16014900 | 1.12036300 | 0.00001000 |
| O |  | 2.17462900 | 0.12491300 | -0.00001700 |
| H |  | 2.54711700 | -0.77317000 | -0.00001200 |
| H |  | -2.88913500 | -0.20499200 | -0.00003500 |
| H |  | 0.66190400 | 2.00021800 | 0.00006600 |

C4\_IM5

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | C | -1.07550200 | -1.36631400 | 0.00020200 |
|  | C | -1.79380900 | -0.12003600 | -0.00041800 |
|  | C | -1.16030500 | 1.08054000 | -0.00080000 |
|  | N | 0.26691600 | -1.16454000 | 0.00027200 |
|  | H | -1.67199400 | 2.04114400 | 0.00008400 |
|  | C | 1.01159300 | 0.01927400 | 0.00107900 |
|  | N | 0.20411500 | 1.14264900 | 0.00075300 |
|  | O | 2.22378800 | 0.06566300 | -0.00088400 |
|  | H | 0.87417400 | -1.98080900 | -0.00108000 |
|  | H | -2.87944400 | -0.13960300 | 0.00012500 |
|  | H | 0.69788500 | 2.02642800 | 0.00038700 |

C4\_PD

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.06916100 | 1.16492100 | -0.00002200 |
| C |  | 1.77644100 | 0.00165600 | 0.00021600 |
| C |  | 1.00700400 | -1.19409600 | -0.00017500 |
| N |  | -0.28102200 | 1.11250600 | -0.00015700 |
| H |  | 2.85933500 | -0.01092100 | 0.00073100 |
| C |  | -1.03312200 | -0.09152800 | 0.00004500 |
| N |  | -0.29555200 | -1.26078800 | -0.00015500 |
| O |  | -2.24449900 | -0.02414900 | 0.00026000 |
| H |  | -0.84102900 | 1.95721500 | -0.00113200 |
| H |  | 1.52418700 | 2.15190700 | 0.00030400 |
| H |  | 1.53261800 | -2.15275700 | -0.00018300 |

C4\_RC

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.39937400 | 0.82187800 | 0.00008800 |
| C |  | 2.07641300 | -0.37542200 | 0.00000700 |
| C |  | 2.70365100 | -1.40771300 | -0.00011800 |
| N |  | 0.88788900 | 1.87006800 | 0.00006300 |
| H |  | 3.25213000 | -2.32439100 | -0.00027600 |
| C |  | -1.37306900 | -0.36985400 | 0.00033200 |
| N |  | -2.42616200 | -1.18600400 | -0.00007400 |
| O |  | -1.82555200 | 0.88322600 | -0.00024400 |
| H |  | -1.05526400 | 1.48184000 | 0.00010700 |
| H |  | -3.38661500 | -0.84365500 | -0.00034400 |
| H |  | -2.27613400 | -2.18138900 | 0.00068100 |

C4\_RCa

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.16116800 | 0.38886800 | -0.00026900 |
| N |  | -1.08179600 | -0.15821300 | -0.00000500 |
| O |  | 1.19435600 | -0.24652600 | 0.00009900 |
| H |  | 0.13639300 | 1.49759900 | 0.00043700 |
| H |  | -1.17417800 | -1.16450100 | 0.00000500 |
| H |  | -1.91149600 | 0.41339300 | 0.00040700 |

C4\_TS1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.14667000 | -0.21665900 | 0.60131500 |
| C |  | 2.36259200 | -0.01431400 | 0.02273800 |
| C |  | 3.47685500 | 0.15201700 | -0.44208200 |
| N |  | -0.04943700 | -0.28443600 | 0.68626400 |
| H |  | 4.45394400 | 0.29675100 | -0.84706100 |
| C |  | -1.34908500 | 0.04442600 | -0.34281700 |
| N |  | -2.00139200 | 1.18928700 | -0.07123600 |
| O |  | -2.22223400 | -0.98199900 | -0.29111200 |
| H |  | -1.74700600 | -1.79847400 | -0.48666700 |
| H |  | -2.91099500 | 1.17785000 | 0.38313400 |
| H |  | -1.48446300 | 2.05308800 | -0.06062700 |

C4\_TS2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.04281300 | -1.14896000 | 0.42609300 |
| C |  | 1.84637900 | -0.33870600 | -0.32458200 |
| C |  | 1.46153800 | 0.90381900 | -0.37362900 |
| N |  | -0.24172600 | -1.22978200 | -0.00799400 |
| H |  | 1.68167300 | 1.89855700 | -0.72159500 |
| C |  | -0.83758000 | -0.10909900 | 0.03242300 |
| N |  | -0.13479500 | 1.07439300 | 0.46202600 |
| O |  | -2.13001700 | 0.13325200 | -0.25934000 |
| H |  | -2.49637100 | -0.67038300 | -0.65645800 |
| H |  | 0.07576800 | 1.03315300 | 1.46589500 |
| H |  | -0.66418500 | 1.91805700 | 0.24682000 |

C4\_TS3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.96503000 | -1.03321800 | 0.40043800 |
| C |  | 1.80927900 | -0.33337100 | -0.37817800 |
| C |  | 1.33233500 | 0.91584200 | -0.35430700 |
| N |  | -0.31672700 | -1.25601400 | -0.07611900 |
| H |  | 1.58746900 | 1.87373500 | -0.78886600 |
| C |  | -0.84232400 | -0.09458600 | 0.00828600 |
| N |  | 0.04336700 | 0.92036400 | 0.50351300 |
| O |  | -2.10300500 | 0.28623600 | -0.22114900 |
| H |  | -2.59519800 | -0.48242000 | -0.54382600 |
| H |  | -0.41293600 | 1.80988100 | 0.72576900 |
| H |  | 0.57230900 | 0.13045700 | 1.32692800 |

C4\_TS4

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.94760300 | -1.28075600 | 0.08265400 |
| C |  | -1.86886600 | -0.23192100 | -0.02221600 |
| C |  | -1.31001800 | 1.00890700 | -0.06733400 |
| N |  | 0.37657000 | -1.08522000 | -0.10774000 |
| H |  | -1.85039200 | 1.93291400 | -0.27031100 |
| C |  | 0.87985300 | 0.16161800 | -0.00808100 |
| N |  | 0.07715300 | 1.22285000 | 0.09943400 |
| O |  | 2.15058300 | 0.06332300 | -0.00331900 |
| H |  | -1.23549000 | -2.30446000 | 0.32581600 |
| H |  | 0.48909200 | 2.14118900 | 0.23028300 |
| H |  | 1.69586900 | -1.18672400 | -0.11123000 |

C4\_TS4a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.06021200 | -1.28224100 | -0.00026500 |
| C |  | 1.86996500 | -0.08452100 | -0.00074100 |
| C |  | 1.22144400 | 1.11286100 | 0.00025400 |
| N |  | -0.30723800 | -1.24737200 | 0.00068900 |
| H |  | 1.66726900 | 2.10677200 | 0.00127500 |
| C |  | -0.84390000 | -0.05303600 | 0.00008600 |
| N |  | -0.16091900 | 1.10893600 | 0.00003200 |
| O |  | -2.16893100 | 0.10409700 | -0.00035700 |
| H |  | -2.54825600 | -0.78979300 | -0.00011800 |
| H |  | -0.69944600 | 1.97032600 | 0.00001200 |
| H |  | 2.36265800 | -1.30939700 | 0.00062800 |

C4\_TS5

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.09626600 | -1.22801600 | -0.12432600 |
| C |  | 1.85668500 | -0.02159400 | -0.11291300 |
| C |  | 1.14812600 | 1.13823900 | 0.08406300 |
| N |  | -0.24550000 | -1.17197100 | 0.11353800 |
| H |  | 1.58338900 | 2.10085800 | 0.35428900 |
| C |  | -1.00210400 | -0.01158100 | 0.00001700 |
| N |  | -0.21310600 | 1.13711100 | -0.04868800 |
| O |  | -2.21429200 | 0.02252200 | -0.03675100 |
| H |  | -0.79481300 | -2.01743300 | 0.23818200 |
| H |  | -0.75372800 | 1.99704700 | -0.07019500 |
| H |  | 2.29588900 | -1.27891200 | 0.23674100 |

C4\_TS5a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.88504500 | -1.48370200 | 0.00009500 |
| C |  | -1.75009200 | -0.29837200 | -0.00015100 |
| C |  | -1.28992100 | 0.97417200 | 0.00000900 |
| N |  | 0.40893400 | -1.10898000 | 0.00012300 |
| H |  | -1.91350200 | 1.86332300 | 0.00003700 |
| C |  | 0.88684600 | 0.15340300 | -0.00001700 |
| N |  | 0.07966800 | 1.21746900 | 0.00009100 |
| O |  | 2.15936000 | 0.08999600 | -0.00015000 |
| H |  | -2.82720900 | -0.44535000 | -0.00036100 |
| H |  | 0.46267500 | 2.15425000 | 0.00032500 |
| H |  | 1.81221000 | -1.12461600 | 0.00009000 |

C4\_TS6

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.11549000 | -1.11357900 | -0.00043800 |
| C |  | -1.81820100 | 0.05170500 | 0.04907700 |
| C |  | -1.07859700 | 1.26658100 | -0.00958700 |
| N |  | 0.24448600 | -1.11297600 | -0.04691500 |
| H |  | -2.90025800 | 0.04621700 | 0.11347500 |
| C |  | 1.04928300 | 0.03749400 | -0.00770900 |
| N |  | 0.28032500 | 1.19831600 | -0.08757900 |
| O |  | 2.25402500 | -0.03280500 | 0.06472700 |
| H |  | 0.76074000 | -1.98522200 | -0.04057800 |
| H |  | -1.58379300 | -2.09653200 | 0.00204300 |
| H |  | -0.20453500 | 2.24739800 | 0.16064400 |

C4\_TSa

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.08414800 | -0.47317400 | -0.00012000 |
| N |  | 1.11014800 | 0.10832500 | 0.00002700 |
| O |  | -1.14761400 | 0.29038600 | -0.00002700 |
| H |  | 1.16023800 | 1.12664900 | 0.00019900 |
| H |  | 1.95958900 | -0.43339900 | -0.00003000 |
| H |  | -1.20506700 | -0.93556100 | 0.00057400 |

Cytosine\_IM1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.19842300 | 1.72400500 | -0.07708800 |
| C |  | 1.02334400 | 1.21198200 | 0.08706000 |
| C |  | 1.15115300 | -0.26780500 | 0.29826800 |
| N |  | -1.30726300 | 0.89143700 | -0.07377200 |
| H |  | 1.14198800 | -0.41591000 | 1.41931600 |
| H |  | 1.91297000 | 1.83214700 | 0.10062000 |
| C |  | -1.23620900 | -0.49804300 | -0.01360100 |
| N |  | 0.03439700 | -1.05746700 | -0.09515400 |
| O |  | -2.24623300 | -1.17537100 | 0.04819000 |
| H |  | -0.39741900 | 2.78099200 | -0.22296700 |
| H |  | -2.24273800 | 1.26714900 | -0.15314300 |
| N |  | 2.35796200 | -0.80336300 | -0.29175200 |
| H |  | 3.18755000 | -0.47790900 | 0.19372400 |
| H |  | 2.33264300 | -1.81859200 | -0.26615900 |

Cytosine\_PD

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.08278600 | -1.82250200 | 0.02826300 |
| C |  | -1.23987700 | -1.11574600 | 0.01771200 |
| C |  | -1.10353100 | 0.31394000 | -0.00853500 |
| N |  | 1.10385800 | -1.17495800 | 0.01382400 |
| H |  | -2.20730100 | -1.60544200 | 0.02522800 |
| C |  | 1.22131800 | 0.24465600 | -0.01467500 |
| N |  | 0.05038300 | 0.94599600 | -0.02236000 |
| O |  | 2.33915200 | 0.72479000 | -0.02811700 |
| H |  | -0.05290700 | -2.90852400 | 0.04799800 |
| H |  | 1.98373000 | -1.67460600 | 0.01951900 |
| N |  | -2.22339500 | 1.07637200 | -0.03054700 |
| H |  | -3.14268400 | 0.67585800 | 0.05360300 |
| H |  | -2.11059800 | 2.07893500 | -0.00186300 |
| H |  | 1.52987900 | 5.98149700 | 0.21744500 |

