

Computational Methods

All DFT calculations were performed with the Gaussian 09 software package.¹ The geometry optimizations were carried out with the B3LYP functional² including the D3 version of Grimme's dispersion correction with the combination of Becke–Johnson damping.³ The 6-31G(d) basis set⁴ was used for all the atoms. All structures were analyzed by harmonic vibrational frequencies at the same level to characterize each stationary point as a minimum (no imaginary frequency) or a transition state (one imaginary frequency) and to obtain the thermodynamic corrections to Gibbs free energy. To have more accurate relative energies, the single point energies were calculated using the M06 functional⁵ with def2-TZVP basis set⁶ and the SMD model⁷ for considering the solvation effect (toluene). The three-dimensional geometry structures displayed in this work were generated with CYLview.⁸ The bond order, localized molecular orbitals and canonical molecular orbitals analysis were performed with Multiwfn software.⁹ All the bond lengths are in Å.

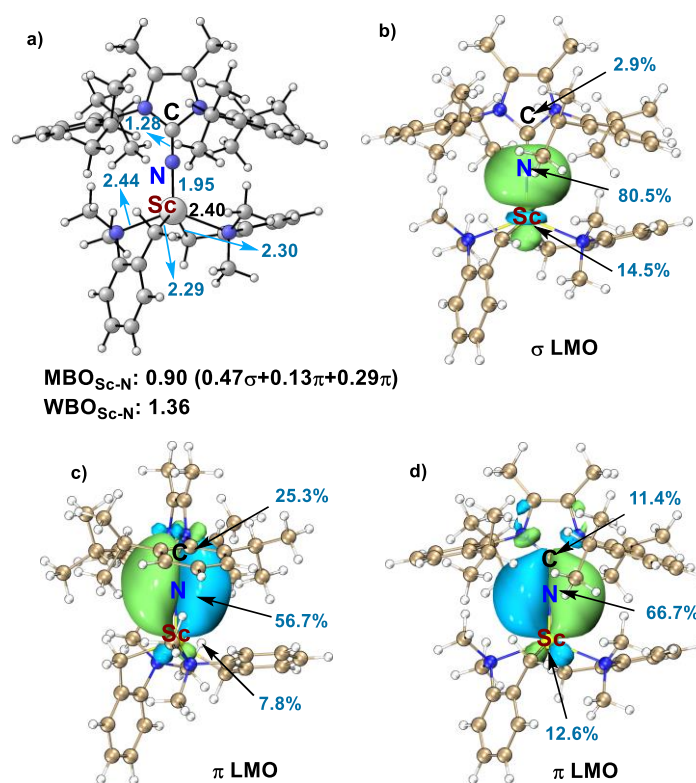


Figure S192. The Mayer bond order (MBO), Wiberg bond order (WBO) and the localized molecular orbitals of σ and π bond between the Sc and N atom (imidazolium) of the catalyst. (isovalue = 0.02)

Note: The calculated Wiberg bond order of Sc–N (1.36) is similar with that of Sc–N^{imido} (1.32) in Chen's work, indicating that a strong interaction between the N atom of NHI and Sc ion. The molecule orbital analysis of **Sc-1** disclosed that except the existence of one σ -bond, two p orbitals of N atom in NHI form two π bonds with two d orbitals of Sc

ion, respectively, providing further evidence for their capability of acting as $2\sigma,4p$ -electron donors (Fig. S192, b-d). The calculated ADCH charges suggested the charge donation from the NHI to the scandium(III) center is -0.91.

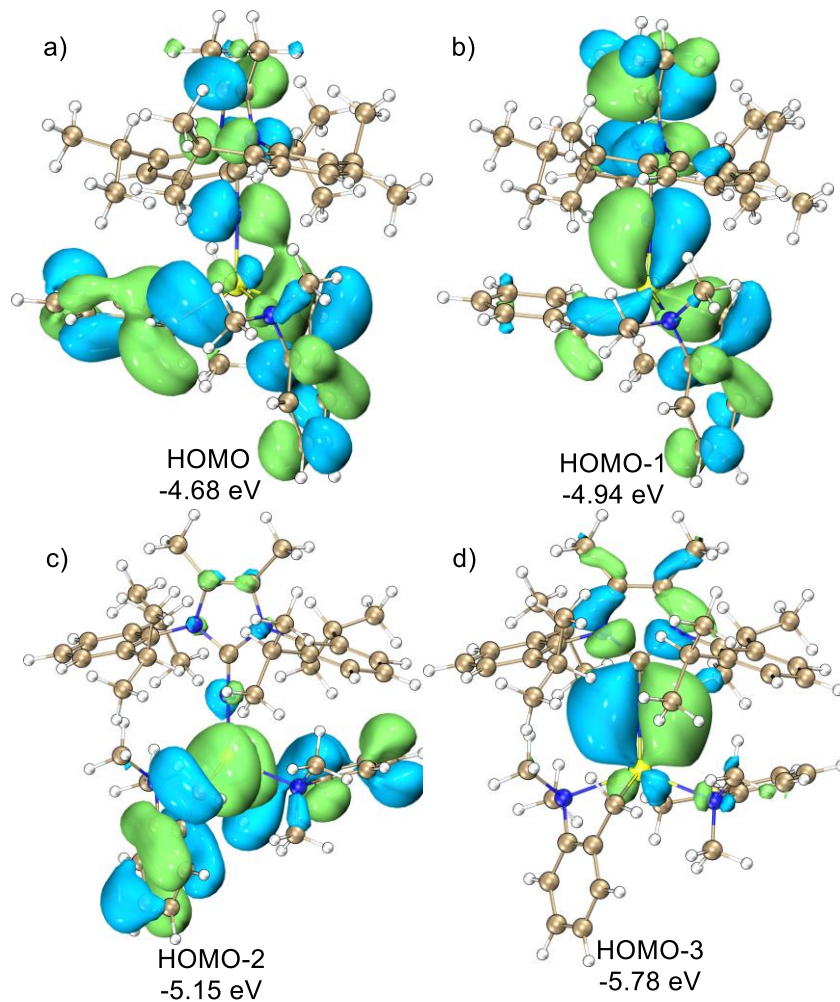


Figure S193. DFT calculated the four highest occupied molecular orbitals of the catalyst.

Note: The HOMO-1 and HOMO-3 point towards the presence of two additional p-bonds between the iminato ligand and the scandium atom. A bonding analysis of the p-orbitals HOMO-1 and HOMO-3 reveals 8.6 and 12.0 % orbital contribution from the metal center, respectively.

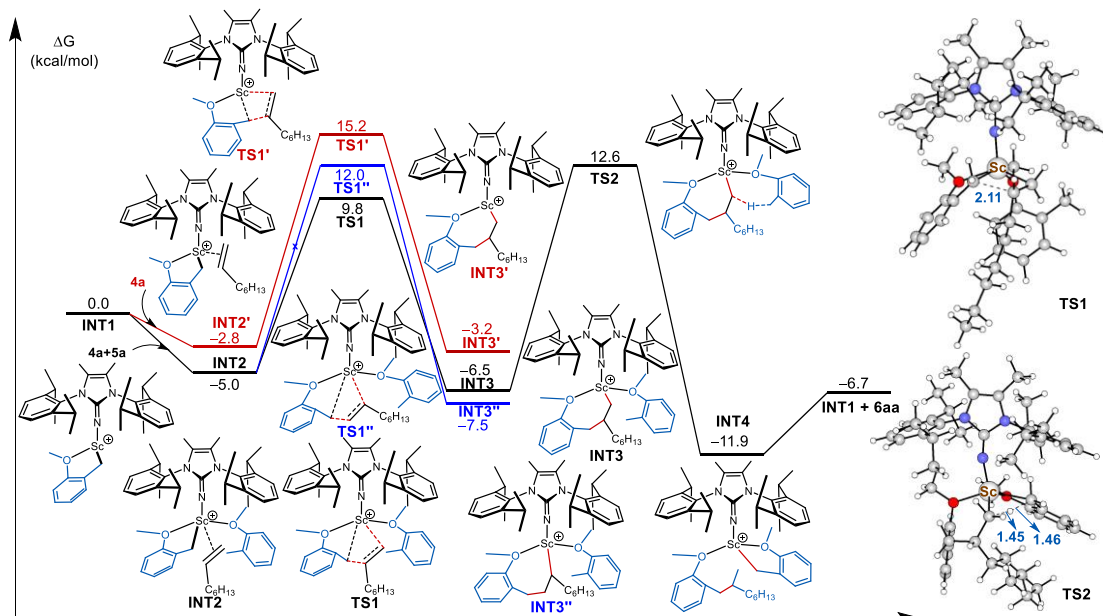


Figure S194. DFT-Calculated relative Gibbs free energies (in kcal/mol) of the anisole C–H alkylation.

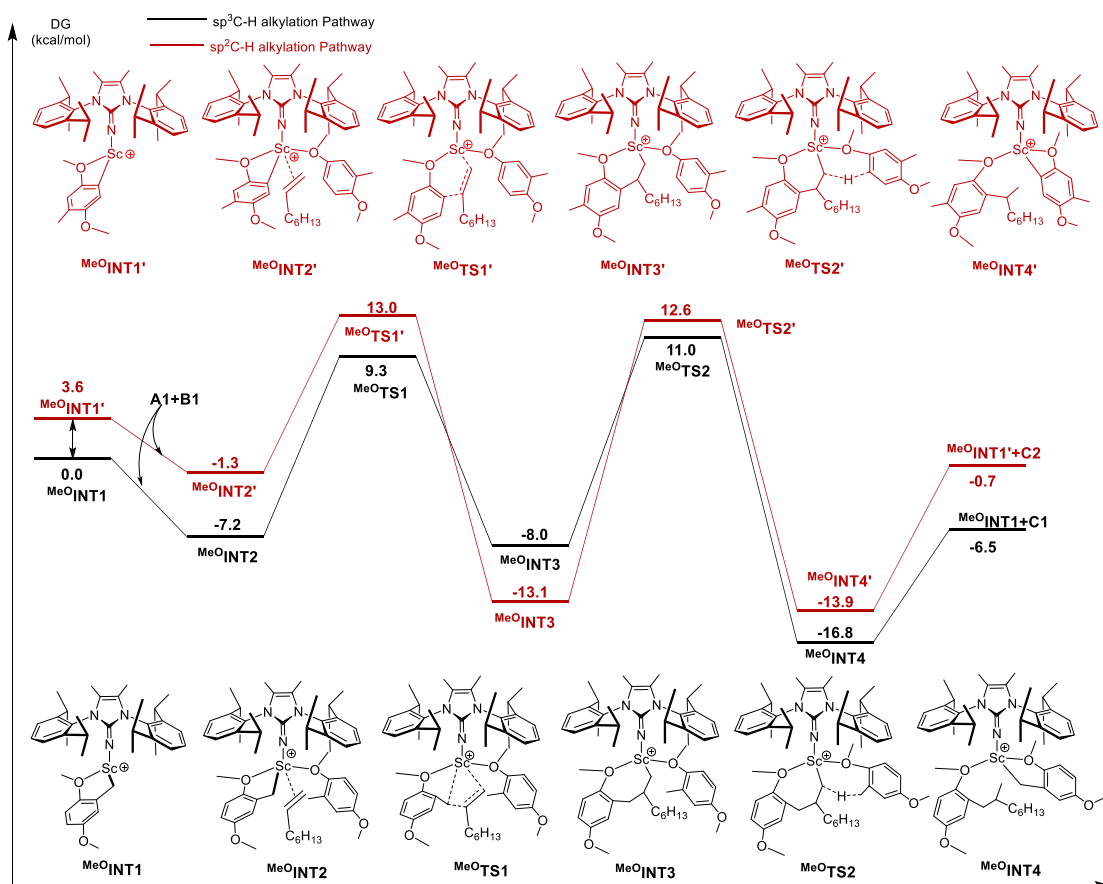


Figure S195. DFT-Calculated relative Gibbs free energies (in kcal/mol) of the $\text{Csp}^3\text{-H}$ and $\text{Csp}^2\text{-H}$ alkylation.

Note: The above results indicated that the $\text{Csp}^3\text{-H}$ activation pathway is more favourable than the $\text{Csp}^2\text{-H}$ activation pathway for the 1,4-dimethoxy-2-methylbenzene (**6ia**) kinetically and

thermodynamically. Therefore, only Csp³–H alkylation product was obtained in current reaction system.

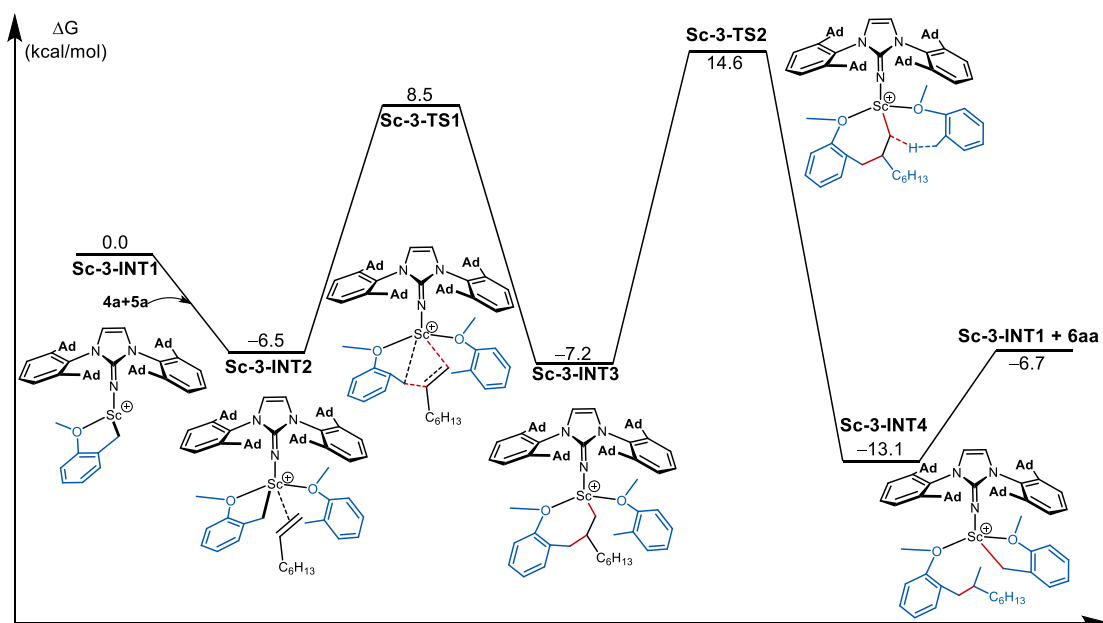


Figure S196. DFT-Calculated relative Gibbs free energies (in kcal/mol) of the **Sc-3** catalyzed anisole C–H alkylation.

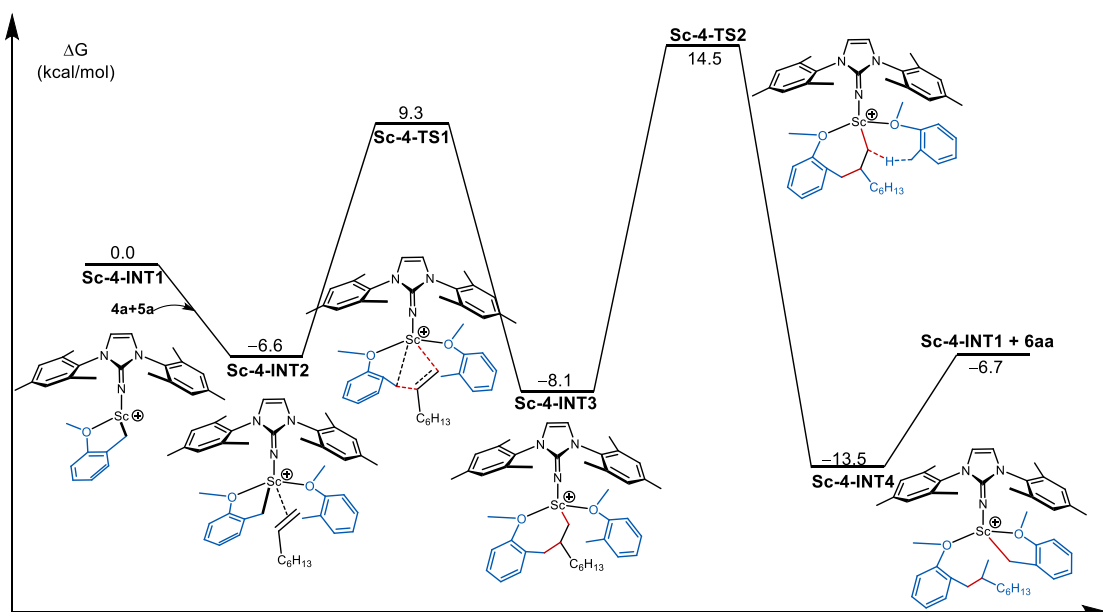


Figure S197. DFT-Calculated relative Gibbs free energies (in kcal/mol) of the **Sc-4** catalyzed anisole C–H alkylation.

Note: As shown in **Figure S196** and **Figure S197**, the activation barrier of **Sc-3** and **Sc-4** catalyzed C–H activation step was 21.8 kcal/mol and 22.6 kcal/mol, respectively, which are higher than that of **Sc-1** catalyzed C–H activation step (19.1 kcal/mol), indicating that the **Sc-3** and **Sc-4** catalysts have low activity.

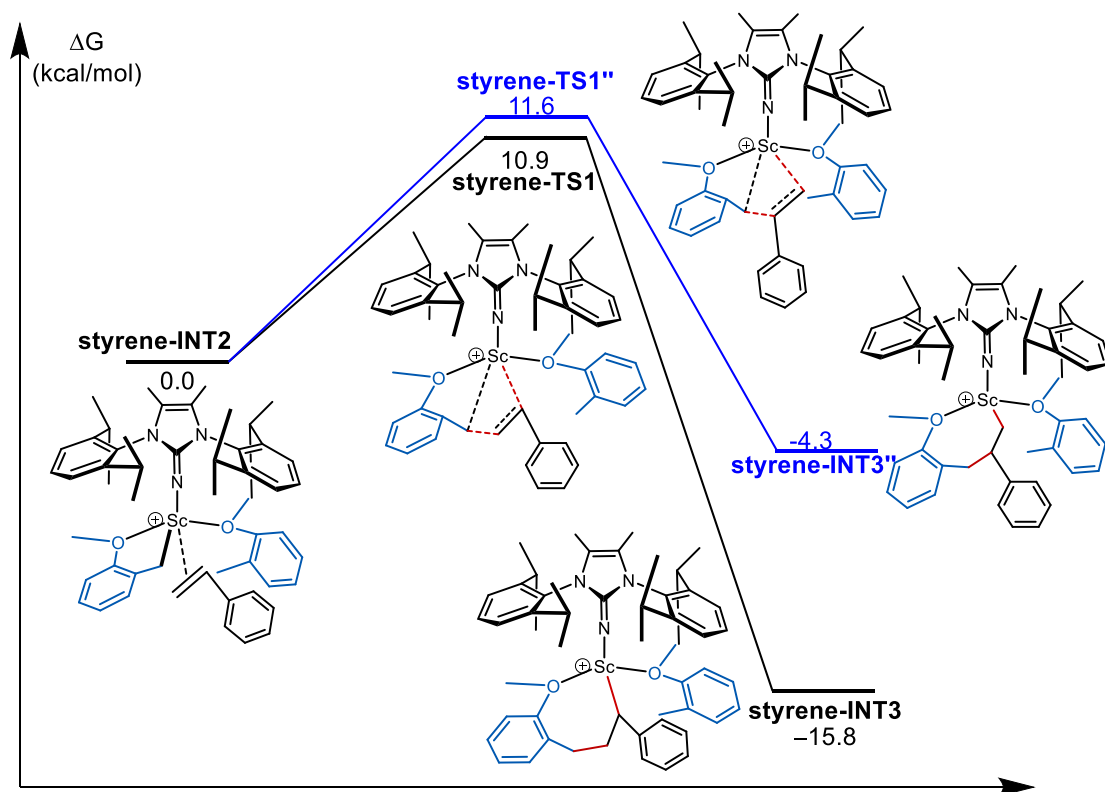


Figure S198. DFT-Calculated relative Gibbs free energies (in kcal/mol) of the reaction of 2-methylanisole with styrene.

