

Electronic Supporting Information For
Insights to highly selective ring expansion of oxaziridine under Lewis
base catalysis: A DFT study

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Part I: Single-point energies of all stationary points

Table S1. The single-point energies of all stationary points involved in the reaction calculated at M06-2X/6-311++G(2df, 2pd)//IEF-PCM_{1,4-dioxane}

	single-point energies/a. u.
<i>p</i> -nitrobenzoic acid	-625.307048
R1	-817.226052
Cat	-1052.231771
HCO₃⁻	-264.519184
R2	-1219.760779
Re-TS1	-1869.474789
Si-TS1	-1869.469038
Re-M1	-1869.480149
Si-M1	-1869.476178
Re-M1'	-2134.022459
Si-M1'	-2134.011214
Re-TS2	-2134.006932
Re-TS2d	-1869.407026
Re-TS2b	-2686.679004
Si-TS2	-2133.995136
Re-M2	-1869.495155
Si-M2	-1869.486990
TS3	-1869.487106
M3	-1244.167464
TS4R	-2463.925530
TS4S	-2463.915221
M4R	-2464.043695
M4S	-2464.046829
TS5R	-2464.039868
TS5S	-2464.031305
M5R	-2464.040516
M5S	-2464.035249
TS6R	-2464.03526
TS6S	-2464.024055
PR/S	-1411.702942
TS4_N	-2463.910575
TS4_C	-2463.902948
M4_N	-2464.001651
M4_C	-2463.959351
TS3'	-1244.133284
R1'	-191.895712
TS4'	-1411.613763

Part II: The Gibbs free energy profiles of stereoselectivity-determining step (Step

4) with different method B3LYP

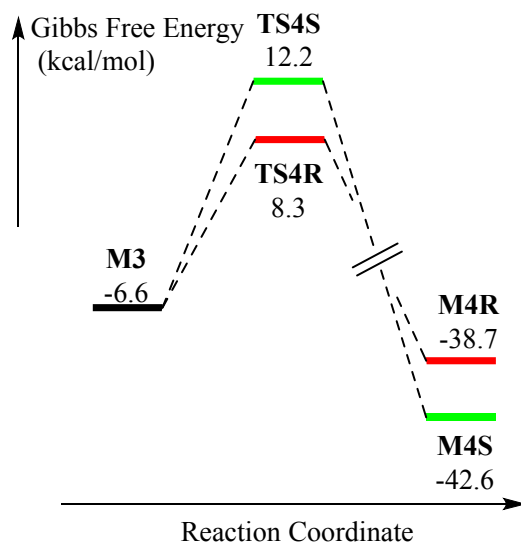
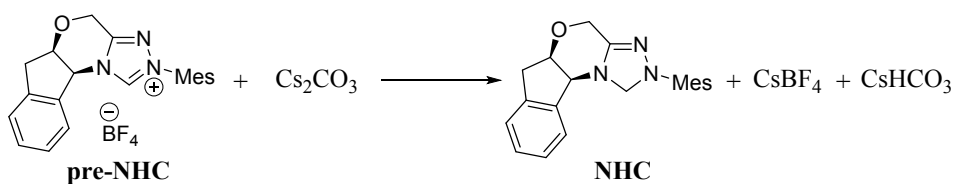


Fig. S1 Gibbs free energy profiles at B3LYP/6-31G(d, p)//IEF-PCM_{1,4-dioxane} level

Part III: Cs₂CO₃-assisted deprotonation process of pre-NHC



Scheme S1 Cs₂CO₃-assisted deprotonation reaction of **pre-NHC**

According to Sunoj's work, the deprotonation process of **pre-NHC** for the formation of NHC has been additionally considered and investigated (Scheme S1). As shown in Fig. S2, the energy barrier for Cs₂CO₃-assisted deprotonation process of **pre-NHC** *via* transition state **TS** is 14.1 kcal/mol, indicating that this process can occur smoothly.

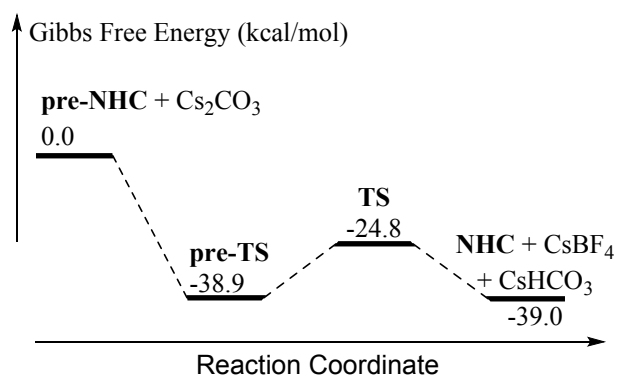


Fig. S2 The Gibbs free energy profile of the deprotonation process of **pre-NHC**

Part IV: Optimized structures and geometrical parameters of reactants, products, and all intermediates

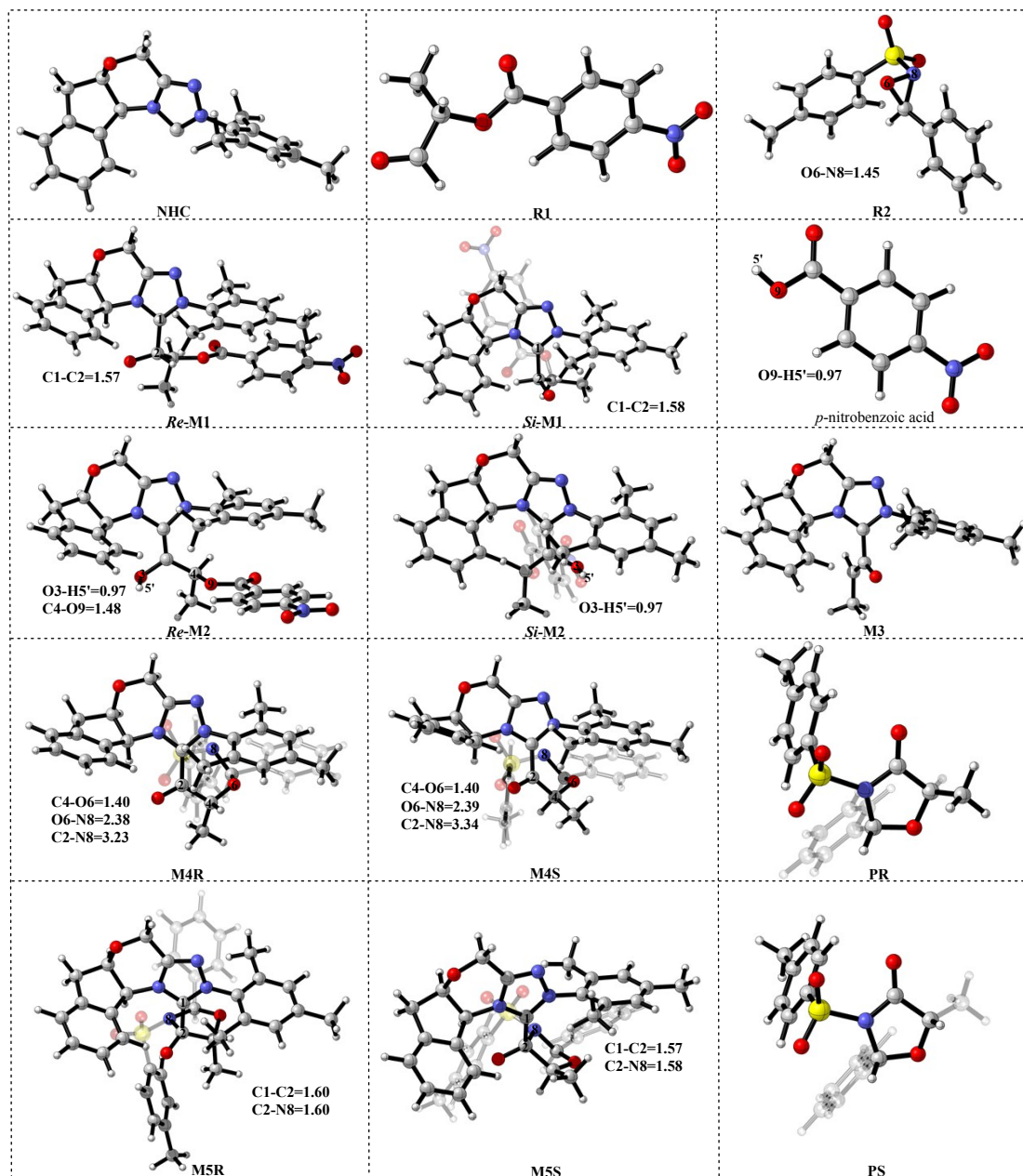


Fig. S3 Optimized structures and geometrical parameters involving with reactants, products, and all intermediates (Units in Å for distances)

Part V: Total energy along IRC of TS4R/S

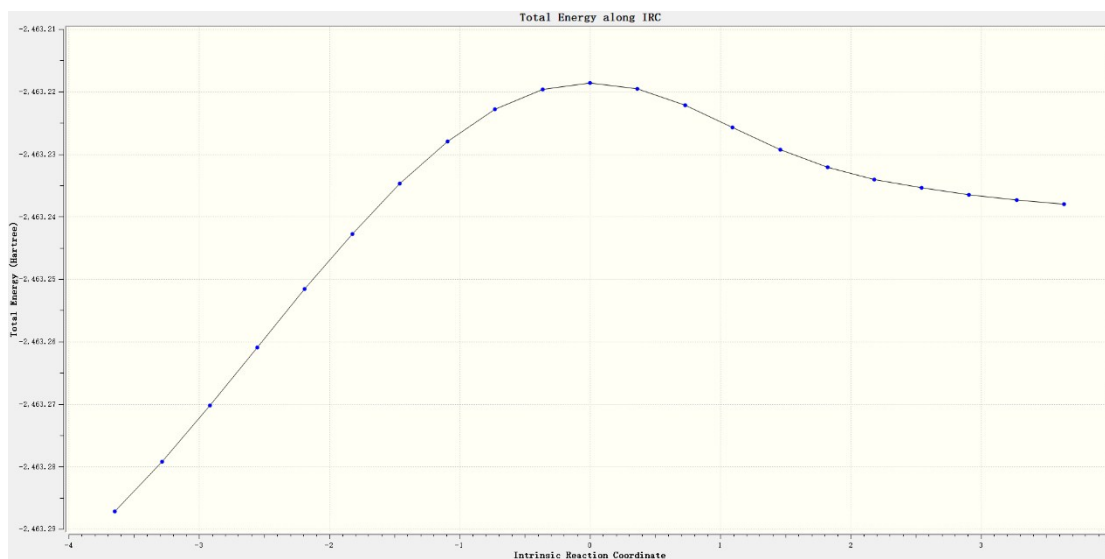


Fig. S4 Total energy along IRC of TS4R

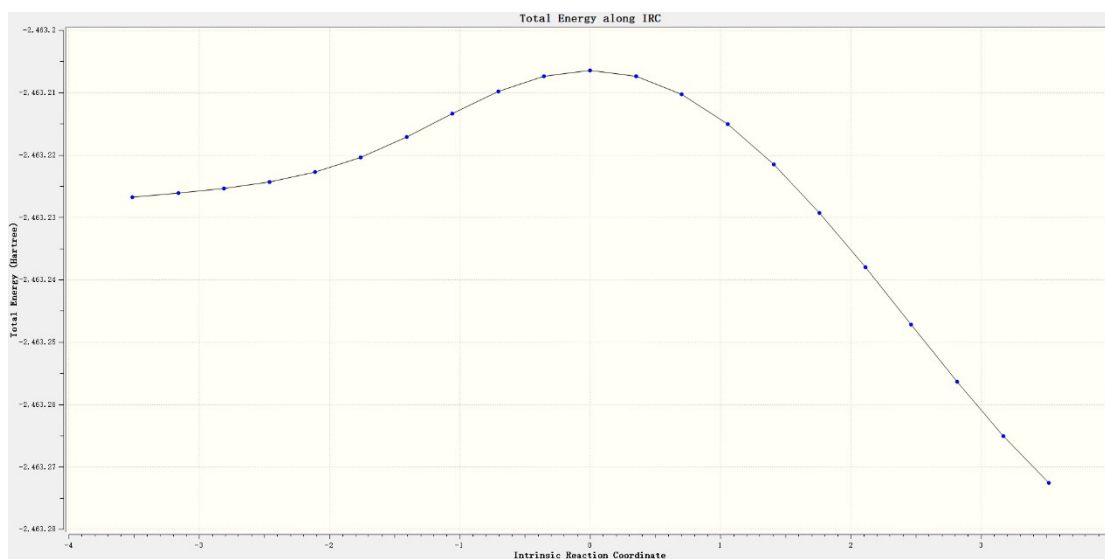


Fig. S5 Total energy along IRC of TS4S

Part VI: The direct reaction pathway between ketene and oxaziridine

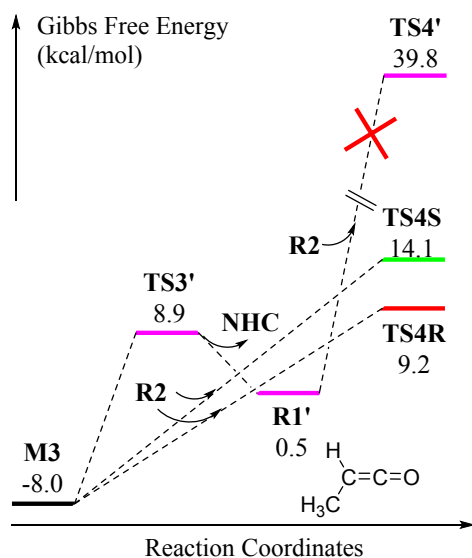


Fig. S6 Gibbs free energy profile associated with the direct reaction between ketene and oxaziridine

In this part, we considered the direct reaction between ketene and oxaziridine. After dissociation of NHC, the ketene molecule **R1'** is formed with an energy barrier of 16.9 kcal/mol *via* the transition state **TS3'**. Then, the **C4** atom of **R1'** attacks on the **O6** atom of **R2** to construct the C–O bond. The transition state of direct reaction pathway (**TS4'**) has a high free energy of 39.8 kcal/mol. Compared with the other two similar processes (**TS4R** and **TS4S**), the direct reaction pathway is impossible to occur. We also calculated the global electrophilicity ω and global nucleophilicity N of **R1'**. From the Table S3, the nucleophilicity index N of **R1'** decreased from 4.76 eV in **M3** to 2.91 eV, which suggests that **R1'** has a poor nucleophilicity. Thus, the NHC organocatalyst are necessary for this kind of reaction.

Table S3. Energies of HOMO and LUMO (Units for a.u.), electric chemical potential (μ , eV), chemical hardness (η , eV), global electrophilicity (ω , eV) and global nucleophilicity (N , eV) of Some Reactants (**SR**) ($E_{\text{HOMO}}(\text{TCE}) = -0.38383$ a. u.)

SR	E_{HOMO}	E_{LUMO}	μ	η	ω	N
R1	-0.34121	-0.06864	-5.576	7.417	2.10	1.16
M3	-0.20890	-0.01177	-2.682	6.005	0.60	4.76
R1'	-0.27702	0.01870	-3.515	8.047	0.77	2.91
R2	-0.31102	-0.01620	-4.452	8.022	1.23	1.98

Part VII: Coordinates of stationary points involved in the reaction

R1

C	4.12803700	-1.18812200	-0.57803200
O	5.27362700	-1.46996300	-0.33720600
H	3.47487800	-1.83976700	-1.19160200
C	3.48117800	0.09508400	-0.09041600
C	4.01352500	0.54839100	1.25488000
H	3.64976200	0.86835300	-0.85097600
H	3.58357600	1.51422000	1.52270000
H	3.76809800	-0.18836500	2.02314500
H	5.09930800	0.63849800	1.19401200
O	2.07368900	-0.18538800	-0.03978400
C	1.25316700	0.87113700	-0.16143200
O	1.63887900	2.00499800	-0.31243100
C	-0.18788200	0.48127100	-0.09256800
C	-0.58255000	-0.84595300	0.08650900
C	-1.13545100	1.49894800	-0.21820400
C	-1.93401700	-1.16214000	0.13981300
H	0.16517100	-1.62338800	0.18513400
C	-2.48893700	1.19625600	-0.16732100
H	-0.79490800	2.51907000	-0.35572300
C	-2.85492000	-0.13140400	0.01063000
H	-2.27966700	-2.17859200	0.27751100
H	-3.25223200	1.95776000	-0.26296800
N	-4.29046300	-0.46199000	0.06650700
O	-5.08385200	0.45316900	-0.04999800
O	-4.59404900	-1.62964900	0.22567500

R2

C	-1.07956600	-0.03477000	-0.20003200
O	-0.67472000	0.61413000	-1.38246300
H	-0.32933600	-0.70175600	0.22705200
N	-0.81867900	1.38090300	-0.16264300
S	0.75610800	1.88797000	0.39482800
O	0.56163900	2.12169400	1.81544400
O	1.13435900	2.95198400	-0.51534000
C	1.86486000	0.52712700	0.16898300
C	2.20170900	-0.25829400	1.26917000
C	2.38360900	0.27620500	-1.09969900
C	3.07989200	-1.31936900	1.08527300
H	1.79224600	-0.02271200	2.24627300

C	3.25563100	-0.79220800	-1.26042500
H	2.11471000	0.91650100	-1.93253500
C	3.61231900	-1.60310300	-0.17666200
H	3.36363100	-1.93237300	1.93547900
H	3.67440400	-0.99748100	-2.24114300
C	4.53974100	-2.77252700	-0.37152200
H	5.07188900	-3.01367600	0.55084100
H	3.97446900	-3.66059300	-0.67238500
H	5.27407800	-2.56819900	-1.15356900
C	-2.49225000	-0.47797400	-0.09930400
C	-3.49727400	0.24514600	-0.74396400
C	-2.80475200	-1.61818000	0.63687900
C	-4.81657700	-0.17704900	-0.64477400
H	-3.23102900	1.12784600	-1.31677500
C	-4.12901400	-2.03747300	0.73603800
H	-2.01443700	-2.17582500	1.13219700
C	-5.13271100	-1.31744100	0.09501100
H	-5.60172500	0.38031000	-1.14466000
H	-4.37500500	-2.92436500	1.31016800
H	-6.16480300	-1.64452000	0.16935800

Cat

C	0.51023300	-1.50213700	0.76789000
C	1.53832900	-2.31766900	1.48713600
C	-0.23735000	-0.13904300	-0.87289800
H	1.48775800	-3.36455000	1.15137600
N	-0.75137300	-1.36290500	1.03076000
N	0.85136300	-0.79612500	-0.35661400
N	-1.17740600	-0.52831600	0.01399100
C	-2.54865600	-0.11920800	-0.00601200
C	-2.99220600	0.78084200	0.96614400
C	-3.39314800	-0.62668800	-0.99662700
C	-4.33020300	1.17078300	0.93041300
C	-4.72150900	-0.20393500	-0.99670300
C	-5.20813700	0.68772500	-0.04012000
H	-4.69287200	1.87597600	1.67475300
H	-5.39407100	-0.58385800	-1.76225200
O	2.82018600	-1.77899500	1.24275500
H	1.36382800	-2.28840100	2.56339200
C	3.13747600	-1.72566800	-0.13979700
H	3.06970600	-2.73257400	-0.57490400
C	2.21159000	-0.71538400	-0.86395900
H	2.18137200	-0.93769200	-1.93644100
C	4.53218600	-1.09778900	-0.24727700
H	5.02481100	-1.42413500	-1.17045600
C	4.23781600	0.38527900	-0.28183800
C	2.90285800	0.60781400	-0.61764300
C	5.08313100	1.46002000	-0.03644300
H	6.12259300	1.29807300	0.23380600
C	4.56822400	2.75390800	-0.12772000