Cytosine\_RC

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.39593700 | -0.75303300 | 0.80817100 |
| C |  | 1.92749600 | 0.36438400 | 0.23885600 |
| C |  | 1.13955900 | 0.98425200 | -0.76499900 |
| N |  | 0.18829000 | -1.19044900 | 0.39428000 |
| H |  | 1.53679100 | 1.86821900 | -1.27062900 |
| H |  | 2.89460500 | 0.75208200 | 0.53364300 |
| C |  | -0.61795500 | -0.50803500 | -0.54436800 |
| N |  | -0.04421200 | 0.59113500 | -1.15218300 |
| O |  | -1.74543800 | -0.91441700 | -0.75841100 |
| H |  | 1.89003900 | -1.33239700 | 1.58319000 |
| H |  | -0.25729000 | -1.99005500 | 0.82888000 |
| N |  | -1.69403000 | 1.27475200 | 1.34721000 |
| H |  | -2.54978600 | 0.72724500 | 1.18143300 |
| H |  | -1.77142300 | 2.03676800 | 0.65966700 |

Cytosine\_TS1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.08872000 | 1.71718100 | 0.20287300 |
| C |  | -1.20398300 | 1.15303000 | -0.30549000 |
| C |  | -1.10500700 | -0.23423000 | -0.70349700 |
| N |  | 1.05059800 | 0.97237000 | 0.32300000 |
| H |  | -1.87954300 | -0.62593700 | -1.36295800 |
| H |  | -2.13663900 | 1.69599800 | -0.39456000 |
| C |  | 1.16281200 | -0.36703700 | -0.10019700 |
| N |  | 0.05006400 | -0.91312700 | -0.71480600 |
| O |  | 2.21278900 | -0.95890400 | 0.06585700 |
| H |  | -0.02937500 | 2.75197600 | 0.52803100 |
| H |  | 1.90282600 | 1.37152600 | 0.69579300 |
| N |  | -1.86270600 | -1.20935000 | 0.84697600 |
| H |  | -1.24842300 | -0.91278200 | 1.61691800 |
| H |  | -1.56746100 | -2.17246500 | 0.64159700 |

Cytosine\_TS2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.22148800 | 1.71918500 | -0.05072200 |
| C |  | 1.02844900 | 1.19970200 | -0.03390300 |
| C |  | 1.11727100 | -0.24966600 | 0.06236700 |
| N |  | -1.29359400 | 0.89131500 | 0.01137900 |
| H |  | 1.91670500 | 1.82004900 | -0.06420300 |
| C |  | -1.20267100 | -0.53156500 | -0.00780900 |
| N |  | 0.05649000 | -1.05915100 | -0.03488200 |
| O |  | -2.23783900 | -1.16994600 | -0.01736200 |
| H |  | -0.42093100 | 2.78530700 | -0.10824900 |
| H |  | -2.23956900 | 1.25047700 | -0.01250700 |
| N |  | 2.34124400 | -0.83752100 | -0.16435400 |
| H |  | 3.16639400 | -0.34339200 | 0.14274200 |
| H |  | 2.35398400 | -1.83895500 | -0.02000000 |
| H |  | 1.06778000 | -0.10236200 | 1.69651700 |

Thymine\_IM1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.60474300 | 1.21257500 | -0.61149100 |
| C |  | -1.44700800 | 0.01573400 | -0.35924900 |
| C |  | -0.56720100 | -1.18973600 | -0.58289000 |
| N |  | 0.69965600 | 1.12207700 | -0.19962100 |
| H |  | -1.03702600 | -2.10294100 | -0.96573500 |
| H |  | -2.28402000 | -0.01375900 | -1.06928200 |
| C |  | 1.34888400 | -0.07357000 | 0.08942400 |
| N |  | 0.68509300 | -1.24134800 | -0.33510900 |
| O |  | 2.44636800 | -0.08347700 | 0.61444500 |
| H |  | -0.97089300 | 2.16392800 | -0.97789600 |
| H |  | 1.27804400 | 1.94786500 | -0.09693700 |
| C |  | -2.02295400 | -0.02815000 | 1.07218500 |
| H |  | -1.21346600 | 0.02379100 | 1.80947300 |
| H |  | -2.69661500 | 0.81917800 | 1.23739000 |
| H |  | -2.58207800 | -0.95646300 | 1.24267000 |

Thymine\_IM2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.93110200 | -1.16755100 | 0.51393600 |
| C |  | -1.49761500 | -0.07391200 | -0.07206900 |
| C |  | -0.58241000 | 0.76668300 | -0.76463800 |
| N |  | 0.39864100 | -1.39165600 | 0.39338900 |
| H |  | -0.97071700 | 1.67748300 | -1.23168600 |
| C |  | 1.28343000 | -0.53642600 | -0.28948300 |
| N |  | 0.70303100 | 0.56744800 | -0.89022700 |
| O |  | 2.47226000 | -0.78851600 | -0.31208800 |
| H |  | -1.49999300 | -1.89310200 | 1.09182800 |
| H |  | 0.83940200 | -2.18257800 | 0.84803000 |
| C |  | -2.95430900 | 0.25275200 | 0.01468500 |
| H |  | -3.41714600 | 0.29948900 | -0.97830000 |
| H |  | -3.49582200 | -0.50042000 | 0.59635000 |
| H |  | -3.11722500 | 1.22398600 | 0.49671400 |
| O |  | 1.27220100 | 2.00535800 | 1.03040800 |
| H |  | 2.08614200 | 1.96059400 | 0.49378700 |

Thymine\_IM3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.49267100 | -1.36095900 | 0.28715200 |
| C |  | -1.24829500 | -0.31426100 | -0.08786100 |
| C |  | -0.51732600 | 0.99446400 | -0.27713800 |
| N |  | 0.89217000 | -1.26472200 | 0.34629400 |
| H |  | -1.09365500 | 1.67424700 | -0.92262800 |
| C |  | 1.54023600 | -0.17799000 | -0.21088300 |
| N |  | 0.69706800 | 0.64593200 | -0.95922400 |
| O |  | 2.73650500 | 0.01680800 | -0.11259300 |
| H |  | -0.91922000 | -2.32631600 | 0.54911400 |
| H |  | 1.45357300 | -1.90149000 | 0.89459200 |
| C |  | -2.72723000 | -0.34603500 | -0.25772500 |
| H |  | -3.02064900 | -0.14513100 | -1.29644500 |
| H |  | -3.13865000 | -1.32180900 | 0.02169700 |
| H |  | -3.20380800 | 0.41975700 | 0.36865600 |
| O |  | -0.31743600 | 1.57453500 | 0.99629400 |
| H |  | 0.11690600 | 2.43020500 | 0.88465200 |

Thymine\_IM4

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.31535800 | 1.35346500 | 0.00192700 |
| C |  | -0.90942400 | 0.76437400 | 0.00055900 |
| C |  | -0.85468500 | -0.66754800 | -0.00069000 |
| N |  | 1.44879100 | 0.60708300 | 0.00194600 |
| C |  | 1.46008300 | -0.80691900 | 0.00010700 |
| N |  | 0.22079200 | -1.40102600 | -0.00097200 |
| O |  | 2.52428900 | -1.39293400 | -0.00036700 |
| H |  | 0.43991400 | 2.43403900 | 0.00308600 |
| H |  | 2.36377000 | 1.03996300 | 0.00294900 |
| C |  | -2.20212700 | 1.51127900 | 0.00048500 |
| H |  | -2.80780700 | 1.26433600 | 0.88010200 |
| H |  | -2.02458000 | 2.59178100 | 0.00088800 |
| H |  | -2.80736000 | 1.26489700 | -0.87957900 |
| O |  | -2.03773600 | -1.29216700 | -0.00161900 |
| H |  | -1.84736800 | -2.24451100 | -0.00220200 |
| H |  | 4.24869500 | 7.75999600 | -0.01050100 |

Thymine\_IM4a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.20631000 | -1.49943200 | -0.04055700 |
| C |  | 1.13589900 | -0.53650400 | 0.03654400 |
| C |  | 0.68330300 | 0.88465600 | 0.25281200 |
| N |  | -1.15450900 | -1.24416300 | 0.01833700 |
| H |  | 0.94027600 | 1.09423600 | 1.34607500 |
| C |  | -1.68870100 | 0.03419000 | -0.00003900 |
| N |  | -0.74648500 | 1.02602100 | 0.07261700 |
| O |  | -2.88614600 | 0.23884700 | -0.08540500 |
| H |  | 0.48080300 | -2.54313900 | -0.17293500 |
| H |  | -1.83092400 | -1.98600500 | -0.08838400 |
| C |  | 2.60327300 | -0.77222700 | -0.03012300 |
| H |  | 3.11274200 | -0.36840900 | 0.85555400 |
| H |  | 2.82839000 | -1.84133400 | -0.09692700 |
| H |  | 3.04437600 | -0.26347300 | -0.89593200 |
| O |  | 1.41179000 | 1.86144200 | -0.28111200 |
| H |  | -1.11436500 | 1.96869700 | 0.03618100 |

Thymine\_IM5a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.20375100 | -1.51884600 | -0.08555500 |
| C |  | 1.16456900 | -0.48048700 | 0.36888700 |
| C |  | 0.65927400 | 0.91785500 | 0.05512400 |
| N |  | -1.15000300 | -1.23690700 | -0.00740900 |
| H |  | 1.22611200 | -0.48994800 | 1.47975300 |
| C |  | -1.67938500 | 0.02995900 | -0.01525200 |
| N |  | -0.71897200 | 1.04169700 | -0.02530600 |
| O |  | -2.87260800 | 0.26422800 | -0.03042200 |
| H |  | 0.48579400 | -2.56158700 | -0.17628300 |
| H |  | -1.84230200 | -1.96941400 | -0.09653800 |
| C |  | 2.56570100 | -0.70100900 | -0.18233200 |
| H |  | 3.24964400 | 0.06663900 | 0.18756100 |
| H |  | 2.94115300 | -1.68449100 | 0.11991000 |
| H |  | 2.56104100 | -0.65525900 | -1.27687500 |
| O |  | 1.38063600 | 1.88501300 | -0.06007700 |
| H |  | -1.08630700 | 1.98177000 | -0.12976100 |

Thymine\_PD

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.23476800 | -1.47939700 | -0.00000200 |
| C |  | -1.15181200 | -0.49016400 | -0.00000600 |
| C |  | -0.67475800 | 0.89208700 | -0.00000300 |
| N |  | 1.12127700 | -1.23739000 | -0.00001100 |
| C |  | 1.67509900 | 0.03076900 | -0.00001600 |
| N |  | 0.72103900 | 1.02869200 | -0.00002100 |
| O |  | 2.87230000 | 0.23281100 | 0.00002700 |
| H |  | -0.51990300 | -2.52855100 | 0.00000600 |
| H |  | 1.79045400 | -1.99485800 | 0.00001500 |
| C |  | -2.62513200 | -0.71774800 | 0.00001000 |
| H |  | -3.09191200 | -0.25562800 | -0.87735600 |
| H |  | -2.86068500 | -1.78668300 | -0.00007700 |
| H |  | -3.09187500 | -0.25578100 | 0.87747700 |
| O |  | -1.38890300 | 1.87854000 | 0.00000700 |
| H |  | 1.07874300 | 1.97829500 | 0.00000100 |

