

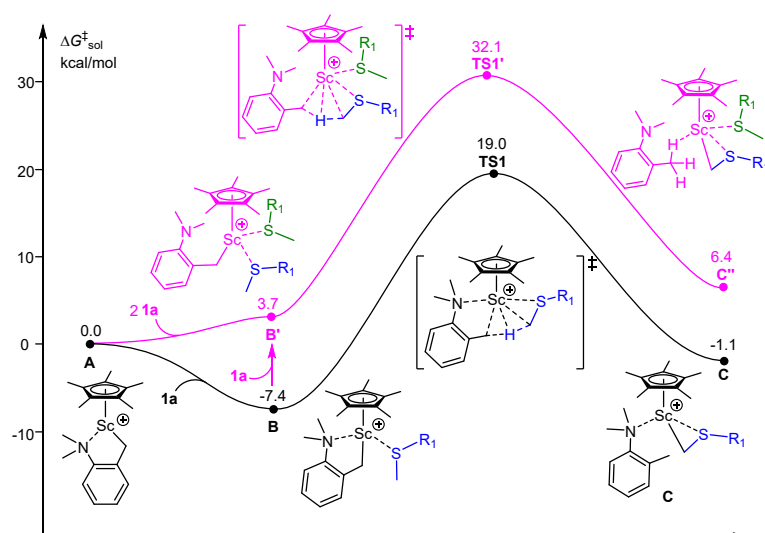
*Electronic Supplementary Information*

**Mechanistic Insights into Rare-Earth-Catalysed C–H Alkylation of  
Sulfides: Sulfide Facilitating Alkene Insertion and Beyond**

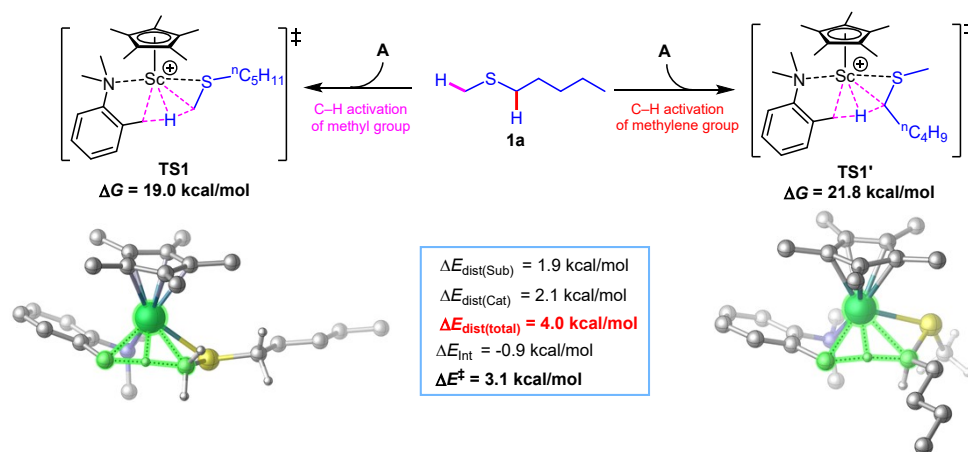
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**Fig. S1** Computed C–H activation of sulfide **1a** by species **A** via *N*-ligated and *N*-dissociated pathways.

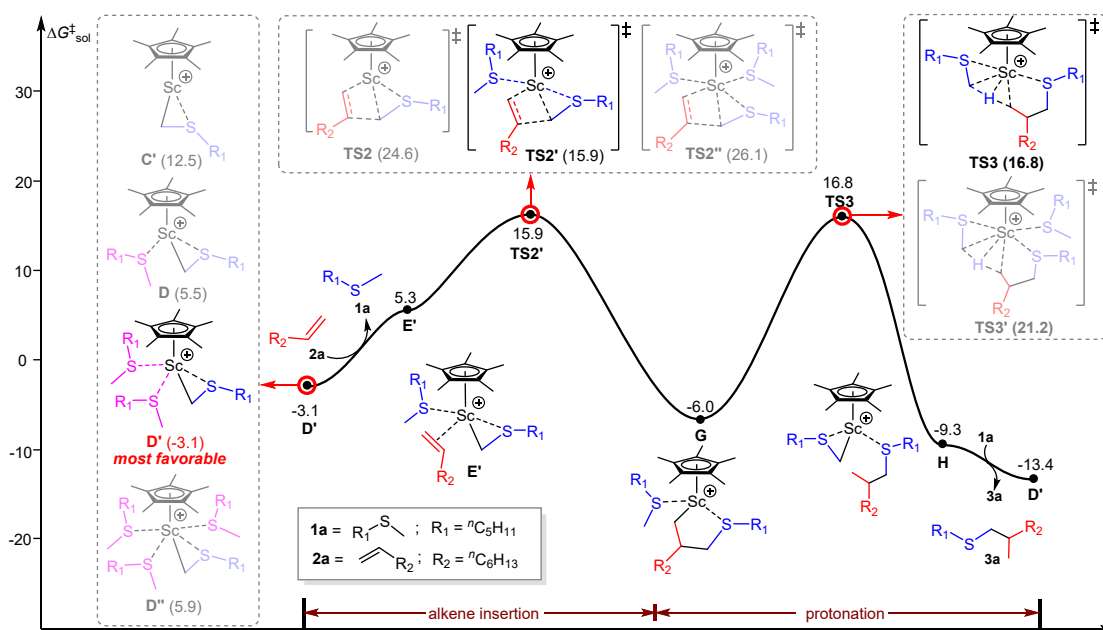


**Fig. S2** Computed C–H activation of sulfide **1a** for both  $\alpha$ -methyl and  $\alpha$ -methylene sites and distortion-interaction analysis for two transition states. All H atoms except for those involved in  $\alpha$ -methyl and  $\alpha$ -methylene are omitted for clarity.

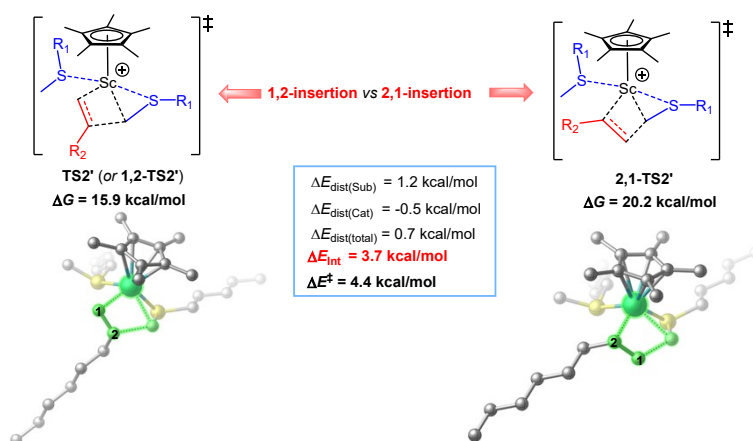
In distortion-interaction analysis (DIA), we divided each structure of transition state into two fragments (*i.e.*, the substrate moiety as fragment Sub and the remaining part as fragment Cat). The energies of the two parts at the geometry they have in the transition states were evaluated through single-point calculations.  $\Delta E_{\text{dist(Sub)}}$  is the energy difference between fragment Sub in the two transition state geometries, whereas  $\Delta E_{\text{dist(Cat)}}$  is the energy difference of fragment Cat in the transition states.  $\Delta E_{\text{dist(total)}}$  denotes the energy sum of  $\Delta E_{\text{dist(Sub)}}$  and  $\Delta E_{\text{dist(Cat)}}$ . The single-point energies of the two fragments and the electronic energy of the corresponding transition state were used to

estimate the interaction energy between the two fragments.  $\Delta E_{\text{int}}$  is the difference in interaction energies between fragments in these transition state geometries. The difference of activation energy between the transition states ( $\Delta E^{\ddagger}$ ) is defined as  $\Delta E^{\ddagger} = \Delta E_{\text{int}} + \Delta E_{\text{dist(Sub)}} + \Delta E_{\text{dist(Cat)}}$ .

As shown in Figure S1, the computational result shows that  $\alpha$ -C(methyl)-H bond activation is more favorable than that of  $\alpha$ -C(methylene)-H bond by 2.8 kcal/mol, which is line with the experimental observation of  $\alpha$ -C(methyl)-H alkylation product. DIA results indicated that the selectivity of this reaction obviously arises from the greater distortion energy in **TS1'** than in **TS1** ( $\Delta E_{\text{dist(total)}} = 4.0$  kcal/mol). Therefore, the selectivity of C-H activation is resulted from steric factors.

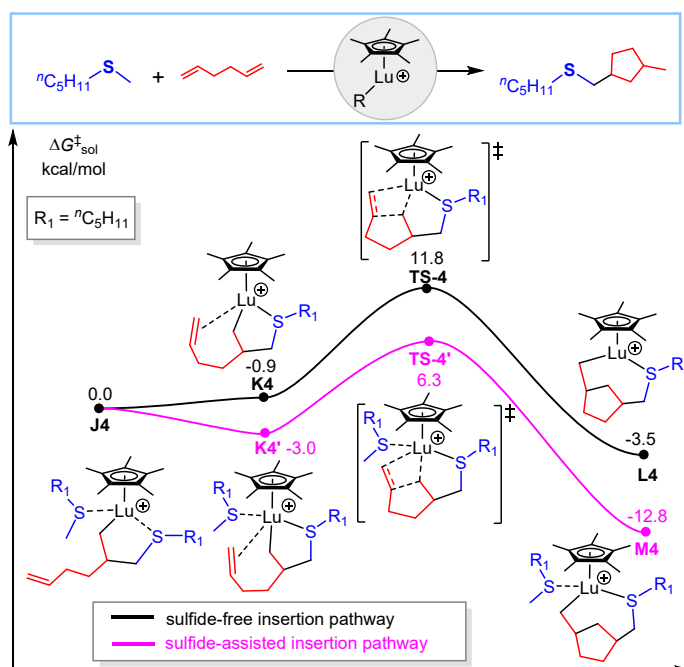


**Fig. S3** Energy profiles for the processes of substrate-assisted/free alkene insertion and protonation. Relative free energies are given in kcal/mol.

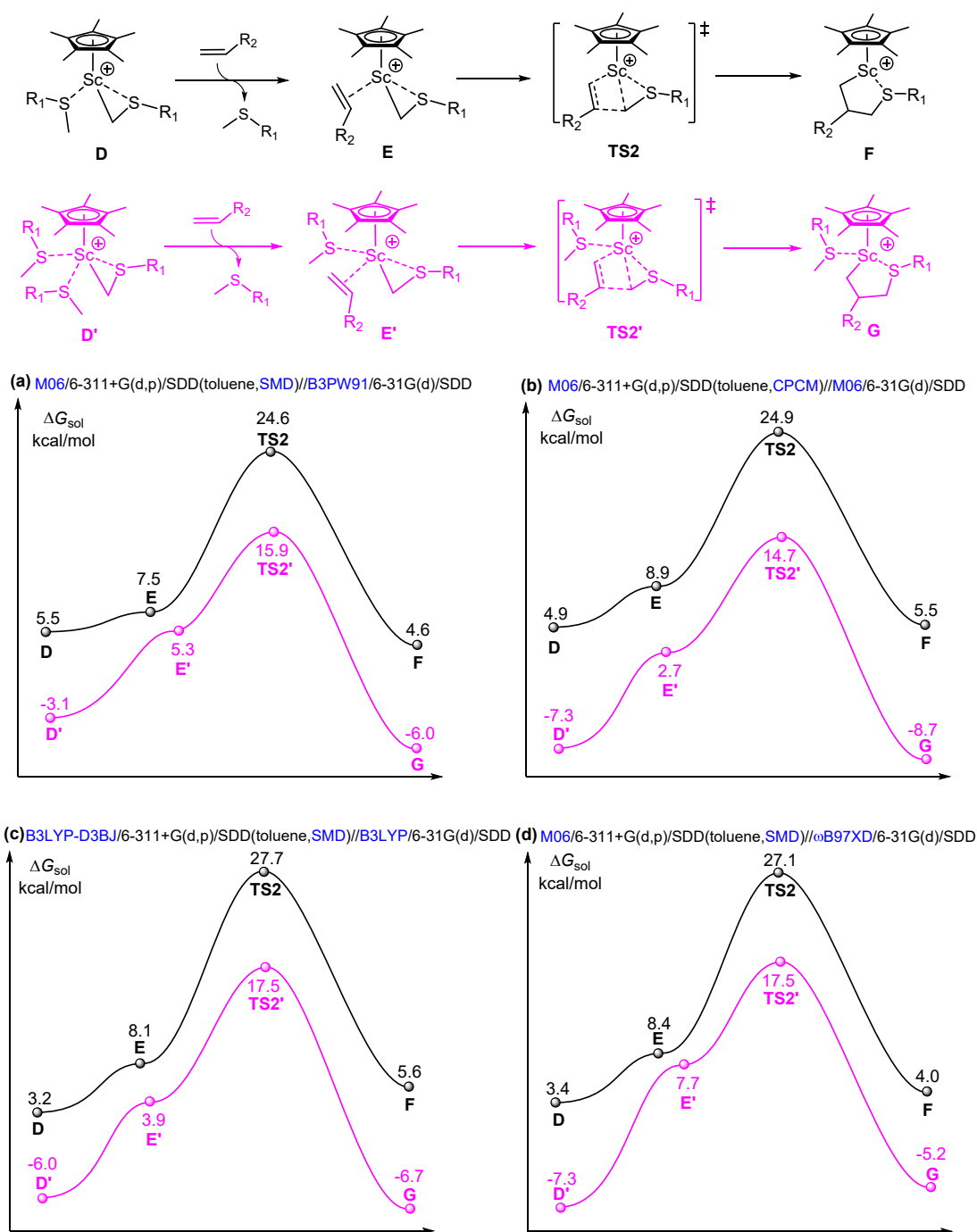


**Fig. S4** Computed alkene insertion via 1,2- and 2,1-insertion modes and distortion-interaction analysis for two transition states. All H atoms in 3D structures are omitted for clarity.

The result shows that alkene insertion through 1,2-insertion mode is more favorable than that 2,1-insertion path by 4.3 kcal/mol, which is line with the experimental observation of regioselectivity. DIA results indicated that the regioselectivity of this reaction is mainly thanks to the stronger interaction in **1,2-TS2'** than in **2,1-TS2'** ( $\Delta E_{\text{int}} = 3.7 \text{ kcal/mol}$ ). Therefore, the regioselectivity of alkene insertion is controlled by electronic factors.



**Fig. S5** Energy profiles for cyclization processes for the case of 1,5-heptadiene catalysed by  $(\text{C}_5\text{Me}_5)\text{LuR}_2$ .



**Fig. S6** Energy profiles for alkene insertion via slide-free and sulfide-facilitated pathways calculated at different functional/basis set/solvation model combinations. The free energies (kcal mol<sup>-1</sup>) are relative to the initial species **A** calculated at their corresponding theoretical level.

## DFT Optimized Cartesian Coordinates of All Structures

Optimized Cartesian coordinates and their corresponding single-point energies ( $E_{(\text{SCRF})}$ , a.u.) calculated at the M06/6-311+G(d,p)-SDD(SMD, toluene)//B3PW91/6-31G(d)-SDD level as well as the imaginary frequency (IF,  $\text{cm}^{-1}$ ) of transition states.

48 (the number of atoms involved in the molecule)

**A,  $E_{(\text{SCF Done})} = -841.276398$  a.u.**

N	-1.581041000	1.768803000	-0.437999000
C	-0.787415000	-0.459681000	-2.057581000
H	-0.917450000	0.353459000	-2.780578000
H	-0.530953000	-1.386508000	-2.568482000
C	-1.828829000	-0.612571000	-1.037101000
C	-2.185870000	0.466750000	-0.162678000
C	-3.058960000	0.265464000	0.921195000
H	-3.346704000	1.099039000	1.553575000
C	-3.578025000	-0.993097000	1.179600000
H	-4.258788000	-1.136245000	2.013087000
C	-3.227118000	-2.070520000	0.354950000
H	-3.637253000	-3.057533000	0.549447000
C	-2.369697000	-1.883058000	-0.714557000
H	-2.115544000	-2.719818000	-1.359508000
C	-1.544561000	2.693895000	0.712157000
H	-2.543787000	3.059853000	0.980015000
H	-0.930991000	3.559359000	0.444934000
H	-1.112565000	2.206443000	1.593949000
C	-2.177737000	2.460942000	-1.605199000
H	-2.286219000	1.770461000	-2.441026000
H	-1.534890000	3.294084000	-1.904397000
H	-3.170138000	2.848686000	-1.343564000
C	2.607367000	0.659239000	0.182313000
C	1.909101000	0.305461000	1.378060000
C	1.368022000	-1.006788000	1.199261000
C	1.753442000	-1.470110000	-0.098058000
C	2.510945000	-0.441376000	-0.728453000
C	1.834105000	1.128746000	2.634088000
H	0.926595000	0.926023000	3.213151000
H	1.874654000	2.205238000	2.434637000
H	2.682602000	0.899982000	3.292123000
C	0.634776000	-1.813531000	2.233964000
H	1.332091000	-2.462342000	2.779838000
H	-0.127239000	-2.460929000	1.788506000
H	0.138897000	-1.181402000	2.977321000
C	1.495989000	-2.841639000	-0.645906000
H	1.503642000	-2.854645000	-1.739507000

H	0.535449000	-3.245357000	-0.310341000
H	2.273568000	-3.539149000	-0.307746000
C	3.161269000	-0.525934000	-2.079089000
H	4.165151000	-0.962519000	-1.995825000
H	3.282193000	0.457604000	-2.545290000
H	2.590881000	-1.153814000	-2.770172000
C	3.381776000	1.927971000	-0.048368000
H	4.429128000	1.798945000	0.254401000
H	3.396020000	2.224264000	-1.103149000
H	2.989187000	2.769965000	0.532289000
Sc	0.288965000	0.455441000	-0.375395000

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**1a,  $E_{(\text{SCF Done})} = -635.125258$  a.u.**

C	-4.215698000	0.346928000	-0.000149000
H	-5.103907000	-0.295093000	0.000077000
H	-4.272428000	0.993395000	0.884342000
H	-4.272392000	0.992726000	-0.885130000
C	-2.930790000	-0.478509000	0.000184000
H	-2.918738000	-1.139421000	0.878430000
H	-2.918653000	-1.139998000	-0.877628000
C	-1.665358000	0.381016000	-0.000040000
H	-1.676340000	1.042623000	0.878939000
H	-1.676333000	1.042183000	-0.879351000
C	-0.376716000	-0.444578000	0.000141000
H	-0.360548000	-1.101968000	-0.879776000
H	-0.360603000	-1.101726000	0.880240000
C	0.875401000	0.428980000	0.000050000
H	0.888081000	1.075277000	0.887170000
H	0.887912000	1.075362000	-0.887013000
S	2.375677000	-0.610254000	-0.000148000
C	3.646250000	0.684712000	0.000088000
H	3.578194000	1.312853000	0.894592000
H	4.618193000	0.183367000	0.000005000
H	3.578197000	1.313195000	-0.894175000

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**B,  $E_{(\text{SCF Done})} = -1476.436922$  a.u.**

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H	1.283881000	-0.613530000	-2.707286000
H	2.519778000	0.661585000	-2.495671000
C	2.713067000	-0.961394000	-1.105892000
C	2.114209000	-1.912348000	-0.226645000
C	2.894424000	-2.674774000	0.657137000
H	2.427133000	-3.415136000	1.298224000

C	4.269310000	-2.508019000	0.707568000
H	4.863862000	-3.112070000	1.386283000
C	4.880901000	-1.566151000	-0.129021000
H	5.959378000	-1.436100000	-0.104361000
C	4.117129000	-0.810234000	-1.001542000
H	4.600888000	-0.098230000	-1.664791000
C	0.045149000	-2.620054000	0.927668000
H	0.282644000	-3.682299000	1.071329000
H	-1.041741000	-2.530853000	0.839857000
H	0.381667000	-2.065514000	1.808414000
C	0.254718000	-2.904123000	-1.452174000
H	0.711849000	-2.530429000	-2.368214000
H	-0.832041000	-2.872797000	-1.560973000
H	0.577413000	-3.941875000	-1.296865000
C	-0.319770000	2.118097000	1.066522000
C	0.293638000	1.204788000	1.981083000
C	1.695031000	1.191872000	1.716944000
C	1.945373000	2.089351000	0.630924000
C	0.703041000	2.664109000	0.238477000
C	-0.410606000	0.519453000	3.119048000
H	0.178633000	-0.304058000	3.534195000
H	-1.391272000	0.119689000	2.833620000
H	-0.587659000	1.224598000	3.942004000
C	2.749343000	0.496565000	2.528791000
H	3.153590000	1.178829000	3.288527000
H	3.588857000	0.159076000	1.914313000
H	2.358452000	-0.376779000	3.059860000
C	3.293373000	2.497086000	0.116296000
H	3.257916000	2.792278000	-0.937168000
H	4.029667000	1.694754000	0.215782000
H	3.673699000	3.358890000	0.681311000
C	0.542227000	3.734068000	-0.801943000
H	0.901548000	4.698961000	-0.420864000
H	-0.504170000	3.877349000	-1.087380000
H	1.114501000	3.519489000	-1.711745000
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H	-1.884171000	3.325687000	1.903287000
H	-2.086846000	3.008509000	0.185089000
H	-2.436572000	1.741560000	1.374331000
Sc	0.601974000	0.241130000	-0.238292000
C	-7.106617000	-1.282966000	1.436494000
H	-7.416872000	-2.040910000	2.163188000
H	-7.259470000	-0.299297000	1.896039000
H	-7.778849000	-1.355482000	0.573574000



C	-5.650503000	-1.481537000	1.021823000
H	-5.006338000	-1.440379000	1.912149000
H	-5.523205000	-2.486897000	0.596308000
C	-5.175554000	-0.440485000	0.005901000
H	-5.299899000	0.566415000	0.429506000
H	-5.818431000	-0.481334000	-0.884613000
C	-3.716505000	-0.640028000	-0.417121000
H	-3.595568000	-1.641417000	-0.851968000
H	-3.072429000	-0.597409000	0.473810000
C	-3.269338000	0.412394000	-1.426493000
H	-3.346182000	1.421160000	-1.010869000
H	-3.885548000	0.363056000	-2.331054000
S	-1.545058000	0.118923000	-1.972265000
C	-1.327469000	1.421386000	-3.221138000
H	-1.508869000	2.411416000	-2.797880000
H	-0.298194000	1.361544000	-3.581596000
H	-2.010557000	1.234971000	-4.053775000

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**TS1,  $E_{(\text{SCF Done})} = -1476.395118$  a.u., IF =  $i1256.314$  cm<sup>-1</sup>**

N	1.135332000	-2.140375000	0.055027000
C	2.180981000	-0.443790000	-2.050923000
H	2.074287000	-1.242193000	-2.798730000
H	2.655460000	0.403152000	-2.555500000
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C	2.530261000	-1.738553000	0.131825000
C	3.366190000	-2.160824000	1.176747000
H	2.984006000	-2.818080000	1.950514000
C	4.695577000	-1.766497000	1.217118000
H	5.337136000	-2.114622000	2.021227000
C	5.203214000	-0.932584000	0.216291000
H	6.246189000	-0.629457000	0.234935000
C	4.376614000	-0.502724000	-0.810718000
H	4.780276000	0.125379000	-1.600120000
C	0.533496000	-2.529330000	1.344479000
H	0.925768000	-3.487126000	1.710209000
H	-0.545087000	-2.633949000	1.203461000
H	0.723432000	-1.762870000	2.102877000
C	0.922145000	-3.230744000	-0.925828000
H	1.343909000	-2.960390000	-1.893593000
H	-0.149252000	-3.407379000	-1.041943000
H	1.409765000	-4.149367000	-0.574628000
C	-0.494301000	2.168638000	0.481377000
C	0.207909000	1.572792000	1.576283000
C	1.603379000	1.649047000	1.298145000

C	1. 761807000	2. 260015000	0. 015102000
C	0. 463866000	2. 586153000	-0. 482449000
C	-0. 428804000	1. 093571000	2. 850795000
H	0. 239326000	0. 448333000	3. 430044000
H	-1. 358314000	0. 540483000	2. 671994000
H	-0. 684873000	1. 942773000	3. 498335000
C	2. 715373000	1. 295878000	2. 242588000
H	3. 011182000	2. 179148000	2. 824443000
H	3. 606187000	0. 937997000	1. 719414000
H	2. 422300000	0. 525391000	2. 962630000
C	3. 055031000	2. 714853000	-0. 593771000
H	3. 037867000	2. 675861000	-1. 688247000
H	3. 903928000	2. 120585000	-0. 246371000
H	3. 256550000	3. 758645000	-0. 317552000
C	0. 195916000	3. 376764000	-1. 730176000
H	0. 378983000	4. 445150000	-1. 555015000
H	-0. 841881000	3. 285664000	-2. 065914000
H	0. 842701000	3. 075395000	-2. 561572000
C	-1. 956282000	2. 500682000	0. 483583000
H	-2. 129454000	3. 423047000	1. 054534000
H	-2. 343455000	2. 681802000	-0. 523646000
H	-2. 563401000	1. 719590000	0. 951791000
Sc	0. 638348000	0. 109429000	-0. 317546000
C	-8. 030621000	-0. 421788000	0. 800143000
H	-8. 654593000	-0. 835591000	1. 599212000
H	-8. 083605000	0. 671294000	0. 869405000
H	-8. 477623000	-0. 716599000	-0. 156632000
C	-6. 590388000	-0. 915943000	0. 914545000
H	-6. 182354000	-0. 636896000	1. 896368000
H	-6. 573748000	-2. 014094000	0. 876610000
C	-5. 683265000	-0. 360407000	-0. 185629000
H	-5. 698520000	0. 738533000	-0. 150298000
H	-6. 088017000	-0. 642477000	-1. 167989000
C	-4. 237289000	-0. 855218000	-0. 071593000
H	-4. 221738000	-1. 952533000	-0. 114908000
H	-3. 827612000	-0. 571323000	0. 907677000
C	-3. 359908000	-0. 285662000	-1. 181609000
H	-3. 312290000	0. 804432000	-1. 138365000
H	-3. 732911000	-0. 580130000	-2. 168122000
S	-1. 653804000	-0. 962138000	-1. 070820000
C	-0. 667240000	-0. 078126000	-2. 298251000
H	-1. 031075000	0. 944236000	-2. 433741000
H	0. 764178000	-0. 205167000	-2. 173161000
H	-0. 670559000	-0. 597236000	-3. 261674000

**C,  $E_{(\text{SCF Done})} = -1476.427369$  a.u.**

N	1.430762000	-1.877930000	0.024281000
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H	3.355150000	0.413580000	-2.551784000
C	3.537999000	-0.929131000	-0.878944000
C	2.861526000	-1.600104000	0.161664000
C	3.564083000	-2.000768000	1.304331000
H	3.060382000	-2.529436000	2.105234000
C	4.924012000	-1.737159000	1.436582000
H	5.447720000	-2.060595000	2.331299000
C	5.601003000	-1.066081000	0.422544000
H	6.661788000	-0.852538000	0.513797000
C	4.905842000	-0.671965000	-0.715482000
H	5.433926000	-0.154856000	-1.513310000
C	0.765679000	-2.258054000	1.290319000
H	1.102567000	-3.236446000	1.656178000
H	-0.311631000	-2.324989000	1.110068000
H	0.959124000	-1.509176000	2.064198000
C	1.199559000	-2.968107000	-0.961926000
H	1.626107000	-2.706631000	-1.929709000
H	0.125371000	-3.127771000	-1.082208000
H	1.669406000	-3.894535000	-0.607899000
C	-0.731294000	2.207577000	0.521085000
C	0.007432000	1.610834000	1.590802000
C	1.394183000	1.701718000	1.273897000
C	1.508665000	2.324217000	-0.008089000
C	0.194546000	2.649678000	-0.466489000
C	-0.585003000	1.119393000	2.881641000
H	0.093704000	0.452752000	3.423185000
H	-1.530582000	0.586150000	2.731906000
H	-0.799044000	1.962414000	3.552004000
C	2.538838000	1.356324000	2.182110000
H	2.821629000	2.232984000	2.780331000
H	3.429209000	1.039802000	1.631319000
H	2.287552000	0.560058000	2.890138000
C	2.789902000	2.744296000	-0.670038000
H	2.692638000	2.798929000	-1.759261000
H	3.619634000	2.070886000	-0.433999000
H	3.082744000	3.746014000	-0.327976000
C	-0.124713000	3.456502000	-1.690991000
H	-0.011382000	4.529060000	-1.484741000
H	-1.153954000	3.303738000	-2.029305000

H	0.536045000	3.217735000	-2.530576000
C	-2.202831000	2.496310000	0.548459000
H	-2.396473000	3.413204000	1.121445000
H	-2.610249000	2.661520000	-0.453363000
H	-2.778177000	1.696334000	1.025300000
Sc	0.382761000	0.201313000	-0.369052000
C	-8.104114000	-0.827388000	0.833704000
H	-8.695283000	-1.306492000	1.621194000
H	-8.202583000	0.257699000	0.957745000
H	-8.555403000	-1.094329000	-0.129223000
C	-6.642224000	-1.263255000	0.900078000
H	-6.228624000	-1.015377000	1.887978000
H	-6.579446000	-2.356466000	0.807325000
C	-5.779509000	-0.615861000	-0.185496000
H	-5.839629000	0.478419000	-0.094606000
H	-6.190816000	-0.865400000	-1.173902000
C	-4.312697000	-1.054870000	-0.121138000
H	-4.253176000	-2.146920000	-0.221105000
H	-3.895848000	-0.804655000	0.864352000
C	-3.478958000	-0.394369000	-1.213611000
H	-3.468495000	0.693304000	-1.110795000
H	-3.858855000	-0.646618000	-2.209084000
S	-1.744946000	-1.003451000	-1.177701000
C	-0.725033000	0.019247000	-2.275608000
H	-1.261424000	0.933171000	-2.549437000
H	1.813770000	-0.353284000	-2.171186000
H	-0.460204000	-0.535196000	-3.180484000

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**RH,  $E_{(\text{SCF Done})} = -405.319575$  a.u.**

N	1.575305000	-0.058062000	-0.178519000
C	-0.057959000	2.325597000	-0.374805000
H	0.205761000	2.841832000	0.558798000
H	-0.772154000	2.967269000	-0.901707000
C	-0.647788000	0.962397000	-0.131466000
C	0.165520000	-0.192855000	-0.057842000
C	-0.443314000	-1.447494000	0.089086000
H	0.173570000	-2.339823000	0.141236000
C	-1.827563000	-1.572731000	0.180112000
H	-2.272531000	-2.558405000	0.293734000
C	-2.630417000	-0.437220000	0.133933000
H	-3.711902000	-0.520614000	0.203173000
C	-2.032689000	0.811574000	-0.024333000
H	-2.658082000	1.700025000	-0.092351000
C	2.296644000	-1.207783000	-0.686138000

H	2.404858000	-2.029953000	0.046078000
H	3.306340000	-0.890933000	-0.973080000
H	1.794788000	-1.599348000	-1.575732000
C	2.240106000	0.518177000	0.981442000
H	1.709739000	1.407608000	1.327275000
H	3.260184000	0.814359000	0.708925000
H	2.301564000	-0.191275000	1.826923000
H	0.855488000	2.247717000	-0.973569000

46

**$C', E_{(\text{SCF Done})} = -1071.058180 \text{ a.u.}$**

C	-2.036743000	1.725832000	0.056366000
C	-2.764688000	1.008969000	-0.939381000
C	-3.212894000	-0.220713000	-0.356692000
C	-2.776483000	-0.259424000	1.003793000
C	-2.033918000	0.937204000	1.251958000
C	-3.062678000	1.485338000	-2.333889000
H	-3.170565000	0.659570000	-3.045380000
H	-2.293014000	2.162651000	-2.719086000
H	-4.009412000	2.040636000	-2.352299000
C	-4.063303000	-1.258058000	-1.032941000
H	-5.127323000	-1.046477000	-0.864664000
H	-3.873220000	-2.264020000	-0.645511000
H	-3.914934000	-1.280078000	-2.117754000
C	-3.147894000	-1.295450000	2.021727000
H	-2.390296000	-1.393489000	2.804520000
H	-3.289782000	-2.282007000	1.571537000
H	-4.090861000	-1.022980000	2.513760000
C	-1.433311000	1.334651000	2.570781000
H	-2.180848000	1.846121000	3.191094000
H	-0.592902000	2.027608000	2.457098000
H	-1.084404000	0.469415000	3.144040000
C	-1.431744000	3.092906000	-0.103129000
H	-2.163089000	3.866678000	0.164139000
H	-0.563395000	3.245892000	0.546740000
H	-1.121375000	3.296832000	-1.133604000
Sc	-0.830275000	-0.290237000	-0.399537000
C	6.976336000	1.223918000	0.357568000
H	7.767626000	1.661657000	-0.259596000
H	6.617966000	2.003585000	1.040379000
H	7.429282000	0.431408000	0.964758000
C	5.843188000	0.679400000	-0.508868000
H	5.434457000	1.487304000	-1.132126000
H	6.239793000	-0.073237000	-1.203962000
C	4.714188000	0.056207000	0.315511000

H	4.314855000	0.807584000	1.013021000
H	5.121610000	-0.754434000	0.935936000
C	3.578202000	-0.492832000	-0.554030000
H	3.974601000	-1.248773000	-1.243981000
H	3.166356000	0.314118000	-1.176772000
C	2.471566000	-1.112359000	0.292667000
H	2.030832000	-0.372153000	0.974982000
H	2.852970000	-1.936630000	0.904775000
S	1.150445000	-1.842600000	-0.767896000
C	-0.210684000	-2.181920000	0.421383000
H	0.183893000	-2.291633000	1.437371000
H	-0.694986000	-3.120590000	0.130255000

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**D,  $E_{(\text{SCF Done})} = -1706.215742$  a.u.**

C	-1.011933000	2.406737000	0.020115000
C	-0.634748000	2.021762000	1.342418000
C	0.791985000	1.981297000	1.399344000
C	1.291664000	2.321139000	0.105172000
C	0.176795000	2.587012000	-0.748811000
C	-1.566943000	1.805542000	2.501437000
H	-1.168706000	1.090119000	3.229386000
H	-2.548797000	1.442188000	2.181575000
H	-1.735189000	2.745866000	3.042847000
C	1.611354000	1.743895000	2.635854000
H	1.741309000	2.679578000	3.195590000
H	2.615644000	1.374505000	2.405127000
H	1.138434000	1.032792000	3.322304000
C	2.735318000	2.483961000	-0.278733000
H	2.926848000	2.183541000	-1.314913000
H	3.405959000	1.910069000	0.368647000
H	3.037892000	3.536185000	-0.195312000
C	0.254798000	3.109843000	-2.153473000
H	0.350562000	4.203811000	-2.151373000
H	-0.639831000	2.865553000	-2.733565000
H	1.117387000	2.711018000	-2.696448000
C	-2.406631000	2.708412000	-0.443456000
H	-2.637082000	3.770458000	-0.285928000
H	-2.540332000	2.513079000	-1.512416000
H	-3.161045000	2.136489000	0.105996000
Sc	0.089601000	0.238770000	-0.143193000
C	-8.204971000	-1.130377000	0.118315000
H	-8.885808000	-1.514996000	0.884887000
H	-8.328862000	-0.041458000	0.079837000
H	-8.528926000	-1.536288000	-0.847272000

C	-6.758980000	-1.514417000	0.423457000
H	-6.475379000	-1.125584000	1.411857000
H	-6.674467000	-2.608046000	0.488918000
C	-5.772693000	-0.995743000	-0.625424000
H	-5.854913000	0.098991000	-0.692862000
H	-6.053912000	-1.386397000	-1.613627000
C	-4.321609000	-1.383268000	-0.321177000
H	-4.238467000	-2.476839000	-0.267848000
H	-4.035645000	-0.996145000	0.666815000
C	-3.362961000	-0.848015000	-1.379237000
H	-3.376276000	0.244570000	-1.417857000
H	-3.615713000	-1.233459000	-2.372525000
S	-1.641702000	-1.408510000	-1.051616000
C	-0.539521000	-0.417439000	-2.126408000
H	-1.131773000	0.280282000	-2.727138000
H	0.020701000	-1.084606000	-2.788807000
C	7.844645000	-0.946370000	-1.030479000
H	8.391285000	-0.777063000	-1.963886000
H	8.058841000	-0.103779000	-0.362224000
H	8.252948000	-1.851818000	-0.566415000
C	6.346107000	-1.083902000	-1.289086000
H	5.973753000	-0.177650000	-1.787685000
H	6.167297000	-1.913370000	-1.987091000
C	5.543253000	-1.322401000	-0.008235000
H	5.719502000	-0.493705000	0.692948000
H	5.913208000	-2.230242000	0.488982000
C	4.039727000	-1.465909000	-0.267067000
H	3.862576000	-2.296474000	-0.962341000
H	3.667828000	-0.555749000	-0.759314000
C	3.268223000	-1.713224000	1.025936000
H	3.388562000	-0.890101000	1.737451000
H	3.607163000	-2.637319000	1.507030000
S	1.481848000	-1.955483000	0.679849000
C	0.826386000	-2.426740000	2.311399000
H	1.026051000	-1.660264000	3.063940000
H	-0.251447000	-2.574240000	2.203586000
H	1.279273000	-3.374537000	2.613272000

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**2a,  $E_{(\text{SCF Done})} = -314.295740$  a.u.**

C	4.295209000	-0.408040000	0.123182000
H	4.278626000	-1.094572000	0.978716000
H	5.203696000	0.200045000	0.202590000
H	4.380583000	-1.016442000	-0.785730000
C	3.040494000	0.462144000	0.089259000

H	3.001004000	1.084396000	0.994843000
H	3.102212000	1.162134000	-0.756366000
C	1.747941000	-0.348244000	-0.021291000
H	1.686143000	-1.049143000	0.824711000
H	1.787373000	-0.971419000	-0.927437000
C	0.486506000	0.515635000	-0.055668000
H	0.548131000	1.216282000	-0.902040000
H	0.448016000	1.138634000	0.850495000
C	-0.804451000	-0.296625000	-0.165418000
H	-0.875033000	-0.996543000	0.678808000
H	-0.769169000	-0.916969000	-1.073222000
C	-2.067160000	0.576852000	-0.197063000
H	-1.981643000	1.285794000	-1.035700000
H	-2.122235000	1.182022000	0.717889000
C	-3.327254000	-0.222947000	-0.350566000
C	-4.332065000	-0.255605000	0.525276000
H	-3.397157000	-0.829159000	-1.256478000
H	-5.218173000	-0.863256000	0.359167000
H	-4.307687000	0.329175000	1.443489000

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**E,  $E_{(\text{SCF Done})} = -1385.382381$  a.u.**

C	-2.781790000	-1.508321000	0.985655000
C	-1.794435000	-0.775752000	1.716928000
C	-2.212279000	0.589844000	1.775043000
C	-3.443814000	0.704371000	1.064281000
C	-3.789872000	-0.592418000	0.567153000
C	-0.611668000	-1.357572000	2.439431000
H	0.234891000	-0.663953000	2.482175000
H	-0.260101000	-2.285823000	1.978822000
H	-0.877469000	-1.599761000	3.476940000
C	-1.528335000	1.679003000	2.551642000
H	-1.844387000	1.654201000	3.602970000
H	-1.772391000	2.677064000	2.173793000
H	-0.437980000	1.575332000	2.548064000
C	-4.300677000	1.935281000	0.968065000
H	-4.909627000	1.951571000	0.057892000
H	-3.715124000	2.860148000	0.999074000
H	-5.000709000	1.978480000	1.812715000
C	-5.045051000	-0.944018000	-0.178486000
H	-5.846106000	-1.216935000	0.521092000
H	-4.897876000	-1.794115000	-0.851346000
H	-5.420386000	-0.108473000	-0.778727000
C	-2.821629000	-2.996639000	0.806292000
H	-3.323168000	-3.467452000	1.662135000



H	-3.374238000	-3.288700000	-0.091352000
H	-1.822131000	-3.439242000	0.744277000
Sc	-1.735884000	0.061867000	-0.546348000
C	5.164120000	-4.550365000	0.713556000
H	6.196792000	-4.345275000	1.014475000
H	4.637245000	-4.953103000	1.586902000
H	5.190929000	-5.336189000	-0.050509000
C	4.483443000	-3.288955000	0.187249000
H	4.504051000	-2.508839000	0.961466000
H	5.052872000	-2.891125000	-0.664152000
C	3.035942000	-3.532364000	-0.245747000
H	2.463990000	-3.931188000	0.604910000
H	3.014716000	-4.309875000	-1.022489000
C	2.352251000	-2.267034000	-0.775020000
H	2.918177000	-1.874392000	-1.629926000
H	2.366923000	-1.488369000	-0.000214000
C	0.914408000	-2.543549000	-1.199237000
H	0.308418000	-2.891897000	-0.357648000
H	0.873129000	-3.298787000	-1.991065000
S	0.133181000	-1.035011000	-1.909340000
C	-1.641454000	-1.430074000	-2.131582000
C	5.889211000	2.973545000	1.468648000
H	5.581254000	3.544897000	2.352583000
H	6.929198000	3.237487000	1.249682000
H	5.866210000	1.909877000	1.735850000
C	4.982124000	3.266128000	0.275758000
H	5.054966000	4.330131000	0.011195000
H	5.337227000	2.709089000	-0.602700000
C	3.516548000	2.913236000	0.537787000
H	3.160163000	3.473601000	1.414871000
H	3.443504000	1.847701000	0.805008000
C	2.603550000	3.201581000	-0.654537000
H	2.955113000	2.638685000	-1.530992000
H	2.677059000	4.265074000	-0.923300000
C	1.137085000	2.857896000	-0.386606000
H	0.778990000	3.427306000	0.482624000
H	1.062757000	1.791766000	-0.116113000
C	0.230201000	3.142436000	-1.595203000
H	0.558571000	2.567960000	-2.469959000
H	0.327282000	4.206680000	-1.860771000
C	-1.216346000	2.892486000	-1.321948000
C	-2.036393000	2.116655000	-2.063123000
H	-1.826414000	-2.476712000	-1.871887000
H	-1.920362000	-1.264297000	-3.177422000

H	-1.636013000	3.410343000	-0.456072000
H	-3.109648000	2.081642000	-1.863090000
H	-1.688459000	1.644025000	-2.983018000

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**TS2,  $E_{(\text{SCF Done})} = -1385.358046$  a.u., IF =  $i287.2534$  cm<sup>-1</sup>**

C	-2.423058000	-1.819188000	0.941029000
C	-2.515456000	-2.408647000	-0.354674000
C	-1.446461000	-3.353156000	-0.492094000
C	-0.688817000	-3.334510000	0.713705000
C	-1.278716000	-2.373918000	1.595164000
C	-3.604865000	-2.168637000	-1.361532000
H	-3.245940000	-2.254608000	-2.392855000
H	-4.060268000	-1.179963000	-1.248921000
H	-4.407518000	-2.908383000	-1.243192000
C	-1.242724000	-4.278396000	-1.656134000
H	-1.818816000	-5.202542000	-1.516874000
H	-0.194426000	-4.567649000	-1.776786000
H	-1.576237000	-3.835658000	-2.600356000
C	0.468213000	-4.229671000	1.050461000
H	1.230753000	-3.724711000	1.654245000
H	0.956909000	-4.624892000	0.155247000
H	0.124260000	-5.092963000	1.635139000
C	-0.853044000	-2.109312000	3.013880000
H	-1.353755000	-2.803895000	3.701067000
H	-1.108491000	-1.097437000	3.346718000
H	0.224082000	-2.246824000	3.157614000
C	-3.416220000	-0.875441000	1.555241000
H	-4.224022000	-1.437149000	2.042718000
H	-2.966339000	-0.241961000	2.327156000
H	-3.886532000	-0.223861000	0.811902000
Sc	-0.457670000	-1.135470000	-0.287832000
C	-5.991298000	5.277553000	0.541702000
H	-6.874584000	5.650473000	0.012989000
H	-6.338521000	4.754053000	1.440508000
H	-5.407549000	6.146805000	0.866864000
C	-5.164208000	4.357257000	-0.352920000
H	-5.785715000	3.516563000	-0.691925000
H	-4.861004000	4.899250000	-1.259249000
C	-3.917520000	3.813106000	0.348716000
H	-4.217884000	3.268754000	1.255796000
H	-3.293363000	4.653156000	0.685130000
C	-3.086273000	2.891758000	-0.551094000
H	-2.780139000	3.436522000	-1.453537000
H	-3.704728000	2.047795000	-0.885935000