As shown in **Figure S198**, the activation barrier of the **branched pathway** is 0.7 kcal/mol higher than that of the **linear pathway** (11.6 kcal/mol vs 10.9 kcal/mol), showing that the linear products is slightly preferred.

References

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Cartesian coordinates**INT1**

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H	4.249788000	-2.306274000	3.001258000
H	3.621944000	-0.881054000	3.795403000
C	2.098285000	-2.085551000	2.856047000
H	1.890172000	-2.417317000	3.884703000
C	1.023659000	-1.058760000	2.449943000
H	1.098040000	-0.188597000	3.122493000
H	0.034245000	-1.494980000	2.673561000
N	-1.092623000	-0.055402000	0.014143000
N	-2.846359000	1.592988000	0.082777000
N	-3.445480000	-0.487080000	-0.209719000
C	-2.333181000	0.313773000	-0.030112000
C	-4.253569000	1.576887000	-0.016020000
C	-4.625093000	0.285100000	-0.208183000
C	-2.066987000	2.763173000	0.350201000
C	-1.377844000	3.384724000	-0.710005000
C	-0.680372000	4.562294000	-0.420740000
H	-0.135525000	5.073112000	-1.205611000
C	-0.670376000	5.092110000	0.868455000
C	-1.331969000	4.439123000	1.904421000
H	-1.297992000	4.853209000	2.906235000
C	-2.038917000	3.254320000	1.667910000
C	-1.368370000	2.768310000	-2.105262000
H	-1.215784000	1.691371000	-1.968129000
C	-0.220430000	3.285859000	-2.982525000
H	0.749472000	3.210837000	-2.480085000
H	-0.368262000	4.332841000	-3.269429000
H	-0.177607000	2.706550000	-3.911748000
C	-2.707646000	2.962215000	-2.840779000
C	-2.681775000	2.476096000	2.807664000

H	-3.507142000	1.887682000	2.395368000
C	-3.263557000	3.370072000	3.910460000
H	-3.950598000	4.119400000	3.502574000
H	-2.480831000	3.897008000	4.466945000
H	-3.815494000	2.758507000	4.631518000
C	-1.662697000	1.474514000	3.385135000
C	-3.392260000	-1.900175000	-0.420500000
C	-3.219501000	-2.749533000	0.689508000
C	-3.385398000	-4.631572000	-0.841586000
C	-3.227345000	-4.127876000	0.448652000
H	-3.105462000	-4.818123000	1.275495000
C	-3.518549000	-3.767202000	-1.925680000
H	-3.623095000	-4.175250000	-2.925059000
C	-3.521016000	-2.380492000	-1.736920000
C	-3.566335000	-1.417371000	-2.916140000
H	-4.020407000	-0.482581000	-2.573694000
C	-4.401641000	-1.927416000	-4.096972000
H	-4.494915000	-1.142082000	-4.854111000
H	-5.409319000	-2.217025000	-3.780758000
H	-3.938982000	-2.792918000	-4.583836000
C	-2.129823000	-1.075727000	-3.361204000
C	-3.004318000	-2.179120000	2.086766000
H	-2.357269000	-1.303720000	1.973820000
C	-2.281747000	-3.151148000	3.028688000
H	-2.007006000	-2.632474000	3.952530000
H	-1.363389000	-3.545032000	2.579894000
H	-2.915808000	-4.000200000	3.307706000
C	-4.323010000	-1.706988000	2.726680000
H	-2.938033000	4.028053000	-2.949935000
H	-2.651742000	2.526357000	-3.844906000

H	-3.536558000	2.481893000	-2.316758000
H	-2.125153000	0.860819000	4.166503000
H	-1.279821000	0.809224000	2.606955000
H	-0.810628000	2.002498000	3.829911000
H	-4.792225000	-0.907394000	2.148373000
H	-5.034438000	-2.536385000	2.810769000
H	-4.133761000	-1.321447000	3.734769000
H	-2.142798000	-0.327683000	-4.162294000
H	-1.550217000	-0.678651000	-2.522029000
H	-1.622659000	-1.971529000	-3.741292000
H	-3.397500000	-5.705666000	-1.003049000
H	-0.133034000	6.015126000	1.066863000
H	5.864751000	-4.349947000	-0.461913000
H	2.521593000	-2.686475000	-2.602510000
C	2.266850000	-3.003249000	-0.495425000
O	0.967538000	-2.441116000	-0.529155000
C	-0.084532000	-3.351452000	-0.957470000
H	-1.005096000	-2.776825000	-0.940723000
H	0.143660000	-3.706022000	-1.965010000
H	-0.136663000	-4.189088000	-0.260547000
C	3.921449000	-0.625774000	1.683357000
H	3.511615000	-1.043880000	0.753854000
H	3.492649000	0.377084000	1.793673000
C	5.434173000	-0.486709000	1.496433000
H	5.870925000	-1.487674000	1.376925000
H	5.877931000	-0.061967000	2.407793000
C	5.800905000	0.378521000	0.289643000
H	5.338244000	-0.051913000	-0.611543000
H	5.359673000	1.377551000	0.408246000
C	7.308513000	0.514960000	0.062108000

H	7.747379000	-0.483624000	-0.070795000
H	7.774319000	0.934498000	0.964168000
C	7.649459000	1.392190000	-1.144698000
H	8.731615000	1.468273000	-1.294239000
H	7.212646000	0.983859000	-2.064931000
H	7.255066000	2.406823000	-1.014912000
C	3.280827000	3.695224000	0.165811000
C	2.487352000	2.553581000	0.020479000
C	2.713195000	1.755941000	-1.107232000
C	3.675107000	2.069887000	-2.060920000
C	4.448289000	3.218796000	-1.889575000
C	4.254367000	4.031438000	-0.774686000
H	3.117116000	4.332666000	1.029814000
H	3.839615000	1.431992000	-2.920622000
H	5.204510000	3.465969000	-2.627039000
H	4.853473000	4.925884000	-0.638954000
O	1.910863000	0.605954000	-1.233399000
C	1.640729000	0.144799000	-2.576407000
H	2.514425000	-0.372547000	-2.976223000
H	0.800309000	-0.545088000	-2.502636000
H	1.368509000	0.994303000	-3.203382000
C	1.427926000	2.201204000	1.025941000
H	1.211882000	3.040604000	1.688591000
H	0.466543000	1.965656000	0.548778000
H	1.735308000	1.376870000	1.685988000
C	-5.965554000	-0.333966000	-0.408436000
H	-6.748874000	0.419108000	-0.298065000
H	-6.063705000	-0.779638000	-1.405224000
H	-6.153603000	-1.129718000	0.320371000
C	-5.059503000	2.824815000	0.097599000

H	-6.114874000	2.609446000	-0.083421000
H	-4.972570000	3.276194000	1.092591000
H	-4.736282000	3.578804000	-0.628340000
INT4			
Sc	-0.878998000	0.434610000	-0.061492000
C	-0.979294000	-3.910036000	-0.622111000
C	-0.812624000	-4.858562000	-1.630821000
H	-0.435705000	-5.843891000	-1.375821000
C	-1.113428000	-4.533155000	-2.951097000
C	-1.586051000	-3.257354000	-3.250844000
H	-1.822659000	-2.998373000	-4.279258000
C	-1.786038000	-2.286013000	-2.262047000
C	-2.398666000	-0.964471000	-2.663920000
H	-2.233336000	-0.164504000	-1.929363000
H	-1.902095000	-0.605717000	-3.572354000
C	-4.709948000	-1.578906000	-1.723120000
H	-4.295367000	-2.554957000	-1.439703000
H	-5.743333000	-1.772064000	-2.037776000
C	-3.922627000	-1.050977000	-2.935408000
H	-4.046379000	-1.789874000	-3.739353000
C	-4.448471000	0.296251000	-3.438760000
H	-5.515690000	0.230954000	-3.677037000
H	-3.920650000	0.613336000	-4.345560000
N	0.945109000	0.207007000	0.239864000
N	3.040565000	1.322420000	-0.142478000
N	3.128837000	-0.699436000	0.675398000
C	2.242109000	0.271498000	0.257443000
C	4.400897000	1.005491000	0.025006000
C	4.456641000	-0.252212000	0.539552000
C	2.520230000	2.524645000	-0.721353000

C	2.341841000	3.647948000	0.106546000
C	1.815958000	4.805356000	-0.474914000
H	1.663702000	5.691084000	0.132163000
C	1.489219000	4.839182000	-1.829586000
C	1.681374000	3.715307000	-2.626434000
H	1.426529000	3.755790000	-3.680990000
C	2.197877000	2.531403000	-2.088487000
C	2.659512000	3.580250000	1.593350000
H	3.430867000	2.816091000	1.736681000
C	1.415185000	3.114397000	2.371167000
H	1.066130000	2.150860000	1.990193000
H	0.602249000	3.842314000	2.260384000
H	1.639860000	3.012029000	3.439559000
C	3.206110000	4.896287000	2.161935000
C	2.404616000	1.313832000	-2.975565000
H	2.745355000	0.487736000	-2.346191000
C	3.496873000	1.573247000	-4.027312000
H	4.445123000	1.851613000	-3.555309000
H	3.211791000	2.384983000	-4.705572000
H	3.668208000	0.675100000	-4.631085000
C	1.092641000	0.870738000	-3.642629000
C	2.716530000	-2.011416000	1.070139000
C	2.713473000	-3.032538000	0.100955000
C	1.835314000	-4.528840000	1.802350000
C	2.264294000	-4.296139000	0.496395000
H	2.248366000	-5.107147000	-0.223242000
C	1.864794000	-3.504028000	2.745460000
H	1.550896000	-3.703483000	3.765695000
C	2.320020000	-2.225441000	2.399825000
C	2.375951000	-1.115143000	3.437103000

H	2.892459000	-0.262953000	2.985305000
C	3.170643000	-1.531800000	4.684615000
H	3.261225000	-0.687035000	5.375914000
H	4.179330000	-1.864646000	4.418278000
H	2.681022000	-2.349654000	5.224309000
C	0.959943000	-0.642751000	3.804661000
C	3.156852000	-2.758377000	-1.329386000
H	3.838098000	-1.901801000	-1.307157000
C	1.956130000	-2.359950000	-2.206099000
H	2.298436000	-2.066544000	-3.204786000
H	1.409109000	-1.521669000	-1.767437000
H	1.262652000	-3.197346000	-2.317892000
C	3.923223000	-3.931751000	-1.955851000
H	2.446097000	5.685049000	2.171647000
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H	4.061123000	5.259372000	1.582032000
H	1.250082000	-0.041887000	-4.226891000
H	0.322045000	0.672106000	-2.891558000
H	0.705233000	1.640258000	-4.319293000
H	4.756882000	-4.254409000	-1.323009000
H	3.274305000	-4.797432000	-2.128102000
H	4.328370000	-3.633728000	-2.928437000
H	1.002390000	0.193792000	4.511597000
H	0.440998000	-0.313129000	2.900186000
H	0.379131000	-1.448443000	4.269960000
H	1.493712000	-5.519208000	2.090633000
H	1.084541000	5.748340000	-2.264315000
H	-0.978211000	-5.262876000	-3.742726000
H	-0.702673000	-4.161036000	0.392304000
C	-1.466987000	-2.646762000	-0.945994000

O	-1.655047000	-1.669033000	0.053215000
C	-1.569305000	-2.105335000	1.428033000
H	-1.881696000	-1.252326000	2.033420000
H	-2.266894000	-2.929078000	1.591606000
H	-0.545923000	-2.391903000	1.677745000
C	-4.724184000	-0.666190000	-0.489672000
H	-3.729364000	-0.230404000	-0.334927000
H	-5.391787000	0.189312000	-0.644821000
C	-5.117864000	-1.417248000	0.785073000
H	-4.495487000	-2.320324000	0.869880000
H	-6.152416000	-1.776437000	0.700754000
C	-4.963514000	-0.581412000	2.056005000
H	-3.941771000	-0.172320000	2.086961000
H	-5.626537000	0.291886000	2.004354000
C	-5.232847000	-1.357394000	3.347327000
H	-4.589637000	-2.249019000	3.377325000
H	-6.265118000	-1.730573000	3.337317000
C	-5.002134000	-0.516589000	4.605011000
H	-5.220857000	-1.082755000	5.516166000
H	-3.958356000	-0.179868000	4.670552000
H	-5.639722000	0.375593000	4.606707000
C	-3.737563000	3.263677000	-1.326281000
C	-2.688152000	2.665079000	-0.603995000
C	-2.965514000	2.396555000	0.751727000
C	-4.153193000	2.738782000	1.383232000
C	-5.156630000	3.355397000	0.632786000
C	-4.949575000	3.600314000	-0.725565000
H	-3.572190000	3.488173000	-2.376096000
H	-4.315514000	2.515615000	2.430890000
H	-6.091122000	3.631549000	1.109926000

H	-5.728030000	4.074305000	-1.315684000
O	-1.951683000	1.653194000	1.432228000
C	-1.809521000	1.866457000	2.851128000
H	-2.627029000	1.379215000	3.387929000
H	-0.857012000	1.425277000	3.136791000
H	-1.804767000	2.939295000	3.053764000
C	-1.385411000	2.263939000	-1.202577000
H	-1.368530000	2.415958000	-2.282945000
H	-0.558958000	2.853285000	-0.771426000
H	-4.322136000	1.080119000	-2.685666000
C	5.605125000	-1.105522000	0.952134000
H	5.635239000	-2.045678000	0.389188000
H	6.548139000	-0.580659000	0.784629000
H	5.546035000	-1.366823000	2.015593000
C	5.472793000	1.974937000	-0.333411000
H	5.399475000	2.896459000	0.255922000
H	6.457104000	1.536238000	-0.155709000
H	5.413033000	2.261963000	-1.389365000

TS1

Sc	0.639109000	0.327168000	-0.042933000
C	3.395266000	-3.087793000	-0.294865000
C	4.384608000	-3.551214000	0.576376000
H	5.144543000	-4.235241000	0.213344000
C	4.384464000	-3.131490000	1.906896000
C	3.404173000	-2.254027000	2.367987000
H	3.398256000	-1.954246000	3.411494000
C	2.404571000	-1.753249000	1.517743000
C	1.367905000	-0.791793000	1.980467000
H	0.360757000	-1.095787000	1.641257000
H	1.301487000	-0.808906000	3.064803000

C	3.245678000	1.174540000	2.502377000
H	3.407974000	0.370951000	3.228501000
H	3.502498000	2.107268000	3.025999000
C	1.772149000	1.267396000	2.161879000
H	1.130507000	1.274255000	3.038377000
C	1.325999000	2.116150000	1.095958000
H	2.102052000	2.619163000	0.520366000
H	0.437093000	2.718530000	1.287913000
N	-1.223406000	0.064989000	-0.177297000
N	-3.345075000	1.011874000	0.425637000
N	-3.328963000	-1.104757000	-0.122724000
C	-2.500090000	-0.006320000	0.021993000
C	-4.669438000	0.548473000	0.537457000
C	-4.662612000	-0.765788000	0.188084000
C	-2.854883000	2.303415000	0.798054000
C	-2.519332000	3.218453000	-0.218179000
C	-2.002203000	4.456040000	0.175295000
H	-1.733176000	5.191480000	-0.574269000
C	-1.823480000	4.763226000	1.524010000
C	-2.153286000	3.835470000	2.506914000
H	-1.999046000	4.084787000	3.551582000
C	-2.672935000	2.581805000	2.163011000
C	-2.714641000	2.857488000	-1.686222000
H	-2.409793000	1.811638000	-1.797248000
C	-1.844231000	3.689103000	-2.636289000
H	-0.791783000	3.672752000	-2.338317000
H	-2.167980000	4.734791000	-2.677035000
H	-1.920902000	3.290213000	-3.653698000
C	-4.192174000	2.957922000	-2.107910000
C	-2.957397000	1.536205000	3.232647000

H	-3.610725000	0.773256000	2.800699000
C	-3.674875000	2.112011000	4.461888000
H	-4.589286000	2.644383000	4.179205000
H	-3.039516000	2.810537000	5.016809000
H	-3.948408000	1.304363000	5.149027000
C	-1.652750000	0.825363000	3.633345000
C	-2.872872000	-2.401146000	-0.524229000
C	-2.236953000	-3.225193000	0.424575000
C	-2.044707000	-4.923449000	-1.305456000
C	-1.831879000	-4.497194000	0.004315000
H	-1.347357000	-5.165550000	0.706932000
C	-2.658359000	-4.081214000	-2.228867000
H	-2.812554000	-4.425080000	-3.245749000
C	-3.085723000	-2.801895000	-1.855954000
C	-3.690423000	-1.840764000	-2.870454000
H	-4.366390000	-1.166333000	-2.336376000
C	-4.505414000	-2.531682000	-3.970315000
H	-5.009104000	-1.780570000	-4.587448000
H	-5.268922000	-3.194113000	-3.548980000
H	-3.872736000	-3.126922000	-4.637825000
C	-2.575430000	-0.964263000	-3.468976000
C	-2.002616000	-2.748344000	1.853025000
H	-1.730201000	-1.690221000	1.793578000
C	-0.850627000	-3.481366000	2.554286000
H	-0.620834000	-2.983361000	3.501823000
H	0.062327000	-3.491787000	1.950226000
H	-1.113864000	-4.518318000	2.790432000
C	-3.280224000	-2.843998000	2.707925000
H	-4.573242000	3.972831000	-1.948418000
H	-4.299927000	2.720050000	-3.172394000