Thymine\_RC

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.18445000 | -0.14618500 | 1.17230200 |
| C |  | 1.86857900 | 0.02820100 | 0.00772000 |
| C |  | 1.14119200 | -0.23181500 | -1.18546000 |
| N |  | -0.10893600 | -0.53103000 | 1.12282600 |
| H |  | 1.65895900 | -0.13792800 | -2.14383500 |
| H |  | 2.90824700 | 0.33124000 | -0.00569400 |
| C |  | -0.83832800 | -0.70974900 | -0.07964300 |
| N |  | -0.11360100 | -0.58246700 | -1.24935600 |
| O |  | -2.02413600 | -0.96336200 | -0.01277500 |
| H |  | 1.61833100 | 0.00006300 | 2.15797900 |
| H |  | -0.65753800 | -0.64391700 | 1.96736000 |
| C |  | -0.86759300 | 2.45709800 | -0.04984500 |
| H |  | -1.83861300 | 1.99201400 | -0.17983000 |
| H |  | -0.57511100 | 2.83170900 | 0.92504700 |
| H |  | -0.29322500 | 2.74289300 | -0.92356500 |

Thymine\_TS1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.47124900 | 1.34984700 | -0.45255200 |
| C |  | -1.28309800 | 0.25566500 | -0.69848200 |
| C |  | -0.58035800 | -1.00221300 | -0.78266700 |
| N |  | 0.78932400 | 1.11866400 | 0.01325300 |
| H |  | -1.12039600 | -1.86389700 | -1.18772800 |
| H |  | -2.22254800 | 0.38334700 | -1.22556100 |
| C |  | 1.37607300 | -0.15428800 | 0.12328400 |
| N |  | 0.63613100 | -1.21458600 | -0.39750300 |
| O |  | 2.47691300 | -0.26833500 | 0.62279500 |
| H |  | -0.79341600 | 2.38309300 | -0.52947300 |
| H |  | 1.39350900 | 1.88310900 | 0.29018300 |
| C |  | -2.33391800 | -0.28028700 | 1.18492000 |
| H |  | -1.48485500 | -0.35840300 | 1.86065100 |
| H |  | -2.97099000 | 0.59186900 | 1.30828100 |
| H |  | -2.83949300 | -1.21333100 | 0.94402400 |

Thymine\_TS2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.55126600 | 1.18554600 | -0.02565600 |
| C |  | 1.28969800 | 0.02842500 | 0.07005200 |
| C |  | 0.50538100 | -1.17899400 | -0.03028100 |
| N |  | -0.80162400 | 1.11337600 | -0.01892000 |
| H |  | 1.05360000 | -2.12728600 | -0.06743200 |
| C |  | -1.53807800 | -0.09150500 | -0.01840600 |
| N |  | -0.78651400 | -1.25778700 | -0.07285800 |
| O |  | -2.74966700 | -0.04757100 | 0.01299700 |
| H |  | 0.99757700 | 2.17651200 | -0.06166000 |
| H |  | -1.37010100 | 1.95207900 | -0.03487900 |
| C |  | 2.77772100 | 0.00039900 | -0.12134300 |
| H |  | 3.04197100 | -0.08624100 | -1.18272500 |
| H |  | 3.24373700 | 0.91060500 | 0.26954300 |
| H |  | 3.22308300 | -0.84984400 | 0.40593300 |
| H |  | 1.40851200 | -0.24760500 | 1.96349000 |

Thymine\_TS3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.44822000 | -1.40754200 | 0.28618400 |
| C |  | -1.23778600 | -0.41649300 | -0.18037900 |
| C |  | -0.53619000 | 0.76659000 | -0.62842300 |
| N |  | 0.91270600 | -1.25942100 | 0.30211700 |
| H |  | -1.09926600 | 1.48541200 | -1.22742300 |
| C |  | 1.58721700 | -0.11736200 | -0.13702400 |
| N |  | 0.79912600 | 0.86876700 | -0.72428900 |
| O |  | 2.79658600 | -0.03622600 | -0.03852100 |
| H |  | -0.83693100 | -2.35005800 | 0.66418300 |
| H |  | 1.51051200 | -1.98925200 | 0.66875400 |
| C |  | -2.72781500 | -0.43467200 | -0.16379600 |
| H |  | -3.14842900 | -0.24960300 | -1.16010000 |
| H |  | -3.11225900 | -1.39667300 | 0.19014200 |
| H |  | -3.11129000 | 0.34898200 | 0.50320300 |
| O |  | -0.56154500 | 1.79485500 | 0.97280500 |
| H |  | 0.11129000 | 2.47361000 | 0.78279900 |

Thymine\_TS4

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.13442400 | -1.53136700 | -0.03924800 |
| C |  | 1.08868600 | -0.55947000 | -0.00833900 |
| C |  | 0.54796400 | 0.78603300 | 0.06400600 |
| N |  | -1.18147500 | -1.20540500 | 0.00219200 |
| C |  | -1.67959800 | 0.12819900 | -0.01076600 |
| N |  | -0.72792000 | 1.10979400 | -0.04138600 |
| O |  | -2.88229500 | 0.29851300 | -0.01775300 |
| H |  | 0.38399100 | -2.58844700 | -0.08842200 |
| H |  | -1.89856800 | -1.91986800 | -0.02387300 |
| C |  | 2.55663400 | -0.80875800 | -0.03426500 |
| H |  | 3.04657300 | -0.36939600 | 0.84316800 |
| H |  | 2.76821100 | -1.88264100 | -0.04360200 |
| H |  | 3.02002100 | -0.35388500 | -0.91736600 |
| O |  | 1.44537300 | 1.77563800 | -0.09494400 |
| H |  | 0.93675900 | 2.60136800 | -0.13235200 |
| H |  | 0.71550100 | 0.50112100 | 1.71005100 |

Thymine\_TS4a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.24094200 | -1.53624100 | 0.01439200 |
| C |  | 1.17510200 | -0.51995500 | 0.03487700 |
| C |  | 0.65859000 | 0.83529500 | 0.35282100 |
| N |  | -1.07023100 | -1.26895000 | 0.13833400 |
| H |  | 0.93471600 | 0.83227800 | 1.46506500 |
| C |  | -1.65622500 | 0.07534700 | 0.01071800 |
| N |  | -0.76976400 | 1.04249900 | 0.24203900 |
| O |  | -2.83198900 | 0.12042100 | -0.28806900 |
| H |  | 0.52582600 | -2.57322200 | -0.15979700 |
| H |  | -1.75596700 | -2.00879900 | 0.02605500 |
| C |  | 2.62363300 | -0.70180000 | -0.18088500 |
| H |  | 3.19847200 | -0.29465100 | 0.66113000 |
| H |  | 2.90083800 | -1.75044400 | -0.32496600 |
| H |  | 2.92755800 | -0.11051800 | -1.05612600 |
| O |  | 1.10044900 | 1.94553600 | -0.25947100 |
| H |  | -0.25140400 | 2.04697600 | -0.28518300 |

Thymine\_TS5

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.27580200 | -1.48845000 | 0.00000100 |
| C |  | 1.19682200 | -0.48500500 | 0.00000500 |
| C |  | 0.60463000 | 0.81189900 | 0.00000500 |
| N |  | -1.06699100 | -1.25498400 | 0.00000400 |
| C |  | -1.66798900 | 0.02857800 | 0.00000100 |
| N |  | -0.72654600 | 1.02032000 | 0.00000500 |
| O |  | -2.87336700 | 0.14942700 | -0.00000700 |
| H |  | 0.57404500 | -2.53487000 | -0.00000500 |
| H |  | -1.72556200 | -2.02353300 | -0.00000400 |
| C |  | 2.67691600 | -0.67034700 | -0.00000400 |
| H |  | 3.13366400 | -0.20312500 | 0.88002600 |
| H |  | 2.94058400 | -1.73286400 | -0.00018400 |
| H |  | 3.13367300 | -0.20282200 | -0.87986900 |
| O |  | 1.14160200 | 1.97059900 | -0.00000200 |
| H |  | -0.16460600 | 2.19959700 | -0.00000400 |

Thymine\_TS5a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.19343600 | -1.52170100 | -0.00825100 |
| C |  | 1.13718700 | -0.51894400 | 0.02276700 |
| C |  | 0.69037900 | 0.89135300 | 0.10681400 |
| N |  | -1.15250100 | -1.23492900 | 0.03822600 |
| C |  | -1.68772400 | 0.05495100 | -0.01413200 |
| N |  | -0.73816200 | 1.04021600 | -0.00859000 |
| O |  | -2.88596600 | 0.24317400 | -0.06891300 |
| H |  | 0.46880500 | -2.57137800 | -0.03761000 |
| H |  | -1.84418500 | -1.97145700 | 0.00462200 |
| C |  | 2.60257900 | -0.75639400 | -0.08769700 |
| H |  | 3.15155900 | -0.17790500 | 0.66220000 |
| H |  | 2.84690400 | -1.81604000 | 0.03106200 |
| H |  | 2.95933100 | -0.40838100 | -1.06465900 |
| O |  | 1.41276400 | 1.88705500 | -0.08009000 |
| H |  | -1.07717400 | 1.99435200 | -0.03697000 |
| H |  | 0.89987300 | 0.37637700 | 1.30892000 |

Thymine\_TS6a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.21787600 | -1.48302400 | -0.06466200 |
| C |  | -1.13718400 | -0.48398500 | 0.06017400 |
| C |  | -0.65309900 | 0.90546800 | -0.01150200 |
| N |  | 1.13254100 | -1.23707000 | -0.04640100 |
| C |  | 1.68840700 | 0.03208500 | -0.00645500 |
| N |  | 0.73983800 | 1.03590900 | 0.00251400 |
| O |  | 2.88563700 | 0.22774100 | 0.00482000 |
| H |  | -0.50816300 | -2.52853800 | -0.12064300 |
| H |  | 1.80485300 | -1.99165000 | -0.07782100 |
| O |  | -1.36820300 | 1.88520200 | -0.07909300 |
| H |  | 1.10341400 | 1.98317100 | -0.00999100 |
| C |  | -2.60903400 | -0.70709400 | -0.07454400 |
| H |  | -2.86166900 | -1.76135700 | 0.07533900 |
| H |  | -2.95761300 | -0.39894700 | -1.06759400 |
| H |  | -3.15852600 | -0.10612700 | 0.65618300 |
| H |  | -1.09569900 | -0.27266500 | 2.02785200 |

Uracil\_IM1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.13974200 | 1.71875600 | -0.07553800 |
| C |  | 1.06831500 | 1.17896900 | 0.09676300 |
| C |  | 1.15090200 | -0.30153000 | 0.31273800 |
| N |  | -1.27336600 | 0.91431900 | -0.08525800 |
| H |  | 1.13620000 | -0.46921500 | 1.42614200 |
| H |  | 1.98038300 | 1.76220600 | 0.13613000 |
| C |  | -1.23581300 | -0.47270400 | -0.02007100 |
| N |  | 0.03108800 | -1.04388000 | -0.14882200 |
| O |  | -2.24827000 | -1.13934500 | 0.07172700 |
| H |  | -0.31200000 | 2.78143300 | -0.21162200 |
| H |  | -2.19919600 | 1.31651800 | -0.14733900 |
| O |  | 2.34668700 | -0.79531400 | -0.21084900 |
| H |  | 2.24126000 | -1.74770100 | -0.33512600 |

Uracil\_IM2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.12090300 | -1.78689900 | 0.01440400 |
| C |  | 1.11364300 | -1.22253700 | 0.00948200 |
| C |  | 1.12614200 | 0.20284700 | -0.00529700 |
| N |  | -1.22335100 | -1.00191700 | 0.00521200 |
| H |  | 2.02969000 | -1.79870100 | 0.01629700 |
| C |  | -1.18171600 | 0.41758300 | -0.00801500 |
| N |  | 0.07464800 | 0.97241800 | -0.01399800 |
| O |  | -2.22720900 | 1.03396700 | -0.01395800 |
| H |  | -0.28250600 | -2.86095000 | 0.02566100 |
| H |  | -2.15517600 | -1.39791100 | 0.00979000 |
| O |  | 2.32907000 | 0.78141000 | -0.01089100 |
| H |  | 2.17797900 | 1.74078600 | -0.02059100 |
| H |  | -0.16694500 | 4.33428600 | 0.16568900 |