C	-1.849012000	2.370840000	0.174464000
H	-2.117391000	1.787018000	1.060326000
H	-1.193645000	3.193697000	0.478479000
S	-0.850434000	1.312757000	-0.962595000
C	0.644073000	0.807019000	-0.078356000
C	8.549678000	2.876766000	0.429122000
H	8.887592000	2.816239000	-0.612403000
H	9.437539000	2.832415000	1.068889000
H	8.086935000	3.860985000	0.570927000
C	7.571903000	1.751537000	0.760078000
H	8.075033000	0.781371000	0.642885000
H	7.280094000	1.817208000	1.817962000
C	6.315477000	1.775213000	-0.112237000
H	6.607232000	1.709364000	-1.170683000
H	5.810804000	2.746011000	0.004412000
C	5.332426000	0.649188000	0.212070000
H	5.039431000	0.713807000	1.270796000
H	5.837784000	-0.320357000	0.093950000
C	4.078878000	0.673066000	-0.663832000
H	4.370241000	0.610796000	-1.721734000
H	3.572535000	1.642652000	-0.544120000
C	3.111470000	-0.472100000	-0.348833000
H	2.834791000	-0.438995000	0.714428000
H	3.633020000	-1.428250000	-0.486760000
C	1.877577000	-0.493670000	-1.246458000
C	1.260564000	-1.724872000	-1.593614000
H	0.429338000	0.574265000	0.992830000
H	1.420763000	1.568423000	-0.089888000
H	1.852189000	0.288620000	-2.005803000
H	0.822827000	-1.812021000	-2.591788000
H	1.705187000	-2.644078000	-1.213310000

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**F,  $E_{(\text{SCF Done})} = -1385.390534$  a.u.**

C	-3.418986000	-1.787714000	0.077514000
C	-2.883520000	-2.388257000	-1.100801000
C	-1.822237000	-3.265410000	-0.706376000
C	-1.700852000	-3.209148000	0.712059000
C	-2.673106000	-2.276794000	1.195668000
C	-3.393244000	-2.193566000	-2.501921000
H	-2.608577000	-2.326544000	-3.254410000
H	-3.837648000	-1.203679000	-2.652452000
H	-4.175583000	-2.929060000	-2.730460000
C	-1.024150000	-4.146271000	-1.623610000
H	-1.510427000	-5.124264000	-1.734537000

H	-0.015103000	-4.329640000	-1.242092000
H	-0.930348000	-3.724838000	-2.630125000
C	-0.809141000	-4.063936000	1.560335000
H	-0.493109000	-3.554075000	2.475597000
H	0.092970000	-4.374394000	1.026042000
H	-1.337124000	-4.977297000	1.864266000
C	-2.928526000	-1.952734000	2.641268000
H	-3.619250000	-2.683360000	3.082074000
H	-3.386485000	-0.966677000	2.774742000
H	-2.012133000	-1.982909000	3.240341000
C	-4.596166000	-0.855168000	0.136817000
H	-5.529554000	-1.425414000	0.232212000
H	-4.552835000	-0.180161000	0.998288000
H	-4.693054000	-0.243984000	-0.767092000
Sc	-1.160610000	-1.005566000	-0.152360000
C	-4.936888000	6.001348000	0.418838000
H	-5.919057000	6.239909000	-0.002004000
H	-5.067007000	5.838136000	1.495267000
H	-4.297814000	6.882712000	0.290217000
C	-4.332044000	4.774787000	-0.260248000
H	-5.011973000	3.918343000	-0.146258000
H	-4.245622000	4.956848000	-1.340390000
C	-2.956315000	4.406296000	0.299927000
H	-3.039532000	4.221372000	1.380730000
H	-2.275675000	5.261454000	0.184693000
C	-2.344180000	3.179342000	-0.384640000
H	-2.247688000	3.368504000	-1.461649000
H	-3.025864000	2.323121000	-0.272142000
C	-0.977070000	2.836485000	0.198996000
H	-1.041159000	2.592605000	1.264965000
H	-0.282369000	3.674319000	0.080046000
S	-0.213324000	1.417877000	-0.688827000
C	1.377915000	1.124309000	0.195322000
C	9.400424000	1.383140000	-0.374246000
H	9.422919000	1.267721000	-1.464741000
H	10.388225000	1.105220000	0.009112000
H	9.247339000	2.447324000	-0.157027000
C	8.301223000	0.526793000	0.250508000
H	8.501895000	-0.534550000	0.046579000
H	8.327182000	0.636005000	1.344049000
C	6.902696000	0.881298000	-0.257929000
H	6.875788000	0.770600000	-1.352292000
H	6.702396000	1.944233000	-0.055377000
C	5.796410000	0.028859000	0.365202000

H	5.821016000	0.142777000	1.459019000
H	5.998460000	-1.033724000	0.165819000
C	4.397255000	0.379403000	-0.148120000
H	4.368557000	0.247398000	-1.240192000
H	4.214969000	1.447779000	0.037344000
C	3.301993000	-0.475627000	0.495904000
H	3.271774000	-0.294558000	1.581142000
H	3.566498000	-1.534955000	0.377492000
C	1.878195000	-0.301458000	-0.076188000
C	0.895785000	-1.357993000	0.475703000
H	1.201566000	1.274232000	1.267692000
H	2.077077000	1.886389000	-0.157334000
H	1.956871000	-0.422192000	-1.170299000
H	1.281189000	-2.361922000	0.251219000
H	0.891464000	-1.295861000	1.582833000

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**D',  $E_{(\text{SCF Done})} = -2341.378307$  a.u.**

C	-3.332207000	-2.181889000	-0.686782000
C	-2.653287000	-2.897850000	0.347524000
C	-2.784250000	-2.152364000	1.555907000
C	-3.536540000	-0.972008000	1.265961000
C	-3.875359000	-0.993529000	-0.118702000
C	-2.055986000	-4.268839000	0.209930000
H	-1.223817000	-4.434077000	0.902395000
H	-1.681109000	-4.449482000	-0.801612000
H	-2.808493000	-5.040320000	0.421204000
C	-2.410915000	-2.616577000	2.935948000
H	-3.309096000	-2.922008000	3.488869000
H	-1.920903000	-1.840951000	3.536859000
H	-1.754424000	-3.491300000	2.906370000
C	-4.038850000	0.004425000	2.290241000
H	-4.193404000	1.005277000	1.873630000
H	-3.361188000	0.088544000	3.147229000
H	-5.008154000	-0.324681000	2.688947000
C	-4.731863000	0.007088000	-0.837567000
H	-5.775059000	-0.334120000	-0.875783000
H	-4.404229000	0.159742000	-1.871231000
H	-4.726977000	0.982098000	-0.341502000
C	-3.581733000	-2.678536000	-2.080258000
H	-4.453283000	-3.346675000	-2.094065000
H	-3.795197000	-1.858957000	-2.772587000
H	-2.735790000	-3.244878000	-2.482500000
Sc	-1.440585000	-0.783324000	0.013960000
C	6.400988000	-3.291197000	-2.539946000

H	7.050135000	-4.158956000	-2.382646000
H	6.491143000	-2.995894000	-3.591978000
H	6.792372000	-2.468386000	-1.929300000
C	4.952989000	-3.612786000	-2.177550000
H	4.602373000	-4.461054000	-2.781332000
H	4.899623000	-3.941829000	-1.129809000
C	4.009164000	-2.426135000	-2.383982000
H	4.059949000	-2.099774000	-3.432491000
H	4.358715000	-1.573682000	-1.781932000
C	2.555306000	-2.748119000	-2.024736000
H	2.498787000	-3.076135000	-0.977029000
H	2.205716000	-3.593408000	-2.631637000
C	1.632364000	-1.554079000	-2.245474000
H	1.656231000	-1.236198000	-3.293535000
H	1.929723000	-0.698645000	-1.628565000
S	-0.118042000	-1.986419000	-1.888073000
C	-1.041447000	-0.435151000	-2.124541000
C	1.962723000	0.246115000	1.383544000
H	2.485542000	-0.362537000	0.637616000
S	0.496504000	-0.696622000	1.959684000
C	1.219105000	-2.338811000	2.253086000
H	1.557778000	1.123218000	0.865671000
C	2.898153000	0.670145000	2.512618000
H	3.263226000	-0.215799000	3.048044000
H	2.338094000	1.266626000	3.244234000
C	4.094025000	1.471244000	1.988343000
H	3.732777000	2.359320000	1.448489000
H	4.645932000	0.868577000	1.252255000
C	5.049887000	1.910230000	3.100294000
H	5.410809000	1.022281000	3.637585000
H	4.497111000	2.509482000	3.837072000
C	6.240160000	2.710923000	2.577515000
H	5.913045000	3.624184000	2.066105000
H	6.904185000	3.009068000	3.395426000
H	6.833325000	2.124679000	1.865573000
H	-1.723918000	-0.519028000	-2.972679000
H	-0.317382000	0.368029000	-2.317914000
H	2.024236000	-2.255685000	2.986458000
H	0.433021000	-2.971321000	2.667679000
H	1.590775000	-2.775089000	1.323376000
C	-0.733951000	2.984893000	-0.743018000
H	0.325314000	2.883484000	-0.477146000
S	-1.734912000	1.931462000	0.374530000
C	-1.297684000	2.581246000	2.016207000

H	-0.875520000	2.533926000	-1.730268000
C	-1.166350000	4.448027000	-0.756220000
H	-1.035310000	4.890967000	0.239545000
H	-2.236766000	4.505903000	-0.991294000
C	-0.363631000	5.261249000	-1.777267000
H	-0.496346000	4.824064000	-2.777571000
H	0.709527000	5.184826000	-1.547704000
C	-0.768577000	6.736767000	-1.812041000
H	-0.636458000	7.172184000	-0.811630000
H	-1.840953000	6.811716000	-2.039233000
C	0.028688000	7.546398000	-2.831955000
H	-0.112304000	7.157220000	-3.847351000
H	-0.283317000	8.595998000	-2.833090000
H	1.102524000	7.519470000	-2.610999000
H	-1.706012000	3.586701000	2.137189000
H	-1.752009000	1.924723000	2.760687000
H	-0.214645000	2.598317000	2.164036000

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**E', E<sub>(SCF Done)</sub> = -2020.535837 a.u.**

C	2.645750000	1.188340000	1.729026000
C	1.768633000	2.294994000	1.519290000
C	0.661472000	2.155506000	2.407431000
C	0.853004000	0.959599000	3.163574000
C	2.086041000	0.373539000	2.758524000
C	2.063239000	3.488599000	0.658520000
H	1.153839000	4.026011000	0.372363000
H	2.601376000	3.220129000	-0.256940000
H	2.697500000	4.204551000	1.198744000
C	-0.413516000	3.180550000	2.632913000
H	-0.077996000	3.929610000	3.362286000
H	-1.333873000	2.742901000	3.032156000
H	-0.671869000	3.727213000	1.719228000
C	-0.015774000	0.457622000	4.280900000
H	-0.136929000	-0.631175000	4.253686000
H	-1.014001000	0.905926000	4.261532000
H	0.423310000	0.707872000	5.255664000
C	2.759059000	-0.778036000	3.442608000
H	3.395432000	-0.411449000	4.259367000
H	3.407489000	-1.349763000	2.771349000
H	2.038663000	-1.472299000	3.885762000
C	4.005001000	1.027044000	1.110040000
H	4.039323000	1.393557000	0.078571000
H	4.756316000	1.595152000	1.675170000
H	4.335350000	-0.015770000	1.102668000

Sc	0. 572266000	0. 272114000	0. 816658000
C	7. 540825000	-3. 736715000	-2. 335371000
H	8. 173368000	-3. 609154000	-3. 220158000
H	8. 097015000	-3. 354202000	-1. 471154000
H	7. 392592000	-4. 812690000	-2. 185542000
C	6. 207166000	-3. 012059000	-2. 501948000
H	6. 389467000	-1. 943717000	-2. 686482000
H	5. 690131000	-3. 393225000	-3. 393649000
C	5. 291445000	-3. 165267000	-1. 285553000
H	5. 806034000	-2. 782416000	-0. 392106000
H	5. 108100000	-4. 233226000	-1. 100580000
C	3. 950299000	-2. 442991000	-1. 452524000
H	3. 431473000	-2. 836267000	-2. 337117000
H	4. 131389000	-1. 374848000	-1. 635704000
C	3. 063177000	-2. 608635000	-0. 223998000
H	3. 522761000	-2. 160938000	0. 661457000
H	2. 874670000	-3. 667158000	-0. 015478000
S	1. 407916000	-1. 848781000	-0. 477153000
C	0. 548751000	-1. 912562000	1. 118640000
C	-8. 397127000	-4. 971658000	-0. 526716000
H	-9. 015203000	-4. 350047000	0. 132368000
H	-8. 736024000	-6. 007721000	-0. 419440000
H	-8. 598257000	-4. 661583000	-1. 559304000
C	-6. 914761000	-4. 835442000	-0. 186380000
H	-6. 739616000	-5. 186723000	0. 840381000
H	-6. 325668000	-5. 495678000	-0. 838606000
C	-6. 399138000	-3. 401483000	-0. 322853000
H	-6. 988040000	-2. 740382000	0. 329948000
H	-6. 573382000	-3. 049119000	-1. 350287000
C	-4. 914819000	-3. 258894000	0. 017488000
H	-4. 324286000	-3. 916418000	-0. 637213000
H	-4. 740687000	-3. 611370000	1. 044550000
C	-4. 406535000	-1. 822304000	-0. 117530000
H	-4. 988978000	-1. 159215000	0. 535960000
H	-4. 569520000	-1. 469527000	-1. 145537000
C	-2. 910635000	-1. 694196000	0. 237519000
H	-2. 338957000	-2. 355392000	-0. 429754000
H	-2. 740185000	-2. 031670000	1. 266677000
C	-2. 438851000	-0. 290317000	0. 065108000
C	-2. 025389000	0. 535885000	1. 048421000
H	-2. 497236000	0. 103564000	-0. 951475000
H	-1. 868416000	1. 597905000	0. 858507000
H	-2. 021750000	0. 212159000	2. 089819000
C	-3. 633757000	6. 613811000	-2. 054936000



H	-4.591617000	6.924952000	-1.625298000
H	-2.883007000	7.360043000	-1.769002000
H	-3.733899000	6.643622000	-3.146274000
C	-3.241504000	5.219028000	-1.572895000
H	-3.185207000	5.212257000	-0.474861000
H	-4.028331000	4.501218000	-1.844144000
C	-1.906260000	4.745176000	-2.150842000
H	-1.116328000	5.459771000	-1.878156000
H	-1.961708000	4.752231000	-3.248572000
C	-1.512898000	3.342290000	-1.675240000
H	-2.294970000	2.627606000	-1.964637000
H	-1.461236000	3.336926000	-0.577834000
C	-0.174121000	2.906556000	-2.257576000
H	0.635527000	3.563610000	-1.925207000
H	-0.209861000	2.935754000	-3.352452000
S	0.263200000	1.174969000	-1.829081000
C	1.809110000	1.013061000	-2.768184000
H	2.564933000	1.717612000	-2.412235000
H	2.166460000	-0.009391000	-2.640532000
H	1.601277000	1.190898000	-3.826662000
H	1.220484000	-2.302231000	1.887759000
H	-0.329998000	-2.557934000	1.041604000

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**TS2',  $E_{(\text{SCF Done})} = -2020.521341$  a.u., IF =  $i249.1046$  cm<sup>-1</sup>**

C	-0.883499000	1.147565000	2.547396000
C	-0.741626000	-0.189992000	3.023685000
C	0.648076000	-0.446057000	3.225011000
C	1.364274000	0.735003000	2.875033000
C	0.421535000	1.718452000	2.451860000
C	-1.876243000	-1.089910000	3.419950000
H	-1.599485000	-2.148171000	3.387248000
H	-2.758556000	-0.949104000	2.786899000
H	-2.190496000	-0.879026000	4.451154000
C	1.239046000	-1.688901000	3.824117000
H	1.331999000	-1.588113000	4.913668000
H	2.240236000	-1.901488000	3.435661000
H	0.618310000	-2.571609000	3.639289000
C	2.833499000	0.970009000	3.069406000
H	3.264419000	1.610907000	2.292309000
H	3.403844000	0.036702000	3.088553000
H	3.014570000	1.472422000	4.029127000
C	0.750855000	3.152890000	2.147977000
H	0.807364000	3.738001000	3.075620000
H	-0.004680000	3.634626000	1.519551000

H	1. 719956000	3. 263499000	1. 648676000
C	-2. 191303000	1. 864906000	2. 375050000
H	-2. 958420000	1. 233407000	1. 913893000
H	-2. 584322000	2. 183160000	3. 350071000
H	-2. 091986000	2. 767480000	1. 765928000
Sc	0. 318305000	-0. 103038000	0. 807996000
C	-5. 623396000	5. 547616000	-1. 765794000
H	-6. 707913000	5. 540985000	-1. 916995000
H	-5. 421151000	6. 088780000	-0. 833752000
H	-5. 177199000	6. 120875000	-2. 587020000
C	-5. 066015000	4. 126956000	-1. 714932000
H	-5. 557372000	3. 567312000	-0. 906435000
H	-5. 314001000	3. 600526000	-2. 647109000
C	-3. 550553000	4. 091217000	-1. 504922000
H	-3. 299886000	4. 617262000	-0. 572234000
H	-3. 057776000	4. 648243000	-2. 314487000
C	-2. 989923000	2. 665700000	-1. 455441000
H	-3. 234822000	2. 142906000	-2. 389471000
H	-3. 474109000	2. 109128000	-0. 641768000
C	-1. 477770000	2. 663600000	-1. 253223000
H	-1. 195531000	3. 140016000	-0. 310859000
H	-0. 973099000	3. 186531000	-2. 072479000
S	-0. 825395000	0. 939768000	-1. 276073000
C	0. 978121000	1. 071599000	-1. 122654000
C	2. 357373000	-0. 509597000	-0. 818015000
C	2. 198079000	-1. 265527000	0. 375983000
C	-0. 765308000	-3. 833827000	0. 785019000
H	-1. 310320000	-3. 788434000	1. 730708000
H	-1. 100746000	-4. 691698000	0. 198561000
S	-0. 996715000	-2. 309388000	-0. 176837000
C	-2. 822158000	-2. 173420000	-0. 259835000
H	-3. 215576000	-2. 228412000	0. 761174000
H	-3. 002647000	-1. 160608000	-0. 635333000
H	1. 249328000	1. 944098000	-0. 506183000
H	1. 414784000	1. 191977000	-2. 110029000
C	-3. 471965000	-3. 210223000	-1. 171273000
H	-3. 258478000	-4. 222279000	-0. 803584000
H	-3. 031749000	-3. 137874000	-2. 173830000
C	-4. 989525000	-3. 014440000	-1. 251005000
H	-5. 208351000	-2. 002075000	-1. 621244000
H	-5. 421939000	-3. 073214000	-0. 241389000
C	-5. 674581000	-4. 042371000	-2. 154555000
H	-5. 454862000	-5. 053188000	-1. 783589000
H	-5. 239735000	-3. 984926000	-3. 162037000

C	-7.186438000	-3.845273000	-2.236888000
H	-7.647064000	-4.594731000	-2.888937000
H	-7.654151000	-3.932377000	-1.248882000
H	-7.438084000	-2.856347000	-2.638500000
H	0.303003000	-3.942868000	0.984906000
H	2.937959000	-1.116413000	1.160268000
H	1.864742000	-2.298907000	0.265110000
H	2.009318000	-0.983804000	-1.735866000
C	3.599875000	0.340834000	-0.985012000
H	3.810556000	0.874596000	-0.048954000
H	3.474361000	1.099120000	-1.766846000
C	4.808375000	-0.539236000	-1.349844000
H	4.583133000	-1.102335000	-2.266837000
H	4.967506000	-1.285097000	-0.560315000
C	6.085273000	0.278569000	-1.555029000
H	5.919475000	1.022789000	-2.347766000
H	6.303416000	0.849437000	-0.640256000
C	7.296694000	-0.583331000	-1.914908000
H	7.462300000	-1.328215000	-1.122476000
H	7.078214000	-1.155160000	-2.828893000
C	8.577186000	0.227971000	-2.120925000
H	8.794361000	0.800000000	-1.207621000
H	8.410969000	0.971636000	-2.913193000
C	9.782426000	-0.638637000	-2.479123000
H	10.682190000	-0.030064000	-2.620271000
H	9.995884000	-1.369012000	-1.689246000
H	9.609371000	-1.196012000	-3.407680000

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**G,  $E_{(\text{SCF Done})} = -2020.556517$  a.u.**

C	-2.597070000	-1.182808000	1.856655000
C	-2.513814000	-2.436568000	1.179049000
C	-1.407046000	-3.155801000	1.720855000
C	-0.806466000	-2.352567000	2.734009000
C	-1.540225000	-1.130035000	2.814358000
C	-3.511415000	-2.951302000	0.181089000
H	-3.087266000	-3.722317000	-0.470355000
H	-3.914042000	-2.155159000	-0.455085000
H	-4.368768000	-3.408493000	0.693028000
C	-0.995370000	-4.558587000	1.377822000
H	-1.373225000	-5.264484000	2.129187000
H	0.093669000	-4.677932000	1.352125000
H	-1.394544000	-4.883230000	0.411988000
C	0.285495000	-2.789688000	3.663647000
H	0.816659000	-1.939332000	4.101706000

H	1.027288000	-3.421325000	3.164833000
H	-0.132088000	-3.372426000	4.495713000
C	-1.291536000	-0.039405000	3.816496000
H	-1.676155000	-0.326851000	4.803837000
H	-1.791318000	0.894151000	3.541211000
H	-0.223702000	0.173551000	3.943670000
C	-3.687826000	-0.167096000	1.665983000
H	-4.598048000	-0.475292000	2.197453000
H	-3.409866000	0.815703000	2.057529000
H	-3.967586000	-0.039840000	0.613464000
Sc	-0.483033000	-1.176637000	0.622855000
C	-3.819434000	6.387410000	1.823811000
H	-4.754834000	6.815237000	1.448240000
H	-3.982163000	6.098381000	2.869005000
H	-3.063154000	7.181094000	1.812106000
C	-3.381830000	5.193086000	0.979104000
H	-4.174368000	4.431147000	0.980466000
H	-3.260200000	5.506747000	-0.067024000
C	-2.075985000	4.564641000	1.470812000
H	-2.194727000	4.250412000	2.518071000
H	-1.282811000	5.325876000	1.467269000
C	-1.632928000	3.368143000	0.622586000
H	-1.508504000	3.680368000	-0.422241000
H	-2.420438000	2.602163000	0.631169000
C	-0.323293000	2.774380000	1.130856000
H	-0.402687000	2.443979000	2.171023000
H	0.482948000	3.513424000	1.066812000
S	0.222936000	1.360773000	0.093527000
C	1.982512000	1.140795000	0.591992000
C	9.673016000	1.787517000	-1.705386000
H	9.467563000	1.661992000	-2.775521000
H	10.732928000	1.563448000	-1.542594000
H	9.515765000	2.845009000	-1.460172000
C	8.777548000	0.884349000	-0.860161000
H	8.983669000	-0.167899000	-1.102540000
H	9.031406000	1.006116000	0.202459000
C	7.286426000	1.163412000	-1.056651000
H	7.031599000	1.041031000	-2.120126000
H	7.080405000	2.217057000	-0.815043000
C	6.383042000	0.263666000	-0.212174000
H	6.636146000	0.388588000	0.851039000
H	6.591090000	-0.789666000	-0.451459000
C	4.890648000	0.539803000	-0.411842000
H	4.635074000	0.399515000	-1.473132000

H	4.698182000	1.599007000	-0.188211000
C	4.000578000	-0.362284000	0.448076000
H	4.198190000	-0.178188000	1.515085000
H	4.283482000	-1.408918000	0.269878000
C	2.480594000	-0.255699000	0.198958000
C	1.682154000	-1.336133000	0.957515000
H	2.040582000	1.272714000	1.679332000
H	2.547141000	1.941794000	0.107293000
H	2.324029000	-0.369836000	-0.886757000
C	-5.537347000	1.254936000	-4.752102000
H	-5.979537000	2.255802000	-4.711308000
H	-5.281509000	1.047626000	-5.797752000
H	-6.309527000	0.537570000	-4.449774000
C	-4.307469000	1.159287000	-3.852145000
H	-3.567031000	1.911093000	-4.159016000
H	-4.588160000	1.408388000	-2.818496000
C	-3.658564000	-0.226178000	-3.879327000
H	-3.378223000	-0.475824000	-4.912355000
H	-4.395755000	-0.980952000	-3.569468000
C	-2.418462000	-0.322191000	-2.984674000
H	-2.695643000	-0.067504000	-1.950576000
H	-1.675040000	0.420020000	-3.303225000
C	-1.801278000	-1.716738000	-3.024221000
H	-1.517945000	-1.985387000	-4.047749000
H	-2.495488000	-2.473858000	-2.646256000
S	-0.259738000	-1.780033000	-2.034282000
C	0.249176000	-3.514623000	-2.230602000
H	0.486595000	-3.697632000	-3.281637000
H	1.151968000	-3.662337000	-1.633405000
H	-0.530731000	-4.201785000	-1.895559000
H	2.050517000	-2.336226000	0.666631000
H	1.917729000	-1.251108000	2.030996000

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**TS3,  $E_{(\text{SCF Done})} = -2020.520639$  a.u., IF =  $i1250.2509$  cm<sup>-1</sup>**

C	-1.803773000	0.424829000	2.571084000
C	-2.605266000	-0.654930000	2.090427000
C	-1.927455000	-1.873435000	2.393381000
C	-0.710407000	-1.547162000	3.066708000
C	-0.638172000	-0.127215000	3.181255000
C	-3.991845000	-0.514910000	1.531868000
H	-4.309335000	-1.405667000	0.983163000
H	-4.088784000	0.344427000	0.859837000
H	-4.715855000	-0.368209000	2.344495000
C	-2.467553000	-3.262665000	2.208308000

H	-3.016670000	-3.582399000	3.103808000
H	-1.674185000	-3.999998000	2.045716000
H	-3.166954000	-3.333117000	1.369294000
C	0.239335000	-2.536720000	3.676388000
H	1.249563000	-2.131187000	3.785300000
H	0.314847000	-3.457021000	3.088018000
H	-0.101091000	-2.824536000	4.679800000
C	0.419388000	0.650775000	3.909845000
H	0.115472000	0.831632000	4.949436000
H	0.601242000	1.632885000	3.459065000
H	1.375076000	0.118481000	3.948971000
C	-2.204074000	1.872523000	2.573422000
H	-2.800493000	2.103676000	3.466394000
H	-1.339543000	2.543799000	2.589904000
H	-2.819380000	2.135209000	1.706547000
Sc	-0.528738000	-0.651794000	0.794687000
C	-2.016368000	7.365693000	-0.467220000
H	-2.914996000	7.822629000	-0.894639000
H	-2.054220000	7.510656000	0.619075000
H	-1.149772000	7.919719000	-0.846841000
C	-1.927716000	5.884484000	-0.827224000
H	-2.825957000	5.363462000	-0.466232000
H	-1.925862000	5.770473000	-1.920100000
C	-0.683940000	5.206200000	-0.248563000
H	-0.683640000	5.318369000	0.845467000
H	0.214701000	5.725503000	-0.611118000
C	-0.592377000	3.720968000	-0.612865000
H	-0.587045000	3.605930000	-1.704234000
H	-1.485744000	3.198597000	-0.244331000
C	0.662547000	3.076692000	-0.032243000
H	0.693549000	3.156434000	1.059056000
H	1.562259000	3.554032000	-0.436077000
S	0.782189000	1.308538000	-0.511389000
C	2.514018000	0.876050000	-0.095929000
C	10.066649000	-0.532298000	-2.405386000
H	9.790143000	-0.782588000	-3.436853000
H	11.060341000	-0.953081000	-2.216971000
H	10.150663000	0.559427000	-2.340802000
C	9.038896000	-1.068283000	-1.411231000
H	9.004109000	-2.165166000	-1.474457000
H	9.361277000	-0.833333000	-0.386874000
C	7.634495000	-0.506215000	-1.638612000
H	7.311057000	-0.741935000	-2.663528000
H	7.669377000	0.591880000	-1.576419000

C	6.599819000	-1.037828000	-0.645837000
H	6.921108000	-0.798270000	0.378602000
H	6.567929000	-2.135691000	-0.705326000
C	5.193177000	-0.480363000	-0.877922000
H	4.864819000	-0.737103000	-1.896392000
H	5.240102000	0.617187000	-0.837002000
C	4.173779000	-1.010927000	0.133788000
H	4.442843000	-0.676652000	1.147063000
H	4.236543000	-2.107720000	0.152289000
C	2.701055000	-0.643358000	-0.141255000
C	1.747730000	-1.327498000	0.853867000
H	2.740163000	1.258834000	0.906969000
H	3.150360000	1.389129000	-0.821738000
H	2.468019000	-0.978274000	-1.166147000
C	-7.817239000	-1.936398000	-3.601623000
H	-8.561794000	-1.287601000	-4.074690000
H	-7.654096000	-2.793533000	-4.265611000
H	-8.251769000	-2.315869000	-2.669022000
C	-6.515716000	-1.181660000	-3.341142000
H	-6.123991000	-0.785101000	-4.288073000
H	-6.716908000	-0.309248000	-2.703460000
C	-5.445866000	-2.053833000	-2.680341000
H	-5.241645000	-2.925181000	-3.318801000
H	-5.835520000	-2.451730000	-1.731902000
C	-4.138951000	-1.296950000	-2.420535000
H	-4.337330000	-0.429652000	-1.776727000
H	-3.746695000	-0.905116000	-3.368089000
C	-3.091347000	-2.194084000	-1.769307000
H	-2.849416000	-3.046368000	-2.412906000
H	-3.429504000	-2.573875000	-0.801376000
S	-1.514996000	-1.274727000	-1.534908000
C	-0.376043000	-2.445164000	-0.747108000
H	0.292219000	-2.900512000	-1.482874000
H	0.654323000	-1.921042000	0.053446000
H	-0.928539000	-3.232147000	-0.221231000
H	2.115187000	-2.332665000	1.102684000
H	1.777158000	-0.782020000	1.812773000

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**H,  $E_{(\text{SCF Done})} = -2020.562265$  a.u.**

C	-1.228419000	-1.219853000	2.393398000
C	-2.391698000	-1.708529000	1.722846000
C	-2.041024000	-2.929035000	1.067035000
C	-0.660948000	-3.181556000	1.314890000
C	-0.158952000	-2.129508000	2.143877000

C	-3.772614000	-1.132537000	1.856769000
H	-4.431839000	-1.445578000	1.042580000
H	-3.768966000	-0.037696000	1.880523000
H	-4.238651000	-1.471595000	2.791574000
C	-2.980708000	-3.867303000	0.369666000
H	-3.394599000	-4.591670000	1.083829000
H	-2.481072000	-4.441144000	-0.416810000
H	-3.831548000	-3.349355000	-0.083441000
C	0.089988000	-4.405674000	0.874386000
H	1.173782000	-4.258910000	0.901104000
H	-0.178768000	-4.713511000	-0.141688000
H	-0.133055000	-5.252004000	1.537403000
C	1.208248000	-2.066390000	2.763572000
H	1.213613000	-2.585988000	3.730997000
H	1.531215000	-1.037862000	2.957405000
H	1.972370000	-2.548090000	2.145170000
C	-1.184722000	-0.026835000	3.305053000
H	-1.502350000	-0.306199000	4.318647000
H	-0.176759000	0.390975000	3.395489000
H	-1.854366000	0.774995000	2.975949000
Sc	-0.769744000	-1.132278000	0.002330000
C	-2.319609000	6.077823000	1.993615000
H	-3.316281000	6.511779000	1.862211000
H	-2.187728000	5.864575000	3.061090000
H	-1.585453000	6.842382000	1.713757000
C	-2.153097000	4.815911000	1.150183000
H	-2.925381000	4.083794000	1.427332000
H	-2.323243000	5.055244000	0.091329000
C	-0.771685000	4.176159000	1.305835000
H	-0.599479000	3.932451000	2.364230000
H	0.000331000	4.908024000	1.028944000
C	-0.598872000	2.914820000	0.453490000
H	-0.756851000	3.157975000	-0.604974000
H	-1.372733000	2.181950000	0.725259000
C	0.785898000	2.301378000	0.635615000
H	0.956217000	1.993943000	1.672403000
H	1.564515000	3.020009000	0.357181000
S	1.022905000	0.851108000	-0.465289000
C	2.754598000	0.359720000	-0.086799000
C	10.627221000	1.748092000	-0.659057000
H	10.546336000	2.306088000	-1.599831000
H	11.664982000	1.411273000	-0.561492000
H	10.427347000	2.449474000	0.160265000
C	9.656026000	0.570073000	-0.628983000



H	9.904280000	-0.131326000	-1.438046000
H	9.785819000	0.010603000	0.308373000
C	8.192801000	0.995413000	-0.763211000
H	8.062058000	1.553514000	-1.702324000
H	7.944666000	1.699386000	0.045487000
C	7.214302000	-0.179405000	-0.731379000
H	7.342518000	-0.734982000	0.209425000
H	7.464812000	-0.884594000	-1.537249000
C	5.750586000	0.245432000	-0.872356000
H	5.618015000	0.781024000	-1.824155000
H	5.518027000	0.967851000	-0.076570000
C	4.784894000	-0.941077000	-0.818563000
H	4.851250000	-1.429458000	0.165638000
H	5.112762000	-1.693227000	-1.549126000
C	3.310223000	-0.617992000	-1.126159000
C	2.483394000	-1.903579000	-1.190989000
H	2.798571000	-0.068787000	0.920914000
H	3.323378000	1.294107000	-0.089964000
H	3.266944000	-0.125732000	-2.108207000
C	-8.760690000	1.280022000	-1.730198000
H	-9.365017000	2.170437000	-1.527286000
H	-8.990256000	0.948303000	-2.749724000
H	-9.088995000	0.491681000	-1.042197000
C	-7.271612000	1.575395000	-1.566107000
H	-6.981295000	2.391008000	-2.242882000
H	-7.078411000	1.939514000	-0.547013000
C	-6.389889000	0.355517000	-1.841966000
H	-6.580938000	-0.007781000	-2.861794000
H	-6.678446000	-0.462318000	-1.165377000
C	-4.895161000	0.651406000	-1.680307000
H	-4.697838000	1.008433000	-0.660500000
H	-4.606071000	1.462822000	-2.361169000
C	-4.043647000	-0.580362000	-1.967103000
H	-4.203264000	-0.940409000	-2.989019000
H	-4.270879000	-1.396292000	-1.275457000
S	-2.251966000	-0.185240000	-1.854508000
C	-1.344466000	-1.760157000	-2.018921000
H	-0.724561000	-1.735240000	-2.919929000
H	1.455768000	-1.724808000	-1.546287000
H	-2.050939000	-2.593906000	-2.084136000
H	2.919323000	-2.618061000	-1.897434000
H	2.444569000	-2.397373000	-0.211410000

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**3a,  $E_{(\text{SCF Done})} = -949.460936$  a.u.**

C	7. 225397000	-2. 400638000	0. 291835000
H	8. 255612000	-2. 375465000	-0. 081228000
H	7. 268140000	-2. 385130000	1. 387925000
H	6. 786585000	-3. 360425000	-0. 007734000
C	6. 408443000	-1. 227716000	-0. 245919000
H	6. 890609000	-0. 282196000	0. 040077000
H	6. 412531000	-1. 250181000	-1. 344901000
C	4. 961945000	-1. 225523000	0. 251838000
H	4. 957117000	-1. 202343000	1. 351806000
H	4. 478477000	-2. 171245000	-0. 035165000
C	4. 141801000	-0. 050531000	-0. 285753000
H	4. 140367000	-0. 074244000	-1. 383986000
H	4. 619187000	0. 895181000	0. 004567000
C	2. 701428000	-0. 064667000	0. 220863000
H	2. 685152000	-0. 015811000	1. 317234000
H	2. 202081000	-0. 994682000	-0. 080721000
S	1. 775523000	1. 355586000	-0. 454004000
C	0. 146056000	1. 046182000	0. 316315000
C	-6. 896039000	-2. 856500000	-0. 254808000
H	-6. 900008000	-2. 899699000	-1. 351008000
H	-7. 926318000	-3. 007473000	0. 087444000
H	-6. 298364000	-3. 702787000	0. 106000000
C	-6. 329795000	-1. 528368000	0. 243294000
H	-6. 968703000	-0. 703835000	-0. 104200000
H	-6. 371088000	-1. 500794000	1. 341673000
C	-4. 891650000	-1. 277124000	-0. 212867000
H	-4. 850157000	-1. 304294000	-1. 312188000
H	-4. 252269000	-2. 103059000	0. 133794000
C	-4. 316969000	0. 050645000	0. 282551000
H	-4. 355823000	0. 075561000	1. 382012000
H	-4. 959250000	0. 875411000	-0. 060923000
C	-2. 880064000	0. 304698000	-0. 178216000
H	-2. 843955000	0. 293284000	-1. 277869000
H	-2. 249574000	-0. 531195000	0. 155524000
C	-2. 318083000	1. 634070000	0. 331109000
H	-2. 298016000	1. 628290000	1. 432032000
H	-3. 016001000	2. 436147000	0. 049653000
C	-0. 923625000	2. 019567000	-0. 195854000
C	-0. 597835000	3. 468069000	0. 180207000
H	0. 238280000	1. 137008000	1. 407551000
H	-0. 138787000	0. 013201000	0. 087538000
H	-0. 945415000	1. 943911000	-1. 293588000
H	0. 375653000	3. 781848000	-0. 210370000
H	-1. 357514000	4. 152353000	-0. 215492000

H -0.572992000 3.590302000 1.271031000

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**2b,  $E_{(\text{SCF Done})} = -273.775586$  a.u.**

C -1.211885000 -0.187319000 0.553399000

H -1.031278000 0.817012000 0.956260000

H -1.094090000 -0.889006000 1.393772000

C -2.608670000 -0.283913000 0.015181000

C -3.485700000 0.719123000 -0.034714000

H -2.901921000 -1.261975000 -0.372849000

H -4.484341000 0.587666000 -0.443887000

H -3.238209000 1.712116000 0.337065000

C -0.142353000 -0.512916000 -0.509401000

H -0.226184000 0.201635000 -1.337923000

H -0.360780000 -1.506690000 -0.930746000

C 1.250610000 -0.496699000 0.047176000

H 1.455644000 -1.213115000 0.847124000

C 2.228651000 0.322954000 -0.347391000

H 2.019434000 1.039775000 -1.144681000

C 3.617595000 0.345374000 0.213039000

H 4.365391000 0.142104000 -0.565646000

H 3.862662000 1.330881000 0.632078000

H 3.744186000 -0.400028000 1.005694000

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**I,  $E_{(\text{SCF Done})} = -1344.862331$  a.u.**

C -2.179408000 -2.016651000 0.797322000

C -1.430779000 -1.135012000 1.639068000

C -2.146533000 0.098715000 1.732541000

C -3.322660000 -0.012949000 0.933199000

C -3.336679000 -1.318215000 0.346603000

C -0.196219000 -1.489531000 2.420252000

H 0.478924000 -0.636405000 2.547674000

H 0.372494000 -2.297946000 1.950615000

H -0.465388000 -1.835653000 3.426934000

C -1.782494000 1.253679000 2.621399000

H -2.191056000 1.101948000 3.629323000

H -2.186566000 2.204388000 2.258515000

H -0.699494000 1.369186000 2.733970000

C -4.426789000 1.001538000 0.833797000

H -4.945420000 0.965030000 -0.130268000

H -4.071809000 2.025778000 0.987914000

H -5.186405000 0.813399000 1.603858000

C -4.430677000 -1.885506000 -0.511321000

H -5.193763000 -2.374035000 0.108900000

H -4.054424000 -2.635148000 -1.213812000

H	-4.943988000	-1.113696000	-1.094508000
C	-1.874132000	-3.462500000	0.542448000
H	-2.299345000	-4.085275000	1.340556000
H	-2.301174000	-3.812450000	-0.401684000
H	-0.798903000	-3.668047000	0.521034000
Sc	-1.409318000	-0.159867000	-0.568283000
C	6.305568000	-3.043719000	0.947242000
H	7.245439000	-2.612624000	1.307573000
H	5.847654000	-3.587339000	1.782309000
H	6.552865000	-3.775678000	0.169328000
C	5.372695000	-1.959958000	0.411829000
H	5.172411000	-1.222516000	1.201989000
H	5.872044000	-1.412094000	-0.399289000
C	4.045337000	-2.520901000	-0.103438000
H	3.543133000	-3.069487000	0.706905000
H	4.244530000	-3.256325000	-0.895792000
C	3.109968000	-1.433545000	-0.643138000
H	3.608729000	-0.892388000	-1.457835000
H	2.904535000	-0.698185000	0.146741000
C	1.799203000	-2.023368000	-1.151219000
H	1.250287000	-2.527831000	-0.350462000
H	1.974445000	-2.743408000	-1.957416000
S	0.725972000	-0.714384000	-1.876087000
C	-0.894234000	-1.504604000	-2.201680000
C	0.637920000	3.023327000	0.025012000
H	0.108617000	3.441030000	0.890924000
H	0.699021000	1.930325000	0.185197000
C	-0.177267000	3.285241000	-1.259657000
H	0.350951000	2.890146000	-2.135646000
H	-0.260544000	4.372718000	-1.398016000
C	-1.559995000	2.724037000	-1.188105000
C	-2.098052000	1.845407000	-2.060256000
H	-0.833430000	-2.578536000	-2.002051000
H	-1.164551000	-1.349751000	-3.251655000
H	-2.178697000	3.075979000	-0.359165000
H	-3.148631000	1.556052000	-1.994059000
H	-1.552006000	1.525320000	-2.949044000
C	2.025361000	3.590569000	-0.049427000
H	2.658457000	3.212452000	-0.854426000
C	2.507574000	4.515762000	0.785464000
H	1.861418000	4.888242000	1.583747000
C	3.881902000	5.102163000	0.724791000
H	4.426299000	4.922947000	1.660914000
H	4.468648000	4.682389000	-0.098379000

H 3.837159000 6.190959000 0.593546000

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**TS4,  $E_{(\text{SCF Done})} = -1344.839776$  a.u., IF =  $i272.1821$  cm $^{-1}$**

C	-1.034450000	-2.090384000	1.169676000
C	-1.057838000	-2.796085000	-0.070234000
C	0.269709000	-3.259151000	-0.344742000
C	1.112265000	-2.826622000	0.719523000
C	0.312399000	-2.089933000	1.649675000
C	-2.276689000	-3.103562000	-0.893605000
H	-3.075790000	-2.372661000	-0.737107000
H	-2.683121000	-4.087633000	-0.625477000
H	-2.058255000	-3.133293000	-1.966539000
C	0.665691000	-4.147379000	-1.487723000
H	0.525979000	-5.202778000	-1.219410000
H	1.716901000	-4.022828000	-1.764635000
H	0.062395000	-3.963775000	-2.382640000
C	2.565708000	-3.160942000	0.892115000
H	3.129981000	-2.353615000	1.372377000
H	3.052481000	-3.389736000	-0.060568000
H	2.680027000	-4.047115000	1.530192000
C	0.782732000	-1.538719000	2.968344000
H	0.699611000	-2.300393000	3.754685000
H	0.189748000	-0.678897000	3.298449000
H	1.833132000	-1.229370000	2.940259000
C	-2.228069000	-1.545026000	1.899649000
H	-2.664093000	-2.316862000	2.547582000
H	-1.970407000	-0.701172000	2.548838000
H	-3.019834000	-1.219216000	1.217598000
Sc	0.309642000	-0.822050000	-0.388396000
C	-7.261366000	2.851922000	0.781157000
H	-8.271790000	2.751890000	0.371471000
H	-7.253742000	2.372380000	1.767287000
H	-7.067458000	3.920884000	0.928837000
C	-6.227031000	2.224195000	-0.150233000
H	-6.468424000	1.163623000	-0.307962000
H	-6.282987000	2.701468000	-1.138260000
C	-4.798281000	2.342864000	0.385678000
H	-4.738555000	1.864423000	1.374055000
H	-4.554705000	3.403531000	0.540805000
C	-3.760272000	1.715664000	-0.551753000
H	-3.814247000	2.198138000	-1.536243000
H	-3.997004000	0.654148000	-0.706526000
C	-2.347392000	1.854496000	0.007612000
H	-2.243466000	1.346866000	0.971551000