C	2.38108800	1.88994800	-0.71272400
H	1.33593000	2.03517900	-0.97045100
C	3.23024600	2.96761900	-0.46075600
H	2.84651000	3.98095100	-0.52159500
H	5.21441300	3.60331000	0.07052000
H	5.15308200	-1.40647700	0.59721500
C	-2.87531200	-1.58978400	-2.03107300
H	-2.10930800	-1.11506900	-2.65005500
H	-2.41056700	-2.45853000	-1.55429100
H	-3.68607600	-1.93782600	-2.67367300
C	-2.04235400	1.31903100	2.00251200
H	-1.74171200	0.53428500	2.70227100
H	-1.12882400	1.69577300	1.53120700
H	-2.50600900	2.13127100	2.56520300
C	-6.65748100	1.10161200	-0.04208600
H	-7.06327300	1.11648100	-1.05647600
H	-7.26197300	0.40249400	0.54524100
H	-6.78582900	2.09505500	0.39409500

p-nitrobenzoic acid

C	0.71902800	-1.21266200	0.00010000
C	-0.67000700	-1.19128100	0.00009200
C	-1.34382600	0.03143600	0.00009500
C	-0.64013100	1.23686500	0.00009000
C	0.74766100	1.22956800	0.00008800
C	1.39403700	0.00038200	0.00009900
H	1.27739000	-2.13985000	0.00010900
H	-1.23169500	-2.11762400	0.00009600
H	-1.19504100	2.16829200	0.00009100
H	1.32711300	2.14372200	0.00008700
N	2.86801200	-0.01726000	0.00010500
O	3.44488900	1.05430400	-0.00021400
O	3.41937500	-1.10226100	-0.00012100
C	-2.83592100	0.10324200	0.00010500
O	-3.46285400	1.13496400	-0.00010400
O	-3.41451000	-1.10613800	-0.00016000
H	-4.37410900	-0.96597900	-0.00033100

Re-TS1

C	-1.44373400	-1.21577800	2.12142000
O	-2.27686300	-2.10829700	2.29489800
H	-1.71152300	-0.14504600	2.24286500
C	0.03104100	-1.48440900	2.39179800
C	0.24324600	-1.61718700	3.89233500
H	0.36017400	-2.38875500	1.87572000
H	1.29430400	-1.81479300	4.10940100
H	-0.06525400	-0.69895400	4.40122900
H	-0.36516300	-2.44472800	4.26251600

O	0.77157700	-0.36216700	1.88313100
C	2.06462200	-0.57390300	1.62019500
O	2.64994700	-1.60874200	1.83926100
C	2.71945900	0.62861700	1.01219000
C	2.04680400	1.84340000	0.87187800
C	4.03534800	0.48874000	0.56755800
C	2.68447600	2.92378300	0.27418900
H	1.02858300	1.93740000	1.23078000
C	4.68393600	1.55685000	-0.03638900
H	4.52696700	-0.46972700	0.69472200
C	3.98800700	2.75220400	-0.17120000
H	2.19456900	3.88057700	0.14654300
H	5.70144900	1.48266500	-0.39856000
N	4.66539000	3.89171100	-0.81310800
O	5.80083500	3.71918100	-1.21652600
O	4.04868400	4.93747400	-0.90299700
C	-2.68082500	-1.11928800	-1.82136200
C	-3.95168400	-0.94794200	-2.59487800
C	-1.38807000	-0.96743500	-0.00785200
H	-4.52490600	-1.88661000	-2.57616700
N	-1.56085600	-1.66929100	-2.18257600
N	-2.61426000	-0.69090100	-0.52318100
N	-0.78807900	-1.56222400	-1.04581100
C	0.53824600	-2.10112000	-1.02862100
C	1.58962000	-1.31762800	-1.50489200
C	0.71619400	-3.39373800	-0.52650600
C	2.87191400	-1.86352900	-1.45152100
C	2.01738800	-3.88690900	-0.47576500
C	3.10416700	-3.13263500	-0.92383700
H	3.70964200	-1.27026100	-1.81150200
H	2.18857500	-4.88128500	-0.07059300
O	-4.70069600	0.10938700	-2.03592400
H	-3.73482800	-0.69165200	-3.63256500
C	-5.00583100	-0.09498000	-0.66319200
H	-5.53984000	-1.04645200	-0.53808700
C	-3.70866200	-0.03943600	0.18120700
H	-3.83993400	-0.57378500	1.13089800
C	-5.80196600	1.12893700	-0.19678200
H	-6.43080400	0.86442800	0.66074400
C	-4.72129300	2.10913300	0.20153500
C	-3.51050300	1.44507900	0.39560200
C	-4.79557500	3.48561800	0.37195600
H	-5.73171800	4.01370700	0.21702300
C	-3.64019900	4.18303000	0.72758600

C	-2.35360000	2.13117600	0.73845700
H	-1.41291800	1.59761000	0.85788700
C	-2.42873000	3.51438500	0.90398200
H	-1.53805500	4.07619800	1.16724700
H	-3.68181900	5.25975600	0.85701800
H	-6.45147900	1.48915000	-0.99807600
C	-0.46783100	-4.20553000	-0.06679000
H	-1.01748200	-3.70987700	0.74275700
H	-1.17401800	-4.34965500	-0.89085100
H	-0.14475700	-5.18668100	0.28537200
C	1.33720400	0.06378100	-2.04609000
H	0.84428000	0.01695200	-3.02232800
H	0.68278500	0.63069900	-1.37641200
H	2.27634400	0.61262400	-2.15446700
C	4.50723100	-3.65997900	-0.78195300
H	4.88184700	-3.44981200	0.22587100
H	4.54382100	-4.74216900	-0.92797600
H	5.18550500	-3.19111300	-1.49857500

Si-TS1

C	1.43450700	1.20425600	1.88556300
O	2.45762200	1.91658300	1.86277200
H	0.43402200	1.68512000	1.95738900
C	1.45869300	-0.08869500	2.73536300
C	2.78812100	-0.79938500	2.70880100
H	1.19501500	0.21749600	3.75335200
H	2.80833300	-1.61966500	3.42936500
H	2.99889300	-1.19202900	1.71165900
H	3.56380800	-0.07276700	2.95393200
O	0.44048100	-1.00961000	2.27481900
C	-0.82836300	-0.72768500	2.56970400
O	-1.18903600	0.07887700	3.39698200
C	-1.79049900	-1.48263200	1.70060000
C	-1.34797400	-2.18877500	0.57988000
C	-3.15295800	-1.38007500	1.98724300
C	-2.26873900	-2.79180500	-0.26752800
H	-0.28565000	-2.24537000	0.37067600
C	-4.08508100	-1.98800600	1.15497300
H	-3.46407400	-0.81355900	2.85817100
C	-3.61828300	-2.67142600	0.03931000
H	-1.96125500	-3.33893100	-1.15071400
H	-5.14937400	-1.93205500	1.34591700
N	-4.60052800	-3.28234300	-0.87330800
O	-5.76512800	-3.29154300	-0.52283600

O	-4.18430300	-3.73203400	-1.92517500
C	-0.32832700	0.00735800	-1.65640700
C	-1.58106200	0.03345700	-2.47627500
C	0.95115700	0.46336100	0.10676300
H	-2.18025000	-0.86553900	-2.26279300
N	0.78885400	-0.60389300	-1.90181200
N	-0.27003400	0.66544600	-0.45305400
N	1.56225900	-0.30864500	-0.79967500
C	2.94305800	-0.70252200	-0.81074200
C	3.91096700	0.29116900	-0.96513100
C	3.25849800	-2.06067300	-0.69502400
C	5.24667100	-0.11632100	-0.98096800
C	4.60283400	-2.41545700	-0.72441000
C	5.60930700	-1.45572800	-0.86651100
H	6.01961200	0.63897500	-1.09273400
H	4.87317100	-3.46432400	-0.62565500
O	-2.30709600	1.20232700	-2.17893200
H	-1.33533500	0.04775500	-3.53862900
C	-2.63295800	1.31179900	-0.80262200
H	-3.19681500	0.42391300	-0.47864500
C	-1.35089800	1.51928600	0.04091800
H	-1.55798400	1.24893700	1.08259000
C	-3.38936500	2.63308900	-0.63761200
H	-4.02777000	2.59490400	0.25238900
C	-2.27521700	3.64137000	-0.46431100
C	-1.09129600	3.00578000	-0.08686600
C	-2.30781900	5.02023600	-0.62230400
H	-3.22233300	5.52282800	-0.92301100
C	-1.13846600	5.74787800	-0.39920100
C	0.07791600	3.71984800	0.14640900
H	1.00134000	3.23435600	0.46074300
C	0.03938900	5.10561500	-0.01887300
H	0.93876100	5.68733300	0.15432200
H	-1.14503000	6.82582300	-0.52569000
H	-4.02450500	2.81836800	-1.50698900
C	2.18033200	-3.08955200	-0.48060300
H	1.65536800	-2.88845200	0.46043600
H	1.44397900	-3.06930300	-1.28882100
H	2.60886600	-4.09097600	-0.41860900
C	3.53645400	1.74307400	-1.09480000
H	2.71798900	1.87844900	-1.80852800
H	3.21652000	2.13079500	-0.12067900
H	4.39321900	2.32351600	-1.44076900
C	7.05647700	-1.87823800	-0.91702600

H	7.25948200	-2.63559400	-0.15684500
H	7.28534300	-2.30784100	-1.89925000
H	7.71001000	-1.01654000	-0.74854500

Re-M1

C	-1.25047000	0.88565200	-1.33084600
O	-2.39175600	1.22140800	-1.88600700
H	-0.56210500	0.21621300	-1.91349100
C	-0.34796300	2.10877400	-0.95565400
C	-0.36969100	3.13230100	-2.06920100
H	-0.65128200	2.56170700	-0.00381200
H	0.23493900	4.00301400	-1.80427800
H	0.01717900	2.68356500	-2.98899000
H	-1.40512400	3.42375200	-2.24286000
O	0.98734700	1.58019100	-0.80707300
C	1.89990200	2.28246800	-0.13766900
O	1.67431300	3.27539800	0.51518700
C	3.24886000	1.64515800	-0.26486200
C	3.51544200	0.75257200	-1.30459200
C	4.21429300	1.92946300	0.70093300
C	4.74662500	0.11662100	-1.36926400
H	2.75057500	0.54544700	-2.04346500
C	5.43965900	1.27620200	0.66618300
H	3.98250400	2.64464900	1.48319100
C	5.67075500	0.37350600	-0.36537100
H	4.98789000	-0.58219000	-2.16040400
H	6.20372900	1.44547300	1.41431000
N	6.94763700	-0.35773900	-0.38725800
O	7.74513400	-0.13156200	0.50417200
O	7.12664400	-1.15676600	-1.28945400
C	-2.50612400	-0.47148000	1.86836300
C	-3.57311900	-0.46045000	2.91780900
C	-1.50051100	0.11712000	0.01099000
H	-3.32983700	0.32080700	3.65435100
N	-1.31767400	-0.98309300	1.96518700
N	-2.67236500	0.19240900	0.68229800
N	-0.70192300	-0.61047200	0.79976600
C	0.62847500	-1.11319000	0.57758600
C	0.82624600	-2.10836400	-0.38510000
C	1.63575300	-0.67907500	1.44202000
C	2.10859400	-2.64811600	-0.48706600
C	2.89063400	-1.27257100	1.31614700
C	3.14727800	-2.25216900	0.35867900
H	2.29005000	-3.42350500	-1.22765700
H	3.69159600	-0.94848700	1.97665400
O	-4.82673600	-0.23422500	2.33338900
H	-3.60311000	-1.42351800	3.42962300
C	-4.87278000	0.94256900	1.53323000
H	-4.61061500	1.82044300	2.13891800
C	-3.96957300	0.78522100	0.28517300
H	-3.74459200	1.73261400	-0.20501200
C	-6.28405800	0.97306200	0.94465200
H	-6.53717100	1.98733100	0.61578300
C	-6.15699000	0.03222100	-0.23183600
C	-4.82118700	-0.08669600	-0.61630000

C	-7.14895200	-0.65795100	-0.91616000
H	-8.19017000	-0.57128100	-0.61973400
C	-6.77982300	-1.47620600	-1.98374700
C	-4.44804100	-0.87439200	-1.69534300
H	-3.41434300	-0.87831000	-2.02327900
C	-5.44335100	-1.58177600	-2.36980300
H	-5.17661500	-2.20941100	-3.21409800
H	-7.54130700	-2.03112200	-2.52289400
H	-7.01622500	0.65870400	1.69203500
C	-0.30079700	-2.61766500	-1.24558700
H	-1.20921300	-2.77580800	-0.65590700
H	-0.54772600	-1.91560200	-2.04842200
H	-0.02406700	-3.56805000	-1.70466100
C	1.37896600	0.38010100	2.48114100
H	0.82376600	-0.03356700	3.32798700
H	2.32351200	0.78417300	2.85154200
H	0.78766700	1.20809100	2.07607200
C	4.51353400	-2.87735800	0.24259500
H	4.96271600	-2.68304600	-0.73668700
H	5.19154500	-2.48579600	1.00551200
H	4.45700600	-3.96287500	0.36539900

Si-M1

C	1.38060800	1.03660400	1.60479900
O	2.46768900	1.76935900	1.56026400
H	0.43949700	1.58177200	1.88061500
C	1.41564100	-0.15202400	2.62855900
C	2.75400100	-0.83755200	2.72584200
H	1.12466700	0.25622900	3.59896500
H	2.80136700	-1.49103000	3.59961100
H	2.98279400	-1.42006600	1.83306600
H	3.50103700	-0.04553200	2.80619300
O	0.40143900	-1.12277200	2.22914100
C	-0.86752100	-0.83187600	2.51736100
O	-1.22764100	-0.03017200	3.34987900
C	-1.84004900	-1.55460100	1.63069200
C	-1.41749700	-2.22449000	0.48015800
C	-3.19939900	-1.44740900	1.93187900
C	-2.35326400	-2.79267000	-0.37601900
H	-0.35919400	-2.28688300	0.25277200
C	-4.14612200	-2.01746600	1.08974600
H	-3.49644000	-0.90644800	2.82365400
C	-3.69822300	-2.67165300	-0.05088800
H	-2.06081000	-3.31739300	-1.27765800
H	-5.20773100	-1.95707500	1.29381600
N	-4.69585100	-3.25396300	-0.96617300
O	-5.86093900	-3.22870700	-0.61827600
O	-4.29063100	-3.71761500	-2.01611300
C	-0.24037500	0.11076900	-1.61576300
C	-1.46538800	0.15267200	-2.47661400
C	0.95554000	0.46954000	0.19678700
H	-2.04971900	-0.76694400	-2.31795400
N	0.89458600	-0.47595400	-1.84441400
N	-0.24228000	0.70712300	-0.38309700
N	1.63075100	-0.23955300	-0.71090800
C	3.01038300	-0.65829100	-0.71207800

C	3.98569700	0.29924100	-0.99078600
C	3.29319900	-2.01857800	-0.54878000
C	5.30985900	-0.14278000	-1.03199300
C	4.62735700	-2.40561400	-0.60504300
C	5.64881600	-1.47879400	-0.83527700
H	6.09311300	0.58301900	-1.23401500
H	4.87672800	-3.45512000	-0.46839500
O	-2.22307400	1.29251700	-2.15536700
H	-1.18302000	0.21505500	-3.52802900
C	-2.59635700	1.34335100	-0.78730100
H	-3.15613800	0.43602200	-0.51425400
C	-1.34732800	1.54199100	0.10531600
H	-1.58046400	1.24018800	1.13163100
C	-3.37368500	2.64880800	-0.59843800
H	-4.02928400	2.57479000	0.27665800
C	-2.27475300	3.66382400	-0.37342700
C	-1.09223000	3.03274700	0.01648500
C	-2.31892400	5.04524300	-0.50052000
H	-3.23198300	5.54532600	-0.80957900
C	-1.16141100	5.77811700	-0.23631200
C	0.06780600	3.74956600	0.28961800
H	0.99412600	3.26584700	0.60724500
C	0.01513000	5.13831500	0.15216400
H	0.90498600	5.72519900	0.35458500
H	-1.17607000	6.85857200	-0.33875700
H	-3.99309700	2.85215800	-1.47499700
C	2.19642500	-3.01851100	-0.29699300
H	1.67543700	-2.79498200	0.64157600
H	1.45995200	-3.00272300	-1.10707300
H	2.60588000	-4.02719300	-0.22479500
C	3.62464400	1.73521400	-1.23984900
H	2.84522000	1.81413600	-2.00598500
H	3.24343700	2.16164200	-0.30289600
H	4.49759100	2.29460700	-1.58036400
C	7.08475900	-1.93228900	-0.87931900
H	7.75306700	-1.10667500	-1.13069300
H	7.39378200	-2.33628200	0.08931800
H	7.22205600	-2.72308200	-1.62236200

Re-TS2

C	-1.12714700	-0.00202400	1.23527400
O	-1.97480800	0.83831600	1.91105600
H	-0.53170900	0.76951800	0.39404900
C	0.04315300	-0.59056100	2.06051100
C	0.00437200	-0.09885400	3.49381500
H	0.08692200	-1.68368900	2.02974900
H	0.83618800	-0.52818800	4.05756800
H	0.06196700	0.99111400	3.49219900
H	-0.94497400	-0.38349000	3.95001500
O	1.27043700	-0.11206500	1.44478600
C	2.40534400	-0.74037300	1.68107600
O	2.53929300	-1.72517400	2.38163700
C	3.54448500	-0.07031100	0.96830700

C	3.32771700	1.03527800	0.13925100
C	4.82686100	-0.58075800	1.17365300
C	4.41693100	1.63285300	-0.48745300
H	2.32323200	1.42927900	-0.01167900
C	5.91931200	0.01161800	0.55671600
H	4.94578800	-1.44080600	1.82396300
C	5.68583000	1.11008900	-0.26335800
H	4.29001700	2.49661500	-1.12787800
H	6.92851500	-0.35437200	0.69443100
N	6.83711800	1.73865700	-0.92727100
O	7.94780900	1.29640900	-0.68210000
O	6.62232000	2.66374000	-1.68963300
C	-3.35465700	-2.08524900	-0.69378200
C	-4.74762100	-2.49017000	-1.06206200
C	-1.80748000	-0.98222900	0.42525000
H	-5.06515000	-3.31558700	-0.40562500
N	-2.25223500	-2.67455800	-1.02699100
N	-3.14779800	-1.04285800	0.17531600
N	-1.28261700	-1.98928600	-0.32277900
C	0.08622100	-2.07432900	-0.74722100
C	0.49565900	-1.19160500	-1.76218200
C	0.94940600	-3.00288600	-0.16805500
C	1.83430200	-1.21934000	-2.13347900
C	2.28509600	-2.99371100	-0.58339400
C	2.74572100	-2.09977500	-1.54374500
H	2.18086700	-0.52449400	-2.89544300
H	2.98107600	-3.68572000	-0.11411800
O	-5.61927800	-1.39440800	-0.94531000
H	-4.77457200	-2.83828200	-2.09570900
C	-5.59696300	-0.80264200	0.34980700
H	-5.86648400	-1.55485100	1.10487900
C	-4.22335500	-0.14960500	0.62958600
H	-4.05735600	0.03369100	1.69165000
C	-6.55419200	0.38859600	0.27890500
H	-6.90288100	0.65344400	1.28388900
C	-5.67817000	1.47749300	-0.29897900
C	-4.32991900	1.16740400	-0.11423800
C	-6.05030600	2.66098900	-0.92317900
H	-7.09892400	2.90435400	-1.07110700
C	-5.04913400	3.52593800	-1.36549700
C	-3.32541800	2.02933900	-0.53461700
H	-2.27474600	1.81840100	-0.35679800
C	-3.70391400	3.21142700	-1.17303100
H	-2.93371400	3.89697300	-1.51197400

H	-5.31962900	4.45287000	-1.86241400
H	-7.42529400	0.14230100	-0.33353200
C	0.23097700	2.81926400	0.69100600
O	1.11754200	3.66178700	0.54068600
O	-0.53251900	2.82723100	1.78413400
O	-0.00839500	1.87495800	-0.19036100
H	-1.23914100	2.01043000	1.82402300
C	0.50844800	-3.97558800	0.89301800
H	0.76838600	-4.99716300	0.60145700
H	1.02539000	-3.75103200	1.83180500
H	-0.56843500	-3.93187500	1.06421300
C	-0.46267100	-0.23509800	-2.42006900
H	-1.47179500	-0.65126900	-2.48373200
H	-0.49629700	0.70554100	-1.85964100
H	-0.12325100	-0.01139400	-3.43416100
C	4.19637500	-2.05492300	-1.94455000
H	4.58821100	-1.03907100	-1.82726400
H	4.80102300	-2.72538800	-1.32976300
H	4.32469500	-2.33944300	-2.99382500