Uracil\_IM2a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.46728300 | 1.56861400 | -0.05151700 |
| C |  | -1.45174300 | 0.71063400 | -0.40747400 |
| C |  | -1.16048800 | -0.75768000 | -0.32052800 |
| N |  | 0.80215100 | 1.13268400 | 0.21197100 |
| H |  | -1.70575700 | -1.36529300 | -1.05921000 |
| H |  | -2.46402300 | 1.04225400 | -0.59476600 |
| C |  | 1.23947600 | -0.17539700 | -0.02601800 |
| N |  | 0.26426700 | -1.00135900 | -0.51097300 |
| O |  | 2.40397000 | -0.48560100 | 0.13735600 |
| H |  | -0.62400100 | 2.64226500 | 0.00449700 |
| H |  | 1.53394000 | 1.77258300 | 0.48828200 |
| O |  | -1.62098500 | -0.90514300 | 0.94819400 |
| H |  | 0.57126100 | -1.96215900 | -0.59697300 |

Uracil\_IM3a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.03218800 | 1.72587200 | -0.17530900 |
| C |  | 1.25190300 | 1.08010800 | 0.18460500 |
| C |  | 1.24929200 | -0.41878100 | -0.00716100 |
| N |  | -1.19362000 | 0.98602000 | -0.01637200 |
| H |  | 1.52044100 | 1.24028500 | 1.24761500 |
| H |  | 2.09104600 | 1.48422200 | -0.39151800 |
| C |  | -1.25235100 | -0.38494600 | 0.01296600 |
| N |  | -0.00393800 | -1.00788500 | -0.03092100 |
| O |  | -2.29091000 | -1.01575600 | 0.06091100 |
| H |  | -0.14492500 | 2.79830200 | -0.26793000 |
| H |  | -2.10127900 | 1.42981700 | -0.06895000 |
| O |  | 2.25946900 | -1.08322900 | -0.08603100 |
| H |  | -0.03079500 | -2.02120500 | -0.07780900 |

Uracil\_PD

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.00417600 | 1.70477500 | 0.00000400 |
| C |  | -1.20185200 | 1.10523100 | -0.00000200 |
| C |  | -1.28803200 | -0.34645700 | -0.00006800 |
| N |  | 1.17249700 | 0.98426000 | 0.00000500 |
| H |  | -2.12535800 | 1.67030200 | 0.00003100 |
| C |  | 1.21808900 | -0.40446200 | -0.00000900 |
| N |  | -0.03297400 | -0.98450500 | -0.00002600 |
| O |  | 2.26001500 | -1.02547200 | 0.00002100 |
| H |  | 0.12114500 | 2.78436000 | 0.00003200 |
| H |  | 2.07549200 | 1.43878100 | 0.00000500 |
| O |  | -2.30961400 | -1.00539200 | 0.00004600 |
| H |  | -0.04543900 | -1.99933900 | 0.00000100 |

Uracil\_RC

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.62549100 | -0.65292700 | 0.53418300 |
| C |  | 1.82135500 | 0.55765600 | -0.06162400 |
| C |  | 0.71477100 | 1.08980500 | -0.76732300 |
| N |  | 0.43340100 | -1.27042200 | 0.40060200 |
| H |  | 0.80698500 | 2.07206300 | -1.23532400 |
| H |  | 2.76051900 | 1.08996100 | 0.02122100 |
| C |  | -0.66433100 | -0.72506800 | -0.30376000 |
| N |  | -0.44751900 | 0.50235700 | -0.90278900 |
| O |  | -1.71274400 | -1.33651500 | -0.33793200 |
| H |  | 2.38156600 | -1.16567400 | 1.12259600 |
| H |  | 0.24537200 | -2.15697200 | 0.85434800 |
| O |  | -1.40030400 | 1.65085900 | 1.06529900 |
| H |  | -2.17495500 | 1.40552200 | 0.52467800 |

Uracil\_TS1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.32347200 | 1.67837800 | 0.19613900 |
| C |  | -1.36980600 | 0.98879000 | -0.30427300 |
| C |  | -1.11832100 | -0.38053800 | -0.66874000 |
| N |  | 0.89689200 | 1.07776700 | 0.30490300 |
| H |  | -1.87108800 | -0.90388600 | -1.25674100 |
| H |  | -2.35894300 | 1.41995700 | -0.38886500 |
| C |  | 1.16554100 | -0.23240100 | -0.11296900 |
| N |  | 0.11612000 | -0.91957200 | -0.71619900 |
| O |  | 2.27781800 | -0.70164600 | 0.02377600 |
| H |  | -0.38359600 | 2.71248200 | 0.52239900 |
| H |  | 1.69184000 | 1.57072500 | 0.69173400 |
| O |  | -1.43057000 | -1.30348500 | 0.95995400 |
| H |  | -1.07093600 | -2.19096400 | 0.77976900 |

Uracil\_TS2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.16806100 | 1.71979600 | -0.05515700 |
| C |  | 1.07484600 | 1.17595100 | -0.02965000 |
| C |  | 1.11483700 | -0.26606500 | 0.06097900 |
| N |  | -1.25507800 | 0.91148100 | 0.00041400 |
| H |  | 1.98783700 | 1.75689600 | -0.04340200 |
| C |  | -1.19746600 | -0.51300300 | -0.00586600 |
| N |  | 0.05862400 | -1.05773500 | -0.03963700 |
| O |  | -2.24050100 | -1.13359800 | -0.00650200 |
| H |  | -0.34770000 | 2.78912300 | -0.11081100 |
| H |  | -2.19369900 | 1.29052700 | -0.02519000 |
| O |  | 2.32378700 | -0.82743800 | -0.10994600 |
| H |  | 2.18193400 | -1.78696900 | -0.14369000 |
| H |  | 1.13557400 | -0.03758200 | 1.70739200 |

Uracil\_TS2a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.13247900 | 1.74238500 | -0.08628500 |
| C |  | 1.13544300 | 1.23112200 | -0.06455400 |
| C |  | 1.26651700 | -0.20797600 | 0.25053000 |
| N |  | -1.21159200 | 0.94350200 | 0.05560300 |
| H |  | 1.58483600 | -0.04414300 | 1.35042700 |
| H |  | 2.01662700 | 1.85520400 | -0.15273600 |
| C |  | -1.16705200 | -0.50806400 | 0.04639000 |
| N |  | 0.06770300 | -0.99323000 | 0.25835300 |
| O |  | -2.20751400 | -1.10015700 | -0.14921800 |
| H |  | -0.32591600 | 2.79782300 | -0.26202300 |
| H |  | -2.14695400 | 1.31582600 | -0.06561800 |
| O |  | 2.11997600 | -1.07277300 | -0.31367100 |
| H |  | 0.96436300 | -1.73797500 | -0.24111400 |

Uracil\_TS3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | C | 0.06335000 | 1.72439700 | 0.00000300 |
|  | C | -1.18863100 | 1.18988800 | -0.00000700 |
|  | C | -1.22046200 | -0.23061700 | -0.00000800 |
|  | N | 1.17737600 | 0.94881400 | 0.00000000 |
|  | H | -2.08663600 | 1.79244500 | 0.00000200 |
|  | C | 1.17630500 | -0.47418300 | -0.00000400 |
|  | N | -0.09345600 | -0.97612100 | -0.00002400 |
|  | O | 2.21966100 | -1.08762900 | 0.00001000 |
|  | H | 0.23356700 | 2.79758900 | 0.00002000 |
|  | H | 2.10092100 | 1.36347000 | 0.00001800 |
|  | O | -2.18558000 | -1.06296200 | 0.00001800 |
|  | H | -1.09130700 | -1.81453600 | 0.00000600 |

Uracil\_TS3a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | C | -0.07094900 | 1.72863300 | -0.05414500 |
|  | C | 1.16190300 | 1.13158900 | -0.03805200 |
|  | C | 1.29439400 | -0.33751100 | 0.07842400 |
|  | N | -1.21598300 | 0.96893100 | 0.01134900 |
|  | H | 2.08641700 | 1.69503600 | -0.08822300 |
|  | C | -1.23340800 | -0.43068200 | 0.00400400 |
|  | N | 0.01150800 | -0.99923800 | 0.03842400 |
|  | O | -2.27718800 | -1.04810800 | -0.03412100 |
|  | H | -0.20074300 | 2.80467400 | -0.08682000 |
|  | H | -2.13167400 | 1.39465300 | -0.03666900 |
|  | O | 2.31992500 | -1.00876900 | -0.13536700 |
|  | H | 0.04202400 | -2.01182600 | 0.02250000 |
|  | H | 1.38176400 | 0.23245400 | 1.25532000 |

Uracil\_TS4a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | C | 0.00639300 | 1.69156100 | -0.10841800 |
|  | C | 1.20461900 | 1.05824400 | -0.01704300 |
|  | C | 1.24922200 | -0.40494300 | -0.04375100 |
|  | N | -1.17390700 | 0.99757000 | -0.04951200 |
|  | H | 2.13984400 | 1.58969800 | -0.14432700 |
|  | C | -1.25394800 | -0.38849400 | 0.01401100 |
|  | N | -0.01863800 | -1.00454200 | 0.01618300 |
|  | O | -2.31092600 | -0.98120100 | 0.05361300 |
|  | H | -0.08254400 | 2.77058400 | -0.18263300 |
|  | H | -2.06737700 | 1.47025100 | -0.07973100 |
|  | O | 2.25281200 | -1.08399300 | -0.10564700 |
|  | H | -0.03612500 | -2.01925700 | 0.02537500 |
|  | H | 1.62120300 | 1.02087200 | 1.96210200 |

RC(A2: H2CCCN→A1: HCCHCN)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.81579400 | -0.00004400 | -0.00012900 |
| C |  | 0.52200000 | 0.00001600 | -0.00004600 |
| C |  | 1.82485600 | -0.00000500 | 0.00003600 |
| N |  | -1.99859600 | 0.00002400 | 0.00009400 |
| H |  | 2.40192900 | 0.92808800 | 0.00008800 |
| H |  | 2.40186900 | -0.92806000 | 0.00008800 |

TS(A2: H2CCCN→A1: HCCHCN)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.79090600 | -0.03051900 | -0.00008200 |
| C |  | 0.57722700 | 0.17884200 | -0.00032800 |
| C |  | 1.83898100 | -0.09895900 | -0.00008500 |
| N |  | -1.96037600 | -0.07739100 | 0.00015000 |
| H |  | 2.58829000 | -0.89056100 | 0.00089700 |
| H |  | 1.38252900 | 1.13611300 | 0.00102700 |

PD(A2: H2CCCN→A1: HCCHCN)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.69088900 | 0.09389400 | -0.00016200 |
| C |  | -0.67907000 | 0.51204700 | -0.00037300 |
| C |  | -1.67524100 | -0.35218900 | 0.00005300 |
| N |  | 1.80514400 | -0.24044700 | 0.00014100 |
| H |  | -1.79480400 | -1.42763000 | 0.00048000 |
| H |  | -0.86066900 | 1.58824600 | 0.00143100 |

RC(A4: H2NCO→A3:HNCHO)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.15990700 | -0.40974900 | -0.00000300 |
| N |  | 1.08203600 | 0.09391900 | -0.00001300 |
| O |  | -1.21659500 | 0.15282300 | 0.00000400 |
| H |  | 1.87948900 | -0.52031600 | 0.00005400 |
| H |  | 1.23846300 | 1.09879400 | 0.00002300 |