H	-2.073382000	2.907372000	0.131750000
S	-1.125320000	1.142341000	-1.178771000
C	0.525515000	1.409127000	-0.479895000
C	3.321521000	0.959617000	-1.028722000
H	3.503821000	0.291842000	-0.174871000
H	4.123508000	0.723959000	-1.746029000
C	2.054708000	0.550460000	-1.753513000
C	1.845678000	-0.829246000	-2.016243000
H	0.524062000	1.268142000	0.627552000
H	0.894796000	2.411722000	-0.676410000
H	1.692791000	1.259491000	-2.497811000
H	1.325926000	-1.103702000	-2.937309000
H	2.632702000	-1.521167000	-1.714781000
C	3.488215000	2.422533000	-0.592579000
H	2.846910000	2.648711000	0.268165000
H	3.165561000	3.077858000	-1.417470000
C	4.913285000	2.732009000	-0.230128000
H	5.645448000	2.633559000	-1.034372000
C	5.325174000	3.109636000	0.983177000
H	4.583020000	3.213565000	1.778828000
C	6.738528000	3.426682000	1.357540000
H	6.826950000	4.460912000	1.714614000
H	7.084721000	2.782570000	2.176315000
H	7.420991000	3.299823000	0.511202000

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**J, E<sub>(SCF Done)</sub> = -1344.870472 a.u.**

C	2.715941000	2.102696000	0.251876000
C	2.185476000	2.678611000	-0.940988000
C	0.989008000	3.386142000	-0.595859000
C	0.778191000	3.248528000	0.806244000
C	1.833945000	2.434701000	1.327752000
C	2.812755000	2.619171000	-2.306220000
H	3.404340000	1.709522000	-2.456084000
H	3.494700000	3.467132000	-2.451577000
H	2.070674000	2.672465000	-3.110070000
C	0.143292000	4.193357000	-1.537745000
H	0.495566000	5.232519000	-1.573828000
H	-0.905931000	4.219453000	-1.228248000
H	0.180631000	3.811898000	-2.563663000
C	-0.280678000	3.934191000	1.615036000
H	-0.584487000	3.345488000	2.486067000
H	-1.178417000	4.141441000	1.026178000
H	0.091946000	4.896842000	1.988959000
C	2.030853000	2.082439000	2.775957000

H	2. 582453000	2. 878530000	3. 292875000
H	2. 609720000	1. 161951000	2. 908108000
H	1. 079884000	1. 961887000	3. 305798000
C	4. 003421000	1. 335587000	0. 365696000
H	4. 840584000	2. 021584000	0. 550241000
H	3. 994163000	0. 622899000	1. 197342000
H	4. 245710000	0. 784175000	-0. 549309000
Sc	0. 609079000	1. 033907000	-0. 174288000
C	5. 236847000	-5. 420833000	0. 544375000
H	6. 274015000	-5. 508979000	0. 204993000
H	5. 253372000	-5. 282935000	1. 632025000
H	4. 737612000	-6. 374488000	0. 336863000
C	4. 528091000	-4. 261570000	-0. 152237000
H	5. 072222000	-3. 326527000	0. 043770000
H	4. 557776000	-4. 412043000	-1. 240260000
C	3. 072988000	-4. 103017000	0. 294572000
H	3. 039551000	-3. 949971000	1. 383014000
H	2. 527972000	-5. 036764000	0. 097321000
C	2. 357880000	-2. 944134000	-0. 408585000
H	2. 378701000	-3. 103466000	-1. 494512000
H	2. 904108000	-2. 009058000	-0. 214171000
C	0. 912693000	-2. 809626000	0. 060927000
H	0. 853017000	-2. 600541000	1. 134521000
H	0. 350829000	-3. 727217000	-0. 141637000
S	0. 041606000	-1. 471883000	-0. 853052000
C	-1. 642493000	-1. 423252000	-0. 104040000
C	-3. 779733000	-0. 101575000	0. 075306000
H	-3. 821376000	-0. 323616000	1. 151361000
H	-4. 175423000	0. 916542000	-0. 035944000
C	-2. 304979000	-0. 066031000	-0. 379848000
C	-1. 521236000	1. 089054000	0. 281146000
H	-1. 537787000	-1. 589242000	0. 975272000
H	-2. 201284000	-2. 256792000	-0. 536587000
H	-2. 311181000	0. 083946000	-1. 473233000
H	-2. 017584000	2. 041309000	0. 049590000
H	-1. 599470000	0. 987699000	1. 382521000
C	-4. 696239000	-1. 071798000	-0. 688846000
H	-4. 403257000	-2. 113942000	-0. 505492000
H	-4. 572734000	-0. 894986000	-1. 769418000
C	-6. 139362000	-0. 897744000	-0. 310636000
H	-6. 575688000	0. 080401000	-0. 525579000
C	-6. 899175000	-1. 833876000	0. 264139000
H	-6. 456537000	-2. 810638000	0. 473900000
C	-8. 336654000	-1. 667494000	0. 646158000

H	-8.970197000	-2.398061000	0.126250000
H	-8.483009000	-1.835952000	1.721266000
H	-8.706523000	-0.665551000	0.405172000

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**K,  $E_{(\text{SCF Done})} = -1344.888590$  a.u.**

C	0.457476000	-2.123287000	1.133153000
C	0.116171000	-2.315122000	-0.239823000
C	1.324158000	-2.296457000	-0.999686000
C	2.409768000	-2.090367000	-0.096877000
C	1.875025000	-1.982338000	1.224479000
C	-1.246991000	-2.624309000	-0.790596000
H	-2.048504000	-2.258159000	-0.142357000
H	-1.384929000	-3.709785000	-0.884041000
H	-1.401885000	-2.201319000	-1.789746000
C	1.424466000	-2.576425000	-2.472858000
H	1.330947000	-3.653410000	-2.664758000
H	2.388191000	-2.267353000	-2.889633000
H	0.633829000	-2.086132000	-3.053741000
C	3.871051000	-2.124642000	-0.445045000
H	4.477917000	-1.553961000	0.265270000
H	4.078448000	-1.740271000	-1.449789000
H	4.245026000	-3.156659000	-0.420634000
C	2.668064000	-1.905963000	2.495216000
H	2.920440000	-2.913884000	2.850444000
H	2.112580000	-1.410265000	3.296806000
H	3.610144000	-1.364465000	2.365463000
C	-0.486238000	-2.163938000	2.300051000
H	-0.476115000	-3.157417000	2.767451000
H	-0.214853000	-1.443792000	3.079494000
H	-1.520551000	-1.965842000	2.002267000
Sc	1.041326000	-0.068437000	-0.012238000
C	-7.350702000	-0.631981000	-0.399192000
H	-8.019117000	-0.923256000	-1.216061000
H	-7.263244000	-1.488366000	0.280084000
H	-7.835716000	0.182115000	0.152212000
C	-5.985449000	-0.203835000	-0.932255000
H	-5.541122000	-1.026541000	-1.510249000
H	-6.109838000	0.631817000	-1.634775000
C	-5.018735000	0.212693000	0.178690000
H	-4.892838000	-0.621874000	0.883896000
H	-5.461540000	1.037471000	0.755222000
C	-3.649485000	0.645430000	-0.356027000
H	-3.771363000	1.480147000	-1.057970000
H	-3.201055000	-0.180913000	-0.923746000



C	-2.717160000	1.071140000	0.773187000
H	-2.565231000	0.271493000	1.504541000
H	-3.123715000	1.942585000	1.297779000
S	-1.083245000	1.611196000	0.124304000
C	-0.407062000	2.640858000	1.506872000
C	1.620405000	3.344837000	0.184120000
H	0.893180000	3.200281000	-0.627537000
H	1.638561000	4.426919000	0.361844000
C	1.125599000	2.634422000	1.471218000
C	1.644856000	1.197558000	1.668059000
H	-0.774025000	2.205493000	2.441884000
H	-0.826458000	3.646144000	1.393472000
C	3.002336000	2.912212000	-0.336440000
C	3.048675000	1.520567000	-0.920199000
C	2.436373000	1.088211000	-2.049055000
H	3.744359000	2.989331000	0.465191000
H	3.313697000	3.623247000	-1.113336000
C	1.608357000	1.894193000	-3.007928000
H	0.579153000	1.519176000	-3.094360000
H	1.561165000	2.952542000	-2.743099000
H	2.044534000	1.815171000	-4.011547000
H	3.700653000	0.803214000	-0.416515000
H	1.434258000	3.258582000	2.325585000
H	1.183247000	0.783949000	2.581020000
H	2.724445000	1.206209000	1.875866000
H	2.655664000	0.065101000	-2.368170000

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**TS5,  $E_{(\text{SCF Done})} = -1344.877298$  a.u.,  $\text{IF} = i297.0203$  cm<sup>-1</sup>**

C	0.085186000	-1.997415000	0.971098000
C	0.191180000	-2.327879000	-0.413220000
C	1.578728000	-2.397460000	-0.747299000
C	2.329298000	-2.108330000	0.429448000
C	1.410622000	-1.854736000	1.489840000
C	-0.938598000	-2.677128000	-1.341033000
H	-1.897166000	-2.281233000	-0.993326000
H	-1.052155000	-3.766850000	-1.414248000
H	-0.775746000	-2.309676000	-2.360802000
C	2.129826000	-2.851455000	-2.067249000
H	2.166972000	-3.948089000	-2.109827000
H	3.150341000	-2.494766000	-2.237746000
H	1.514533000	-2.523353000	-2.912131000
C	3.822174000	-2.171524000	0.566555000
H	4.198807000	-1.479646000	1.327350000
H	4.338127000	-1.950276000	-0.373196000

H	4.137006000	-3.178563000	0.870598000
C	1.770028000	-1.642921000	2.933283000
H	1.878871000	-2.606975000	3.447351000
H	1.002237000	-1.080277000	3.475305000
H	2.719144000	-1.110073000	3.052407000
C	-1.173650000	-1.976727000	1.789673000
H	-1.330343000	-2.948923000	2.275706000
H	-1.141019000	-1.228167000	2.589335000
H	-2.060604000	-1.781628000	1.179586000
Sc	1.075762000	-0.073797000	-0.136169000
C	-7.308525000	-0.633354000	-0.226527000
H	-7.971889000	-1.082327000	-0.973003000
H	-7.225456000	-1.337015000	0.610372000
H	-7.796740000	0.273891000	0.148420000
C	-5.939939000	-0.318779000	-0.825997000
H	-5.492612000	-1.239909000	-1.225785000
H	-6.059656000	0.359827000	-1.681818000
C	-4.979901000	0.311648000	0.185510000
H	-4.858236000	-0.365260000	1.043721000
H	-5.425798000	1.234549000	0.583139000
C	-3.607551000	0.631057000	-0.416601000
H	-3.725924000	1.310183000	-1.270562000
H	-3.156307000	-0.290426000	-0.808934000
C	-2.679298000	1.269076000	0.611118000
H	-2.520895000	0.619677000	1.477082000
H	-3.095071000	2.219884000	0.962591000
S	-1.052541000	1.692826000	-0.131772000
C	-0.369872000	2.854904000	1.122356000
C	1.637766000	3.512741000	-0.318363000
H	0.964557000	3.192455000	-1.126443000
H	1.621579000	4.608050000	-0.318434000
C	1.154272000	2.936915000	1.027179000
C	1.832508000	1.575323000	1.243610000
H	-0.678291000	2.494508000	2.109828000
H	-0.830527000	3.832942000	0.948473000
C	3.039710000	2.975237000	-0.576504000
C	3.099089000	1.456872000	-0.467806000
C	2.702453000	0.567495000	-1.501031000
H	3.737310000	3.413173000	0.147269000
H	3.395073000	3.266741000	-1.573063000
C	1.774244000	0.952278000	-2.631800000
H	0.686554000	0.914995000	-2.379242000
H	1.928565000	1.974817000	-2.998297000
H	1.898863000	0.268564000	-3.475552000

H	3.955897000	1.087432000	0.093625000
H	1.465905000	3.624987000	1.826139000
H	1.155525000	0.876115000	1.803275000
H	2.705144000	1.653429000	1.894791000
H	3.364594000	-0.273294000	-1.683505000

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**L,  $E_{(\text{SCF Done})} = -1344.896210$  a.u.**

C	-0.126117000	-2.104228000	0.898072000
C	0.058734000	-2.488429000	-0.463628000
C	1.464140000	-2.586164000	-0.708534000
C	2.149284000	-2.263250000	0.497430000
C	1.168100000	-1.947410000	1.486946000
C	-1.026967000	-2.838958000	-1.442874000
H	-1.974897000	-2.344863000	-1.206983000
H	-1.220896000	-3.919628000	-1.431314000
H	-0.763174000	-2.578469000	-2.473927000
C	2.103324000	-3.041312000	-1.988049000
H	2.261373000	-4.127752000	-1.974537000
H	3.081627000	-2.576841000	-2.147144000
H	1.482077000	-2.823887000	-2.863286000
C	3.626620000	-2.365321000	0.730366000
H	3.988013000	-1.619706000	1.446181000
H	4.196271000	-2.241575000	-0.194793000
H	3.882125000	-3.352169000	1.138859000
C	1.444103000	-1.660221000	2.937077000
H	1.459061000	-2.591927000	3.517937000
H	0.680250000	-1.018632000	3.390484000
H	2.416606000	-1.179604000	3.085240000
C	-1.433068000	-2.034875000	1.634082000
H	-1.666253000	-3.006433000	2.090013000
H	-1.414351000	-1.303597000	2.449659000
H	-2.270593000	-1.786522000	0.974944000
Sc	0.961884000	-0.259661000	-0.225923000
C	-7.253293000	-0.349428000	-0.171403000
H	-7.937024000	-0.797096000	-0.900018000
H	-7.189705000	-1.029619000	0.686340000
H	-7.706513000	0.585728000	0.177966000
C	-5.878463000	-0.102343000	-0.787983000
H	-5.466742000	-1.050768000	-1.161469000
H	-5.979715000	0.553426000	-1.663710000
C	-4.890258000	0.524332000	0.198430000
H	-4.787071000	-0.129494000	1.076695000
H	-5.300585000	1.474413000	0.569359000
C	-3.511319000	0.776543000	-0.420156000

H	-3.610342000	1.432247000	-1.294566000
H	-3.094948000	-0.172631000	-0.785647000
C	-2.554608000	1.412955000	0.582466000
H	-2.418242000	0.786899000	1.469253000
H	-2.931728000	2.390270000	0.903464000
S	-0.917807000	1.746245000	-0.185823000
C	-0.205684000	2.965324000	0.998794000
C	1.780419000	3.601463000	-0.548746000
H	1.135369000	3.185728000	-1.335025000
H	1.739922000	4.690367000	-0.652831000
C	1.302413000	3.133013000	0.840589000
C	2.142794000	1.861116000	1.144834000
H	-0.454808000	2.626732000	2.010772000
H	-0.721281000	3.913851000	0.816488000
C	3.197011000	3.036367000	-0.668475000
C	3.113907000	1.612081000	-0.073910000
C	2.772221000	0.463150000	-1.054046000
H	3.884271000	3.642068000	-0.063051000
H	3.585206000	3.045258000	-1.691654000
C	2.008467000	0.760002000	-2.339226000
H	0.885432000	0.764734000	-2.234551000
H	2.195361000	1.741368000	-2.793699000
H	2.220988000	-0.003051000	-3.094305000
H	4.080874000	1.330239000	0.353473000
H	1.577996000	3.900543000	1.575581000
H	1.508769000	1.012389000	1.491959000
H	2.758851000	2.027895000	2.034340000
H	3.663215000	-0.123394000	-1.271276000

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**$\mathbf{I}, E_{(\text{SCF Done})} = -1980.014870 \text{ a.u.}$**

C	-1.627027000	-2.009739000	1.673578000
C	-0.356647000	-2.619680000	1.445129000
C	0.578879000	-2.046541000	2.356256000
C	-0.113516000	-1.079116000	3.145770000
C	-1.477787000	-1.070075000	2.737433000
C	-0.104384000	-3.793862000	0.544936000
H	0.951350000	-3.885045000	0.271547000
H	-0.691851000	-3.747167000	-0.378399000
H	-0.382682000	-4.729789000	1.048250000
C	1.991567000	-2.512567000	2.566845000
H	2.011475000	-3.368724000	3.254054000
H	2.626682000	-1.739073000	3.009865000
H	2.468122000	-2.845729000	1.638104000
C	0.448247000	-0.291560000	4.294433000

H	0.089678000	0.744024000	4.301139000
H	1.542317000	-0.267031000	4.282983000
H	0.152994000	-0.739639000	5.252351000
C	-2.584334000	-0.348626000	3.445967000
H	-2.991241000	-0.978190000	4.248805000
H	-3.420964000	-0.102905000	2.784549000
H	-2.239905000	0.579924000	3.911342000
C	-2.919976000	-2.433507000	1.037057000
H	-2.789645000	-2.740304000	-0.006163000
H	-3.349141000	-3.292435000	1.570606000
H	-3.671865000	-1.639344000	1.057830000
Sc	-0.153243000	-0.254544000	0.826106000
C	-8.161510000	0.339969000	-2.325499000
H	-8.670206000	-0.036898000	-3.219048000
H	-8.491764000	-0.267079000	-1.474046000
H	-8.506335000	1.366752000	-2.155320000
C	-6.644463000	0.285611000	-2.490416000
H	-6.333503000	-0.748810000	-2.695184000
H	-6.348538000	0.874384000	-3.369905000
C	-5.894133000	0.804534000	-1.261906000
H	-6.188114000	0.215928000	-0.380567000
H	-6.203129000	1.839419000	-1.057215000
C	-4.371354000	0.753835000	-1.426030000
H	-4.077873000	1.353564000	-2.298131000
H	-4.060180000	-0.280182000	-1.628867000
C	-3.652578000	1.270677000	-0.185246000
H	-3.873062000	0.652093000	0.689092000
H	-3.948392000	2.300928000	0.039650000
S	-1.830521000	1.318191000	-0.428508000
C	-1.093841000	1.708454000	1.181839000
C	3.403035000	3.847163000	0.047579000
H	4.204628000	3.477768000	0.702983000
H	3.714783000	3.641987000	-0.984617000
C	2.108161000	3.055265000	0.364588000
H	1.320521000	3.411933000	-0.312738000
H	1.786580000	3.263908000	1.391553000
C	2.315879000	1.591834000	0.168840000
C	2.295876000	0.649383000	1.133929000
H	2.564152000	1.284822000	-0.848987000
H	2.630336000	-0.368005000	0.930665000
H	2.126172000	0.916118000	2.177555000
C	6.477141000	-3.942479000	-2.143976000
H	7.479867000	-3.788204000	-1.732112000
H	6.145596000	-4.944130000	-1.845594000

H	6.561808000	-3.931716000	-3.236985000
C	5.509289000	-2.868313000	-1.653012000
H	5.474425000	-2.879724000	-0.554134000
H	5.885940000	-1.875844000	-1.937650000
C	4.093797000	-3.047509000	-2.205994000
H	3.713124000	-4.038775000	-1.920514000
H	4.128229000	-3.036117000	-3.304572000
C	3.121001000	-1.966979000	-1.721106000
H	3.495501000	-0.979073000	-2.020693000
H	3.089087000	-1.979755000	-0.623032000
C	1.720797000	-2.178905000	-2.283430000
H	1.298204000	-3.131538000	-1.949515000
H	1.750495000	-2.183856000	-3.378860000
S	0.558705000	-0.829359000	-1.833241000
C	-0.889280000	-1.338269000	-2.804411000
H	-1.263272000	-2.312240000	-2.479327000
H	-1.661000000	-0.579975000	-2.666724000
H	-0.610614000	-1.378382000	-3.860784000
H	-0.588556000	2.676425000	1.134054000
H	-1.871932000	1.741097000	1.948765000
C	3.215089000	5.323515000	0.241101000
H	2.999823000	5.652224000	1.260001000
C	3.296344000	6.233129000	-0.733886000
H	3.518846000	5.893989000	-1.748285000
C	3.121715000	7.708497000	-0.556524000
H	2.901380000	7.969483000	0.483614000
H	4.027220000	8.250244000	-0.859296000
H	2.305657000	8.087946000	-1.185387000

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**TS4',  $E_{(\text{SCF Done})} = -1980.001341$  a.u., IF =  $i260.6422$  cm<sup>-1</sup>**

C	-1.487427000	-1.669019000	1.923839000
C	-0.206530000	-2.284907000	1.788351000
C	0.740799000	-1.508687000	2.520370000
C	0.044526000	-0.412163000	3.108229000
C	-1.331624000	-0.516326000	2.749976000
C	0.046209000	-3.623595000	1.157778000
H	1.096200000	-3.759133000	0.882082000
H	-0.564977000	-3.789199000	0.264110000
H	-0.201542000	-4.429897000	1.861431000
C	2.179428000	-1.866730000	2.753411000
H	2.282387000	-2.481694000	3.657396000
H	2.811738000	-0.984523000	2.894149000
H	2.600850000	-2.445391000	1.925319000
C	0.617045000	0.600071000	4.057905000

H	0.211906000	1.605994000	3.897471000
H	1.706475000	0.664886000	3.983767000
H	0.385282000	0.327473000	5.096086000
C	-2.433599000	0.328082000	3.323739000
H	-2.752438000	-0.076006000	4.293891000
H	-3.323825000	0.353976000	2.688099000
H	-2.120790000	1.362451000	3.505260000
C	-2.781979000	-2.253640000	1.435984000
H	-2.688628000	-2.704321000	0.441800000
H	-3.126698000	-3.046544000	2.113445000
H	-3.581242000	-1.508592000	1.388498000
Sc	-0.074640000	-0.100263000	0.666157000
C	-8.285163000	-0.447084000	-1.810672000
H	-8.860093000	-1.040722000	-2.529090000
H	-8.507974000	-0.831511000	-0.808142000
H	-8.654311000	0.584064000	-1.861298000
C	-6.789779000	-0.515491000	-2.111834000
H	-6.457288000	-1.563052000	-2.089384000
H	-6.603178000	-0.156368000	-3.133485000
C	-5.948391000	0.302436000	-1.129518000
H	-6.132823000	-0.055561000	-0.106135000
H	-6.278063000	1.350821000	-1.152925000
C	-4.447416000	0.236481000	-1.432274000
H	-4.263528000	0.603185000	-2.450967000
H	-4.114372000	-0.810161000	-1.404146000
C	-3.634576000	1.060728000	-0.438581000
H	-3.750030000	0.687987000	0.582178000
H	-3.937897000	2.112822000	-0.461147000
S	-1.847117000	1.035769000	-0.891041000
C	-0.960340000	2.016178000	0.336106000
C	1.185699000	2.186303000	0.311156000
C	1.887863000	1.033195000	0.732083000
H	2.517422000	0.535388000	-0.008453000
H	2.264649000	1.001609000	1.751182000
C	6.971507000	-3.448518000	-1.454482000
H	7.939563000	-3.057598000	-1.124291000
H	6.782896000	-4.377774000	-0.903757000
H	7.061414000	-3.703724000	-2.516955000
C	5.858294000	-2.429589000	-1.221885000
H	5.816984000	-2.166890000	-0.155190000
H	6.092964000	-1.499329000	-1.757840000
C	4.486135000	-2.936739000	-1.670945000
H	4.247993000	-3.866809000	-1.134660000
H	4.526441000	-3.198665000	-2.737800000

C	3.368494000	-1.913058000	-1.442639000
H	3.599594000	-0.991028000	-1.992526000
H	3.329674000	-1.650563000	-0.377335000
C	2.016883000	-2.453409000	-1.894848000
H	1.725109000	-3.337092000	-1.319133000
H	2.054438000	-2.732797000	-2.953914000
S	0.677448000	-1.203135000	-1.771325000
C	-0.687361000	-2.114295000	-2.549753000
H	-0.915897000	-3.032976000	-2.004144000
H	-1.561227000	-1.460527000	-2.556686000
H	-0.413302000	-2.351375000	-3.581168000
H	-0.989431000	3.076411000	0.097418000
H	-1.393513000	1.873776000	1.341182000
C	1.368041000	2.711550000	-1.096186000
H	1.344355000	1.876405000	-1.808317000
H	0.559973000	3.397169000	-1.371675000
C	2.714003000	3.461352000	-1.253203000
H	3.535888000	2.761404000	-1.047868000
H	2.802052000	3.753467000	-2.306923000
C	2.844777000	4.677421000	-0.380993000
H	2.992795000	4.504909000	0.687408000
C	2.808047000	5.936816000	-0.827119000
H	2.680612000	6.106923000	-1.898814000
C	2.945705000	7.161918000	0.020968000
H	3.811498000	7.760252000	-0.291387000
H	2.066537000	7.812421000	-0.076381000
H	3.070668000	6.911857000	1.079761000
H	1.021247000	2.951865000	1.068807000

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**$J'$ ,  $E_{(\text{SCF Done})} = -1980.035852$  a.u.**

C	-2.065241000	-1.909210000	1.573398000
C	-1.050366000	-2.823001000	1.157522000
C	0.148592000	-2.494528000	1.856812000
C	-0.123422000	-1.384270000	2.712452000
C	-1.490772000	-1.021959000	2.533752000
C	-1.254690000	-4.000942000	0.248224000
H	-0.333299000	-4.296581000	-0.264649000
H	-2.019792000	-3.811966000	-0.513031000
H	-1.591145000	-4.876575000	0.819354000
C	1.441317000	-3.258019000	1.815599000
H	1.468064000	-4.009578000	2.616001000
H	2.310708000	-2.608825000	1.964434000
H	1.579001000	-3.797152000	0.872788000
C	0.817040000	-0.811100000	3.730063000



H	0.538784000	0.207195000	4.015971000
H	1.851248000	-0.781034000	3.372214000
H	0.807425000	-1.418480000	4.644949000
C	-2.209427000	0.051742000	3.298666000
H	-2.478557000	-0.302790000	4.302358000
H	-3.141133000	0.352745000	2.809800000
H	-1.594196000	0.948512000	3.432057000
C	-3.511426000	-1.973402000	1.171102000
H	-3.643685000	-2.293818000	0.131522000
H	-4.052848000	-2.696940000	1.795088000
H	-4.018284000	-1.011114000	1.290781000
Sc	-0.358279000	-0.587049000	0.420876000
C	-8.379280000	1.268185000	-1.297065000
H	-9.120015000	0.758469000	-1.921967000
H	-8.601397000	1.023283000	-0.251540000
H	-8.524203000	2.347493000	-1.424031000
C	-6.959868000	0.851621000	-1.675490000
H	-6.856328000	-0.238030000	-1.573042000
H	-6.779924000	1.078366000	-2.735555000
C	-5.891618000	1.542489000	-0.824931000
H	-6.070012000	1.317852000	0.236811000
H	-5.992709000	2.632235000	-0.929224000
C	-4.466764000	1.127125000	-1.205323000
H	-4.285196000	1.352596000	-2.264067000
H	-4.361069000	0.039739000	-1.089775000
C	-3.425309000	1.844990000	-0.353042000
H	-3.567116000	1.651115000	0.714535000
H	-3.477594000	2.927482000	-0.513265000
S	-1.718505000	1.359936000	-0.829967000
C	-0.680214000	2.719201000	-0.142925000
C	3.145576000	3.292050000	0.266584000
H	3.407823000	2.487427000	0.969031000
H	3.430364000	2.943889000	-0.736383000
C	1.628919000	3.523589000	0.314648000
H	1.385853000	4.342266000	-0.377916000
H	1.343679000	3.868082000	1.319888000
C	0.786437000	2.279498000	-0.042160000
C	0.930082000	1.107572000	0.948741000
H	1.103913000	1.954863000	-1.047270000
H	1.976554000	0.758046000	0.969094000
H	0.729327000	1.479583000	1.966576000
C	6.834872000	-3.459930000	-0.996578000
H	7.751568000	-3.080473000	-0.533383000
H	6.564343000	-4.390965000	-0.484285000

H	7.067998000	-3.708857000	-2.038562000
C	5.709557000	-2.431459000	-0.911102000
H	5.524443000	-2.174948000	0.141744000
H	6.023376000	-1.500138000	-1.402463000
C	4.407469000	-2.922394000	-1.547906000
H	4.090425000	-3.854195000	-1.057443000
H	4.591195000	-3.176132000	-2.601666000
C	3.279228000	-1.889130000	-1.465347000
H	3.592094000	-0.960048000	-1.958789000
H	3.090287000	-1.639335000	-0.412103000
C	1.998697000	-2.401970000	-2.116849000
H	1.635838000	-3.315925000	-1.635765000
H	2.164013000	-2.614557000	-3.178955000
S	0.678634000	-1.128111000	-2.059845000
C	-0.618500000	-1.878677000	-3.090751000
H	-0.946925000	-2.840099000	-2.689686000
H	-1.458326000	-1.179773000	-3.122381000
H	-0.233567000	-2.007121000	-4.105704000
H	-0.809091000	3.582389000	-0.803771000
H	-1.075593000	2.968688000	0.848849000
C	3.923868000	4.528926000	0.611163000
H	3.777889000	4.921431000	1.620339000
C	4.754637000	5.168405000	-0.216527000
H	4.897095000	4.770638000	-1.224197000
C	5.531140000	6.403346000	0.119682000
H	5.333760000	6.739457000	1.142979000
H	6.611177000	6.231426000	0.020992000
H	5.282349000	7.226528000	-0.563181000

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**TS5'',  $E_{(\text{SCF Done})} = -1980.000374$  a.u., IF =  $i1252.0078$  cm<sup>-1</sup>**

C	-1.321065000	-1.940103000	2.372773000
C	-0.007062000	-1.686982000	2.873472000
C	0.140682000	-0.276775000	3.027473000
C	-1.076288000	0.342471000	2.613542000
C	-1.983371000	-0.686004000	2.215682000
C	0.978532000	-2.735897000	3.299505000
H	0.931372000	-3.630454000	2.669859000
H	0.773356000	-3.057265000	4.329140000
H	2.009773000	-2.371393000	3.277413000
C	1.323881000	0.433467000	3.619035000
H	1.496408000	1.413199000	3.159052000
H	2.246865000	-0.147177000	3.525167000
H	1.169052000	0.610903000	4.691557000
C	-1.409513000	1.802482000	2.728468000

H	-2.144599000	2.120912000	1.982048000
H	-0.526079000	2.440889000	2.626465000
H	-1.844158000	2.019805000	3.713569000
C	-3.427805000	-0.471539000	1.866543000
H	-3.857908000	-1.327436000	1.339559000
H	-3.581264000	0.416287000	1.243760000
H	-4.022595000	-0.328824000	2.778610000
C	-1.940303000	-3.299731000	2.218156000
H	-2.369224000	-3.635724000	3.171464000
H	-2.754472000	-3.309901000	1.486618000
H	-1.210130000	-4.058457000	1.916849000
Sc	-0.116853000	-0.704153000	0.633209000
C	-1.465669000	7.411344000	-0.035606000
H	-2.395995000	7.919906000	-0.309221000
H	-1.346899000	7.497483000	1.051117000
H	-0.638732000	7.957119000	-0.505016000
C	-1.486620000	5.950092000	-0.478014000
H	-2.346107000	5.439294000	-0.020874000
H	-1.640728000	5.896278000	-1.564621000
C	-0.202505000	5.201285000	-0.114323000
H	-0.046114000	5.253425000	0.973032000
H	0.657067000	5.710363000	-0.573310000
C	-0.221182000	3.735950000	-0.560957000
H	-0.371833000	3.680188000	-1.646549000
H	-1.074587000	3.223326000	-0.096563000
C	1.075820000	3.021296000	-0.194847000
H	1.261542000	3.042668000	0.883832000
H	1.928675000	3.489775000	-0.698412000
S	1.057410000	1.277673000	-0.769879000
C	2.814422000	0.773209000	-0.634552000
C	4.420988000	-1.168918000	-0.725909000
H	4.857477000	-0.883760000	0.241856000
H	4.450172000	-2.266470000	-0.758488000
C	2.937751000	-0.747768000	-0.764289000
C	2.120219000	-1.446292000	0.335962000
H	3.200816000	1.105733000	0.336750000
H	3.354513000	1.297290000	-1.427497000
H	2.543915000	-1.032117000	-1.754895000
C	5.296256000	-0.622536000	-1.865624000
H	5.401424000	0.467284000	-1.786399000
H	4.790841000	-0.821989000	-2.824324000
C	6.662720000	-1.245794000	-1.876080000
H	6.695095000	-2.326291000	-2.034102000
C	7.808640000	-0.582214000	-1.701552000

H	7.768553000	0.498677000	-1.546706000
C	9.173944000	-1.195316000	-1.709474000
H	9.797597000	-0.759272000	-2.500906000
H	9.696967000	-1.010345000	-0.761910000
H	9.131201000	-2.277681000	-1.869080000
C	-8.000651000	-1.580364000	-2.704378000
H	-8.778840000	-0.889661000	-3.045609000
H	-7.968771000	-2.419143000	-3.409785000
H	-8.311750000	-1.976410000	-1.730247000
C	-6.646142000	-0.881518000	-2.612869000
H	-6.378568000	-0.466664000	-3.594537000
H	-6.718891000	-0.025052000	-1.927755000
C	-5.528380000	-1.813231000	-2.139091000
H	-5.452730000	-2.668804000	-2.825260000
H	-5.793710000	-2.229414000	-1.156186000
C	-4.168561000	-1.112361000	-2.049070000
H	-4.238233000	-0.260523000	-1.359441000
H	-3.900100000	-0.703329000	-3.031846000
C	-3.075563000	-2.067381000	-1.580237000
H	-2.960971000	-2.905325000	-2.275809000
H	-3.288274000	-2.467399000	-0.585098000
S	-1.447169000	-1.211147000	-1.547673000
C	-0.250924000	-2.444644000	-0.969093000
H	0.287374000	-2.895097000	-1.807302000
H	-0.749747000	-3.231497000	-0.391933000
H	0.902694000	-1.979664000	-0.312113000
H	2.308146000	-0.942548000	1.299714000
H	2.487652000	-2.470286000	0.489943000

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**$N', E_{(\text{SCF Done})} = -1980.041238 \text{ a.u.}$**

C	-1.371411000	-2.911186000	1.214850000
C	0.035604000	-3.020835000	1.411001000
C	0.468996000	-1.884261000	2.163697000
C	-0.671229000	-1.066511000	2.418056000
C	-1.809394000	-1.695749000	1.826189000
C	0.882125000	-4.189924000	0.994981000
H	0.598096000	-4.578038000	0.011092000
H	0.774821000	-5.015607000	1.710756000
H	1.946236000	-3.938487000	0.958154000
C	1.849813000	-1.658460000	2.710975000
H	2.079184000	-0.594771000	2.836654000
H	2.628338000	-2.098402000	2.079583000
H	1.949543000	-2.121734000	3.701583000
C	-0.703388000	0.171303000	3.268391000

H	-1.467974000	0.883449000	2.940164000
H	0.259608000	0.692130000	3.282201000
H	-0.938061000	-0.084868000	4.310319000
C	-3.232100000	-1.242906000	1.991880000
H	-3.891556000	-1.665524000	1.228851000
H	-3.331710000	-0.153065000	1.951895000
H	-3.624909000	-1.565095000	2.965456000
C	-2.246247000	-3.966604000	0.606114000
H	-2.573385000	-4.679716000	1.374516000
H	-3.152440000	-3.551685000	0.153923000
H	-1.722103000	-4.541241000	-0.163564000
Sc	-0.320116000	-1.063707000	0.007548000
C	-2.396847000	6.042277000	1.755007000
H	-3.435092000	6.376737000	1.659580000
H	-2.191775000	5.894222000	2.821966000
H	-1.752498000	6.855931000	1.401993000
C	-2.155961000	4.761133000	0.959867000
H	-2.841327000	3.976145000	1.311069000
H	-2.401358000	4.931994000	-0.097476000
C	-0.714736000	4.258109000	1.067066000
H	-0.466905000	4.082892000	2.123990000
H	-0.029404000	5.042580000	0.716075000
C	-0.468830000	2.977607000	0.262531000
H	-0.701571000	3.153893000	-0.795378000
H	-1.157719000	2.192564000	0.607899000
C	0.973770000	2.499836000	0.395527000
H	1.223468000	2.259286000	1.433934000
H	1.668235000	3.270630000	0.043746000
S	1.285381000	1.024053000	-0.651777000
C	3.070660000	0.703461000	-0.343753000
C	5.179408000	-0.416808000	-1.146473000
H	5.360944000	-0.835468000	-0.146088000
H	5.541791000	-1.170896000	-1.858066000
C	3.664620000	-0.258413000	-1.376761000
C	2.974093000	-1.622996000	-1.342372000
H	3.201042000	0.319436000	0.674247000
H	3.549589000	1.685033000	-0.406738000
H	3.515864000	0.183341000	-2.372580000
C	6.013131000	0.862122000	-1.323174000
H	5.771432000	1.595642000	-0.542609000
H	5.746021000	1.325554000	-2.286287000
C	7.488597000	0.583077000	-1.289439000
H	7.869305000	-0.073793000	-2.074774000
C	8.339395000	1.069088000	-0.381855000

H	7.951337000	1.728030000	0.398726000
C	9.810506000	0.796787000	-0.341367000
H	10.386354000	1.727692000	-0.426327000
H	10.102041000	0.334633000	0.611020000
H	10.121614000	0.130449000	-1.152464000
C	-8.543048000	0.569199000	-1.423406000
H	-9.210753000	1.415287000	-1.229678000
H	-8.796084000	0.166039000	-2.411122000
H	-8.765372000	-0.206452000	-0.680742000
C	-7.078614000	0.996627000	-1.358324000
H	-6.895752000	1.796729000	-2.089023000
H	-6.864713000	1.429125000	-0.370560000
C	-6.110066000	-0.157922000	-1.624180000
H	-6.321272000	-0.589299000	-2.613017000
H	-6.291398000	-0.960190000	-0.893843000
C	-4.640317000	0.270533000	-1.560497000
H	-4.423415000	0.698391000	-0.572388000
H	-4.457410000	1.064772000	-2.296209000
C	-3.700556000	-0.899269000	-1.830888000
H	-3.878448000	-1.326795000	-2.823348000
H	-3.821739000	-1.692156000	-1.087675000
S	-1.946626000	-0.349459000	-1.832953000
C	-0.916107000	-1.851995000	-1.949423000
H	-0.334066000	-1.826893000	-2.875381000
H	-1.551998000	-2.743014000	-1.941665000
H	1.910670000	-1.563195000	-1.623848000
H	3.055872000	-2.081651000	-0.348630000
H	3.431957000	-2.314125000	-2.058054000

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**$K'$ ,  $E_{(\text{SCF Done})} = -1980.034321$  a.u.**

C	-1.112968000	0.470652000	2.596239000
C	-0.641681000	-0.825009000	2.228849000
C	0.783299000	-0.782448000	2.193040000
C	1.191643000	0.549310000	2.491235000
C	0.016615000	1.322677000	2.747569000
C	-1.472928000	-2.070583000	2.104103000
H	-2.528577000	-1.841064000	1.935622000
H	-1.419282000	-2.664854000	3.026382000
H	-1.137862000	-2.722755000	1.289034000
C	1.668865000	-1.988056000	2.103202000
H	1.781500000	-2.444289000	3.096492000
H	2.675121000	-1.746053000	1.750946000
H	1.251065000	-2.759017000	1.447932000
C	2.603499000	1.016434000	2.708028000

H	2.749463000	2.064125000	2.423080000
H	3.330497000	0.414497000	2.153371000
H	2.874190000	0.939852000	3.769713000
C	-0.001012000	2.731582000	3.262456000
H	0.098150000	2.738115000	4.356239000
H	-0.932138000	3.250392000	3.018969000
H	0.826593000	3.331803000	2.868693000
C	-2.535071000	0.822750000	2.916551000
H	-2.795832000	0.465647000	3.921791000
H	-2.702607000	1.902822000	2.904837000
H	-3.248130000	0.369594000	2.219867000
Sc	-0.055836000	0.653514000	0.365730000
C	-7.748220000	-2.722481000	0.048014000
H	-8.504831000	-2.605269000	0.830886000
H	-8.246205000	-2.582556000	-0.918707000
H	-7.385201000	-3.756399000	0.088706000
C	-6.606305000	-1.725635000	0.232170000
H	-7.006223000	-0.702014000	0.221662000
H	-6.151403000	-1.866489000	1.222955000
C	-5.525199000	-1.854878000	-0.843339000
H	-5.980559000	-1.713756000	-1.834102000
H	-5.122556000	-2.878313000	-0.834063000
C	-4.379867000	-0.852371000	-0.662004000
H	-3.910658000	-0.995895000	0.318783000
H	-4.790533000	0.165037000	-0.669109000
C	-3.327542000	-1.005941000	-1.752466000
H	-3.764219000	-0.871680000	-2.748608000
H	-2.890025000	-2.010150000	-1.728335000
S	-1.885306000	0.128943000	-1.677628000
C	-2.619553000	1.797213000	-1.924378000
C	-0.446780000	3.085125000	-2.189585000
H	-0.049278000	2.129074000	-2.565453000
H	-0.739981000	3.658186000	-3.078845000
C	-1.687934000	2.844210000	-1.311359000
C	-1.351579000	2.438642000	0.127912000
H	-3.587892000	1.811539000	-1.416271000
H	-2.777843000	1.939643000	-2.998714000
C	0.685400000	3.825546000	-1.453351000
C	1.492888000	2.938290000	-0.534986000
C	2.484658000	2.113062000	-0.935706000
H	0.266419000	4.661884000	-0.881633000
H	1.358484000	4.272675000	-2.194216000
C	2.986091000	1.954736000	-2.338374000
H	4.066347000	2.145337000	-2.365174000

H	2.830852000	0.937360000	-2.714898000
H	2.503467000	2.642564000	-3.036560000
H	-2.267798000	3.783060000	-1.312110000
C	7.766444000	-2.237576000	0.112918000
H	8.640560000	-1.624405000	0.355704000
H	7.583441000	-2.906740000	0.962078000
H	8.027114000	-2.860132000	-0.751076000
C	6.546807000	-1.366829000	-0.180182000
H	6.333416000	-0.729015000	0.689681000
H	6.773099000	-0.685055000	-1.011957000
C	5.301081000	-2.185934000	-0.524746000
H	5.073616000	-2.870634000	0.305186000
H	5.514043000	-2.821251000	-1.396295000
C	4.074867000	-1.315583000	-0.821040000
H	4.303720000	-0.632927000	-1.648255000
H	3.853702000	-0.691085000	0.054846000
C	2.862733000	-2.166548000	-1.176798000
H	2.630962000	-2.874139000	-0.375560000
H	3.066540000	-2.742048000	-2.087042000
S	1.350736000	-1.188887000	-1.555819000
C	0.299768000	-2.552928000	-2.137330000
H	0.020990000	-3.227677000	-1.323405000
H	-0.591476000	-2.116628000	-2.590568000
H	0.840728000	-3.109481000	-2.907662000
H	-0.953260000	3.304250000	0.674670000
H	-2.292844000	2.184307000	0.640978000
H	3.044610000	1.580052000	-0.165526000
H	1.336107000	3.050683000	0.540029000

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**TS5',  $E_{(\text{SCF Done})} = -1980.018088$  a.u., IF =  $i316.0547$  cm<sup>-1</sup>**

C	-1.147691000	1.276637000	2.385169000
C	-0.350789000	0.104907000	2.533703000
C	1.019242000	0.489622000	2.429676000
C	1.067559000	1.895650000	2.213010000
C	-0.270990000	2.384960000	2.194172000
C	-0.875733000	-1.245467000	2.927394000
H	-1.783521000	-1.524496000	2.380157000
H	-1.137302000	-1.257968000	3.994081000
H	-0.136230000	-2.035018000	2.772604000
C	2.213728000	-0.374432000	2.705009000
H	2.624764000	-0.150728000	3.698563000
H	3.023795000	-0.220082000	1.983914000
H	1.956394000	-1.436695000	2.700282000
C	2.308698000	2.738794000	2.235213000