Si-TS2

C	1.41690300	0.27537600	1.28861200
O	2.21100300	-0.77182500	1.67051500
H	2.24350100	1.24931700	1.11183800
C	0.44186800	0.72762300	2.36830800
C	1.08417900	0.69684100	3.73377200
H	0.01355600	1.71722400	2.17653400
H	0.37567000	1.01802000	4.50099300
H	1.44692600	-0.31260500	3.92563300
H	1.94545400	1.37052500	3.72035500
O	-0.68803000	-0.23290700	2.32257000
C	-1.92123400	0.21568500	2.45527400
O	-2.24680100	1.24510400	3.01171100
C	-2.90599900	-0.64163400	1.70822300
C	-2.46481500	-1.62488800	0.81714200
C	-4.26610700	-0.35488000	1.83433700
C	-3.38477900	-2.32357900	0.04484000
H	-1.40259100	-1.83205900	0.73222900
C	-5.19764800	-1.05089700	1.07515400
H	-4.57394600	0.42583800	2.52128900
C	-4.73238400	-2.01761900	0.19158700
H	-3.07537200	-3.08744100	-0.65826400
H	-6.26000400	-0.85588300	1.14835800
N	-5.71199800	-2.74906000	-0.62813100

O	-6.89189600	-2.49881700	-0.45829400
O	-5.28568500	-3.56040100	-1.42956000
C	-0.59129100	-0.12343200	-1.74103500
C	-1.78809700	0.18145700	-2.58563300
C	0.73272900	-0.00299000	0.02799300
H	-2.61428700	-0.48290900	-2.28471600
N	0.25479100	-1.08649800	-1.90425600
N	-0.34416900	0.58559300	-0.59093200
N	1.07588900	-1.00688500	-0.80495400
C	2.24824800	-1.84465300	-0.79770000
C	3.40483000	-1.34214300	-1.38546000
C	2.15431600	-3.12708100	-0.26418500
C	4.50470300	-2.19681100	-1.45653000
C	3.27351600	-3.94607900	-0.36093100
C	4.45534300	-3.49604900	-0.95560900
H	5.42844500	-1.82505700	-1.89301500
H	3.23179200	-4.94912500	0.05806900
O	-2.15912400	1.53054200	-2.43783700
H	-1.55853300	0.00242800	-3.63666200
C	-2.40079400	1.87447300	-1.08395800
H	-3.18312000	1.22307900	-0.66490900
C	-1.09125300	1.79893100	-0.26020900
H	-1.36585400	1.77845500	0.79648500
C	-2.74340500	3.36520600	-1.06488300
H	-3.32228000	3.60563000	-0.16554800
C	-1.38065200	4.02002100	-1.02770600
C	-0.41222800	3.11408300	-0.58782800
C	-1.02494700	5.32176600	-1.35065400
H	-1.77056000	6.02881000	-1.70329500
C	0.31289800	5.70092700	-1.22689100
C	0.92043200	3.47990200	-0.45669500
H	1.69115800	2.79707600	-0.10638000
C	1.27201100	4.79109500	-0.78594800
H	2.30876700	5.09549200	-0.68993800
H	0.60868600	6.71417000	-1.48121400
H	-3.34121600	3.63068300	-1.94023300
C	4.47078000	1.44958800	1.05494300
O	5.53917300	2.04479400	0.90817900
O	4.45520000	0.12085000	1.17358400
O	3.31021200	2.06480100	1.08022700
H	3.48981900	-0.29018900	1.42048500
C	3.45589700	0.07842400	-1.87605900
H	2.71518000	0.25229900	-2.66495300
H	3.25051500	0.77085000	-1.05244200

H	4.44662100	0.31457900	-2.26725400
C	0.91224900	-3.52741400	0.47763500
H	0.79151900	-2.82054200	1.30836900
H	0.02606400	-3.47473800	-0.16553300
H	0.99427800	-4.54234300	0.87160700
C	5.67680100	-4.37913200	-0.99914800
H	6.31379300	-4.19412400	-0.12795700
H	5.40341400	-5.43742400	-0.99364800
H	6.27615600	-4.18191800	-1.89169600

Re-TS2d

C	-1.12140600	0.26372600	1.26129300
O	-2.00684300	1.16330300	1.97864900
H	-1.13755100	1.40561100	1.00481500
C	0.06027000	-0.30930300	2.01861200
C	-0.02575700	0.01341000	3.49793900
H	0.14006100	-1.39052700	1.87390100
H	0.81541600	-0.43632100	4.02841000
H	-0.03841000	1.09417700	3.63916600
H	-0.96425800	-0.37835100	3.89513100
O	1.29396700	0.25995300	1.47694500
C	2.40479100	-0.44400500	1.67828800
O	2.46102000	-1.49371500	2.28297600
C	3.61357500	0.21084700	1.07805600
C	3.51668700	1.38056500	0.32175600
C	4.85054300	-0.39754400	1.29402200
C	4.66264000	1.95229400	-0.21647200
H	2.54465300	1.83117500	0.15800500
C	6.00565400	0.16454900	0.76585000
H	4.88728200	-1.30943300	1.87950900
C	5.88303300	1.33124600	0.02284600
H	4.62875900	2.85916200	-0.80674700
H	6.98187000	-0.27881000	0.91562900
N	7.10018900	1.93395700	-0.54575200
O	8.15595300	1.35660800	-0.36128200
O	6.97848200	2.97340500	-1.16816600
C	-3.23604000	-1.70601600	-0.88387100
C	-4.59814300	-2.20486500	-1.26143500
C	-1.75966200	-0.61015300	0.32983800
H	-4.77624500	-3.15883900	-0.74205000
N	-2.09601600	-2.17943600	-1.27320300
N	-3.09503700	-0.73285200	0.07561500
N	-1.17263100	-1.49292400	-0.51549900
C	0.21364200	-1.53166200	-0.88071200

C	0.68838600	-0.50145700	-1.70939200
C	1.02797900	-2.57174500	-0.43779100
C	2.02879400	-0.52579400	-2.06840100
C	2.37217800	-2.55053800	-0.82707500
C	2.88762900	-1.54064800	-1.63096700
H	2.42141100	0.26930500	-2.69868200
H	3.02996300	-3.33834600	-0.46730200
O	-5.58050900	-1.25813800	-0.92749000
H	-4.65004600	-2.38105100	-2.33687900
C	-5.53043700	-0.85136500	0.43465000
H	-5.62537600	-1.72488100	1.09390000
C	-4.23749700	-0.04523900	0.69464100
H	-4.01917500	0.05056600	1.75860300
C	-6.63731700	0.19188700	0.60071400
H	-6.90730800	0.29262000	1.65811300
C	-5.97354800	1.44721800	0.08004700
C	-4.58522400	1.30563800	0.10343500
C	-6.55308500	2.61843300	-0.38864800
H	-7.63289300	2.73180000	-0.41307400
C	-5.72183500	3.64106500	-0.84636800
C	-3.75345900	2.31998500	-0.34499500
H	-2.67610400	2.20371700	-0.31439500
C	-4.33535400	3.49109200	-0.83009200
H	-3.70308100	4.29466300	-1.19346200
H	-6.15764700	4.55979900	-1.22595900
H	-7.52932900	-0.10185500	0.04273500
C	-0.22363800	0.60598600	-2.16145600
H	-1.17511700	0.21452900	-2.53481500
H	-0.44604200	1.27198000	-1.32000600
H	0.24376300	1.19236900	-2.95397000
C	0.53026000	-3.66296300	0.47102300
H	-0.55769600	-3.66654400	0.55189700
H	0.85065600	-4.64039600	0.10214400
H	0.95972100	-3.52645600	1.46959900
C	4.34129500	-1.51148400	-2.02044000
H	4.76097700	-0.51489500	-1.84933100
H	4.92352600	-2.23237800	-1.44272600
H	4.46639200	-1.74388800	-3.08270700

Re-TS2b

C	-1.60697100	-0.45171000	-0.56552900
O	-2.12726900	-1.74696600	-0.45507000
H	-1.22482000	-0.33827900	0.62392600
C	-0.33168500	-0.36016600	-1.42249000

C	0.15750500	-1.72522100	-1.86681200
H	-0.46680700	0.29168800	-2.29055000
H	1.08001400	-1.61583800	-2.44036100
H	0.33571000	-2.35392900	-0.99238300
H	-0.60151800	-2.20566200	-2.48626800
O	0.67884900	0.26567700	-0.58805100
C	1.72013100	0.82497300	-1.19998000
O	1.89621700	0.83447500	-2.39914100
C	2.68853400	1.41193300	-0.21762200
C	2.42907500	1.39816200	1.15627800
C	3.86964600	1.95958800	-0.71852800
C	3.36301200	1.92969700	2.03712200
H	1.50017000	0.97281800	1.52340100
C	4.81273700	2.49160700	0.15224200
H	4.03427300	1.95913700	-1.79067700
C	4.53611900	2.46025300	1.51251900
H	3.20033100	1.93704100	3.10770400
H	5.74257100	2.92014600	-0.19953500
N	5.52999600	3.02320100	2.44359800
O	6.54539300	3.49498200	1.96659300
O	5.27429100	2.98380100	3.63279100
C	-4.54196800	1.42277100	-1.59915100
C	-5.98803300	1.47354300	-1.99027900
C	-2.65403000	0.47886200	-0.98624100
H	-6.06610400	1.35552600	-3.08149200
N	-3.66626000	2.37486300	-1.67341600
N	-3.97919000	0.24367600	-1.17644800
N	-2.49260700	1.77984900	-1.28802900
C	-1.34269100	2.59319100	-1.00558900
C	-1.13811700	2.96057300	0.33406200
C	-0.51191100	3.00696500	-2.04498000
C	-0.01556800	3.72955000	0.61762000
C	0.60126600	3.78116200	-1.70303300
C	0.86973100	4.13778400	-0.38542100
H	0.17671300	4.01860100	1.64850600
H	1.28011200	4.09317100	-2.49339000
O	-6.70612600	0.46833800	-1.32026100
H	-6.41243200	2.43895000	-1.71184600
C	-6.18281200	-0.83112700	-1.55418300
H	-6.18013100	-1.04733800	-2.63110400
C	-4.77797400	-0.96255300	-0.92032600
H	-4.23867000	-1.81246200	-1.34150700
C	-7.03110700	-1.79926300	-0.72096400
H	-6.95909700	-2.81233200	-1.13284900

C	-6.38871000	-1.70768900	0.64604500
C	-5.10004600	-1.18495800	0.53912200
C	-6.90330300	-2.03489200	1.89306900
H	-7.90625900	-2.43949300	1.99121600
C	-6.11437200	-1.81473100	3.02432800
C	-4.31748900	-0.94166000	1.65582900
H	-3.33268200	-0.49056900	1.58776400
C	-4.83812200	-1.26385600	2.90936800
H	-4.23458400	-1.07609700	3.79146500
H	-6.50728100	-2.05947700	4.00612700
H	-8.08048200	-1.49615100	-0.73798600
C	-2.10148500	2.55170000	1.41610500
H	-1.99746500	3.21211000	2.27892800
H	-3.13714200	2.61289400	1.06739500
H	-1.92225200	1.52885400	1.76834100
C	-0.74570400	2.62957300	-3.48351000
H	-0.71587200	3.52057700	-4.11556700
H	0.04830600	1.95455700	-3.81998500
H	-1.71063700	2.14246700	-3.63278200
C	2.08894300	4.94534000	-0.02844300
H	2.77300200	5.02982600	-0.87525800
H	1.80950200	5.95485600	0.28843100
H	2.62574200	4.47639900	0.80231500
C	-0.95697800	-0.94388600	2.14346700
O	-1.53503000	-0.33088100	3.03779300
H	-1.91272700	-1.99015200	0.47860300
C	0.15248600	-1.90091800	2.63740400
C	0.91475600	-1.41178900	3.85394300
H	-0.33678600	-2.86052300	2.85034000
H	1.58959000	-2.18078800	4.23591000
H	1.49711700	-0.52088100	3.60037200
H	0.19207300	-1.14047900	4.62545100
O	1.06262800	-2.10719100	1.53245800
C	1.74212000	-3.25851300	1.52118000
O	1.55691700	-4.17685300	2.28562200
C	2.77460200	-3.28927100	0.43637800
C	3.12562700	-2.12480000	-0.24626200
C	3.39532100	-4.50289600	0.14027800
C	4.08874700	-2.16259700	-1.24477700
H	2.63122600	-1.20021000	0.02075800
C	4.36002200	-4.55960600	-0.85712600
H	3.11321100	-5.38898300	0.69779700
C	4.68212200	-3.38599900	-1.52802600
H	4.37549000	-1.27638200	-1.79798500

H	4.86093300	-5.48264600	-1.11954700
N	5.70411800	-3.44104600	-2.58731400
O	6.20341200	-4.52322400	-2.83514800
O	5.98880700	-2.40084700	-3.15195500

Re-M2

C	-1.28045400	-0.48032700	1.68946100
O	-2.04894100	0.38469100	2.47291100
C	0.01152800	-0.96044700	2.23667200
C	0.04550600	-1.00131900	3.75535100
H	0.25297900	-1.94562500	1.83111800
H	1.01277600	-1.37933000	4.09170600
H	-0.12248300	-0.00531300	4.16859700
H	-0.74350700	-1.66123800	4.12284500
O	1.09876400	-0.06566100	1.78936900
C	2.29311300	-0.63330100	1.62453100
O	2.55854100	-1.78084700	1.90553000
C	3.29621800	0.30846900	1.02704100
C	2.98091400	1.63673300	0.73726400
C	4.56068300	-0.20322900	0.73139700
C	3.92703700	2.45767000	0.13509200
H	1.99692300	2.02030800	0.98002400
C	5.51580300	0.60368200	0.13032300
H	4.76921800	-1.24109000	0.96756900
C	5.17250300	1.91949600	-0.15815600
H	3.71776200	3.49164900	-0.10794700
H	6.50409100	0.23753100	-0.11794800
N	6.17717100	2.78240600	-0.80076200
O	7.27002500	2.29926200	-1.03430000
O	5.85617500	3.92762300	-1.06154400
C	-3.25453800	-1.53723300	-1.07734200
C	-4.58508800	-1.59855700	-1.76248100
C	-1.82694100	-0.97550600	0.54523600
H	-5.15124600	-2.46035000	-1.37708600
N	-2.19799500	-2.20549300	-1.37121700
N	-3.11313800	-0.76248400	0.05154100
N	-1.28059000	-1.87793900	-0.36519700
C	0.10237800	-2.03855900	-0.69166800
C	0.83478000	-0.95974000	-1.19791100
C	0.66901800	-3.31285800	-0.55014300
C	2.17363600	-1.17677800	-1.53315500
C	2.00406300	-3.48328900	-0.90047400
C	2.77413200	-2.42506100	-1.38895800
H	2.75960300	-0.34211800	-1.91421400

H	2.45904800	-4.46401700	-0.78160600
O	-5.29929300	-0.40219300	-1.54696500
H	-4.44742400	-1.72296000	-2.83715900
C	-5.48837900	-0.12804900	-0.16775900
H	-6.01321000	-0.96593700	0.31167300
C	-4.12986400	0.17089300	0.50967700
H	-4.22628400	0.07100900	1.59417900
C	-6.23766300	1.20568400	-0.08169600
H	-6.76790700	1.27970100	0.87470900
C	-5.12044700	2.22129000	-0.16961500
C	-3.89854800	1.62101600	0.13635700
C	-5.17552300	3.56530800	-0.51350500
H	-6.12294500	4.03689900	-0.75768900
C	-3.98797400	4.29727400	-0.56250000
C	-2.71241800	2.33954900	0.07538200
H	-1.75941400	1.85091500	0.26079300
C	-2.76596000	3.68826300	-0.27986400
H	-1.84912900	4.26554900	-0.34379300
H	-4.01372800	5.34636500	-0.83929800
H	-6.97130300	1.28727500	-0.88720500
H	-1.71377900	1.28615500	2.37499900
C	4.21785000	-2.64057800	-1.76230800
H	4.72098000	-1.69088400	-1.95962200
H	4.75582500	-3.15544100	-0.96064100
H	4.30126000	-3.25984900	-2.66116300
C	0.22046800	0.40359700	-1.35172700
H	-0.81356700	0.34420500	-1.70618300
H	0.21062000	0.91309100	-0.38089100
H	0.79646800	1.00947500	-2.05440300
C	-0.16347400	-4.44972500	-0.02348500
H	-1.01895800	-4.63838900	-0.67852200
H	0.43010500	-5.36221300	0.05451000
H	-0.56725200	-4.21001300	0.96586600

Si-M2

C	0.43250800	0.46772500	-0.89637900
O	0.12224400	1.77738300	-1.26879900
C	-0.27298100	-0.56289000	-1.70251700
C	-0.08727500	-0.37851900	-3.20087500
H	0.00997300	-1.57476700	-1.40885500
H	-0.71187600	-1.08168000	-3.75561200
H	-0.36090300	0.64071800	-3.47995500
H	0.95822200	-0.55343000	-3.46782400
O	-1.73032800	-0.44155200	-1.52072500

C	-2.24294700	-0.83424600	-0.36354600
O	-1.62507700	-1.39326100	0.51880600
C	-3.70708000	-0.52966800	-0.25428000
C	-4.38694800	0.16382900	-1.25745000
C	-4.37584000	-0.96301200	0.89157900
C	-5.74426200	0.42479300	-1.11906600
H	-3.84857200	0.49638700	-2.13678100
C	-5.73214400	-0.71084000	1.04261800
H	-3.81769300	-1.49430300	1.65403100
C	-6.38524000	-0.02122100	0.02895000
H	-6.30418700	0.95984300	-1.87527500
H	-6.28364200	-1.03211700	1.91695700
N	-7.82529200	0.24863900	0.17895600
O	-8.37541300	-0.16361800	1.18380600
O	-8.38078900	0.86607300	-0.71109000
C	2.22606200	-0.44951100	2.06338900
C	2.63949300	-1.45092400	3.09628500
C	1.16799100	0.28737500	0.23722200
H	1.86498900	-1.50979700	3.87622700
N	2.40697700	0.82053100	2.11155800
N	1.50668800	-0.85962300	0.96129500
N	1.75548200	1.30872500	0.98055500
C	2.12880400	2.60585000	0.52467900
C	3.02054800	2.74547200	-0.54397400
C	1.60524500	3.71713300	1.19772000
C	3.35441100	4.03897800	-0.95633900
C	1.98278800	4.98468300	0.76783700
C	2.85220100	5.16618500	-0.31155800
H	4.04145800	4.16224900	-1.79061900
H	1.57741600	5.85626500	1.27721600
O	2.83384500	-2.71391900	2.50069800
H	3.57861800	-1.14191900	3.55651600
C	1.66536200	-3.16748400	1.83787600
H	0.82555500	-3.20760100	2.54517600
C	1.34541500	-2.26478700	0.62240000
H	0.29924900	-2.43036800	0.35133300
C	2.00922500	-4.51797500	1.20274500
H	1.09573600	-5.10322900	1.04588400
C	2.63661200	-4.11862600	-0.11362600
C	2.28670500	-2.80593400	-0.43667700
C	3.46940600	-4.84873300	-0.95017200
H	3.75088400	-5.86739000	-0.69958900
C	3.95821900	-4.24450900	-2.10985300
C	2.78080200	-2.19478300	-1.58131200

H	2.52943300	-1.16242700	-1.80608500
C	3.62354600	-2.92719000	-2.41956900
H	4.02587900	-2.46542500	-3.31555400
H	4.61669100	-4.80137800	-2.76886500
H	2.67526200	-5.09040300	1.85272100
H	0.88033200	2.19548900	-1.70006300
C	3.60334900	1.54178200	-1.23915300
H	3.83392800	0.74511000	-0.52500300
H	2.90224400	1.11849700	-1.97064200
H	4.51855900	1.81121500	-1.76950300
C	0.63721900	3.51655400	2.33038400
H	-0.22423600	2.93520800	1.98718500
H	1.10190700	2.95351700	3.14476800
H	0.28586400	4.47486100	2.71713700
C	3.25045100	6.55370600	-0.74509600
H	2.38194600	7.21637700	-0.78905800
H	3.96124900	6.99273500	-0.03774700
H	3.72298900	6.54171800	-1.72968200