TS(A4: H2NCO→A3:HNCHO)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.09837600 | 0.35411800 | -0.00573800 |
| N |  | 1.15623600 | -0.21506600 | -0.12704100 |
| O |  | -1.14549200 | -0.24439900 | 0.02552400 |
| H |  | 1.70132400 | -0.13516600 | 0.73938200 |
| H |  | -0.04079000 | 1.47111200 | -0.01986200 |

PD(A4: H2NCO→A3:HNCHO)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.11049300 | 0.23649700 | 0.12348600 |
| N |  | 1.14299800 | -0.24572400 | -0.10015300 |
| O |  | -1.23732400 | -0.10743500 | -0.01997500 |
| H |  | 1.79132200 | 0.16302400 | 0.58036800 |
| H |  | 0.76923700 | 0.99753600 | -0.46041100 |

RC(B1: HNCHO→B4: H2NCO)/RC(B2: HNCHO→B4: H2NCO)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.11049300 | 0.23649700 | 0.12348600 |
| N |  | 1.14299800 | -0.24572400 | -0.10015300 |
| O |  | -1.23732400 | -0.10743500 | -0.01997500 |
| H |  | 1.79132200 | 0.16302400 | 0.58036800 |
| H |  | 0.76923700 | 0.99753600 | -0.46041100 |

TS(B1: HNCHO→B4: H2NCO)/TS(B2: HNCHO→B4: H2NCO)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.09837600 | 0.35411800 | -0.00573800 |
| N |  | 1.15623600 | -0.21506600 | -0.12704100 |
| O |  | -1.14549200 | -0.24439900 | 0.02552400 |
| H |  | 1.70132400 | -0.13516600 | 0.73938200 |
| H |  | -0.04079000 | 1.47111200 | -0.01986200 |

PD(B1: HNCHO→B4: H2NCO)/PD(B2: HNCHO→B4: H2NCO)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.15990700 | -0.40974900 | -0.00000300 |
| N |  | 1.08203600 | 0.09391900 | -0.00001300 |
| O |  | -1.21659500 | 0.15282300 | 0.00000400 |
| H |  | 1.87948900 | -0.52031600 | 0.00005400 |
| H |  | 1.23846300 | 1.09879400 | 0.00002300 |

RC’(B1: HCCHCN→B4: H2CCCN)/RC(B3: HCCHCN→B4: H2CCCN)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.69088900 | 0.09389400 | -0.00016200 |
| C |  | -0.67907000 | 0.51204700 | -0.00037300 |
| C |  | -1.67524100 | -0.35218900 | 0.00005300 |
| N |  | 1.80514400 | -0.24044700 | 0.00014100 |
| H |  | -1.79480400 | -1.42763000 | 0.00048000 |
| H |  | -0.86066900 | 1.58824600 | 0.00143100 |

TS’(B1: HCCHCN→B4: H2CCCN)/TS(B3: HCCHCN→B4: H2CCCN)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.79090600 | -0.03051900 | -0.00008200 |
| C |  | 0.57722700 | 0.17884200 | -0.00032800 |
| C |  | 1.83898100 | -0.09895900 | -0.00008500 |
| N |  | -1.96037600 | -0.07739100 | 0.00015000 |
| H |  | 2.58829000 | -0.89056100 | 0.00089700 |
| H |  | 1.38252900 | 1.13611300 | 0.00102700 |

PD(B1: HCCHCN→B4: H2CCCN)/PD(B3: HCCHCN→B4: H2CCCN)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.81579400 | -0.00004400 | -0.00012900 |
| C |  | 0.52200000 | 0.00001600 | -0.00004600 |
| C |  | 1.82485600 | -0.00000500 | 0.00003600 |
| N |  | -1.99859600 | 0.00002400 | 0.00009400 |
| H |  | 2.40192900 | 0.92808800 | 0.00008800 |
| H |  | 2.40186900 | -0.92806000 | 0.00008800 |

RC(C1: NCHO→C2: HNCO)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.09813100 | 0.57724100 | -0.00001200 |
| N |  | -0.88988100 | -0.40201000 | 0.00000300 |
| O |  | 0.86454500 | -0.28924400 | 0.00000200 |
| H |  | -0.09840700 | 1.66457300 | 0.00003300 |

TS(C1: NCHO→C2: HNCO)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.04448700 | 0.02319700 | 0.00000000 |
| N |  | 1.15894500 | -0.11953600 | 0.00000000 |
| O |  | -1.21464100 | 0.01334700 | 0.00000000 |
| H |  | 1.87142800 | 0.59079700 | 0.00000000 |

PD(C1: NCHO→C2: HNCO)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.00000000 | 0.35256800 | 0.00000000 |
| N |  | 1.18213100 | -0.16108200 | 0.00000000 |
| O |  | -1.04737000 | -0.30868600 | 0.00000000 |
| H |  | 0.10403800 | 1.48165800 | 0.00000000 |

RC(C3: CCHCN→C2: HCCCH)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.64411600 | 0.06174600 | -0.00000600 |
| C |  | -0.74289200 | 0.33696200 | -0.00002300 |
| C |  | -1.79980300 | -0.44247300 | 0.00001000 |
| N |  | 1.78513800 | -0.15942900 | 0.00000800 |
| H |  | -1.10448700 | 1.37859300 | 0.00006000 |

TS(C3: CCHCN→C2: HCCCH)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.70061300 | -0.00918300 | 0.00000200 |
| C |  | -0.69079800 | -0.00673900 | 0.00000100 |
| C |  | -1.95551400 | -0.13887700 | -0.00000100 |
| N |  | 1.86391700 | -0.01515200 | -0.00000100 |
| H |  | -1.37322400 | 1.03485400 | -0.00000100 |

PD(C3: CCHCN→C2: HCCCH)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.02061100 | -0.09010200 | 0.73488500 |
| C |  | -0.01767200 | 0.07751200 | -0.63014500 |
| C |  | -0.05122100 | 0.22456300 | -1.82896100 |
| N |  | 0.05293500 | -0.23232300 | 1.89064300 |
| H |  | -0.08085400 | 0.35442300 | -2.88917600 |

### Molecular coordinates were optimized at MP2/6-311++G(2d,2p) level.

0\_IM1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| N |  | -1.80560600 | 1.10716000 | 0.23227100 |
| O |  | -2.15516100 | -1.09508100 | -0.07422400 |
| H |  | -1.59876000 | -1.86540300 | -0.27077300 |
| H |  | -2.78708400 | 1.26028100 | 0.36216100 |
| H |  | -1.07850600 | 1.82385800 | 0.26439700 |
| C |  | 0.76103700 | 0.75018300 | -0.10511300 |
| C |  | 2.18815500 | 0.46530600 | -0.24635100 |
| C |  | 2.77311300 | -0.61791200 | 0.30300700 |
| N |  | 0.00197900 | -0.34963000 | -0.21125000 |
| H |  | 2.16945500 | -1.37900100 | 0.77543800 |
| H |  | 3.84742900 | -0.72833400 | 0.32993500 |
| H |  | 2.80812900 | 1.25188600 | -0.65715200 |

0\_IM2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.75849600 | -0.63824800 | -0.23043900 |
| C |  | 2.21373600 | -0.46282100 | -0.21645200 |
| C |  | 2.81769600 | 0.63257500 | 0.26649200 |
| N |  | -0.04420000 | 0.32125700 | 0.06121900 |
| H |  | 2.23221200 | 1.44538600 | 0.67004100 |
| H |  | 3.89288400 | 0.72040900 | 0.26483100 |
| H |  | 2.80280300 | -1.28185400 | -0.60460700 |
| C |  | -1.42281800 | -0.00119900 | 0.05828800 |
| N |  | -1.88334000 | -1.15565700 | 0.31784700 |
| O |  | -2.18904200 | 1.08752600 | -0.21603800 |
| H |  | 0.35801900 | -1.61851100 | -0.48745500 |
| H |  | -1.58461900 | 1.83197500 | -0.31805900 |
| H |  | -2.89884300 | -1.13865500 | 0.28275100 |

0\_IM3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.00028700 | 1.27433700 | -0.05557000 |
| C |  | -1.78906500 | 0.18663500 | -0.05531500 |
| C |  | -1.18223000 | -1.16857000 | 0.17906300 |
| N |  | 0.39569100 | 1.23414700 | 0.11348100 |
| H |  | -1.67727100 | -1.92794400 | -0.42097900 |
| H |  | -1.27020300 | -1.46593600 | 1.23038500 |
| H |  | -2.85635000 | 0.27886200 | -0.18298600 |
| C |  | 0.90268400 | 0.05496000 | -0.00751600 |
| N |  | 0.21904800 | -1.09698800 | -0.23569500 |
| O |  | 2.24290000 | -0.12699100 | 0.02458600 |
| H |  | -1.41231800 | 2.26219200 | -0.19844800 |
| H |  | 2.61382700 | 0.76295100 | 0.07901100 |
| H |  | 0.76933000 | -1.93848000 | -0.21214500 |

0\_IM4a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.12040900 | -1.29200500 | 0.00001100 |
| C |  | 1.80429700 | -0.08276100 | -0.00002000 |
| C |  | 1.02814000 | 1.07132500 | -0.00001300 |
| N |  | -0.21751400 | -1.35268500 | 0.00001700 |
| H |  | 1.47949200 | 2.05448500 | -0.00002900 |
| H |  | 2.88174200 | -0.04194700 | -0.00005700 |
| C |  | -0.85270300 | -0.17612900 | 0.00004300 |
| N |  | -0.31002100 | 1.04063600 | 0.00002500 |
| O |  | -2.20048200 | -0.20754500 | -0.00003700 |
| H |  | 1.64209700 | -2.23916600 | -0.00001700 |
| H |  | -2.44494700 | -1.14103300 | -0.00004500 |
| H |  | -0.53621900 | 3.69060100 | -0.00002700 |
| H |  | -0.32642200 | 4.39918300 | 0.00004200 |

0\_PD

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.07171900 | 1.16721700 | 0.00002900 |
| C |  | 1.77808500 | 0.00155500 | 0.00002300 |
| C |  | 1.01513800 | -1.19645600 | 0.00003000 |
| N |  | -0.28039400 | 1.11010900 | -0.00003800 |
| H |  | 1.53246300 | -2.14936000 | 0.00005800 |
| H |  | 2.85425200 | -0.00311900 | 0.00006100 |
| C |  | -1.03546500 | -0.08318100 | -0.00018200 |
| N |  | -0.29559300 | -1.26392200 | -0.00001300 |
| O |  | -2.25255600 | -0.02627900 | 0.00009500 |
| H |  | 1.51949700 | 2.14915300 | 0.00008300 |
| H |  | -0.83070900 | 1.95543300 | -0.00000200 |

0\_RC

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.65331800 | -0.31713600 | -0.00088900 |
| N |  | 1.64775600 | 1.00104100 | 0.00035100 |
| O |  | 2.95275500 | -0.71970000 | 0.00017300 |
| H |  | 2.93843100 | -1.67766600 | -0.00093000 |
| H |  | 2.50501500 | 1.53921700 | 0.00205100 |
| H |  | 0.76562500 | 1.48622100 | 0.00003700 |
| C |  | -1.81975200 | 0.75537500 | -0.00015500 |
| C |  | -2.44033500 | -0.53659500 | 0.00010200 |
| C |  | -1.70176000 | -1.65449000 | 0.00029100 |
| N |  | -1.31182900 | 1.81256200 | -0.00022600 |
| H |  | -0.62113800 | -1.59608900 | 0.00006500 |
| H |  | -2.19034400 | -2.61665400 | 0.00038500 |
| H |  | -3.51993900 | -0.55557500 | 0.00004500 |

0\_RCa

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.15963000 | 0.38953100 | 0.00006600 |
| N |  | -1.08537500 | -0.15937600 | 0.00001800 |
| O |  | 1.19857200 | -0.24606400 | -0.00011900 |
| H |  | 0.13579000 | 1.48769600 | 0.00025600 |
| H |  | -1.18118100 | -1.15826500 | -0.00009000 |
| H |  | -1.90334300 | 0.41752700 | 0.00026400 |