H	2. 245184000	3. 607037000	1. 569845000
H	3. 199428000	2. 168022000	1. 953712000
H	2. 488140000	3. 129783000	3. 245916000
C	-0. 663780000	3. 831740000	2. 222196000
H	-0. 583971000	4. 222866000	3. 245416000
H	-1. 698372000	3. 991388000	1. 903719000
H	-0. 017496000	4. 458219000	1. 597145000
C	-2. 636649000	1. 343945000	2. 573125000
H	-2. 886060000	1. 453443000	3. 637324000
H	-3. 084640000	2. 198143000	2. 054691000
H	-3. 142021000	0. 438055000	2. 221041000
Sc	-0. 027127000	0. 879321000	0. 208010000
C	-6. 816321000	-3. 719245000	0. 611002000
H	-7. 442924000	-3. 696249000	1. 508673000
H	-7. 475291000	-3. 601126000	-0. 257191000
H	-6. 360050000	-4. 714378000	0. 549354000
C	-5. 753887000	-2. 623244000	0. 652709000
H	-6. 240921000	-1. 642562000	0. 748496000
H	-5. 133688000	-2. 746768000	1. 552134000
C	-4. 854013000	-2. 619902000	-0. 585035000
H	-5. 474034000	-2. 499449000	-1. 484831000
H	-4. 362941000	-3. 599190000	-0. 681570000
C	-3. 792060000	-1. 515637000	-0. 550542000
H	-3. 170288000	-1. 626985000	0. 348792000
H	-4. 287584000	-0. 539554000	-0. 464961000
C	-2. 903513000	-1. 543674000	-1. 788036000
H	-3. 496485000	-1. 461711000	-2. 706245000
H	-2. 348275000	-2. 484338000	-1. 862558000
S	-1. 632353000	-0. 224881000	-1. 908235000
C	-2. 658342000	1. 223088000	-2. 366294000
C	-0. 717786000	2. 703604000	-3. 148691000
H	-0. 304319000	1. 731735000	-3. 445173000
H	-1. 066702000	3. 190092000	-4. 066358000
C	-1. 866269000	2. 508567000	-2. 140447000
C	-1. 300924000	2. 577677000	-0. 719894000
H	-3. 562781000	1. 214559000	-1. 749493000
H	-2. 947930000	1. 106391000	-3. 416210000
C	0. 358182000	3. 534674000	-2. 457966000
C	0. 787339000	2. 925479000	-1. 134155000
C	1. 666908000	1. 818615000	-1. 034624000
H	-0. 020400000	4. 549126000	-2. 283631000
H	1. 245333000	3. 633421000	-3. 097259000
C	2. 079635000	1. 031986000	-2. 266909000
H	2. 919612000	0. 374734000	-2. 034642000

H	1. 289213000	0. 395882000	-2. 685534000
H	2. 411376000	1. 698017000	-3. 077052000
H	-2. 583479000	3. 330835000	-2. 280471000
C	7. 774596000	-2. 427844000	-0. 374816000
H	8. 637444000	-1. 880697000	-0. 768889000
H	7. 883414000	-2. 479849000	0. 715114000
H	7. 825265000	-3. 451925000	-0. 763250000
C	6. 464719000	-1. 749952000	-0. 770064000
H	6. 459424000	-0. 715206000	-0. 398605000
H	6. 401129000	-1. 682454000	-1. 865094000
C	5. 231570000	-2. 483570000	-0. 238329000
H	5. 292467000	-2. 551447000	0. 857583000
H	5. 235610000	-3. 517950000	-0. 610903000
C	3. 916147000	-1. 806025000	-0. 637382000
H	3. 852069000	-1. 747146000	-1. 731263000
H	3. 909857000	-0. 775114000	-0. 258795000
C	2. 712836000	-2. 566536000	-0. 097002000
H	2. 751930000	-2. 638694000	0. 994193000
H	2. 699539000	-3. 584142000	-0. 504341000
S	1. 094886000	-1. 836180000	-0. 578939000
C	0. 029886000	-3. 190564000	0. 004670000
H	0. 292731000	-3. 482800000	1. 024368000
H	-1. 007983000	-2. 853412000	-0. 001810000
H	0. 132436000	-4. 052310000	-0. 660745000
H	-1. 372706000	3. 588633000	-0. 317292000
H	-1. 928266000	1. 966763000	-0. 025515000
H	2. 437408000	1. 927141000	-0. 270264000
H	0. 878038000	3. 644285000	-0. 321787000

86

**M,  $E_{(\text{SCF Done})} = -1980.052402$  a.u.**

C	0. 552824000	0. 278488000	2. 575278000
C	-0. 676348000	-0. 440422000	2. 671179000
C	-0. 374126000	-1. 837452000	2. 660422000
C	1. 038086000	-1. 979579000	2. 548585000
C	1. 610760000	-0. 671261000	2. 492490000
C	-2. 009550000	0. 178058000	2. 980996000
H	-2. 178394000	1. 114006000	2. 436389000
H	-2. 074369000	0. 421501000	4. 050228000
H	-2. 841756000	-0. 499929000	2. 766608000
C	-1. 349327000	-2. 958161000	2. 880317000
H	-1. 398148000	-3. 220549000	3. 945374000
H	-1. 064536000	-3. 866895000	2. 339838000
H	-2. 365309000	-2. 693986000	2. 569704000
C	1. 821441000	-3. 254425000	2. 663890000

H	2. 708620000	-3. 258861000	2. 021438000
H	1. 222382000	-4. 133847000	2. 409010000
H	2. 171066000	-3. 394975000	3. 695774000
C	3. 086941000	-0. 397660000	2. 533441000
H	3. 510068000	-0. 742072000	3. 486070000
H	3. 307834000	0. 670499000	2. 459902000
H	3. 638214000	-0. 914323000	1. 738590000
C	0. 680653000	1. 770120000	2. 686919000
H	0. 566430000	2. 088799000	3. 731887000
H	1. 658222000	2. 127905000	2. 351361000
H	-0. 085602000	2. 299052000	2. 108751000
Sc	0. 277792000	-0. 988462000	0. 442894000
C	3. 188738000	6. 762611000	0. 197204000
H	2. 625722000	7. 697472000	0. 107064000
H	3. 475815000	6. 647702000	1. 249257000
H	4. 109071000	6. 871593000	-0. 388654000
C	2. 362145000	5. 573059000	-0. 285692000
H	1. 431086000	5. 511211000	0. 295458000
H	2. 061124000	5. 733854000	-1. 330322000
C	3. 113385000	4. 244188000	-0. 177584000
H	3. 418534000	4. 082756000	0. 866705000
H	4. 042961000	4. 303727000	-0. 761964000
C	2. 284892000	3. 049657000	-0. 660412000
H	1. 974427000	3. 209242000	-1. 701238000
H	1. 364624000	2. 978311000	-0. 065204000
C	3. 069698000	1. 744822000	-0. 567187000
H	3. 433248000	1. 558601000	0. 446281000
H	3. 938975000	1. 772031000	-1. 233600000
S	2. 071196000	0. 303682000	-1. 120587000
C	3. 331496000	-0. 684355000	-2. 037496000
C	1. 461200000	-1. 842122000	-3. 414530000
H	0. 870174000	-1. 014452000	-3. 002794000
H	1. 601482000	-1. 623964000	-4. 478768000
C	2. 805407000	-1. 977425000	-2. 659656000
C	2. 628841000	-3. 174253000	-1. 680446000
H	4. 159232000	-0. 888992000	-1. 350736000
H	3. 689081000	-0. 001838000	-2. 816456000
C	0. 743810000	-3. 168429000	-3. 163439000
C	1. 138594000	-3. 572104000	-1. 732548000
C	0. 371157000	-2. 905681000	-0. 579699000
H	1. 125660000	-3. 931164000	-3. 854489000
H	-0. 336576000	-3. 111605000	-3. 335774000
H	1. 039321000	-4. 664209000	-1. 637457000
H	3. 584053000	-2. 247158000	-3. 385329000

H	2.945910000	-2.928497000	-0.659091000
H	3.259978000	-4.006743000	-2.012673000
C	-8.242658000	1.245557000	-0.670933000
H	-8.989311000	2.020959000	-0.871608000
H	-8.432687000	0.414971000	-1.361174000
H	-8.412134000	0.877324000	0.347942000
C	-6.825966000	1.790815000	-0.835323000
H	-6.698645000	2.184343000	-1.853484000
H	-6.677714000	2.642573000	-0.157081000
C	-5.749121000	0.737554000	-0.564031000
H	-5.894300000	-0.114150000	-1.244500000
H	-5.875742000	0.342616000	0.454604000
C	-4.327337000	1.286105000	-0.725071000
H	-4.172034000	2.129104000	-0.039842000
H	-4.205930000	1.679571000	-1.742498000
C	-3.280792000	0.211117000	-0.448573000
H	-3.387780000	-0.643293000	-1.126574000
H	-3.375070000	-0.162770000	0.575016000
S	-1.551172000	0.818365000	-0.579663000
C	-1.378307000	0.984299000	-2.383360000
H	-0.347127000	1.278945000	-2.586624000
H	-1.597075000	0.039829000	-2.888190000
H	-2.052124000	1.766056000	-2.740292000
H	0.635036000	-3.496398000	0.312919000
C	-1.155661000	-2.901289000	-0.672428000
H	-1.514021000	-2.559509000	-1.650404000
H	-1.632911000	-3.868651000	-0.457119000
H	-1.638318000	-2.221758000	0.077121000

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**TS6,  $E_{(\text{SCF Done})} = -1980.014688$  a.u., IF =  $i1173.205$  cm<sup>-1</sup>**

C	-0.243903000	-0.288092000	2.321259000
C	-0.226776000	-1.690121000	2.056646000
C	1.125856000	-2.138231000	2.126760000
C	1.945786000	-1.016226000	2.435277000
C	1.101471000	0.129072000	2.548069000
C	-1.429400000	-2.581780000	1.952668000
H	-2.305157000	-2.053793000	1.565437000
H	-1.701966000	-2.964965000	2.945447000
H	-1.249889000	-3.458145000	1.320245000
C	1.580293000	-3.567001000	2.056413000
H	1.523950000	-4.033009000	3.049460000
H	2.617803000	-3.657594000	1.720297000
H	0.959385000	-4.172266000	1.387391000
C	3.403680000	-1.063929000	2.786520000

H	3.869029000	-0.074876000	2.743828000
H	3.978856000	-1.730515000	2.133805000
H	3.533263000	-1.437437000	3.811084000
C	1.552692000	1.480246000	3.025080000
H	1.848154000	1.431574000	4.081224000
H	0.754346000	2.223778000	2.957439000
H	2.418531000	1.862781000	2.471946000
C	-1.477413000	0.550514000	2.488906000
H	-1.872045000	0.455284000	3.509530000
H	-1.283319000	1.613714000	2.320190000
H	-2.277913000	0.249748000	1.805638000
Sc	0.932011000	-0.624848000	0.184241000
C	-4.237173000	5.743907000	0.642447000
H	-5.302898000	5.751002000	0.390769000
H	-4.153902000	5.704832000	1.735191000
H	-3.811639000	6.698282000	0.310539000
C	-3.524219000	4.562595000	-0.011526000
H	-3.995408000	3.623330000	0.311676000
H	-3.654429000	4.611206000	-1.101535000
C	-2.029755000	4.515186000	0.314425000
H	-1.897171000	4.466262000	1.405357000
H	-1.558076000	5.454299000	-0.009078000
C	-1.313676000	3.332503000	-0.345591000
H	-1.441008000	3.379794000	-1.434381000
H	-1.775952000	2.392984000	-0.017496000
C	0.174778000	3.326200000	-0.013648000
H	0.353382000	3.275951000	1.063713000
H	0.651286000	4.237721000	-0.392084000
S	1.058293000	1.944853000	-0.842527000
C	2.760750000	2.640812000	-0.951714000
C	3.396000000	0.916199000	-2.772678000
H	2.310465000	0.767398000	-2.825583000
H	3.671383000	1.505603000	-3.653794000
C	3.776758000	1.621528000	-1.456544000
C	4.090065000	0.488341000	-0.446306000
H	3.039740000	3.017901000	0.038357000
H	2.683119000	3.491696000	-1.637291000
C	4.112583000	-0.431811000	-2.702122000
C	4.058033000	-0.856006000	-1.218023000
C	2.864443000	-1.737939000	-0.796288000
H	5.161580000	-0.303772000	-2.998006000
H	3.687457000	-1.176241000	-3.383306000
H	4.967412000	-1.431422000	-0.989551000
H	4.697512000	2.195140000	-1.627755000

H	3.366266000	0.486309000	0.387240000
H	5.062769000	0.658351000	0.027834000
C	-7.211236000	-3.269344000	-0.840483000
H	-8.213346000	-2.924964000	-0.564440000
H	-7.267741000	-3.673677000	-1.858063000
H	-6.946678000	-4.094581000	-0.168562000
C	-6.195104000	-2.133143000	-0.751253000
H	-6.505487000	-1.308853000	-1.408225000
H	-6.187372000	-1.725332000	0.269488000
C	-4.778954000	-2.572578000	-1.129983000
H	-4.784770000	-2.976716000	-2.152391000
H	-4.465976000	-3.398049000	-0.474244000
C	-3.758734000	-1.432671000	-1.041029000
H	-3.746215000	-1.032282000	-0.018053000
H	-4.067395000	-0.607905000	-1.696413000
C	-2.362080000	-1.898731000	-1.438460000
H	-2.352088000	-2.240512000	-2.478817000
H	-2.012246000	-2.713900000	-0.799242000
S	-1.165577000	-0.498780000	-1.370005000
C	0.338680000	-1.182688000	-2.119436000
H	0.591132000	-0.618574000	-3.019712000
H	1.536688000	-1.318619000	-1.481464000
H	0.156620000	-2.228473000	-2.387209000
H	3.051822000	-1.975782000	0.259771000
C	2.837243000	-3.091619000	-1.518485000
H	2.635625000	-2.995442000	-2.592987000
H	3.796804000	-3.618502000	-1.420843000
H	2.065894000	-3.755247000	-1.106324000

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**N,  $E_{(\text{SCF Done})} = -1980.064567$  a.u.**

C	-0.428808000	-0.019845000	2.866261000
C	-1.152936000	-1.160681000	2.400474000
C	-0.217249000	-2.221458000	2.194319000
C	1.082052000	-1.729572000	2.507843000
C	0.951814000	-0.370214000	2.933149000
C	-2.649821000	-1.268984000	2.328935000
H	-3.122095000	-0.335639000	2.004912000
H	-3.063612000	-1.510418000	3.317104000
H	-2.975284000	-2.060155000	1.647551000
C	-0.548105000	-3.644266000	1.854713000
H	-0.726389000	-4.222339000	2.771251000
H	0.265834000	-4.138825000	1.316037000
H	-1.453427000	-3.730991000	1.246006000
C	2.348045000	-2.537300000	2.500394000

H	3. 238680000	-1. 909178000	2. 401409000
H	2. 365869000	-3. 269210000	1. 686548000
H	2. 454367000	-3. 095096000	3. 440340000
C	2. 056530000	0. 488161000	3. 480669000
H	2. 201964000	0. 289213000	4. 550774000
H	1. 836782000	1. 556772000	3. 386485000
H	3. 018225000	0. 296295000	2. 992805000
C	-1. 039598000	1. 275991000	3. 318466000
H	-1. 340483000	1. 211924000	4. 372743000
H	-0. 340745000	2. 115372000	3. 241310000
H	-1. 939600000	1. 533758000	2. 750079000
Sc	0. 307699000	-0. 453477000	0. 586856000
C	-4. 452653000	5. 341741000	-0. 201629000
H	-5. 496379000	5. 178492000	-0. 489567000
H	-4. 436704000	5. 585896000	0. 867238000
H	-4. 091039000	6. 220004000	-0. 749092000
C	-3. 599512000	4. 111849000	-0. 503497000
H	-4. 008378000	3. 241021000	0. 029219000
H	-3. 662210000	3. 873698000	-1. 574381000
C	-2. 131303000	4. 298071000	-0. 114518000
H	-2. 064534000	4. 532593000	0. 957720000
H	-1. 722669000	5. 169039000	-0. 646199000
C	-1. 270841000	3. 069299000	-0. 426413000
H	-1. 324524000	2. 841645000	-1. 498677000
H	-1. 681646000	2. 194549000	0. 099805000
C	0. 183443000	3. 285580000	-0. 021122000
H	0. 279136000	3. 452613000	1. 056668000
H	0. 603130000	4. 152738000	-0. 542623000
S	1. 231915000	1. 854801000	-0. 498077000
C	2. 886137000	2. 388359000	0. 119229000
C	4. 218565000	1. 833078000	-2. 047286000
H	3. 261921000	2. 076935000	-2. 523883000
H	4. 889860000	2. 675799000	-2. 242050000
C	4. 038039000	1. 620877000	-0. 523888000
C	4. 032995000	0. 097811000	-0. 345234000
H	2. 899779000	2. 293171000	1. 209093000
H	2. 952798000	3. 453254000	-0. 131458000
C	4. 777662000	0. 497417000	-2. 595753000
C	5. 073971000	-0. 385208000	-1. 365251000
C	5. 058825000	-1. 890697000	-1. 627453000
H	5. 661881000	0. 643672000	-3. 222742000
H	4. 024612000	0. 001901000	-3. 223078000
H	6. 066125000	-0. 113522000	-0. 971435000
H	4. 936274000	2. 000699000	-0. 014987000

H	3.050144000	-0.325918000	-0.625137000
H	4.256323000	-0.217750000	0.681219000
C	-7.496323000	-2.610094000	-1.942125000
H	-8.445250000	-2.078594000	-2.069641000
H	-7.395628000	-3.314366000	-2.776403000
H	-7.565572000	-3.196788000	-1.018215000
C	-6.321248000	-1.636223000	-1.894572000
H	-6.299161000	-1.040477000	-2.817675000
H	-6.468191000	-0.921614000	-1.072249000
C	-4.973502000	-2.339079000	-1.717623000
H	-4.824358000	-3.051865000	-2.541150000
H	-4.993319000	-2.936304000	-0.794123000
C	-3.793690000	-1.362506000	-1.671385000
H	-3.935586000	-0.651144000	-0.846568000
H	-3.769273000	-0.772606000	-2.597109000
C	-2.465807000	-2.091264000	-1.497613000
H	-2.287423000	-2.788427000	-2.323177000
H	-2.435683000	-2.653196000	-0.559979000
S	-1.057150000	-0.910751000	-1.528223000
C	0.439268000	-1.860905000	-1.084010000
H	1.156407000	-1.817532000	-1.908868000
H	4.069323000	-2.173606000	-2.018061000
H	0.174422000	-2.903805000	-0.883573000
H	5.175935000	-2.421483000	-0.671992000
C	6.143073000	-2.358795000	-2.597111000
H	6.024323000	-1.903598000	-3.586719000
H	7.142764000	-2.099714000	-2.228377000
H	6.110225000	-3.445555000	-2.728094000

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**3b,  $E_{(\text{SCF Done})} = -908.963841$  a.u.**

C	7.217668000	-0.464381000	0.127097000
H	7.951076000	-1.229864000	0.405109000
H	7.414494000	-0.177511000	-0.913308000
H	7.403376000	0.417080000	0.753215000
C	5.787956000	-0.973004000	0.299020000
H	5.642631000	-1.874816000	-0.312453000
H	5.631638000	-1.284753000	1.341455000
C	4.731477000	0.066750000	-0.078940000
H	4.886805000	0.378573000	-1.122552000
H	4.875877000	0.969300000	0.533472000
C	3.298074000	-0.441344000	0.092747000
H	3.138545000	-0.748451000	1.135304000
H	3.149296000	-1.339077000	-0.522437000
C	2.257702000	0.609233000	-0.288297000



H	2.387543000	0.907930000	-1.336474000
H	2.378189000	1.506209000	0.333007000
S	0.572163000	-0.051711000	-0.060018000
C	-0.388708000	1.410906000	-0.601517000
C	-2.296809000	1.194126000	1.155404000
H	-1.471090000	0.797998000	1.756498000
H	-2.525693000	2.191197000	1.548822000
C	-1.889439000	1.274276000	-0.338561000
C	-2.586024000	0.070513000	-0.988972000
H	-0.210314000	1.568427000	-1.672768000
H	-0.001464000	2.288290000	-0.067045000
C	-3.522483000	0.250433000	1.213745000
C	-3.927802000	-0.011991000	-0.251484000
C	-4.698983000	-1.310677000	-0.485342000
H	-4.343482000	0.664091000	1.809154000
H	-3.240949000	-0.702867000	1.681880000
H	-4.553807000	0.828491000	-0.594447000
H	-2.344172000	2.181045000	-0.766040000
H	-2.009824000	-0.848358000	-0.807332000
H	-2.693425000	0.177598000	-2.075447000
H	-4.080639000	-2.155044000	-0.145987000
H	-4.841258000	-1.452471000	-1.566149000
C	-6.058627000	-1.360747000	0.210593000
H	-5.956364000	-1.290147000	1.299718000
H	-6.701331000	-0.533483000	-0.116117000
H	-6.584272000	-2.296557000	-0.011759000

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**O,  $E_{(\text{SCF Done})} = -1129.198134$  a.u.**

C	2.341228000	-1.084489000	1.043032000
C	1.263460000	-1.928242000	1.446259000
C	0.810780000	-2.645559000	0.296135000
C	1.602992000	-2.235904000	-0.816432000
C	2.549490000	-1.269216000	-0.356363000
C	0.753306000	-2.116343000	2.847607000
H	1.237583000	-2.979886000	3.321978000
H	-0.326215000	-2.304990000	2.880707000
H	0.962131000	-1.249693000	3.482498000
C	-0.236103000	-3.722240000	0.291085000
H	0.216280000	-4.699658000	0.505082000
H	-0.736126000	-3.810861000	-0.679112000
H	-1.004623000	-3.558144000	1.054357000
C	1.543173000	-2.808783000	-2.204143000
H	1.819316000	-2.075233000	-2.969948000
H	0.551293000	-3.201962000	-2.450676000

H	2.247803000	-3.644779000	-2.304639000
C	3.661543000	-0.666552000	-1.162082000
H	4.565404000	-1.286189000	-1.089530000
H	3.919636000	0.336988000	-0.813054000
H	3.407759000	-0.592094000	-2.224134000
C	3.169245000	-0.200061000	1.928837000
H	4.122224000	-0.686517000	2.174564000
H	3.407583000	0.754091000	1.447196000
H	2.669170000	0.018348000	2.877239000
Sc	0.350088000	-0.285933000	-0.089008000
C	0.571845000	2.280325000	0.436073000
C	1.082811000	1.657087000	-0.708051000
C	0.673429000	3.631700000	0.734941000
C	1.741753000	2.503113000	-1.609736000
C	1.336909000	4.430484000	-0.201765000
H	0.268679000	4.069728000	1.642034000
C	1.864935000	3.874207000	-1.367155000
H	2.174553000	2.091898000	-2.520264000
H	1.439786000	5.494933000	-0.010272000
H	2.377897000	4.511496000	-2.082420000
C	-0.480598000	1.740857000	2.607459000
H	-0.870160000	0.850746000	3.101660000
H	0.384045000	2.128208000	3.154334000
H	-1.264231000	2.501447000	2.548265000
O	-0.089574000	1.341065000	1.292846000
H	-2.450458000	1.894735000	-1.053684000
C	-2.647354000	-0.224484000	-0.713307000
C	-3.057485000	1.103086000	-0.622554000
C	-3.389879000	-1.270917000	-0.175768000
C	-4.254725000	1.384387000	0.034716000
C	-4.582643000	-0.971161000	0.483750000
H	-3.044839000	-2.295073000	-0.282806000
C	-5.013955000	0.351335000	0.586918000
H	-4.594649000	2.413142000	0.111296000
H	-5.177585000	-1.775022000	0.907258000
H	-5.946980000	0.577712000	1.094454000
C	-1.489073000	-0.538386000	-2.802194000
H	-0.493566000	-0.801192000	-3.161066000
H	-2.217877000	-1.288532000	-3.118233000
H	-1.772241000	0.452442000	-3.164359000
O	-1.424670000	-0.526935000	-1.354488000

16

**1c,  $E_{(\text{SCF Done})} = -346.614132$  a.u.**

C	-2.278527000	0.331566000	0.000046000
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C	-1.330982000	1.350048000	0.000011000
C	0.035782000	1.060870000	-0.000092000
C	0.456969000	-0.272573000	-0.000072000
C	-0.493583000	-1.302389000	0.000002000
C	-1.848362000	-0.998210000	0.000036000
H	-3.339036000	0.567174000	0.000092000
H	-1.649447000	2.389770000	-0.000001000
H	0.753877000	1.874019000	-0.000172000
H	-0.142994000	-2.330304000	0.000009000
H	-2.575432000	-1.806591000	0.000072000
O	1.757774000	-0.671826000	-0.000106000
C	2.756536000	0.325138000	0.000121000
H	2.696245000	0.959310000	0.895229000
H	3.711121000	-0.204949000	0.000195000
H	2.696471000	0.959475000	-0.894888000

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**P,  $E_{(\text{SCF Done})} = -1096.869823$  a.u.**

C	-3.297973000	-0.687965000	0.991478000
C	-3.430333000	-1.425827000	-0.224114000
C	-2.412466000	-2.428315000	-0.246582000
C	-1.643132000	-2.298904000	0.948729000
C	-2.189495000	-1.222206000	1.714578000
C	-4.516912000	-1.265171000	-1.250029000
H	-5.354661000	-1.940208000	-1.031405000
H	-4.175520000	-1.508549000	-2.262756000
H	-4.925585000	-0.249937000	-1.265802000
C	-2.271316000	-3.498695000	-1.291275000
H	-2.983551000	-4.312348000	-1.101618000
H	-1.273831000	-3.948450000	-1.295373000
H	-2.477489000	-3.131310000	-2.303131000
C	-0.524262000	-3.198486000	1.391782000
H	-0.038591000	-3.705728000	0.552116000
H	-0.905338000	-3.983357000	2.058118000
H	0.247730000	-2.658734000	1.951304000
C	-1.756589000	-0.809073000	3.090435000
H	-2.308339000	-1.376330000	3.851837000
H	-1.942547000	0.252879000	3.274026000
H	-0.691655000	-0.995941000	3.262007000
C	-4.201287000	0.410298000	1.471248000
H	-4.960077000	0.008352000	2.155445000
H	-3.651449000	1.185869000	2.013275000
H	-4.737678000	0.893474000	0.648875000
Sc	-1.320413000	-0.244242000	-0.308043000
C	-1.260876000	2.366490000	-0.478775000

C	-0.720844000	1.626929000	0.581438000
C	-1.258164000	3.750044000	-0.584485000
C	-0.134089000	2.385802000	1.605086000
C	-0.655010000	4.454332000	0.461750000
H	-1.693631000	4.281723000	-1.424664000
C	-0.094857000	3.780424000	1.548670000
H	0.299539000	1.883141000	2.467970000
H	-0.627996000	5.539598000	0.420904000
H	0.366958000	4.347712000	2.352153000
C	-2.677375000	2.087880000	-2.488655000
H	-3.103492000	1.256902000	-3.051179000
H	-3.473862000	2.675013000	-2.022691000
H	-2.081189000	2.717631000	-3.154806000
O	-1.838221000	1.513737000	-1.480834000
C	8.802715000	-0.235210000	0.074775000
H	9.013263000	-0.959745000	-0.721078000
H	9.563515000	-0.365493000	0.851830000
H	8.928785000	0.768553000	-0.348634000
C	7.396768000	-0.425661000	0.639422000
H	7.313008000	-1.425848000	1.087635000
H	7.228919000	0.289678000	1.457015000
C	6.301414000	-0.252484000	-0.414671000
H	6.468007000	-0.968762000	-1.232575000
H	6.384410000	0.748139000	-0.863838000
C	4.890648000	-0.441422000	0.145546000
H	4.721255000	0.276852000	0.961023000
H	4.807166000	-1.442119000	0.593942000
C	3.801512000	-0.268357000	-0.914761000
H	3.958628000	-0.985697000	-1.731050000
H	3.875858000	0.733820000	-1.359012000
C	2.384425000	-0.464950000	-0.334567000
H	2.233510000	0.267082000	0.470924000
H	2.296547000	-1.468116000	0.101218000
C	1.344796000	-0.258475000	-1.385608000
C	0.516870000	-1.208794000	-1.875226000
H	0.578421000	-2.242096000	-1.536196000
H	-0.110562000	-1.015053000	-2.748102000
H	1.300978000	0.743365000	-1.819255000

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**TS7,  $E_{(\text{SCF Done})} = -1096.850099$  a.u., IF =  $i264.2062$  cm<sup>-1</sup>**

C	-3.640810000	0.114177000	0.668692000
C	-3.755975000	-0.742819000	-0.468072000
C	-3.064917000	-1.960450000	-0.179932000
C	-2.515436000	-1.849662000	1.133309000

C	-2.869765000	-0.569541000	1.658776000
C	-4.561302000	-0.480022000	-1.709032000
H	-5.549042000	-0.953365000	-1.633776000
H	-4.086076000	-0.886944000	-2.608861000
H	-4.736337000	0.587949000	-1.872911000
C	-3.063478000	-3.187881000	-1.042749000
H	-3.978322000	-3.772411000	-0.878568000
H	-2.219817000	-3.847848000	-0.819570000
H	-3.024335000	-2.947273000	-2.110336000
C	-1.759599000	-2.923846000	1.863243000
H	-1.170115000	-3.550523000	1.185592000
H	-2.452785000	-3.591350000	2.391751000
H	-1.079335000	-2.514550000	2.617694000
C	-2.572440000	-0.061379000	3.042349000
H	-3.389210000	-0.319112000	3.729450000
H	-2.464084000	1.028147000	3.071690000
H	-1.658559000	-0.497237000	3.458741000
C	-4.301156000	1.451412000	0.853122000
H	-5.236808000	1.343025000	1.417055000
H	-3.675395000	2.154615000	1.414547000
H	-4.561578000	1.919567000	-0.101249000
Sc	-1.393802000	-0.176447000	-0.196584000
C	-0.230098000	2.095463000	-0.480808000
C	0.462283000	1.005539000	0.083469000
C	-0.038977000	3.421047000	-0.105623000
C	1.371907000	1.312251000	1.105889000
C	0.893046000	3.674046000	0.902769000
H	-0.579897000	4.239498000	-0.569663000
C	1.581073000	2.627973000	1.520119000
H	1.938564000	0.516263000	1.583801000
H	1.073259000	4.699937000	1.210763000
H	2.289655000	2.841302000	2.315179000
C	-1.978061000	2.659404000	-2.109317000
H	-2.629864000	2.101891000	-2.780863000
H	-2.572583000	3.250841000	-1.407340000
H	-1.312598000	3.304530000	-2.688746000
O	-1.198361000	1.677553000	-1.410569000
C	8.493443000	-0.355196000	0.142898000
H	8.742725000	-0.367267000	-0.924994000
H	9.317608000	-0.835488000	0.681169000
H	8.454537000	0.693419000	0.462220000
C	7.168368000	-1.065586000	0.409903000
H	7.250784000	-2.120455000	0.112365000
H	6.964616000	-1.069698000	1.490277000

C	5.987873000	-0.426760000	-0.323796000
H	6.191608000	-0.423052000	-1.404688000
H	5.904177000	0.629589000	-0.027144000
C	4.657267000	-1.134489000	-0.063384000
H	4.455345000	-1.143506000	1.018760000
H	4.741432000	-2.189067000	-0.364040000
C	3.477995000	-0.491578000	-0.794947000
H	3.685245000	-0.475344000	-1.874432000
H	3.380571000	0.558006000	-0.486204000
C	2.159231000	-1.232247000	-0.561354000
H	1.962061000	-1.341885000	0.513720000
H	2.259128000	-2.259596000	-0.937102000
C	0.966421000	-0.621994000	-1.276704000
C	-0.160443000	-1.419083000	-1.596433000
H	-0.154920000	-2.464292000	-1.288430000
H	-0.672176000	-1.224672000	-2.543066000
H	1.210562000	0.178648000	-1.974310000

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**O',  $E_{(\text{SCF Done})} = -1475.842473$  a.u.**

C	-1.083334000	0.739960000	2.255932000
C	-1.392171000	-0.648925000	2.327621000
C	-0.163401000	-1.375466000	2.301470000
C	0.903642000	-0.435646000	2.214621000
C	0.335230000	0.873185000	2.191130000
C	-2.762525000	-1.220459000	2.536673000
H	-3.024026000	-1.204092000	3.603269000
H	-2.830852000	-2.261309000	2.206769000
H	-3.527804000	-0.652102000	2.000567000
C	-0.005226000	-2.855480000	2.497808000
H	0.222240000	-3.079728000	3.548541000
H	0.815021000	-3.272959000	1.903193000
H	-0.918839000	-3.402825000	2.249739000
C	2.367166000	-0.737454000	2.356273000
H	2.993782000	-0.086904000	1.737447000
H	2.603932000	-1.771110000	2.092035000
H	2.682774000	-0.588831000	3.398157000
C	1.116258000	2.141520000	2.372605000
H	1.311881000	2.299152000	3.442354000
H	0.583098000	3.023062000	2.008987000
H	2.088097000	2.109634000	1.871919000
C	-2.074678000	1.857928000	2.379165000
H	-2.306778000	2.050934000	3.435339000
H	-1.689495000	2.792139000	1.959631000
H	-3.016589000	1.623652000	1.873955000

Sc	-0.404269000	-0.280861000	0.117634000
C	-2.776777000	-1.291086000	-0.901767000
C	-2.440551000	0.045085000	-0.673035000
C	-3.981597000	-1.744665000	-1.423964000
C	-3.431086000	0.975562000	-1.012149000
C	-4.933461000	-0.772160000	-1.749243000
H	-4.201284000	-2.797121000	-1.576523000
C	-4.662937000	0.579971000	-1.546396000
H	-3.259121000	2.039881000	-0.852211000
H	-5.890385000	-1.082428000	-2.159809000
H	-5.414017000	1.323908000	-1.799245000
C	-1.908866000	-3.545051000	-0.548647000
H	-0.989028000	-3.997897000	-0.178473000
H	-2.745540000	-3.826382000	0.099712000
H	-2.106291000	-3.891973000	-1.569556000
O	-1.711624000	-2.137831000	-0.527768000
H	2.769798000	2.413720000	-1.030607000
C	0.661356000	2.794273000	-0.843678000
C	2.003796000	3.151232000	-0.812625000
C	-0.346407000	3.715426000	-0.577024000
C	2.345023000	4.463598000	-0.484342000
C	0.006633000	5.024682000	-0.251894000
H	-1.386992000	3.408911000	-0.621162000
C	1.349987000	5.398972000	-0.203935000
H	3.391445000	4.753005000	-0.451099000
H	-0.771146000	5.752177000	-0.037934000
H	1.620202000	6.420070000	0.048314000
C	-0.058826000	1.391067000	-2.587558000
H	-0.410568000	0.378589000	-2.780285000
H	-0.869526000	2.092068000	-2.797178000
H	0.814382000	1.621256000	-3.205308000
O	0.312283000	1.472470000	-1.191507000
H	2.078454000	-3.731030000	-0.269746000
C	2.390965000	-1.735978000	-1.017526000
C	2.806767000	-2.957670000	-0.496843000
C	3.298195000	-0.733451000	-1.339412000
C	4.167123000	-3.167189000	-0.274723000
C	4.656839000	-0.952759000	-1.108436000
H	2.942058000	0.196195000	-1.771327000
C	5.090968000	-2.165936000	-0.575949000
H	4.503891000	-4.115656000	0.133668000
H	5.376026000	-0.176746000	-1.354689000
H	6.149474000	-2.334543000	-0.401881000
C	0.599771000	-2.119597000	-2.504566000

H	-0.467436000	-1.930727000	-2.615649000
H	1.161828000	-1.671594000	-3.329113000
H	0.784301000	-3.196788000	-2.475706000
O	1.018769000	-1.520698000	-1.256213000

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**P', E<sub>(SCF Done)</sub> = -1443.515897 a.u.**

C	3.151228000	-0.926325000	1.105353000
C	2.424952000	-2.155135000	1.077567000
C	1.358372000	-2.062020000	2.017273000
C	1.424299000	-0.775649000	2.627615000
C	2.531577000	-0.070614000	2.064705000
C	2.779547000	-3.388949000	0.301533000
H	3.496626000	-3.178951000	-0.497259000
H	1.899090000	-3.862418000	-0.145985000
H	3.246392000	-4.132604000	0.960612000
C	0.450480000	-3.181373000	2.428161000
H	-0.510717000	-2.815319000	2.802538000
H	0.909905000	-3.765569000	3.237398000
H	0.243653000	-3.865208000	1.600988000
C	0.606031000	-0.344343000	3.811829000
H	0.963682000	-0.850028000	4.718383000
H	-0.455887000	-0.595883000	3.712527000
H	0.682059000	0.730351000	4.004567000
C	3.058883000	1.256392000	2.529438000
H	2.263645000	1.930947000	2.865205000
H	3.622364000	1.775377000	1.749123000
H	3.737548000	1.119191000	3.382089000
C	4.431624000	-0.639913000	0.374469000
H	4.554754000	0.423793000	0.149526000
H	5.294328000	-0.941500000	0.983503000
H	4.504508000	-1.193153000	-0.567637000
Sc	0.926560000	-0.424630000	0.231899000
C	0.083975000	-2.145743000	-1.707686000
C	-0.569717000	-1.866748000	-0.505057000
C	-0.334144000	-3.062132000	-2.664759000
C	-1.741460000	-2.602180000	-0.281327000
C	-1.514786000	-3.760562000	-2.393837000
H	0.211936000	-3.245308000	-3.585199000
C	-2.215550000	-3.534626000	-1.209514000
H	-2.305721000	-2.460522000	0.640223000
H	-1.880293000	-4.485691000	-3.115634000
H	-3.128248000	-4.089743000	-1.009186000
C	2.179784000	-1.663584000	-2.874236000
H	3.053447000	-1.031775000	-2.712670000



H	2.473451000	-2.717154000	-2.832943000
H	1.738555000	-1.439884000	-3.851406000
O	1.256796000	-1.362202000	-1.833898000
C	-1.842726000	0.625621000	1.052029000
C	-0.830020000	1.496989000	1.220659000
H	3.570118000	1.385614000	-2.395289000
C	2.334474000	2.416048000	-0.965729000
C	3.468706000	2.257006000	-1.755454000
C	2.162382000	3.529815000	-0.150888000
C	4.463839000	3.233173000	-1.711404000
C	3.165182000	4.498952000	-0.114834000
H	1.263626000	3.637964000	0.447907000
C	4.313796000	4.351699000	-0.891683000
H	5.355040000	3.118200000	-2.321520000
H	3.043636000	5.371157000	0.520895000
H	5.090238000	5.110244000	-0.861625000
C	0.379208000	1.657308000	-2.086476000
H	-0.375649000	0.869490000	-2.029257000
H	-0.088067000	2.637912000	-1.961390000
H	0.896695000	1.607535000	-3.047835000
O	1.323552000	1.433715000	-1.013354000
H	-0.759955000	2.388926000	0.602591000
H	-0.145741000	1.426960000	2.063858000
C	-2.953050000	0.774279000	0.061918000
H	-2.750642000	1.621117000	-0.606982000
H	-3.011176000	-0.130199000	-0.557340000
C	-4.307858000	0.983884000	0.765171000
H	-4.502638000	0.136980000	1.438290000
H	-4.252391000	1.878188000	1.400333000
C	-5.464609000	1.124601000	-0.225868000
H	-5.263870000	1.969109000	-0.901548000
H	-5.509675000	0.228021000	-0.861403000
C	-6.817264000	1.333323000	0.456799000
H	-7.019285000	0.488501000	1.131779000
H	-6.769349000	2.227834000	1.095231000
C	-7.976779000	1.479259000	-0.530481000
H	-7.774018000	2.323666000	-1.204555000
H	-8.023771000	0.585291000	-1.168505000
C	-9.324361000	1.687301000	0.156989000
H	-9.571901000	0.842240000	0.810759000
H	-9.319882000	2.593580000	0.774612000
H	-10.133004000	1.788546000	-0.574937000
H	-1.920064000	-0.225211000	1.731630000

**TS7',  $E_{(\text{SCF Done})} = -1443.497081$  a.u., IF =  $i266.0481$  cm<sup>-1</sup>**

C	-3.223950000	0.297744000	0.874566000
C	-3.017184000	1.573649000	0.266653000
C	-2.116894000	2.313958000	1.085941000
C	-1.731985000	1.480643000	2.178145000
C	-2.421730000	0.238201000	2.052591000
C	-3.763045000	2.113778000	-0.920485000
H	-4.005649000	1.334734000	-1.651804000
H	-3.200156000	2.900336000	-1.434441000
H	-4.716935000	2.560942000	-0.609361000
C	-1.799738000	3.769951000	0.917691000
H	-0.947920000	4.075973000	1.528556000
H	-2.660195000	4.377464000	1.228720000
H	-1.571598000	4.037079000	-0.119516000
C	-0.867064000	1.888262000	3.335051000
H	-1.474733000	2.326785000	4.137833000
H	-0.125200000	2.640446000	3.049524000
H	-0.331777000	1.038995000	3.773045000
C	-2.438766000	-0.861961000	3.073606000
H	-1.486388000	-0.950830000	3.606930000
H	-2.665941000	-1.835055000	2.628200000
H	-3.208668000	-0.667675000	3.832505000
C	-4.297587000	-0.675428000	0.484587000
H	-4.093145000	-1.690932000	0.832236000
H	-5.252795000	-0.365618000	0.930511000
H	-4.452184000	-0.719516000	-0.597748000
Sc	-0.870350000	0.401985000	0.139827000
C	0.403113000	2.106293000	-1.516298000
C	0.805893000	2.005452000	-0.176638000
C	0.603406000	3.226081000	-2.317929000
C	1.443967000	3.142342000	0.340372000
C	1.265690000	4.319053000	-1.758468000
H	0.269977000	3.262382000	-3.350062000
C	1.677231000	4.282006000	-0.426867000
H	1.799400000	3.136323000	1.370230000
H	1.454509000	5.197595000	-2.368569000
H	2.186656000	5.136653000	0.009218000
C	-0.926768000	0.997260000	-3.246690000
H	-1.472492000	0.058171000	-3.333523000
H	-1.619834000	1.840150000	-3.320877000
H	-0.166716000	1.060059000	-4.030843000
O	-0.299322000	0.971303000	-1.961636000
C	1.683168000	0.393480000	0.902309000
C	0.811524000	-0.661642000	1.256115000

H	-3.086531000	-2.378515000	-2.617268000
C	-1.976528000	-2.681093000	-0.798707000
C	-2.980311000	-2.974836000	-1.715166000
C	-1.800484000	-3.431439000	0.358890000
C	-3.845605000	-4.035570000	-1.450465000
C	-2.674735000	-4.488995000	0.614451000
H	-0.995762000	-3.192220000	1.047778000
C	-3.695797000	-4.790124000	-0.286716000
H	-4.637488000	-4.270829000	-2.155668000
H	-2.550781000	-5.080553000	1.517059000
H	-4.371477000	-5.615961000	-0.084903000
C	0.026455000	-2.083496000	-1.861602000
H	0.661035000	-1.222670000	-2.068635000
H	0.582015000	-2.843655000	-1.304476000
H	-0.342201000	-2.513370000	-2.797497000
O	-1.093427000	-1.616772000	-1.075004000
H	0.968116000	-1.625124000	0.770120000
H	0.467146000	-0.718095000	2.287392000
C	2.861057000	0.141823000	-0.015238000
H	2.550732000	-0.476604000	-0.867835000
H	3.243052000	1.082366000	-0.424000000
C	3.990229000	-0.576451000	0.744910000
H	4.273664000	0.022831000	1.621962000
H	3.621401000	-1.534696000	1.133753000
C	5.223901000	-0.811006000	-0.129586000
H	4.938976000	-1.405863000	-1.010479000
H	5.585195000	0.152974000	-0.516415000
C	6.359897000	-1.517318000	0.612321000
H	6.644223000	-0.922557000	1.492858000
H	5.998719000	-2.481212000	1.000661000
C	7.596074000	-1.754085000	-0.257282000
H	7.311540000	-2.348375000	-1.137397000
H	7.955763000	-0.790310000	-0.644714000
C	8.726768000	-2.457738000	0.489913000
H	9.057771000	-1.870041000	1.354667000
H	8.408499000	-3.440111000	0.859489000
H	9.596155000	-2.612674000	-0.158194000
H	1.880155000	1.120114000	1.687874000

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**Q,  $E_{(\text{SCF Done})} = -1089.505919$  a.u.**

Sc	0.102928000	0.356962000	0.065368000
C	1.387152000	2.086752000	-1.052095000
C	0.089646000	2.089700000	-1.649581000
C	-0.856354000	2.487709000	-0.656682000