TS3

C	1.26839100	0.80052600	1.70802600
O	1.82631100	-0.28445600	2.36419100
C	0.19774200	1.47337900	2.29098100
C	-0.01575700	1.34097000	3.77182400
H	-0.10956300	2.41080100	1.84191400
H	-0.95915400	1.80094200	4.06368300
H	-0.01973600	0.29064400	4.06430800
H	0.80623800	1.83757800	4.29793600
O	-1.49784200	0.71841800	1.77984400
C	-1.50396400	-0.53770100	1.58401800
O	-0.59154000	-1.34694100	1.83789300
C	-2.76330200	-1.07223000	0.92956100
C	-3.80741000	-0.20821300	0.59264200
C	-2.85589000	-2.43488800	0.64533700
C	-4.94427100	-0.69954700	-0.03678100
H	-3.70772800	0.84592700	0.82718900
C	-3.98619800	-2.94433200	0.01992600
H	-2.02774700	-3.07731700	0.92234800
C	-5.00648300	-2.06077300	-0.30996800
H	-5.77241500	-0.05889900	-0.31293500
H	-4.08991800	-3.99602700	-0.21508500
N	-6.20455000	-2.59034300	-0.97813200
O	-6.24694900	-3.78710400	-1.20183600
O	-7.08668600	-1.80282300	-1.27189700

C	3.16699200	1.25978800	-1.29048100
C	4.43289100	1.03098400	-2.05747300
C	1.79250000	1.10576200	0.43665700
H	5.15053800	1.82558300	-1.80223800
N	2.23065900	2.10689200	-1.55943000
N	2.95263600	0.60638000	-0.10106100
N	1.36472600	2.00749000	-0.48896100
C	0.06825700	2.60598600	-0.59707400
C	-0.98323500	1.82044100	-1.07364200
C	-0.08281200	3.94960800	-0.24930400
C	-2.23711600	2.42107400	-1.17597600
C	-1.35502500	4.50509400	-0.36187900
C	-2.44194800	3.75283100	-0.81472600
H	-3.07262300	1.83161500	-1.54698100
H	-1.50209300	5.54810400	-0.09225700
O	4.96313400	-0.23683600	-1.75949900
H	4.23322800	1.07277400	-3.12892100
C	5.17746200	-0.43265500	-0.36909700
H	5.85132700	0.34240600	0.02105700
C	3.82338800	-0.46850000	0.37979000
H	3.97252700	-0.32467400	1.45213100
C	5.70384300	-1.86126000	-0.21554400
H	6.24040900	-1.96677400	0.73427500
C	4.43155200	-2.67856900	-0.22376300
C	3.33469700	-1.87454400	0.09160700
C	4.25736900	-4.02659300	-0.50454400
H	5.10706100	-4.65430000	-0.75639600
C	2.96649600	-4.55586500	-0.47754700
C	2.04722500	-2.39156700	0.11801600
H	1.18828400	-1.77447600	0.36515000
C	1.87336100	-3.74521100	-0.17444500
H	0.87389300	-4.16801800	-0.16221000
H	2.81066800	-5.60608700	-0.70298000
H	6.39153800	-2.10499500	-1.02859400
H	1.10136700	-0.94916100	2.36424500
C	-3.81736900	4.36372700	-0.88880900
H	-4.33811500	4.25255500	0.06805900
H	-3.76556200	5.43149800	-1.11362800
H	-4.42520600	3.87816600	-1.65555300
C	-0.74877900	0.39133200	-1.47955800
H	-0.00910300	0.33454400	-2.28519000
H	-0.36369200	-0.20132800	-0.64246100
H	-1.67594000	-0.07099700	-1.82381000
C	1.09899000	4.74258900	0.24038300

H	1.88718100	4.77202000	-0.51769300
H	0.80736400	5.76608300	0.48102200
H	1.53166400	4.28693300	1.13818500

M3

C	-0.09381900	-1.35560800	2.41994800
C	-0.20565300	-2.65323700	3.16059400
H	0.18581200	-0.44997500	2.95461900
H	0.74987100	-2.96947400	3.59720700
H	-0.93165100	-2.60512100	3.98098500
H	-0.53200200	-3.42812500	2.46301700
O	-0.72508700	-2.14101900	0.22588400
C	-0.37478000	-1.27215700	1.08649400
C	0.58835900	1.99040500	-0.29782300
C	1.63121800	3.03992000	-0.52845900
C	-0.21046900	0.11591300	0.50739700
H	1.54591700	3.81379900	0.24884500
N	-0.66646600	1.99074600	-0.63832300
N	0.91043900	0.85813600	0.40389200
N	-1.14390200	0.81330600	-0.13311500
C	-2.52357900	0.44404500	-0.29828000
C	-2.88494300	-0.24774900	-1.45511900
C	-3.42169700	0.79079300	0.70823000
C	-4.23036000	-0.57348500	-1.60028300
C	-4.75717500	0.43946400	0.51700000
C	-5.17665600	-0.23377100	-0.63046700
H	-4.54527400	-1.11860400	-2.48671700
H	-5.48301800	0.69243600	1.28571300
O	2.90591000	2.44301100	-0.51342300
H	1.48658900	3.50463800	-1.50427500
C	3.18938900	1.75319200	0.69605300
H	3.09379500	2.43882000	1.54874500
C	2.27033200	0.51375400	0.83003600
H	2.21018800	0.17824300	1.86959500
C	4.58546500	1.14609700	0.53163100
H	5.04016600	0.97365000	1.51366500
C	4.30323000	-0.15835800	-0.17965100
C	2.96268200	-0.51869300	-0.03546900
C	5.16936000	-0.96738200	-0.90266300
H	6.21231700	-0.69177600	-1.02764200
C	4.66831400	-2.13430800	-1.48039300
C	2.45062800	-1.68039800	-0.60019700
H	1.40339100	-1.96149600	-0.49003500

C	3.32645600	-2.48391600	-1.33270100
H	2.95438300	-3.39421400	-1.79133800
H	5.32909000	-2.77377700	-2.05722200
H	5.23050300	1.82618900	-0.02964000
C	-1.83907700	-0.65537800	-2.45359800
H	-1.28109100	0.21201800	-2.82040900
H	-1.13915400	-1.33679600	-1.95624300
H	-2.29404700	-1.16112500	-3.30665600
C	-2.94776800	1.48623900	1.95621900
H	-2.27337100	0.83094200	2.51926700
H	-2.40122600	2.40324900	1.71424800
H	-3.79132900	1.74665400	2.59722400
C	-6.62899900	-0.58147700	-0.83183200
H	-7.10472400	0.12889800	-1.51575100
H	-6.73763200	-1.57830300	-1.26616200
H	-7.17733900	-0.55543500	0.11208900

TS4R

C	1.17561700	-0.36437700	-1.78398600
C	1.39334900	0.56898400	-2.93521000
H	2.01729700	-0.91435300	-1.38546100
H	2.35364500	1.08460600	-2.84422300
H	1.38878900	0.04341700	-3.89900500
H	0.58881000	1.31049800	-2.97423900
O	-1.18570500	-0.30774100	-2.01370200
C	-0.13612000	-0.71524600	-1.45636900
C	-1.27495500	-1.96991100	1.76015300
C	-2.27445000	-1.88403900	2.86927900
C	-0.36043200	-1.45737100	-0.15748400
H	-1.97837900	-1.04674600	3.51781600
N	-0.08925600	-2.49755600	1.80887200
N	-1.50161300	-1.35914300	0.55966400
N	0.47126700	-2.17052400	0.61129300
C	1.80087000	-2.63256500	0.33187500
C	2.00209000	-3.51300600	-0.73544900
C	2.83101700	-2.20223500	1.17664500
C	3.30994100	-3.92993800	-0.98023200
C	4.11735200	-2.65286400	0.88437900
C	4.37776200	-3.50337400	-0.19145700
H	3.49496900	-4.61033700	-1.80750500
H	4.93903500	-2.32542800	1.51767300
O	-3.56083100	-1.68948700	2.33974900
H	-2.27604500	-2.80837600	3.44821700

C	-3.63312700	-0.52894900	1.52082800
H	-3.31290900	0.35422800	2.08531200
C	-2.79082800	-0.72425700	0.23654600
H	-2.57949300	0.23780200	-0.22873200
C	-5.06851700	-0.47499700	0.99223900
H	-5.32097900	0.54744300	0.68892100
C	-5.01795100	-1.40147000	-0.20127400
C	-3.70194500	-1.56106000	-0.63714000
C	-6.05606100	-2.05234600	-0.85499400
H	-7.08182800	-1.93623700	-0.51769300
C	-5.75499600	-2.87292200	-1.94239000
C	-3.39490800	-2.36457500	-1.72568400
H	-2.37161400	-2.45102100	-2.07515700
C	-4.43743000	-3.02891200	-2.37244800
H	-4.22061800	-3.66825000	-3.22214300
H	-6.55393000	-3.39710700	-2.45734100
H	-5.77232900	-0.78709600	1.76734700
C	1.79467400	2.03134500	-0.00009300
O	1.22252100	0.76480300	0.08323300
H	1.21257100	2.75327900	-0.58333400
N	1.48847200	1.91235600	1.40002500
S	-0.08496900	2.24921000	1.90346100
O	0.06655600	3.11165500	3.07029900
O	-0.80735000	0.98237700	2.06681300
C	-0.91609400	3.18286000	0.63708300
C	-1.29238200	2.56049900	-0.55365700
C	-1.18008800	4.52832600	0.86400900
C	-1.95083700	3.30462000	-1.52251100
H	-1.05632700	1.51814600	-0.74234900
C	-1.85085000	5.25539200	-0.11654000
H	-0.87521900	4.98382300	1.80002800
C	-2.24303700	4.65925200	-1.31721200
H	-2.24069300	2.81797400	-2.45017900
H	-2.07492500	6.30378200	0.05692900
C	-2.94964700	5.45253900	-2.38444700
H	-2.27816400	5.64586400	-3.22686400
H	-3.81125400	4.90325500	-2.77274100
H	-3.29618300	6.41405000	-2.00076000
C	3.25876700	2.08401600	-0.31820300
C	4.06469700	0.97221000	-0.07773300
C	3.81262000	3.24161500	-0.86009000
C	5.42216900	1.02189700	-0.37252100
H	3.61251300	0.07169800	0.32320900
C	5.17452400	3.29412500	-1.14704400

H	3.17832000	4.10173500	-1.05923300
C	5.97986500	2.18436900	-0.90373900
H	6.04470600	0.15080300	-0.19011300
H	5.60417700	4.19791600	-1.56661900
H	7.03986100	2.22294400	-1.13385000
C	2.57389800	-1.29048000	2.34709700
H	1.89086500	-0.47926800	2.07995200
H	2.12641800	-1.84785300	3.17452000
H	3.51166100	-0.84955100	2.69182200
C	0.87088000	-3.98180100	-1.61166800
H	-0.02608100	-4.20984300	-1.02842700
H	0.60689300	-3.21312800	-2.34646300
H	1.16307200	-4.88158100	-2.15543300
C	5.78798800	-3.93462800	-0.49861900
H	6.31753200	-3.14984800	-1.04867500
H	6.34876700	-4.12933700	0.41876300
H	5.80238900	-4.83842600	-1.11110200

TS4S

C	-0.94736100	-0.79819800	1.46746800
C	-0.47642800	-0.81433100	2.89072800
H	-1.04356400	-1.73470000	0.92960300
H	-1.31091800	-0.98219200	3.58397300
H	0.25610600	-1.60771200	3.05811200
H	-0.02867900	0.14891000	3.15273800
O	-1.71672600	1.46020800	1.51433800
C	-1.57946100	0.34037300	0.97474000
C	-3.44482300	-0.31410900	-2.11932500
C	-4.46831300	-1.11164700	-2.86675100
C	-2.17578000	0.21533600	-0.41774500
H	-3.96043100	-1.88183700	-3.46539200
N	-2.71133200	0.67356200	-2.54100000
N	-3.15004800	-0.62631700	-0.81806900
N	-1.93511100	0.99610900	-1.46787300
C	-0.89873700	1.99042000	-1.57286200
C	-1.15397600	3.27936300	-1.10010900
C	0.31047000	1.59504000	-2.14898500
C	-0.09326700	4.18176900	-1.14250000
C	1.33976200	2.53455700	-2.15443700
C	1.16309600	3.81638500	-1.63226400
H	-0.24950000	5.19133100	-0.76960000
H	2.30645800	2.24469300	-2.55677800
O	-5.36914500	-1.69004800	-1.95226300
H	-5.03423800	-0.46164500	-3.53474200

C	-4.73012100	-2.51372100	-0.98868000
H	-4.14223500	-3.29360500	-1.49016500
C	-3.86362700	-1.64658500	-0.04076200
H	-3.11177300	-2.26563900	0.45683100
C	-5.83172300	-3.05054400	-0.07123900
H	-5.50611400	-3.98304100	0.40329900
C	-5.99276500	-1.94509000	0.94743100
C	-4.87388900	-1.11049500	0.95259500
C	-7.05134100	-1.69829900	1.81096600
H	-7.92849400	-2.33824400	1.80903900
C	-6.97364900	-0.60294900	2.67132000
C	-4.78353300	-0.01828100	1.80623600
H	-3.91625400	0.63747900	1.81037400
C	-5.85486900	0.22932600	2.66581100
H	-5.81366700	1.08072700	3.33687500
H	-7.79624600	-0.39193100	3.34709400
H	-6.73642300	-3.25801700	-0.64720300
C	1.92053900	-0.29309400	0.99625500
O	0.77199400	-0.45879700	0.22555500
H	2.10772800	-1.13509900	1.67386900
N	2.45771400	-0.41443800	-0.32864300
S	2.81955700	-2.00603200	-0.73992800
O	2.64584700	-2.12481100	-2.18399400
O	2.16854600	-2.97518500	0.14324000
C	4.56059900	-2.03693100	-0.38398700
C	5.45213000	-1.50175400	-1.31135400
C	5.00089500	-2.55673800	0.82889500
C	6.80683200	-1.49113600	-1.00984900
H	5.07889300	-1.11248600	-2.25284300
C	6.36266500	-2.53530300	1.11385500
H	4.28424600	-2.98334400	1.52316000
C	7.28048900	-2.00525500	0.20347900
H	7.51301800	-1.07939700	-1.72547300
H	6.72023900	-2.94158200	2.05566600
C	8.75674500	-2.00962400	0.50203400
H	9.22646600	-1.07878700	0.17462500
H	8.94554700	-2.13519900	1.57011400
H	9.25330400	-2.83110700	-0.02434600
C	2.15817700	1.04013300	1.64031900
C	1.39211400	2.15067500	1.29654100
C	3.18803600	1.16153100	2.57352100
C	1.66604700	3.38410800	1.88204900
H	0.57640400	2.04295300	0.59167800
C	3.46441600	2.39630900	3.15187300

H	3.77828500	0.28735700	2.83984300
C	2.70197200	3.51094600	2.80481800
H	1.05985700	4.24486400	1.61373300
H	4.26801600	2.48930300	3.87547300
H	2.91024100	4.47389400	3.26100000
C	2.32024700	4.77483200	-1.54708200
H	2.82958400	4.64449100	-0.58525400
H	3.05083100	4.59297300	-2.33832400
H	1.98539400	5.81293500	-1.61104200
C	0.47212200	0.23603900	-2.76985500
H	0.11759200	-0.55309100	-2.10225800
H	-0.09786800	0.18111700	-3.70367100
H	1.52062100	0.02543300	-2.97710000
C	-2.50848200	3.66378400	-0.57235700
H	-3.29335400	3.41071000	-1.29233600
H	-2.70378300	3.12437000	0.35845100
H	-2.55212500	4.73723000	-0.38081700

M4R

C	0.17578100	1.17029400	2.14974700
C	0.56337800	0.35222400	3.37905200
H	-0.07409600	2.19192000	2.48070000
H	1.51589900	0.72576400	3.76159600
H	-0.20114400	0.46872600	4.14814300
H	0.64125300	-0.70715200	3.13038500
O	-2.02463000	0.21330300	2.27288000
C	-1.14400100	0.65330200	1.57410000
C	-1.92619100	0.07119800	-1.91201900
C	-2.36640900	-0.91843400	-2.94370500
C	-1.40611300	0.73296100	0.08486600
H	-1.49341700	-1.54035400	-3.18548900
N	-1.31772400	1.21330000	-2.07951600
N	-2.06254000	-0.22663000	-0.58853600
N	-1.00809100	1.62115500	-0.82440200
C	-0.39015800	2.89589000	-0.59385600
C	-1.02428200	3.78946800	0.27436600
C	0.82258300	3.18097200	-1.23823300
C	-0.36478800	4.98962000	0.55088400
C	1.42732200	4.39339700	-0.92555500
C	0.86346700	5.30015200	-0.02471400
H	-0.83623900	5.70134900	1.22391600
H	2.38415100	4.62478100	-1.38803700
O	-3.42617800	-1.69122300	-2.43514400
H	-2.71701200	-0.40373800	-3.83919000

C	-3.08358500	-2.38917600	-1.23897400
H	-2.21164700	-3.02644200	-1.40197400
C	-2.84609700	-1.37293600	-0.09250500
H	-2.26781500	-1.82675800	0.71929100
C	-4.35480800	-3.11712700	-0.80068600
H	-4.10103600	-3.94636300	-0.13085200
C	-5.12189900	-2.03791700	-0.07369800
C	-4.26262800	-1.00845300	0.31662700
C	-6.48033300	-1.96229900	0.20158300
H	-7.15042100	-2.75991300	-0.10527100
C	-6.97330100	-0.83391700	0.85668000
C	-4.74810600	0.11851200	0.96483400
H	-4.08042200	0.91720100	1.26968900
C	-6.11578700	0.20014000	1.22856000
H	-6.51428500	1.07713800	1.72819500
H	-8.03481400	-0.75477100	1.06866600
H	-4.88134700	-3.52368000	-1.66734200
C	1.92463600	0.24991600	0.68971800
O	1.18474900	1.37053900	1.20234200
H	2.18532100	-0.40207500	1.54055900
N	1.21388000	-0.43887600	-0.35076600
S	0.66850400	-1.87656700	-0.02317500
O	-0.06411400	-2.36629600	-1.20837500
O	-0.08120800	-1.94232200	1.26186600
C	2.04477200	-2.99997800	0.20273300
C	2.50451400	-3.30019300	1.48170400
C	2.69761300	-3.49916000	-0.92107600
C	3.63165500	-4.10176300	1.63054500
H	1.96603800	-2.92219000	2.34518800
C	3.82052900	-4.30236100	-0.75688600
H	2.31461600	-3.26280400	-1.90920500
C	4.30460000	-4.61271400	0.51750800
H	3.99343500	-4.34012000	2.62744300
H	4.32967800	-4.69901100	-1.63108000
C	5.51022800	-5.49879300	0.69566200
H	6.20733500	-5.07354800	1.42261000
H	5.21499400	-6.48639800	1.06412900
H	6.04193700	-5.63867300	-0.24781600
C	3.21547500	0.85374300	0.14256500
C	3.64546400	2.12940300	0.50880500
C	3.98734000	0.10659600	-0.74860200
C	4.82003700	2.65731300	-0.02574700
H	3.04156200	2.71718100	1.19012200
C	5.16644000	0.62802600	-1.27131700

H	3.64037300	-0.87827700	-1.04538800
C	5.58419400	1.90995700	-0.91722200
H	5.13565700	3.65788500	0.25588900
H	5.75584400	0.03642100	-1.96521700
H	6.49881300	2.32138800	-1.33295800
C	-2.38470600	3.53063100	0.87890500
H	-3.03065100	2.96730500	0.19928800
H	-2.33018500	2.97771200	1.82379800
H	-2.87542700	4.48139600	1.09418700
C	1.46524900	2.24217700	-2.22205300
H	1.00532200	2.35853400	-3.20840100
H	2.53159700	2.46822100	-2.30060900
H	1.35135400	1.19969300	-1.91243600
C	1.57680500	6.58593800	0.30200200
H	0.97011500	7.22651800	0.94497200
H	2.52022200	6.38198100	0.81802700
H	1.81741200	7.14190800	-0.60833900