H	-4.820338000	2.262043000	-1.547671000
H	-1.853040000	0.020372000	4.349787000
H	-1.167443000	0.393803000	2.753890000
H	-0.953983000	1.530138000	4.099236000
H	-4.078161000	-2.208062000	2.318097000
H	-3.646577000	-3.876056000	2.745835000
H	-3.070113000	-2.522545000	3.734310000
H	-2.993581000	-0.201099000	-4.135661000
H	-2.019688000	-0.467752000	-2.669128000
H	-1.873106000	-1.575709000	-4.049381000
H	-1.730562000	-5.918698000	-1.606833000
H	-1.421815000	5.731634000	1.807607000
H	5.143194000	-3.496740000	2.591701000
H	3.379197000	-3.404306000	-1.332547000
C	2.440798000	-2.203867000	0.187449000
O	1.466350000	-1.644884000	-0.655018000
C	0.795486000	-2.513512000	-1.600125000
H	-0.150489000	-2.028729000	-1.835904000
H	1.409227000	-2.632013000	-2.497300000
H	0.602839000	-3.478935000	-1.131278000
C	4.198479000	0.979810000	1.316811000
H	3.808743000	0.195626000	0.657214000
H	4.251294000	1.890677000	0.708502000
C	5.605098000	0.572178000	1.767929000
H	5.520458000	-0.268666000	2.469249000
H	6.068308000	1.395884000	2.328944000
C	6.513156000	0.154234000	0.610843000
H	6.014540000	-0.644530000	0.042180000
H	6.633286000	0.994922000	-0.085663000
C	7.890967000	-0.337691000	1.060417000

H	7.763339000	-1.180166000	1.754569000
H	8.393719000	0.454744000	1.631386000
C	8.775357000	-0.767992000	-0.112012000
H	9.754622000	-1.119997000	0.228976000
H	8.307589000	-1.582112000	-0.680004000
H	8.944430000	0.065172000	-0.805325000
C	4.442117000	2.944285000	-2.331249000
C	3.066390000	2.720774000	-2.188365000
C	2.647455000	1.385660000	-2.198770000
C	3.525235000	0.316427000	-2.346874000
C	4.886954000	0.572064000	-2.496039000
C	5.342280000	1.890316000	-2.487521000
H	4.807104000	3.967386000	-2.320210000
H	3.140665000	-0.696615000	-2.332035000
H	5.584822000	-0.251265000	-2.603281000
H	6.401753000	2.099152000	-2.596479000
O	1.273665000	1.098373000	-2.022724000
C	0.510166000	1.056446000	-3.251702000
H	0.824333000	0.195529000	-3.848255000
H	-0.532748000	0.965301000	-2.960032000
H	0.671652000	1.980961000	-3.808670000
C	2.094729000	3.864146000	-2.049545000
H	1.302559000	3.638291000	-1.331524000
H	2.611261000	4.769090000	-1.718935000
H	1.613218000	4.096683000	-3.007882000
C	-5.767862000	-1.761133000	0.092326000
H	-5.935474000	-2.088382000	-0.940512000
H	-5.554350000	-2.658217000	0.683176000
H	-6.699322000	-1.326407000	0.461613000
C	-5.775668000	1.434613000	0.998307000

H	-6.733796000	0.916330000	0.918613000
H	-5.642728000	1.738285000	2.043087000
H	-5.834254000	2.351164000	0.402120000
TS2			
Sc	0.650324000	-0.252817000	0.338730000
C	2.943376000	-3.052046000	-1.437522000
C	4.252240000	-3.529509000	-1.420410000
H	4.791689000	-3.670047000	-2.351426000
C	4.852640000	-3.837220000	-0.198036000
C	4.147607000	-3.667630000	0.991346000
H	4.618095000	-3.926583000	1.934831000
C	2.837988000	-3.163707000	1.010146000
C	2.107410000	-2.961489000	2.318263000
H	1.038795000	-3.169638000	2.190884000
H	2.484875000	-3.724871000	3.006739000
C	3.702049000	-1.051954000	3.034342000
H	4.383794000	-1.888175000	3.236961000
H	3.825700000	-0.361305000	3.877867000
C	2.255203000	-1.585717000	3.044592000
H	2.025819000	-1.832638000	4.090662000
C	1.218519000	-0.519646000	2.628337000
H	1.156537000	0.217336000	3.440274000
H	0.209189000	-0.968553000	2.627439000
N	-1.208479000	-0.104088000	0.091296000
N	-2.918640000	1.589727000	0.113760000
N	-3.563424000	-0.464522000	-0.245890000
C	-2.437602000	0.299287000	-0.002451000
C	-4.321178000	1.615557000	-0.028892000
C	-4.720422000	0.337132000	-0.256878000
C	-2.090129000	2.732845000	0.351265000

C	-1.376636000	3.292387000	-0.727950000
C	-0.597093000	4.423440000	-0.464746000
H	-0.027410000	4.883739000	-1.263131000
C	-0.527225000	4.963921000	0.817650000
C	-1.223828000	4.377141000	1.869456000
H	-1.147308000	4.802550000	2.864003000
C	-2.019055000	3.245027000	1.658639000
C	-1.427353000	2.660809000	-2.115473000
H	-1.356864000	1.577529000	-1.969774000
C	-0.250779000	3.074195000	-3.009255000
H	0.713554000	2.936039000	-2.511072000
H	-0.321603000	4.123497000	-3.316168000
H	-0.259626000	2.474129000	-3.926248000
C	-2.753847000	2.949605000	-2.842775000
C	-2.720777000	2.543251000	2.813587000
H	-3.607760000	2.040349000	2.415700000
C	-3.193781000	3.500199000	3.915500000
H	-3.800451000	4.316062000	3.508163000
H	-2.353751000	3.943682000	4.461080000
H	-3.800769000	2.955294000	4.645802000
C	-1.805958000	1.445465000	3.389144000
C	-3.523939000	-1.868515000	-0.511368000
C	-3.560080000	-2.766350000	0.567925000
C	-3.402003000	-4.583774000	-1.035762000
C	-3.494108000	-4.134610000	0.278853000
H	-3.518241000	-4.854049000	1.091716000
C	-3.378105000	-3.671924000	-2.090754000
H	-3.312953000	-4.036790000	-3.110501000
C	-3.442382000	-2.296078000	-1.850721000
C	-3.358558000	-1.291755000	-2.990842000

H	-3.766692000	-0.341735000	-2.632105000
C	-4.172737000	-1.704838000	-4.224307000
H	-4.164945000	-0.897866000	-4.964492000
H	-5.214580000	-1.917098000	-3.962479000
H	-3.759689000	-2.595616000	-4.709912000
C	-1.883226000	-1.039207000	-3.353866000
C	-3.627611000	-2.285054000	2.007446000
H	-3.737080000	-1.196751000	1.993131000
C	-2.312339000	-2.602946000	2.738155000
H	-2.318386000	-2.182527000	3.749704000
H	-1.468313000	-2.172825000	2.192108000
H	-2.154302000	-3.684493000	2.822832000
C	-4.839922000	-2.866079000	2.751843000
H	-2.903968000	4.028847000	-2.959453000
H	-2.739196000	2.502778000	-3.843632000
H	-3.612853000	2.537589000	-2.309141000
H	-2.311822000	0.905850000	4.198100000
H	-1.524482000	0.726075000	2.616013000
H	-0.887627000	1.884382000	3.796818000
H	-5.775864000	-2.623214000	2.237337000
H	-4.778492000	-3.956652000	2.834988000
H	-4.893067000	-2.458343000	3.767004000
H	-1.799570000	-0.261028000	-4.121418000
H	-1.328444000	-0.718321000	-2.467439000
H	-1.420066000	-1.954131000	-3.744755000
H	-3.357189000	-5.649308000	-1.241859000
H	0.083415000	5.843802000	0.997784000
H	5.868059000	-4.219547000	-0.172276000
H	2.440292000	-2.826547000	-2.371576000
C	2.271498000	-2.871456000	-0.232272000

O	0.967186000	-2.327739000	-0.269076000
C	-0.093013000	-3.286314000	-0.558422000
H	-1.018898000	-2.719275000	-0.541953000
H	0.085495000	-3.726248000	-1.541533000
H	-0.090819000	-4.060561000	0.211156000
C	4.125287000	-0.339907000	1.740061000
H	3.601967000	-0.778338000	0.880086000
H	3.812258000	0.707600000	1.776876000
C	5.624784000	-0.396725000	1.442185000
H	5.963188000	-1.441169000	1.477238000
H	6.179853000	0.134909000	2.227751000
C	5.953962000	0.200195000	0.072666000
H	5.391025000	-0.351321000	-0.696166000
H	5.590195000	1.234253000	0.030097000
C	7.442042000	0.173157000	-0.282282000
H	7.807655000	-0.862827000	-0.248993000
H	8.008341000	0.720826000	0.483332000
C	7.726538000	0.776735000	-1.659823000
H	8.795026000	0.753866000	-1.898807000
H	7.195676000	0.227233000	-2.447584000
H	7.393235000	1.820409000	-1.705409000
C	3.443968000	3.318226000	0.285501000
C	2.551691000	2.266808000	0.036482000
C	2.679832000	1.620278000	-1.202001000
C	3.599445000	2.002926000	-2.168966000
C	4.461897000	3.067466000	-1.890258000
C	4.389186000	3.717419000	-0.660214000
H	3.374668000	3.838216000	1.236756000
H	3.671831000	1.488099000	-3.118766000
H	5.190442000	3.370866000	-2.634618000

H	5.061206000	4.540316000	-0.438048000
O	1.798389000	0.529529000	-1.387624000
C	1.692905000	-0.029554000	-2.708918000
H	2.639539000	-0.494209000	-2.992790000
H	0.906458000	-0.780547000	-2.660641000
H	1.416077000	0.752892000	-3.417605000
C	1.506146000	1.844684000	1.010598000
H	1.590669000	2.424333000	1.933570000
H	0.501452000	2.089638000	0.624586000
H	1.547555000	0.607569000	1.784235000
C	-6.067641000	-0.255699000	-0.481198000
H	-6.834295000	0.521698000	-0.456036000
H	-6.128999000	-0.762592000	-1.451439000
H	-6.311823000	-0.998658000	0.287402000
C	-5.096817000	2.882555000	0.086657000
H	-6.149796000	2.701902000	-0.140913000
H	-5.037353000	3.306501000	1.095711000
H	-4.724269000	3.644720000	-0.606140000
INT1'			
Sc	0.110467000	1.739949000	-0.179934000
C	1.805519000	4.822216000	0.945642000
C	1.714017000	5.983309000	0.187749000
H	2.552742000	6.668967000	0.133554000
C	0.524820000	6.252734000	-0.510612000
C	-0.558460000	5.388376000	-0.444024000
H	-1.471985000	5.619369000	-0.984540000
C	-0.526563000	4.205402000	0.338140000
C	-1.548839000	3.161129000	0.289132000
H	-1.858345000	2.751325000	1.256881000
H	-2.421612000	3.398465000	-0.316566000

C	2.616986000	2.066973000	-2.428569000
H	3.467045000	2.668306000	-2.772790000
H	2.495082000	1.233568000	-3.127831000
C	1.382046000	2.928640000	-2.407745000
H	1.491541000	3.914674000	-1.951762000
C	0.168271000	2.563247000	-2.861850000
H	0.005486000	1.612664000	-3.364964000
H	-0.679352000	3.240664000	-2.800766000
N	-0.314016000	-0.066855000	-0.109213000
N	-0.293906000	-2.473078000	-0.041076000
N	-2.232898000	-1.486248000	0.124084000
C	-0.886016000	-1.232049000	-0.012146000
C	-1.261478000	-3.486816000	0.082125000
C	-2.470643000	-2.872306000	0.190148000
C	1.106822000	-2.680663000	-0.252062000
C	1.950659000	-2.788570000	0.866427000
C	3.313621000	-2.995563000	0.629997000
H	3.995858000	-3.091203000	1.467698000
C	3.808882000	-3.082580000	-0.669344000
C	2.949682000	-2.971136000	-1.759896000
H	3.348205000	-3.050966000	-2.766350000
C	1.576340000	-2.780079000	-1.573125000
C	1.408115000	-2.643537000	2.280252000
H	0.323875000	-2.788675000	2.236806000
C	1.653644000	-1.214841000	2.801992000
H	1.236842000	-0.479681000	2.106412000
H	2.726123000	-1.017629000	2.910826000
H	1.182878000	-1.079849000	3.782872000
C	1.975733000	-3.691621000	3.248043000
C	0.635130000	-2.661141000	-2.762474000

H	-0.390166000	-2.756259000	-2.391693000
C	0.850908000	-3.772750000	-3.800216000
H	0.776673000	-4.764589000	-3.342016000
H	1.832255000	-3.698580000	-4.280873000
H	0.093554000	-3.703603000	-4.588286000
C	0.758422000	-1.267012000	-3.401771000
C	-3.227904000	-0.458320000	0.205449000
C	-3.635667000	0.183984000	-0.978183000
C	-5.170897000	1.498017000	0.371217000
C	-4.626212000	1.164660000	-0.867332000
H	-4.976866000	1.678424000	-1.755195000
C	-4.724690000	0.868711000	1.529535000
H	-5.146536000	1.151819000	2.487780000
C	-3.738187000	-0.121577000	1.470336000
C	-3.170437000	-0.746028000	2.737038000
H	-2.757142000	-1.726081000	2.479729000
C	-4.217076000	-0.964762000	3.837286000
H	-3.773863000	-1.521175000	4.669719000
H	-5.076415000	-1.533088000	3.465950000
H	-4.589824000	-0.017969000	4.242627000
C	-1.997958000	0.112564000	3.247703000
C	-3.007223000	-0.171165000	-2.320652000
H	-1.943713000	-0.354162000	-2.136902000
C	-3.092331000	0.970755000	-3.341988000
H	-2.477424000	0.733565000	-4.217056000
H	-2.739259000	1.916004000	-2.916286000
H	-4.115449000	1.125228000	-3.701295000
C	-3.606493000	-1.459416000	-2.913492000
H	3.049274000	-3.553297000	3.415945000
H	1.480903000	-3.611148000	4.221673000

H	1.823406000	-4.708252000	2.870486000
H	0.040872000	-1.151403000	-4.222693000
H	0.562155000	-0.495861000	-2.651751000
H	1.765325000	-1.110949000	-3.807478000
H	-3.437050000	-2.321091000	-2.262889000
H	-4.686040000	-1.351016000	-3.066780000
H	-3.148084000	-1.679829000	-3.884418000
H	-1.534042000	-0.346477000	4.128559000
H	-1.235928000	0.223245000	2.470426000
H	-2.351371000	1.111661000	3.530181000
H	-5.943072000	2.259241000	0.433297000
H	4.869467000	-3.249507000	-0.832101000
H	0.448716000	7.156915000	-1.107320000
H	2.711351000	4.561659000	1.484841000
C	0.706316000	3.966551000	0.998871000
O	0.853280000	2.702764000	1.637341000
C	0.543584000	2.660173000	3.052163000
H	0.679281000	1.625583000	3.364119000
H	1.235865000	3.317608000	3.581936000
H	-0.488255000	2.980992000	3.212425000
C	2.927068000	1.522542000	-1.019254000
H	2.876943000	2.346175000	-0.290295000
H	2.175040000	0.756673000	-0.748420000
C	4.290893000	0.838449000	-0.881732000
H	5.074448000	1.529438000	-1.220364000
H	4.322828000	-0.033692000	-1.547155000
C	4.563174000	0.399273000	0.558262000
H	4.522043000	1.277861000	1.219847000
H	3.758866000	-0.272895000	0.881596000
C	5.909347000	-0.306030000	0.739542000

H	6.718451000	0.358345000	0.407666000
H	5.944028000	-1.183782000	0.081328000
C	6.158035000	-0.735729000	2.186880000
H	7.119923000	-1.247487000	2.294060000
H	6.163571000	0.129146000	2.860895000
H	5.374783000	-1.419953000	2.536042000
C	-3.842887000	-3.424594000	0.369054000
H	-3.824047000	-4.514084000	0.293476000
H	-4.262526000	-3.161086000	1.346850000
H	-4.531186000	-3.041156000	-0.391484000
C	-0.875866000	-4.924823000	0.077746000
H	-0.201246000	-5.162522000	0.908743000
H	-1.761855000	-5.556715000	0.169279000
H	-0.356605000	-5.197245000	-0.848445000

INT2'

Sc	-0.927991000	-1.213405000	-0.725247000
C	-1.702110000	-3.371354000	1.726561000
C	-2.954901000	-3.445502000	2.330838000
H	-3.036332000	-3.370125000	3.410178000
C	-4.094891000	-3.622887000	1.542853000
C	-3.981010000	-3.718447000	0.158139000
H	-4.871778000	-3.865002000	-0.445257000
C	-2.740870000	-3.635750000	-0.496087000
C	-2.662806000	-3.682904000	-2.009416000
H	-1.760562000	-4.222773000	-2.314501000
H	-3.520226000	-4.273484000	-2.348235000
C	-3.815046000	-1.366068000	-2.317845000
H	-4.732151000	-1.932410000	-2.111431000
H	-4.055895000	-0.685331000	-3.143224000
C	-2.689879000	-2.320031000	-2.791361000

H	-2.968610000	-2.627752000	-3.809675000
C	-1.323459000	-1.598833000	-2.835887000
H	-1.407944000	-0.701088000	-3.462723000
H	-0.573225000	-2.248454000	-3.307730000
N	0.438090000	-0.063990000	-0.198179000
N	1.289835000	2.161538000	0.103959000
N	2.696003000	0.516734000	0.382723000
C	1.381601000	0.787029000	0.068976000
C	2.534541000	2.735517000	0.422714000
C	3.411710000	1.711770000	0.596280000
C	0.082911000	2.861965000	-0.211293000
C	-0.800505000	3.187215000	0.833190000
C	-2.004498000	3.810441000	0.489192000
H	-2.707827000	4.087433000	1.266694000
C	-2.314206000	4.083287000	-0.842311000
C	-1.408176000	3.773516000	-1.853612000
H	-1.649165000	4.017790000	-2.883513000
C	-0.179066000	3.172854000	-1.556461000
C	-0.465934000	2.849817000	2.279135000
H	0.615810000	2.691480000	2.338715000
C	-1.138909000	1.531799000	2.705778000
H	-0.881646000	0.725800000	2.011118000
H	-2.228335000	1.638477000	2.725233000
H	-0.810536000	1.241707000	3.710273000
C	-0.817774000	3.985566000	3.250946000
C	0.833991000	2.886805000	-2.655144000
H	1.775783000	2.601887000	-2.175381000
C	1.115467000	4.135679000	-3.506717000
H	1.421830000	4.983568000	-2.884561000
H	0.234189000	4.443323000	-4.079761000

H	1.917773000	3.929386000	-4.223097000
C	0.392924000	1.702213000	-3.529593000
C	3.239245000	-0.804559000	0.442812000
C	3.676032000	-1.410934000	-0.747145000
C	4.325947000	-3.347959000	0.569481000
C	4.221286000	-2.697977000	-0.657912000
H	4.578182000	-3.189501000	-1.558010000
C	3.877696000	-2.726313000	1.734285000
H	3.966785000	-3.243268000	2.684356000
C	3.325183000	-1.441627000	1.694323000
C	2.780775000	-0.781479000	2.952455000
H	2.686861000	0.290687000	2.754865000
C	3.703066000	-0.948255000	4.168195000
H	3.317907000	-0.368895000	5.013803000
H	4.717861000	-0.599571000	3.949762000
H	3.769992000	-1.992415000	4.492413000
C	1.364484000	-1.309532000	3.250085000
C	3.571637000	-0.712450000	-2.093376000
H	3.133251000	0.275872000	-1.929001000
C	2.632502000	-1.476807000	-3.040805000
H	2.526628000	-0.940151000	-3.989564000
H	1.636075000	-1.578032000	-2.600938000
H	3.017346000	-2.478529000	-3.264419000
C	4.957661000	-0.505140000	-2.726641000
H	-1.899753000	4.140790000	3.323304000
H	-0.456775000	3.744322000	4.256321000
H	-0.362565000	4.932421000	2.942014000
H	1.135748000	1.504412000	-4.310668000
H	0.278586000	0.797789000	-2.927679000
H	-0.564087000	1.911262000	-4.022426000