C	-0.138687000	2.726845000	0.556193000
C	1.246356000	2.489866000	0.309724000
C	-0.201744000	1.841352000	-3.103430000
H	0.023954000	2.735888000	-3.698770000
H	-1.256824000	1.607938000	-3.280050000
H	0.402385000	1.028320000	-3.524029000
H	-1.247269000	-0.552747000	2.227184000
C	-0.717943000	3.238217000	1.844763000
H	-0.198037000	2.834309000	2.720184000
H	-1.781368000	2.999333000	1.946311000
H	-0.632564000	4.331567000	1.899615000
C	2.370964000	2.744176000	1.269758000
H	2.743128000	3.771653000	1.159482000
H	3.217338000	2.072318000	1.098363000
H	2.057573000	2.621605000	2.310574000
C	2.686951000	1.843049000	-1.763943000
H	3.427527000	1.361939000	-1.117236000
H	2.559220000	1.214303000	-2.651023000
H	3.123315000	2.791248000	-2.105037000
C	2.639573000	-1.949579000	-0.125837000
C	3.435048000	-2.441251000	0.904748000
C	3.218446000	-2.011276000	2.218591000
C	2.211009000	-1.091756000	2.493729000
C	1.430435000	-0.607849000	1.438467000
N	1.672171000	-1.057098000	0.180416000
H	3.846160000	-2.396909000	3.018585000
H	4.222395000	-3.155102000	0.680625000
H	2.038352000	-0.748222000	3.509845000
C	2.779384000	-2.396310000	-1.554778000
H	3.806833000	-2.736208000	-1.726265000
H	2.614426000	-1.534536000	-2.212833000
C	1.800784000	-3.521694000	-1.918067000
H	1.924029000	-3.812000000	-2.966436000
H	1.971333000	-4.409011000	-1.299273000
H	0.761169000	-3.206240000	-1.772129000
C	-2.575893000	-1.361089000	0.744576000
C	-3.638017000	-2.221374000	0.449267000
C	-3.944671000	-2.520151000	-0.871604000
C	-3.180377000	-1.949388000	-1.890332000
C	-2.141402000	-1.108707000	-1.530741000
N	-1.837040000	-0.817454000	-0.247907000
H	-4.766821000	-3.189965000	-1.107022000
H	-4.213318000	-2.652614000	1.262958000
H	-3.382597000	-2.151617000	-2.936748000

C	-2.252005000	-0.996849000	2.169505000
H	-2.197296000	-1.916927000	2.764770000
C	-3.286673000	-0.048743000	2.791232000
H	-4.281518000	-0.505313000	2.814277000
H	-3.005691000	0.193394000	3.820686000
H	-3.361528000	0.887414000	2.228239000
H	-1.521066000	-0.640503000	-2.292233000
C	-2.321175000	2.735313000	-0.880657000
H	-2.906925000	2.609396000	0.035546000
H	-2.490974000	3.762940000	-1.227978000
H	-2.747569000	2.068221000	-1.637314000

18

**2c,  $E_{(\text{SCF Done})} = -235.712232$  a.u.**

C	3.264327000	0.037283000	-0.000014000
H	3.496913000	1.101306000	-0.000021000
H	4.111531000	-0.643762000	-0.000026000
C	2.008470000	-0.409888000	0.000007000
H	1.839729000	-1.488625000	0.000013000
C	0.770241000	0.456006000	0.000013000
H	0.785558000	1.120401000	-0.876403000
H	0.785553000	1.120403000	0.876428000
C	-0.532044000	-0.347275000	0.000009000
H	-0.549540000	-1.008986000	0.878778000
H	-0.549529000	-1.008994000	-0.878754000
C	-1.785204000	0.527572000	-0.000002000
H	-1.764548000	1.189182000	-0.877980000
H	-1.764561000	1.189187000	0.877972000
C	-3.081739000	-0.279510000	-0.000010000
H	-3.961169000	0.374577000	-0.000017000
H	-3.147115000	-0.924907000	-0.884680000
H	-3.147127000	-0.924904000	0.884662000

17

**1d,  $E_{(\text{SCF Done})} = -326.750564$  a.u.**

H	1.988545000	-1.342799000	-0.871185000
C	0.377024000	-0.279490000	0.000033000
C	-0.041680000	1.054856000	0.000051000
C	-1.406071000	1.339487000	0.000019000
C	-2.313354000	0.286064000	-0.000030000
C	-1.801078000	-1.011421000	-0.000046000
N	-0.499789000	-1.297823000	-0.000018000
H	-1.750906000	2.370815000	0.000030000
H	0.684824000	1.861241000	0.000087000
H	-3.386051000	0.457086000	-0.000059000
C	1.832616000	-0.692699000	0.000071000

H	1.988568000	-1.342593000	0.871478000
C	2.860117000	0.433804000	-0.000069000
H	2.764291000	1.071828000	0.886489000
H	3.874830000	0.021830000	-0.000064000
H	2.764224000	1.071663000	-0.886738000
H	-2.475250000	-1.867922000	-0.000083000

60

**R,  $E_{(\text{SCF Done})} = -998.438446$  a.u.**

Sc	0.617672000	-0.418040000	-0.308726000
C	2.662268000	-0.464235000	0.971597000
C	1.707391000	-1.248346000	1.682105000
C	1.395226000	-2.396516000	0.885054000
C	2.150101000	-2.310019000	-0.322051000
C	2.925786000	-1.109778000	-0.276073000
C	1.189885000	-0.985415000	3.068553000
H	1.799887000	-1.512409000	3.814072000
H	0.159353000	-1.333460000	3.204139000
H	1.220736000	0.077704000	3.326496000
C	0.528269000	-3.543508000	1.321657000
H	1.082841000	-4.205424000	1.999665000
H	0.200556000	-4.160558000	0.479320000
H	-0.364380000	-3.215496000	1.867324000
C	2.211473000	-3.339114000	-1.414961000
H	2.341634000	-2.887473000	-2.404652000
H	1.317001000	-3.969125000	-1.447972000
H	3.066691000	-4.009977000	-1.260742000
C	3.952674000	-0.688946000	-1.287276000
H	4.921243000	-1.157817000	-1.068424000
H	4.105766000	0.393769000	-1.286252000
H	3.675226000	-0.982481000	-2.304613000
C	3.340469000	0.778716000	1.468265000
H	4.307090000	0.529079000	1.925058000
H	3.538949000	1.489657000	0.660145000
H	2.749134000	1.295561000	2.229975000
C	-0.019188000	2.922503000	0.146866000
C	0.302919000	3.973618000	-0.703715000
C	0.949043000	3.716269000	-1.920757000
C	1.273977000	2.413613000	-2.280855000
C	0.939396000	1.374074000	-1.406260000
N	0.305751000	1.666378000	-0.241936000
H	1.196738000	4.546840000	-2.577611000
H	0.056355000	4.992008000	-0.424185000
H	1.778842000	2.204540000	-3.219474000
C	-0.709791000	3.076050000	1.478312000

H	-0.079542000	2.593566000	2.238433000
H	-1.636531000	2.484704000	1.447725000
C	-2.023710000	-0.846479000	-1.253521000
C	-1.170047000	-1.829107000	-1.611668000
H	-2.046091000	0.064487000	-1.857492000
H	-0.563669000	-1.746539000	-2.516087000
H	-1.156851000	-2.787130000	-1.093594000
C	-1.029187000	4.505084000	1.905062000
H	-1.519264000	4.501831000	2.883088000
H	-0.122638000	5.113532000	1.993599000
H	-1.706980000	4.998301000	1.199849000
C	-3.011349000	-0.916669000	-0.132023000
C	-4.459988000	-0.894435000	-0.663462000
H	-2.879549000	-0.050827000	0.534811000
H	-2.849625000	-1.823181000	0.465195000
C	-5.494687000	-0.928919000	0.463126000
H	-4.609811000	0.006392000	-1.274554000
H	-4.607250000	-1.753206000	-1.331358000
C	-6.929385000	-0.916443000	-0.059498000
H	-5.333645000	-1.826239000	1.076522000
H	-5.335904000	-0.067980000	1.127795000
H	-7.647053000	-0.942028000	0.766868000
H	-7.131882000	-0.014084000	-0.648220000
H	-7.128024000	-1.784345000	-0.698921000

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**TS8,  $E_{(\text{SCF Done})} = -998.419052$  a.u.,  $IF = i262.3178$  cm<sup>-1</sup>**

Sc	0.575010000	-0.487546000	-0.184754000
C	2.975980000	-0.192392000	-0.075857000
C	2.566358000	-0.661102000	1.205661000
C	2.052745000	-1.989849000	1.046662000
C	2.154029000	-2.343682000	-0.328696000
C	2.694552000	-1.221341000	-1.029958000
C	2.754897000	0.035388000	2.523897000
H	3.647971000	-0.347586000	3.034801000
H	1.911505000	-0.120664000	3.206383000
H	2.891540000	1.113836000	2.406582000
C	1.600592000	-2.886739000	2.163300000
H	2.457059000	-3.409721000	2.609112000
H	0.901356000	-3.654465000	1.818005000
H	1.115594000	-2.331173000	2.973837000
C	1.864499000	-3.691465000	-0.920420000
H	1.549108000	-3.627939000	-1.967221000
H	1.087741000	-4.228818000	-0.367982000
H	2.766374000	-4.317256000	-0.898796000

C	3.037045000	-1.177204000	-2.494256000
H	4.046625000	-1.572772000	-2.667214000
H	3.024505000	-0.157039000	-2.892772000
H	2.353639000	-1.781325000	-3.101029000
C	3.677443000	1.100228000	-0.381209000
H	4.756567000	0.931349000	-0.491647000
H	3.332635000	1.558299000	-1.315244000
H	3.551500000	1.836463000	0.417481000
C	-0.107818000	2.867055000	0.135036000
C	-0.741385000	3.703619000	-0.780379000
C	-1.428737000	3.157867000	-1.869447000
C	-1.529119000	1.778172000	-2.008298000
C	-0.880666000	0.977775000	-1.066572000
N	-0.176138000	1.527480000	-0.061562000
H	-1.892602000	3.817827000	-2.598161000
H	-0.692380000	4.779052000	-0.652086000
H	-2.095502000	1.337373000	-2.824193000
C	0.648575000	3.347625000	1.344452000
H	1.660327000	2.924770000	1.293001000
H	0.184718000	2.888370000	2.228561000
C	-1.887682000	-0.846029000	-0.878115000
C	-1.093797000	-1.953718000	-0.479490000
H	-2.132511000	-0.783875000	-1.938441000
H	-0.784969000	-2.674234000	-1.236293000
H	-1.285632000	-2.385513000	0.506470000
C	0.725988000	4.859717000	1.527908000
H	1.295096000	5.094218000	2.432067000
H	1.230403000	5.347495000	0.686599000
H	-0.267144000	5.307465000	1.642367000
C	-2.981893000	-0.353922000	0.053771000
C	-4.196784000	-1.296212000	0.005329000
H	-3.304524000	0.658666000	-0.211256000
H	-2.599079000	-0.306402000	1.083850000
C	-5.339279000	-0.820232000	0.905836000
H	-4.555477000	-1.372084000	-1.031130000
H	-3.888518000	-2.307809000	0.299432000
C	-6.548808000	-1.751468000	0.862050000
H	-4.975519000	-0.737160000	1.939800000
H	-5.642656000	0.192188000	0.604780000
H	-7.348740000	-1.387689000	1.515252000
H	-6.956779000	-1.826944000	-0.152759000
H	-6.284894000	-2.763342000	1.191382000

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**Q',  $E_{(\text{SCF Done})} = -1416.297765$  a.u.**



Sc	-0.114255000	0.336446000	-0.301561000
C	0.295795000	2.201392000	-1.884028000
C	0.463976000	0.998949000	-2.628039000
C	-0.803342000	0.343343000	-2.698833000
C	-1.750632000	1.149723000	-1.997096000
C	-1.069716000	2.296441000	-1.493444000
C	1.714759000	0.624263000	-3.372792000
H	1.889014000	1.326501000	-4.198702000
H	1.647888000	-0.372572000	-3.817715000
H	2.611970000	0.651051000	-2.743200000
H	1.287962000	-1.756671000	-2.070607000
C	-3.235655000	0.933552000	-1.978343000
H	-3.706845000	1.366123000	-1.089971000
H	-3.503734000	-0.127236000	-2.012106000
H	-3.703504000	1.410421000	-2.850290000
C	-1.701226000	3.487263000	-0.833315000
H	-1.926698000	4.264964000	-1.575701000
H	-1.045364000	3.935035000	-0.080409000
H	-2.646951000	3.235365000	-0.342880000
C	1.337374000	3.260890000	-1.684504000
H	1.218794000	3.779836000	-0.727925000
H	2.350992000	2.849860000	-1.717756000
H	1.270143000	4.020634000	-2.475279000
C	2.657354000	1.716831000	1.278903000
C	2.683634000	2.611988000	2.348112000
C	1.485168000	3.030078000	2.930677000
C	0.272256000	2.549793000	2.441416000
C	0.280580000	1.653816000	1.366908000
N	1.463795000	1.275907000	0.835984000
H	1.507099000	3.733432000	3.760201000
H	3.636227000	2.983455000	2.715650000
H	-0.665183000	2.874491000	2.886020000
C	3.914194000	1.207546000	0.625857000
H	4.601889000	2.047225000	0.465319000
H	3.656209000	0.810629000	-0.362282000
C	4.621752000	0.126827000	1.454239000
H	5.533577000	-0.208248000	0.948771000
H	4.906771000	0.506668000	2.441235000
H	3.974363000	-0.744020000	1.603939000
C	1.613947000	-2.716658000	-0.204930000
C	2.114062000	-3.805230000	0.520232000
C	1.939539000	-3.866353000	1.895250000
C	1.263315000	-2.825211000	2.530482000
C	0.789566000	-1.783658000	1.750022000

N	0.948324000	-1.718312000	0.411887000
H	2.322798000	-4.709225000	2.463573000
H	2.635091000	-4.599089000	-0.006290000
H	1.103346000	-2.818534000	3.603581000
C	1.810854000	-2.641861000	-1.694837000
H	1.333810000	-3.514860000	-2.161571000
C	3.284674000	-2.591684000	-2.115889000
H	3.826422000	-3.488743000	-1.798932000
H	3.365443000	-2.525360000	-3.205244000
H	3.791480000	-1.723095000	-1.683386000
H	0.258045000	-0.953276000	2.209523000
C	-1.148071000	-0.841395000	-3.557405000
H	-1.984527000	-1.420096000	-3.151281000
H	-1.453371000	-0.511968000	-4.559905000
H	-0.305230000	-1.526475000	-3.695637000
H	-2.564960000	1.522699000	1.254606000
C	-3.036275000	-0.543511000	1.239013000
C	-4.133151000	-1.391714000	1.420613000
C	-4.206861000	-2.601751000	0.741384000
C	-3.170253000	-2.951106000	-0.119258000
C	-2.112074000	-2.064783000	-0.249988000
N	-2.029521000	-0.890093000	0.401219000
H	-5.060333000	-3.259386000	0.880815000
H	-4.929935000	-1.096681000	2.093407000
H	-3.176320000	-3.881664000	-0.677165000
C	-2.914994000	0.769548000	1.969857000
H	-2.095841000	0.674653000	2.696054000
C	-4.173094000	1.262775000	2.679418000
H	-4.474762000	0.599376000	3.497273000
H	-3.987220000	2.248240000	3.117330000
H	-5.018419000	1.362939000	1.989389000
H	-1.283708000	-2.304885000	-0.911385000

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**R',  $E_{(\text{SCF Done})} = -1325.233588$  a.u.**

Sc	-0.640230000	-0.062720000	-0.436431000
C	-2.897503000	-0.987965000	-0.682796000
C	-3.019506000	0.420513000	-0.881638000
C	-2.334617000	0.754409000	-2.089456000
C	-1.778356000	-0.449606000	-2.620455000
C	-2.139512000	-1.525172000	-1.762469000
C	-3.885591000	1.321887000	-0.046536000
H	-4.946685000	1.096253000	-0.215747000
H	-3.743566000	2.377976000	-0.290142000
H	-3.706472000	1.203369000	1.029023000

H	-1.415735000	2.740542000	-0.429154000
C	-1.103969000	-0.596890000	-3.954435000
H	-0.253949000	-1.288027000	-3.922494000
H	-0.746505000	0.359758000	-4.348704000
H	-1.807188000	-0.997723000	-4.696705000
C	-1.916325000	-2.980788000	-2.044340000
H	-2.755902000	-3.390277000	-2.622699000
H	-1.836082000	-3.572064000	-1.127332000
H	-1.006345000	-3.150389000	-2.627630000
C	-3.617499000	-1.782270000	0.366385000
H	-3.077627000	-2.695735000	0.633052000
H	-3.777682000	-1.206507000	1.283356000
H	-4.608180000	-2.087555000	0.002776000
C	-0.487525000	-2.419589000	2.103522000
C	0.218675000	-3.621680000	2.117995000
C	1.029393000	-3.965722000	1.032471000
C	1.128612000	-3.109361000	-0.061275000
C	0.397244000	-1.917271000	-0.051172000
N	-0.367099000	-1.621690000	1.020209000
H	1.575602000	-4.906211000	1.048163000
H	0.133367000	-4.286885000	2.972361000
H	1.754664000	-3.371325000	-0.910317000
C	-1.361422000	-1.973966000	3.247746000
H	-2.173267000	-2.701925000	3.378405000
H	-1.833367000	-1.025518000	2.969761000
C	2.015181000	0.132590000	-1.771755000
C	1.225923000	1.212935000	-1.943266000
H	0.502395000	1.259812000	-2.752110000
H	1.401406000	2.127288000	-1.379277000
C	-0.612341000	-1.816965000	4.576410000
H	-1.302408000	-1.500164000	5.364878000
H	-0.152974000	-2.757704000	4.897079000
H	0.180869000	-1.065014000	4.501576000
C	3.197906000	0.062375000	-0.857572000
C	4.514261000	0.021298000	-1.657925000
H	3.133886000	-0.842456000	-0.239201000
H	3.205242000	0.926168000	-0.180535000
C	5.746088000	-0.084549000	-0.756774000
H	4.493523000	-0.832065000	-2.350454000
H	4.586727000	0.923007000	-2.280652000
C	7.052872000	-0.124631000	-1.545685000
H	5.761222000	0.767474000	-0.062445000
H	5.662851000	-0.986741000	-0.134272000
H	7.916006000	-0.199537000	-0.875888000

H	7.082432000	-0.985964000	-2.223446000
H	7.179875000	0.780119000	-2.151748000
C	-0.011091000	2.926989000	1.150436000
C	0.663602000	3.733235000	2.073223000
C	1.519713000	3.164855000	3.005989000
C	1.687700000	1.782309000	2.999146000
C	0.988533000	1.041499000	2.059617000
N	0.151179000	1.582534000	1.147081000
H	2.047770000	3.787829000	3.722443000
H	0.515933000	4.807894000	2.047227000
H	2.345383000	1.283067000	3.703081000
C	-0.911792000	3.545430000	0.115394000
H	-0.289770000	4.073803000	-0.621584000
C	-1.952210000	4.518863000	0.679471000
H	-1.485924000	5.391985000	1.146528000
H	-2.594275000	4.890182000	-0.125591000
H	-2.587724000	4.034913000	1.427930000
H	1.855541000	-0.734734000	-2.413201000
H	1.092454000	-0.036751000	2.025390000
C	-2.380681000	2.069780000	-2.817280000
H	-1.397418000	2.422280000	-3.152236000
H	-3.004478000	1.980684000	-3.716044000
H	-2.821945000	2.862824000	-2.207274000

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**TS8',  $E_{(\text{SCF Done})} = -1325.223391$  a.u., IF =  $i239.0532$  cm<sup>-1</sup>**

Sc	-0.401778000	-0.236985000	-0.428820000
C	-2.440743000	-1.623311000	-0.417219000
C	-2.761750000	-0.441964000	-1.152485000
C	-1.971584000	-0.432266000	-2.338340000
C	-1.155467000	-1.603811000	-2.329687000
C	-1.466825000	-2.351097000	-1.155239000
C	-3.900218000	0.481004000	-0.825303000
H	-4.859363000	-0.032247000	-0.975867000
H	-3.910276000	1.363138000	-1.471284000
H	-3.885638000	0.824321000	0.215775000
H	-1.766278000	2.336592000	-1.112778000
C	-0.246191000	-2.050213000	-3.438178000
H	0.536593000	-2.723758000	-3.075421000
H	0.244985000	-1.207879000	-3.938097000
H	-0.807104000	-2.594259000	-4.210008000
C	-0.954344000	-3.723536000	-0.835009000
H	-1.519335000	-4.481596000	-1.393596000
H	-1.060418000	-3.965133000	0.226636000
H	0.099994000	-3.848245000	-1.102385000

C	-3.142941000	-2.068632000	0.833440000
H	-2.573864000	-2.827363000	1.379201000
H	-3.339594000	-1.236144000	1.519337000
H	-4.117732000	-2.515067000	0.593802000
C	1.153447000	-2.502017000	1.715918000
C	2.193381000	-3.388459000	1.447569000
C	2.917338000	-3.273783000	0.259787000
C	2.610608000	-2.252675000	-0.631482000
C	1.568916000	-1.378391000	-0.314072000
N	0.872464000	-1.520819000	0.823750000
H	3.710643000	-3.982804000	0.036101000
H	2.421172000	-4.176095000	2.159849000
H	3.173449000	-2.136096000	-1.554005000
C	0.357717000	-2.596237000	2.989386000
H	0.198127000	-3.654147000	3.229530000
H	-0.635680000	-2.162930000	2.828778000
C	1.953165000	0.429247000	-1.371047000
C	0.839051000	1.233609000	-1.678600000
H	0.434516000	1.219773000	-2.687246000
H	0.758576000	2.184581000	-1.153280000
C	1.056850000	-1.915310000	4.175429000
H	0.445058000	-1.999725000	5.079475000
H	2.025198000	-2.382934000	4.381528000
H	1.240527000	-0.852504000	3.981059000
C	3.001709000	0.964589000	-0.412021000
C	3.895758000	2.003646000	-1.109592000
H	3.632208000	0.159845000	-0.019294000
H	2.506937000	1.431509000	0.451816000
C	4.993650000	2.542825000	-0.190011000
H	4.355443000	1.547946000	-1.998455000
H	3.277051000	2.833261000	-1.475804000
C	5.885277000	3.574728000	-0.877297000
H	4.532103000	2.990408000	0.701865000
H	5.609111000	1.706939000	0.170990000
H	6.659830000	3.943416000	-0.196551000
H	6.388373000	3.145894000	-1.752011000
H	5.303704000	4.439196000	-1.219102000
C	-1.576516000	2.646921000	0.978544000
C	-1.944767000	3.421656000	2.082736000
C	-1.793711000	2.928538000	3.372600000
C	-1.266546000	1.651769000	3.542510000
C	-0.919426000	0.937085000	2.406960000
N	-1.067038000	1.401211000	1.149298000
H	-2.081021000	3.531677000	4.229262000

H	-2.351517000	4.413951000	1.923970000
H	-1.125003000	1.215982000	4.525837000
C	-1.701503000	3.185386000	-0.424156000
H	-0.764375000	3.702995000	-0.675940000
C	-2.868910000	4.144575000	-0.663667000
H	-2.743089000	5.091934000	-0.129840000
H	-2.933190000	4.387760000	-1.728762000
H	-3.824073000	3.705173000	-0.358273000
H	2.340589000	-0.197155000	-2.173431000
H	-0.497129000	-0.057749000	2.493611000
C	-2.116434000	0.518375000	-3.491277000
H	-1.217672000	0.549446000	-4.115226000
H	-2.942083000	0.204316000	-4.143870000
H	-2.334347000	1.544213000	-3.175196000

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**D'', E<sub>(SCF Done)</sub> = -2976.513701 a.u.**

S	-1.885818000	-2.209801000	-0.386077000
S	1.753815000	-2.560120000	-0.087306000
S	1.371519000	1.678527000	-0.786044000
S	-2.029747000	1.404921000	-0.667703000
Sc	0.037007000	-0.240552000	0.422400000
C	1.614530000	1.934636000	2.767424000
H	1.319524000	2.834257000	2.218902000
H	2.621995000	1.659945000	2.440354000
H	1.687918000	2.208832000	3.829205000
C	-1.550490000	2.213048000	2.651504000
H	-1.832834000	2.356840000	3.703754000
H	-2.481971000	2.217769000	2.074745000
H	-0.960638000	3.088583000	2.364796000
C	-2.798231000	-0.679840000	2.713715000
H	-3.430907000	0.022503000	2.160431000
H	-3.094697000	-0.606763000	3.769874000
C	-0.474377000	-2.762827000	3.016253000
H	-1.224859000	-2.874201000	3.808184000
H	0.445028000	-3.216633000	3.396519000
H	-0.821532000	-3.355738000	2.162007000
C	2.325905000	-1.104985000	3.006411000
H	2.633666000	-0.799383000	4.015264000
H	2.366256000	-2.196484000	2.976444000
H	3.089653000	-0.737706000	2.311921000
C	-0.276243000	-1.307319000	2.697352000
C	7.393913000	4.333190000	0.367665000
H	7.785321000	5.328929000	0.601663000
H	7.705775000	3.656264000	1.172238000

H	7.877336000	3.995341000	-0.556873000
C	5.874215000	4.357495000	0.221266000
H	5.420941000	4.733591000	1.149274000
H	5.591673000	5.069260000	-0.566887000
C	5.284925000	2.983952000	-0.106756000
H	5.567886000	2.269921000	0.680887000
H	5.735397000	2.608409000	-1.037172000
C	3.760285000	3.006934000	-0.252444000
H	3.474157000	3.718248000	-1.038371000
H	3.309155000	3.371700000	0.679217000
C	3.201976000	1.629539000	-0.596848000
H	3.470971000	0.888430000	0.163779000
H	3.597088000	1.287217000	-1.559614000
C	-0.775880000	0.937195000	2.502777000
C	0.965262000	0.093499000	-1.592060000
C	-3.706440000	7.868899000	-1.285449000
H	-4.618278000	8.441333000	-1.486109000
H	-3.309490000	8.204427000	-0.319816000
H	-2.972312000	8.132540000	-2.056266000
C	-3.987565000	6.368083000	-1.277834000
H	-4.751131000	6.140212000	-0.520993000
H	-4.416848000	6.069324000	-2.244522000
C	-2.737755000	5.529550000	-1.001030000
H	-2.307322000	5.827237000	-0.033635000
H	-1.973347000	5.755342000	-1.758843000
C	-3.018892000	4.023470000	-0.991329000
H	-3.449508000	3.731282000	-1.958203000
H	-3.773471000	3.789992000	-0.228945000
C	-1.752878000	3.218631000	-0.715026000
H	-1.333951000	3.473814000	0.260878000
H	-0.973426000	3.412608000	-1.460113000
C	-1.338687000	-0.370666000	2.558223000
C	-2.226816000	1.084273000	-2.444477000
H	-1.425078000	1.564766000	-3.012122000
H	-2.173338000	0.005950000	-2.598325000
H	-3.196352000	1.451209000	-2.789320000
C	-1.549944000	-2.964987000	-2.001789000
C	0.952098000	-0.576643000	2.698797000
C	-3.665164000	-1.797216000	-0.587434000
H	-3.866026000	-0.986886000	0.117936000
H	-3.806948000	-1.391317000	-1.595630000
C	2.142512000	-3.054636000	-1.817352000
C	3.605734000	-2.870658000	-2.218940000
H	3.878711000	-1.811716000	-2.114820000

H	3.668297000	-3.098161000	-3.293468000
C	4.613043000	-3.733522000	-1.460750000
H	4.329513000	-4.793184000	-1.551101000
H	4.575841000	-3.486219000	-0.390057000
C	6.047437000	-3.553610000	-1.962937000
H	6.089251000	-3.797983000	-3.033507000
H	6.328275000	-2.493978000	-1.880900000
C	7.057426000	-4.410241000	-1.203057000
H	6.823876000	-5.477669000	-1.296219000
H	7.065258000	-4.163508000	-0.134352000
H	0.428847000	0.287828000	-2.525292000
H	1.915195000	-0.386814000	-1.847030000
H	-3.042774000	-1.695637000	2.386815000
H	-0.559749000	-3.417696000	-1.950761000
H	-1.568520000	-2.228545000	-2.809537000
H	1.836686000	-4.102623000	-1.921041000
H	-2.285312000	-3.749880000	-2.195930000
C	-4.590502000	-2.984184000	-0.335212000
H	-4.331471000	-3.814600000	-1.005785000
H	-4.435222000	-3.352295000	0.687067000
C	-6.062220000	-2.610510000	-0.536931000
H	-6.322149000	-1.775056000	0.129547000
H	-6.210288000	-2.241502000	-1.562588000
C	-7.015485000	-3.779406000	-0.278171000
H	-6.753346000	-4.614135000	-0.943349000
H	-6.866613000	-4.147243000	0.746612000
C	-8.482232000	-3.406008000	-0.479867000
H	-8.669740000	-3.068071000	-1.506160000
H	-9.138237000	-4.261530000	-0.287431000
H	-8.783928000	-2.597474000	0.196770000
C	0.639096000	0.810502000	2.583281000
H	8.072401000	-4.259176000	-1.585472000
C	1.776088000	-4.188989000	0.724005000
H	0.936063000	-4.804797000	0.390837000
H	2.720214000	-4.693330000	0.508317000
H	1.697531000	-4.035675000	1.799725000
H	1.494571000	-2.455028000	-2.461602000

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**TS2'',  $E_{(\text{SCF Done})} = -2655.655314$  a.u., IF =  $i226.6671$  cm<sup>-1</sup>**

C	0.988075000	-0.098880000	2.894528000
C	0.492618000	1.213764000	2.646454000
C	-0.916612000	1.125445000	2.466922000
C	-1.292941000	-0.242658000	2.605915000
C	-0.119600000	-1.001981000	2.878942000



C	1. 271782000	2. 488248000	2. 781986000
H	0. 908294000	3. 270329000	2. 107902000
H	2. 339592000	2. 345679000	2. 589504000
H	1. 186710000	2. 879088000	3. 805329000
C	-1. 865980000	2. 286006000	2. 433249000
H	-2. 193341000	2. 533151000	3. 452855000
H	-2. 772752000	2. 073193000	1. 857209000
H	-1. 401310000	3. 189752000	2. 026565000
C	-2. 704230000	-0. 747955000	2. 669603000
H	-3. 362587000	-0. 223193000	1. 969026000
H	-3. 118746000	-0. 593155000	3. 675532000
C	-0. 102949000	-2. 449176000	3. 272755000
H	-0. 379858000	-2. 559282000	4. 329736000
H	0. 885760000	-2. 902145000	3. 155439000
H	-0. 811929000	-3. 044286000	2. 687555000
C	2. 400800000	-0. 428759000	3. 286069000
H	2. 579873000	-0. 164477000	4. 336865000
H	2. 620379000	-1. 495843000	3. 188367000
H	3. 144810000	0. 117491000	2. 693782000
Sc	0. 167344000	-0. 114521000	0. 577820000
C	6. 564976000	5. 632539000	0. 393223000
H	6. 783367000	6. 702523000	0. 474574000
H	6. 874710000	5. 158083000	1. 332158000
H	7. 193088000	5. 225539000	-0. 408200000
C	5. 083428000	5. 392493000	0. 112556000
H	4. 479290000	5. 841972000	0. 913122000
H	4. 795800000	5. 908359000	-0. 814085000
C	4. 734048000	3. 907589000	-0. 009205000
H	5. 021319000	3. 389712000	0. 917802000
H	5. 336074000	3. 457188000	-0. 811828000
C	3. 247820000	3. 666587000	-0. 290788000
H	2. 956995000	4. 181457000	-1. 215793000
H	2. 646627000	4. 106114000	0. 515574000
C	2. 932332000	2. 179632000	-0. 423901000
H	3. 207881000	1. 632777000	0. 483262000
H	3. 483313000	1. 742864000	-1. 263708000
S	1. 143597000	1. 927664000	-0. 779986000
C	1. 160722000	0. 275245000	-1. 531485000
C	-4. 987832000	6. 899863000	-2. 002536000
H	-5. 993740000	7. 284780000	-2. 200737000
H	-4. 607210000	7. 409918000	-1. 109473000
H	-4. 349862000	7. 187304000	-2. 846908000
C	-5. 004771000	5. 385119000	-1. 810887000
H	-5. 678473000	5. 126198000	-0. 982153000

H	-5.423914000	4.905591000	-2.706626000
C	-3.616559000	4.804709000	-1.531736000
H	-3.196209000	5.283439000	-0.635118000
H	-2.941663000	5.061809000	-2.361266000
C	-3.632282000	3.285170000	-1.337420000
H	-4.052523000	2.811196000	-2.234309000
H	-4.297405000	3.022812000	-0.504430000
C	-2.235162000	2.738787000	-1.059322000
H	-1.822504000	3.173658000	-0.145835000
H	-1.539061000	2.975248000	-1.872138000
S	-2.195553000	0.920738000	-0.796755000
C	-2.363052000	0.371298000	-2.521367000
H	-1.631374000	0.870514000	-3.164968000
H	-2.196928000	-0.707594000	-2.545963000
H	-3.370296000	0.585929000	-2.885723000
C	-1.608065000	-3.729153000	-1.610782000
S	-2.085593000	-2.569934000	-0.295097000
C	-3.886253000	-2.421698000	-0.598731000
H	-4.188195000	-1.514856000	-0.063932000
H	-4.041970000	-2.232749000	-1.668177000
C	1.795231000	-1.693880000	-0.834107000
C	1.246220000	-2.137417000	0.381497000
C	3.297941000	-1.531548000	-0.930977000
H	3.675904000	-1.033365000	-0.027807000
H	3.587119000	-0.908917000	-1.785736000
C	3.984469000	-2.900588000	-1.074704000
H	3.574806000	-3.419999000	-1.953277000
H	3.738910000	-3.524888000	-0.205902000
C	5.503646000	-2.784388000	-1.215893000
H	5.743409000	-2.159531000	-2.089007000
H	5.911090000	-2.256310000	-0.340818000
C	6.198826000	-4.139499000	-1.357614000
H	5.791439000	-4.667906000	-2.232278000
H	5.958170000	-4.765146000	-0.485365000
C	7.718344000	-4.030145000	-1.496706000
H	8.124764000	-3.501484000	-0.622689000
H	7.958039000	-3.405103000	-2.368708000
C	8.405045000	-5.386843000	-1.637122000
H	8.213279000	-6.021785000	-0.763642000
H	8.045505000	-5.924644000	-2.522772000
H	9.490417000	-5.275531000	-1.734529000
H	0.421191000	-2.846762000	0.386864000
H	1.928017000	-2.240958000	1.222466000
H	0.234350000	0.164061000	-2.104141000

H	1.992101000	0.213974000	-2.230659000
H	-2.764866000	-1.819390000	2.459704000
H	-0.539033000	-3.932972000	-1.501898000
H	-1.795940000	-3.311889000	-2.605341000
H	1.316118000	-2.026288000	-1.756898000
H	-2.146504000	-4.673845000	-1.502515000
C	-4.701628000	-3.622997000	-0.127717000
H	-4.356222000	-4.534170000	-0.633811000
H	-4.527387000	-3.777981000	0.944721000
C	-6.198884000	-3.436056000	-0.391124000
H	-6.547152000	-2.521450000	0.111252000
H	-6.365921000	-3.276852000	-1.466753000
C	-7.041375000	-4.623434000	0.080098000
H	-6.692080000	-5.536633000	-0.421885000
H	-6.872847000	-4.782497000	1.154348000
C	-8.533942000	-4.435325000	-0.181388000
H	-8.737994000	-4.309404000	-1.251554000
H	-9.109016000	-5.300127000	0.166259000
H	-8.920378000	-3.549512000	0.337033000

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**TS3',  $E_{(\text{SCF Done})} = -2655.660931$  a.u., IF =  $i1185.0239$  cm<sup>-1</sup>**

C	-1.404868000	1.140604000	2.743995000
C	-2.268409000	0.016181000	2.590281000
C	-1.554971000	-1.144055000	3.016289000
C	-0.263080000	-0.737636000	3.450353000
C	-0.161607000	0.671137000	3.266423000
C	-3.737076000	0.039785000	2.271485000
H	-4.000171000	-0.553510000	1.389149000
H	-4.098556000	1.058444000	2.108416000
H	-4.312341000	-0.363458000	3.114612000
C	-2.152255000	-2.502178000	3.238877000
H	-2.529344000	-2.586101000	4.267599000
H	-1.425665000	-3.311165000	3.107125000
H	-3.001570000	-2.696255000	2.577494000
C	0.712960000	-1.607409000	4.184275000
H	1.727570000	-1.199880000	4.172315000
H	0.757353000	-2.624010000	3.780047000
H	0.414750000	-1.693777000	5.237970000
C	0.979066000	1.532034000	3.725842000
H	0.942396000	1.669928000	4.814877000
H	0.942046000	2.529192000	3.277823000
H	1.958264000	1.095657000	3.496898000
C	-1.771048000	2.587595000	2.572895000
H	-2.660350000	2.722196000	1.951411000

H	-1.989570000	3.043607000	3.547734000
H	-0.966406000	3.174925000	2.118450000
Sc	-0.385558000	-0.273562000	1.000543000
C	1.872744000	3.027330000	0.285538000
H	2.276249000	3.009561000	1.303712000
S	1.537174000	1.299630000	-0.220414000
C	3.135428000	0.445542000	-0.015893000
C	9.725416000	-3.286190000	-2.629674000
H	9.304852000	-3.509856000	-3.617719000
H	10.567239000	-3.967732000	-2.465480000
H	10.126185000	-2.265725000	-2.663988000
C	8.671505000	-3.430266000	-1.534029000
H	8.316002000	-4.469965000	-1.500855000
H	9.130897000	-3.235371000	-0.554526000
C	7.475899000	-2.495236000	-1.724315000
H	7.015200000	-2.690580000	-2.704323000
H	7.831980000	-1.454578000	-1.758802000
C	6.416517000	-2.632321000	-0.629985000
H	6.876747000	-2.433822000	0.349270000
H	6.062763000	-3.673280000	-0.593435000
C	5.218318000	-1.699789000	-0.823142000
H	4.746940000	-1.911683000	-1.794966000
H	5.583673000	-0.664402000	-0.878385000
C	4.174704000	-1.836867000	0.288376000
H	4.613327000	-1.537779000	1.252286000
H	3.910858000	-2.898512000	0.394187000
C	2.862495000	-1.055921000	0.075022000
C	1.847901000	-1.311588000	1.198958000
H	3.607697000	0.802778000	0.908086000
H	3.771951000	0.706448000	-0.864452000
H	2.447868000	-1.381478000	-0.895418000
C	-3.286613000	-2.735703000	-0.556191000
H	-3.428526000	-2.923303000	0.512140000
S	-1.771178000	-1.717213000	-0.771781000
C	-0.456559000	-2.569184000	0.110351000
H	0.884867000	3.499596000	0.319638000
C	2.798021000	3.775280000	-0.669482000
H	3.770824000	3.268919000	-0.720425000
H	2.374489000	3.748506000	-1.681690000
C	3.005721000	5.227940000	-0.229308000
H	3.416904000	5.247918000	0.790606000
H	2.032090000	5.736998000	-0.178223000
C	3.935236000	6.005832000	-1.163690000
H	4.907346000	5.495648000	-1.213802000

H	3. 525099000	5. 983090000	-2. 182990000
C	4. 139843000	7. 454380000	-0. 726313000
H	4. 581923000	7. 509212000	0. 275719000
H	4. 808484000	7. 983893000	-1. 413180000
H	3. 189372000	8. 000750000	-0. 700835000
H	-4. 105196000	-2. 088832000	-0. 894032000
C	-3. 246572000	-4. 033681000	-1. 354318000
H	-2. 390063000	-4. 637984000	-1. 027128000
H	-3. 083355000	-3. 804075000	-2. 415210000
C	-4. 537655000	-4. 841634000	-1. 187815000
H	-5. 395121000	-4. 232961000	-1. 510165000
H	-4. 699888000	-5. 060312000	-0. 122100000
C	-4. 524335000	-6. 153421000	-1. 976201000
H	-3. 666702000	-6. 760394000	-1. 653918000
H	-4. 360868000	-5. 933872000	-3. 040445000
C	-5. 811656000	-6. 957757000	-1. 811087000
H	-5. 772171000	-7. 889078000	-2. 385845000
H	-5. 984090000	-7. 222593000	-0. 760983000
H	-6. 683225000	-6. 390041000	-2. 158316000
C	-7. 634105000	3. 978388000	-2. 557763000
H	-8. 055000000	4. 816646000	-3. 122934000
H	-7. 992390000	3. 051777000	-3. 022233000
H	-8. 046203000	4. 022511000	-1. 542446000
C	-6. 108396000	4. 036137000	-2. 540102000
H	-5. 727728000	4. 026424000	-3. 571036000
H	-5. 780897000	4. 989468000	-2. 102536000
C	-5. 477280000	2. 881000000	-1. 759534000
H	-5. 803108000	1. 926273000	-2. 198332000
H	-5. 857699000	2. 889869000	-0. 727405000
C	-3. 946446000	2. 939399000	-1. 739962000
H	-3. 614833000	3. 885075000	-1. 292290000
H	-3. 574006000	2. 932959000	-2. 772189000
C	-3. 346938000	1. 774784000	-0. 956071000
H	-3. 637555000	0. 808743000	-1. 387263000
H	-3. 702342000	1. 788497000	0. 077340000
S	-1. 521079000	1. 808138000	-0. 838385000
C	-1. 092664000	1. 392056000	-2. 556834000
H	-1. 437639000	2. 183542000	-3. 225660000
H	-1. 533640000	0. 433630000	-2. 844199000
H	-0. 005060000	1. 325206000	-2. 617581000
H	0. 603050000	-1. 872683000	0. 635155000
H	2. 043199000	-0. 616224000	2. 025047000
H	2. 017024000	-2. 308085000	1. 633551000
H	-0. 862594000	-3. 184552000	0. 917980000

H 0.139012000 -3.191461000 -0.564537000

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**TS2<sup>N</sup>,  $E_{(\text{SCF Done})} = -1790.708887$  a.u., IF =  $i232.3759$  cm<sup>-1</sup>**

C	-1.018393000	0.382508000	2.209063000
C	-0.665029000	-0.983270000	2.420826000
C	0.763051000	-1.067151000	2.429070000
C	1.284285000	0.247243000	2.246778000
C	0.188968000	1.141636000	2.086671000
C	-1.575471000	-2.058210000	2.941911000
H	-1.232166000	-3.065877000	2.686102000
H	-2.599830000	-1.957741000	2.576371000
H	-1.607420000	-2.002837000	4.038254000
C	1.552983000	-2.285051000	2.816940000
H	1.597656000	-2.379338000	3.910440000
H	2.586957000	-2.239823000	2.460971000
H	1.113540000	-3.215552000	2.442292000
C	2.715744000	0.655584000	2.415611000
H	2.955555000	1.566809000	1.859892000
H	3.419379000	-0.126747000	2.116142000
H	2.916797000	0.871429000	3.474245000
C	0.269354000	2.638425000	2.093574000
H	0.442442000	3.000705000	3.115991000
H	-0.662863000	3.092599000	1.748665000
H	1.085222000	3.032961000	1.478020000
C	-2.398101000	0.975133000	2.230136000
H	-2.527860000	1.620379000	3.108604000
H	-2.599196000	1.588917000	1.346972000
H	-3.166110000	0.201088000	2.284431000
Sc	0.060056000	-0.392788000	0.136852000
C	-6.106492000	5.786963000	-0.535950000
H	-7.149292000	5.767609000	-0.201887000
H	-5.567563000	6.501526000	0.097650000
H	-6.093281000	6.176104000	-1.560928000
C	-5.477507000	4.397389000	-0.463525000
H	-5.539029000	4.019581000	0.567149000
H	-6.057804000	3.697926000	-1.081519000
C	-4.017411000	4.380983000	-0.920909000
H	-3.433428000	5.077511000	-0.301797000
H	-3.954665000	4.759939000	-1.950901000
C	-3.384657000	2.986820000	-0.854043000
H	-3.962672000	2.295893000	-1.483322000
H	-3.447895000	2.603973000	0.172111000
C	-1.932493000	3.004788000	-1.318138000
H	-1.293790000	3.619850000	-0.675272000