0\_TS1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.34661500 | -0.10492500 | 0.34145100 |
| N |  | 2.22201000 | 0.93411000 | 0.45429600 |
| O |  | 2.05335500 | -1.19452900 | -0.09770100 |
| H |  | 1.47052100 | -1.95528500 | -0.04691500 |
| H |  | 3.03359200 | 0.94899900 | -0.15062300 |
| H |  | 1.82898600 | 1.83047600 | 0.66890000 |
| C |  | -1.05052600 | 0.40314500 | -0.65512600 |
| C |  | -2.30751500 | 0.50715800 | -0.01025300 |
| C |  | -2.98184400 | -0.57198300 | 0.44098300 |
| N |  | 0.12879500 | 0.18805700 | -0.69910100 |
| H |  | -2.58275400 | -1.56833100 | 0.32872600 |
| H |  | -3.94345900 | -0.45375900 | 0.91435600 |
| H |  | -2.72974300 | 1.49860100 | 0.07846600 |

0\_TS2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.35365300 | -0.06586500 | 0.00202400 |
| N |  | -1.64856400 | 1.16984100 | 0.23778400 |
| O |  | -2.25810800 | -1.02618800 | -0.05770300 |
| H |  | -1.75250900 | -1.83099900 | -0.25519600 |
| H |  | -2.58742300 | 1.50334000 | 0.36224700 |
| H |  | -0.60208200 | 1.62579400 | 0.17168400 |
| C |  | 0.72047800 | 0.65703300 | -0.12583900 |
| C |  | 2.16190600 | 0.44731300 | -0.24133900 |
| C |  | 2.79176100 | -0.61587700 | 0.29243400 |
| N |  | -0.03054100 | -0.42551300 | -0.20687200 |
| H |  | 2.22294800 | -1.40543300 | 0.76170200 |
| H |  | 3.86949700 | -0.68791900 | 0.29822000 |
| H |  | 2.74521700 | 1.25879600 | -0.65710000 |

0\_TS3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.90511000 | -1.28121100 | 0.01402300 |
| C |  | -1.79752900 | -0.25631200 | -0.35723800 |
| C |  | -1.60550100 | 0.98239300 | 0.21605900 |
| N |  | 0.35146400 | -1.07111100 | 0.38501700 |
| H |  | -1.31700200 | 1.02825200 | 1.25163800 |
| H |  | -2.12168400 | 1.85387100 | -0.16315500 |
| H |  | -2.49568100 | -0.41304700 | -1.16712700 |
| C |  | 0.95602500 | 0.12583000 | 0.08317600 |
| N |  | 0.43864500 | 1.31474600 | 0.01590600 |
| O |  | 2.27517300 | -0.03127700 | -0.21820800 |
| H |  | -1.18354000 | -2.32603400 | -0.08292100 |
| H |  | 2.43554200 | -0.98228400 | -0.16775800 |
| H |  | 1.06290500 | 1.95981800 | -0.46759900 |

0\_TS4a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.97215000 | -1.30873600 | 0.07305100 |
| C |  | 1.78716500 | -0.19392900 | -0.06087300 |
| C |  | 1.17547800 | 1.05797400 | -0.10068800 |
| N |  | -0.37399500 | -1.25926400 | 0.08206500 |
| H |  | 1.65775900 | 2.00596500 | -0.22621700 |
| H |  | 0.72770400 | 2.69234800 | 1.26803800 |
| H |  | 2.85931400 | -0.28667000 | -0.09890200 |
| C |  | -0.90035900 | -0.04581200 | -0.03744900 |
| N |  | -0.18497900 | 1.06706800 | -0.13022100 |
| O |  | -2.22480800 | 0.11664800 | -0.03468300 |
| H |  | 1.40059900 | -2.29704700 | 0.16761300 |
| H |  | -2.60769000 | -0.76091400 | 0.09536000 |
| H |  | -0.53300300 | 2.00153100 | 0.16441900 |

0\_TS5a

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.92343300 | 1.26714400 | 0.00000600 |
| C |  | 1.74863700 | 0.15167800 | -0.00000400 |
| C |  | 1.14041800 | -1.11137400 | -0.00001000 |
| N |  | -0.39286800 | 1.05755600 | 0.00000800 |
| H |  | 1.75800700 | -2.00026600 | -0.00001700 |
| H |  | 2.82084200 | 0.25289700 | -0.00000600 |
| C |  | -0.92006400 | -0.20994000 | 0.00000100 |
| N |  | -0.17937800 | -1.32984500 | -0.00000800 |
| O |  | -2.19440100 | -0.05557500 | 0.00000600 |
| H |  | 1.28245900 | 2.28543100 | 0.00001100 |
| H |  | -1.65492200 | 1.22751800 | 0.00001200 |

0\_TSa

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.07624000 | -0.47955200 | 0.00004500 |
| N |  | 1.11345600 | 0.11136800 | -0.00013700 |
| O |  | -1.15262000 | 0.29094200 | 0.00011700 |
| H |  | -1.23090000 | -0.92177700 | 0.00002600 |
| H |  | 1.16009900 | 1.12221700 | -0.00018700 |
| H |  | 1.95500900 | -0.43024100 | -0.00009000 |

B4\_IM1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.81585100 | -0.45637600 | -0.00065200 |
| C |  | -2.05905800 | -0.18390200 | 0.00002000 |
| C |  | -3.32715400 | 0.19301300 | 0.00086300 |
| N |  | 0.36784300 | -0.84981600 | -0.00122700 |
| H |  | -3.59804200 | 1.24156900 | 0.00230600 |
| H |  | -4.13116700 | -0.53233700 | 0.00014900 |
| C |  | 1.39819400 | 0.18060300 | -0.00020400 |
| N |  | 2.61446300 | -0.41596900 | 0.00125900 |
| O |  | 1.19486400 | 1.37608500 | -0.00058200 |
| H |  | 3.43604800 | 0.15730300 | 0.00134200 |
| H |  | 2.68132000 | -1.41474400 | 0.00046900 |

B4\_IM2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.82247100 | -0.42673800 | 0.02525500 |
| C |  | 2.06968800 | -0.18434400 | 0.00013500 |
| C |  | 3.33560400 | 0.20087200 | -0.03351500 |
| N |  | -0.36254200 | -0.81930400 | 0.05800200 |
| H |  | 4.14478800 | -0.51698700 | 0.01243400 |
| H |  | 3.59635800 | 1.24936500 | -0.10803700 |
| C |  | -1.41061700 | 0.14581400 | 0.00698000 |
| N |  | -1.22060600 | 1.39835100 | 0.03078700 |
| O |  | -2.62262600 | -0.45888300 | -0.05804800 |
| H |  | -2.46664200 | -1.41029400 | -0.04907900 |
| H |  | -2.11432800 | 1.88202400 | -0.00558600 |

B4\_IM3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.77077100 | 1.33434900 | 0.00006600 |
| C |  | -1.74844800 | 0.58468100 | 0.00008400 |
| C |  | -1.56717600 | -0.88827600 | 0.00005500 |
| N |  | 0.59071900 | 1.28473000 | -0.00008100 |
| H |  | -1.97133700 | -1.37929500 | 0.88372000 |
| H |  | -1.97145500 | -1.37930100 | -0.88355300 |
| C |  | 0.83205800 | -0.00964700 | -0.00028900 |
| N |  | -0.07064300 | -1.02556900 | -0.00009200 |
| O |  | 2.10656500 | -0.44807700 | 0.00017600 |
| H |  | 2.64830200 | 0.35192300 | 0.00028200 |
| H |  | 0.32745700 | -1.94947700 | -0.00014400 |

B4\_IM4

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.20008700 | -0.40621200 | 0.03362200 |
| C |  | -2.43796100 | -0.83261800 | -0.13440700 |
| C |  | -0.96764900 | 1.12053800 | 0.12675800 |
| N |  | 0.03866300 | -1.08720600 | 0.09690300 |
| H |  | -1.55466400 | 1.69564000 | -0.57857400 |
| H |  | -1.14443400 | 1.47615300 | 1.14023600 |
| C |  | 0.91458700 | -0.14224400 | -0.01747800 |
| N |  | 0.46572900 | 1.14318300 | -0.20663500 |
| O |  | 2.23738500 | -0.32631400 | -0.01255500 |
| H |  | 2.38061700 | -1.27558300 | 0.08956400 |
| H |  | 1.03531100 | 1.88568300 | 0.16637400 |

B4\_IM5

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.02317700 | -0.74453200 | -0.27165100 |
| C |  | 1.99260200 | -0.26851000 | 0.49175300 |
| C |  | 1.20360500 | 0.72809600 | -0.34927300 |
| N |  | -0.30133500 | -1.18390700 | -0.27411400 |
| H |  | 2.45665000 | -0.39563200 | 1.45469500 |
| H |  | 1.60424000 | 1.29729800 | -1.17644900 |
| C |  | -0.90446000 | -0.04513200 | -0.02482400 |
| N |  | -0.13367000 | 1.08332200 | 0.10670700 |
| O |  | -2.22187000 | 0.07517100 | 0.19958000 |
| H |  | -2.58396900 | -0.81813300 | 0.15724900 |
| H |  | -0.54647000 | 1.99966600 | 0.06367400 |

B4\_IM6

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.01811200 | -0.72440600 | 0.19847300 |
| C |  | -1.99458300 | -0.17035100 | -0.49492100 |
| C |  | -1.13425400 | 0.72971600 | 0.37478700 |
| N |  | 0.28384000 | -1.14507700 | 0.31797700 |
| H |  | -2.65883700 | -0.24869300 | -1.33600900 |
| H |  | -1.48116500 | 1.19763500 | 1.28612400 |
| C |  | 1.06789400 | 0.03330600 | -0.01084500 |
| N |  | 0.19537700 | 1.10353300 | -0.07494200 |
| O |  | 2.25971100 | 0.01189200 | -0.22859800 |
| H |  | 0.60831800 | -1.99610100 | -0.11354500 |
| H |  | 0.57380600 | 2.03324100 | -0.11399200 |

B4\_IM7

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.07603200 | -1.36658100 | -0.00027200 |
| C |  | 1.79409900 | -0.12106200 | -0.00033300 |
| C |  | 1.15968700 | 1.08434700 | -0.00011300 |
| N |  | -0.26142000 | -1.16329600 | 0.00000700 |
| H |  | 2.87171200 | -0.13543700 | -0.00054600 |
| H |  | 1.66610300 | 2.03939700 | -0.00010100 |
| C |  | -1.01209500 | 0.02212900 | 0.00015800 |
| N |  | -0.20370700 | 1.14114000 | 0.00016100 |
| O |  | -2.22955200 | 0.06163900 | 0.00031000 |
| H |  | -0.86074800 | -1.97782800 | 0.00010100 |
| H |  | -0.69110300 | 2.02285300 | 0.00025100 |

B4\_PD

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.07171100 | 1.16720900 | -0.00005200 |
| C |  | 1.77808700 | 0.00150200 | -0.00041700 |
| C |  | 1.01507000 | -1.19643900 | -0.00007300 |
| N |  | -0.28029700 | 1.11016100 | 0.00030500 |
| H |  | 1.53244100 | -2.14932700 | -0.00026800 |
| H |  | 2.85425500 | -0.00330500 | -0.00079800 |
| C |  | -1.03550200 | -0.08337600 | -0.00002700 |
| N |  | -0.29563200 | -1.26384300 | 0.00013000 |
| O |  | -2.25253500 | -0.02618400 | 0.00012400 |
| H |  | -0.83072800 | 1.95541000 | 0.00047700 |
| H |  | 1.51962400 | 2.14910200 | -0.00003600 |