M4S

C	0.26507300	0.92043500	2.16228800
C	0.18402800	2.05520600	3.18138300
H	0.51446500	-0.02324300	2.66768800
H	-0.63405300	1.88144600	3.88325500
H	1.12564700	2.10404800	3.73097000
H	0.03666400	3.00876400	2.66655700
O	-2.05404800	0.33388800	2.29441300
C	-1.12560200	0.64421500	1.58748800
C	-1.88887700	0.03320000	-1.90264400
C	-2.33298100	-0.96263400	-2.92685600
C	-1.36902300	0.70545600	0.09215300
H	-1.46382100	-1.59460100	-3.15604200
N	-1.25873700	1.16207000	-2.07716800
N	-2.03944100	-0.24784500	-0.57662500
N	-0.94776400	1.57548100	-0.82398000
C	-0.32586100	2.84992500	-0.60271000
C	-0.96559000	3.75889400	0.24523200
C	0.88784500	3.12657300	-1.24909800
C	-0.30297000	4.96043400	0.51135700
C	1.49707000	4.33861600	-0.94407300
C	0.93183200	5.25792300	-0.05679000
H	-0.77727300	5.68192100	1.17212600
H	2.45762800	4.56026900	-1.40359400
O	-3.40286300	-1.72077500	-2.41753300
H	-2.67344200	-0.45392600	-3.82966500

C	-3.07905300	-2.40491300	-1.20816400
H	-2.21000000	-3.05082700	-1.35169400
C	-2.84799300	-1.37322800	-0.07399000
H	-2.28737400	-1.82169200	0.75303600
C	-4.36197600	-3.11459000	-0.77550600
H	-4.12517200	-3.93268500	-0.08598800
C	-5.13021400	-2.01498000	-0.08092300
C	-4.26763600	-0.98619900	0.30504200
C	-6.49216100	-1.92260300	0.17013400
H	-7.16409100	-2.71970200	-0.13404700
C	-6.98567200	-0.77846400	0.79694400
C	-4.75341200	0.15594000	0.92634300
H	-4.08409900	0.95279700	1.23203400
C	-6.12475500	0.25376700	1.16543400
H	-6.52324800	1.14283800	1.64321600
H	-8.04984500	-0.68585600	0.98927100
H	-4.87908700	-3.53348000	-1.64193300
C	1.98820100	0.16810500	0.64085000
O	1.22161000	1.25068400	1.20132100
H	2.27229300	-0.48605300	1.48699000
N	1.28637400	-0.53128800	-0.39563900
S	0.67504700	-1.93252400	-0.02732900
O	-0.04704200	-2.44035500	-1.21111600
O	-0.10899800	-1.92528200	1.24036500
C	2.00352200	-3.09266000	0.27721300
C	2.71551100	-3.59611800	-0.81144900
C	2.36631000	-3.42532300	1.57637500
C	3.79685600	-4.43635900	-0.58760000
H	2.40688900	-3.33243700	-1.81873500
C	3.45650300	-4.26853200	1.78595000
H	1.78476100	-3.03831100	2.40676600
C	4.18426200	-4.78332200	0.71352500
H	4.35230600	-4.83598000	-1.43223900
H	3.74222000	-4.53288100	2.80044400
C	5.34877900	-5.71273400	0.93768900
H	6.20575800	-5.42540400	0.32261700
H	5.66186600	-5.71037200	1.98388100
H	5.08303500	-6.74020900	0.66920600
C	3.25462100	0.80806600	0.08541300
C	3.67053200	2.07964100	0.48053700
C	4.01925700	0.09912300	-0.84212800
C	4.82236400	2.64386200	-0.06600600
H	3.07129000	2.63670800	1.19179200
C	5.17594700	0.65660900	-1.37707200

H	3.67939400	-0.88233400	-1.15750600
C	5.57778700	1.93631700	-0.99686100
H	5.12724200	3.64165700	0.23662900
H	5.75930700	0.09636000	-2.10140500
H	6.47416600	2.37665500	-1.42256300
C	1.63925600	6.55322600	0.24434500
H	1.14660800	7.09807900	1.05198100
H	2.67698000	6.36868900	0.53645100
H	1.65883600	7.19895000	-0.63885900
C	1.52164200	2.18498600	-2.23590600
H	1.06327000	2.31456900	-3.22145300
H	2.59065900	2.39910500	-2.31292000
H	1.39445100	1.14147800	-1.93600000
C	-2.33362900	3.51821900	0.83937400
H	-2.96776900	2.92675300	0.17277500
H	-2.28866000	3.00305100	1.80560900
H	-2.82962900	4.47556400	1.00913500
TS5R			
C	0.86455900	1.11405800	-1.46817100
C	0.25513200	2.30326200	-2.18961400
H	1.50655300	0.56966900	-2.16984000
H	1.05262400	2.89063800	-2.64951400
H	-0.42758200	1.94888500	-2.96486900
H	-0.31274600	2.94483400	-1.51458200
O	-1.28895100	-0.03188500	-1.50909600
C	-0.19977600	0.13341200	-0.96213100
C	0.45934600	-2.81177300	1.12557300
C	-0.02651400	-3.69087900	2.23885300
C	0.36724800	-1.10366500	-0.22852900
H	0.29976100	-3.23809000	3.18768300
N	1.67043700	-2.68856000	0.66737800
N	-0.37868600	-1.89234500	0.56257900
N	1.59583900	-1.62582400	-0.19026100
C	2.71244200	-1.37701000	-1.06542900
C	2.54832200	-1.67106200	-2.42397900
C	3.91920300	-0.93838400	-0.51679300
C	3.63867800	-1.44615900	-3.26203000
C	4.97688300	-0.73290800	-1.40068600
C	4.85367200	-0.96720300	-2.77035800
H	3.53738700	-1.66083400	-4.32271800
H	5.92545300	-0.38092900	-1.00310600
O	-1.42196100	-3.82834000	2.19143000
H	0.41588800	-4.68470200	2.15712300
C	-2.13084400	-2.59048400	2.13113100

H	-1.89887900	-1.96812200	3.00470300
C	-1.82433000	-1.87458200	0.80101600
H	-2.13905100	-0.82917200	0.84847900
C	-3.60520800	-2.96692500	1.98248300
H	-4.23376500	-2.11059800	2.25123800
C	-3.70353100	-3.27683200	0.50445400
C	-2.65313000	-2.66946300	-0.18837800
C	-4.63953600	-4.04332900	-0.17494600
H	-5.45598400	-4.52164900	0.35792500
C	-4.50204100	-4.20478500	-1.55465200
C	-2.51354000	-2.81838500	-1.55954000
H	-1.70960000	-2.31889900	-2.08889400
C	-3.44784500	-3.60194600	-2.23891900
H	-3.35460600	-3.73867100	-3.31155000
H	-5.21994900	-4.80974200	-2.09942200
H	-3.86084200	-3.80786400	2.63088500
C	0.95271700	1.93888100	0.72315300
O	1.71017400	1.44452200	-0.38875900
H	0.73235700	3.00758600	0.54852200
N	-0.24962600	1.13996300	0.79041200
S	-1.54136200	1.90275600	1.40151400
O	-1.12135300	2.74279400	2.52701100
O	-2.59018600	0.90099500	1.63156100
C	-2.18792500	3.01708900	0.17011200
C	-2.97680900	2.51025800	-0.86112900
C	-1.82881600	4.36056000	0.20866900
C	-3.39348900	3.36731700	-1.87062800
H	-3.23887000	1.45794200	-0.87464800
C	-2.25163400	5.20401100	-0.81599900
H	-1.23477800	4.72982900	1.03833500
C	-3.03373200	4.72066600	-1.86667700
H	-4.00721300	2.98254400	-2.68073400
H	-1.97356800	6.25418800	-0.79619100
C	-3.51324100	5.63990000	-2.95984800
H	-3.48922700	5.14192200	-3.93242700
H	-4.54663600	5.95130800	-2.77561400
H	-2.89912700	6.54116000	-3.01760700
C	1.86904600	1.82102100	1.92490900
C	3.07553600	2.52271200	1.91024500
C	1.57192500	0.98558100	2.99793900
C	3.98731700	2.37539700	2.94940800
H	3.30396300	3.17067100	1.06809100
C	2.48639000	0.83573100	4.03959100
H	0.62466100	0.45607500	3.00343100

C	3.69650600	1.52339500	4.01460200
H	4.92546100	2.92139900	2.92967400
H	2.25094300	0.18292300	4.87458200
H	4.40781000	1.40506100	4.82597700
C	1.24905400	-2.20467100	-2.97403900
H	0.84624900	-3.00366400	-2.34280200
H	0.48136900	-1.42455300	-3.04871400
H	1.40415200	-2.61086900	-3.97457000
C	4.08655300	-0.73817800	0.96200700
H	4.22973400	-1.70287300	1.45868200
H	4.95344300	-0.10842200	1.16857100
H	3.20712000	-0.26321600	1.39918500
C	6.00722600	-0.69748200	-3.70043300
H	5.93372600	-1.29913500	-4.60891900
H	6.02056600	0.35583000	-3.99863700
H	6.96258900	-0.91476900	-3.21731300

TS5S

C	-0.54369200	-0.16078800	2.14544300
C	-0.23460600	-1.24965000	3.15544400
H	-0.49128900	0.81821400	2.64989200
H	-0.46875400	-2.23335800	2.74843800
H	0.81721100	-1.20556700	3.45155600
H	-0.84900400	-1.09894200	4.04531700
O	1.43907000	0.82500900	1.33593100
C	0.52154300	0.04523300	1.05099600
C	2.05116700	-1.74201200	-1.74159800
C	3.05587400	-1.73410700	-2.85264500
C	0.93680300	-0.97871000	-0.02320900
H	2.58797900	-1.27022700	-3.73382300
N	1.04340900	-2.55190700	-1.61082800
N	2.04943800	-0.78252400	-0.76994100
N	0.36045300	-2.06922600	-0.53662400
C	-0.76060300	-2.85350500	-0.08758500
C	-0.50590900	-3.82955500	0.88230700
C	-1.97359700	-2.74628600	-0.76785300
C	-1.57119100	-4.63620400	1.27285100
C	-3.00162300	-3.59296600	-0.34951400
C	-2.82925800	-4.52038600	0.67587000
H	-1.40962200	-5.38751900	2.04176500
H	-3.96763900	-3.51104400	-0.84193900
O	4.20779100	-1.03797900	-2.46162900
H	3.33903500	-2.75751000	-3.10304100
C	3.91398600	0.27815500	-2.00604900

H	3.37598200	0.83951700	-2.78024300
C	3.12408700	0.22937000	-0.68164100
H	2.64105600	1.18637600	-0.49467300
C	5.25381400	0.88509700	-1.58521300
H	5.18634600	1.97869300	-1.57767800
C	5.43292800	0.33829600	-0.18606300
C	4.20333400	-0.06985900	0.33583300
C	6.59243500	0.20904200	0.56572000
H	7.55086500	0.52325900	0.16295700
C	6.50753200	-0.34739200	1.84250600
C	4.11094200	-0.61533600	1.60734300
H	3.14929800	-0.91043500	2.01450100
C	5.27888800	-0.75906600	2.35704000
H	5.22878800	-1.19056800	3.35154500
H	7.40690200	-0.46449700	2.43882300
H	6.04375600	0.59207400	-2.28060700
C	-2.11162100	0.68356300	0.71320800
O	-1.82974100	-0.35487500	1.63106700
H	-2.17487700	1.64095900	1.26673800
N	-0.94376300	0.69091800	-0.16272500
S	-0.59985800	1.88494800	-1.17816200
O	-1.52125100	1.94643500	-2.31733700
O	0.82587100	1.74003700	-1.50913400
C	-0.81285600	3.42077400	-0.28823100
C	-1.67014700	4.39121700	-0.79103000
C	-0.12140700	3.61814400	0.90773000
C	-1.84294100	5.57848100	-0.08297500
H	-2.18663200	4.20965000	-1.72798900
C	-0.30842500	4.80656600	1.60076700
H	0.55028900	2.84662600	1.28047500
C	-1.16972000	5.80120100	1.11833300
H	-2.51336000	6.34063800	-0.46995300
H	0.22037900	4.97081500	2.53609000
C	-1.34994600	7.08462500	1.88631700
H	-0.42830600	7.67467300	1.87742200
H	-2.14635800	7.69573800	1.45710100
H	-1.59772700	6.88307900	2.93220900
C	-3.47210400	0.40204500	0.09559100
C	-4.20204300	-0.72720700	0.46806600
C	-4.04331800	1.31410500	-0.79461800
C	-5.45693100	-0.97113900	-0.08727800
H	-3.77848600	-1.41887300	1.18567100
C	-5.29454900	1.06921900	-1.34998000
H	-3.50475500	2.21330800	-1.06928700

C	-6.00303500	-0.08063900	-1.00672900
H	-6.00947700	-1.85963400	0.20590900
H	-5.71773200	1.78097700	-2.05160500
H	-6.97909200	-0.27098700	-1.44223100
C	-3.96276200	-5.42125400	1.09301700
H	-3.97636500	-6.33130900	0.48457200
H	-3.86492600	-5.72262000	2.13832100
H	-4.92735600	-4.92434000	0.96533600
C	-2.15614700	-1.82687800	-1.94369400
H	-1.67852600	-2.26257200	-2.82825600
H	-3.21967400	-1.69000600	-2.15274000
H	-1.71457000	-0.84451100	-1.76330900
C	0.88468200	-4.05692100	1.41913400
H	1.53018200	-4.45747500	0.63043500
H	1.35159000	-3.13861900	1.78593300
H	0.86443200	-4.77465100	2.24092800

M5R

C	-0.26486000	-1.86736200	-0.77834400
C	0.77471600	-2.88921900	-1.19898300
H	-1.07594100	-1.88097300	-1.50465900
H	0.27912100	-3.82354400	-1.47213100
H	1.32630200	-2.50208300	-2.05921500
H	1.49175900	-3.10248100	-0.40406000
O	1.17765500	0.00459300	-1.45609200
C	0.31956900	-0.43649500	-0.62367600
C	-1.95236200	2.40840900	0.21475200
C	-2.12415400	3.72087100	0.91567700
C	-0.88544300	0.59367800	-0.40571500
H	-2.39767100	3.50844900	1.96120500
N	-2.88671200	1.60051300	-0.18269900
N	-0.71392600	1.85185600	0.05705600
N	-2.20782300	0.48052300	-0.57768300
C	-2.97212900	-0.53260500	-1.25521500
C	-2.80677500	-0.64971500	-2.64030500
C	-3.88455600	-1.28807700	-0.52148000
C	-3.57525400	-1.60998100	-3.29173500
C	-4.62999900	-2.23486200	-1.22483400
C	-4.48449600	-2.41436100	-2.59946600
H	-3.46430800	-1.73061800	-4.36644500
H	-5.34395000	-2.84649100	-0.67868200
O	-0.94776400	4.48057800	0.84333600
H	-2.93008000	4.29268400	0.45360400
C	0.21040400	3.77878300	1.28418500

H	0.08422400	3.45608100	2.32740400
C	0.51735100	2.60396400	0.32831100
H	1.24038900	1.91794100	0.77300000
C	1.38436200	4.72868700	1.05004400
H	2.24432400	4.41752300	1.65365000
C	1.65449900	4.53615400	-0.42531000
C	1.13382300	3.31587300	-0.86179900
C	2.30557500	5.38010700	-1.31340600
H	2.70768500	6.33175300	-0.97838900
C	2.41799100	4.98985100	-2.64832700
C	1.25183700	2.91253600	-2.18354300
H	0.88537700	1.93817500	-2.48867600
C	1.89484400	3.77084000	-3.07730300
H	1.99453100	3.48096000	-4.11854900
H	2.91482900	5.64276500	-3.35923500
H	1.11532900	5.75136400	1.32415000
C	0.00988000	-1.66329000	1.51195100
O	-0.85967700	-2.13733700	0.48454400
H	0.66739700	-2.47833900	1.85184200
N	0.79356500	-0.58969600	0.89957400
S	2.38638600	-0.48044200	1.36113000
O	2.38649800	-0.86008000	2.77218000
O	2.88030600	0.83234200	0.96416300
C	3.36876300	-1.68341100	0.50163300
C	3.78033000	-1.42320900	-0.80383300
C	3.68110100	-2.87615800	1.14576100
C	4.50841900	-2.39783600	-1.47218100
H	3.48881800	-0.49292700	-1.27899200
C	4.40682600	-3.84110100	0.45331400
H	3.36441500	-3.03386900	2.17140600
C	4.82639500	-3.61673800	-0.85977300
H	4.83308800	-2.21599100	-2.49311400
H	4.65460400	-4.77913900	0.94177700
C	5.63390900	-4.65066900	-1.59968400
H	5.33573600	-4.70478700	-2.64965300
H	6.69858500	-4.39681800	-1.57344600
H	5.51543300	-5.64063100	-1.15438700
C	-0.87086900	-1.20288100	2.65388600
C	-1.67842000	-2.14709900	3.29016400
C	-0.95664700	0.13624000	3.02670300
C	-2.58236200	-1.75181200	4.26971100
H	-1.61161300	-3.19095500	2.99526100
C	-1.86558400	0.53409300	4.00581500
H	-0.29630400	0.85737300	2.55475000

C	-2.68488400	-0.40663600	4.62296300
H	-3.21108500	-2.49095400	4.75609600
H	-1.92521600	1.57930800	4.29498400
H	-3.39185000	-0.09613200	5.38567600
C	-1.81177200	0.20407400	-3.38361900
H	-1.95977900	1.26632700	-3.16036800
H	-0.77735400	-0.04435700	-3.11098300
H	-1.92332500	0.06400900	-4.45990400
C	-4.08308800	-1.06878400	0.95226800
H	-4.79999400	-0.25890400	1.12108800
H	-4.46935600	-1.97426800	1.42440600
H	-3.14719800	-0.79820600	1.44422100
C	-5.27688000	-3.47017900	-3.32539200
H	-5.48640100	-3.16940700	-4.35449000
H	-4.71884200	-4.41135100	-3.36281300
H	-6.22608400	-3.66762600	-2.82250700

M5S

C	-0.39737100	-0.32554100	2.21263500
C	-0.10470900	-1.63097200	2.91151600
H	-0.05299400	0.51475900	2.83347200
H	-0.64172400	-2.44778700	2.43149600
H	0.96949200	-1.83878100	2.90365000
H	-0.43118500	-1.57593000	3.95220700
O	1.37597300	0.77208000	1.08686900
C	0.35137900	0.01686600	0.87366700
C	2.01307900	-2.23666300	-1.53697800
C	3.12563300	-2.47680500	-2.51044500
C	0.79265200	-1.16262200	-0.06802800
H	2.77472000	-2.18149900	-3.51074100
N	0.91845400	-2.92938500	-1.44906300
N	1.99573600	-1.15964100	-0.69685300
N	0.16786600	-2.24990300	-0.53707800
C	-1.12118600	-2.82360900	-0.24178400
C	-1.14554300	-3.93461000	0.61470900
C	-2.23348700	-2.41074900	-0.97335400
C	-2.37677600	-4.53284800	0.85643700
C	-3.44226200	-3.06391600	-0.71052500
C	-3.54139400	-4.09495200	0.21738900
H	-2.42467900	-5.38030000	1.53601700
H	-4.32717300	-2.74585900	-1.25760600
O	4.26755100	-1.75715900	-2.13799600
H	3.37905700	-3.53808700	-2.52959700
C	3.99115200	-0.37529000	-1.93632700