H	-1. 867837000	3. 407196000	-2. 335339000
S	-1. 204454000	1. 312267000	-1. 434328000
C	0. 563941000	1. 373535000	-1. 186977000
C	9. 561913580	3. 195215170	-1. 466718710
H	9. 958628630	2. 381582400	-0. 847365570
H	10. 161577640	4. 089194380	-1. 264107120
H	9. 720358750	2. 919933130	-2. 516417910
C	8. 083157640	3. 441945940	-1. 176525370
H	7. 960770450	3. 750818760	-0. 128567840
H	7. 724799400	4. 283953770	-1. 785483400
C	7. 207240960	2. 216992090	-1. 446537730
H	7. 562811930	1. 374341320	-0. 834964180
H	7. 331292580	1. 906032870	-2. 494277040
C	5. 723931230	2. 460609710	-1. 163218240
H	5. 367761760	3. 296435360	-1. 782907680
H	5. 599505260	2. 780754810	-0. 117963320
C	4. 853028570	1. 231047300	-1. 424420900
H	5. 191030410	0. 394843830	-0. 797511790
H	4. 977984020	0. 905929640	-2. 466128260
C	3. 359180210	1. 501436800	-1. 150387860
H	3. 027285330	2. 333349660	-1. 782580360
H	3. 241772460	1. 825858550	-0. 113231400
C	2. 504616370	0. 297620830	-1. 420303490
C	2. 486799820	-0. 941561640	-0. 695893640
H	1. 957468830	-1. 762796810	-1. 165008530
H	3. 142900880	-1. 174858360	0. 137931860
N	-1. 233072000	-2. 368309000	-1. 008420000
C	-3. 579103000	-4. 529772000	-2. 310231000
H	-4. 209805000	-4. 025874000	-3. 058165000
H	-4. 094308000	-5. 457531000	-2. 047028000
C	-3. 556007000	-3. 590824000	-1. 110123000
C	-2. 682367000	-2. 535941000	-0. 715296000
C	-3. 221930000	-1. 435008000	-0. 039596000
H	-2. 591920000	-0. 557955000	0. 072863000
C	-4. 496322000	-1. 427944000	0. 511982000
H	-4. 851521000	-0. 569150000	1. 073641000
C	-5. 289997000	-2. 553361000	0. 331974000
H	-6. 284305000	-2. 616735000	0. 764623000
C	-4. 826944000	-3. 567902000	-0. 492851000
H	-5. 514352000	-4. 370807000	-0. 749815000
H	-2. 682522000	-4. 794648000	-2. 852056000
C	-1. 108704000	-2. 192938000	-2. 480851000
H	-1. 886378000	-1. 509253000	-2. 821142000
H	-0. 131390000	-1. 763475000	-2. 731982000

H	-1.204335000	-3.145324000	-3.016453000
C	-0.391201000	-3.452183000	-0.490343000
H	-0.059031000	-3.148055000	0.505088000
H	-0.901712000	-4.418145000	-0.441513000
H	0.488833000	-3.581391000	-1.124561000
H	2.620421640	0.052392930	-2.455365040
H	0.766438650	2.217181450	-0.560753900
H	0.694381680	1.826429640	-2.147587050

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**TS2<sup>C</sup>,  $E_{(\text{SCF Done})} = -1699.680619$  a.u., IF =  $i258.5404$  cm<sup>-1</sup>**

C	-2.591462000	-1.759344000	1.582582000
C	-1.472173000	-2.624342000	1.390653000
C	-0.395536000	-2.146389000	2.196478000
C	-0.853296000	-0.989170000	2.892633000
C	-2.211162000	-0.755523000	2.521545000
C	-1.522484000	-3.931921000	0.651990000
H	-0.529055000	-4.371373000	0.525356000
H	-1.991195000	-3.855010000	-0.336290000
H	-2.115817000	-4.660395000	1.220401000
C	0.930347000	-2.823755000	2.386212000
H	1.722168000	-2.117283000	2.653068000
H	1.257340000	-3.356992000	1.487900000
H	0.874356000	-3.562995000	3.196278000
C	-0.104547000	-0.226697000	3.947447000
H	-0.245148000	0.857618000	3.866548000
H	0.970325000	-0.425769000	3.914450000
H	-0.450474000	-0.517254000	4.948152000
C	-3.121956000	0.242185000	3.178088000
H	-3.580169000	-0.198497000	4.073617000
H	-3.944275000	0.559724000	2.529589000
H	-2.589859000	1.140409000	3.510177000
C	-3.970026000	-2.012623000	1.043853000
H	-3.956413000	-2.366858000	0.007145000
H	-4.476071000	-2.786832000	1.636578000
H	-4.601975000	-1.121263000	1.083590000
Sc	-0.841305000	-0.402598000	0.506002000
C	-8.860439000	0.967998000	-2.246282000
H	-9.486669000	0.558935000	-3.046016000
H	-9.200419000	0.529053000	-1.300608000
H	-9.046645000	2.047435000	-2.198073000
C	-7.383861000	0.671008000	-2.497299000
H	-7.234778000	-0.415113000	-2.576627000
H	-7.082766000	1.093050000	-3.466120000
C	-6.471941000	1.227018000	-1.401260000



H	-6.771162000	0.805814000	-0.430331000
H	-6.617584000	2.313865000	-1.323242000
C	-4.989760000	0.930148000	-1.653843000
H	-4.689882000	1.356954000	-2.620002000
H	-4.839191000	-0.155457000	-1.726441000
C	-4.105638000	1.499783000	-0.548491000
H	-4.341536000	1.059986000	0.423623000
H	-4.217281000	2.586731000	-0.475614000
S	-2.328856000	1.193690000	-0.933974000
C	-1.339489000	1.870734000	0.411255000
C	0.803010000	1.654742000	0.452289000
C	1.276174000	0.356999000	0.752304000
H	1.826681000	-0.167300000	-0.031325000
H	1.605668000	0.146312000	1.766133000
H	-1.827989000	1.709779000	1.386187000
H	-1.165073000	2.936391000	0.285550000
C	1.130593000	2.282045000	-0.887312000
H	0.466765000	3.127036000	-1.103118000
H	0.968793000	1.543575000	-1.684674000
C	2.591538000	2.768141000	-0.952420000
H	2.779118000	3.101354000	-1.982083000
H	3.267930000	1.921988000	-0.772217000
C	2.925910000	3.909186000	0.010488000
H	2.209907000	4.731799000	-0.136774000
H	2.801923000	3.574523000	1.050829000
C	4.349062000	4.440880000	-0.170271000
H	4.477784000	4.786889000	-1.206420000
H	5.065245000	3.616980000	-0.033728000
C	4.699366000	5.579020000	0.789782000
H	4.571496000	5.232039000	1.825257000
H	3.982336000	6.401047000	0.653457000
C	6.120327000	6.105050000	0.599998000
H	6.862429000	5.314325000	0.764089000
H	6.268209000	6.492673000	-0.415138000
H	0.745428000	2.350050000	1.288585000
H	6.340713000	6.917626000	1.300644000
C	-0.493996000	-1.493103000	-1.872999000
H	-0.403125000	-0.562372000	-2.432895000
H	-1.508242000	-1.822347000	-1.634700000
C	0.552646000	-2.331130000	-1.729470000
H	0.378332000	-3.295029000	-1.250211000
C	1.935352000	-2.104533000	-2.248927000
H	1.990349000	-2.638509000	-3.212282000
H	2.086927000	-1.043848000	-2.488567000

C	3.054756000	-2.636254000	-1.343798000
H	2.877278000	-3.702797000	-1.143767000
H	3.019116000	-2.131282000	-0.368488000
C	4.444350000	-2.459505000	-1.957856000
H	4.618414000	-1.393542000	-2.166271000
H	4.476306000	-2.969351000	-2.931763000
C	5.568147000	-2.992331000	-1.067962000
H	5.393757000	-4.058396000	-0.860013000
H	5.535167000	-2.482596000	-0.093172000
C	6.959205000	-2.818991000	-1.680548000
H	7.132671000	-1.753804000	-1.889689000
H	6.991728000	-3.329032000	-2.653533000
C	8.076357000	-3.352803000	-0.786868000
H	7.950414000	-4.424288000	-0.589947000
H	9.057946000	-3.214638000	-1.252667000
H	8.092622000	-2.837343000	0.181191000

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**J1,  $E_{(\text{SCF Done})} = -1940.738969$  a.u.**

C	-1.585046000	-2.088063000	1.491841000
C	-0.394271000	-2.774940000	1.106866000
C	0.690127000	-2.224673000	1.852585000
C	0.172591000	-1.204135000	2.705939000
C	-1.232940000	-1.117925000	2.478704000
C	-0.328495000	-3.958769000	0.184857000
H	0.648371000	-4.056138000	-0.300491000
H	-1.093408000	-3.919756000	-0.598646000
H	-0.497126000	-4.890891000	0.740598000
C	2.111523000	-2.709332000	1.847276000
H	2.264514000	-3.459387000	2.634797000
H	2.824449000	-1.900451000	2.039495000
H	2.387132000	-3.185347000	0.900698000
C	0.942575000	-0.472184000	3.764220000
H	0.446555000	0.456371000	4.060896000
H	1.956374000	-0.214748000	3.440763000
H	1.036365000	-1.091453000	4.666256000
C	-2.175447000	-0.218391000	3.225274000
H	-2.372931000	-0.613948000	4.230196000
H	-3.144350000	-0.130717000	2.724432000
H	-1.770597000	0.791752000	3.355403000
C	-2.973377000	-2.429651000	1.030085000
H	-3.002590000	-2.735480000	-0.021992000
H	-3.378315000	-3.267581000	1.613019000
H	-3.667867000	-1.593343000	1.153377000
Sc	-0.136332000	-0.435735000	0.414251000

C	-8.345006000	0.116988000	-1.295517000
H	-8.992193000	-0.503726000	-1.923886000
H	-8.524902000	-0.165995000	-0.251483000
H	-8.664036000	1.158777000	-1.417613000
C	-6.876398000	-0.060526000	-1.673860000
H	-6.596523000	-1.119179000	-1.576426000
H	-6.735128000	0.197740000	-2.732562000
C	-5.935812000	0.791153000	-0.818361000
H	-6.076121000	0.535137000	0.242000000
H	-6.213146000	1.850323000	-0.917563000
C	-4.461910000	0.615516000	-1.198343000
H	-4.318134000	0.875240000	-2.255045000
H	-4.181373000	-0.441161000	-1.090477000
C	-3.552225000	1.486755000	-0.338201000
H	-3.662650000	1.265211000	0.727672000
H	-3.778876000	2.547490000	-0.492027000
S	-1.788112000	1.288262000	-0.812612000
C	-0.984865000	2.785234000	-0.097804000
C	2.696755000	3.952642000	0.356384000
H	3.077393000	3.200346000	1.062313000
H	3.044837000	3.658659000	-0.643622000
C	1.162483000	3.941983000	0.390120000
H	0.799087000	4.719536000	-0.297007000
H	0.816691000	4.224588000	1.395602000
C	0.532596000	2.584135000	0.010183000
C	0.854852000	1.435807000	0.986294000
H	0.904573000	2.329605000	-0.996402000
H	1.943572000	1.257557000	1.013332000
H	0.587013000	1.753290000	2.007044000
C	7.462892000	-1.966097000	-0.986539000
H	8.295106000	-1.437246000	-0.510531000
H	7.360541000	-2.939083000	-0.491288000
H	7.741294000	-2.151544000	-2.030634000
C	6.171813000	-1.156318000	-0.892893000
H	5.939121000	-0.955148000	0.162528000
H	6.316785000	-0.175673000	-1.366825000
C	4.981131000	-1.860462000	-1.547386000
H	4.832775000	-2.841947000	-1.074034000
H	5.212262000	-2.059808000	-2.603506000
C	3.686390000	-1.046138000	-1.457709000
H	3.831292000	-0.068269000	-1.934519000
H	3.450504000	-0.851489000	-0.402278000
C	2.521401000	-1.768391000	-2.127313000
H	2.324705000	-2.739952000	-1.662724000

H	2.728022000	-1.931419000	-3.190944000
S	0.994915000	-0.751171000	-2.063754000
C	-0.142342000	-1.705384000	-3.114910000
H	-0.292462000	-2.717197000	-2.731734000
H	-1.094670000	-1.169422000	-3.139777000
H	0.262224000	-1.744417000	-4.129592000
H	-1.245754000	3.626649000	-0.747726000
H	-1.421470000	2.953700000	0.893799000
C	3.263978000	5.296514000	0.712145000
H	3.034945000	5.659075000	1.716054000
C	3.999752000	6.055948000	-0.099259000
H	4.254442000	5.736141000	-1.108418000
H	4.381443000	7.023925000	0.214015000

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**K1,  $E_{(\text{SCF Done})} = -1305.593224$  a.u.**

C	0.593943000	-1.959296000	1.228821000
C	0.197775000	-2.312701000	-0.097082000
C	1.368854000	-2.339530000	-0.913115000
C	2.485645000	-2.002687000	-0.091725000
C	2.009265000	-1.768757000	1.234835000
C	-1.179259000	-2.715846000	-0.543059000
H	-1.960342000	-2.310166000	0.106933000
H	-1.283993000	-3.808754000	-0.520684000
H	-1.397573000	-2.401000000	-1.569965000
C	1.411301000	-2.758461000	-2.355739000
H	1.374092000	-3.852558000	-2.439294000
H	2.331653000	-2.437832000	-2.854040000
H	0.563722000	-2.371862000	-2.934425000
C	3.928517000	-2.008048000	-0.509257000
H	4.527843000	-1.296130000	0.067974000
H	4.059765000	-1.777939000	-1.572021000
H	4.371898000	-2.998974000	-0.345003000
C	2.858894000	-1.529911000	2.447418000
H	3.162676000	-2.484819000	2.896378000
H	2.326675000	-0.965765000	3.219131000
H	3.774377000	-0.979372000	2.210112000
C	-0.296961000	-1.892519000	2.435874000
H	-0.266339000	-2.839874000	2.990073000
H	0.009660000	-1.106519000	3.134497000
H	-1.343878000	-1.716541000	2.168713000
Sc	1.050371000	-0.031567000	-0.160414000
C	-7.271256000	-0.710888000	-0.217715000
H	-7.943024000	-1.144117000	-0.965984000
H	-7.159045000	-1.442464000	0.591400000

H	-7.765993000	0.173969000	0.199737000
C	-5.920987000	-0.352015000	-0.833640000
H	-5.467134000	-1.250535000	-1.275281000
H	-6.069873000	0.354601000	-1.661763000
C	-4.950099000	0.258158000	0.179956000
H	-4.800145000	-0.446779000	1.010744000
H	-5.401992000	1.158932000	0.619293000
C	-3.595445000	0.620193000	-0.438164000
H	-3.741310000	1.327037000	-1.264841000
H	-3.138512000	-0.280592000	-0.869808000
C	-2.657660000	1.238625000	0.593199000
H	-2.480499000	0.568536000	1.440239000
H	-3.073284000	2.176330000	0.977617000
S	-1.042072000	1.688970000	-0.160988000
C	-0.317466000	2.860212000	1.074316000
C	1.669851000	3.464007000	-0.374603000
H	0.933728000	3.253308000	-1.163491000
H	1.684189000	4.556385000	-0.287944000
C	1.212584000	2.858629000	0.981069000
C	1.761102000	1.451564000	1.286885000
H	-0.642905000	2.526449000	2.064988000
H	-0.747991000	3.846932000	0.873354000
C	3.047510000	2.987271000	-0.842014000
C	3.088932000	1.597659000	-1.411627000
C	2.158612000	1.022890000	-2.209248000
H	3.779334000	3.072370000	-0.031711000
H	3.410234000	3.654306000	-1.639319000
H	3.996944000	1.025801000	-1.213403000
H	1.542576000	3.558162000	1.766367000
H	1.344888000	1.123128000	2.256166000
H	2.847471000	1.486759000	1.449880000
H	2.365805000	0.073490000	-2.702386000
H	1.269741000	1.564190000	-2.540035000

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**TS-1,  $E_{(\text{SCF Done})} = -1305.583617$  a.u., IF =  $i268.7241$  cm<sup>-1</sup>**

C	0.343494000	-1.988306000	1.056844000
C	0.249505000	-2.335036000	-0.324831000
C	1.569888000	-2.344042000	-0.870607000
C	2.478884000	-2.004230000	0.174263000
C	1.725111000	-1.781379000	1.364400000
C	-0.991028000	-2.743978000	-1.068207000
H	-1.903924000	-2.418923000	-0.560733000
H	-1.044904000	-3.837684000	-1.149227000
H	-1.017302000	-2.353293000	-2.092337000

C	1. 930277000	-2. 787890000	-2. 258679000
H	1. 943784000	-3. 884239000	-2. 318079000
H	2. 924931000	-2. 443526000	-2. 557582000
H	1. 215508000	-2. 437230000	-3. 011514000
C	3. 976099000	-1. 988026000	0. 068286000
H	4. 435585000	-1. 332441000	0. 814970000
H	4. 322546000	-1. 667539000	-0. 920105000
H	4. 383736000	-2. 993690000	0. 235495000
C	2. 289539000	-1. 526610000	2. 733103000
H	2. 521730000	-2. 474822000	3. 235341000
H	1. 586357000	-0. 990197000	3. 379296000
H	3. 218128000	-0. 947577000	2. 700054000
C	-0. 782447000	-1. 969975000	2. 051679000
H	-0. 834638000	-2. 924026000	2. 592672000
H	-0. 661036000	-1. 186813000	2. 808983000
H	-1. 755206000	-1. 825552000	1. 571448000
Sc	1. 055041000	-0. 043917000	-0. 208315000
C	-7. 241318000	-0. 690096000	-0. 146715000
H	-7. 913208000	-1. 163817000	-0. 869854000
H	-7. 133176000	-1. 373696000	0. 703832000
H	-7. 733629000	0. 219345000	0. 217354000
C	-5. 888817000	-0. 372491000	-0. 780127000
H	-5. 437616000	-1. 296706000	-1. 168144000
H	-6. 033745000	0. 285384000	-1. 648101000
C	-4. 917555000	0. 292210000	0. 198250000
H	-4. 770113000	-0. 364182000	1. 068293000
H	-5. 367638000	1. 217916000	0. 584372000
C	-3. 561617000	0. 615448000	-0. 438507000
H	-3. 705923000	1. 274875000	-1. 303740000
H	-3. 106190000	-0. 308733000	-0. 819346000
C	-2. 623203000	1. 287666000	0. 558005000
H	-2. 438090000	0. 658483000	1. 433995000
H	-3. 043153000	2. 240397000	0. 898635000
S	-1. 015339000	1. 712562000	-0. 227735000
C	-0. 289671000	2. 895153000	0. 986250000
C	1. 655020000	3. 579203000	-0. 532668000
H	0. 938448000	3. 293601000	-1. 316342000
H	1. 664210000	4. 673940000	-0. 506835000
C	1. 230254000	2. 985814000	0. 829465000
C	1. 933403000	1. 632191000	1. 020622000
H	-0. 559424000	2. 548665000	1. 989607000
H	-0. 762890000	3. 867307000	0. 813961000
C	3. 029121000	3. 018464000	-0. 876685000
C	3. 010379000	1. 502555000	-0. 899795000

C	2.343965000	0.750587000	-1.891026000
H	3.768077000	3.371249000	-0.147653000
H	3.359741000	3.367459000	-1.862549000
H	3.888782000	1.025464000	-0.465618000
H	1.562303000	3.676480000	1.618360000
H	1.337139000	0.961635000	1.697292000
H	2.885450000	1.739153000	1.544543000
H	2.854027000	-0.116601000	-2.304179000
H	1.685183000	1.277816000	-2.588109000

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**M1,  $E_{(\text{SCF Done})} = -1305.605231$  a.u.**

C	0.092081000	-2.189301000	0.898552000
C	0.218491000	-2.525819000	-0.483275000
C	1.607371000	-2.482907000	-0.827697000
C	2.335021000	-2.106078000	0.335018000
C	1.400538000	-1.913292000	1.401431000
C	-0.890959000	-2.954338000	-1.403367000
H	-1.870751000	-2.598897000	-1.068531000
H	-0.949948000	-4.049709000	-1.449134000
H	-0.740518000	-2.606464000	-2.431881000
C	2.190267000	-2.870594000	-2.154092000
H	2.344910000	-3.956753000	-2.201749000
H	3.159305000	-2.395442000	-2.328699000
H	1.535399000	-2.604070000	-2.990306000
C	3.828132000	-2.014862000	0.444227000
H	4.145601000	-1.321402000	1.229675000
H	4.287928000	-1.691388000	-0.494514000
H	4.255486000	-2.995007000	0.693715000
C	1.742748000	-1.620936000	2.836098000
H	1.864124000	-2.555337000	3.399598000
H	0.961066000	-1.045748000	3.345124000
H	2.682563000	-1.068337000	2.934077000
C	-1.170510000	-2.219320000	1.712302000
H	-1.304382000	-3.205383000	2.176609000
H	-1.158659000	-1.488204000	2.528384000
H	-2.062769000	-2.033443000	1.105773000
Sc	0.893358000	-0.232817000	-0.269215000
C	-7.164931000	-0.429147000	-0.105051000
H	-7.830696000	-0.954703000	-0.797307000
H	-7.097011000	-1.028607000	0.810595000
H	-7.641443000	0.523380000	0.154796000
C	-5.788760000	-0.208188000	-0.728494000
H	-5.353460000	-1.176908000	-1.012556000
H	-5.893863000	0.365319000	-1.659720000

C	-4.824915000	0.524584000	0.207684000
H	-4.715386000	-0.047714000	1.140328000
H	-5.259658000	1.493813000	0.490377000
C	-3.446157000	0.754131000	-0.420440000
H	-3.553315000	1.331633000	-1.347494000
H	-3.007155000	-0.214042000	-0.701104000
C	-2.511666000	1.493040000	0.532233000
H	-2.352695000	0.934592000	1.460355000
H	-2.920402000	2.477080000	0.786286000
S	-0.886967000	1.817571000	-0.265587000
C	-0.104011000	2.982787000	0.931019000
C	1.842019000	3.692398000	-0.644378000
H	1.129486000	3.404039000	-1.428924000
H	1.885373000	4.785699000	-0.644006000
C	1.402800000	3.129931000	0.726276000
C	2.232065000	1.823679000	0.899685000
H	-0.326564000	2.618799000	1.940448000
H	-0.604385000	3.947185000	0.795545000
C	3.200746000	3.037168000	-0.903834000
C	3.009364000	1.572150000	-0.449209000
C	2.339356000	0.681264000	-1.522139000
H	3.972248000	3.523488000	-0.290745000
H	3.518202000	3.099636000	-1.948595000
H	3.969684000	1.110971000	-0.196728000
H	1.716722000	3.832569000	1.508841000
H	1.628834000	1.001645000	1.358350000
H	2.986216000	1.968601000	1.680552000
H	3.094160000	0.198251000	-2.146070000
H	1.702183000	1.290791000	-2.193755000

83

**K1',  $E_{(\text{SCF Done})} = -1940.740914$  a.u.**

C	-1.059259000	1.465139000	2.124806000
C	-0.566799000	0.142371000	2.335027000
C	0.858303000	0.198146000	2.337321000
C	1.245829000	1.547780000	2.095824000
C	0.058091000	2.331559000	1.964348000
C	-1.394905000	-1.064792000	2.671986000
H	-2.413908000	-0.983007000	2.282575000
H	-1.477563000	-1.187864000	3.760410000
H	-0.960824000	-1.992065000	2.281527000
C	1.770089000	-0.925720000	2.730264000
H	1.899985000	-0.946183000	3.821027000
H	2.768638000	-0.824993000	2.294475000
H	1.369856000	-1.902866000	2.441186000



C	2.643535000	2.092620000	2.179167000
H	2.793826000	2.964727000	1.533443000
H	3.400321000	1.345291000	1.917228000
H	2.866395000	2.419469000	3.203649000
C	0.007581000	3.826165000	1.847437000
H	0.011449000	4.289760000	2.843037000
H	-0.893758000	4.171051000	1.332929000
H	0.871891000	4.228889000	1.308665000
C	-2.496021000	1.887013000	2.207659000
H	-2.812124000	1.954788000	3.257177000
H	-2.660263000	2.870028000	1.758298000
H	-3.171462000	1.180680000	1.714305000
Sc	0.090227000	0.757916000	0.060791000
C	-7.869515000	-2.284396000	0.859515000
H	-8.684132000	-1.809329000	1.416091000
H	-8.280792000	-2.639347000	-0.092855000
H	-7.545297000	-3.162911000	1.430045000
C	-6.714702000	-1.310765000	0.635882000
H	-7.078345000	-0.426873000	0.093401000
H	-6.348310000	-0.945520000	1.605731000
C	-5.553015000	-1.935379000	-0.140427000
H	-5.919177000	-2.298816000	-1.111367000
H	-5.187588000	-2.820565000	0.400395000
C	-4.393105000	-0.958704000	-0.366407000
H	-4.014591000	-0.602749000	0.599390000
H	-4.767280000	-0.077829000	-0.902755000
C	-3.261871000	-1.614097000	-1.148226000
H	-3.614024000	-1.985381000	-2.117250000
H	-2.863785000	-2.475747000	-0.600689000
S	-1.785461000	-0.583026000	-1.511077000
C	-2.432139000	0.799508000	-2.532465000
C	-0.186770000	1.694794000	-3.313050000
H	0.210478000	0.688600000	-3.105072000
H	-0.445561000	1.697430000	-4.379476000
C	-1.445434000	1.968541000	-2.470974000
C	-1.125945000	2.295841000	-1.006658000
H	-3.395425000	1.103350000	-2.113402000
H	-2.587447000	0.426514000	-3.550445000
C	0.920650000	2.729801000	-3.061665000
C	1.604990000	2.584244000	-1.726660000
C	2.278687000	1.485971000	-1.323959000
H	0.508154000	3.740201000	-3.158263000
H	1.687574000	2.629479000	-3.841183000
H	-1.971317000	2.813043000	-2.948502000

C	8.018210000	-1.772654000	0.223645000
H	8.853400000	-1.075000000	0.102056000
H	7.990761000	-2.078295000	1.276360000
H	8.239810000	-2.663557000	-0.375710000
C	6.699093000	-1.132686000	-0.203004000
H	6.523471000	-0.223290000	0.389528000
H	6.769783000	-0.807096000	-1.250287000
C	5.503990000	-2.075627000	-0.048147000
H	5.428993000	-2.399995000	0.999941000
H	5.680063000	-2.985587000	-0.639216000
C	4.179419000	-1.439104000	-0.483164000
H	4.250639000	-1.132684000	-1.535064000
H	4.006973000	-0.528191000	0.105006000
C	3.013507000	-2.402970000	-0.303555000
H	2.890853000	-2.679060000	0.748238000
H	3.195337000	-3.319818000	-0.876050000
S	1.413516000	-1.753122000	-0.935368000
C	0.405755000	-3.244111000	-0.689579000
H	0.262539000	-3.467113000	0.371079000
H	-0.558067000	-3.078042000	-1.173038000
H	0.897068000	-4.088465000	-1.181013000
H	2.880881000	1.501680000	-0.418849000
H	1.611283000	3.455964000	-1.072757000
H	2.391633000	0.626515000	-1.982353000
H	-0.734449000	3.319359000	-0.927699000
H	-2.069710000	2.312605000	-0.437053000

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**TS-1',  $E_{(\text{SCF Done})} = -1940.732017$  a.u.,  $\text{IF} = i280.4899$  cm<sup>-1</sup>**

C	-1.078098000	1.369642000	2.116684000
C	-0.697267000	0.005990000	2.277085000
C	0.726997000	-0.044565000	2.359038000
C	1.225875000	1.283099000	2.231881000
C	0.109553000	2.156738000	2.066040000
C	-1.621114000	-1.156998000	2.500372000
H	-2.613393000	-0.982539000	2.073994000
H	-1.763086000	-1.340320000	3.574160000
H	-1.230501000	-2.087144000	2.072013000
C	1.532534000	-1.252098000	2.736474000
H	1.548727000	-1.373624000	3.828300000
H	2.573682000	-1.169506000	2.411428000
H	1.118548000	-2.177221000	2.321796000
C	2.647143000	1.709971000	2.453895000
H	2.878300000	2.660535000	1.962284000
H	3.368939000	0.966476000	2.099474000

H	2.839367000	1.854606000	3.525488000
C	0.166833000	3.656257000	2.033656000
H	0.105970000	4.067521000	3.050186000
H	-0.660211000	4.092470000	1.464368000
H	1.101900000	4.025647000	1.599997000
C	-2.478264000	1.908613000	2.166959000
H	-2.780964000	2.081280000	3.208486000
H	-2.574248000	2.866691000	1.646477000
H	-3.210681000	1.219553000	1.734486000
Sc	0.154734000	0.685359000	0.070559000
C	-7.763453000	-2.112555000	0.939085000
H	-8.629986000	-1.584639000	1.350635000
H	-8.117141000	-2.733850000	0.107843000
H	-7.382585000	-2.783893000	1.717968000
C	-6.688894000	-1.130347000	0.478437000
H	-7.110623000	-0.450291000	-0.274764000
H	-6.381244000	-0.498378000	1.323619000
C	-5.458476000	-1.828117000	-0.105750000
H	-5.765953000	-2.454675000	-0.955224000
H	-5.036718000	-2.513304000	0.643992000
C	-4.375983000	-0.843552000	-0.564820000
H	-4.038944000	-0.238129000	0.285597000
H	-4.815948000	-0.151393000	-1.293153000
C	-3.192703000	-1.576998000	-1.182601000
H	-3.495497000	-2.112659000	-2.088708000
H	-2.795652000	-2.321299000	-0.483291000
S	-1.714192000	-0.582590000	-1.645089000
C	-2.379476000	0.856244000	-2.563132000
C	-0.114935000	1.779872000	-3.351369000
H	0.268332000	0.758758000	-3.197283000
H	-0.312751000	1.882608000	-4.424681000
C	-1.381363000	2.015266000	-2.512300000
C	-0.961432000	2.354037000	-1.076909000
H	-3.319141000	1.153840000	-2.090402000
H	-2.584785000	0.544121000	-3.592214000
C	0.922079000	2.790556000	-2.872152000
C	1.235299000	2.601281000	-1.399274000
C	2.045151000	1.552933000	-0.941210000
H	0.546165000	3.806275000	-3.046027000
H	1.857037000	2.692313000	-3.436537000
H	-1.909667000	2.874342000	-2.953211000
C	8.017310000	-1.492204000	0.104889000
H	8.820062000	-0.757181000	-0.015470000
H	8.015601000	-1.814021000	1.153182000

H	8.270397000	-2.363946000	-0.510057000
C	6.666686000	-0.904335000	-0.297406000
H	6.458329000	-0.012159000	0.310334000
H	6.710745000	-0.560628000	-1.340316000
C	5.515379000	-1.900533000	-0.144002000
H	5.467773000	-2.244129000	0.899687000
H	5.724054000	-2.792909000	-0.751288000
C	4.159742000	-1.314543000	-0.553256000
H	4.205493000	-0.985564000	-1.599777000
H	3.949845000	-0.423315000	0.051309000
C	3.040545000	-2.334136000	-0.383841000
H	2.943621000	-2.645007000	0.660887000
H	3.251600000	-3.226349000	-0.984738000
S	1.407153000	-1.734643000	-0.975315000
C	0.462357000	-3.272592000	-0.771803000
H	0.353884000	-3.547491000	0.280793000
H	-0.520251000	-3.126647000	-1.224035000
H	0.971426000	-4.076306000	-1.311082000
H	2.729467000	1.745559000	-0.119883000
H	1.230020000	3.504524000	-0.793143000
H	2.380396000	0.816488000	-1.672415000
H	-0.991210000	3.428415000	-0.885235000
H	-1.677455000	1.928125000	-0.339166000

83

**L1,  $E_{(\text{SCF Done})} = -1940.761514$  a.u.**

C	-0.950769000	-0.503778000	2.567699000
C	-0.875804000	-1.748363000	1.874007000
C	0.498363000	-2.112931000	1.772956000
C	1.273283000	-1.091573000	2.399411000
C	0.381183000	-0.099830000	2.897975000
C	-2.038521000	-2.603007000	1.456786000
H	-2.965654000	-2.026655000	1.390760000
H	-2.213490000	-3.401738000	2.190057000
H	-1.879994000	-3.094891000	0.489521000
C	1.013912000	-3.433519000	1.279553000
H	1.106767000	-4.141640000	2.114068000
H	2.006496000	-3.356958000	0.824151000
H	0.338505000	-3.895144000	0.552164000
C	2.760713000	-1.111190000	2.597753000
H	3.186866000	-0.103190000	2.608150000
H	3.274635000	-1.683616000	1.818303000
H	3.017321000	-1.580081000	3.557237000
C	0.767798000	1.067451000	3.756118000
H	0.791296000	0.772619000	4.813963000

H	0.063069000	1.899454000	3.669573000
H	1.761150000	1.448401000	3.502092000
C	-2.215329000	0.170793000	3.021028000
H	-2.603226000	-0.312923000	3.927317000
H	-2.052692000	1.223705000	3.268498000
H	-3.010832000	0.125497000	2.269250000
Sc	0.202026000	-0.046998000	0.461785000
C	-7.737465000	-1.836755000	-1.217914000
H	-8.593388000	-1.887457000	-0.536935000
H	-8.094066000	-1.424732000	-2.169284000
H	-7.400500000	-2.863335000	-1.405098000
C	-6.616611000	-0.982847000	-0.629687000
H	-6.994774000	0.027639000	-0.421071000
H	-6.306104000	-1.399615000	0.338965000
C	-5.398792000	-0.884180000	-1.551402000
H	-5.708887000	-0.462440000	-2.518213000
H	-5.020327000	-1.894677000	-1.764788000
C	-4.271293000	-0.029920000	-0.960728000
H	-3.939282000	-0.459551000	-0.007363000
H	-4.661374000	0.971000000	-0.739082000
C	-3.089497000	0.068270000	-1.917415000
H	-3.381427000	0.541963000	-2.861481000
H	-2.708263000	-0.928182000	-2.168276000
S	-1.611522000	0.986451000	-1.330504000
C	-2.292785000	2.657387000	-0.958063000
C	-0.051429000	3.956555000	-1.263946000
H	0.195207000	3.108474000	-1.916797000
H	-0.246809000	4.811923000	-1.918845000
C	-1.264744000	3.619430000	-0.367658000
C	-0.661610000	3.162858000	0.989233000
H	-3.128428000	2.527946000	-0.264272000
H	-2.681764000	3.033688000	-1.910813000
C	1.088094000	4.204525000	-0.268389000
C	0.876462000	3.115753000	0.804848000
C	1.423134000	1.738909000	0.379811000
H	0.977800000	5.202181000	0.179300000
H	2.080493000	4.158623000	-0.729021000
H	-1.836374000	4.542118000	-0.199834000
C	7.914242000	-0.359474000	-1.176085000
H	8.601599000	0.474035000	-0.997660000
H	8.077905000	-1.100510000	-0.384510000
H	8.195119000	-0.823088000	-2.129148000
C	6.464157000	0.118232000	-1.198484000
H	6.223571000	0.610137000	-0.245340000

H	6.340180000	0.883026000	-1.977681000
C	5.468714000	-1.017462000	-1.445661000
H	5.589082000	-1.783085000	-0.665258000
H	5.708502000	-1.509792000	-2.399016000
C	4.013941000	-0.536883000	-1.473931000
H	3.890261000	0.219514000	-2.259630000
H	3.771868000	-0.046416000	-0.522284000
C	3.050788000	-1.692051000	-1.724671000
H	3.113308000	-2.448379000	-0.935756000
H	3.274117000	-2.177383000	-2.681677000
S	1.313835000	-1.111813000	-1.864926000
C	0.487483000	-2.636100000	-2.411735000
H	0.622714000	-3.447555000	-1.693890000
H	-0.577538000	-2.421163000	-2.527952000
H	0.889606000	-2.927347000	-3.385735000
H	2.450861000	1.615270000	0.750799000
H	1.362085000	3.398564000	1.744994000
H	1.517038000	1.705947000	-0.730443000
H	-0.924237000	3.886795000	1.769778000
H	-1.083253000	2.203963000	1.329149000

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**J2,  $E_{(\text{SCF Done})} = -1744.257941$  a.u.**

C	-1.698925000	-1.867532000	1.816418000
C	-0.702422000	-2.745818000	1.322024000
C	0.534133000	-2.376967000	1.910227000
C	0.301713000	-1.274699000	2.773554000
C	-1.076647000	-0.960577000	2.713060000
Sc	-0.136657000	-0.487075000	0.509502000
C	-8.231764000	-0.973923000	-0.088430000
H	-8.856586000	-1.754435000	-0.534784000
H	-8.234179000	-1.126597000	0.997385000
H	-8.711382000	-0.008948000	-0.290182000
C	-6.813371000	-1.016127000	-0.652175000
H	-6.373029000	-2.006327000	-0.466871000
H	-6.847076000	-0.894749000	-1.743769000
C	-5.905284000	0.060658000	-0.053814000
H	-5.870337000	-0.057733000	1.038955000
H	-6.343004000	1.051228000	-0.242030000
C	-4.481971000	0.020633000	-0.620190000
H	-4.513521000	0.145561000	-1.710239000
H	-4.040336000	-0.967638000	-0.428133000
C	-3.604586000	1.109159000	-0.011177000
H	-3.540146000	1.018425000	1.077802000
H	-3.997105000	2.102685000	-0.252867000

S	-1.905015000	1.060621000	-0.710646000
C	-1.135702000	2.630423000	-0.118336000
C	2.519565000	3.948692000	0.105377000
H	2.952472000	3.263421000	0.848444000
H	2.841387000	3.594186000	-0.883701000
C	0.988797000	3.891435000	0.199353000
H	0.573137000	4.603970000	-0.527259000
H	0.669458000	4.234323000	1.194596000
C	0.392034000	2.490786000	-0.058005000
C	0.793233000	1.425979000	0.982770000
H	0.736633000	2.177536000	-1.058987000
H	1.888414000	1.291215000	0.984645000
H	0.538122000	1.790852000	1.990701000
C	7.087856000	-2.893415000	0.479420000
H	7.894731000	-2.390366000	1.022155000
H	6.791447000	-3.772360000	1.064159000
H	7.499568000	-3.249470000	-0.472225000
C	5.907388000	-1.951445000	0.254513000
H	5.540687000	-1.582884000	1.223242000
H	6.243181000	-1.066382000	-0.303292000
C	4.755266000	-2.616142000	-0.502376000
H	4.415699000	-3.501871000	0.054107000
H	5.120255000	-2.983061000	-1.472079000
C	3.572117000	-1.670220000	-0.733942000
H	3.907796000	-0.791427000	-1.299549000
H	3.207097000	-1.300688000	0.235933000
C	2.440082000	-2.360969000	-1.488281000
H	2.047386000	-3.219680000	-0.933547000
H	2.781681000	-2.707968000	-2.469547000
S	1.063142000	-1.189908000	-1.813402000
C	-0.114922000	-2.227702000	-2.735077000
H	-0.418706000	-3.103435000	-2.156594000
H	-0.987670000	-1.611395000	-2.965568000
H	0.349947000	-2.540823000	-3.673383000
H	-1.454372000	3.420928000	-0.804715000
H	-1.542245000	2.839670000	0.878070000
C	3.050533000	5.333283000	0.341603000
H	2.846049000	5.760155000	1.325235000
C	3.728383000	6.054609000	-0.550864000
H	3.957348000	5.670083000	-1.543436000
H	4.086889000	7.054775000	-0.323124000
H	-2.755329000	-1.903019000	1.576049000
H	-1.567552000	-0.161896000	3.257716000
H	1.045447000	-0.761701000	3.371198000

H	1.487655000	-2.869024000	1.752712000
H	-0.863180000	-3.568701000	0.634085000

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**K2,  $E_{(\text{SCF Done})} = -1109.111856$  a.u.**

C	-0.072790000	2.337334000	1.349632000
C	0.397882000	2.592815000	0.034900000
C	-0.697728000	3.048787000	-0.739976000
C	-1.843362000	3.073181000	0.095833000
C	-1.457120000	2.636474000	1.389858000
Sc	-1.195091000	0.728402000	-0.085539000
C	6.884158000	0.140274000	-0.183765000
H	7.595269000	0.579270000	-0.891088000
H	6.883332000	0.764802000	0.717491000
H	7.263210000	-0.849426000	0.096808000
C	5.488573000	0.046118000	-0.796002000
H	5.151779000	1.047406000	-1.100153000
H	5.528685000	-0.556098000	-1.714133000
C	4.461696000	-0.563255000	0.161416000
H	4.418927000	0.037909000	1.081232000
H	4.796236000	-1.565813000	0.463450000
C	3.061440000	-0.660769000	-0.453981000
H	3.099361000	-1.267242000	-1.367879000
H	2.723668000	0.341289000	-0.753210000
C	2.064534000	-1.275473000	0.522121000
H	1.983720000	-0.692362000	1.444952000
H	2.357431000	-2.298267000	0.781777000
S	0.394914000	-1.416370000	-0.239257000
C	-0.551957000	-2.431828000	0.987364000
C	-2.713613000	-2.382993000	-0.329190000
H	-2.013637000	-2.272048000	-1.170848000
H	-2.968548000	-3.448739000	-0.315938000
C	-2.026973000	-2.013207000	1.012202000
C	-2.149971000	-0.530489000	1.413902000
H	-0.087380000	-2.263772000	1.964286000
H	-0.418478000	-3.482053000	0.708628000
C	-3.979333000	-1.571720000	-0.626689000
C	-3.738780000	-0.164964000	-1.097943000
C	-2.799876000	0.235078000	-1.988542000
H	-4.640060000	-1.558816000	0.246356000
H	-4.548918000	-2.070513000	-1.425507000
H	-4.433558000	0.592644000	-0.730857000
H	-2.489336000	-2.643183000	1.789344000
H	-1.582797000	-0.369400000	2.347256000
H	-3.189300000	-0.280689000	1.670271000



H	-2.815679000	1.248538000	-2.389068000
H	-2.138976000	-0.479340000	-2.486062000
H	1.420233000	2.485858000	-0.309776000
H	-0.660502000	3.344151000	-1.783261000
H	-2.838038000	3.392893000	-0.195881000
H	-2.102347000	2.552736000	2.255739000
H	0.523257000	1.983570000	2.183658000

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**TS-2,  $E_{(\text{SCF Done})} = -1109.102797$  a.u., IF =  $i259.0755$  cm<sup>-1</sup>**

C	0.456402000	2.267937000	0.937489000
C	0.386869000	2.619960000	-0.436235000
C	-0.908454000	3.134139000	-0.694042000
C	-1.640319000	3.098775000	0.520449000
C	-0.797646000	2.569654000	1.529515000
Sc	-1.188477000	0.775494000	-0.083960000
C	6.825185000	-0.000931000	-0.101335000
H	7.546688000	0.478468000	-0.770838000
H	6.835626000	0.549110000	0.847152000
H	7.182854000	-1.017759000	0.098748000
C	5.429305000	-0.015935000	-0.719898000
H	5.114241000	1.013437000	-0.942440000
H	5.458675000	-0.543185000	-1.683397000
C	4.387844000	-0.678630000	0.184943000
H	4.355279000	-0.151909000	1.149791000
H	4.700942000	-1.708766000	0.406317000
C	2.987616000	-0.697555000	-0.438232000
H	3.016274000	-1.233040000	-1.395817000
H	2.671693000	0.331360000	-0.658858000
C	1.974870000	-1.363236000	0.486804000
H	1.891939000	-0.839813000	1.444785000
H	2.253613000	-2.404322000	0.681748000
S	0.311031000	-1.432012000	-0.296509000
C	-0.655362000	-2.450046000	0.901951000
C	-2.812725000	-2.427091000	-0.480943000
H	-2.106152000	-2.271045000	-1.310000000
H	-3.112987000	-3.479146000	-0.526685000
C	-2.143109000	-2.088986000	0.869485000
C	-2.410427000	-0.607808000	1.188137000
H	-0.231709000	-2.272884000	1.896155000
H	-0.497860000	-3.500756000	0.639131000
C	-4.008123000	-1.497450000	-0.655281000
C	-3.582913000	-0.043047000	-0.593009000
C	-2.833963000	0.587452000	-1.611082000
H	-4.753999000	-1.701481000	0.121662000

H	-4.497769000	-1.665809000	-1.622055000
H	-4.248562000	0.611183000	-0.030229000
H	-2.611619000	-2.712010000	1.645079000
H	-1.587623000	-0.173198000	1.822588000
H	-3.302064000	-0.476636000	1.804017000
H	-3.114583000	1.598936000	-1.896882000
H	-2.436685000	-0.030691000	-2.422907000
H	1.189984000	2.532206000	-1.160233000
H	-1.267703000	3.507425000	-1.645532000
H	-2.663340000	3.432142000	0.657282000
H	-1.058607000	2.439273000	2.573964000
H	1.324686000	1.872523000	1.452460000

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**L2,  $E_{(\text{SCF Done})} = -1109.122476$  a.u.**