H	5.619043000	0.060466000	-2.061482000
H	5.445276000	-1.460807000	-2.948123000
H	4.866209000	0.048229000	-3.667374000
H	0.930646000	-0.795835000	4.114945000
H	0.707555000	-1.147231000	2.389383000
H	1.394358000	-2.383087000	3.478219000
H	4.763928000	-4.340707000	0.620716000
H	-3.258616000	4.559932000	-1.089164000
H	-5.072130000	-3.692612000	2.009604000
H	-0.807178000	-3.236943000	2.323505000
C	-1.613940000	-3.478249000	0.333679000
O	-0.385108000	-3.280793000	-0.323093000
C	0.830089000	-3.834917000	0.244887000
H	1.598360000	-3.677155000	-0.508731000
H	1.109165000	-3.306404000	1.155492000
H	0.674194000	-4.898949000	0.433237000
C	-3.500414000	-0.490736000	-1.091756000
H	-3.228977000	-1.124325000	-0.224491000
H	-2.669566000	0.203447000	-1.326085000
C	-4.668104000	0.381614000	-0.617780000
H	-5.568190000	-0.242155000	-0.543471000
H	-4.875114000	1.140821000	-1.382710000
C	-4.386223000	1.049368000	0.728798000
H	-4.270583000	0.268643000	1.496610000
H	-3.426440000	1.577934000	0.674841000
C	-5.477788000	2.031287000	1.163421000
H	-6.454248000	1.529417000	1.129152000
H	-5.530168000	2.851654000	0.434696000
C	-5.246661000	2.598703000	2.565797000
H	-6.038020000	3.300355000	2.848332000

H	-5.225348000	1.799621000	3.316554000
H	-4.291220000	3.133023000	2.627634000
C	4.860124000	1.695366000	0.939931000
H	5.237485000	2.715299000	1.040901000
H	5.046547000	1.169810000	1.884062000
H	5.449551000	1.189397000	0.166462000
C	2.701139000	4.212428000	0.508752000
H	3.732814000	4.465603000	0.762515000
H	2.455329000	4.698701000	-0.442576000
H	2.046293000	4.646929000	1.273339000

TS1'

Sc	0.951143000	-0.763849000	0.254749000
C	4.516953000	1.464169000	-1.085867000
C	5.586866000	1.117236000	-1.914471000
H	6.449425000	1.772439000	-1.975254000
C	5.541272000	-0.065758000	-2.650600000
C	4.428245000	-0.900324000	-2.560344000
H	4.390588000	-1.814196000	-3.146317000
C	3.333535000	-0.585875000	-1.740080000
C	2.155466000	-1.503719000	-1.644085000
H	1.208103000	-0.963890000	-1.880632000
H	2.207412000	-2.241395000	-2.440832000
C	3.645083000	-3.057071000	0.086727000
H	4.238364000	-2.949588000	-0.826326000
H	3.855301000	-4.064677000	0.469491000
C	2.163369000	-3.005626000	-0.238654000
H	1.858371000	-3.712183000	-1.006614000
C	1.225454000	-2.857475000	0.858379000
H	1.654310000	-2.900949000	1.862234000
H	0.283258000	-3.398724000	0.766535000

N	-0.760543000	-0.042538000	0.187930000
N	-3.078455000	-0.639328000	0.024950000
N	-2.595176000	1.487655000	-0.032456000
C	-2.021997000	0.241369000	0.069928000
C	-4.296092000	0.054201000	-0.092266000
C	-3.995370000	1.381220000	-0.133761000
C	-2.891627000	-2.055304000	0.120895000
C	-2.728930000	-2.627429000	1.392801000
C	-2.490246000	-4.004956000	1.457989000
H	-2.364952000	-4.480513000	2.425940000
C	-2.411805000	-4.772154000	0.299127000
C	-2.578446000	-4.178180000	-0.951319000
H	-2.522662000	-4.791494000	-1.844226000
C	-2.823884000	-2.806549000	-1.066869000
C	-2.804645000	-1.800563000	2.666467000
H	-2.960760000	-0.755157000	2.384923000
C	-1.489089000	-1.869613000	3.459022000
H	-0.648008000	-1.547063000	2.836454000
H	-1.280447000	-2.887702000	3.805245000
H	-1.537434000	-1.218970000	4.338823000
C	-3.998966000	-2.228875000	3.536294000
C	-2.962390000	-2.138851000	-2.428195000
H	-3.544486000	-1.221072000	-2.293554000
C	-3.705583000	-3.005064000	-3.454517000
H	-4.670461000	-3.347378000	-3.066130000
H	-3.125314000	-3.888574000	-3.741777000
H	-3.889470000	-2.427960000	-4.366681000
C	-1.578996000	-1.718818000	-2.959956000
C	-1.827533000	2.695145000	-0.044839000
C	-1.274729000	3.132719000	-1.259771000

C	-0.320793000	5.016367000	-0.058922000
C	-0.523112000	4.313702000	-1.243749000
H	-0.093724000	4.685860000	-2.169247000
C	-0.866619000	4.550724000	1.136843000
H	-0.699680000	5.107756000	2.052652000
C	-1.636151000	3.382867000	1.168214000
C	-2.193735000	2.839057000	2.475514000
H	-3.028970000	2.174443000	2.231882000
C	-2.735053000	3.935084000	3.403931000
H	-3.228082000	3.480722000	4.269506000
H	-3.463869000	4.571323000	2.890757000
H	-1.936339000	4.579170000	3.787378000
C	-1.126985000	1.984339000	3.187550000
C	-1.446454000	2.350843000	-2.551905000
H	-2.059699000	1.471267000	-2.336996000
C	-0.086484000	1.847702000	-3.066475000
H	-0.219309000	1.208995000	-3.946233000
H	0.424372000	1.265571000	-2.293323000
H	0.565895000	2.680099000	-3.353991000
C	-2.178268000	3.175530000	-3.623113000
H	-3.896455000	-3.266665000	3.871758000
H	-4.071276000	-1.594569000	4.426513000
H	-4.941171000	-2.149582000	2.983396000
H	-1.672197000	-1.214125000	-3.928328000
H	-1.088494000	-1.035198000	-2.261258000
H	-0.935530000	-2.596834000	-3.095442000
H	-3.159074000	3.507098000	-3.265994000
H	-1.606885000	4.067004000	-3.903983000
H	-2.329519000	2.577168000	-4.528056000
H	-1.533617000	1.545280000	4.105350000

H	-0.785567000	1.172234000	2.537854000
H	-0.261524000	2.599705000	3.462709000
H	0.260638000	5.933912000	-0.065646000
H	-2.226897000	-5.840117000	0.368927000
H	6.367568000	-0.337355000	-3.299247000
H	4.553265000	2.375019000	-0.500065000
C	3.422586000	0.613588000	-1.011893000
O	2.337709000	0.880931000	-0.158090000
C	2.026289000	2.262693000	0.168679000
H	1.009013000	2.255246000	0.557061000
H	2.729685000	2.629759000	0.918965000
H	2.070811000	2.863714000	-0.739640000
C	4.094407000	-2.008403000	1.119796000
H	3.496891000	-1.089137000	1.003183000
H	3.891465000	-2.362763000	2.137377000
C	5.563936000	-1.602731000	0.990017000
H	5.763573000	-1.327982000	-0.052642000
H	6.205156000	-2.466243000	1.212952000
C	5.938013000	-0.425864000	1.893807000
H	5.236929000	0.402394000	1.704632000
H	5.805538000	-0.705471000	2.948782000
C	7.366970000	0.076115000	1.668929000
H	7.486450000	0.340606000	0.608872000
H	8.073599000	-0.742235000	1.861437000
C	7.721342000	1.280033000	2.543965000
H	8.745960000	1.620340000	2.361363000
H	7.048901000	2.124229000	2.345146000
H	7.636494000	1.034086000	3.608992000
C	-4.855453000	2.589979000	-0.258937000
H	-4.594403000	3.176358000	-1.147794000

H	-5.906020000	2.302489000	-0.339117000
H	-4.749971000	3.252478000	0.608328000
C	-5.596744000	-0.669007000	-0.137945000
H	-5.749358000	-1.270540000	0.765717000
H	-6.424157000	0.039376000	-0.217854000
H	-5.649654000	-1.351815000	-0.993949000

TS1''

Sc	0.666972000	0.288386000	0.237599000
C	3.958616000	-0.148829000	2.973156000
C	4.917043000	0.812374000	3.303852000
H	5.888917000	0.497122000	3.668432000
C	4.621035000	2.168040000	3.155535000
C	3.369805000	2.567176000	2.690398000
H	3.137149000	3.624582000	2.599252000
C	2.380062000	1.629641000	2.350119000
C	1.064890000	2.021750000	1.799458000
H	0.242129000	1.379993000	2.163242000
H	0.789171000	3.034537000	2.077201000
C	2.781665000	1.668073000	-1.833293000
H	3.047894000	2.532545000	-2.462399000
H	2.794050000	0.801533000	-2.504597000
C	1.145312000	2.758914000	-0.202443000
H	0.167992000	3.227496000	-0.132869000
C	1.379651000	1.852876000	-1.262296000
H	1.961804000	3.380713000	0.154499000
H	0.554511000	1.766880000	-1.968772000
N	-1.201340000	0.047567000	0.101559000
N	-3.331058000	1.058003000	-0.424148000
N	-3.363979000	-0.970198000	0.380870000
C	-2.494320000	0.048822000	0.023312000

C	-4.680421000	0.663882000	-0.352084000
C	-4.702718000	-0.594640000	0.158978000
C	-2.838722000	2.308495000	-0.909478000
C	-2.397023000	2.384600000	-2.240097000
C	-1.821673000	3.588104000	-2.664371000
H	-1.460054000	3.679053000	-3.684180000
C	-1.725321000	4.675138000	-1.800556000
C	-2.229655000	4.591917000	-0.502245000
H	-2.182567000	5.462045000	0.143572000
C	-2.802406000	3.406975000	-0.029683000
C	-2.588659000	1.231198000	-3.214451000
H	-3.109921000	0.427936000	-2.685185000
C	-1.253342000	0.656724000	-3.707512000
H	-0.678162000	0.261470000	-2.867275000
H	-0.649693000	1.418587000	-4.214189000
H	-1.425625000	-0.160339000	-4.416697000
C	-3.477817000	1.658227000	-4.395445000
C	-3.370808000	3.298202000	1.380282000
H	-4.163260000	2.543281000	1.357397000
C	-4.003200000	4.605950000	1.875741000
H	-4.732287000	4.998017000	1.158881000
H	-3.251062000	5.382862000	2.051708000
H	-4.517588000	4.433323000	2.826791000
C	-2.310125000	2.793205000	2.371798000
C	-2.894322000	-2.234798000	0.844896000
C	-2.498410000	-2.353310000	2.188225000
C	-1.796741000	-4.626727000	1.695578000
C	-1.933554000	-3.568918000	2.593013000
H	-1.624275000	-3.697753000	3.626439000
C	-2.244011000	-4.498397000	0.380821000

H	-2.158105000	-5.341618000	-0.296547000
C	-2.803177000	-3.298618000	-0.072930000
C	-3.268611000	-3.131919000	-1.514497000
H	-3.986713000	-2.307707000	-1.536683000
C	-3.985095000	-4.376429000	-2.057148000
H	-4.405913000	-4.163577000	-3.045339000
H	-4.801946000	-4.688622000	-1.397950000
H	-3.302205000	-5.225379000	-2.171758000
C	-2.104878000	-2.720944000	-2.433936000
C	-2.741309000	-1.233625000	3.189216000
H	-3.136620000	-0.375214000	2.640015000
C	-1.457248000	-0.771537000	3.891195000
H	-1.674267000	0.061479000	4.568218000
H	-0.718431000	-0.429324000	3.162220000
H	-1.010559000	-1.574529000	4.488905000
C	-3.805883000	-1.659262000	4.216467000
H	-2.995053000	2.432255000	-5.001852000
H	-3.681206000	0.801876000	-5.047748000
H	-4.436080000	2.058641000	-4.047686000
H	-2.748334000	2.656124000	3.367031000
H	-1.890313000	1.840029000	2.042562000
H	-1.491516000	3.516091000	2.461534000
H	-4.735458000	-1.962027000	3.723193000
H	-3.459720000	-2.505224000	4.820754000
H	-4.033634000	-0.830945000	4.896111000
H	-2.476883000	-2.492088000	-3.438604000
H	-1.588483000	-1.837170000	-2.048972000
H	-1.378867000	-3.537296000	-2.526711000
H	-1.364439000	-5.566031000	2.028633000
H	-1.277233000	5.602144000	-2.146176000

H	5.363165000	2.916521000	3.414186000
H	4.183438000	-1.204428000	3.079235000
C	2.726081000	0.274229000	2.493571000
O	1.743522000	-0.630012000	2.045834000
C	1.632864000	-1.894330000	2.725097000
H	0.667265000	-2.313853000	2.447069000
H	2.437352000	-2.567095000	2.415420000
H	1.674237000	-1.728894000	3.803946000
C	3.877555000	1.482354000	-0.777724000
H	3.929217000	2.360806000	-0.123841000
H	3.617475000	0.642117000	-0.118278000
C	5.260634000	1.209576000	-1.367604000
H	5.580566000	2.069754000	-1.972264000
H	5.196706000	0.356008000	-2.053756000
C	6.306487000	0.915090000	-0.289551000
H	6.417980000	1.790947000	0.365485000
H	5.934134000	0.107667000	0.357204000
C	7.671972000	0.516798000	-0.853852000
H	8.057613000	1.328800000	-1.485033000
H	7.545165000	-0.349598000	-1.518545000

INT3''

Sc	0.673826000	-0.064096000	0.029599000
C	3.876393000	1.652095000	2.268552000
C	4.853458000	2.619322000	2.052332000
H	5.810669000	2.540272000	2.556976000
C	4.593870000	3.681646000	1.183202000
C	3.370891000	3.756958000	0.524194000
H	3.177185000	4.574473000	-0.164692000
C	2.368335000	2.791354000	0.707670000
C	1.105591000	2.862866000	-0.115860000

H	0.268177000	2.351031000	0.382054000
H	0.776385000	3.905510000	-0.155703000
C	2.874808000	0.464215000	-2.304530000
H	3.134148000	1.070621000	-3.190533000
H	2.864701000	-0.575794000	-2.658863000
C	1.256856000	2.358909000	-1.586821000
H	0.339737000	2.680414000	-2.089697000
C	1.465202000	0.837474000	-1.808740000
H	2.079616000	2.931156000	-2.041966000
H	0.763805000	0.529394000	-2.597454000
N	-1.218412000	-0.063902000	0.066416000
N	-3.305170000	1.148800000	-0.107906000
N	-3.425355000	-1.019895000	0.110440000
C	-2.511372000	0.019388000	0.023586000
C	-4.672237000	0.807255000	-0.104705000
C	-4.747727000	-0.540839000	0.025096000
C	-2.805046000	2.467566000	-0.348848000
C	-2.654975000	2.893956000	-1.681866000
C	-2.130846000	4.172991000	-1.895726000
H	-1.992605000	4.533431000	-2.909509000
C	-1.803527000	5.000945000	-0.823580000
C	-2.016476000	4.575114000	0.485105000
H	-1.788185000	5.243128000	1.309359000
C	-2.532174000	3.301594000	0.748339000
C	-3.064165000	2.002099000	-2.846641000
H	-3.788522000	1.274863000	-2.465278000
C	-1.866827000	1.201759000	-3.383748000
H	-1.405622000	0.612605000	-2.588409000
H	-1.104035000	1.870126000	-3.798998000
H	-2.189069000	0.522303000	-4.181253000

C	-3.757101000	2.781468000	-3.974063000
C	-2.786765000	2.837467000	2.174259000
H	-3.460474000	1.975640000	2.125647000
C	-3.471320000	3.910594000	3.033258000
H	-4.386380000	4.278448000	2.557402000
H	-2.817242000	4.770852000	3.211800000
H	-3.737858000	3.495108000	4.011010000
C	-1.480796000	2.351554000	2.822397000
C	-3.074125000	-2.400152000	0.217430000
C	-3.091477000	-3.003485000	1.490672000
C	-2.468292000	-5.094980000	0.423924000
C	-2.780372000	-4.364320000	1.570690000
H	-2.788949000	-4.862489000	2.534040000
C	-2.455408000	-4.474488000	-0.821855000
H	-2.213003000	-5.053650000	-1.707827000
C	-2.759918000	-3.113896000	-0.951542000
C	-2.721778000	-2.446368000	-2.316286000
H	-3.041742000	-1.408306000	-2.194652000
C	-3.687779000	-3.115369000	-3.307144000
H	-3.683338000	-2.578270000	-4.261743000
H	-4.712931000	-3.116340000	-2.921557000
H	-3.405828000	-4.154506000	-3.509137000
C	-1.284905000	-2.421338000	-2.863606000
C	-3.372385000	-2.176020000	2.736858000
H	-4.022012000	-1.344334000	2.445326000
C	-2.058658000	-1.558373000	3.255758000
H	-2.251594000	-0.901679000	4.111847000
H	-1.576042000	-0.973919000	2.466384000
H	-1.368174000	-2.347298000	3.580782000
C	-4.090627000	-2.956481000	3.844769000

H	-3.064496000	3.452778000	-4.493111000
H	-4.151794000	2.083862000	-4.720227000
H	-4.589728000	3.383779000	-3.595107000
H	-1.664733000	1.981603000	3.838005000
H	-1.052990000	1.541682000	2.227295000
H	-0.747675000	3.165557000	2.881326000
H	-4.999717000	-3.439313000	3.471197000
H	-3.451450000	-3.731686000	4.281628000
H	-4.374266000	-2.277097000	4.655139000
H	-1.246398000	-1.906019000	-3.828710000
H	-0.625910000	-1.889347000	-2.170491000
H	-0.893665000	-3.435303000	-3.005503000
H	-2.239981000	-6.153915000	0.504368000
H	-1.403503000	5.993366000	-1.011001000
H	5.347134000	4.444860000	1.015991000
H	4.071107000	0.812457000	2.926234000
C	2.655243000	1.763292000	1.609057000
O	1.670701000	0.759619000	1.804746000
C	1.326283000	0.463228000	3.177873000
H	0.453223000	-0.188008000	3.146296000
H	2.155315000	-0.046756000	3.672386000
H	1.086210000	1.392269000	3.696921000
C	4.007191000	0.613677000	-1.285145000
H	4.072671000	1.655436000	-0.954838000
H	3.776472000	0.024999000	-0.385356000
C	5.376562000	0.174493000	-1.804600000
H	5.640603000	0.763287000	-2.694480000
H	5.320351000	-0.871714000	-2.135465000
C	6.476345000	0.313263000	-0.748815000
H	6.599245000	1.374053000	-0.486882000