B4\_RC

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -5.12970500 | -0.77893500 | 0.02967400 |
| C |  | -4.49987300 | 0.50718300 | -0.03051400 |
| C |  | -4.89710500 | 1.71607900 | -0.07565000 |
| N |  | -5.59928600 | -1.80273700 | 0.07737700 |
| H |  | -5.95634500 | 1.94998700 | -0.07287400 |
| H |  | -4.19970500 | 2.53932000 | -0.11751500 |
| C |  | 5.57257900 | -0.27397200 | -0.02375600 |
| N |  | 5.77693300 | 1.04946800 | 0.11413500 |
| O |  | 6.36640900 | -1.16658700 | -0.11008500 |
| H |  | 6.71027500 | 1.42490700 | 0.15951900 |
| H |  | 4.99560300 | 1.66923900 | 0.17242400 |

B4\_TS1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.83493800 | -0.47166700 | 0.00001100 |
| C |  | 2.07117200 | -0.17655200 | 0.00000000 |
| C |  | 3.31585700 | 0.27357400 | -0.00001600 |
| N |  | -0.33039300 | -0.92806800 | 0.00002400 |
| H |  | 3.52444300 | 1.33620400 | -0.00004700 |
| H |  | 4.15969800 | -0.40464800 | 0.00000100 |
| C |  | -1.38763400 | -0.00192800 | 0.00000400 |
| N |  | -2.65554000 | -0.31511300 | -0.00002800 |
| O |  | -1.27575700 | 1.28551800 | 0.00001700 |
| H |  | -2.58034800 | 1.00859600 | -0.00001500 |
| H |  | -3.00219800 | -1.26258500 | -0.00004000 |

B4\_TS2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.81767700 | -1.09924600 | 0.03978900 |
| C |  | -1.93433600 | -0.60038200 | -0.30571000 |
| C |  | -1.89932200 | 0.74055300 | 0.08085900 |
| N |  | 0.44487300 | -1.17372300 | 0.17976700 |
| H |  | -2.16668700 | 1.50824800 | -0.63437500 |
| H |  | -1.94900000 | 1.04112600 | 1.11879600 |
| C |  | 0.95274000 | 0.10182300 | 0.02712000 |
| N |  | 0.21646100 | 1.16550400 | 0.04854300 |
| O |  | 2.29267100 | 0.17165100 | -0.10583200 |
| H |  | 2.61082000 | -0.73936200 | -0.13974200 |
| H |  | 0.72573600 | 2.01782700 | -0.14854700 |

B4\_TS3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.06196400 | -0.81177500 | 0.01557200 |
| C |  | -2.28856600 | -0.54757000 | -0.25311500 |
| C |  | -1.16019200 | 0.94274800 | 0.23061300 |
| N |  | 0.24514100 | -1.17848900 | 0.13956200 |
| H |  | -1.80829100 | 1.58906700 | -0.34097000 |
| H |  | -1.26441000 | 1.10421600 | 1.30051600 |
| C |  | 0.92071100 | -0.07929100 | -0.01028100 |
| N |  | 0.22940800 | 1.07859000 | -0.21732800 |
| O |  | 2.25132300 | -0.00785400 | -0.03229100 |
| H |  | 2.58101800 | -0.91385700 | 0.02237900 |
| H |  | 0.69932200 | 1.95803000 | -0.07596400 |

B4\_TS4

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.06022700 | -0.69897800 | 0.22579500 |
| C |  | -2.08171800 | -0.50205200 | -0.61920800 |
| C |  | -1.14186700 | 0.78075300 | 0.32954700 |
| N |  | 0.26196000 | -1.16196600 | 0.29395800 |
| H |  | -2.23177400 | 0.79737400 | -0.39355700 |
| H |  | -1.48680400 | 1.22003600 | 1.25879100 |
| C |  | 0.90949500 | -0.06320800 | 0.02323800 |
| N |  | 0.16370800 | 1.09298600 | -0.14570600 |
| O |  | 2.22782800 | 0.02887100 | -0.17691000 |
| H |  | 2.57627400 | -0.86983400 | -0.12542100 |
| H |  | 0.58591200 | 2.00523200 | -0.11852700 |

B4\_TS5

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.93498200 | -0.80005300 | -0.23023400 |
| C |  | 1.93037000 | -0.36584300 | 0.52233500 |
| C |  | 1.24048000 | 0.66079200 | -0.33976400 |
| N |  | -0.41278600 | -1.05407200 | -0.36581900 |
| H |  | 2.51124400 | -0.52923700 | 1.41205600 |
| H |  | 1.68269400 | 1.14850300 | -1.19676600 |
| C |  | -0.95962900 | 0.15076600 | -0.03791300 |
| N |  | -0.08914200 | 1.17517500 | 0.04890600 |
| O |  | -2.19187400 | -0.02507400 | 0.27541400 |
| H |  | -1.65987000 | -1.25789400 | 0.04889100 |
| H |  | -0.36279300 | 2.11752700 | 0.26435600 |

B4\_TS6

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.03214300 | 0.95587800 | 0.01244500 |
| C |  | 1.95417500 | 0.10088400 | -0.40863400 |
| C |  | 1.15238600 | -0.83583500 | 0.32693100 |
| N |  | -0.27434200 | 1.11395500 | 0.28655700 |
| H |  | 2.93647000 | 0.17651000 | -0.84090100 |
| H |  | 1.38668000 | -1.14501300 | 1.34197300 |
| C |  | -1.07544300 | -0.04434600 | -0.00765100 |
| N |  | -0.18702100 | -1.09687200 | -0.09108500 |
| O |  | -2.27063300 | -0.02494000 | -0.19656800 |
| H |  | -0.72771400 | 2.01006500 | 0.21288300 |
| H |  | -0.58038800 | -2.02111100 | -0.04826000 |

B4\_TS7

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.08732200 | 1.26919500 | -0.01357000 |
| C |  | 1.82332200 | 0.04909600 | 0.05014800 |
| C |  | 1.11717000 | -1.11652100 | 0.00014800 |
| N |  | -0.27229400 | 1.19626700 | -0.08016500 |
| H |  | 1.57545800 | -2.09570400 | -0.00158900 |
| H |  | 2.89826900 | 0.03451300 | 0.10930900 |
| C |  | -1.05511400 | 0.02865500 | -0.00630000 |
| N |  | -0.24616100 | -1.10917600 | -0.04510100 |
| O |  | -2.26514600 | -0.02699500 | 0.06117600 |
| H |  | 0.19325800 | 2.26632800 | 0.14370700 |
| H |  | -0.75283100 | -1.98136300 | -0.04652700 |

C2\_IM1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.75373900 | -1.19170200 | -0.04457500 |
| C |  | -1.77463400 | -0.40395900 | -0.34357900 |
| C |  | -1.29810500 | 0.93209700 | 0.24132100 |
| N |  | 0.38722100 | -1.22979400 | 0.42329800 |
| H |  | -1.77640400 | 1.72942500 | -0.32118900 |
| H |  | -1.53658300 | 1.04760900 | 1.29749300 |
| H |  | -2.49375300 | -0.51546900 | -1.13138300 |
| C |  | 1.06887500 | 0.02270800 | -0.00684000 |
| N |  | 0.16046900 | 1.05613600 | 0.03386800 |
| O |  | 2.24547900 | 0.10455700 | -0.24711400 |
| H |  | 0.55469600 | 1.96272400 | -0.14613800 |

C2\_IM2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.07611400 | -1.36654300 | 0.00001700 |
| C |  | 1.79409500 | -0.12102100 | -0.00005500 |
| C |  | 1.15962100 | 1.08438900 | 0.00000300 |
| N |  | -0.26140500 | -1.16329600 | 0.00003900 |
| H |  | 1.66603100 | 2.03943700 | 0.00001400 |
| H |  | -0.86060100 | -1.97790900 | -0.00001200 |
| H |  | 2.87169900 | -0.13537500 | -0.00012400 |
| C |  | -1.01210400 | 0.02203100 | 0.00006400 |
| N |  | -0.20371900 | 1.14112500 | 0.00003000 |
| O |  | -2.22955200 | 0.06163900 | -0.00007400 |
| H |  | -0.69119900 | 2.02279000 | 0.00005400 |

C2\_PD

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.01493100 | -1.19649900 | 0.00020100 |
| C |  | 1.77806500 | 0.00161300 | 0.00041300 |
| C |  | 1.07171500 | 1.16716900 | 0.00008700 |
| N |  | -0.29551700 | -1.26386800 | -0.00002800 |
| H |  | 1.51950100 | 2.14922700 | 0.00011900 |
| H |  | 1.53256600 | -2.14942600 | 0.00052700 |
| H |  | 2.85430100 | -0.00326100 | 0.00077100 |
| C |  | -1.03541500 | -0.08318200 | -0.00020500 |
| N |  | -0.28046500 | 1.11016100 | -0.00024500 |
| O |  | -2.25242200 | -0.02633400 | -0.00026100 |
| H |  | -0.83089500 | 1.95548300 | -0.00039700 |

C2\_RC

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.83793800 | 0.85592000 | 0.00033700 |
| C |  | 2.63669700 | -0.33372600 | 0.00095800 |
| C |  | 2.06415400 | -1.54463000 | -0.00030500 |
| N |  | 1.15473600 | 1.80914700 | -0.00006800 |
| H |  | 2.67722000 | -2.43186700 | 0.00015800 |
| H |  | 0.98975200 | -1.65223000 | -0.00181600 |
| H |  | 3.70861300 | -0.20591100 | 0.00246200 |
| C |  | -2.53356100 | -0.08257400 | -0.00009900 |
| N |  | -1.31403800 | -0.04670300 | -0.00242700 |
| O |  | -3.69133200 | -0.27701200 | 0.00160000 |
| H |  | -0.76118600 | 0.79905600 | -0.00148900 |

C2\_TS1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.87747200 | 1.18554400 | -0.06433500 |
| C |  | 1.83412100 | 0.25492400 | -0.39419000 |
| C |  | 1.40572800 | -0.90794400 | 0.31273100 |
| N |  | -0.18512000 | 1.51701200 | 0.37336200 |
| H |  | 1.81408500 | -1.85869600 | -0.01225400 |
| H |  | 1.33744100 | -0.82926500 | 1.38903800 |
| H |  | 2.24826000 | 0.21053400 | -1.38654200 |
| C |  | -1.22414500 | -0.27066200 | -0.04395600 |
| N |  | -0.30308100 | -1.15199600 | 0.03205900 |
| O |  | -2.34689000 | 0.05486500 | -0.18202300 |
| H |  | -0.56631500 | -2.08778200 | -0.23350700 |

C2\_TS2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.80844100 | -1.18731100 | -0.32348000 |
| C |  | -1.79067900 | -0.27790000 | -0.34798300 |
| C |  | -1.10698600 | 0.92714100 | 0.27055800 |
| N |  | 0.06906700 | -0.96089300 | 0.61444600 |
| H |  | -1.64697300 | 1.87059600 | 0.22468300 |
| H |  | -0.54605700 | -0.15999500 | 1.29076700 |
| H |  | -2.74501800 | -0.22067200 | -0.84370800 |
| C |  | 1.06619400 | -0.00266300 | 0.03510200 |
| N |  | 0.29025600 | 1.14551900 | 0.00481400 |
| O |  | 2.20737600 | -0.18108900 | -0.27952500 |
| H |  | 0.60324900 | 1.91079300 | -0.57555100 |

C2\_TS3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.08732200 | 1.26919500 | -0.01357000 |
| C |  | -1.82332200 | 0.04909500 | 0.05014600 |
| C |  | -1.11717000 | -1.11652100 | 0.00014800 |
| N |  | 0.27229400 | 1.19626600 | -0.08016100 |
| H |  | -1.57545800 | -2.09570400 | -0.00158900 |
| H |  | -0.19325900 | 2.26632900 | 0.14370000 |
| H |  | -2.89826900 | 0.03451300 | 0.10930300 |
| C |  | 1.05511400 | 0.02865500 | -0.00630000 |
| N |  | 0.24616100 | -1.10917600 | -0.04509800 |
| O |  | 2.26514600 | -0.02699500 | 0.06117300 |
| H |  | 0.75283100 | -1.98136300 | -0.04652400 |