C	0.549962000	2.550648000	0.726022000
C	0.210013000	2.961784000	-0.590656000
C	-1.171796000	3.289344000	-0.610045000
C	-1.686975000	3.063119000	0.688463000
C	-0.625830000	2.608014000	1.515551000
Sc	-0.987659000	0.903305000	-0.202337000
C	6.813507000	-0.121059000	-0.064936000
H	7.540139000	0.354798000	-0.731343000
H	6.834772000	0.418353000	0.889441000
H	7.156516000	-1.145209000	0.122916000
C	5.415970000	-0.108681000	-0.679819000
H	5.115761000	0.927594000	-0.890938000
H	5.435009000	-0.626307000	-1.648751000
C	4.367287000	-0.765376000	0.221068000
H	4.343693000	-0.248126000	1.191257000
H	4.665937000	-1.802056000	0.431224000
C	2.965685000	-0.759556000	-0.399072000
H	2.985930000	-1.285824000	-1.362003000
H	2.664826000	0.277065000	-0.610064000
C	1.944044000	-1.419710000	0.521422000
H	1.866631000	-0.900247000	1.482276000
H	2.210794000	-2.464799000	0.711241000
S	0.284223000	-1.458052000	-0.272292000
C	-0.720240000	-2.401749000	0.955062000
C	-2.855375000	-2.555752000	-0.526682000
H	-2.133799000	-2.439272000	-1.347030000
H	-3.172008000	-3.602886000	-0.532224000
C	-2.221441000	-2.148217000	0.821300000
C	-2.675718000	-0.673170000	1.035320000
H	-0.364663000	-2.121408000	1.952906000

H	-0.495858000	-3.461202000	0.796098000
C	-4.017257000	-1.577231000	-0.708076000
C	-3.438167000	-0.208586000	-0.278120000
C	-2.649170000	0.493418000	-1.412481000
H	-4.847642000	-1.856246000	-0.045129000
H	-4.403554000	-1.547482000	-1.730538000
H	-4.231418000	0.477358000	0.034766000
H	-2.673669000	-2.754119000	1.616772000
H	-1.869895000	-0.046007000	1.497284000
H	-3.417927000	-0.631436000	1.839070000
H	-3.293876000	1.174246000	-1.969302000
H	-2.237954000	-0.247146000	-2.126117000
H	0.893376000	3.042355000	-1.430173000
H	-1.731887000	3.645028000	-1.465387000
H	-2.714440000	3.217635000	0.998814000
H	-0.695712000	2.376724000	2.573202000
H	1.537194000	2.264616000	1.071540000

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**K2',  $E_{(\text{SCF Done})} = -1744.265904$  a.u.**

C	-1.023995000	-0.689305000	2.433684000
C	-0.252713000	-1.629309000	1.706664000
C	1.113246000	-1.288090000	1.867317000
C	1.182669000	-0.133439000	2.685269000
C	-0.140120000	0.237401000	3.034498000
Sc	0.054514000	0.551088000	0.611824000
C	-7.067740000	-3.064315000	0.592573000
H	-7.552984000	-3.324129000	1.539127000
H	-7.812678000	-2.562027000	-0.035762000
H	-6.788472000	-4.000245000	0.094290000
C	-5.848803000	-2.174586000	0.825254000
H	-6.155391000	-1.262161000	1.355921000
H	-5.138230000	-2.690429000	1.486775000
C	-5.139080000	-1.787146000	-0.474207000
H	-5.849770000	-1.273787000	-1.137582000
H	-4.827894000	-2.698687000	-1.004944000
C	-3.919321000	-0.888418000	-0.242284000
H	-3.206414000	-1.395028000	0.420651000
H	-4.236427000	0.026227000	0.276100000
C	-3.224596000	-0.537823000	-1.551207000
H	-3.918207000	-0.081185000	-2.266359000
H	-2.819340000	-1.434424000	-2.032715000
S	-1.801566000	0.620213000	-1.442243000
C	-2.601259000	2.241096000	-1.085584000
C	-0.469109000	3.606992000	-0.969272000

H	-0.017841000	2.802737000	-1.573598000
H	-0.787056000	4.372229000	-1.688282000
C	-1.688940000	3.081271000	-0.190301000
C	-1.296210000	2.267219000	1.047190000
H	-3.545827000	2.031830000	-0.574516000
H	-2.817274000	2.721764000	-2.045291000
C	0.609353000	4.195230000	-0.046811000
C	1.375248000	3.160479000	0.737057000
C	2.117565000	2.172876000	0.189140000
H	0.153208000	4.917194000	0.639186000
H	1.333125000	4.754725000	-0.654125000
H	-2.290840000	3.959994000	0.097351000
C	7.694107000	-1.951480000	0.422921000
H	8.509921000	-1.408266000	0.911033000
H	7.464404000	-2.829533000	1.038160000
H	8.065936000	-2.310317000	-0.544003000
C	6.466863000	-1.059986000	0.247805000
H	6.140662000	-0.687384000	1.229539000
H	6.737078000	-0.173514000	-0.342879000
C	5.300999000	-1.781749000	-0.431425000
H	5.026145000	-2.666879000	0.160504000
H	5.626698000	-2.156630000	-1.412025000
C	4.070960000	-0.886228000	-0.616106000
H	4.340879000	-0.014502000	-1.226680000
H	3.752953000	-0.505744000	0.363791000
C	2.924058000	-1.640366000	-1.278230000
H	2.586376000	-2.478597000	-0.658500000
H	3.248778000	-2.045477000	-2.243388000
S	1.480031000	-0.571169000	-1.660285000
C	0.464238000	-1.780408000	-2.560257000
H	0.112070000	-2.581400000	-1.904562000
H	-0.382319000	-1.245673000	-2.994846000
H	1.060925000	-2.203602000	-3.372915000
H	2.775023000	1.563729000	0.805905000
H	1.387793000	3.264965000	1.821925000
H	2.230955000	2.081995000	-0.890411000
H	-0.974277000	2.933859000	1.859206000
H	-2.193786000	1.761378000	1.444317000
H	-0.637416000	-2.474019000	1.145737000
H	1.957134000	-1.831268000	1.461646000
H	2.089541000	0.361439000	3.014627000
H	-0.427690000	1.075826000	3.656163000
H	-2.104230000	-0.672022000	2.511451000

**TS-2',  $E_{(\text{SCF Done})} = -1744.256503$  a.u.,  $\text{IF} = i278.4026$  cm<sup>-1</sup>**

C	-1.060526000	-0.675982000	2.428101000
C	-0.397313000	-1.673631000	1.674275000
C	0.998852000	-1.468149000	1.814320000
C	1.196420000	-0.342715000	2.648055000
C	-0.076997000	0.154667000	3.020009000
Sc	0.112262000	0.485482000	0.589952000
C	-7.069887000	-2.924716000	0.610733000
H	-7.556813000	-3.165416000	1.561420000
H	-7.810169000	-2.424153000	-0.024401000
H	-6.800658000	-3.870756000	0.126300000
C	-5.841642000	-2.044274000	0.829444000
H	-6.138566000	-1.120992000	1.346776000
H	-5.135862000	-2.557673000	1.497938000
C	-5.129396000	-1.683553000	-0.476300000
H	-5.835126000	-1.172385000	-1.146532000
H	-4.828282000	-2.605919000	-0.993805000
C	-3.899237000	-0.794938000	-0.258864000
H	-3.190271000	-1.300178000	0.408820000
H	-4.208565000	0.128591000	0.249022000
C	-3.205603000	-0.469031000	-1.574427000
H	-3.894997000	-0.007729000	-2.290685000
H	-2.820972000	-1.378293000	-2.048844000
S	-1.756381000	0.660983000	-1.494564000
C	-2.535274000	2.278636000	-1.105196000
C	-0.380395000	3.666764000	-1.029561000
H	0.047844000	2.871632000	-1.661010000
H	-0.644896000	4.491266000	-1.701276000
C	-1.602312000	3.143121000	-0.256729000
C	-1.109853000	2.402218000	0.991047000
H	-3.463255000	2.072645000	-0.563259000
H	-2.785361000	2.764581000	-2.053632000
C	0.646458000	4.095291000	0.012967000
C	1.049957000	2.926527000	0.892846000
C	1.908612000	1.913783000	0.433900000
H	0.226172000	4.899793000	0.628538000
H	1.550627000	4.492509000	-0.463309000
H	-2.199477000	4.016957000	0.044846000
C	7.729005000	-1.689032000	0.375755000
H	8.515230000	-1.101833000	0.861610000
H	7.557794000	-2.584229000	0.985401000
H	8.113128000	-2.017402000	-0.597220000
C	6.448950000	-0.871596000	0.218268000
H	6.109515000	-0.526643000	1.205536000

H	6.660106000	0.034134000	-0.367201000
C	5.322254000	-1.656427000	-0.457131000
H	5.106393000	-2.560993000	0.130014000
H	5.661741000	-2.003831000	-1.443292000
C	4.039632000	-0.834331000	-0.623155000
H	4.251784000	0.057631000	-1.227145000
H	3.702568000	-0.481303000	0.359671000
C	2.936099000	-1.650756000	-1.284213000
H	2.654282000	-2.512053000	-0.668177000
H	3.273731000	-2.028670000	-2.256087000
S	1.426858000	-0.668096000	-1.642953000
C	0.436503000	-1.957527000	-2.455124000
H	0.142022000	-2.744838000	-1.755782000
H	-0.447921000	-1.480977000	-2.882807000
H	1.021135000	-2.389308000	-3.272108000
H	2.654789000	1.521519000	1.119289000
H	1.073630000	3.122539000	1.963105000
H	2.203203000	1.931776000	-0.617221000
H	-1.170531000	3.019160000	1.889892000
H	-1.763859000	1.529369000	1.221359000
H	-0.871131000	-2.470569000	1.111776000
H	1.778693000	-2.083462000	1.384013000
H	2.152025000	0.052953000	2.969076000
H	-0.267733000	1.004101000	3.664973000
H	-2.132950000	-0.568939000	2.541604000

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**M2,  $E_{(\text{SCF Done})} = -1744.283619$  a.u.**

C	-1.290137000	-0.352239000	2.674956000
C	-0.944467000	-1.636537000	2.186794000
C	0.456209000	-1.797793000	2.341856000
C	0.973439000	-0.616596000	2.930384000
C	-0.102564000	0.276090000	3.134251000
Sc	0.124993000	0.014401000	0.708271000
C	-7.291791000	-2.369164000	-0.256606000
H	-7.944500000	-2.590168000	0.594215000
H	-7.883061000	-1.812353000	-0.992971000
H	-7.005555000	-3.324225000	-0.712927000
C	-6.064746000	-1.574188000	0.183825000
H	-6.385339000	-0.640674000	0.667157000
H	-5.513819000	-2.141403000	0.947761000
C	-5.123656000	-1.242904000	-0.976744000
H	-5.674058000	-0.675220000	-1.740422000
H	-4.801180000	-2.175648000	-1.462263000
C	-3.892696000	-0.442298000	-0.537589000

H	-3.337055000	-1.004381000	0.225315000
H	-4.220681000	0.490900000	-0.061351000
C	-2.972134000	-0.136281000	-1.712629000
H	-3.497984000	0.409704000	-2.504235000
H	-2.590853000	-1.056211000	-2.169960000
S	-1.470404000	0.854795000	-1.343436000
C	-2.180577000	2.534471000	-1.060635000
C	0.071352000	3.832078000	-1.266117000
H	0.362248000	2.965822000	-1.876007000
H	-0.086286000	4.664533000	-1.959220000
C	-1.194057000	3.517213000	-0.435716000
C	-0.671444000	3.097633000	0.964311000
H	-3.059761000	2.416158000	-0.419571000
H	-2.510220000	2.881814000	-2.045693000
C	1.146235000	4.118853000	-0.211191000
C	0.879268000	3.060030000	0.879525000
C	1.469826000	1.678230000	0.535488000
H	1.001828000	5.127682000	0.199961000
H	2.165128000	4.067785000	-0.608511000
H	-1.773938000	4.443337000	-0.326003000
C	7.800910000	-0.858152000	-0.376694000
H	8.523836000	-0.051730000	-0.537916000
H	7.869039000	-1.160113000	0.675268000
H	8.114042000	-1.711927000	-0.989163000
C	6.386514000	-0.408092000	-0.734925000
H	6.115218000	0.469611000	-0.131333000
H	6.358608000	-0.079877000	-1.783181000
C	5.343030000	-1.507481000	-0.523865000
H	5.368540000	-1.836771000	0.525184000
H	5.611875000	-2.385067000	-1.129074000
C	3.923875000	-1.055719000	-0.885115000
H	3.893190000	-0.735545000	-1.934528000
H	3.653429000	-0.181817000	-0.278462000
C	2.912451000	-2.175825000	-0.666802000
H	2.892119000	-2.504094000	0.377753000
H	3.151977000	-3.040775000	-1.295647000
S	1.217369000	-1.663039000	-1.161978000
C	0.336221000	-3.252771000	-1.082619000
H	0.395695000	-3.697092000	-0.086445000
H	-0.710417000	-3.073271000	-1.340140000
H	0.765260000	-3.932815000	-1.823237000
H	2.481460000	1.584051000	0.950614000
H	1.300648000	3.373498000	1.841176000
H	1.591017000	1.580719000	-0.568579000

H	-0.983970000	3.833097000	1.714704000
H	-1.125633000	2.150682000	1.306803000
H	-1.632440000	-2.374907000	1.789822000
H	1.026685000	-2.685746000	2.095285000
H	2.010868000	-0.424356000	3.176448000
H	-0.029274000	1.267577000	3.564114000
H	-2.289343000	0.067355000	2.713333000

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**J3,  $E_{(\text{SCF Done})} = -1932.296067$  a.u.**

C	-1.638633000	-2.286509000	1.372006000
C	-0.383960000	-2.916083000	1.105274000
C	0.605971000	-2.282519000	1.915334000
C	-0.032815000	-1.264986000	2.687470000
C	-1.420777000	-1.267020000	2.348694000
C	-0.184060000	-4.132290000	0.244721000
H	0.836076000	-4.202687000	-0.148728000
H	-0.875819000	-4.161110000	-0.605284000
H	-0.361145000	-5.049724000	0.822179000
C	2.044248000	-2.698401000	2.047491000
H	2.163894000	-3.419546000	2.867272000
H	2.701234000	-1.851562000	2.274492000
H	2.423698000	-3.185722000	1.142646000
C	0.601496000	-0.477256000	3.795899000
H	0.062882000	0.453518000	3.997477000
H	1.641148000	-0.212669000	3.577612000
H	0.602676000	-1.058725000	4.727777000
C	-2.475774000	-0.429955000	3.016046000
H	-2.751184000	-0.858268000	3.989001000
H	-3.395336000	-0.373707000	2.424469000
H	-2.135407000	0.594350000	3.206812000
C	-2.966217000	-2.728873000	0.821671000
H	-2.905583000	-3.044860000	-0.227054000
H	-3.351790000	-3.589122000	1.385170000
H	-3.724894000	-1.942678000	0.887897000
C	-8.371285000	0.342654000	-1.174387000
H	-9.023177000	-0.334237000	-1.736395000
H	-8.538164000	0.155037000	-0.106971000
H	-8.695562000	1.368205000	-1.386628000
C	-6.906302000	0.135984000	-1.552077000
H	-6.621482000	-0.908966000	-1.362447000
H	-6.778088000	0.297824000	-2.631418000
C	-5.959373000	1.064195000	-0.788212000
H	-6.086043000	0.904809000	0.292569000
H	-6.241557000	2.109131000	-0.979885000



C	-4.489162000	0.860044000	-1.167979000
H	-4.359370000	1.027868000	-2.245095000
H	-4.204614000	-0.183854000	-0.972857000
C	-3.571263000	1.801304000	-0.394618000
H	-3.654624000	1.650212000	0.686438000
H	-3.814942000	2.845738000	-0.617027000
S	-1.818966000	1.575824000	-0.890953000
C	-0.950946000	2.967272000	-0.049460000
C	2.768351000	4.003192000	0.411632000
H	3.135037000	3.211112000	1.080336000
H	3.098330000	3.743985000	-0.604183000
C	1.234901000	4.032895000	0.461848000
H	0.887842000	4.848731000	-0.188415000
H	0.907404000	4.282519000	1.482136000
C	0.561173000	2.708827000	0.035576000
C	0.863361000	1.511372000	0.959398000
H	0.916230000	2.492438000	-0.987986000
H	1.954507000	1.344577000	0.997944000
H	0.582599000	1.784740000	1.989566000
C	7.546052000	-1.572289000	-0.587189000
H	8.273403000	-0.964609000	-0.039049000
H	7.480184000	-2.545141000	-0.085561000
H	7.946921000	-1.742665000	-1.593294000
C	6.184959000	-0.882501000	-0.642828000
H	5.826886000	-0.692115000	0.379098000
H	6.290214000	0.101968000	-1.119372000
C	5.136701000	-1.699619000	-1.401301000
H	5.026835000	-2.684468000	-0.924520000
H	5.493307000	-1.889761000	-2.423517000
C	3.772313000	-1.005017000	-1.464351000
H	3.878919000	-0.026473000	-1.950067000
H	3.416068000	-0.813997000	-0.441518000
C	2.750364000	-1.843202000	-2.226138000
H	2.580008000	-2.810744000	-1.742342000
H	3.087838000	-2.024469000	-3.252421000
S	1.148035000	-0.958668000	-2.367772000
C	0.166378000	-2.114389000	-3.373713000
H	0.062530000	-3.085902000	-2.884705000
H	-0.819675000	-1.667944000	-3.527872000
H	0.647270000	-2.233837000	-4.347933000
H	-1.180441000	3.871077000	-0.622808000
H	-1.378512000	3.067349000	0.955244000
C	3.376265000	5.314134000	0.818997000
H	3.165922000	5.639081000	1.839767000

C	4.126446000	6.087346000	0.034190000
H	4.363276000	5.804884000	-0.990383000
H	4.537877000	7.029833000	0.385286000
Y	-0.171517000	-0.469584000	0.204364000

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**K3,  $E_{(\text{SCF Done})} = -1297.156956$  a.u.**

C	0.250001000	-2.108004000	1.063623000
C	0.260302000	-2.526173000	-0.302359000
C	1.610827000	-2.481285000	-0.766638000
C	2.433763000	-2.039236000	0.313009000
C	1.595999000	-1.807763000	1.446481000
C	-0.912269000	-3.043489000	-1.089229000
H	-1.868828000	-2.677326000	-0.701932000
H	-0.953332000	-4.140037000	-1.044229000
H	-0.858240000	-2.777675000	-2.151962000
C	2.081423000	-2.948276000	-2.116417000
H	2.169943000	-4.042586000	-2.137321000
H	3.068473000	-2.549547000	-2.372917000
H	1.390601000	-2.676936000	-2.924291000
C	3.934733000	-1.965324000	0.312710000
H	4.309576000	-1.191631000	0.991350000
H	4.345876000	-1.768668000	-0.683636000
H	4.367266000	-2.917101000	0.648740000
C	2.066320000	-1.504811000	2.838882000
H	2.318102000	-2.433056000	3.369022000
H	1.300933000	-0.993891000	3.431292000
H	2.960705000	-0.874166000	2.846663000
C	-0.936435000	-2.117243000	1.987258000
H	-0.993255000	-3.068285000	2.533360000
H	-0.881670000	-1.323969000	2.741201000
H	-1.884161000	-2.005164000	1.449795000
C	-7.308789000	-0.830243000	-0.193958000
H	-7.907763000	-1.437102000	-0.880829000
H	-7.216472000	-1.386034000	0.746762000
H	-7.871373000	0.087192000	0.015140000
C	-5.938781000	-0.515694000	-0.790286000
H	-5.414890000	-1.453866000	-1.023413000
H	-6.065437000	0.010518000	-1.746574000
C	-5.067582000	0.332277000	0.139182000
H	-4.937076000	-0.192549000	1.096747000
H	-5.590311000	1.270929000	0.371191000
C	-3.695095000	0.654478000	-0.461176000
H	-3.824354000	1.188115000	-1.411730000
H	-3.170007000	-0.283609000	-0.693490000

C	-2.850933000	1.500224000	0.486275000
H	-2.666828000	0.983621000	1.434077000
H	-3.348289000	2.451973000	0.700430000
S	-1.237161000	1.930740000	-0.278068000
C	-0.473229000	3.065617000	0.969048000
C	1.622581000	3.473832000	-0.382830000
H	1.016480000	3.106580000	-1.226784000
H	1.522607000	4.565263000	-0.421941000
C	1.057948000	2.964550000	0.965174000
C	1.518291000	1.546652000	1.351967000
H	-0.869651000	2.773731000	1.947110000
H	-0.821601000	4.076998000	0.735596000
C	3.090782000	3.097241000	-0.629822000
C	3.316776000	1.680643000	-1.086816000
C	2.668460000	1.060743000	-2.099844000
H	3.684542000	3.293153000	0.268970000
H	3.499407000	3.750648000	-1.414081000
H	4.120047000	1.130670000	-0.594878000
H	1.381497000	3.689570000	1.731730000
H	0.997936000	1.250592000	2.280070000
H	2.582260000	1.561248000	1.630825000
H	3.010369000	0.092271000	-2.465856000
H	1.932784000	1.585427000	-2.714393000
Y	0.897644000	-0.012806000	-0.298362000

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**TS-3,  $E_{(\text{SCF Done})} = -1297.141648$  a.u.,  $\text{IF} = i294.8351$  cm<sup>-1</sup>**

C	0.427688000	-2.134957000	1.140872000
C	0.330130000	-2.573634000	-0.214413000
C	1.631733000	-2.483628000	-0.804539000
C	2.530460000	-1.993372000	0.186515000
C	1.788923000	-1.766224000	1.386724000
C	-0.890520000	-3.152452000	-0.876475000
H	-1.820858000	-2.799625000	-0.418222000
H	-0.893599000	-4.247318000	-0.790725000
H	-0.937347000	-2.924947000	-1.948131000
C	2.003194000	-2.961908000	-2.179812000
H	2.238268000	-4.034540000	-2.165414000
H	2.885856000	-2.447355000	-2.572672000
H	1.192142000	-2.827203000	-2.904474000
C	4.020947000	-1.881299000	0.045635000
H	4.444627000	-1.117723000	0.706431000
H	4.328008000	-1.646055000	-0.978692000
H	4.503210000	-2.831552000	0.310758000
C	2.371176000	-1.402096000	2.723782000

H	2.693550000	-2.303439000	3.261570000
H	1.648472000	-0.890232000	3.368719000
H	3.249262000	-0.754357000	2.632300000
C	-0.667770000	-2.182070000	2.170259000
H	-0.658471000	-3.143370000	2.701156000
H	-0.558627000	-1.402206000	2.932546000
H	-1.663981000	-2.078522000	1.726106000
C	-7.275572000	-0.963539000	-0.122331000
H	-7.859744000	-1.601034000	-0.793941000
H	-7.170239000	-1.493887000	0.831603000
H	-7.859811000	-0.054865000	0.064316000
C	-5.913442000	-0.631537000	-0.727151000
H	-5.367570000	-1.562472000	-0.937615000
H	-6.052512000	-0.131784000	-1.695774000
C	-5.062586000	0.259096000	0.181111000
H	-4.918938000	-0.239484000	1.150760000
H	-5.607274000	1.190411000	0.390893000
C	-3.698597000	0.599431000	-0.428619000
H	-3.841615000	1.109032000	-1.390295000
H	-3.153179000	-0.331898000	-0.641406000
C	-2.872756000	1.484807000	0.499368000
H	-2.671089000	0.989907000	1.455397000
H	-3.394894000	2.426337000	0.699599000
S	-1.276089000	1.942593000	-0.286060000
C	-0.522877000	3.068223000	0.965170000
C	1.486643000	3.709578000	-0.500242000
H	0.840746000	3.369028000	-1.323731000
H	1.445390000	4.804122000	-0.507129000
C	1.002651000	3.130087000	0.844483000
C	1.705271000	1.777534000	1.062070000
H	-0.818709000	2.703970000	1.955092000
H	-0.965031000	4.058113000	0.813931000
C	2.903601000	3.195404000	-0.723521000
C	2.932138000	1.675631000	-0.708821000
C	2.449488000	0.905465000	-1.805421000
H	3.565425000	3.590753000	0.056703000
H	3.302009000	3.536196000	-1.686306000
H	3.780626000	1.239936000	-0.182890000
H	1.317542000	3.823279000	1.638642000
H	1.073927000	1.093042000	1.690099000
H	2.604451000	1.894593000	1.670235000
H	3.085052000	0.093293000	-2.155807000
H	1.925394000	1.443703000	-2.602752000
Y	0.831473000	-0.042425000	-0.319790000

**L3,  $E_{(\text{SCF Done})} = -1297.166110$  a.u.**

C	0.317676000	-2.447293000	1.006338000
C	0.379711000	-2.813656000	-0.372565000
C	1.712998000	-2.569697000	-0.837107000
C	2.470899000	-2.047604000	0.247733000
C	1.605421000	-1.954716000	1.386418000
C	-0.724734000	-3.457543000	-1.165988000
H	-1.720290000	-3.168183000	-0.810627000
H	-0.669503000	-4.551415000	-1.087134000
H	-0.668225000	-3.219570000	-2.234424000
C	2.247014000	-2.903460000	-2.200668000
H	2.674949000	-3.914695000	-2.210601000
H	3.038358000	-2.213928000	-2.510766000
H	1.468222000	-2.883693000	-2.970878000
C	3.947369000	-1.783791000	0.240588000
H	4.235857000	-1.018795000	0.968462000
H	4.300096000	-1.457048000	-0.742010000
H	4.500704000	-2.696588000	0.499092000
C	2.027152000	-1.587850000	2.783356000
H	2.366602000	-2.478867000	3.327882000
H	1.208916000	-1.154093000	3.369443000
H	2.858534000	-0.875498000	2.791968000
C	-0.854883000	-2.649351000	1.925519000
H	-0.808562000	-3.640131000	2.397015000
H	-0.879953000	-1.916494000	2.740074000
H	-1.814455000	-2.597671000	1.399077000
C	-7.187944000	-0.747653000	-0.077849000
H	-7.731905000	-1.496626000	-0.662442000
H	-7.173256000	-1.085886000	0.965032000
H	-7.761939000	0.185424000	-0.117706000
C	-5.773460000	-0.550692000	-0.618213000
H	-5.236467000	-1.510240000	-0.600227000
H	-5.821338000	-0.244882000	-1.672564000
C	-4.976699000	0.489481000	0.172393000
H	-4.923338000	0.184688000	1.227544000
H	-5.512500000	1.448804000	0.154580000
C	-3.560009000	0.696682000	-0.373455000
H	-3.613287000	1.017161000	-1.422280000
H	-3.025771000	-0.266645000	-0.360469000
C	-2.785346000	1.729685000	0.439469000
H	-2.661778000	1.409993000	1.480040000
H	-3.306083000	2.692879000	0.434329000
S	-1.129192000	2.030563000	-0.294268000

C	-0.402264000	3.243594000	0.891223000
C	1.588434000	3.959162000	-0.629196000
H	0.940674000	3.596043000	-1.438655000
H	1.566215000	5.052491000	-0.672833000
C	1.107034000	3.424047000	0.737560000
C	1.972885000	2.156170000	0.994275000
H	-0.651612000	2.900520000	1.901916000
H	-0.919663000	4.191833000	0.713162000
C	2.996136000	3.375785000	-0.781623000
C	2.852805000	1.921836000	-0.278828000
C	2.294531000	0.956529000	-1.350180000
H	3.699037000	3.931975000	-0.145352000
H	3.372813000	3.419489000	-1.807948000
H	3.821237000	1.525060000	0.044501000
H	1.364868000	4.164328000	1.506434000
H	1.356336000	1.301020000	1.358715000
H	2.633672000	2.328532000	1.850939000
H	3.119636000	0.538955000	-1.935644000
H	1.667070000	1.521799000	-2.073678000
Y	0.647303000	-0.260181000	-0.302073000

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**K3',  $E_{(\text{SCF Done})} = -1932.308301$  a.u.**

C	-1.002133000	1.075503000	2.416373000
C	-0.499058000	-0.261248000	2.464221000
C	0.927026000	-0.197290000	2.425721000
C	1.303981000	1.175739000	2.334720000
C	0.109908000	1.962501000	2.328117000
C	-1.307229000	-1.504594000	2.714196000
H	-2.349453000	-1.388407000	2.401180000
H	-1.323578000	-1.747622000	3.785399000
H	-0.900655000	-2.383524000	2.199535000
C	1.854468000	-1.355937000	2.655169000
H	2.011517000	-1.515732000	3.730836000
H	2.842999000	-1.193336000	2.213456000
H	1.454749000	-2.293816000	2.253675000
C	2.704283000	1.711536000	2.448246000
H	2.824376000	2.679027000	1.948469000
H	3.451563000	1.025306000	2.033891000
H	2.972337000	1.867947000	3.501842000
C	0.045051000	3.460827000	2.398444000
H	0.038818000	3.798588000	3.443613000
H	-0.857703000	3.857778000	1.924526000
H	0.907307000	3.936346000	1.918500000
C	-2.435049000	1.484625000	2.598872000

H	-2.683739000	1.540349000	3.667351000
H	-2.636930000	2.470244000	2.169557000
H	-3.136406000	0.776841000	2.144740000
C	-7.743872000	-2.350226000	0.957521000
H	-8.395863000	-2.016374000	1.771473000
H	-8.332520000	-2.334401000	0.032671000
H	-7.467989000	-3.392265000	1.158556000
C	-6.507600000	-1.461413000	0.842262000
H	-6.817392000	-0.420199000	0.675173000
H	-5.959408000	-1.469041000	1.795181000
C	-5.566999000	-1.894154000	-0.284739000
H	-6.115438000	-1.888265000	-1.237639000
H	-5.253644000	-2.935138000	-0.117894000
C	-4.328087000	-1.000084000	-0.405509000
H	-3.772604000	-1.005083000	0.540876000
H	-4.646000000	0.036265000	-0.577628000
C	-3.410505000	-1.463731000	-1.529324000
H	-3.938844000	-1.502428000	-2.488720000
H	-3.034057000	-2.474164000	-1.334016000
S	-1.905504000	-0.455935000	-1.827374000
C	-2.571475000	1.116359000	-2.519759000
C	-0.338395000	2.142903000	-3.132011000
H	0.085755000	1.127301000	-3.055226000
H	-0.601716000	2.268299000	-4.190367000
C	-1.602257000	2.273799000	-2.261898000
C	-1.282677000	2.387563000	-0.765771000
H	-3.525751000	1.311881000	-2.022099000
H	-2.754300000	0.952351000	-3.587056000
C	0.754635000	3.161451000	-2.767905000
C	1.480710000	2.870684000	-1.478602000
C	2.260144000	1.789122000	-1.256226000
H	0.317442000	4.165133000	-2.725262000
H	1.501280000	3.178495000	-3.572645000
H	-2.141307000	3.168497000	-2.620746000
C	7.964410000	-1.676466000	0.253453000
H	8.777649000	-0.943407000	0.268430000
H	7.869854000	-2.089118000	1.264952000
H	8.266093000	-2.493476000	-0.412470000
C	6.656772000	-1.038882000	-0.210412000
H	6.400979000	-0.200845000	0.454067000
H	6.793224000	-0.606018000	-1.211309000
C	5.491719000	-2.030328000	-0.244926000
H	5.350492000	-2.462265000	0.756504000
H	5.747598000	-2.868907000	-0.907941000

C	4.180176000	-1.395156000	-0.718596000
H	4.318294000	-0.977526000	-1.724724000
H	3.924770000	-0.556323000	-0.056458000
C	3.040572000	-2.406851000	-0.735892000
H	2.847149000	-2.803365000	0.265644000
H	3.289443000	-3.245575000	-1.395786000
S	1.484435000	-1.697688000	-1.403851000
C	0.463347000	-3.199544000	-1.474013000
H	0.268033000	-3.603798000	-0.477249000
H	-0.475555000	-2.934783000	-1.964453000
H	0.975323000	-3.948141000	-2.084651000
H	2.882027000	1.725128000	-0.364453000
H	1.427358000	3.629100000	-0.698055000
H	2.436101000	1.049068000	-2.036816000
Y	0.081790000	0.606309000	0.068246000
H	-0.944858000	3.407824000	-0.535720000
H	-2.220727000	2.273253000	-0.193103000

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**TS-3',  $E_{(\text{SCF Done})} = -1932.295079$  a.u., IF =  $i291.4027$  cm<sup>-1</sup>**

C	1.043920000	0.562840000	-2.538733000
C	0.503971000	-0.748246000	-2.383711000
C	-0.921465000	-0.640312000	-2.387486000
C	-1.261575000	0.735995000	-2.545084000
C	-0.047263000	1.481268000	-2.628464000
C	1.278321000	-2.036828000	-2.396678000
H	2.317008000	-1.899025000	-2.079801000
H	1.310816000	-2.460191000	-3.409863000
H	0.832482000	-2.803621000	-1.751809000
C	-1.881603000	-1.793900000	-2.446178000
H	-2.050460000	-2.101602000	-3.487354000
H	-2.861729000	-1.540740000	-2.028941000
H	-1.504893000	-2.675330000	-1.915509000
C	-2.640559000	1.274260000	-2.795932000
H	-2.741300000	2.320544000	-2.488839000
H	-3.414061000	0.699761000	-2.274889000
H	-2.880605000	1.233484000	-3.867023000
C	0.064464000	2.940944000	-2.963721000
H	0.090879000	3.085899000	-4.052170000
H	0.977268000	3.392505000	-2.561330000
H	-0.786394000	3.519528000	-2.588688000
C	2.490519000	0.905839000	-2.760188000
H	2.734684000	0.863689000	-3.830342000
H	2.734744000	1.918310000	-2.420948000
H	3.169742000	0.213695000	-2.252328000



C	7. 586744000	-2. 474139000	-0. 524675000
H	8. 190672000	-2. 346222000	-1. 429032000
H	8. 218241000	-2. 220953000	0. 335045000
H	7. 327170000	-3. 536508000	-0. 445664000
C	6. 336003000	-1. 599352000	-0. 569638000
H	6. 627972000	-0. 545816000	-0. 683528000
H	5. 743296000	-1. 851798000	-1. 460573000
C	5. 461772000	-1. 748123000	0. 677668000
H	6. 055105000	-1. 497808000	1. 568728000
H	5. 166703000	-2. 801380000	0. 792006000
C	4. 207691000	-0. 867816000	0. 639078000
H	3. 605530000	-1. 117558000	-0. 244003000
H	4. 507771000	0. 182526000	0. 529108000
C	3. 359858000	-1. 047376000	1. 891057000
H	3. 934565000	-0. 837232000	2. 800318000
H	3. 005039000	-2. 080465000	1. 976776000
S	1. 840515000	-0. 023493000	2. 017670000
C	2. 520053000	1. 660831000	2. 292333000
C	0. 275685000	2. 797656000	2. 812812000
H	-0. 105969000	1. 782523000	3. 007170000
H	0. 503442000	3. 238687000	3. 790144000
C	1. 515162000	2. 746190000	1. 904246000
C	1. 032964000	2. 643522000	0. 449965000
H	3. 428839000	1. 753394000	1. 689935000
H	2. 791354000	1. 735367000	3. 350521000
C	-0. 776915000	3. 601459000	2. 058215000
C	-1. 102101000	2. 950349000	0. 722367000
C	-1. 972197000	1. 833574000	0. 641822000
H	-0. 405233000	4. 621209000	1. 896708000
H	-1. 703888000	3. 684242000	2. 637315000
H	2. 057572000	3. 694451000	2. 039525000
C	-7. 943096000	-1. 463386000	0. 238632000
H	-8. 729723000	-0. 703780000	0. 181103000
H	-7. 914319000	-1. 985939000	-0. 725018000
H	-8. 239756000	-2. 191330000	1. 002963000
C	-6. 591950000	-0. 833483000	0. 569068000
H	-6. 339525000	-0. 083322000	-0. 194162000
H	-6. 662304000	-0. 289538000	1. 521347000
C	-5. 462503000	-1. 861978000	0. 659142000
H	-5. 389134000	-2. 406452000	-0. 293715000
H	-5. 714152000	-2. 611944000	1. 422560000
C	-4. 107020000	-1. 231547000	0. 995209000
H	-4. 176532000	-0. 700157000	1. 953483000
H	-3. 853192000	-0. 481267000	0. 234869000

C	-3.006132000	-2.282885000	1.072956000
H	-2.882335000	-2.800309000	0.116720000
H	-3.244656000	-3.028459000	1.840003000
S	-1.392799000	-1.562576000	1.570280000
C	-0.403826000	-3.078417000	1.734226000
H	-0.289274000	-3.595177000	0.777767000
H	0.577017000	-2.796118000	2.123513000
H	-0.882459000	-3.742009000	2.459504000
H	-2.721071000	1.839050000	-0.148006000
H	-1.140866000	3.630497000	-0.126279000
H	-2.304761000	1.393006000	1.585233000
Y	-0.109835000	0.515905000	-0.168659000
H	1.072581000	3.611973000	-0.051919000
H	1.724694000	2.012860000	-0.159962000

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**M3,  $E_{(\text{SCF Done})} = -1932.322581$  a.u.**

C	-1.181060000	-0.568528000	2.688887000
C	-0.986286000	-1.833199000	2.056601000
C	0.411858000	-2.124268000	2.077707000
C	1.078972000	-1.044324000	2.734471000
C	0.099236000	-0.087658000	3.117932000
C	-2.072078000	-2.761726000	1.589178000
H	-2.988035000	-2.225147000	1.320015000
H	-2.344940000	-3.470307000	2.382974000
H	-1.771317000	-3.362229000	0.722620000
C	1.046748000	-3.432704000	1.697986000
H	1.198743000	-4.057416000	2.588490000
H	2.031796000	-3.308725000	1.233269000
H	0.418608000	-4.011688000	1.013771000
C	2.539042000	-0.999477000	3.081085000
H	2.916145000	0.026132000	3.135533000
H	3.154351000	-1.540489000	2.353591000
H	2.720513000	-1.465800000	4.059071000
C	0.344217000	1.114149000	3.982421000
H	0.273232000	0.840137000	5.043937000
H	-0.386734000	1.910191000	3.809881000
H	1.340326000	1.537144000	3.822716000
C	-2.508811000	0.055129000	3.023501000
H	-2.880332000	-0.320486000	3.986450000
H	-2.443967000	1.144645000	3.114051000
H	-3.278787000	-0.170595000	2.277448000
C	-7.425938000	-1.705925000	-1.759446000
H	-8.175763000	-2.041694000	-1.035619000
H	-7.911026000	-0.988276000	-2.431424000

H	-7.129531000	-2.575051000	-2.358705000
C	-6.223483000	-1.080275000	-1.056405000
H	-6.557642000	-0.234891000	-0.438601000
H	-5.782069000	-1.811229000	-0.363552000
C	-5.148770000	-0.596671000	-2.032730000
H	-5.590170000	0.133075000	-2.726345000
H	-4.811534000	-1.441305000	-2.651378000
C	-3.942859000	0.036802000	-1.331045000
H	-3.495710000	-0.689646000	-0.637542000
H	-4.283475000	0.883636000	-0.721106000
C	-2.887380000	0.500837000	-2.328068000
H	-3.303102000	1.214545000	-3.048566000
H	-2.495870000	-0.340071000	-2.911920000
S	-1.397342000	1.305080000	-1.624438000
C	-2.054183000	2.935789000	-1.075487000
C	0.257579000	4.141368000	-1.059996000
H	0.541718000	3.346114000	-1.762193000
H	0.132846000	5.055168000	-1.650092000
C	-1.031059000	3.761380000	-0.297910000
C	-0.542012000	3.119867000	1.030206000
H	-2.944526000	2.755751000	-0.464645000
H	-2.358208000	3.457799000	-1.989384000
C	1.312675000	4.270017000	0.043621000
C	1.012671000	3.079947000	0.981314000
C	1.615212000	1.744037000	0.498242000
H	1.173885000	5.220990000	0.577618000
H	2.339048000	4.252696000	-0.337011000
H	-1.567160000	4.687531000	-0.050674000
C	7.664710000	-0.232075000	-1.728241000
H	8.294245000	0.663618000	-1.707460000
H	7.925259000	-0.841733000	-0.854791000
H	7.930863000	-0.804179000	-2.624907000
C	6.183017000	0.136824000	-1.725820000
H	5.954827000	0.739175000	-0.835030000
H	5.960846000	0.774659000	-2.592637000
C	5.266334000	-1.088167000	-1.754451000
H	5.485079000	-1.726496000	-0.885946000
H	5.492709000	-1.691309000	-2.645297000
C	3.779338000	-0.717647000	-1.756607000
H	3.556788000	-0.089679000	-2.629109000
H	3.552868000	-0.115332000	-0.866516000
C	2.896227000	-1.960283000	-1.786804000
H	3.062633000	-2.594968000	-0.910046000
H	3.096205000	-2.554395000	-2.685466000

S	1.114091000	-1.521501000	-1.865798000
C	0.356471000	-3.160736000	-2.079249000
H	0.638791000	-3.837554000	-1.270490000
H	-0.729121000	-3.034902000	-2.088554000
H	0.668747000	-3.574254000	-3.041718000
H	2.631719000	1.635334000	0.899858000
H	1.401138000	3.275049000	1.986686000
H	1.747907000	1.780607000	-0.608308000
Y	0.124373000	-0.046944000	0.493922000
H	-0.875357000	3.728136000	1.878990000
H	-1.018339000	2.136346000	1.213544000

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**TS1',  $E_{(\text{SCF Done})} = -1476.39064714$  a.u., IF =  $i1270.7113$  cm<sup>-1</sup>**

N	1.441586000	0.604160000	-1.947280000
C	-0.162542000	1.975414000	0.061408000
C	1.334322000	2.081455000	0.013552000
C	2.130751000	1.409644000	-0.950058000
C	3.528311000	1.539781000	-0.943124000
H	4.129033000	1.030863000	-1.689460000
C	4.153852000	2.349570000	-0.005784000
H	5.234210000	2.458913000	-0.023500000
C	3.387606000	3.032268000	0.943351000
H	3.869151000	3.679630000	1.670589000
C	2.009847000	2.882944000	0.955972000
H	1.416874000	3.419398000	1.692185000
C	2.269628000	-0.437734000	-2.584729000
H	3.021150000	-0.010579000	-3.261743000
H	1.616734000	-1.090815000	-3.169620000
H	2.782991000	-1.035884000	-1.826273000
C	0.839570000	1.456274000	-2.996506000
H	0.185554000	2.206704000	-2.553174000
H	0.258186000	0.837145000	-3.682642000
H	1.627500000	1.968536000	-3.564099000
C	-0.563019000	-1.981646000	1.525828000
C	0.550926000	-2.580930000	0.862134000
C	1.710097000	-1.807334000	1.159063000
C	1.317919000	-0.741969000	2.028934000
C	-0.087681000	-0.837422000	2.236513000
C	0.532720000	-3.886574000	0.122733000
H	1.233492000	-3.903234000	-0.719731000
H	-0.462386000	-4.120934000	-0.265462000
H	0.821590000	-4.707542000	0.792626000
C	3.126017000	-2.156300000	0.793737000
H	3.605563000	-2.718720000	1.606233000

H	3.743918000	-1.268251000	0.618682000
H	3.178326000	-2.791207000	-0.097354000
C	2.268021000	0.143133000	2.777671000
H	1.791317000	1.058801000	3.135987000
H	3.135380000	0.431225000	2.177376000
H	2.646757000	-0.389939000	3.660652000
C	-0.901596000	0.013188000	3.168763000
H	-0.985099000	-0.462358000	4.155018000
H	-1.921090000	0.172747000	2.802444000
H	-0.448792000	0.996855000	3.326655000
C	-1.918859000	-2.608812000	1.683019000
H	-1.859781000	-3.445304000	2.392197000
H	-2.649746000	-1.904136000	2.089017000
H	-2.319613000	-3.009209000	0.746580000
Sc	0.281082000	-0.356339000	-0.171157000
C	-5.608312000	2.957402000	0.897446000
H	-6.628881000	2.968237000	1.294022000
H	-4.949447000	3.377784000	1.667080000
H	-5.581869000	3.630797000	0.032303000
C	-5.181835000	1.542829000	0.512458000
H	-5.253430000	0.884778000	1.389837000
H	-5.881593000	1.136607000	-0.230832000
C	-3.759740000	1.479241000	-0.050577000
H	-3.061497000	1.892011000	0.691904000
H	-3.693917000	2.133296000	-0.933573000
C	-3.335623000	0.057533000	-0.432621000
H	-4.078620000	-0.358725000	-1.128641000
H	-3.359628000	-0.583320000	0.455054000
C	-1.950483000	0.004794000	-1.075040000
S	-1.435329000	-1.651895000	-1.632681000
C	-1.565290000	-1.620206000	-3.451289000
H	-1.008685000	-0.793834000	-3.896100000
H	-2.619380000	-1.549236000	-3.730500000
H	-1.164161000	-2.568916000	-3.818999000
H	-1.061105000	0.942571000	-0.376030000
H	-1.929843000	0.640371000	-1.973118000
H	-0.525996000	2.281548000	1.046680000
H	-0.629358000	2.648367000	-0.671249000