H	6.150248000	-0.187689000	0.173586000
C	7.823258000	-0.268996000	-1.183466000
H	8.160463000	0.232718000	-2.100603000
H	7.686052000	-1.326903000	-1.450871000
C	8.900870000	-0.149333000	-0.103672000
H	9.853508000	-0.577065000	-0.433835000
H	9.080183000	0.899924000	0.160036000
H	8.599633000	-0.672207000	0.813215000
C	4.644242000	-3.212876000	-0.792321000
C	3.264842000	-2.967273000	-0.830064000
C	2.694609000	-2.445335000	0.334393000
C	3.428225000	-2.186568000	1.488041000
C	4.797679000	-2.442174000	1.495222000
C	5.404056000	-2.954669000	0.347435000
H	5.126551000	-3.607417000	-1.681906000
H	2.921943000	-1.792825000	2.362470000
H	5.384583000	-2.241275000	2.385651000
H	6.472060000	-3.146686000	0.336482000
O	1.315864000	-2.127243000	0.352093000
C	0.436478000	-3.239433000	0.684684000
H	0.721066000	-3.632129000	1.663312000
H	-0.569420000	-2.832103000	0.700179000
H	0.526426000	-4.010999000	-0.079941000
C	2.449006000	-3.266497000	-2.060847000
H	1.627970000	-2.557897000	-2.189612000
H	3.075208000	-3.227468000	-2.955765000
H	2.011308000	-4.271846000	-2.011213000
C	-5.913110000	-1.466805000	0.071077000
H	-5.955239000	-2.024827000	1.013999000
H	-6.845403000	-0.907274000	-0.032168000

H	-5.868513000	-2.205090000	-0.738343000
C	-5.728413000	1.850486000	-0.222557000
H	-6.719535000	1.392943000	-0.186388000
H	-5.661572000	2.581546000	0.591965000
H	-5.644805000	2.407174000	-1.163110000

MeOINT1

Sc	1.597201000	-0.506171000	-0.050135000
C	4.959530000	0.970877000	0.839927000
C	6.162602000	0.305513000	0.633604000
H	6.994277000	0.482485000	1.303015000
C	6.268177000	-0.600304000	-0.440562000
C	5.181483000	-0.817369000	-1.295602000
H	5.307273000	-1.513611000	-2.118249000
C	3.966590000	-0.131179000	-1.140968000
C	2.747255000	-0.408706000	-1.934746000
H	2.322674000	0.483937000	-2.411369000
H	2.885861000	-1.189253000	-2.684002000
N	-0.206426000	-0.156236000	-0.139071000
N	-2.359867000	-1.084089000	0.296802000
N	-2.250894000	1.088341000	0.108650000
C	-1.487166000	-0.049764000	0.053494000
C	-3.660380000	-0.588761000	0.513261000
C	-3.593029000	0.764935000	0.391043000
C	-1.945215000	-2.453689000	0.273544000
C	-1.216164000	-2.962278000	1.362523000
C	-0.815710000	-4.302359000	1.311471000
H	-0.266646000	-4.731403000	2.144714000
C	-1.124912000	-5.096849000	0.210560000
C	-1.822679000	-4.559635000	-0.869447000
H	-2.037869000	-5.185680000	-1.728292000

C	-2.237545000	-3.224102000	-0.867053000
C	-0.856314000	-2.100145000	2.561773000
H	-1.160741000	-1.073535000	2.350279000
C	0.660152000	-2.085734000	2.816935000
H	1.225731000	-1.871155000	1.888115000
H	1.033985000	-3.053726000	3.164410000
H	0.932227000	-1.325900000	3.555966000
C	-1.601558000	-2.552805000	3.829348000
C	-2.883701000	-2.592830000	-2.091866000
H	-3.487476000	-1.742915000	-1.759123000
C	-3.815236000	-3.544478000	-2.853740000
H	-4.569319000	-3.985758000	-2.193033000
H	-3.264461000	-4.361771000	-3.331585000
H	-4.335019000	-2.998881000	-3.647854000
C	-1.784074000	-2.031161000	-3.016398000
C	-1.700887000	2.404016000	-0.022172000
C	-1.526702000	2.938082000	-1.308878000
C	-0.605778000	4.931222000	-0.268300000
C	-0.966207000	4.217518000	-1.408000000
H	-0.817410000	4.660128000	-2.387953000
C	-0.788504000	4.375636000	0.997835000
H	-0.501030000	4.943007000	1.876819000
C	-1.338284000	3.098428000	1.147481000
C	-1.480543000	2.459627000	2.521702000
H	-2.211715000	1.648657000	2.442342000
C	-1.994590000	3.435289000	3.589872000
H	-2.184282000	2.900146000	4.526178000
H	-2.927356000	3.915367000	3.276072000
H	-1.267342000	4.224568000	3.808106000
C	-0.142814000	1.824951000	2.949219000

C	-1.896886000	2.157388000	-2.559345000
H	-2.418919000	1.247993000	-2.246462000
C	-0.629217000	1.721139000	-3.315249000
H	-0.893090000	1.119728000	-4.191864000
H	0.013736000	1.118706000	-2.667064000
H	-0.059519000	2.590789000	-3.663468000
C	-2.851360000	2.947496000	-3.468638000
H	-1.342305000	-3.582233000	4.098778000
H	-1.353972000	-1.906214000	4.678538000
H	-2.684240000	-2.510788000	3.673769000
H	-2.231419000	-1.507004000	-3.868532000
H	-1.132190000	-1.333021000	-2.482310000
H	-1.160905000	-2.843650000	-3.408190000
H	-3.755134000	3.251392000	-2.929343000
H	-2.378366000	3.852571000	-3.864752000
H	-3.153740000	2.332591000	-4.322939000
H	-0.246844000	1.315327000	3.914213000
H	0.190390000	1.097069000	2.202297000
H	0.635530000	2.590163000	3.051755000
H	-0.181693000	5.926529000	-0.364792000
H	-0.815627000	-6.137603000	0.190282000
H	4.839694000	1.658494000	1.671600000
C	3.896193000	0.749256000	-0.027111000
O	2.626557000	1.328826000	0.264884000
C	2.341308000	2.642923000	-0.288315000
H	1.303189000	2.855569000	-0.041617000
H	3.012817000	3.368105000	0.175287000
H	2.488255000	2.620823000	-1.370430000
C	-4.633034000	1.824547000	0.499799000
H	-5.609225000	1.380214000	0.705466000

H	-4.405523000	2.534238000	1.303770000
H	-4.710588000	2.401329000	-0.429348000
C	-4.794852000	-1.498378000	0.833842000
H	-5.703759000	-0.921213000	1.016873000
H	-4.998207000	-2.202017000	0.018621000
H	-4.583360000	-2.093715000	1.730081000
O	7.384071000	-1.307847000	-0.727596000
C	8.544260000	-1.115118000	0.077038000
H	8.357767000	-1.402402000	1.118926000
H	9.308398000	-1.765848000	-0.347972000
H	8.886282000	-0.074166000	0.036864000

MeO^{INT2}

Sc	0.147327000	0.216832000	0.118119000
C	2.533555000	3.509395000	0.906041000
C	3.853987000	3.691516000	0.483793000
H	4.521526000	4.313532000	1.065797000
C	4.285426000	3.044922000	-0.684814000
C	3.400476000	2.251675000	-1.429483000
H	3.769013000	1.788182000	-2.337474000
C	2.069786000	2.063302000	-1.033485000
C	1.100451000	1.155435000	-1.699004000
H	0.227823000	1.712337000	-2.069282000
H	1.545114000	0.622221000	-2.541262000
C	2.988809000	-2.467157000	-1.096500000
H	3.216633000	-3.386005000	-1.659406000
H	3.315818000	-2.640392000	-0.065057000
N	-1.731276000	0.035270000	0.022861000
N	-3.585289000	-1.389302000	-0.550170000
N	-4.073310000	0.657248000	0.023646000
C	-2.996612000	-0.200326000	-0.148236000

C	-4.984968000	-1.264437000	-0.628287000
C	-5.289544000	0.006884000	-0.268199000
C	-2.862122000	-2.569874000	-0.901487000
C	-2.729965000	-3.589704000	0.060018000
C	-2.040162000	-4.747379000	-0.312394000
H	-1.917785000	-5.553818000	0.402643000
C	-1.505586000	-4.879666000	-1.592800000
C	-1.654590000	-3.858240000	-2.526207000
H	-1.242057000	-3.978003000	-3.523486000
C	-2.342711000	-2.682878000	-2.202712000
C	-3.266475000	-3.405195000	1.472158000
H	-4.072272000	-2.665494000	1.429987000
C	-2.165715000	-2.823408000	2.379165000
H	-1.787009000	-1.880166000	1.973108000
H	-1.328954000	-3.526802000	2.462115000
H	-2.552922000	-2.636432000	3.387380000
C	-3.852208000	-4.690892000	2.071233000
C	-2.529738000	-1.589264000	-3.242789000
H	-3.079966000	-0.768067000	-2.775401000
C	-3.368170000	-2.092316000	-4.430254000
H	-4.341545000	-2.469812000	-4.099336000
H	-2.860160000	-2.903316000	-4.963559000
H	-3.542752000	-1.280102000	-5.144314000
C	-1.181496000	-1.023886000	-3.715235000
C	-3.979539000	2.042627000	0.362321000
C	-3.923502000	2.986814000	-0.679516000
C	-3.804618000	4.724621000	1.013913000
C	-3.823350000	4.336480000	-0.324518000
H	-3.772053000	5.093121000	-1.100172000
C	-3.908164000	3.772217000	2.025657000

H	-3.922443000	4.092700000	3.062128000
C	-4.011998000	2.410695000	1.719351000
C	-4.142570000	1.361137000	2.813169000
H	-4.570583000	0.462278000	2.357250000
C	-5.080894000	1.794423000	3.948341000
H	-5.236799000	0.961874000	4.642465000
H	-6.057727000	2.105572000	3.563467000
H	-4.666862000	2.626975000	4.527516000
C	-2.755032000	0.975377000	3.353406000
C	-3.956560000	2.551472000	-2.138050000
H	-4.439138000	1.569230000	-2.177915000
C	-2.530275000	2.374310000	-2.686800000
H	-2.558099000	2.007182000	-3.718801000
H	-1.967906000	1.659944000	-2.081015000
H	-1.992940000	3.330570000	-2.687275000
C	-4.776643000	3.497827000	-3.026216000
H	-3.080059000	-5.445510000	2.256527000
H	-4.328681000	-4.472069000	3.032573000
H	-4.604519000	-5.134712000	1.410602000
H	-1.336797000	-0.221237000	-4.444080000
H	-0.618756000	-0.607774000	-2.875242000
H	-0.569367000	-1.795431000	-4.196678000
H	-5.780907000	3.661333000	-2.620961000
H	-4.294821000	4.475205000	-3.138333000
H	-4.878506000	3.070816000	-4.029329000
H	-2.835700000	0.185705000	4.109167000
H	-2.123806000	0.612724000	2.537106000
H	-2.270883000	1.843058000	3.819360000
H	-3.729939000	5.777736000	1.269307000
H	-0.972752000	-5.786368000	-1.863735000

H	2.180870000	3.973800000	1.822292000
C	1.683582000	2.706445000	0.164373000
O	0.392675000	2.383064000	0.653514000
C	-0.616874000	3.403747000	0.459657000
H	-1.543562000	2.991197000	0.845665000
H	-0.327936000	4.300496000	1.012608000
H	-0.712976000	3.628880000	-0.604027000
C	3.775302000	-1.302843000	-1.711718000
H	3.404052000	-1.099755000	-2.725805000
H	3.580614000	-0.398920000	-1.127461000
C	5.283143000	-1.559937000	-1.760465000
H	5.496311000	-2.374501000	-2.466854000
H	5.618550000	-1.915851000	-0.776751000
C	6.075470000	-0.309390000	-2.149567000
H	5.701815000	0.075300000	-3.109871000
H	5.882260000	0.487318000	-1.418706000
C	7.585563000	-0.536495000	-2.258450000
H	7.787415000	-1.298702000	-3.023033000
H	7.962457000	-0.952656000	-1.312579000
C	8.350226000	0.746818000	-2.590904000
H	9.428487000	0.567939000	-2.659363000
H	8.017602000	1.165450000	-3.547858000
H	8.181498000	1.511402000	-1.822786000
C	3.953255000	-2.377697000	2.843456000
C	2.674452000	-1.824635000	2.823710000
C	2.517454000	-0.601882000	2.154726000
C	3.584814000	0.060461000	1.565380000
C	4.861744000	-0.497130000	1.608486000
C	5.046938000	-1.729544000	2.247346000
H	4.131479000	-3.326888000	3.338985000

H	3.426378000	1.009950000	1.070934000
H	5.682852000	0.025638000	1.135076000
O	1.230381000	-0.010559000	2.081674000
C	0.942794000	0.848092000	3.214903000
H	1.660803000	1.670694000	3.230527000
H	-0.067438000	1.227306000	3.081868000
H	1.010749000	0.260000000	4.132441000
C	1.527252000	-2.505771000	3.526887000
H	1.518703000	-2.251922000	4.594453000
H	0.561676000	-2.210513000	3.111534000
H	1.616917000	-3.593874000	3.456686000
C	1.503860000	-2.277210000	-1.139735000
H	1.080477000	-2.027502000	-2.112408000
C	0.666877000	-2.449473000	-0.101616000
H	1.043423000	-2.748064000	0.872105000
H	-0.410317000	-2.420888000	-0.232878000
C	-5.845307000	-2.406419000	-1.044504000
H	-6.894001000	-2.101930000	-1.066286000
H	-5.575120000	-2.768096000	-2.043203000
H	-5.752827000	-3.256382000	-0.358190000
C	-6.593331000	0.716732000	-0.149715000
H	-6.643275000	1.586209000	-0.815534000
H	-7.414681000	0.044804000	-0.408220000
H	-6.761561000	1.081852000	0.870483000
O	5.551130000	3.122775000	-1.178389000
O	6.233361000	-2.376148000	2.344420000
C	6.493481000	3.941472000	-0.497783000
H	6.666325000	3.585629000	0.526074000
H	7.418980000	3.865881000	-1.069322000
H	6.165289000	4.987479000	-0.468820000

C	7.402345000	-1.719488000	1.864104000
H	7.554727000	-0.760842000	2.374798000
H	8.231850000	-2.389853000	2.089662000
H	7.351623000	-1.554069000	0.781890000

MeOINT3

Sc	0.251839000	-0.494429000	0.397322000
C	2.687235000	-2.848536000	-1.502930000
C	4.039289000	-3.179995000	-1.436344000
H	4.655010000	-3.108280000	-2.323752000
C	4.568406000	-3.605730000	-0.210204000
C	3.732337000	-3.718786000	0.909286000
H	4.172698000	-4.070114000	1.836028000
C	2.386105000	-3.355897000	0.870954000
C	1.558798000	-3.393861000	2.135896000
H	0.524786000	-3.674850000	1.904895000
H	1.967347000	-4.196648000	2.759087000
C	2.914736000	-1.450196000	3.178805000
H	3.645892000	-2.244643000	3.378250000
H	2.893414000	-0.835861000	4.087455000
C	1.521209000	-2.088479000	2.997309000
H	1.229778000	-2.452328000	3.994759000
C	0.459076000	-1.083450000	2.514541000
H	0.460340000	-0.217649000	3.196320000
H	-0.534860000	-1.543474000	2.658479000
N	-1.538348000	-0.072377000	-0.008005000
N	-3.308513000	1.557488000	0.017291000
N	-3.875474000	-0.523914000	-0.332486000
C	-2.778796000	0.284488000	-0.095371000
C	-4.710481000	1.529819000	-0.137089000
C	-5.061742000	0.238112000	-0.364784000

C	-2.550762000	2.724605000	0.352225000
C	-1.821318000	3.381797000	-0.658194000
C	-1.144831000	4.554018000	-0.304826000
H	-0.571739000	5.092199000	-1.050375000
C	-1.188683000	5.042556000	0.999842000
C	-1.887956000	4.354189000	1.986701000
H	-1.896145000	4.735939000	3.001875000
C	-2.580553000	3.175861000	1.684001000
C	-1.747429000	2.807051000	-2.069095000
H	-1.599874000	1.726486000	-1.957095000
C	-0.560204000	3.350937000	-2.875239000
H	0.385596000	3.254969000	-2.331109000
H	-0.693096000	4.407558000	-3.132443000
H	-0.475520000	2.804050000	-3.821079000
C	-3.052007000	3.022295000	-2.858690000
C	-3.272101000	2.365780000	2.771667000
H	-4.065249000	1.774699000	2.303831000
C	-3.926370000	3.230090000	3.857562000
H	-4.602229000	3.976745000	3.426660000
H	-3.183242000	3.758345000	4.464765000
H	-4.506502000	2.596912000	4.536706000
C	-2.271117000	1.367371000	3.383789000
C	-3.801473000	-1.935026000	-0.551295000
C	-3.666873000	-2.791882000	0.558299000
C	-3.764444000	-4.664233000	-0.990618000
C	-3.658249000	-4.168656000	0.307847000
H	-3.564851000	-4.863928000	1.134184000
C	-3.860407000	-3.792734000	-2.072946000
H	-3.925130000	-4.194144000	-3.078327000
C	-3.877199000	-2.407505000	-1.874772000

C	-3.885603000	-1.435336000	-3.047223000
H	-4.373750000	-0.512555000	-2.719105000
C	-4.652927000	-1.949929000	-4.271233000
H	-4.724895000	-1.159237000	-5.025141000
H	-5.668912000	-2.261700000	-4.006828000
H	-4.150354000	-2.801653000	-4.742697000
C	-2.436287000	-1.062313000	-3.418516000
C	-3.511993000	-2.231775000	1.967608000
H	-2.868232000	-1.350525000	1.888065000
C	-2.820182000	-3.206510000	2.929723000
H	-2.584889000	-2.693138000	3.867297000
H	-1.882407000	-3.591135000	2.514235000
H	-3.459110000	-4.061625000	3.177472000
C	-4.858665000	-1.774907000	2.558317000
H	-3.279622000	4.090765000	-2.946128000
H	-2.950454000	2.616443000	-3.871835000
H	-3.902311000	2.525671000	-2.386546000
H	-2.765458000	0.730576000	4.126259000
H	-1.837062000	0.725067000	2.613572000
H	-1.452078000	1.897698000	3.884235000
H	-5.310321000	-0.973600000	1.968558000
H	-5.566647000	-2.610109000	2.606908000
H	-4.712528000	-1.396827000	3.576376000
H	-2.423797000	-0.306118000	-4.212045000
H	-1.907098000	-0.664465000	-2.547368000
H	-1.894261000	-1.944932000	-3.781179000
H	-3.765106000	-5.737228000	-1.159742000
H	-0.663788000	5.960395000	1.248941000
H	2.247935000	-2.532716000	-2.443140000
C	1.891312000	-2.919381000	-0.366973000