H	3.53651900	0.05595500	-2.83812600
C	3.10560000	-0.17717400	-0.68417700
H	2.63668200	0.80595500	-0.67970400
C	5.32252600	0.25526200	-1.52882900
H	5.29810100	1.33678400	-1.70293900
C	5.38492600	-0.05755700	-0.05143400
C	4.10623700	-0.32059400	0.44412000
C	6.48930400	-0.09505900	0.78908400
H	7.48462000	0.10583500	0.40342900
C	6.29874800	-0.40911500	2.13469000
C	3.90780700	-0.60943000	1.78636600
H	2.90238300	-0.74536000	2.16655600
C	5.01923500	-0.66310700	2.62778500
H	4.88459000	-0.89493900	3.67956300
H	7.15264000	-0.45292500	2.80347100
H	6.14303200	-0.17100700	-2.11065700
C	-1.93647500	0.89605600	1.12906200
O	-1.78804200	-0.19526600	1.99392000
H	-1.67779300	1.83432900	1.65479200
N	-0.89557500	0.61792900	0.10333500
S	-0.62870500	1.65913900	-1.14872900
O	-1.82918000	1.73300800	-1.97489800
O	0.60912400	1.19862400	-1.78167300
C	-0.40990500	3.30745400	-0.49051000
C	-1.12185700	4.33963400	-1.09741700
C	0.46406800	3.55196600	0.56799500
C	-0.94965100	5.64078700	-0.63640000
H	-1.80079700	4.11505600	-1.91273000
C	0.61485000	4.85998800	1.01387400
H	0.99409900	2.71594200	1.02387500
C	-0.08279300	5.91907500	0.42275000
H	-1.49686800	6.45218400	-1.10791000
H	1.29031500	5.06523000	1.84027600
C	0.08360300	7.32398300	0.93978800
H	-0.45151400	7.45260200	1.88612200
H	1.13630100	7.55081300	1.12675700
H	-0.30711800	8.05705000	0.23122600
C	-3.35860600	0.97184800	0.63377400
C	-4.16076000	-0.16778900	0.63436100
C	-3.88946600	2.18967700	0.21052500
C	-5.47271200	-0.09741400	0.17339600
H	-3.75003400	-1.10045500	1.00303200
C	-5.19936000	2.25965500	-0.25132700
H	-3.27180200	3.08434000	0.23364200

C	-5.99226300	1.11392600	-0.27636500
H	-6.09140200	-0.99038900	0.17458700
H	-5.60287900	3.20882500	-0.58881300
H	-7.01520400	1.16904900	-0.63529900
C	-4.86915400	-4.73584900	0.52473800
H	-5.58702000	-4.56641000	-0.28063200
H	-4.76389400	-5.81331800	0.67424900
H	-5.29200200	-4.31655400	1.44366500
C	-2.17570800	-1.36444900	-2.04857100
H	-2.63175900	-1.75979200	-2.96066800
H	-2.72650300	-0.46885200	-1.75242300
H	-1.15439600	-1.05734500	-2.28021200
C	0.11904100	-4.53026500	1.18025800
H	0.89081300	-3.78114000	1.36815200
H	-0.08756200	-5.05309800	2.11656900
H	0.53302900	-5.25318200	0.47006200

TS6R

C	-0.59010156	-0.11421320	0.00000000
C	0.59800844	-0.96883720	-0.41662700
H	-1.39300156	-0.20286120	-0.73097100
H	0.27154044	-1.99890020	-0.57487800
H	1.01938944	-0.57393220	-1.34421500
H	1.38685244	-0.96585820	0.34081900
O	0.49911644	1.99856680	-0.60526000
C	-0.16504356	1.34767880	0.19877500
C	-3.43133056	3.61663180	1.32730700
C	-3.84568456	4.83459580	2.09213500
C	-1.98323656	2.17945780	0.44896200
H	-3.92556956	4.57108080	3.15841000
N	-4.16661956	2.62127080	0.93852600
N	-2.11178956	3.39733180	1.03151600
N	-3.25187056	1.75058680	0.39494300
C	-3.74016056	0.57447680	-0.26047900
C	-3.57600356	0.47330080	-1.64856000
C	-4.37944856	-0.40280020	0.50134100
C	-4.05873556	-0.67586720	-2.26851000
C	-4.84829356	-1.53364220	-0.16970400
C	-4.69569456	-1.68839220	-1.54526700
H	-3.93941456	-0.78250020	-3.34433000
H	-5.34209356	-2.31419720	0.40380700
O	-2.91289056	5.86928780	1.89690300
H	-4.81828856	5.18754480	1.74678400
C	-1.58063156	5.49372080	2.22485900

H	-1.52838056	5.17643180	3.27639100
C	-1.07443056	4.40168980	1.25284900
H	-0.19421056	3.90053880	1.66441200
C	-0.70414056	6.70267380	1.88920300
H	0.23699844	6.65019880	2.44817500
C	-0.46338756	6.52991280	0.40624000
C	-0.69036256	5.20606880	0.02872500
C	-0.07053556	7.46865680	-0.53772700
H	0.10364744	8.50241880	-0.25367500
C	0.08407544	7.06180680	-1.86344800
C	-0.52809856	4.78824380	-1.28336700
H	-0.66964856	3.74528980	-1.55152800
C	-0.14251356	5.73600780	-2.23236300
H	-0.01266356	5.43681380	-3.26752300
H	0.38352444	7.78505180	-2.61570900
H	-1.21417156	7.63210080	2.15321400
C	-0.35044556	0.13155780	2.27937500
O	-1.12679256	-0.48453120	1.26061100
H	0.48283044	-0.52845820	2.57146100
N	0.17463244	1.36029180	1.66457500
S	1.67143044	1.88964780	2.19523400
O	1.69857344	1.52670880	3.60718800
O	1.82024244	3.27729080	1.78604400
C	2.91682544	0.93420580	1.37123800
C	3.31981744	1.30130380	0.08870600
C	3.42997244	-0.19297520	2.00717900
C	4.24641944	0.50248380	-0.56735900
H	2.88868544	2.18014180	-0.37626000
C	4.35538644	-0.97939820	1.32849000
H	3.11512944	-0.43453320	3.01715500
C	4.77203744	-0.64570620	0.03683900
H	4.56847344	0.77197080	-1.56921600
H	4.76496444	-1.86228020	1.81066900
C	5.79557844	-1.48442620	-0.68182800
H	5.82275944	-2.50212120	-0.28687200
H	5.58392544	-1.53253120	-1.75254300
H	6.79474744	-1.05316620	-0.56230200
C	-1.25968856	0.36595780	3.46241800
C	-1.78659356	-0.74998820	4.11340100
C	-1.63920256	1.64302780	3.86684200
C	-2.70752756	-0.59128220	5.14317600
H	-1.48868156	-1.74478920	3.79297900
C	-2.56421156	1.80251880	4.89692700
H	-1.19799056	2.50618980	3.37823500

C	-3.10532756	0.68748080	5.53101400
H	-3.11921556	-1.46359620	5.64072900
H	-2.85426556	2.80049580	5.21201400
H	-3.82716056	0.81348180	6.33146200
C	-2.87427056	1.54811880	-2.44027900
H	-3.23499456	2.54457280	-2.16708300
H	-1.79145956	1.53731080	-2.26206000
H	-3.04315056	1.40077880	-3.50843000
C	-4.56715956	-0.23769320	1.98387300
H	-5.43814356	0.39123780	2.19232200
H	-4.71780656	-1.20865820	2.46021800
H	-3.69726356	0.24096280	2.43942500
C	-5.20754956	-2.91620920	-2.25327100
H	-5.95516256	-2.64742720	-3.00563400
H	-4.39535356	-3.43521320	-2.77050500
H	-5.66640256	-3.61516520	-1.55125500
TS6S			
C	-0.40102300	0.05932800	2.38409600
C	-0.40709700	-1.35863200	2.89929500
H	0.10540700	0.72937300	3.09467700
H	-1.00378000	-1.98264000	2.23297900
H	0.60659300	-1.75914700	2.96575700
H	-0.85500700	-1.37995300	3.89566000
O	1.44192700	0.84327300	1.03819500
C	0.30584200	0.37845800	1.04640100
C	1.62486800	-2.62772300	-1.60490200
C	2.71638700	-2.97489400	-2.56928100
C	0.57313200	-1.45043200	-0.02669000
H	2.45821400	-2.57178300	-3.56014400
N	0.45138300	-3.17238800	-1.53194500
N	1.74794000	-1.59417700	-0.71363300
N	-0.17421700	-2.43120100	-0.55854000
C	-1.54386000	-2.76472300	-0.29334300
C	-1.80738000	-3.80123700	0.61433500
C	-2.54371400	-2.15312900	-1.04744200
C	-3.13526500	-4.15378200	0.82711000
C	-3.86086600	-2.56718600	-0.82040900
C	-4.17691400	-3.53964200	0.12199300
H	-3.36376300	-4.94280900	1.53987900
H	-4.65572400	-2.10076900	-1.39881000
O	3.94396600	-2.45664300	-2.12094700
H	2.81532400	-4.05857400	-2.64983300
C	3.87177700	-1.05914000	-1.87867100
H	3.52938200	-0.53934600	-2.78401100

C	2.95839800	-0.76561100	-0.66494500
H	2.62776600	0.27356700	-0.68876400
C	5.26180100	-0.63252200	-1.39942600
H	5.41449900	0.43638600	-1.58747900
C	5.20611300	-0.92119400	0.08328700
C	3.88021600	-1.01408100	0.50754400
C	6.24573700	-1.08132900	0.99040500
H	7.28016600	-1.01631800	0.66550800
C	5.93759200	-1.34326000	2.32577700
C	3.56739500	-1.26147600	1.83505900
H	2.53028300	-1.30466100	2.14887100
C	4.61004500	-1.43386000	2.74488900
H	4.38808200	-1.63702300	3.78771800
H	6.73806000	-1.48118200	3.04579400
H	6.03737300	-1.18801300	-1.93207300
C	-1.80071800	1.43685500	1.18870600
O	-1.74597400	0.47681800	2.20954800
H	-1.46433000	2.42359600	1.55697000
N	-0.79114900	0.92029200	0.21833300
S	-0.38217000	1.81117100	-1.13580300
O	-1.62679300	2.09776300	-1.83431900
O	0.67620300	1.05872400	-1.79727700
C	0.26372600	3.38619400	-0.60666000
C	-0.57961600	4.49183500	-0.67445700
C	1.58461000	3.51098100	-0.17575600
C	-0.09888000	5.73629600	-0.27721300
H	-1.58538100	4.37505500	-1.06306600
C	2.04459700	4.76156800	0.21146100
H	2.22364600	2.63838600	-0.13382000
C	1.21290400	5.88777700	0.17406300
H	-0.75084900	6.60327600	-0.32930400
H	3.07158500	4.86987000	0.54926400
C	1.73779400	7.23100400	0.60714800
H	2.03320600	7.20979200	1.66033500
H	2.62197200	7.50829200	0.02620500
H	0.98566500	8.01166300	0.47943600
C	-3.21623700	1.52862900	0.68611300
C	-3.99716700	0.37656600	0.62266200
C	-3.76408000	2.75859000	0.33338400
C	-5.31109600	0.45259600	0.17230800
H	-3.57013400	-0.56854700	0.94011300
C	-5.07746900	2.83560800	-0.12007100
H	-3.16045900	3.65865200	0.41542200
C	-5.85119000	1.68058000	-0.20551000

H	-5.91590200	-0.44879700	0.12691400
H	-5.49843000	3.79570600	-0.40031200
H	-6.87701100	1.73953500	-0.55533700
C	-5.60994800	-3.92068200	0.38993500
H	-6.25633700	-3.63755600	-0.44391100
H	-5.71051300	-4.99651700	0.55441700
H	-5.98094000	-3.41544300	1.28801500
C	-2.25870600	-1.09819100	-2.08037100
H	-2.66640500	-1.40552500	-3.04793200
H	-2.73334500	-0.15275300	-1.80070400
H	-1.19092800	-0.90722700	-2.20050900
C	-0.67989500	-4.54701800	1.27823700
H	0.08527000	-3.86895700	1.66498300
H	-1.05266700	-5.15964000	2.10114100
H	-0.18911200	-5.20458900	0.55332800
PR			
C	0.52713221	2.02026033	0.04732792
C	0.83826112	4.10242661	-0.72030567
C	-0.19310061	4.04589363	0.40385019
H	-0.36470018	1.83128107	-0.51287010
H	-0.21206467	4.94174710	0.98864666
O	1.08779292	5.08635247	-1.46407602
N	1.47999391	2.80318193	-0.75776578
O	0.21329859	2.88989935	1.16401443
C	-1.59889881	3.81598809	-0.18136332
H	-2.30525068	3.71604978	0.61611983
H	-1.87009550	4.64900139	-0.79572575
H	-1.59810614	2.92317356	-0.77109340
C	1.12719710	0.67242898	0.48877185
C	2.05550967	0.01661640	-0.33102548
C	0.74494362	0.10171499	1.71028315
C	2.60156950	-1.20990961	0.07068895
H	2.34736597	0.45236738	-1.26367814
C	1.29100468	-1.12481023	2.11199827
H	0.03615631	0.60244233	2.33621662
C	2.21931696	-1.78062292	1.29220081
H	3.31035567	-1.71063776	-0.55524514
H	0.99914604	-1.56056281	3.04464942
H	2.63624666	-2.71710215	1.59891930
S	3.01933430	2.86593633	-0.01574624
O	3.90204302	3.74744528	-0.79259336
O	3.59540162	1.51480490	0.03236264
C	2.85479875	3.50007290	1.63930629
C	3.25496109	2.71906990	2.73192994

C	2.32509706	4.78033377	1.84971108
C	3.12541871	3.21832646	4.03495856
H	3.65939865	1.74156171	2.57128132
C	2.19555452	5.27959027	3.15273973
H	2.01956295	5.37664637	1.01546877
C	2.59571395	4.49858603	4.24536356
H	3.43094778	2.62201172	4.86920118
H	1.79111408	6.25709724	3.31338858
C	2.45335650	5.04721832	5.67726334
H	2.29148600	4.23576332	6.35567231
H	3.34755477	5.56750858	5.95040702
H	1.62211802	5.71957563	5.72060208

PS

C	-1.89665200	1.07276200	0.34218000
C	-2.31222800	-1.12373700	-0.46540200
C	-3.28852200	-0.13947600	-1.09719800
H	-2.40246600	1.41606800	1.25287700
H	-4.26433700	-0.27764400	-0.60787100
O	-2.17730500	-2.29362600	-0.72742900
N	-1.61242200	-0.37472000	0.46539100
O	-2.75176600	1.13836700	-0.78058200
C	-3.40846300	-0.31391500	-2.59466200
H	-3.75929000	-1.32524800	-2.81025800
H	-4.11615700	0.40787000	-3.00502900
H	-2.43593800	-0.16885800	-3.07108600
C	-0.64567300	1.87744600	0.08049800
C	-0.13538700	2.73748300	1.04810100
C	0.02534800	1.71039400	-1.13110500
C	1.05185100	3.42801600	0.80710800
H	-0.65357300	2.84683300	1.99647700
C	1.21000700	2.39484900	-1.37026300
H	-0.38406200	1.03457500	-1.87706300
C	1.72497900	3.25410000	-0.39889800
H	1.44986800	4.09826500	1.56193300
H	1.73522700	2.25666100	-2.30972300
H	2.65095000	3.78909000	-0.58510200
S	-0.52503400	-0.99038900	1.60922400
O	-0.98145700	-2.32185000	1.94352600
O	-0.43049100	0.05629100	2.61216700
C	0.99638900	-1.09391200	0.71892300
C	1.96973100	-0.12338600	0.92399100
C	1.15548000	-2.12247600	-0.20810800
C	3.13899800	-0.19100900	0.17532800

H	1.80029100	0.67368600	1.64073300
C	2.32998000	-2.16467700	-0.94715200
H	0.36781800	-2.85735800	-0.34555600
C	3.33475300	-1.20585400	-0.76498300
H	3.90615500	0.56467800	0.31706300
H	2.47319800	-2.95424500	-1.67897300
C	4.61523400	-1.28533600	-1.55318100
H	5.07419900	-0.30063600	-1.66385500
H	5.33661800	-1.93317700	-1.04463300
H	4.44220300	-1.70238800	-2.54777800

TS4_N

C	0.54717000	0.15059000	1.44363200
C	1.18792500	-0.67718400	2.52329400
H	0.84918400	1.17871200	1.33081100
H	1.91767200	-0.08313100	3.07605100
H	0.42780900	-1.05793800	3.21426100
H	1.70700900	-1.56087600	2.12546600
O	-1.32422900	-1.29571900	1.36918500
C	-0.72130400	-0.25546000	1.02289100
C	-3.01040100	1.13872300	-1.44895900
C	-4.24452700	0.97477200	-2.28153700
C	-1.46833500	0.58847600	0.00576000
H	-3.96233600	0.53305500	-3.24959800
N	-2.11915400	2.08107900	-1.53658400
N	-2.66648300	0.21412100	-0.50598500
N	-1.16343300	1.72787300	-0.63098200
C	-0.08999400	2.65880400	-0.38989200
C	-0.13776300	3.40080800	0.79741400
C	0.89331000	2.83602100	-1.36496600
C	0.90373100	4.29069500	1.03672700
C	1.90793100	3.74875500	-1.07364900
C	1.94605100	4.45823000	0.12280600
H	0.90146400	4.86589400	1.95904700
H	2.70557300	3.87905700	-1.79952400
O	-5.17478700	0.16836000	-1.60719200
H	-4.70146600	1.94875700	-2.46143200
C	-4.63446100	-1.09450900	-1.24142000
H	-4.26247500	-1.61510700	-2.13378200
C	-3.53910500	-0.92461700	-0.16406200
H	-2.90006500	-1.80614500	-0.10043300
C	-5.74535900	-1.83769900	-0.49648100
H	-5.55518100	-2.91713100	-0.52016200
C	-5.61903200	-1.29118600	0.90768800

C	-4.35063800	-0.74165700	1.10112300
C	-6.55396100	-1.27750900	1.93381100
H	-7.54341600	-1.70076100	1.78801500
C	-6.20470100	-0.69296900	3.15130800
C	-3.99297300	-0.16634800	2.31159100
H	-2.99858700	0.24046900	2.46052200
C	-4.93813800	-0.13923400	3.33684000
H	-4.68313900	0.31308600	4.28968100
H	-6.92722600	-0.66342400	3.96073800
H	-6.71454000	-1.64821500	-0.96352500
C	1.76494100	-1.52069200	-0.80893400
O	2.47609100	-1.00487600	-1.85260200
H	2.32436300	-2.15437300	-0.10304500
N	1.72704800	-0.10640100	-0.50142800
S	3.28603400	0.59501100	-0.04044300
O	3.08200000	1.34702700	1.19287400
O	3.77808600	1.31827300	-1.20261300
C	4.40793300	-0.73848200	0.32333200
C	5.10692100	-1.35907500	-0.71199700
C	4.60678500	-1.09570100	1.65220300
C	6.00280500	-2.37002400	-0.39583700
H	4.93024500	-1.04925200	-1.73456200
C	5.51054800	-2.11264500	1.94651800
H	4.07399100	-0.57330000	2.43842500
C	6.21478200	-2.76318400	0.93192700
H	6.55236500	-2.86507300	-1.19171300
H	5.67578300	-2.39832700	2.98112500
C	7.19963800	-3.85769400	1.24759100
H	8.21588000	-3.55097300	0.98226600
H	7.18762100	-4.10990800	2.30957200
H	6.97223600	-4.76229500	0.67674300
C	0.43309800	-2.11276600	-1.18790800
C	-0.26989400	-1.53520900	-2.24712000
C	-0.05167900	-3.26610400	-0.58010000
C	-1.44752900	-2.11727400	-2.70192200
H	0.14368500	-0.64895900	-2.71981100
C	-1.22644000	-3.85795900	-1.04151800
H	0.49150800	-3.70576300	0.25200500
C	-1.92056600	-3.28901500	-2.10636800
H	-1.98236000	-1.67695800	-3.53957500
H	-1.59486400	-4.76552000	-0.57443800
H	-2.82699700	-3.76048400	-2.47677300
C	0.91723800	2.08611300	-2.66962500
H	1.58404700	1.22146900	-2.58811900

H	-0.07635200	1.74387800	-2.96429100
H	1.29904200	2.73764300	-3.45909300
C	-1.25596000	3.22529900	1.79181000
H	-2.23394300	3.20520900	1.29984700
H	-1.13991400	2.28674200	2.34594600
H	-1.25339000	4.04458300	2.51228900
C	3.10949000	5.35895600	0.43817100
H	3.91732200	4.77058300	0.88566700
H	3.50424800	5.82898700	-0.46547400
H	2.83030500	6.14212000	1.14674900