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**2,1-TS2',  $E_{(\text{SCF Done})} = -2020.51522117$  a.u., IF =  $i254.5565$  cm<sup>-1</sup>**

C	1.093931000	-2.111895000	1.745123000
C	-0.041986000	-1.566309000	2.415675000
C	-1.191776000	-2.317817000	2.028634000
C	-0.765336000	-3.328568000	1.118613000

C	0.644528000	-3.207226000	0.948545000
C	0.003313000	-0.522099000	3.493197000
H	-0.959330000	-0.017365000	3.619466000
H	0.766683000	0.240064000	3.305062000
H	0.247406000	-0.981681000	4.460535000
C	-2.571310000	-2.163981000	2.599175000
H	-2.681704000	-2.770354000	3.508013000
H	-3.349522000	-2.489749000	1.902284000
H	-2.792630000	-1.128774000	2.879599000
C	-1.606467000	-4.434031000	0.549473000
H	-1.360300000	-4.656865000	-0.495388000
H	-2.675759000	-4.209233000	0.599237000
H	-1.451419000	-5.362443000	1.115183000
C	1.504586000	-4.209783000	0.233420000
H	1.641592000	-5.101450000	0.859786000
H	2.505150000	-3.826241000	0.014938000
H	1.063773000	-4.558346000	-0.707890000
C	2.519130000	-1.710802000	1.995770000
H	2.626732000	-0.630738000	2.142205000
H	2.902082000	-2.194623000	2.904522000
H	3.183692000	-2.001913000	1.177207000
Sc	-0.366396000	-1.151368000	0.018756000
C	8.104118000	-0.700988000	-1.516238000
H	8.910724000	-0.001047000	-1.274307000
H	8.210864000	-1.571413000	-0.857917000
H	8.258548000	-1.042091000	-2.546703000
C	6.736167000	-0.043319000	-1.349615000
H	6.625399000	0.319599000	-0.317876000
H	6.672990000	0.843506000	-1.995507000
C	5.578975000	-0.988924000	-1.679204000
H	5.639525000	-1.877308000	-1.033810000
H	5.687337000	-1.350562000	-2.711580000
C	4.205277000	-0.329060000	-1.515152000
H	4.142652000	0.552772000	-2.166413000
H	4.092146000	0.027301000	-0.482109000
C	3.074319000	-1.295245000	-1.854020000
H	3.069596000	-2.160691000	-1.187488000
H	3.161574000	-1.651047000	-2.886015000
S	1.440468000	-0.447596000	-1.747766000
C	0.192417000	-1.670575000	-2.215544000
H	-2.397369000	2.086353000	1.376164000
H	4.802357000	6.001637000	1.988683000
C	-1.370752000	2.399368000	1.572775000
H	-1.079208000	2.104586000	2.583106000

H	-1.311124000	3.484420000	1.464572000
S	-0.304632000	1.616035000	0.326384000
C	1.347251000	2.239455000	0.822274000
H	1.465432000	2.068261000	1.898306000
H	2.060105000	1.592992000	0.301237000
H	0.500837000	-2.677620000	-1.897672000
H	0.052043000	-1.670306000	-3.294083000
H	5.420045000	5.506621000	0.404704000
C	1.579207000	3.702601000	0.456444000
H	0.832049000	4.338788000	0.948265000
H	1.439861000	3.830526000	-0.624368000
C	2.981070000	4.168609000	0.862623000
H	3.733974000	3.534017000	0.372331000
H	3.117144000	4.027093000	1.944872000
C	3.246422000	5.633494000	0.507271000
H	2.494137000	6.266404000	0.998222000
H	3.106352000	5.774472000	-0.573449000
C	4.644925000	6.097282000	0.907701000
H	4.803660000	7.147447000	0.641289000
C	-2.499316000	-1.272113000	-0.804764000
H	-1.926743000	-2.421780000	-2.542635000
C	-1.873070000	-1.448492000	-2.058317000
H	-1.880385000	-0.613186000	-2.757992000
H	-2.918851000	-2.176885000	-0.365824000
C	-3.277917000	-0.001267000	-0.500870000
H	-3.308714000	0.181024000	0.584216000
H	-2.781577000	0.868699000	-0.957070000
C	-4.728620000	-0.058122000	-1.011762000
H	-4.714099000	-0.215603000	-2.099311000
H	-5.223761000	-0.940105000	-0.581212000
C	-5.535614000	1.197186000	-0.679401000
H	-5.034221000	2.078025000	-1.108474000
H	-5.542386000	1.348513000	0.411048000
C	-6.977835000	1.141340000	-1.187019000
H	-6.973809000	0.989655000	-2.276462000
H	-7.479667000	0.260738000	-0.759567000
C	-7.788369000	2.395411000	-0.854856000
H	-7.286096000	3.274943000	-1.282492000
H	-7.791893000	2.546405000	0.234195000
C	-9.226196000	2.330766000	-1.365234000
H	-9.779917000	3.241532000	-1.112597000
H	-9.256038000	2.215426000	-2.455452000
H	-9.765439000	1.481924000	-0.927651000

**B',  $E_{(\text{SCF Done})} = -2111.565494$  a.u.**

Sc	0.258615000	-1.353456000	0.291078000
C	-1.946012000	-1.723457000	0.025336000
H	1.771432000	-0.745300000	-3.316958000
C	2.465184000	-0.160943000	-2.711384000
C	-1.570446000	-0.614992000	-3.595533000
H	-1.938799000	0.132671000	-4.290666000
C	-0.623097000	-1.541009000	-4.054769000
H	-0.278755000	-1.488730000	-5.084189000
C	-0.176406000	-2.541441000	-3.207149000
H	0.519909000	-3.299677000	-3.554914000
C	-0.659906000	-2.585329000	-1.890601000
H	-0.392805000	-3.434970000	-1.264969000
C	1.679461000	-3.361967000	0.542535000
C	2.383030000	-2.282210000	1.151342000
C	1.632734000	-1.851938000	2.285185000
C	0.461342000	-2.665728000	2.375022000
C	0.500615000	-3.608665000	1.311299000
C	3.772983000	-1.846455000	0.790018000
H	4.003295000	-0.843784000	1.161667000
H	3.946607000	-1.856537000	-0.291510000
H	4.513600000	-2.526490000	1.232782000
C	2.114016000	-0.903412000	3.344596000
H	1.288144000	-0.418360000	3.874399000
H	2.774240000	-0.126201000	2.944220000
H	2.695919000	-1.447474000	4.100828000
C	-0.562012000	-2.620861000	3.471360000
H	-1.555989000	-2.910453000	3.115838000
H	-0.650780000	-1.621685000	3.907626000
H	-0.292924000	-3.311168000	4.282244000
C	-0.436034000	-4.769330000	1.145558000
H	-0.036089000	-5.650701000	1.664548000
H	-0.582619000	-5.062064000	0.100217000
H	-1.421902000	-4.568522000	1.575237000
C	2.206347000	-4.210851000	-0.579427000
H	2.961105000	-4.915328000	-0.204793000
H	1.421688000	-4.811930000	-1.049084000
H	2.686892000	-3.617669000	-1.365564000
N	-3.105208000	0.228598000	-1.869382000
C	5.600480000	5.720127000	-0.196191000
H	5.773678000	6.705995000	-0.640109000
H	5.353198000	5.871171000	0.861501000
H	6.545232000	5.165383000	-0.241019000
C	4.485084000	4.975935000	-0.926547000



H	3. 562377000	5. 572224000	-0. 896047000
H	4. 746199000	4. 871668000	-1. 988826000
C	4. 209768000	3. 590156000	-0. 338135000
H	3. 949888000	3. 692909000	0. 726084000
H	5. 132050000	2. 992020000	-0. 371042000
C	3. 089805000	2. 842815000	-1. 068774000
H	3. 356008000	2. 736084000	-2. 128564000
H	2. 164188000	3. 432561000	-1. 041084000
C	2. 833304000	1. 468246000	-0. 457110000
H	2. 508483000	1. 558935000	0. 583393000
H	3. 738438000	0. 852337000	-0. 462702000
S	1. 515884000	0. 526979000	-1. 322772000
C	-2. 094639000	-0. 662651000	-2. 303123000
C	-1. 630630000	-1. 675653000	-1. 396134000
C	-2. 029412000	1. 801167000	1. 180347000
S	-0. 627754000	0. 785261000	1. 799099000
C	0. 472111000	2. 119841000	2. 365080000
C	-4. 410664000	-0. 415807000	-1. 682424000
H	-4. 302637000	-1. 340127000	-1. 112404000
H	-5. 073501000	0. 257364000	-1. 129817000
H	-4. 884325000	-0. 656829000	-2. 648110000
C	-3. 241335000	1. 460194000	-2. 631887000
H	-3. 908527000	2. 136738000	-2. 088786000
H	-2. 267320000	1. 947304000	-2. 736403000
H	-3. 673116000	1. 310753000	-3. 636535000
C	-2. 923330000	2. 268099000	2. 330658000
C	-3. 991454000	3. 285974000	1. 909172000
C	-5. 107992000	2. 725221000	1. 027392000
C	-6. 176214000	3. 765561000	0. 696572000
H	-5. 747646000	4. 620163000	0. 159225000
H	-6. 967621000	3. 340495000	0. 069890000
H	-6. 646996000	4. 151225000	1. 608412000
H	3. 277734000	-0. 798230000	-2. 353717000
H	2. 866482000	0. 657393000	-3. 313757000
H	0. 727493000	2. 793469000	1. 542670000
H	-0. 025764000	2. 684235000	3. 157160000
H	1. 377158000	1. 674099000	2. 778740000
H	-2. 121754000	-2. 726251000	0. 420108000
H	-2. 694200000	-1. 019236000	0. 380944000
H	-1. 597737000	2. 648802000	0. 634473000
H	-2. 556915000	1. 181689000	0. 448858000
H	-2. 301829000	2. 724787000	3. 111418000
H	-3. 400466000	1. 393389000	2. 791137000
H	-4. 439325000	3. 699235000	2. 822826000

H	-3.509904000	4.134791000	1.401137000
H	-4.682927000	2.330993000	0.094363000
H	-5.572875000	1.869566000	1.537714000

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**TS1',  $E_{(\text{SCF Done})} = -2111.515125$  a.u., IF =  $i1222.7897$  cm<sup>-1</sup>**

Sc	0.400250000	-0.982056000	0.503502000
C	-1.788258000	-1.249575000	-0.146500000
H	-0.634784000	-1.028554000	-1.069038000
C	0.454968000	-0.651062000	-1.855619000
C	-4.788028000	-0.896891000	-2.475778000
H	-5.701439000	-0.317572000	-2.565784000
C	-4.479642000	-1.827603000	-3.465225000
H	-5.147218000	-1.951899000	-4.313505000
C	-3.330702000	-2.604113000	-3.352389000
H	-3.084630000	-3.341939000	-4.110942000
C	-2.487058000	-2.414806000	-2.260604000
H	-1.577104000	-3.006349000	-2.181313000
C	0.686509000	-3.404817000	0.776456000
C	1.951964000	-2.880578000	0.368584000
C	2.436251000	-2.033049000	1.410737000
C	1.467700000	-2.030967000	2.459035000
C	0.385688000	-2.873452000	2.061885000
C	2.724333000	-3.327280000	-0.839264000
H	3.468828000	-2.590847000	-1.156521000
H	2.078462000	-3.542469000	-1.697285000
H	3.272640000	-4.252945000	-0.619376000
C	3.795239000	-1.396441000	1.470869000
H	3.788739000	-0.442229000	2.007705000
H	4.207494000	-1.210276000	0.475003000
H	4.505150000	-2.052279000	1.992373000
C	1.634121000	-1.448096000	3.834027000
H	0.743935000	-0.914800000	4.187396000
H	2.487743000	-0.766443000	3.890994000
H	1.828116000	-2.249928000	4.558655000
C	-0.793032000	-3.222238000	2.924261000
H	-0.510338000	-3.975320000	3.672114000
H	-1.618856000	-3.646450000	2.345044000
H	-1.178480000	-2.356893000	3.475979000
C	-0.100485000	-4.453653000	0.046613000
H	0.193816000	-5.454821000	0.388897000
H	-1.178629000	-4.362909000	0.210508000
H	0.073955000	-4.423408000	-1.033201000
N	-4.273080000	0.222875000	-0.332051000
C	7.757323000	2.569979000	-2.311135000

H	8.424477000	3.353387000	-1.936699000
H	8.243908000	1.604249000	-2.129440000
H	7.669397000	2.699437000	-3.396300000
C	6.391313000	2.639802000	-1.632434000
H	6.515309000	2.543322000	-0.544451000
H	5.945283000	3.629405000	-1.803785000
C	5.426409000	1.560478000	-2.128368000
H	5.869761000	0.568825000	-1.956808000
H	5.300064000	1.657246000	-3.216023000
C	4.053875000	1.632340000	-1.450101000
H	3.609105000	2.620341000	-1.628580000
H	4.175908000	1.528174000	-0.363262000
C	3.114077000	0.549132000	-1.968609000
H	3.502978000	-0.452396000	-1.766331000
H	2.953871000	0.649470000	-3.047055000
S	1.452267000	0.707309000	-1.194175000
C	-3.956551000	-0.711553000	-1.363703000
C	-2.766411000	-1.472153000	-1.263095000
C	-1.020961000	2.459370000	1.174798000
S	-0.165933000	1.143765000	2.138695000
C	1.427921000	1.949193000	2.479731000
C	-4.777638000	-0.417484000	0.883876000
H	-4.108482000	-1.222599000	1.197919000
H	-4.830386000	0.322270000	1.690738000
H	-5.783959000	-0.846200000	0.741126000
C	-5.140524000	1.323936000	-0.725166000
H	-5.142429000	2.072299000	0.073964000
H	-4.760463000	1.792333000	-1.637452000
H	-6.188518000	1.022232000	-0.895367000
C	-1.421528000	3.652038000	2.043872000
C	-1.921373000	4.848854000	1.222798000
C	-3.218972000	4.612449000	0.448805000
C	-3.709053000	5.868218000	-0.269593000
H	-2.966831000	6.227941000	-0.992212000
H	-4.638974000	5.677416000	-0.815702000
H	-3.901405000	6.680973000	0.440530000
H	1.090210000	-1.481366000	-2.179121000
H	-0.168855000	-0.318282000	-2.689074000
H	1.929780000	2.223585000	1.548464000
H	1.266806000	2.834394000	3.098381000
H	2.042382000	1.242554000	3.038861000
H	-1.852358000	-2.060757000	0.596891000
H	-2.056814000	-0.308850000	0.368141000
H	-0.355205000	2.759001000	0.356865000

H	-1.897072000	1.971065000	0.734320000
H	-0.561677000	3.983458000	2.638479000
H	-2.191213000	3.334684000	2.758794000
H	-2.068443000	5.688454000	1.915216000
H	-1.131163000	5.167768000	0.527076000
H	-3.078581000	3.808047000	-0.286224000
H	-3.993685000	4.262457000	1.146338000

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**C'', E<sub>(SCF Done)</sub> = -2111.556644 a.u.**

Sc	0.680999000	-1.034374000	-0.162046000
C	-2.077164000	-1.451901000	-1.122354000
H	-1.183535000	-1.115681000	-1.678849000
C	1.100082000	0.002771000	-2.071165000
C	-5.340535000	0.493670000	-0.816224000
H	-6.184556000	0.586481000	-0.139793000
C	-5.309050000	1.267201000	-1.974450000
H	-6.124319000	1.954846000	-2.182651000
C	-4.247242000	1.145861000	-2.866974000
H	-4.218934000	1.738602000	-3.776695000
C	-3.214392000	0.256395000	-2.578389000
H	-2.377922000	0.163777000	-3.268728000
C	0.956289000	-3.419095000	-0.620398000
C	2.255301000	-2.832378000	-0.650347000
C	2.558231000	-2.358949000	0.664048000
C	1.445495000	-2.662360000	1.505180000
C	0.454735000	-3.314875000	0.712004000
C	3.193262000	-2.884425000	-1.819968000
H	3.933252000	-2.078894000	-1.802061000
H	2.663448000	-2.831539000	-2.776299000
H	3.754017000	-3.828835000	-1.815447000
C	3.879854000	-1.816033000	1.127001000
H	3.771463000	-1.059276000	1.910887000
H	4.448488000	-1.365479000	0.309078000
H	4.500420000	-2.621777000	1.541364000
C	1.386956000	-2.507960000	2.998179000
H	0.408632000	-2.163304000	3.352986000
H	2.149993000	-1.817593000	3.370368000
H	1.575854000	-3.473586000	3.486114000
C	-0.816759000	-3.904721000	1.251245000
H	-0.605134000	-4.845168000	1.777365000
H	-1.534752000	-4.136356000	0.460124000
H	-1.313679000	-3.242595000	1.969417000
C	0.308933000	-4.126248000	-1.776799000
H	0.803124000	-5.089361000	-1.959254000

H	-0.746426000	-4.341702000	-1.589550000
H	0.373237000	-3.552911000	-2.708724000
N	-4.320473000	-1.215016000	0.654796000
C	8.319954000	3.026880000	-0.253185000
H	8.894470000	3.616864000	0.468651000
H	8.796060000	2.042132000	-0.331428000
H	8.409363000	3.517919000	-1.229440000
C	6.858954000	2.904643000	0.173506000
H	6.803618000	2.442459000	1.169373000
H	6.420443000	3.907061000	0.276228000
C	6.019093000	2.086732000	-0.810038000
H	6.455765000	1.082701000	-0.914266000
H	6.071870000	2.549536000	-1.805803000
C	4.552082000	1.965276000	-0.384107000
H	4.115040000	2.967999000	-0.286606000
H	4.494868000	1.495644000	0.607353000
C	3.739627000	1.151840000	-1.385614000
H	4.121136000	0.131226000	-1.477194000
H	3.755559000	1.616286000	-2.377185000
S	1.968822000	1.079863000	-0.896519000
C	-4.314363000	-0.414623000	-0.522458000
C	-3.224210000	-0.521438000	-1.416822000
C	-1.235149000	1.945011000	0.963045000
S	-0.522601000	0.458824000	1.783793000
C	0.857564000	1.182620000	2.724100000
C	-4.700849000	-2.607523000	0.418598000
H	-4.139797000	-3.026623000	-0.419816000
H	-4.481068000	-3.201850000	1.312156000
H	-5.774791000	-2.711209000	0.188975000
C	-5.048920000	-0.670803000	1.791669000
H	-4.780676000	-1.242725000	2.686394000
H	-4.764440000	0.372722000	1.952771000
H	-6.145804000	-0.723000000	1.681534000
C	-1.867964000	2.923247000	1.951010000
C	-2.361984000	4.209951000	1.274263000
C	-3.519927000	4.025850000	0.291900000
C	-4.027284000	5.354423000	-0.265434000
H	-3.234431000	5.889712000	-0.801669000
H	-4.855603000	5.200830000	-0.965202000
H	-4.386143000	6.010742000	0.536222000
H	1.821953000	-0.518720000	-2.708280000
H	0.420970000	0.593437000	-2.692341000
H	1.508454000	1.766572000	2.069042000
H	0.463070000	1.807283000	3.527950000

H	1.420414000	0.359540000	3.167795000
H	-2.262665000	-2.481694000	-1.449088000
H	-1.918627000	-1.506568000	-0.031645000
H	-0.439575000	2.422217000	0.379199000
H	-1.978468000	1.544289000	0.265818000
H	-1.134298000	3.199268000	2.718037000
H	-2.697754000	2.427826000	2.471117000
H	-2.674700000	4.902145000	2.067589000
H	-1.519118000	4.699412000	0.764303000
H	-3.216024000	3.379004000	-0.541802000
H	-4.342650000	3.501670000	0.798477000

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**J4,  $E_{(\text{SCF Done})} = -1933.922654$  a.u.**

C	-1.593904000	-2.259077000	1.292689000
C	-0.334761000	-2.871441000	1.009648000
C	0.649446000	-2.262230000	1.846571000
C	0.001532000	-1.275255000	2.650467000
C	-1.385874000	-1.271442000	2.304342000
C	-0.124398000	-4.058476000	0.111835000
H	0.893189000	-4.102849000	-0.291925000
H	-0.822799000	-4.072024000	-0.732879000
H	-0.283200000	-4.995362000	0.662662000
C	2.087918000	-2.680002000	1.972559000
H	2.202660000	-3.439386000	2.757622000
H	2.740190000	-1.843399000	2.245431000
H	2.477571000	-3.122058000	1.048976000
C	0.628114000	-0.512886000	3.781510000
H	0.095968000	0.419503000	3.992747000
H	1.672797000	-0.254665000	3.581338000
H	0.611999000	-1.110048000	4.703210000
C	-2.449257000	-0.465370000	2.996630000
H	-2.739555000	-0.938537000	3.944047000
H	-3.360280000	-0.379078000	2.395401000
H	-2.111388000	0.548164000	3.241289000
C	-2.917690000	-2.691573000	0.725767000
H	-2.854289000	-2.971379000	-0.332775000
H	-3.298612000	-3.572503000	1.259556000
H	-3.681543000	-1.913061000	0.817725000
C	-8.333979000	0.319662000	-1.203210000
H	-8.984986000	-0.334663000	-1.792326000
H	-8.495937000	0.084029000	-0.144601000
H	-8.663832000	1.352073000	-1.368426000
C	-6.869618000	0.136738000	-1.595232000
H	-6.579117000	-0.914042000	-1.453578000

H	-6.746377000	0.346890000	-2.666770000
C	-5.924315000	1.034937000	-0.794277000
H	-6.045401000	0.826898000	0.278752000
H	-6.212998000	2.085866000	-0.937555000
C	-4.454657000	0.855936000	-1.189353000
H	-4.330469000	1.071474000	-2.258416000
H	-4.163004000	-0.193494000	-1.041516000
C	-3.539854000	1.769029000	-0.379457000
H	-3.618402000	1.573570000	0.694609000
H	-3.789786000	2.820596000	-0.557054000
S	-1.786819000	1.580797000	-0.894084000
C	-0.940111000	2.979324000	-0.037953000
C	2.748014000	4.121989000	0.404827000
H	3.141921000	3.334553000	1.063154000
H	3.080135000	3.882544000	-0.614930000
C	1.214611000	4.104676000	0.464009000
H	0.837984000	4.917812000	-0.173136000
H	0.886242000	4.331521000	1.489305000
C	0.580864000	2.765731000	0.024992000
C	0.939142000	1.565328000	0.927189000
H	0.929573000	2.574223000	-1.004811000
H	2.033518000	1.425437000	0.921601000
H	0.698097000	1.832779000	1.969721000
C	7.520095000	-1.722454000	-0.702695000
H	8.279406000	-1.170311000	-0.139304000
H	7.422763000	-2.714366000	-0.245500000
H	7.898936000	-1.861362000	-1.722094000
C	6.187201000	-0.977614000	-0.703541000
H	5.852090000	-0.821067000	0.331583000
H	6.324613000	0.023207000	-1.135651000
C	5.096194000	-1.716577000	-1.481686000
H	4.954497000	-2.717974000	-1.050068000
H	5.429718000	-1.871945000	-2.517492000
C	3.759655000	-0.966983000	-1.488738000
H	3.897503000	0.028968000	-1.928786000
H	3.425935000	-0.811746000	-0.452629000
C	2.694394000	-1.727742000	-2.272205000
H	2.493038000	-2.710363000	-1.833180000
H	3.007939000	-1.871850000	-3.311924000
S	1.126042000	-0.775593000	-2.345897000
C	0.082355000	-1.843887000	-3.385937000
H	-0.049205000	-2.833953000	-2.943248000
H	-0.888015000	-1.352918000	-3.497753000
H	0.541049000	-1.932962000	-4.373944000

H	-1.202156000	3.884560000	-0.594981000
H	-1.358997000	3.053504000	0.972590000
C	3.317746000	5.446854000	0.822243000
H	3.102449000	5.755823000	1.846898000
C	4.040600000	6.249876000	0.041689000
H	4.281160000	5.984404000	-0.986502000
H	4.425157000	7.200932000	0.400125000
Lu	-0.124818000	-0.390108000	0.231958000

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**K4,  $E_{(\text{SCF Done})} = -1298.778641$  a.u.**

C	0.005029000	-2.099592000	1.024364000
C	0.058020000	-2.465122000	-0.356180000
C	1.428726000	-2.467321000	-0.759656000
C	2.222552000	-2.106628000	0.371826000
C	1.345485000	-1.878520000	1.476805000
C	-1.099054000	-2.901646000	-1.211606000
H	-2.055414000	-2.511522000	-0.848701000
H	-1.185730000	-3.996396000	-1.214421000
H	-0.989978000	-2.595096000	-2.258791000
C	1.937892000	-2.911794000	-2.103037000
H	1.983127000	-4.007636000	-2.155964000
H	2.950744000	-2.547782000	-2.304991000
H	1.294110000	-2.587034000	-2.929504000
C	3.724081000	-2.096785000	0.437757000
H	4.101428000	-1.357397000	1.152356000
H	4.185046000	-1.891443000	-0.534585000
H	4.102823000	-3.074241000	0.764699000
C	1.766384000	-1.638744000	2.897636000
H	1.956029000	-2.592126000	3.408668000
H	0.997374000	-1.113820000	3.472744000
H	2.684860000	-1.047473000	2.963893000
C	-1.219662000	-2.094132000	1.896689000
H	-1.340277000	-3.062715000	2.399729000
H	-1.165306000	-1.335257000	2.685377000
H	-2.136981000	-1.919215000	1.324652000
C	-7.407407000	-0.722817000	-0.197859000
H	-8.031414000	-1.280045000	-0.904240000
H	-7.309691000	-1.329858000	0.710072000
H	-7.946845000	0.193103000	0.070554000
C	-6.042239000	-0.404435000	-0.803142000
H	-5.542423000	-1.338798000	-1.095893000
H	-6.175032000	0.174312000	-1.727653000
C	-5.137037000	0.375327000	0.153257000
H	-5.001474000	-0.201434000	1.079655000



H	-5.635515000	1.310930000	0.443818000
C	-3.768385000	0.699900000	-0.455055000
H	-3.901258000	1.283184000	-1.375173000
H	-3.266406000	-0.234763000	-0.743456000
C	-2.892905000	1.480431000	0.519300000
H	-2.711231000	0.919001000	1.441377000
H	-3.362506000	2.434558000	0.780770000
S	-1.277561000	1.910996000	-0.245090000
C	-0.515636000	3.044134000	1.008486000
C	1.578093000	3.448310000	-0.346246000
H	0.949594000	3.104106000	-1.182860000
H	1.504624000	4.541784000	-0.378302000
C	1.016887000	2.949274000	1.009434000
C	1.479622000	1.537092000	1.420735000
H	-0.913899000	2.748920000	1.984624000
H	-0.867764000	4.054224000	0.775068000
C	3.031908000	3.038403000	-0.620727000
C	3.220228000	1.630972000	-1.119096000
C	2.495806000	1.022983000	-2.086452000
H	3.645217000	3.197810000	0.271928000
H	3.449542000	3.697994000	-1.395973000
H	4.060137000	1.075354000	-0.699137000
H	1.334647000	3.684855000	1.767834000
H	1.002333000	1.287196000	2.383680000
H	2.555556000	1.554678000	1.652782000
H	2.808214000	0.059790000	-2.489795000
H	1.715048000	1.554415000	-2.636287000
Lu	0.835624000	-0.000899000	-0.192683000

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**TS-4,  $E_{(\text{SCF Done})} = -1298.763439$  a.u., IF =  $i296.1285$  cm<sup>-1</sup>**

C	0.048449000	-2.119019000	1.054703000
C	0.094004000	-2.505475000	-0.320246000
C	1.461518000	-2.482020000	-0.742951000
C	2.258754000	-2.081778000	0.371073000
C	1.388829000	-1.850658000	1.481144000
C	-1.064293000	-2.992491000	-1.147483000
H	-2.024004000	-2.600358000	-0.794427000
H	-1.136293000	-4.087380000	-1.103188000
H	-0.965316000	-2.729752000	-2.207130000
C	1.971538000	-2.951184000	-2.076320000
H	2.102550000	-4.041461000	-2.077370000
H	2.943845000	-2.514291000	-2.324268000
H	1.284407000	-2.714712000	-2.896416000
C	3.759813000	-2.040775000	0.409971000

H	4.136169000	-1.328435000	1.151711000
H	4.195237000	-1.775887000	-0.559241000
H	4.165650000	-3.024291000	0.681426000
C	1.818561000	-1.561783000	2.892654000
H	1.998994000	-2.496284000	3.440052000
H	1.059303000	-1.007937000	3.456024000
H	2.747827000	-0.984296000	2.934603000
C	-1.165030000	-2.137480000	1.942692000
H	-1.270324000	-3.114030000	2.433853000
H	-1.109396000	-1.389953000	2.742266000
H	-2.092282000	-1.964005000	1.385982000
C	-7.365803000	-0.763374000	-0.127326000
H	-7.983997000	-1.345213000	-0.818727000
H	-7.262040000	-1.345401000	0.796165000
H	-7.914477000	0.153817000	0.116844000
C	-6.004019000	-0.447511000	-0.741461000
H	-5.494860000	-1.384182000	-1.009570000
H	-6.142674000	0.105391000	-1.680749000
C	-5.106839000	0.366220000	0.194044000
H	-4.964911000	-0.184849000	1.135004000
H	-5.614683000	1.304033000	0.460093000
C	-3.741837000	0.688869000	-0.423591000
H	-3.881329000	1.247967000	-1.357594000
H	-3.231345000	-0.248172000	-0.689027000
C	-2.873363000	1.501256000	0.531382000
H	-2.681670000	0.960475000	1.463913000
H	-3.354660000	2.454322000	0.775235000
S	-1.267671000	1.935309000	-0.252302000
C	-0.505680000	3.059700000	0.997033000
C	1.520024000	3.659113000	-0.462628000
H	0.867984000	3.327142000	-1.284755000
H	1.501060000	4.754158000	-0.477343000
C	1.021454000	3.099604000	0.886320000
C	1.699683000	1.738101000	1.120020000
H	-0.813655000	2.706868000	1.987222000
H	-0.935059000	4.053329000	0.834165000
C	2.927154000	3.116596000	-0.685338000
C	2.928909000	1.598410000	-0.668886000
C	2.414821000	0.827771000	-1.750515000
H	3.598113000	3.502247000	0.091562000
H	3.328724000	3.446676000	-1.650828000
H	3.764525000	1.145477000	-0.136428000
H	1.340336000	3.796992000	1.675122000
H	1.058472000	1.073784000	1.762079000

H	2.602843000	1.846466000	1.723791000
H	3.024726000	-0.009335000	-2.088948000
H	1.912401000	1.373050000	-2.556594000
Lu	0.797221000	-0.031824000	-0.249344000

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**L4,  $E_{(\text{SCF Done})} = -1298.788080$  a.u.**

C	0.036168000	-2.359083000	1.032653000
C	0.127416000	-2.735722000	-0.342709000
C	1.491919000	-2.586146000	-0.754015000
C	2.239638000	-2.109551000	0.360730000
C	1.338313000	-1.954577000	1.464485000
C	-0.984034000	-3.312413000	-1.177332000
H	-1.972138000	-2.957820000	-0.863151000
H	-1.002202000	-4.407014000	-1.093294000
H	-0.870520000	-3.084132000	-2.243188000
C	2.057391000	-2.967932000	-2.092195000
H	2.400677000	-4.010923000	-2.082623000
H	2.915530000	-2.347009000	-2.366691000
H	1.318470000	-2.886803000	-2.896691000
C	3.729334000	-1.936335000	0.407718000
H	4.038173000	-1.199033000	1.155596000
H	4.135981000	-1.620811000	-0.557645000
H	4.217546000	-2.883590000	0.672970000
C	1.726779000	-1.610683000	2.876943000
H	1.983576000	-2.519237000	3.437307000
H	0.916297000	-1.120327000	3.427945000
H	2.602817000	-0.955307000	2.919004000
C	-1.182266000	-2.478581000	1.905270000
H	-1.218176000	-3.466456000	2.383616000
H	-1.192781000	-1.739350000	2.714180000
H	-2.114837000	-2.370268000	1.340670000
C	-7.238343000	-0.521297000	-0.088195000
H	-7.805261000	-1.239414000	-0.689470000
H	-7.233207000	-0.884403000	0.946370000
H	-7.783906000	0.429377000	-0.105096000
C	-5.819035000	-0.354850000	-0.626071000
H	-5.311408000	-1.330163000	-0.632001000
H	-5.858254000	-0.023017000	-1.672804000
C	-4.990696000	0.641818000	0.187868000
H	-4.945959000	0.311338000	1.235503000
H	-5.497074000	1.617151000	0.193057000
C	-3.568584000	0.817907000	-0.355394000
H	-3.612693000	1.164412000	-1.396175000
H	-3.063778000	-0.160839000	-0.365807000

C	-2.762355000	1.807015000	0.481065000
H	-2.646918000	1.459979000	1.513498000
H	-3.251632000	2.786419000	0.499132000
S	-1.099236000	2.076260000	-0.251223000
C	-0.331118000	3.248317000	0.950526000
C	1.666975000	3.929586000	-0.577332000
H	0.998620000	3.603289000	-1.385505000
H	1.682419000	5.023569000	-0.602864000
C	1.181354000	3.389096000	0.786232000
C	2.011290000	2.092621000	1.015614000
H	-0.582850000	2.896360000	1.957453000
H	-0.824497000	4.212371000	0.790382000
C	3.051846000	3.299841000	-0.755349000
C	2.863268000	1.844510000	-0.272261000
C	2.252283000	0.916188000	-1.352879000
H	3.781442000	3.822356000	-0.120798000
H	3.417057000	3.345016000	-1.785571000
H	3.820137000	1.406884000	0.031930000
H	1.466748000	4.109681000	1.563899000
H	1.374600000	1.250075000	1.381744000
H	2.687629000	2.232781000	1.865962000
H	3.056636000	0.459784000	-1.937783000
H	1.669956000	1.524147000	-2.076920000
Lu	0.598680000	-0.225741000	-0.275899000

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**K4',  $E_{(\text{SCF Done})} = -1933.934212$  a.u.**

C	-1.023605000	0.953557000	2.405554000
C	-0.543786000	-0.392697000	2.412100000
C	0.883770000	-0.351806000	2.387865000
C	1.285770000	1.016427000	2.346887000
C	0.105304000	1.823703000	2.355369000
C	-1.372035000	-1.630457000	2.620686000
H	-2.417774000	-1.477552000	2.337580000
H	-1.370493000	-1.924356000	3.679126000
H	-0.996991000	-2.492344000	2.055677000
C	1.785793000	-1.534378000	2.592523000
H	1.909932000	-1.742273000	3.664210000
H	2.788618000	-1.369495000	2.185516000
H	1.382823000	-2.447654000	2.140522000
C	2.693294000	1.524642000	2.492253000
H	2.833879000	2.507510000	2.029189000
H	3.433874000	0.842117000	2.060219000
H	2.954053000	1.639031000	3.552996000
C	0.065285000	3.320472000	2.468282000

H	0.061569000	3.629475000	3.522243000
H	-0.829037000	3.745580000	2.003110000
H	0.936657000	3.795239000	2.004213000
C	-2.450343000	1.383114000	2.589159000
H	-2.709861000	1.403688000	3.656192000
H	-2.628720000	2.387589000	2.194976000
H	-3.160283000	0.707374000	2.101026000
C	-7.762257000	-2.364704000	0.871926000
H	-8.427645000	-2.023850000	1.672034000
H	-8.335905000	-2.358188000	-0.062425000
H	-7.488952000	-3.404580000	1.087175000
C	-6.525008000	-1.475828000	0.768453000
H	-6.832708000	-0.436517000	0.586820000
H	-5.992300000	-1.473721000	1.730009000
C	-5.566349000	-1.918566000	-0.339294000
H	-6.099295000	-1.921460000	-1.300946000
H	-5.255642000	-2.957890000	-0.158395000
C	-4.325601000	-1.025158000	-0.447905000
H	-3.785291000	-1.021322000	0.506908000
H	-4.641000000	0.009412000	-0.634087000
C	-3.390860000	-1.499707000	-1.552591000
H	-3.904087000	-1.545792000	-2.519780000
H	-3.019311000	-2.508894000	-1.342129000
S	-1.878440000	-0.498683000	-1.838922000
C	-2.532595000	1.081295000	-2.525718000
C	-0.292066000	2.118575000	-3.088777000
H	0.132331000	1.102567000	-3.016978000
H	-0.537763000	2.256012000	-4.149672000
C	-1.569794000	2.237437000	-2.237874000
C	-1.275586000	2.330423000	-0.734463000
H	-3.495459000	1.270762000	-2.042588000
H	-2.697150000	0.928140000	-3.597479000
C	0.793998000	3.133608000	-2.693924000
C	1.507139000	2.818373000	-1.403670000
C	2.269365000	1.724122000	-1.188619000
H	0.353439000	4.134890000	-2.636257000
H	1.549889000	3.168275000	-3.489540000
H	-2.104734000	3.135598000	-2.593794000
C	7.958268000	-1.729218000	0.197840000
H	8.770416000	-0.995887000	0.238364000
H	7.872525000	-2.185742000	1.191096000
H	8.256077000	-2.515914000	-0.505301000
C	6.645937000	-1.074629000	-0.227397000
H	6.393811000	-0.266950000	0.474707000

H	6.773617000	-0.598037000	-1.209387000
C	5.482723000	-2.066499000	-0.296102000
H	5.350254000	-2.542334000	0.686346000
H	5.735018000	-2.874741000	-0.997058000
C	4.165991000	-1.414074000	-0.731075000
H	4.295079000	-0.954082000	-1.719618000
H	3.914906000	-0.605405000	-0.031400000
C	3.029104000	-2.427245000	-0.779297000
H	2.843571000	-2.860755000	0.208053000
H	3.276742000	-3.240709000	-1.470611000
S	1.461515000	-1.708736000	-1.412627000
C	0.449270000	-3.216578000	-1.482171000
H	0.259138000	-3.623038000	-0.485403000
H	-0.492071000	-2.959153000	-1.971265000
H	0.966141000	-3.960930000	-2.093857000
H	2.880305000	1.638966000	-0.291576000
H	1.454120000	3.565607000	-0.612353000
H	2.444453000	0.995071000	-1.979186000
H	-0.923190000	3.343922000	-0.493674000
H	-2.230460000	2.240405000	-0.186407000
Lu	0.060238000	0.564730000	0.075599000

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**TS-4',  $E_{(\text{SCF Done})} = -1933.921056$  a.u., IF =  $i293.9991$  cm<sup>-1</sup>**

C	-1.066850000	0.564083000	2.480178000
C	-0.540390000	-0.754965000	2.342237000
C	0.886292000	-0.662599000	2.355309000
C	1.240781000	0.712024000	2.498984000
C	0.033913000	1.471526000	2.566935000
C	-1.326309000	-2.036186000	2.374663000
H	-2.369322000	-1.889072000	2.077783000
H	-1.343260000	-2.455520000	3.389839000
H	-0.901843000	-2.810099000	1.724012000
C	1.831222000	-1.826535000	2.444374000
H	1.981437000	-2.120384000	3.492320000
H	2.820371000	-1.591921000	2.037768000
H	1.451179000	-2.711434000	1.921990000
C	2.624250000	1.239018000	2.749256000
H	2.738806000	2.278919000	2.425819000
H	3.394394000	0.647716000	2.242312000
H	2.858256000	1.213446000	3.822115000
C	-0.063580000	2.936418000	2.883379000
H	-0.092745000	3.096137000	3.969628000
H	-0.969696000	3.392490000	2.471417000
H	0.794745000	3.501382000	2.504596000

C	-2.509937000	0.927167000	2.691465000
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H	-8.225752000	-2.277124000	-0.359800000
H	-7.346964000	-3.564767000	0.479055000
C	-6.362353000	-1.621919000	0.560272000
H	-6.658467000	-0.566167000	0.635421000
H	-5.786058000	-1.844103000	1.469693000
C	-5.464705000	-1.807866000	-0.665265000
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C	-4.213005000	-0.923719000	-0.630256000
H	-3.627711000	-1.143748000	0.271353000
H	-4.516935000	0.128743000	-0.559564000
C	-3.341385000	-1.142413000	-1.859223000
H	-3.900238000	-0.966704000	-2.785478000
H	-2.980673000	-2.176025000	-1.901944000
S	-1.825291000	-0.114241000	-1.999380000
C	-2.511067000	1.558468000	-2.323664000
C	-0.271517000	2.687647000	-2.872266000
H	0.106602000	1.668779000	-3.052772000
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C	-1.508376000	2.653374000	-1.958705000
C	-1.025047000	2.571528000	-0.504422000
H	-3.422038000	1.664878000	-1.726967000
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C	0.788037000	3.499415000	-2.135715000
C	1.125929000	2.865535000	-0.796741000
C	1.976035000	1.736012000	-0.703553000
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H	1.710699000	3.572024000	-2.723344000
H	-2.051977000	3.598402000	-2.110477000
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H	8.204090000	-2.296393000	-0.999026000
C	6.570206000	-0.922902000	-0.561123000
H	6.328950000	-0.166643000	0.199426000
H	6.638200000	-0.384501000	-1.516679000
C	5.432318000	-1.943160000	-0.637908000
H	5.361378000	-2.482353000	0.318019000

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H	4.145588000	-0.779033000	-1.929725000
H	3.837380000	-0.547044000	-0.210383000
C	2.970475000	-2.347460000	-1.028719000
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H	3.199539000	-3.102696000	-1.789222000
S	1.356299000	-1.627669000	-1.527007000
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C	1.078819000	-1.108857000	2.590964000
C	0.127185000	-0.137448000	3.013158000
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C	0.967427000	-3.477995000	1.513718000
H	1.111005000	-4.124701000	2.389725000
H	1.950552000	-3.374562000	1.040096000
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C	0.418363000	1.041737000	3.894667000
H	0.379337000	0.746472000	4.951978000
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H	1.414274000	1.455275000	3.710467000
C	-2.478624000	0.062840000	2.973285000
H	-2.846666000	-0.334940000	3.928462000
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H	-3.263707000	-0.118409000	2.230964000
C	-7.480551000	-1.729235000	-1.718180000
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H	-7.187384000	-2.595105000	-2.323698000
C	-6.274395000	-1.106819000	-1.018676000
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H	-5.828636000	-1.840739000	-0.332067000
C	-5.205980000	-0.617586000	-1.999147000
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H	-4.333545000	0.855660000	-0.684281000
C	-2.948508000	0.482336000	-2.303188000
H	-3.371234000	1.195973000	-3.019630000
H	-2.558146000	-0.355824000	-2.891686000
S	-1.456704000	1.295752000	-1.611995000
C	-2.126852000	2.912875000	-1.037073000
C	0.158407000	4.167485000	-1.085295000
H	0.428291000	3.389385000	-1.811639000
H	0.001139000	5.089813000	-1.653917000
C	-1.098575000	3.756182000	-0.286330000
C	-0.556781000	3.115234000	1.021080000
H	-2.996116000	2.713818000	-0.402438000
H	-2.466216000	3.429034000	-1.941795000
C	1.250560000	4.290646000	-0.016993000
C	0.992879000	3.084591000	0.911987000
C	1.580804000	1.758755000	0.378948000
H	1.122854000	5.232816000	0.534859000
H	2.262797000	4.287884000	-0.433866000
H	-1.647653000	4.668480000	-0.017256000
C	7.716637000	-0.268638000	-1.632881000
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H	7.991662000	-0.840839000	-2.526820000
C	6.244588000	0.135695000	-1.664616000
H	6.008198000	0.737376000	-0.775763000
H	6.059289000	0.784599000	-2.531795000
C	5.300505000	-1.067151000	-1.725503000
H	5.483288000	-1.717708000	-0.857903000
H	5.534373000	-1.668271000	-2.615828000
C	3.823103000	-0.661252000	-1.759901000
H	3.636415000	-0.019294000	-2.630379000

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C	2.913149000	-1.882929000	-1.825012000
H	3.043991000	-2.531342000	-0.952520000
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S	1.143404000	-1.402276000	-1.944811000
C	0.357022000	-3.018522000	-2.223886000
H	0.599295000	-3.722964000	-1.425950000
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H	0.690111000	-3.412756000	-3.187408000
H	2.609604000	1.648933000	0.747872000
H	1.420017000	3.264125000	1.904551000
H	1.688564000	1.828718000	-0.727459000
H	-0.863039000	3.720083000	1.882490000
H	-1.014428000	2.125686000	1.218546000
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