C4\_IM1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.04619200 | 0.02889000 | 0.79679800 |
| C |  | 2.26145600 | 0.01867800 | 0.04805300 |
| C |  | 3.40401300 | 0.02016500 | -0.38604000 |
| N |  | -0.03309800 | -0.01244700 | 0.09914500 |
| H |  | 4.38251500 | 0.02007300 | -0.79612200 |
| C |  | -1.29745500 | -0.01090200 | -0.02263800 |
| N |  | -2.07736300 | 1.11518500 | -0.06443600 |
| O |  | -2.02373700 | -1.14957300 | -0.15312500 |
| H |  | -1.42480600 | -1.89368200 | -0.02366500 |
| H |  | -1.57023900 | 1.97299600 | -0.19047000 |
| H |  | -2.90958200 | 1.03704900 | -0.62474700 |

C4\_IM2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.06546500 | -1.19089200 | 0.38425900 |
| C |  | 1.76089900 | -0.29246700 | -0.27420800 |
| C |  | 1.31325100 | 0.96065600 | -0.33672500 |
| N |  | -0.26914300 | -1.29839300 | -0.08757700 |
| H |  | 1.58495300 | 1.86249400 | -0.85449400 |
| C |  | -0.80334500 | -0.14504500 | -0.01074200 |
| N |  | -0.00194600 | 1.04074900 | 0.43219700 |
| O |  | -2.09958600 | 0.21329100 | -0.17115100 |
| H |  | -2.56409000 | -0.57440900 | -0.48232000 |
| H |  | 0.19318900 | 0.92163200 | 1.43601800 |
| H |  | -0.53735600 | 1.89394500 | 0.28215300 |

C4\_IM3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.11503800 | -1.18347800 | 0.00040800 |
| C |  | 1.95823000 | -0.05209500 | -0.00022100 |
| C |  | 1.20270600 | 1.11485800 | -0.00030700 |
| N |  | -0.25136100 | -1.21028800 | -0.00045800 |
| H |  | 1.61627000 | 2.11630900 | -0.00109200 |
| C |  | -0.84626400 | -0.04543100 | -0.00007400 |
| N |  | -0.17401100 | 1.11456300 | 0.00051100 |
| O |  | -2.18919100 | 0.07336500 | -0.00019000 |
| H |  | -2.53329600 | -0.82944300 | 0.00047100 |
| H |  | 1.53854800 | -2.18106500 | 0.00144200 |
| H |  | -0.70864800 | 1.97423600 | 0.00149200 |

C4\_IM4

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.14610800 | 1.13915000 | 0.00022800 |
| C |  | -1.94577100 | -0.00000500 | 0.00000900 |
| C |  | -1.14610200 | -1.13915100 | -0.00011900 |
| N |  | 0.22297500 | 1.13845500 | 0.00002700 |
| H |  | -1.55245200 | -2.14502100 | 0.00073800 |
| C |  | 1.01059900 | -0.00000200 | -0.00029900 |
| N |  | 0.22298400 | -1.13845400 | -0.00011500 |
| O |  | 2.23155700 | 0.00000700 | 0.00016600 |
| H |  | 0.74752600 | 2.00329800 | -0.00009100 |
| H |  | -1.55247500 | 2.14501500 | -0.00055000 |
| H |  | 0.74753100 | -2.00330100 | 0.00028200 |

C4\_IM5

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.07586800 | -1.36655600 | 0.00022200 |
| C |  | 1.79438900 | -0.12124400 | 0.00012300 |
| C |  | 1.15984700 | 1.08437600 | -0.00007500 |
| N |  | -0.26173000 | -1.16342400 | 0.00009800 |
| H |  | 1.66626500 | 2.03913300 | -0.00050100 |
| C |  | -1.01217600 | 0.02214200 | 0.00031200 |
| N |  | -0.20344900 | 1.14104200 | -0.00022300 |
| O |  | -2.22975900 | 0.06199100 | -0.00017900 |
| H |  | -0.86074900 | -1.97801700 | 0.00000000 |
| H |  | 2.87188400 | -0.13546500 | -0.00023400 |
| H |  | -0.69064600 | 2.02278700 | -0.00044400 |

C4\_PD

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.07168100 | 1.16718200 | -0.00010500 |
| C |  | -1.77807100 | 0.00157400 | -0.00024500 |
| C |  | -1.01505500 | -1.19641700 | -0.00022900 |
| N |  | 0.28043200 | 1.11011500 | 0.00008600 |
| H |  | -2.85432200 | -0.00316100 | -0.00033100 |
| C |  | 1.03542500 | -0.08324200 | 0.00007000 |
| N |  | 0.29558000 | -1.26388800 | 0.00000400 |
| O |  | 2.25245900 | -0.02628000 | 0.00034800 |
| H |  | 0.83086000 | 1.95543200 | 0.00021400 |
| H |  | -1.51952000 | 2.14919300 | -0.00007300 |
| H |  | -1.53248100 | -2.14939600 | -0.00017700 |

C4\_RC

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.47802300 | 0.80474800 | -0.00010400 |
| C |  | 2.22258500 | -0.35033600 | -0.00006100 |
| C |  | 2.90226400 | -1.35972000 | -0.00002700 |
| N |  | 0.86899700 | 1.81130300 | -0.00013100 |
| H |  | 3.48612300 | -2.24676900 | 0.00001100 |
| C |  | -1.49334600 | -0.41205700 | 0.00000600 |
| N |  | -2.59722300 | -1.15119800 | 0.00005600 |
| O |  | -1.86934000 | 0.87701500 | 0.00016600 |
| H |  | -1.05827800 | 1.40488000 | 0.00012000 |
| H |  | -3.52337700 | -0.74372300 | 0.00021900 |
| H |  | -2.50932000 | -2.14705700 | -0.00003500 |

C4\_RCa

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.15963000 | 0.38953100 | 0.00006600 |
| N |  | -1.08537500 | -0.15937600 | 0.00001800 |
| O |  | 1.19857200 | -0.24606400 | -0.00011900 |
| H |  | 0.13579000 | 1.48769600 | 0.00025600 |
| H |  | -1.18118100 | -1.15826500 | -0.00009000 |
| H |  | -1.90334300 | 0.41752700 | 0.00026400 |

C4\_TS1

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.12742300 | -0.10060500 | 0.51614200 |
| C |  | 2.39564300 | -0.00744600 | 0.01379000 |
| C |  | 3.56349100 | 0.06706700 | -0.34046500 |
| N |  | -0.06774700 | -0.13582500 | 0.55546500 |
| H |  | 4.56991900 | 0.13372200 | -0.67205300 |
| C |  | -1.37652200 | 0.00843200 | -0.38108100 |
| N |  | -2.07479400 | 1.15819200 | -0.13655400 |
| O |  | -2.21232100 | -1.05100300 | -0.12829100 |
| H |  | -1.78537200 | -1.84241200 | -0.46410300 |
| H |  | -2.79117800 | 1.14108500 | 0.57857300 |
| H |  | -1.55722200 | 2.01438000 | -0.19877300 |

C4\_TS2

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.06068900 | -1.13497600 | 0.44243100 |
| C |  | 1.82969500 | -0.31683500 | -0.33110300 |
| C |  | 1.42772400 | 0.90799100 | -0.40307300 |
| N |  | -0.23125400 | -1.24165300 | -0.02291700 |
| H |  | 1.65075100 | 1.89394000 | -0.75537700 |
| C |  | -0.83127900 | -0.11760600 | 0.04167300 |
| N |  | -0.13160100 | 1.06654700 | 0.48398100 |
| O |  | -2.12859400 | 0.13671700 | -0.26384200 |
| H |  | -2.47865500 | -0.66980500 | -0.66369200 |
| H |  | 0.15982600 | 0.96995200 | 1.45861000 |
| H |  | -0.68416400 | 1.90647600 | 0.34418300 |

C4\_TS3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 0.99941800 | -1.08976500 | 0.38360700 |
| C |  | 1.75237200 | -0.30848600 | -0.35738400 |
| C |  | 1.30480100 | 0.95200100 | -0.35754100 |
| N |  | -0.32661200 | -1.28436900 | -0.09918100 |
| H |  | 1.59265800 | 1.89473100 | -0.78630000 |
| C |  | -0.82613500 | -0.10601500 | -0.00771000 |
| N |  | 0.07162100 | 0.92436900 | 0.50268300 |
| O |  | -2.09646800 | 0.30834000 | -0.19382500 |
| H |  | -2.59886500 | -0.46199300 | -0.48856300 |
| H |  | 0.58327400 | 0.13448600 | 1.30947100 |
| H |  | -0.40312100 | 1.79964000 | 0.72564500 |

C4\_TS4

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.97576100 | -1.27276700 | 0.00000900 |
| C |  | -1.90949100 | -0.21443000 | -0.00000300 |
| C |  | -1.29153800 | 1.02530600 | -0.00000700 |
| N |  | 0.36382800 | -1.08674000 | -0.00001100 |
| H |  | -1.82616500 | 1.96709700 | -0.00002700 |
| C |  | 0.89461500 | 0.14973000 | -0.00000100 |
| N |  | 0.09202400 | 1.21748900 | 0.00001000 |
| O |  | 2.17515400 | 0.04863100 | -0.00000100 |
| H |  | 1.69575900 | -1.22448700 | -0.00001200 |
| H |  | -1.27644300 | -2.31347500 | 0.00003700 |
| H |  | 0.50770700 | 2.13953600 | 0.00002800 |

C4\_TS5

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | 1.09427100 | -1.23956600 | -0.10900500 |
| C |  | 1.85704800 | -0.02411000 | -0.15375000 |
| C |  | 1.15147400 | 1.13860700 | 0.07976300 |
| N |  | -0.24723000 | -1.16981100 | 0.12370600 |
| H |  | 1.58606200 | 2.09295800 | 0.35147600 |
| C |  | -1.00635900 | -0.01201600 | -0.00164600 |
| N |  | -0.20731700 | 1.13300000 | -0.02109200 |
| O |  | -2.22246400 | 0.02816900 | -0.06172900 |
| H |  | -0.78830800 | -2.00836700 | 0.28385300 |
| H |  | 2.32354500 | -1.22320200 | 0.26232000 |
| H |  | -0.73835500 | 1.99343900 | -0.01428800 |

C4\_TS6

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -1.11717000 | -1.11652100 | 0.00014800 |
| C |  | -1.82332200 | 0.04909600 | 0.05014900 |
| C |  | -1.08732200 | 1.26919500 | -0.01357100 |
| N |  | 0.24616100 | -1.10917600 | -0.04510200 |
| H |  | -2.89826900 | 0.03451300 | 0.10931100 |
| C |  | 1.05511400 | 0.02865500 | -0.00630000 |
| N |  | 0.27229500 | 1.19626700 | -0.08016700 |
| O |  | 2.26514600 | -0.02699500 | 0.06117700 |
| H |  | 0.75283100 | -1.98136300 | -0.04652800 |
| H |  | -1.57545900 | -2.09570400 | -0.00158900 |
| H |  | -0.19325800 | 2.26632700 | 0.14371000 |

C4\_TSa

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| C |  | -0.07624000 | -0.47955200 | 0.00004500 |
| N |  | 1.11345600 | 0.11136800 | -0.00013700 |
| O |  | -1.15262000 | 0.29094200 | 0.00011700 |
| H |  | -1.23090000 | -0.92177700 | 0.00002600 |
| H |  | 1.16009900 | 1.12221700 | -0.00018700 |
| H |  | 1.95500900 | -0.43024100 | -0.00009000 |