O	0.555870000	-2.456814000	-0.463993000
C	-0.423110000	-3.425480000	-0.926217000
H	-1.369867000	-2.896087000	-0.979048000
H	-0.119542000	-3.792375000	-1.909414000
H	-0.478756000	-4.249139000	-0.212570000
C	3.418273000	-0.583528000	2.009494000
H	2.990261000	-0.938037000	1.062197000
H	3.075543000	0.450125000	2.133840000
C	4.940867000	-0.580381000	1.845638000
H	5.301391000	-1.616910000	1.829238000
H	5.407079000	-0.105923000	2.720247000
C	5.390544000	0.122343000	0.564242000
H	4.871069000	-0.338568000	-0.289496000
H	5.069679000	1.172372000	0.582464000
C	6.900069000	0.049665000	0.323053000
H	7.213281000	-1.003873000	0.330588000
H	7.428513000	0.528267000	1.158392000
C	7.322635000	0.703860000	-0.994265000
H	8.404249000	0.636324000	-1.152633000
H	6.827349000	0.225264000	-1.849435000
H	7.045874000	1.764948000	-1.010347000
C	2.979535000	3.539329000	0.376375000
C	2.127955000	2.460982000	0.162902000
C	2.371749000	1.649617000	-0.954842000
C	3.412886000	1.910023000	-1.832168000
C	4.253768000	3.002903000	-1.610819000
C	4.042864000	3.820322000	-0.495699000
H	2.826430000	4.194766000	1.227393000
H	3.595584000	1.269184000	-2.686489000
H	5.063665000	3.192319000	-2.303213000

O	1.512690000	0.546011000	-1.138750000
C	1.214953000	0.182561000	-2.504210000
H	2.070976000	-0.325878000	-2.950929000
H	0.360658000	-0.492982000	-2.467154000
H	0.958677000	1.078770000	-3.069695000
C	0.988793000	2.169524000	1.100167000
H	0.773433000	3.021277000	1.747170000
H	0.050379000	1.974293000	0.563991000
H	1.216740000	1.334074000	1.779174000
C	-6.387898000	-0.389534000	-0.624722000
H	-7.181381000	0.355838000	-0.536670000
H	-6.443367000	-0.824699000	-1.629422000
H	-6.597603000	-1.195142000	0.087239000
C	-5.532806000	2.767695000	-0.030776000
H	-6.577717000	2.547077000	-0.259919000
H	-5.491302000	3.197947000	0.976503000
H	-5.187310000	3.540413000	-0.726086000
O	5.869288000	-3.919900000	-0.001746000
C	6.777615000	-3.796326000	-1.091368000
H	6.819436000	-2.762203000	-1.455062000
H	7.752704000	-4.082813000	-0.697346000
H	6.504649000	-4.467364000	-1.914706000
O	4.793949000	4.902176000	-0.175312000
C	5.909904000	5.213796000	-1.001528000
H	5.594916000	5.443547000	-2.026978000
H	6.371304000	6.095813000	-0.557125000
H	6.634423000	4.389876000	-1.016682000
MeOINT4			
Sc	0.402275000	-0.746117000	0.130096000
C	0.433653000	3.017250000	0.536874000

C	-0.076408000	4.080301000	-0.197542000
H	-0.689744000	4.817527000	0.300402000
C	0.164974000	4.136011000	-1.577742000
C	0.924231000	3.136973000	-2.195594000
H	1.083830000	3.205218000	-3.266803000
C	1.480180000	2.079618000	-1.471243000
C	2.341057000	1.056517000	-2.182800000
H	2.576101000	0.210239000	-1.531778000
H	1.775018000	0.647658000	-3.028776000
C	4.556845000	2.219473000	-1.604565000
H	3.984246000	2.978488000	-1.053201000
H	5.393182000	2.756484000	-2.071412000
C	3.668273000	1.645873000	-2.723442000
H	3.398359000	2.488575000	-3.374771000
C	4.400824000	0.608994000	-3.582907000
H	5.320582000	1.034645000	-3.999406000
H	3.774988000	0.282186000	-4.421321000
N	-1.429336000	-0.428654000	0.331856000
N	-3.468204000	-1.579641000	-0.189002000
N	-3.650657000	0.335003000	0.849737000
C	-2.719064000	-0.539798000	0.326419000
C	-4.840783000	-1.354074000	0.017140000
C	-4.956042000	-0.168236000	0.672493000
C	-2.877337000	-2.682371000	-0.883269000
C	-2.670053000	-3.886646000	-0.185806000
C	-2.063033000	-4.940169000	-0.875903000
H	-1.890045000	-5.885018000	-0.372376000
C	-1.679641000	-4.794659000	-2.208413000
C	-1.897003000	-3.592828000	-2.874417000
H	-1.596598000	-3.492866000	-3.912951000

C	-2.498091000	-2.509121000	-2.224922000
C	-3.043825000	-4.010827000	1.284660000
H	-3.875404000	-3.326094000	1.479959000
C	-1.867855000	-3.549059000	2.165278000
H	-1.595116000	-2.515351000	1.930732000
H	-0.991133000	-4.184554000	1.991720000
H	-2.131994000	-3.610785000	3.227884000
C	-3.505981000	-5.419026000	1.681474000
C	-2.735962000	-1.204779000	-2.968984000
H	-3.158521000	-0.484499000	-2.264541000
C	-3.759330000	-1.393874000	-4.101826000
H	-4.707881000	-1.784660000	-3.717820000
H	-3.392022000	-2.095590000	-4.858788000
H	-3.960601000	-0.438473000	-4.599280000
C	-1.424805000	-0.605910000	-3.503095000
C	-3.321657000	1.640101000	1.335178000
C	-3.590818000	2.748412000	0.506684000
C	-2.761907000	4.180068000	2.287270000
C	-3.318736000	4.019699000	1.019159000
H	-3.542816000	4.896625000	0.421252000
C	-2.465499000	3.065998000	3.066822000
H	-2.034502000	3.201290000	4.054574000
C	-2.749971000	1.772948000	2.609888000
C	-2.455681000	0.569484000	3.490202000
H	-2.738521000	-0.330015000	2.938176000
C	-3.287296000	0.604433000	4.783161000
H	-3.103348000	-0.293872000	5.383030000
H	-4.358252000	0.650922000	4.559225000
H	-3.037530000	1.475611000	5.398713000
C	-0.952753000	0.462295000	3.795990000

C	-4.090279000	2.558388000	-0.919470000
H	-4.646287000	1.617687000	-0.960904000
C	-2.896377000	2.412746000	-1.883148000
H	-3.246724000	2.107433000	-2.875733000
H	-2.179723000	1.669137000	-1.522736000
H	-2.366319000	3.362579000	-1.995664000
C	-5.040682000	3.666290000	-1.391558000
H	-2.686817000	-6.145265000	1.641916000
H	-3.883710000	-5.412411000	2.709245000
H	-4.306267000	-5.777761000	1.025821000
H	-1.613059000	0.364092000	-3.975291000
H	-0.705149000	-0.459493000	-2.691415000
H	-0.958077000	-1.258798000	-4.248944000
H	-5.876633000	3.806712000	-0.697804000
H	-4.527022000	4.628323000	-1.499741000
H	-5.451798000	3.410394000	-2.373476000
H	-0.744483000	-0.437165000	4.386920000
H	-0.384681000	0.408055000	2.861299000
H	-0.594472000	1.324919000	4.369785000
H	-2.562238000	5.177428000	2.669247000
H	-1.210652000	-5.624742000	-2.728419000
H	0.196193000	2.930718000	1.591525000
C	1.213823000	2.053162000	-0.093444000
O	1.690294000	0.945662000	0.653812000
C	2.483026000	1.225624000	1.828050000
H	3.019612000	0.305037000	2.057933000
H	3.190119000	2.022028000	1.595076000
H	1.835595000	1.515118000	2.659580000
C	5.120557000	1.197069000	-0.611050000
H	4.309906000	0.592185000	-0.186189000

H	5.772388000	0.486265000	-1.132904000
C	5.905758000	1.861327000	0.524528000
H	5.269847000	2.610637000	1.021317000
H	6.747724000	2.428000000	0.103379000
C	6.429090000	0.873609000	1.569710000
H	5.592161000	0.273796000	1.957072000
H	7.105061000	0.155576000	1.083047000
C	7.159650000	1.540112000	2.738367000
H	6.484794000	2.259346000	3.223976000
H	8.001640000	2.129126000	2.350800000
C	7.668430000	0.533231000	3.772394000
H	8.184245000	1.031667000	4.599661000
H	6.841113000	-0.049022000	4.197927000
H	8.372613000	-0.175345000	3.319817000
C	3.646920000	-2.431992000	-1.386561000
C	2.467487000	-2.416605000	-0.629166000
C	2.644404000	-2.318745000	0.776000000
C	3.890274000	-2.308899000	1.383999000
C	5.044402000	-2.366860000	0.597964000
C	4.914965000	-2.397031000	-0.796280000
H	3.584910000	-2.494949000	-2.467665000
H	3.987394000	-2.254865000	2.462871000
H	6.013411000	-2.358639000	1.078306000
O	1.440784000	-2.103488000	1.511069000
C	1.408379000	-2.463486000	2.900013000
H	2.024393000	-1.777370000	3.489043000
H	0.368488000	-2.386627000	3.210622000
H	1.768400000	-3.488595000	3.015532000
C	1.116124000	-2.341286000	-1.227201000
H	1.130191000	-2.361582000	-2.316460000

H	0.444958000	-3.132821000	-0.860863000
H	4.678132000	-0.278986000	-3.006861000
C	-6.146459000	0.550711000	1.205925000
H	-6.275491000	1.536471000	0.744993000
H	-7.053018000	-0.029613000	1.020542000
H	-6.059728000	0.709059000	2.287662000
C	-5.866021000	-2.324699000	-0.456673000
H	-5.743943000	-3.308884000	0.010331000
H	-6.869886000	-1.961721000	-0.225608000
H	-5.798813000	-2.471979000	-1.540935000
O	-0.323574000	5.098703000	-2.399359000
C	-1.063220000	6.168194000	-1.820479000
H	-0.460787000	6.715827000	-1.085744000
H	-1.322735000	6.830290000	-2.646648000
H	-1.980699000	5.803358000	-1.342606000
O	5.961129000	-2.389836000	-1.664969000
C	7.280321000	-2.417457000	-1.133042000
H	7.444453000	-3.314693000	-0.524064000
H	7.947591000	-2.435555000	-1.995109000
H	7.485641000	-1.523716000	-0.531064000

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Sc	-0.195348000	-0.254420000	-0.048626000
C	-3.115205000	2.702895000	-1.232401000
C	-4.203666000	3.250982000	-0.549407000
H	-5.022905000	3.683860000	-1.108494000
C	-4.210028000	3.219345000	0.851708000
C	-3.132655000	2.654469000	1.548039000
H	-3.168091000	2.665443000	2.631571000
C	-2.052945000	2.067192000	0.881744000
C	-0.969542000	1.350135000	1.606314000

H	0.030367000	1.585463000	1.199026000
H	-0.924821000	1.671410000	2.643051000
C	-2.766804000	-0.463082000	2.708905000
H	-2.939293000	0.499768000	3.200077000
H	-2.957690000	-1.226832000	3.477623000
C	-1.303181000	-0.597927000	2.339910000
H	-0.635967000	-0.357398000	3.162460000
C	-0.866226000	-1.688728000	1.517556000
H	-1.645430000	-2.334522000	1.116703000
H	0.039347000	-2.208618000	1.832781000
N	1.674735000	-0.029628000	-0.147104000
N	3.748688000	-1.013989000	0.559946000
N	3.836619000	1.029043000	-0.211282000
C	2.953340000	-0.003455000	0.048385000
C	5.095752000	-0.609234000	0.621519000
C	5.153098000	0.658144000	0.132580000
C	3.202328000	-2.238605000	1.057024000
C	2.827341000	-3.235949000	0.136397000
C	2.255134000	-4.403108000	0.651475000
H	1.953421000	-5.198375000	-0.020430000
C	2.066276000	-4.564783000	2.023774000
C	2.441940000	-3.560237000	2.910136000
H	2.281308000	-3.697993000	3.974117000
C	3.014951000	-2.371380000	2.443174000
C	3.039003000	-3.033800000	-1.360295000
H	2.740377000	-2.003743000	-1.583178000
C	2.174504000	-3.957657000	-2.226320000
H	1.118453000	-3.897168000	-1.950690000
H	2.488193000	-5.004123000	-2.144305000
H	2.272583000	-3.675207000	-3.280068000

C	4.518539000	-3.186724000	-1.759472000
C	3.352068000	-1.235153000	3.399338000
H	4.074691000	-0.577986000	2.908072000
C	3.989041000	-1.716993000	4.710199000
H	4.862228000	-2.350896000	4.522302000
H	3.284075000	-2.290008000	5.322051000
H	4.312813000	-0.857715000	5.306855000
C	2.097515000	-0.386230000	3.671402000
C	3.449384000	2.290338000	-0.765144000
C	2.873130000	3.258645000	0.079620000
C	2.761629000	4.742436000	-1.843936000
C	2.541950000	4.493322000	-0.490102000
H	2.105110000	5.270051000	0.127023000
C	3.309902000	3.757918000	-2.661560000
H	3.467885000	3.964597000	-3.714411000
C	3.666994000	2.510606000	-2.136971000
C	4.203386000	1.398020000	-3.028269000
H	4.838980000	0.751586000	-2.415663000
C	5.055302000	1.901678000	-4.199873000
H	5.508393000	1.053069000	-4.722745000
H	5.860486000	2.560129000	-3.857214000
H	4.458072000	2.452743000	-4.934580000
C	3.035622000	0.525432000	-3.525387000
C	2.610512000	2.963791000	1.552391000
H	2.248725000	1.932110000	1.607937000
C	1.527542000	3.862132000	2.166209000
H	1.268353000	3.493927000	3.164292000
H	0.612465000	3.877636000	1.565095000
H	1.874612000	4.894753000	2.283176000
C	3.894997000	3.046953000	2.398293000

H	4.893663000	-4.179107000	-1.485067000
H	4.630715000	-3.072146000	-2.843732000
H	5.148740000	-2.434693000	-1.280915000
H	2.342868000	0.476359000	4.301582000
H	1.670014000	-0.020938000	2.733258000
H	1.334399000	-0.980280000	4.187551000
H	4.635342000	2.306244000	2.088466000
H	4.346831000	4.042419000	2.321986000
H	3.661980000	2.862650000	3.453106000
H	3.407990000	-0.334417000	-4.094489000
H	2.449720000	0.158804000	-2.677547000
H	2.372735000	1.104354000	-4.180649000
H	2.501506000	5.710136000	-2.263174000
H	1.622336000	-5.480925000	2.402272000
H	-3.092334000	2.716186000	-2.317900000
C	-2.075957000	2.125143000	-0.524365000
O	-1.011352000	1.490597000	-1.204257000
C	-0.118056000	2.389908000	-1.917951000
H	0.714792000	1.785694000	-2.269232000
H	-0.655726000	2.840195000	-2.755457000
H	0.248811000	3.160175000	-1.238445000
C	-3.773575000	-0.632917000	1.564459000
H	-3.442057000	-0.055549000	0.694791000
H	-3.811726000	-1.678192000	1.235388000
C	-5.177732000	-0.156992000	1.955637000
H	-5.099289000	0.823766000	2.442751000
H	-5.606492000	-0.837418000	2.704914000
C	-6.124160000	-0.027536000	0.761811000
H	-5.657418000	0.633765000	0.017495000
H	-6.249557000	-0.998927000	0.267817000

C	-7.500099000	0.532113000	1.130072000
H	-7.370739000	1.484687000	1.662399000
H	-7.994992000	-0.146369000	1.838248000
C	-8.392637000	0.737920000	-0.096002000
H	-9.383216000	1.114893000	0.180200000
H	-7.943311000	1.457130000	-0.793645000
H	-8.529947000	-0.202081000	-0.643872000
C	-3.937231000	-3.406984000	-1.355594000
C	-2.563338000	-3.131623000	-1.392284000
C	-2.177328000	-1.849920000	-1.787725000
C	-3.102513000	-0.874537000	-2.158417000
C	-4.456744000	-1.166330000	-2.131047000
C	-4.881316000	-2.439134000	-1.721515000
H	-4.254709000	-4.393224000	-1.038989000
H	-2.755099000	0.109704000	-2.448446000
H	-5.200807000	-0.425574000	-2.398703000
O	-0.801581000	-1.511929000	-1.773930000
C	-0.174794000	-1.490421000	-3.076780000
H	-0.603809000	-0.686886000	-3.682015000
H	0.885495000	-1.317130000	-2.905219000
H	-0.330996000	-2.454879000	-3.564095000
C	-1.554501000	-4.192163000	-1.033198000
H	-0.738805000	-3.790988000	-0.426686000
H	-2.029396000	-5.004996000	-0.477332000
H	-1.107718000	-4.628644000	-1.935120000
C	6.306042000	1.579543000	-0.074292000
H	6.475183000	1.788985000	-1.137087000
H	6.146219000	2.542766000	0.421831000
H	7.219200000	1.137470000	0.330333000
C	6.159055000	-1.496522000	1.172799000

H	7.141344000	-1.038688000	1.036545000
H	6.018942000	-1.680468000	2.244307000
H	6.167324000	-2.472918000	0.677319000
O	-5.216760000	3.696666000	1.626114000
C	-6.343581000	4.281128000	0.981148000
H	-6.855243000	3.553109000	0.340304000
H	-7.014009000	4.593077000	1.782144000
H	-6.051400000	5.155423000	0.386876000
O	-6.223605000	-2.629758000	-1.700598000
C	-6.725190000	-3.887891000	-1.260550000
H	-6.424795000	-4.093464000	-0.225945000
H	-7.810885000	-3.808623000	-1.316052000
H	-6.383679000	-4.701232000	-1.911875000

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Sc	0.201338000	-0.263649000	0.358286000
C	2.616796000	-2.909815000	-1.312922000
C	3.960803000	-3.276157000	-1.263443000
H	4.532570000	-3.344865000	-2.180001000
C	4.541243000	-3.551847000	-0.017584000
C	3.761687000	-3.483324000	1.145605000
H	4.237686000	-3.726150000	2.089199000
C	2.427842000	-3.079456000	1.117577000
C	1.646939000	-2.935837000	2.404474000
H	0.593326000	-3.187700000	2.237737000
H	2.035830000	-3.690938000	3.095581000
C	3.137977000	-0.996451000	3.256742000
H	3.817591000	-1.816017000	3.523558000
H	3.171353000	-0.299615000	4.103468000
C	1.707996000	-1.564729000	3.150527000
H	1.405869000	-1.828264000	4.174221000