TS4_c

C	1.18393000	-1.01449700	-1.63044200
C	1.51405800	-0.88588200	-3.09725200
H	1.85725000	-1.61176300	-1.02508400
H	2.59209300	-0.92649700	-3.26248700
H	1.03565800	-1.68108000	-3.68142100
H	1.14194600	0.06601700	-3.49284500
O	-1.12677200	-1.17135900	-2.17118700
C	-0.19225800	-1.21533300	-1.36172500
C	-1.85136300	-1.10517400	1.87284400
C	-2.99342500	-0.57013600	2.67646800
C	-0.62624500	-1.38071400	0.08975400
H	-2.71599900	0.44281700	3.00615000
N	-0.71706400	-1.55467500	2.31944500
N	-1.85712500	-1.02703900	0.51121300
N	0.04050500	-1.72483300	1.20034900
C	1.34057600	-2.31998800	1.35519600
C	1.60908100	-3.53161900	0.70384600
C	2.25122400	-1.70362800	2.22402500
C	2.86860200	-4.09564900	0.89773500
C	3.48822700	-2.32714900	2.39305400
C	3.82045300	-3.50892400	1.73217000
H	3.10305700	-5.03008200	0.39443200
H	4.21543300	-1.86343300	3.05495800
O	-4.16569300	-0.55365200	1.90567700
H	-3.16818800	-1.19419900	3.55394000
C	-4.01638300	0.15736000	0.68144000
H	-3.70280200	1.19120300	0.87795200
C	-3.03334200	-0.57956100	-0.25494000
H	-2.66708400	0.08261900	-1.04017700
C	-5.35705300	0.01945300	-0.04369300
H	-5.46719500	0.81442800	-0.78956600
C	-5.22978800	-1.33481900	-0.70528400

C	-3.88640600	-1.69674400	-0.81597400
C	-6.22435200	-2.18148300	-1.17548400
H	-7.27178100	-1.90786500	-1.08913000
C	-5.85411600	-3.39887000	-1.74783100
C	-3.50899900	-2.89885000	-1.39564600
H	-2.45952500	-3.15164800	-1.50513500
C	-4.51010200	-3.75484300	-1.85544400
H	-4.23959500	-4.70380200	-2.30717100
H	-6.61950900	-4.07695700	-2.11182000
H	-6.18523400	0.09253700	0.66483800
C	2.05014300	0.69283800	-0.54135100
O	2.26338600	2.35093700	0.19005700
H	1.83243200	0.20905500	0.40240000
N	1.37845000	1.90781000	-0.82014200
S	-0.20617100	2.02365100	-0.15965600
O	-0.30977500	1.32563600	1.13118900
O	-1.15823200	1.66909000	-1.21086200
C	-0.29645100	3.76341300	0.13817000
C	-0.97833700	4.55766800	-0.77868800
C	0.29148500	4.29720200	1.28064400
C	-1.07437300	5.92174600	-0.53523800
H	-1.42351900	4.10485100	-1.65811800
C	0.18466700	5.66505400	1.50269800
H	0.82637400	3.64765200	1.96322100
C	-0.49720600	6.49149000	0.60472000
H	-1.60511400	6.55634500	-1.23943900
H	0.64040400	6.10040600	2.38697600
C	-0.62651300	7.97058900	0.85777100
H	-1.66407800	8.23310000	1.08671700
H	-0.00470700	8.28574000	1.69771000
H	-0.33113700	8.54483900	-0.02435600
C	3.36963700	0.50943400	-1.18848600
C	4.18973100	-0.54747400	-0.78970300
C	3.79477600	1.36788200	-2.20463500
C	5.41642300	-0.75577500	-1.41120100
H	3.85977500	-1.21529300	0.00288500
C	5.02101500	1.15526600	-2.82447700
H	3.15746100	2.19620200	-2.49481600
C	5.83397100	0.09196400	-2.43461600
H	6.04567100	-1.58263500	-1.09642900
H	5.34499700	1.82324700	-3.61628300
H	6.78934100	-0.07187800	-2.92273700
C	1.94303600	-0.43200800	2.97315300
H	1.28597600	0.23962500	2.41533800

H	1.44270000	-0.66581100	3.91755400
H	2.87195700	0.09673200	3.19509400
C	0.59986100	-4.22118300	-0.17682900
H	-0.41085600	-4.15621100	0.23698300
H	0.58100600	-3.77939900	-1.17946400
H	0.85634800	-5.27659000	-0.28092300
C	5.18458100	-4.12520200	1.89782500
H	5.88829000	-3.69546000	1.17734900
H	5.58310500	-3.94072300	2.89784600
H	5.15453000	-5.20370800	1.72904200

M4_N

C	0.88936700	-0.28187100	1.14135800
C	1.34543100	-1.34301000	2.14628600
H	1.04503200	0.70859100	1.59818300
H	2.42210700	-1.26037900	2.29853500
H	0.84096800	-1.19878800	3.10323700
H	1.11661200	-2.34968600	1.79292800
O	-1.31230500	-1.05141200	1.69945700
C	-0.61366600	-0.37172800	0.98219400
C	-2.92265200	0.98897600	-1.46799900
C	-4.19980500	0.84587200	-2.23767600
C	-1.35735300	0.43878900	-0.06253400
H	-3.98563500	0.30277300	-3.17025700
N	-1.96975200	1.85877600	-1.65607400
N	-2.60628600	0.12094400	-0.46639400
N	-1.00320800	1.50874400	-0.77116900
C	0.07819500	2.43549500	-0.53935700
C	0.06159300	3.14838100	0.66580200
C	0.99472700	2.66209800	-1.56721400
C	1.06078200	4.09843800	0.84904400
C	1.96371600	3.63369400	-1.32687500
C	2.02511900	4.34150300	-0.12905700
H	1.08364300	4.66352100	1.77717500
H	2.71730200	3.80686000	-2.08970400
O	-5.15322200	0.17239400	-1.45831300
H	-4.59450200	1.83181700	-2.48670300
C	-4.69463900	-1.09183700	-0.99804200
H	-4.38716800	-1.71331200	-1.84553700
C	-3.55441200	-0.89426900	0.03060800
H	-2.99417900	-1.82302200	0.17034300
C	-5.82335100	-1.67983000	-0.15174500
H	-5.69951300	-2.76536400	-0.06336800
C	-5.62166100	-0.99012200	1.17755000

C	-4.31959900	-0.49547000	1.27976800
C	-6.53031800	-0.79672400	2.20840700
H	-7.54344800	-1.17920500	2.13024400
C	-6.12542700	-0.08252900	3.33614500
C	-3.91331800	0.22256900	2.39546400
H	-2.90567200	0.61542700	2.47413900
C	-4.83228000	0.43025700	3.42448300
H	-4.53525100	0.99531200	4.30167000
H	-6.82738500	0.08601500	4.14631800
H	-6.79343000	-1.47926600	-0.61166800
C	1.65883400	-1.63210100	-1.05520700
O	2.30524800	-1.40821300	-2.13874400
H	2.11882100	-2.33529000	-0.31306900
N	1.57052700	-0.24716500	-0.15375200
S	3.07119800	0.52050600	-0.05811100
O	2.97114900	1.46551400	1.06491000
O	3.46644800	1.03795700	-1.35734000
C	4.31736500	-0.67820200	0.41811900
C	4.73195400	-1.66588900	-0.47644900
C	4.90859000	-0.54083200	1.67031400
C	5.74659700	-2.53010300	-0.08283300
H	4.22728700	-1.74483100	-1.43962600
C	5.92724200	-1.41457800	2.03913100
H	4.57460300	0.24912100	2.33476800
C	6.36090000	-2.41703600	1.16974900
H	6.07510500	-3.30993300	-0.76529600
H	6.39630400	-1.31015700	3.01364600
C	7.48073300	-3.34878500	1.55403000
H	8.39036000	-3.11051700	0.99361800
H	7.71298700	-3.27443200	2.61851200
H	7.22248500	-4.38719000	1.32931000
C	0.20921100	-2.09621300	-1.29501000
C	-0.48828400	-1.54545900	-2.37722600
C	-0.33778000	-3.19712400	-0.63671100
C	-1.70290800	-2.08170500	-2.78703500
H	-0.02020800	-0.73030200	-2.92045500
C	-1.55075400	-3.75223100	-1.05277100
H	0.21157300	-3.66091600	0.17979500
C	-2.23044800	-3.20087900	-2.13462900
H	-2.21849400	-1.66462600	-3.64931100
H	-1.94618800	-4.63043300	-0.55114200
H	-3.15459400	-3.65332800	-2.48451500
C	1.00333600	1.85117000	-2.83177600
H	1.42942700	0.85862800	-2.62691100

H	0.00038800	1.74352300	-3.25258300
H	1.64000300	2.33371000	-3.57527500
C	-0.99487500	2.93545500	1.72333100
H	-1.99321200	2.81197100	1.28983200
H	-0.78589500	2.05670200	2.34662900
H	-1.02827900	3.79651000	2.39245700
C	3.14437600	5.31423100	0.12441800
H	4.00600100	4.77844000	0.53606500
H	3.46599700	5.80070900	-0.79918400
H	2.85215100	6.08383000	0.84262800

M4_C

C	1.11619200	-0.49937100	-1.78343800
C	1.00791600	0.19136300	-3.14309300
H	1.72443100	-1.41103800	-1.91256400
H	2.00385400	0.50704700	-3.45988100
H	0.59238100	-0.48712400	-3.88872700
H	0.36454100	1.06799900	-3.05952300
O	-1.06442900	-1.42026300	-2.18750900
C	-0.22878200	-1.07431500	-1.38572300
C	-1.81648800	-1.21884900	1.87495100
C	-2.94461800	-0.73983900	2.73362300
C	-0.61100100	-1.30732700	0.07303400
H	-2.63571700	0.23252800	3.14562500
N	-0.65815500	-1.66875200	2.26530200
N	-1.84994100	-1.04614200	0.52447500
N	0.08712700	-1.71542500	1.13337900
C	1.40599100	-2.29554200	1.19293900
C	1.62885600	-3.48175800	0.48538800
C	2.37137300	-1.68303100	2.01110800
C	2.89856600	-4.05377800	0.58441100
C	3.61467300	-2.30780600	2.06961400
C	3.89987800	-3.47996700	1.36553500
H	3.10001700	-4.97612000	0.04632400
H	4.39200400	-1.85029900	2.67626500
O	-4.12512700	-0.62980000	1.98238500
H	-3.12584100	-1.43542900	3.55403500
C	-3.98151200	0.14782400	0.79873100
H	-3.62737100	1.15801200	1.03967100
C	-3.04480400	-0.57730100	-0.19254100
H	-2.69759700	0.11123000	-0.96576500
C	-5.33829100	0.07976100	0.09530500
H	-5.43244600	0.90035600	-0.62464800
C	-5.26842500	-1.26064900	-0.60340400

C	-3.93972200	-1.66810500	-0.74543600
C	-6.29996800	-2.06546900	-1.06566900
H	-7.33504900	-1.75658600	-0.95463300
C	-5.98407000	-3.28905300	-1.65758700
C	-3.61723300	-2.88192200	-1.33359400
H	-2.58245700	-3.18671600	-1.44851200
C	-4.65698400	-3.69568300	-1.78542800
H	-4.42961700	-4.65304200	-2.24278500
H	-6.78005900	-3.93473700	-2.01443200
H	-6.15174800	0.15930000	0.81970000
C	1.89528500	0.32223800	-0.72886100
O	2.23970800	2.22260300	0.55108200
H	1.83830700	-0.18692300	0.23137500
N	1.48201800	1.72717200	-0.49961200
S	-0.11005600	1.88819600	0.01915800
O	-0.38592300	1.29545400	1.34314900
O	-1.01251400	1.43300100	-1.06667900
C	-0.27510800	3.64744000	0.15472100
C	-1.08339400	4.30076700	-0.76579400
C	0.35520900	4.33246300	1.19364900
C	-1.26153100	5.67725800	-0.64649300
H	-1.55872800	3.73584800	-1.56024900
C	0.16509600	5.70301600	1.29169100
H	0.99535400	3.78373500	1.87235900
C	-0.64232800	6.39326800	0.37816300
H	-1.88800000	6.20116500	-1.36270500
H	0.65670500	6.25429700	2.08878100
C	-0.83693800	7.88080900	0.51514400
H	-1.40031500	8.11706900	1.42325700
H	0.12567800	8.39478900	0.58624900
H	-1.38205800	8.29108900	-0.33736400
C	3.36681700	0.33507900	-1.12742600
C	4.07590500	-0.86603300	-1.09288000
C	4.01378400	1.49215200	-1.56423500
C	5.40835600	-0.92217900	-1.49454200
H	3.58500600	-1.77140800	-0.74080700
C	5.34393700	1.43486400	-1.97133800
H	3.47655400	2.43229100	-1.53458000
C	6.04594900	0.23139100	-1.94065900
H	5.94320700	-1.86688800	-1.45930000
H	5.83927900	2.34124100	-2.30617700
H	7.08422400	0.19588400	-2.25583300
C	2.13559400	-0.38469000	2.73733900
H	2.22585200	0.47942700	2.05604100

H	1.14226200	-0.34061900	3.18402600
H	2.88261800	-0.27356100	3.52571600
C	0.55166500	-4.15538900	-0.33013100
H	-0.40796700	-4.16181100	0.19647800
H	0.39680000	-3.67077400	-1.30054900
H	0.83128700	-5.19095800	-0.52890500
C	5.27327200	-4.09169700	1.44533400
H	6.02188600	-3.39566700	1.05493700
H	5.54205100	-4.31290700	2.48202300
H	5.33177900	-5.01741400	0.86986700

M3_{CatI}

C	1.19831400	-0.23744300	2.77371400
C	1.36368000	-0.28101200	4.26425100
H	2.05956500	-0.39709300	2.13495600
H	1.74862700	-1.24930700	4.60531900
H	2.06165500	0.48429800	4.62395400
H	0.39603000	-0.11202500	4.74217300
O	-1.17890100	0.20372100	2.68957400
C	-0.02256600	-0.00651000	2.21946500
P	-0.02857600	0.00600000	0.34693800
C	1.56693700	-0.31046800	-0.44864100
C	1.95131300	-1.62061400	-0.75383200
C	2.47352800	0.74170200	-0.62677200
C	3.22682900	-1.87119100	-1.24977000
H	1.25541500	-2.44061700	-0.60454800
C	3.74664600	0.48353100	-1.12318600
H	2.18168000	1.75810300	-0.37878100
C	4.12267100	-0.82108700	-1.43666200
H	3.52110300	-2.88786700	-1.48800500
H	4.44516400	1.30141100	-1.26391900
H	5.11683000	-1.01971400	-1.82385800
C	-0.60447600	1.62333200	-0.24433500
C	-0.41666000	2.00200400	-1.57902100
C	-1.25440300	2.48454800	0.64617500
C	-0.87011900	3.24048400	-2.01849600
H	0.10013100	1.34258800	-2.27116600
C	-1.70307800	3.72353200	0.19525300
H	-1.41149400	2.16522500	1.67240400
C	-1.51344500	4.10151900	-1.13085000
H	-0.71831200	3.53371400	-3.05207500
H	-2.20377100	4.39377500	0.88607700
H	-1.86702800	5.06791600	-1.47574600
C	-1.18249300	-1.25965500	-0.25384700

C	-2.01017800	-1.92502000	0.65540000
C	-1.24784200	-1.56234900	-1.61907500
C	-2.89154200	-2.89925100	0.19134300
H	-1.97135400	-1.65149000	1.70532400
C	-2.13089500	-2.53538000	-2.07154700
H	-0.59931700	-1.05278600	-2.32692300
C	-2.95246300	-3.20440800	-1.16490700
H	-3.53487300	-3.41651100	0.89545400
H	-2.17754600	-2.77265100	-3.12921000
H	-3.64119700	-3.96433700	-1.52005000

TS4_{Cat1}

C	1.30562100	1.76801000	1.20514900
C	1.00108900	3.20642600	1.49764200
H	1.42905600	1.09447300	2.04529500
H	0.02212200	3.32418300	1.97108500
H	1.75316900	3.61672300	2.18215100
H	1.01122200	3.79659000	0.57988700
O	1.86207700	1.93724200	-1.13413600
C	1.81907600	1.37396600	-0.02685600
C	-1.32886700	1.35069800	-0.28034800
O	-0.58094300	0.79858200	0.77232000
H	-0.99662200	1.02014200	-1.27107800
N	-2.28883800	0.52752600	0.39083100
S	-2.48520700	-1.01100500	-0.23962700
O	-1.88834100	-2.00159400	0.65616300
O	-2.12529800	-1.05948600	-1.66163800
C	-4.24840300	-1.15317200	-0.11511200
C	-5.02662000	-1.01845200	-1.25841000
C	-4.81938900	-1.39115800	1.13271400
C	-6.40877800	-1.12656100	-1.14321600
H	-4.54947300	-0.83809100	-2.21560400
C	-6.20042100	-1.49036000	1.22750400
H	-4.18538900	-1.49687000	2.00701000
C	-7.01243400	-1.36204900	0.09433000
H	-7.02922900	-1.02644500	-2.02924200
H	-6.66034300	-1.67157500	2.19484800
C	-8.50739800	-1.50580000	0.20603600
H	-8.79689100	-2.56027900	0.14925400
H	-8.87199900	-1.11514600	1.15887300
H	-9.01726100	-0.97774000	-0.60248900
C	-1.60728700	2.82183000	-0.24294700
C	-2.41426800	3.37169500	0.75341900
C	-1.01570400	3.64496800	-1.19854400

C	-2.62190200	4.74576900	0.79552300
H	-2.87010600	2.71192000	1.48506100
C	-1.22525400	5.02165000	-1.15507600
H	-0.35965600	3.20669100	-1.94590100
C	-2.02659500	5.57178700	-0.15806500
H	-3.24975900	5.17544500	1.56978600
H	-0.76016700	5.66393400	-1.89609700
H	-2.19059600	6.64438800	-0.12403200
P	2.68720500	-0.30529600	0.01264500
C	2.29266800	-1.27157600	1.48904900
C	1.10203800	-2.00400300	1.50166600
C	3.06361700	-1.15942800	2.65290700
C	0.69197800	-2.63333500	2.67177900
H	0.47052800	-2.07080400	0.62231100
C	2.65216000	-1.80461900	3.81426100
H	3.97423900	-0.56818200	2.65522100
C	1.46852600	-2.54103300	3.82361400
H	-0.24438500	-3.18028300	2.67219700
H	3.25220900	-1.72507600	4.71466900
H	1.14773800	-3.03470200	4.73544200
C	4.46711800	0.01872900	-0.02377200
C	5.38033400	-0.96634500	0.37292800
C	4.92402600	1.25049400	-0.50443500
C	6.74591700	-0.71379000	0.29601300
H	5.02533300	-1.92320800	0.74648500
C	6.29292300	1.49352200	-0.57452700
H	4.20924700	1.99963500	-0.83199600
C	7.20085200	0.51665900	-0.17488500
H	7.45290200	-1.47581900	0.60657500
H	6.64908500	2.44903100	-0.94437100
H	8.26675100	0.71253200	-0.23089800
C	2.27048800	-1.24251000	-1.47215000
C	0.93646000	-1.24340000	-1.88307900
C	3.23065300	-1.96282900	-2.18804800
C	0.55129000	-1.98518300	-2.99412900
H	0.19357200	-0.67842700	-1.33189800
C	2.84153700	-2.69504700	-3.30524700
H	4.27264100	-1.94662700	-1.88439100
C	1.50617200	-2.70845000	-3.70496600
H	-0.49339300	-1.98610600	-3.28367600
H	3.58388900	-3.25383600	-3.86542600
H	1.21136700	-3.28419000	-4.57651700