C	0.684794000	-0.516631000	2.665166000
H	0.565495000	0.226815000	3.464649000
H	-0.316976000	-0.979412000	2.609268000
N	-1.650890000	-0.115828000	0.063291000
N	-3.377642000	1.559556000	0.048465000
N	-3.990348000	-0.499127000	-0.344533000
C	-2.879820000	0.274837000	-0.063421000
C	-4.775670000	1.571783000	-0.134080000
C	-5.155137000	0.290913000	-0.381521000
C	-2.570543000	2.703104000	0.348696000
C	-1.816574000	3.295274000	-0.684130000
C	-1.059940000	4.426076000	-0.359992000
H	-0.461291000	4.911107000	-1.121653000
C	-1.047926000	4.933446000	0.937631000
C	-1.782165000	4.313577000	1.943856000
H	-1.750625000	4.713124000	2.951466000
C	-2.558780000	3.181866000	1.670653000
C	-1.800531000	2.696357000	-2.086871000
H	-1.724646000	1.610529000	-1.963131000
C	-0.590083000	3.141890000	-2.917786000
H	0.353777000	2.987810000	-2.385508000
H	-0.652036000	4.200595000	-3.192734000
H	-0.559810000	2.572861000	-3.853875000
C	-3.097825000	2.988978000	-2.863323000
C	-3.306272000	2.448811000	2.776710000
H	-4.169705000	1.947848000	2.327910000
C	-3.838241000	3.378014000	3.875650000
H	-4.433048000	4.197448000	3.458038000
H	-3.028249000	3.816671000	4.468473000
H	-4.473086000	2.812559000	4.565586000

C	-2.409989000	1.345988000	3.371008000
C	-3.932472000	-1.906087000	-0.590029000
C	-3.958600000	-2.788762000	0.501835000
C	-3.795705000	-4.628074000	-1.076197000
C	-3.887808000	-4.160900000	0.231756000
H	-3.908317000	-4.868803000	1.054877000
C	-3.775658000	-3.730857000	-2.144037000
H	-3.709210000	-4.110114000	-3.158236000
C	-3.847379000	-2.352357000	-1.923353000
C	-3.768282000	-1.359727000	-3.074195000
H	-4.234268000	-0.425961000	-2.743763000
C	-4.511390000	-1.823376000	-4.333759000
H	-4.517561000	-1.021556000	-5.079468000
H	-5.549948000	-2.089452000	-4.110830000
H	-4.032619000	-2.693179000	-4.796737000
C	-2.293406000	-1.040178000	-3.382637000
C	-4.033378000	-2.290595000	1.935202000
H	-4.073417000	-1.198053000	1.910704000
C	-2.766858000	-2.685229000	2.712074000
H	-2.773115000	-2.241049000	3.713321000
H	-1.876022000	-2.331109000	2.185933000
H	-2.688211000	-3.772401000	2.827079000
C	-5.303447000	-2.788740000	2.643515000
H	-3.255175000	4.069121000	-2.961000000
H	-3.036197000	2.566055000	-3.872756000
H	-3.973622000	2.555399000	-2.375918000
H	-2.949058000	0.784448000	4.142881000
H	-2.085089000	0.646497000	2.596750000
H	-1.516201000	1.782944000	3.831733000
H	-6.205700000	-2.480838000	2.104245000

H	-5.317757000	-3.881519000	2.720379000
H	-5.357966000	-2.381746000	3.659022000
H	-2.216539000	-0.263943000	-4.152918000
H	-1.786641000	-0.689699000	-2.478983000
H	-1.775080000	-1.935912000	-3.748359000
H	-3.746853000	-5.696185000	-1.267543000
H	-0.452677000	5.812662000	1.165962000
H	2.140210000	-2.709478000	-2.266317000
C	1.880369000	-2.799162000	-0.141327000
O	0.548262000	-2.330722000	-0.221240000
C	-0.459282000	-3.332004000	-0.537776000
H	-1.407264000	-2.802314000	-0.567901000
H	-0.223759000	-3.777932000	-1.506427000
H	-0.460582000	-4.096383000	0.241917000
C	3.653363000	-0.284994000	1.993500000
H	3.147910000	-0.687711000	1.106894000
H	3.385227000	0.774989000	2.027136000
C	5.160986000	-0.412231000	1.758850000
H	5.463812000	-1.460127000	1.881468000
H	5.708477000	0.157539000	2.522370000
C	5.561429000	0.060330000	0.360398000
H	4.978797000	-0.507925000	-0.380501000
H	5.272491000	1.110020000	0.228249000
C	7.050861000	-0.104000000	0.052552000
H	7.340563000	-1.150955000	0.219584000
H	7.640398000	0.490790000	0.763144000
C	7.402598000	0.308254000	-1.378829000
H	8.472546000	0.195914000	-1.584299000
H	6.854167000	-0.299877000	-2.110460000
H	7.132538000	1.355548000	-1.562432000

C	3.109383000	3.193186000	0.390943000
C	2.174015000	2.201617000	0.100704000
C	2.308272000	1.544804000	-1.135545000
C	3.287752000	1.877697000	-2.054462000
C	4.207797000	2.887505000	-1.747930000
C	4.125409000	3.538609000	-0.513751000
H	3.054948000	3.731467000	1.331591000
H	3.370711000	1.365580000	-3.005191000
H	4.975087000	3.136297000	-2.469281000
O	1.375063000	0.501201000	-1.353925000
C	1.245996000	-0.005742000	-2.691527000
H	2.171334000	-0.500923000	-2.993938000
H	0.427797000	-0.723536000	-2.671014000
H	1.007667000	0.813393000	-3.372577000
C	1.077095000	1.829091000	1.037780000
H	1.140547000	2.419684000	1.955242000
H	0.095864000	2.092673000	0.606516000
H	1.065293000	0.600630000	1.824338000
C	-6.490277000	-0.312914000	-0.645547000
H	-7.265027000	0.456719000	-0.631396000
H	-6.523518000	-0.810707000	-1.621877000
H	-6.745684000	-1.065975000	0.109359000
C	-5.567665000	2.829945000	-0.033226000
H	-6.612402000	2.639283000	-0.288936000
H	-5.538924000	3.249905000	0.978821000
H	-5.185530000	3.599430000	-0.712633000
O	5.840357000	-3.884379000	0.169091000
C	6.694183000	-3.942589000	-0.969667000
H	6.749100000	-2.969059000	-1.471629000
H	7.678988000	-4.210136000	-0.586843000

H	6.357443000	-4.707688000	-1.679490000
O	4.967985000	4.520592000	-0.100133000
C	6.040083000	4.887021000	-0.958349000
H	6.590567000	5.667041000	-0.431648000
H	6.705491000	4.035144000	-1.149234000
H	5.671272000	5.282290000	-1.913251000

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Sc	-1.151006000	-1.180610000	-0.855786000
C	-4.327932000	0.747153000	-2.233473000
C	-5.274016000	1.236061000	-1.336289000
C	-5.091926000	0.981514000	0.046186000
C	-3.995411000	0.249672000	0.509849000
H	-3.878796000	0.074818000	1.573751000
C	-3.031967000	-0.248096000	-0.381344000
N	0.315117000	-0.008647000	-0.559282000
N	1.773288000	-1.383327000	0.728947000
N	2.379692000	0.704706000	0.513914000
C	1.396828000	-0.173484000	0.140994000
C	2.948147000	-1.231507000	1.488364000
C	3.326266000	0.067553000	1.345672000
C	0.814140000	-2.426543000	0.623584000
C	0.777799000	-3.178109000	-0.578745000
C	-0.364380000	-3.963119000	-0.831571000
H	-0.424517000	-4.540911000	-1.748594000
C	-1.426476000	-4.003573000	0.081681000
C	-1.349420000	-3.286595000	1.280720000
H	-2.177558000	-3.326817000	1.979931000
C	-0.228301000	-2.490352000	1.581549000
C	1.904320000	-3.110343000	-1.597228000
H	2.646105000	-2.403500000	-1.217307000

C	1.409147000	-2.579122000	-2.954120000
H	0.982797000	-1.574445000	-2.845780000
H	0.662390000	-3.243207000	-3.404978000
H	2.244332000	-2.499408000	-3.656485000
C	2.581077000	-4.484833000	-1.741608000
C	-0.181539000	-1.684473000	2.868701000
H	0.748625000	-1.110608000	2.868296000
C	-0.157614000	-2.623386000	4.088898000
H	0.679891000	-3.327215000	4.039997000
H	-1.082590000	-3.205704000	4.164922000
H	-0.057098000	-2.036483000	5.007147000
C	-1.345160000	-0.681914000	2.953193000
C	2.396111000	2.087247000	0.131506000
C	1.597011000	2.995300000	0.842548000
C	2.457252000	4.748720000	-0.600836000
C	1.645644000	4.338608000	0.451713000
H	1.040566000	5.069629000	0.979027000
C	3.229670000	3.821353000	-1.298619000
H	3.847503000	4.155617000	-2.124938000
C	3.210402000	2.468645000	-0.950502000
C	3.967610000	1.427285000	-1.761480000
H	4.166020000	0.569448000	-1.109410000
C	5.321239000	1.922390000	-2.287028000
H	5.863069000	1.097509000	-2.761671000
H	5.944605000	2.320614000	-1.479285000
H	5.204239000	2.708183000	-3.040816000
C	3.073644000	0.926320000	-2.913473000
C	0.686804000	2.562273000	1.980874000
H	0.839974000	1.491534000	2.149668000
C	-0.791178000	2.762775000	1.600357000

H	-1.444156000	2.441540000	2.419960000
H	-1.044148000	2.182577000	0.708182000
H	-1.006836000	3.817892000	1.399210000
C	1.034886000	3.285819000	3.292049000
H	1.890141000	-5.234105000	-2.143808000
H	3.430954000	-4.412624000	-2.427427000
H	2.950341000	-4.849568000	-0.777556000
H	-1.239803000	-0.068952000	3.854034000
H	-1.362543000	-0.015675000	2.086548000
H	-2.311961000	-1.194549000	3.009872000
H	2.083084000	3.127168000	3.568898000
H	0.871857000	4.365796000	3.211226000
H	0.405719000	2.916372000	4.109689000
H	3.566101000	0.112733000	-3.459558000
H	2.110960000	0.569173000	-2.534195000
H	2.874745000	1.738408000	-3.622312000
H	2.485433000	5.796507000	-0.885115000
H	-2.310029000	-4.594159000	-0.139823000
H	-4.453477000	0.925433000	-3.297107000
C	-3.247276000	0.034608000	-1.725155000
O	-2.218053000	-0.505045000	-2.606764000
C	-1.661123000	0.422728000	-3.570123000
H	-0.809521000	-0.081436000	-4.029014000
H	-2.407812000	0.646864000	-4.333527000
H	-1.338618000	1.334674000	-3.061160000
C	4.485517000	0.819138000	1.900207000
H	5.135690000	1.202219000	1.105480000
H	4.150457000	1.681956000	2.487091000
H	5.083600000	0.175415000	2.548977000
C	3.555249000	-2.375951000	2.221476000

H	3.824941000	-3.192831000	1.539916000
H	4.463402000	-2.059661000	2.738890000
H	2.869469000	-2.788444000	2.972073000
O	-6.060978000	1.506072000	0.846606000
C	-5.944207000	1.330531000	2.250307000
H	-5.019162000	1.781061000	2.632485000
H	-6.804508000	1.838686000	2.687371000
H	-5.970271000	0.267877000	2.523733000
C	-6.472585000	2.018270000	-1.797859000
H	-7.403297000	1.524657000	-1.496738000
H	-6.489061000	3.014775000	-1.342570000
H	-6.474055000	2.131258000	-2.885348000

MeO^{INT2'}

Sc	0.342022000	-0.059605000	-0.567242000
C	2.785830000	2.583041000	1.374670000
C	2.879309000	3.892775000	0.881766000
C	2.035424000	4.260569000	-0.181810000
C	1.147091000	3.344879000	-0.757477000
H	0.537200000	3.699616000	-1.585440000
C	1.052829000	2.024555000	-0.306177000
C	2.436083000	1.428653000	-3.236444000
H	2.399218000	2.432638000	-2.806150000
H	2.851170000	1.551354000	-4.248113000
C	1.023106000	0.933369000	-3.374395000
H	0.273613000	1.698173000	-3.573494000
C	0.609477000	-0.347275000	-3.297958000
H	1.313617000	-1.165045000	-3.170615000
H	-0.426865000	-0.616960000	-3.484517000
N	-1.472592000	-0.342263000	-0.217056000
N	-3.454423000	0.855935000	0.453879000

N	-3.564725000	-1.322254000	0.451186000
C	-2.704989000	-0.272931000	0.187625000
C	-4.753484000	0.508616000	0.867675000
C	-4.821014000	-0.848401000	0.873643000
C	-2.988124000	2.193221000	0.246841000
C	-3.104893000	2.751036000	-1.036192000
C	-2.650129000	4.061130000	-1.218507000
H	-2.730069000	4.525264000	-2.196941000
C	-2.113367000	4.781593000	-0.156731000
C	-2.017280000	4.208069000	1.109162000
H	-1.600433000	4.786879000	1.926075000
C	-2.459126000	2.902549000	1.339736000
C	-3.709710000	1.980016000	-2.198659000
H	-4.062880000	1.015722000	-1.821207000
C	-2.644996000	1.688547000	-3.267002000
H	-1.819272000	1.128780000	-2.821383000
H	-2.245467000	2.616584000	-3.692188000
H	-3.066162000	1.095721000	-4.086453000
C	-4.920856000	2.711182000	-2.800075000
C	-2.362161000	2.262512000	2.717516000
H	-3.132438000	1.485762000	2.777504000
C	-2.623293000	3.253392000	3.860579000
H	-3.564503000	3.794539000	3.716961000
H	-1.819932000	3.992620000	3.951416000
H	-2.679262000	2.717398000	4.813927000
C	-1.002388000	1.564980000	2.897175000
C	-3.204941000	-2.699626000	0.322319000
C	-2.574874000	-3.338272000	1.402885000
C	-2.508991000	-5.366623000	0.070381000
C	-2.232202000	-4.686899000	1.253526000

H	-1.747002000	-5.209794000	2.072271000
C	-3.137914000	-4.710650000	-0.987131000
H	-3.352645000	-5.255174000	-1.900406000
C	-3.505593000	-3.365222000	-0.880910000
C	-4.154237000	-2.627495000	-2.043175000
H	-4.698495000	-1.771125000	-1.631556000
C	-5.165068000	-3.485093000	-2.816533000
H	-5.687025000	-2.869292000	-3.556261000
H	-5.913626000	-3.923852000	-2.148307000
H	-4.678646000	-4.301883000	-3.360832000
C	-3.068959000	-2.065571000	-2.981388000
C	-2.238027000	-2.593981000	2.684166000
H	-2.679386000	-1.595250000	2.620852000
C	-0.715783000	-2.410838000	2.810008000
H	-0.474260000	-1.813154000	3.696188000
H	-0.327140000	-1.898131000	1.925281000
H	-0.206372000	-3.377620000	2.902661000
C	-2.824371000	-3.282941000	3.926041000
H	-4.634297000	3.673784000	-3.237133000
H	-5.374515000	2.107494000	-3.593758000
H	-5.685519000	2.905341000	-2.040347000
H	-0.940835000	1.097105000	3.887351000
H	-0.858007000	0.793452000	2.137352000
H	-0.184543000	2.287640000	2.801732000
H	-3.909732000	-3.399431000	3.838434000
H	-2.393383000	-4.278282000	4.079408000
H	-2.616814000	-2.689732000	4.823183000
H	-3.523893000	-1.491950000	-3.796600000
H	-2.388060000	-1.409448000	-2.431417000
H	-2.485249000	-2.881081000	-3.426198000

H	-2.240556000	-6.414570000	-0.027691000
H	-1.781695000	5.803404000	-0.313793000
H	3.439308000	2.270133000	2.183166000
C	1.877967000	1.721994000	0.774670000
O	1.719125000	0.360713000	1.188427000
C	2.137685000	0.017824000	2.511453000
H	1.638934000	-0.912016000	2.775033000
H	3.222916000	-0.117634000	2.540263000
H	1.834041000	0.804474000	3.206513000
C	3.351347000	0.539498000	-2.384871000
H	2.753732000	0.058594000	-1.598033000
H	3.757701000	-0.288714000	-2.977026000
C	4.478323000	1.294078000	-1.675688000
H	4.059868000	2.191388000	-1.204682000
H	5.225325000	1.637383000	-2.403958000
C	5.135952000	0.424868000	-0.600941000
H	4.349059000	0.046166000	0.067212000
H	5.582498000	-0.464456000	-1.064674000
C	6.193328000	1.143703000	0.237694000
H	5.766310000	2.072876000	0.639231000
H	7.032292000	1.444376000	-0.403874000
C	6.704216000	0.271399000	1.387689000
H	7.501253000	0.766484000	1.952222000
H	5.892144000	0.041068000	2.090333000
H	7.093848000	-0.685228000	1.018577000
C	4.600369000	-3.118148000	-1.392472000
C	3.255483000	-2.800076000	-1.594873000
C	2.441940000	-2.580445000	-0.495174000
C	2.930835000	-2.726188000	0.800700000
C	4.270207000	-3.024929000	1.027327000

C	5.111929000	-3.202762000	-0.093693000
H	5.240094000	-3.275439000	-2.251677000
H	2.253437000	-2.603515000	1.637077000
O	1.099581000	-2.182142000	-0.667214000
C	0.185674000	-3.277802000	-0.953650000
H	0.267041000	-4.024493000	-0.163052000
H	-0.811843000	-2.847088000	-0.964769000
H	0.441066000	-3.716521000	-1.921703000
C	-5.920449000	-1.785587000	1.234109000
H	-6.199405000	-2.426457000	0.389321000
H	-5.629551000	-2.447193000	2.058721000
H	-6.807543000	-1.228667000	1.543564000
C	-5.764233000	1.550326000	1.199913000
H	-6.708609000	1.084692000	1.490314000
H	-5.430101000	2.187867000	2.026714000
H	-5.956842000	2.207293000	0.343941000
O	2.129176000	5.525313000	-0.731458000
C	1.427740000	6.537082000	-0.013211000
H	1.831376000	6.673872000	0.997899000
H	1.553702000	7.463112000	-0.577948000
H	0.361280000	6.293013000	0.061390000
O	6.413774000	-3.451084000	0.200503000
C	7.331778000	-3.628579000	-0.873117000
H	7.381703000	-2.731596000	-1.502403000
H	8.301984000	-3.801770000	-0.407399000
H	7.060531000	-4.495152000	-1.487891000
C	3.881319000	4.860465000	1.456014000
H	4.225723000	5.558754000	0.688825000
H	3.451969000	5.454528000	2.273152000
H	4.748438000	4.330218000	1.862346000

C	4.833992000	-3.151061000	2.415683000
H	5.293672000	-4.133529000	2.567582000
H	5.621635000	-2.408773000	2.585622000
H	4.053850000	-3.012454000	3.169659000
H	2.861092000	-2.714855000	-2.601686000

MeOINT3'

Sc	-0.420760000	-0.268547000	0.120825000
C	-0.892772000	3.111168000	-2.298784000
C	-0.596285000	4.466778000	-2.235689000
C	-0.637706000	5.079121000	-0.966495000
C	-0.997591000	4.345501000	0.164594000
H	-1.036565000	4.828787000	1.133084000
C	-1.328056000	2.979915000	0.111620000
C	-3.307262000	2.128182000	1.487713000
H	-3.765855000	3.126398000	1.503046000
H	-3.530531000	1.672286000	2.462080000
C	-1.768304000	2.303696000	1.416023000
H	-1.552765000	3.056917000	2.187203000
C	-0.974174000	1.029006000	1.791374000
H	-1.477779000	0.541574000	2.640382000
H	0.005809000	1.345593000	2.173764000
N	1.427633000	-0.619028000	0.051371000
N	3.569404000	0.208043000	0.780571000
N	3.565604000	-1.523922000	-0.549648000
C	2.719598000	-0.638611000	0.094025000
C	4.913104000	-0.154414000	0.570485000
C	4.912458000	-1.228161000	-0.263344000
C	3.090942000	1.274645000	1.605183000
C	2.666496000	0.980272000	2.910370000
C	2.149804000	2.031055000	3.677354000