C	0.47352600	-0.59788100	2.79141000
C	0.33286200	-1.63224900	3.86455300
H	0.92474400	0.36233300	3.02705700
H	1.30434600	-1.95922100	4.25499500
H	-0.24951300	-1.26944700	4.72002200
H	-0.17679700	-2.50447900	3.44899500
O	-0.61688800	-1.79767600	1.00270100
C	-0.01782300	-0.81182300	1.53538100
C	0.98511400	1.93640400	-0.69828200
C	2.03875500	2.86451600	-1.21774200
C	0.18986600	0.34590000	0.59040800
H	2.02452500	3.79549700	-0.63218800
N	-0.26621400	1.84908600	-1.03066700
N	1.30713500	1.03065600	0.28368100
N	-0.74171400	0.84770100	-0.22663900
C	-2.08790800	0.41900600	-0.31663500
C	-2.40285300	-0.74027700	-1.01914700
C	-3.08939900	1.15501400	0.30199800
C	-3.72167700	-1.16081500	-1.09509500
C	-4.41158300	0.74250700	0.22191100
C	-4.72022900	-0.41896700	-0.47396600
O	3.29268400	2.23045200	-1.13520700
H	1.84409600	3.10126000	-2.26393400
C	3.63941300	1.84643000	0.18808600
H	3.64056700	2.72671100	0.84437400
C	2.68542500	0.73781400	0.69598200
H	2.70485500	0.68545300	1.78701000
C	4.99041700	1.13151200	0.09495600
H	5.51169900	1.18369800	1.05744700
C	4.59809400	-0.28947200	-0.24243200
C	3.25825700	-0.51995000	0.07374300
C	5.36861800	-1.30250600	-0.79660800
H	6.40964100	-1.12986400	-1.05290600
C	4.77270900	-2.54122500	-1.03517000
C	2.65116000	-1.74861400	-0.15856800
H	1.60222900	-1.93235200	0.06861500
C	3.43065400	-2.75864000	-0.72508100
H	2.98196900	-3.72594500	-0.92527800
H	5.35758800	-3.34179500	-1.47690000
H	5.61945900	1.60811600	-0.66045300
F	-2.78344100	2.26057100	0.96931400
F	-1.46268400	-1.42093500	-1.64401100
F	-4.03938400	-2.26151600	-1.76671600
F	-5.37511100	1.44951400	0.80281600

F	-5.98166900	-0.81589600	-0.56136400
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TS4_{Cat2}

C	1.84240500	-0.32113700	1.87770100
C	1.82519900	-0.68781700	3.32834500
H	2.59239300	-0.78528300	1.25747200
H	1.11803200	-0.05703600	3.86836300
H	1.53591700	-1.73437800	3.47371300
H	2.81997200	-0.55641400	3.77065700
O	0.34567400	1.51634400	2.08832900
C	1.14537500	0.80507600	1.43302200
C	0.60438500	1.87492000	-2.01148100
C	-0.31381500	2.47929800	-3.02541300
C	1.20598600	1.13286600	-0.04266700
H	-0.90717000	1.65893000	-3.45446400
N	1.64219100	1.13573800	-2.25176700
N	0.32486500	1.93397300	-0.67149800
N	2.00875300	0.68456500	-1.01834200
C	3.10980300	-0.19808100	-0.93732800
C	4.31251700	0.21980400	-0.37835400
C	2.97966300	-1.48806700	-1.44101000
C	5.38348500	-0.65609600	-0.30125500
C	4.05370400	-2.36601500	-1.37550300
C	5.24902300	-1.94594300	-0.80500900
O	-1.13312300	3.44487100	-2.41973600
H	0.25871100	2.96385800	-3.81741400
C	-1.85137800	2.92393400	-1.30991100
H	-2.42348000	2.03784700	-1.61177500
C	-0.87569700	2.61270000	-0.14875200
H	-1.32894900	1.93301500	0.57561600
C	-2.68733000	4.08338600	-0.76610800
H	-3.53181100	3.70109200	-0.18096100
C	-1.70047800	4.81571000	0.11424700
C	-0.64071700	3.97705000	0.46351400
C	-1.74163300	6.12446200	0.57579500
H	-2.56180000	6.78184600	0.30291000
C	-0.70127600	6.58341500	1.38325700
C	0.39066600	4.42112500	1.27843900
H	1.18843600	3.74847700	1.57268600
C	0.35463200	5.74036400	1.73000200
H	1.15395000	6.11206300	2.36276800
H	-0.71230300	7.60701300	1.74409400
H	-3.08386300	4.68550600	-1.58686600
C	-0.86752100	-1.34404000	1.15338600

O	0.43576700	-1.49200000	0.68368800
H	-1.27800100	-0.34532200	0.96030000
N	-1.02066100	-2.32480600	0.11923100
S	-1.44568800	-1.67655700	-1.36630300
O	-0.90889500	-2.54250300	-2.40442100
O	-1.17898000	-0.22989000	-1.43296800
C	-3.20990000	-1.87577700	-1.32316200
C	-4.00563100	-0.85164200	-0.81857600
C	-3.76404400	-3.07651300	-1.76025400
C	-5.38184200	-1.03821100	-0.75482200
H	-3.55018400	0.07741600	-0.48951100
C	-5.14059800	-3.24312300	-1.69085000
H	-3.11731600	-3.85327400	-2.15444000
C	-5.96673700	-2.23119100	-1.18835000
H	-6.01361500	-0.24560600	-0.36463400
H	-5.58522500	-4.17381400	-2.03213700
C	-7.45963700	-2.42238800	-1.14041100
H	-7.71510200	-3.42716600	-0.79505700
H	-7.93128000	-1.69792000	-0.47355900
H	-7.89627500	-2.29650400	-2.13629500
C	-1.13903400	-1.81015400	2.54933400
C	-0.94266600	-3.14524000	2.90462400
C	-1.52861100	-0.87895900	3.50858000
C	-1.14230300	-3.54449500	4.22115600
H	-0.63702900	-3.85475100	2.14171200
C	-1.72717200	-1.28090000	4.82766500
H	-1.62767600	0.16612100	3.22595900
C	-1.53485800	-2.61276100	5.18311800
H	-0.99235500	-4.58253100	4.50067000
H	-2.02503500	-0.55403400	5.57661900
H	-1.68865100	-2.92774900	6.21055000
F	1.83830800	-1.87827300	-1.97246000
F	3.94729800	-3.59807400	-1.85314700
F	6.27352100	-2.78213000	-0.73846700
F	6.53202600	-0.27433100	0.24342300
F	4.41966200	1.44495300	0.11771200

M3_{Cat3}

C	-2.41117500	1.63961100	0.21464300
C	-2.73553000	3.09041600	0.06314200
H	-3.03953200	1.01945400	0.84632300
H	-3.70025900	3.24857900	-0.43596200
H	-2.79203300	3.60656700	1.02930800
H	-1.95926100	3.56566200	-0.54083700

O	-0.43317300	1.61531000	-1.15083000
C	-1.31394100	1.09274700	-0.41426400
C	-1.13560300	-0.36503900	-0.08637500
N	0.04694100	-0.98556900	0.02549100
S	-2.41478800	-1.50291400	0.02497200
C	-1.30603900	-2.80360800	0.30042300
H	-1.64131200	-3.81478900	0.47264900
C	-0.03821100	-2.35519500	0.26197700
H	0.87352500	-2.91276200	0.41922800
C	1.32876300	-0.32336500	0.04613600
C	2.37877400	-0.88908600	-0.66581000
C	1.50066200	0.81497900	0.82496000
C	3.63798700	-0.30002900	-0.59124600
H	2.20858600	-1.76118700	-1.28946700
C	2.76158800	1.39271900	0.88973300
H	0.65602100	1.23495800	1.36045300
C	3.82997400	0.83688600	0.18712900
H	4.46327400	-0.72925200	-1.14889600
H	2.90937900	2.28428700	1.48932900
H	4.81152400	1.29539800	0.24383800

TS4_{Cat3}

C	-2.55563900	1.52892600	-0.08396200
C	-2.56937500	2.97766800	-0.45547800
H	-3.04714800	0.82851400	-0.74355500
H	-3.59677100	3.36039600	-0.50403600
H	-2.01748500	3.56393300	0.28183400
H	-2.11370400	3.13141400	-1.43862900
O	-1.74337400	1.87437100	2.13030800
C	-2.19713000	1.14482300	1.21063400
C	-2.15796100	-0.31588000	1.57093000
N	-2.54844000	-1.44152700	0.96810900
C	0.41882900	1.16538700	-0.08234200
O	-0.68255600	0.68476700	-0.78971200
H	0.47092700	0.79381200	0.94753000
N	1.00501700	0.34722000	-1.10920200
S	1.18289100	-1.26294600	-0.67623300
O	0.87022300	-2.06502600	-1.85609900
O	0.50007900	-1.58312400	0.58256600
C	2.93035000	-1.35230500	-0.38894800
C	3.41653700	-1.21929900	0.90879800
C	3.78542800	-1.52419200	-1.47371900
C	4.78995800	-1.26012600	1.11559900
H	2.72319800	-1.10506900	1.73568800

C	5.15520900	-1.56246900	-1.24552500
H	3.37402300	-1.64095400	-2.47084600
C	5.67539500	-1.42641800	0.04582100
H	5.18398600	-1.16690400	2.12362000
H	5.83437700	-1.70471400	-2.08112800
C	7.16287900	-1.43794900	0.28080900
H	7.55526600	-0.41600000	0.30024300
H	7.40754500	-1.90324800	1.23850300
H	7.68497200	-1.97902300	-0.51104000
C	0.69665800	2.63138500	-0.20036600
C	0.82767200	3.21682300	-1.46063400
C	0.76363800	3.41614500	0.94784100
C	1.03189300	4.58676600	-1.56867300
H	0.76735700	2.58660500	-2.34280300
C	0.96818700	4.79045300	0.83702400
H	0.61193000	2.95365800	1.91841300
C	1.10238200	5.37489400	-0.41894200
H	1.13589300	5.04422200	-2.54751700
H	1.01281000	5.40380500	1.73121200
H	1.25921100	6.44571100	-0.50513000
S	-1.41933800	-0.65264900	3.07271800
C	-1.62934900	-2.34599100	2.84015200
H	-1.28705900	-3.06825200	3.56519300
C	-2.24405700	-2.59948500	1.66663900
H	-2.51402400	-3.55032600	1.22997300
C	-3.22499500	-1.51413100	-0.30603600
C	-2.48731600	-1.85558100	-1.43125200
C	-4.59085900	-1.25855500	-0.35551700
C	-3.14794200	-1.92426500	-2.65503100
H	-1.42160000	-2.04288300	-1.35215500
C	-5.23463000	-1.32936400	-1.58632600
H	-5.12583400	-0.99206500	0.55024600
C	-4.51291500	-1.65854000	-2.73329000
H	-2.58583500	-2.17825600	-3.54680900
H	-6.29812900	-1.12640600	-1.64884600
H	-5.01884100	-1.70850800	-3.69181500

M3_{Cat4}

C	2.88737400	-1.42578400	-0.43113200
C	4.12268500	-2.25523100	-0.24207800
H	2.07487600	-1.81311900	-1.03556700
H	3.91826000	-3.20392900	0.26933800
H	4.61595800	-2.50556300	-1.19072900
H	4.84080300	-1.69627200	0.36324900

O	3.69649800	0.66877500	0.45328000
C	2.87426900	-0.11919200	-0.03218300
C	-0.10862500	2.19935600	-0.63743600
H	-0.55812000	3.00802400	-0.06076200
H	-0.20997800	2.38434800	-1.71009800
C	0.30243000	0.00610100	-0.12294900
N	1.50067100	0.53312700	-0.23574200
N	-0.68736000	0.90074700	-0.29440300
C	1.35426300	1.98059500	-0.20743300
H	2.10983500	2.46102500	-0.82600800
S	-0.25893700	-1.58957500	0.22111400
C	-1.97244900	0.39235400	-0.15470100
C	-1.92918300	-0.97773300	0.14008700
C	-3.17919800	1.07132000	-0.27330800
H	-3.20062400	2.13193600	-0.49883000
C	-3.10080800	-1.69940600	0.31923800
H	-3.07167300	-2.75956900	0.54596800
C	-4.31352400	-1.02469900	0.20018800
H	-5.24085600	-1.56932600	0.33629900
C	-4.34949500	0.34109200	-0.09133700
H	-5.30573200	0.84482900	-0.17890300
F	1.48651700	2.42565200	1.08125100

TS4_{Cat4}

C	2.07067500	0.57428300	-0.46954900
O	1.29923600	0.51545600	0.68868400
H	1.97480400	-0.31205300	-1.10574800
N	1.08806400	1.61161800	-0.63498100
S	-0.24052000	1.13430100	-1.53778300
O	-0.55237900	-0.29619300	-1.41129300
O	-0.04699200	1.65632000	-2.88933600
C	-1.53981100	2.03680200	-0.73453000
C	-2.79168500	1.44105200	-0.64609400
C	-1.32049800	3.33607300	-0.27863200
C	-3.84164200	2.15970800	-0.07934100
H	-2.93743600	0.42816700	-1.00939400
C	-2.37792400	4.03278900	0.28786100
H	-0.33313900	3.77796900	-0.35587700
C	-3.65115100	3.45775300	0.39498700
H	-4.82297000	1.69886300	-0.00444100
H	-2.21739800	5.04242300	0.65595100
C	-4.78201700	4.23647500	1.01417200
H	-4.55355900	4.49394900	2.05269900
H	-4.94963100	5.17378900	0.47596700

H	-5.71244800	3.66548000	1.00120600
C	3.48475700	1.02564500	-0.29044400
C	3.76188100	2.19629500	0.41677600
C	4.52322800	0.23304700	-0.77077900
C	5.08004000	2.57474400	0.63751800
H	2.93540300	2.79377600	0.79025500
C	5.84519300	0.61395300	-0.54766900
H	4.28948600	-0.69747400	-1.27902200
C	6.12317200	1.78276800	0.15480400
H	5.29955100	3.48447600	1.18747400
H	6.65600200	-0.00663300	-0.91533000
H	7.15309900	2.07748000	0.33136600
C	2.11285700	-1.03380000	2.06406000
C	3.35670800	-0.48744100	2.69736700
H	1.19478800	-0.99164300	2.63655700
H	4.18979500	-0.54581000	1.99232200
H	3.22262100	0.56362200	2.97347000
H	3.63956300	-1.03695300	3.60456500
O	3.20894200	-2.33870800	0.38507900
C	2.22238500	-1.92164400	1.00030900
C	-0.46290800	-3.51198200	-1.14141900
H	-0.70656800	-3.19658800	-2.15786000
H	-0.68090700	-4.57185700	-0.99682000
C	-0.33073400	-2.05753000	0.63736900
N	0.93490600	-2.37020100	0.39327500
N	-1.18249000	-2.70600100	-0.16459700
C	1.00413100	-3.15096300	-0.83731900
H	1.68041200	-3.99383000	-0.70768500
S	-1.12571300	-1.01414500	1.75828600
C	-2.51546600	-2.36071900	-0.01764100
C	-2.67848300	-1.46540800	1.04567600
C	-3.59858800	-2.79815300	-0.77218900
H	-3.45873300	-3.48391900	-1.60050100
C	-3.93860000	-0.99288300	1.38905300
H	-4.06619600	-0.28930000	2.20435200
C	-5.02726900	-1.42918900	0.63897300
H	-6.02053500	-1.07102800	0.88596500
C	-4.85663200	-2.31477000	-0.43016400
H	-5.71959200	-2.63176700	-1.00504000
F	1.49108600	-2.37755300	-1.85581900
TS3'			
C	-0.69025200	2.52932400	-1.79058300
C	-1.04625900	3.91776500	-2.26739600

H	-0.32439600	1.77260300	-2.46404400
H	-0.18387200	4.41532300	-2.72326500
H	-1.84668700	3.89026500	-3.01412100
H	-1.38867800	4.54286200	-1.43959800
O	-1.04935000	2.33142200	0.64894300
C	-0.82611200	2.22610900	-0.50528000
C	0.74040100	-2.09687500	-0.15790600
C	1.82735500	-3.12636800	-0.14261800
C	-0.13272600	-0.07314700	-0.57563400
H	1.76428700	-3.74317100	-1.05170300
N	-0.51185700	-2.22189500	0.15884100
N	1.00358200	-0.82735900	-0.60327300
N	-1.01804100	-0.96566100	-0.10558100
C	-2.40320900	-0.69890400	0.14851900
C	-2.80267100	-0.46797600	1.46727100
C	-3.29085900	-0.66212800	-0.92624900
C	-4.15233200	-0.21565200	1.69802600
C	-4.63302200	-0.40232100	-0.64748900
C	-5.08046200	-0.18571600	0.65499100
H	-4.48662900	-0.02913600	2.71602200
H	-5.34370400	-0.36833000	-1.46978500
O	3.08374400	-2.48916600	-0.05844000
H	1.72546900	-3.77675000	0.72710000
C	3.30827500	-1.55825600	-1.10740900
H	3.21685800	-2.06154600	-2.07992900
C	2.33182200	-0.36410200	-0.97113000
H	2.24481900	0.16602200	-1.92655400
C	4.68509600	-0.93539100	-0.85514100
H	5.10511800	-0.55561300	-1.79363300
C	4.37413000	0.19421300	0.10149300
C	3.01532700	0.50835100	0.06044500
C	5.22641100	0.88950100	0.94881700
H	6.28429400	0.64748100	0.99294100
C	4.69478400	1.89540100	1.75673100
C	2.47450100	1.50310000	0.86328500
H	1.41090300	1.72568700	0.84371600
C	3.33295200	2.19507000	1.71874700
H	2.93512500	2.97170500	2.36377000
H	5.34600700	2.44406900	2.42989600
H	5.37329600	-1.68113900	-0.45031000
C	-1.78814900	-0.46437500	2.57737400
H	-1.27092500	-1.42604600	2.64079600
H	-1.03401300	0.30724900	2.39038800
H	-2.26538900	-0.25897600	3.53710600

C	-2.80354900	-0.86873100	-2.33500300
H	-2.18939000	-0.01808700	-2.64822600
H	-2.18543800	-1.76831400	-2.41043100
H	-3.64397000	-0.96383500	-3.02485900
C	-6.54013400	0.05849800	0.94043100
H	-6.66872500	0.82443400	1.70938200
H	-7.07136700	0.38057500	0.04213900
H	-7.02185400	-0.85531800	1.30352300

RI'

O	1.86751300	-0.26901500	0.00004600
C	0.76662900	0.12431000	-0.00005300
C	-0.46907500	0.56876100	-0.00015000
H	-0.56791400	1.64746000	0.00044500
C	-1.68671300	-0.33310700	0.00003000
H	-1.72742600	-0.97145100	0.88599100
H	-2.58248200	0.28824900	-0.00018300
H	-1.72733300	-0.97192400	-0.88559000

TS4'

C	0.41010200	2.19726300	-0.49676200
H	1.43399200	2.49431900	-0.71430300
C	-0.45547200	2.47038600	-1.50933200
C	-0.10502800	2.28941100	0.92795700
H	0.66734000	1.89574100	1.59106300
H	-0.30834900	3.32210600	1.21938900
H	-1.01229400	1.69036500	1.04461200
O	-1.19631100	2.57732200	-2.37806100
C	1.15107700	-0.39374600	0.10131800
O	0.50018100	0.35777000	-0.92670500
H	0.59454600	-0.36134900	1.04961900
N	0.89898800	-1.48401700	-0.75356400
S	-0.52758900	-2.28963300	-0.43474600
O	-0.31321000	-3.15449700	0.72727400
O	-0.96610100	-2.87603900	-1.69422600
C	-1.76200400	-1.08916300	0.05843300
C	-2.11927000	-0.99532900	1.39639900
C	-2.36150300	-0.27885900	-0.90589300
C	-3.09268300	-0.07061500	1.77736600
H	-1.64869500	-1.65316600	2.11998600
C	-3.32236000	0.64060300	-0.51105200
H	-2.06817700	-0.37482400	-1.94683800
C	-3.70551900	0.75477300	0.83470100
H	-3.38313100	0.00202900	2.82152100

H	-3.79675400	1.27502000	-1.25563200
C	-4.77832800	1.73277000	1.23568500
H	-4.60500000	2.71497200	0.78760300
H	-5.75832600	1.38727100	0.89239900
H	-4.82459600	1.85086600	2.31996200
C	2.59312000	-0.02407500	0.29145900
C	3.40610500	0.17230500	-0.82699800
C	3.11822800	0.13362200	1.57143200
C	4.74021600	0.52189200	-0.65930700
H	2.97699600	0.03882800	-1.81559100
C	4.45796700	0.48143500	1.73869100
H	2.48161200	-0.02914900	2.43818400
C	5.26716700	0.67665300	0.62427600
H	5.37462200	0.67100500	-1.52722500
H	4.86717600	0.59811900	2.73686300
H	6.31019300	0.94770800	0.75278300