H	1.811336000	1.836897000	4.690565000
C	2.057607000	3.317630000	3.155467000
C	2.498115000	3.585284000	1.860184000
H	2.431766000	4.595566000	1.471282000
C	3.032663000	2.570984000	1.060731000
C	2.758843000	-0.421975000	3.491097000
H	3.183556000	-1.077748000	2.725767000
C	1.370809000	-0.977047000	3.850240000
H	0.723906000	-0.989655000	2.968029000
H	0.881343000	-0.368442000	4.618373000
H	1.456511000	-1.999889000	4.233346000
C	3.702027000	-0.458587000	4.705549000
C	3.501870000	2.839498000	-0.362191000
H	4.291826000	2.117869000	-0.595398000
C	4.091159000	4.243891000	-0.551550000
H	4.867047000	4.461970000	0.189982000
H	3.320981000	5.019966000	-0.476238000
H	4.537189000	4.328758000	-1.548029000
C	2.351389000	2.602609000	-1.354074000
C	3.075141000	-2.621696000	-1.319769000
C	2.622644000	-2.384286000	-2.628820000
C	2.040092000	-4.737912000	-2.775365000
C	2.099031000	-3.468081000	-3.343687000
H	1.745270000	-3.317531000	-4.359430000
C	2.498492000	-4.948498000	-1.475243000
H	2.446869000	-5.943420000	-1.045835000
C	3.019511000	-3.893926000	-0.718179000
C	3.436156000	-4.092218000	0.732824000
H	4.144092000	-3.299153000	0.991040000
C	4.138823000	-5.432799000	0.985696000

H	4.518333000	-5.467054000	2.012193000
H	4.983900000	-5.577983000	0.304327000
H	3.458185000	-6.282594000	0.864118000
C	2.216898000	-3.921167000	1.659475000
C	2.690906000	-1.004001000	-3.262731000
H	3.144124000	-0.322822000	-2.538129000
C	1.285506000	-0.463677000	-3.576110000
H	1.346409000	0.556248000	-3.972195000
H	0.684595000	-0.438542000	-2.661724000
H	0.771530000	-1.086549000	-4.317648000
C	3.579682000	-1.006664000	-4.517414000
H	3.322213000	0.159881000	5.526208000
H	3.805122000	-1.483397000	5.079263000
H	4.699439000	-0.088617000	4.444438000
H	2.691968000	2.751221000	-2.385978000
H	1.947491000	1.590931000	-1.263368000
H	1.540750000	3.308083000	-1.160031000
H	4.587660000	-1.366254000	-4.284977000
H	3.168346000	-1.651820000	-5.301631000
H	3.664813000	0.005751000	-4.927247000
H	2.522486000	-3.979478000	2.710084000
H	1.729622000	-2.955511000	1.494331000
H	1.482488000	-4.715837000	1.479431000
H	1.641236000	-5.569950000	-3.348688000
H	1.648568000	4.119335000	3.763821000
H	-0.821661000	2.603642000	-3.255164000
C	-1.243935000	2.391835000	-1.156552000
O	-1.463276000	0.990376000	-1.293087000
C	-2.244284000	0.535253000	-2.418860000
H	-2.643134000	-0.442775000	-2.143485000

H	-3.064422000	1.232813000	-2.592559000
H	-1.613715000	0.449980000	-3.306520000
C	-3.989823000	1.320113000	0.385106000
H	-3.855835000	1.844372000	-0.569447000
H	-3.519516000	0.335101000	0.278077000
C	-5.489436000	1.122016000	0.624772000
H	-5.942194000	2.074815000	0.933275000
H	-5.632576000	0.428112000	1.464860000
C	-6.223566000	0.598866000	-0.612868000
H	-6.153403000	1.353554000	-1.410436000
H	-5.708818000	-0.295375000	-0.992505000
C	-7.697154000	0.266306000	-0.358767000
H	-8.178941000	1.119364000	0.138401000
H	-7.756070000	-0.576046000	0.342651000
C	-8.465307000	-0.071859000	-1.638718000
H	-9.506725000	-0.334219000	-1.424505000
H	-8.470429000	0.778621000	-2.330760000
H	-8.011073000	-0.919502000	-2.166765000
C	-4.286039000	-2.214793000	2.014324000
C	-2.956812000	-2.134201000	1.589855000
C	-2.657915000	-2.406559000	0.264577000
C	-3.647772000	-2.783775000	-0.644025000
C	-4.971806000	-2.898339000	-0.232865000
C	-5.285122000	-2.593050000	1.113703000
H	-4.523867000	-1.987698000	3.045602000
H	-3.386907000	-2.996873000	-1.676713000
O	-1.328681000	-2.220336000	-0.174139000
C	-0.613690000	-3.405903000	-0.629342000
H	-1.100861000	-3.803739000	-1.521227000
H	0.396681000	-3.073788000	-0.852969000

H	-0.614534000	-4.144902000	0.173653000
C	6.023671000	-2.016813000	-0.863983000
H	5.985121000	-3.071540000	-0.567122000
H	5.983898000	-1.988270000	-1.959715000
H	6.988946000	-1.613286000	-0.550192000
C	6.026077000	0.587557000	1.224880000
H	6.988534000	0.149405000	0.951341000
H	6.038188000	1.644291000	0.933610000
H	5.935940000	0.555287000	2.317165000
O	-0.297928000	6.395635000	-0.948066000
C	-0.291904000	7.076155000	0.299836000
H	0.417777000	6.616077000	0.999507000
H	0.022056000	8.097041000	0.080546000
H	-1.290989000	7.089624000	0.752307000
O	-6.598903000	-2.699477000	1.432347000
C	-7.004776000	-2.395050000	2.763697000
H	-6.772108000	-1.354187000	3.018045000
H	-8.084435000	-2.542458000	2.783496000
H	-6.528176000	-3.068831000	3.485390000
C	-0.191083000	5.257587000	-3.448137000
H	-0.851896000	6.118243000	-3.597937000
H	0.822248000	5.658699000	-3.331625000
H	-0.217282000	4.637605000	-4.348591000
C	-6.062388000	-3.332412000	-1.171918000
H	-6.531802000	-4.258249000	-0.821111000
H	-6.856732000	-2.581965000	-1.226009000
H	-5.670510000	-3.501632000	-2.178467000
H	-2.173597000	-1.849543000	2.284817000
MeOINT4'			
Sc	0.302748000	-0.475402000	-0.079848000

C	2.099964000	-3.858684000	-1.189510000
C	3.315783000	-4.475100000	-1.430772000
C	4.290978000	-4.386273000	-0.410163000
C	4.032555000	-3.685725000	0.765178000
H	4.802223000	-3.622446000	1.522093000
C	2.805437000	-3.035192000	1.010619000
C	3.925714000	-1.388198000	2.601301000
H	4.788992000	-2.013292000	2.856273000
H	3.718274000	-0.799390000	3.504107000
C	2.674927000	-2.274354000	2.336864000
H	2.649114000	-3.040179000	3.125019000
C	1.422530000	-1.405080000	2.551102000
H	1.426304000	-1.022056000	3.576006000
H	0.477145000	-1.932839000	2.417338000
N	-1.525958000	-0.186133000	0.092763000
N	-3.175908000	1.566179000	0.075797000
N	-3.901005000	-0.491807000	0.089245000
C	-2.744803000	0.258283000	0.087114000
C	-4.581950000	1.624039000	0.072747000
C	-5.035355000	0.341590000	0.074900000
C	-2.287792000	2.690082000	0.068435000
C	-1.954337000	3.276427000	-1.165842000
C	-1.072490000	4.360619000	-1.151057000
H	-0.777635000	4.826559000	-2.085029000
C	-0.567416000	4.855860000	0.048558000
C	-0.924370000	4.263866000	1.255611000
H	-0.525265000	4.656949000	2.186073000
C	-1.780437000	3.158580000	1.290314000
C	-2.502259000	2.723624000	-2.473845000
H	-3.419776000	2.170294000	-2.247289000

C	-1.507346000	1.722154000	-3.087081000
H	-1.317040000	0.895067000	-2.398045000
H	-0.551971000	2.216125000	-3.296295000
H	-1.901058000	1.312708000	-4.025272000
C	-2.868742000	3.821526000	-3.482535000
C	-2.110901000	2.483622000	2.611418000
H	-2.815108000	1.670795000	2.410900000
C	-2.788751000	3.450192000	3.595577000
H	-3.701487000	3.877267000	3.166224000
H	-2.126964000	4.281071000	3.863607000
H	-3.058713000	2.928117000	4.520195000
C	-0.849085000	1.853373000	3.225859000
C	-3.895964000	-1.921199000	0.095071000
C	-4.047309000	-2.589230000	1.325035000
C	-3.865130000	-4.688573000	0.115283000
C	-4.029713000	-3.987781000	1.309778000
H	-4.148464000	-4.536362000	2.237931000
C	-3.703512000	-4.002303000	-1.085181000
H	-3.572383000	-4.558841000	-2.008435000
C	-3.712237000	-2.602948000	-1.119511000
C	-3.496944000	-1.865208000	-2.431177000
H	-3.562298000	-0.792226000	-2.231726000
C	-4.580643000	-2.211970000	-3.464609000
H	-4.433648000	-1.631139000	-4.381689000
H	-5.580377000	-1.989386000	-3.076939000
H	-4.556236000	-3.273542000	-3.734079000
C	-2.087944000	-2.140326000	-2.985227000
C	-4.144443000	-1.810386000	2.629153000
H	-4.550982000	-0.820407000	2.398423000
C	-2.734413000	-1.594318000	3.214867000

H	-2.785428000	-0.987020000	4.125651000
H	-2.084724000	-1.086817000	2.495575000
H	-2.277070000	-2.556696000	3.476700000
C	-5.076936000	-2.461031000	3.659449000
H	-1.982624000	4.348192000	-3.852821000
H	-3.371298000	3.380869000	-4.350132000
H	-3.540123000	4.564603000	-3.039403000
H	-1.098768000	1.296853000	4.136188000
H	-0.382880000	1.165349000	2.514331000
H	-0.110680000	2.618948000	3.490194000
H	-6.067428000	-2.659312000	3.236341000
H	-4.675016000	-3.407973000	4.036165000
H	-5.200749000	-1.797172000	4.521239000
H	-1.909201000	-1.549509000	-3.890234000
H	-1.330926000	-1.869795000	-2.241785000
H	-1.957848000	-3.198370000	-3.240674000
H	-3.864116000	-5.774787000	0.122612000
H	0.122648000	5.693912000	0.036558000
H	1.308909000	-3.908437000	-1.933226000
C	1.850107000	-3.169654000	0.002949000
O	0.554229000	-2.609715000	0.122497000
C	-0.492017000	-3.545000000	0.504638000
H	-1.409486000	-2.964982000	0.562207000
H	-0.572726000	-4.322212000	-0.256516000
H	-0.237144000	-3.985383000	1.471965000
C	4.293035000	-0.446307000	1.447544000
H	4.772120000	-1.019122000	0.643500000
H	3.387302000	-0.012770000	1.007128000
C	5.205124000	0.706612000	1.874171000
H	6.123875000	0.313810000	2.333581000

H	4.697130000	1.286731000	2.659108000
C	5.557217000	1.641266000	0.713358000
H	6.125388000	1.087082000	-0.047781000
H	4.629059000	1.964004000	0.225720000
C	6.355513000	2.875158000	1.146025000
H	7.338551000	2.562621000	1.523728000
H	5.845781000	3.354216000	1.994802000
C	6.527373000	3.898183000	0.020504000
H	7.149158000	4.742660000	0.337137000
H	7.003456000	3.444642000	-0.857343000
H	5.554822000	4.296137000	-0.290927000
C	1.939324000	2.559245000	0.429544000
C	1.538636000	1.337263000	-0.122326000
C	1.752337000	1.199698000	-1.491555000
C	2.292856000	2.170612000	-2.324214000
C	2.681445000	3.384642000	-1.751699000
C	2.504585000	3.562632000	-0.363733000
H	1.791570000	2.735953000	1.489181000
H	2.426321000	2.020888000	-3.390850000
O	1.289147000	-0.079303000	-1.976612000
C	1.400027000	-0.401108000	-3.362141000
H	2.451554000	-0.380961000	-3.662139000
H	0.999663000	-1.408508000	-3.477244000
H	0.819153000	0.302893000	-3.964055000
C	-6.412144000	-0.224890000	0.054524000
H	-7.152652000	0.577335000	0.023532000
H	-6.567418000	-0.865019000	-0.822200000
H	-6.612664000	-0.837538000	0.941481000
C	-5.300535000	2.928018000	0.072193000
H	-6.380847000	2.767756000	0.087263000

H	-5.032279000	3.530288000	0.948004000
H	-5.056302000	3.523084000	-0.815488000
O	5.461103000	-5.016031000	-0.681204000
C	6.505490000	-4.963831000	0.284214000
H	6.197715000	-5.431199000	1.227459000
H	7.335170000	-5.524637000	-0.146406000
H	6.819605000	-3.929745000	0.472076000
O	2.912101000	4.780523000	0.112164000
C	2.944086000	4.970012000	1.518751000
H	3.379736000	5.957388000	1.677526000
H	1.936638000	4.941850000	1.951400000
H	3.568085000	4.210786000	2.006191000
C	3.613238000	-5.216946000	-2.703448000
H	4.479728000	-4.785163000	-3.216436000
H	3.863882000	-6.263464000	-2.497964000
H	2.756525000	-5.191231000	-3.382632000
H	1.462789000	-0.493188000	1.929127000
C	3.274994000	4.489489000	-2.582268000
H	2.702233000	5.417050000	-2.471911000
H	4.298912000	4.717032000	-2.264673000
H	3.295870000	4.216917000	-3.641298000

MeO⁺TS1'

Sc	-0.432755000	-0.079749000	0.118974000
C	-1.374737000	3.199177000	-2.043560000
C	-0.964334000	4.480991000	-1.655365000
C	-0.410006000	4.622817000	-0.368148000
C	-0.383888000	3.536786000	0.513311000
H	0.005325000	3.732861000	1.507941000
C	-0.869066000	2.270542000	0.178810000
C	-2.955553000	2.041796000	1.918592000

H	-2.933000000	3.099334000	1.636608000
H	-3.294096000	2.002456000	2.965622000
C	-1.542107000	1.479219000	1.940845000
H	-0.836902000	2.120625000	2.463617000
C	-1.336874000	0.075492000	2.149042000
H	-2.225013000	-0.550275000	2.196544000
H	-0.552255000	-0.199829000	2.851115000
N	1.405173000	-0.501708000	0.024995000
N	3.656066000	0.243355000	0.464128000
N	3.395853000	-1.845440000	-0.109527000
C	2.683857000	-0.679504000	0.117082000
C	4.937586000	-0.340334000	0.437837000
C	4.775799000	-1.642174000	0.090372000
C	3.387241000	1.611548000	0.776941000
C	3.267909000	1.984860000	2.129131000
C	2.999494000	3.328395000	2.409023000
H	2.898763000	3.653436000	3.438835000
C	2.882819000	4.263336000	1.381952000
C	3.036217000	3.870201000	0.056960000
H	2.966962000	4.608469000	-0.733823000
C	3.290588000	2.536199000	-0.274264000
C	3.418370000	0.954617000	3.240411000
H	4.085529000	0.167428000	2.872775000
C	2.066375000	0.287429000	3.545854000
H	1.655828000	-0.183610000	2.649921000
H	1.344034000	1.030382000	3.905646000
H	2.179619000	-0.477970000	4.322569000
C	4.048418000	1.527487000	4.517068000
C	3.447710000	2.118995000	-1.727847000
H	3.789808000	1.079758000	-1.745511000

C	4.503485000	2.963333000	-2.458915000
H	5.467355000	2.932447000	-1.939747000
H	4.200800000	4.013414000	-2.537130000
H	4.651755000	2.586692000	-3.476878000
C	2.093188000	2.168167000	-2.453964000
C	2.800985000	-3.093006000	-0.467228000
C	2.778213000	-3.462159000	-1.826307000
C	1.720729000	-5.545670000	-1.161298000
C	2.225791000	-4.704723000	-2.152946000
H	2.195551000	-5.024239000	-3.189046000
C	1.746234000	-5.151883000	0.173624000
H	1.346478000	-5.813389000	0.936544000
C	2.283651000	-3.914634000	0.547970000
C	2.271755000	-3.480127000	2.004271000
H	2.763277000	-2.505958000	2.070077000
C	3.054509000	-4.455720000	2.897516000
H	3.073451000	-4.093752000	3.931242000
H	4.089398000	-4.562371000	2.555053000
H	2.599943000	-5.452543000	2.901882000
C	0.827763000	-3.298171000	2.504205000
C	3.274350000	-2.504408000	-2.900535000
H	4.030660000	-1.856402000	-2.445761000
C	2.119922000	-1.592733000	-3.363754000
H	2.478457000	-0.862241000	-4.098017000
H	1.688023000	-1.050535000	-2.516975000
H	1.329390000	-2.188448000	-3.837759000
C	3.930940000	-3.211298000	-4.093367000
H	3.378498000	2.230740000	5.023914000
H	4.259914000	0.717570000	5.222959000
H	4.987529000	2.049223000	4.304286000

H	2.203338000	1.852473000	-3.498186000
H	1.381108000	1.502666000	-1.960172000
H	1.672226000	3.179057000	-2.443376000
H	4.720786000	-3.897089000	-3.769040000
H	3.205475000	-3.785426000	-4.680231000
H	4.377039000	-2.471200000	-4.765771000
H	0.822194000	-2.917016000	3.531211000
H	0.290575000	-2.583605000	1.873291000
H	0.280665000	-4.248435000	2.495143000
H	1.307091000	-6.512635000	-1.433046000
H	2.672086000	5.301560000	1.619178000
H	-1.770943000	3.059103000	-3.043850000
C	-1.314988000	2.143054000	-1.145882000
O	-1.641286000	0.817366000	-1.531262000
C	-1.591377000	0.489040000	-2.928319000
H	-1.556970000	-0.598423000	-2.981781000
H	-2.488223000	0.858548000	-3.432201000
H	-0.694107000	0.916013000	-3.385056000
C	-3.968968000	1.296195000	1.047554000
H	-3.656968000	1.342623000	-0.003106000
H	-3.992796000	0.232913000	1.315157000
C	-5.384595000	1.866143000	1.181973000
H	-5.386361000	2.925041000	0.887202000
H	-5.684981000	1.842955000	2.239406000
C	-6.409822000	1.095233000	0.348690000
H	-6.118846000	1.136611000	-0.711579000
H	-6.375722000	0.034874000	0.629633000
C	-7.847212000	1.599030000	0.502000000
H	-7.901873000	2.655722000	0.206808000
H	-8.128286000	1.564172000	1.563724000

C	-8.844989000	0.778265000	-0.319107000
H	-9.873229000	1.123913000	-0.168914000
H	-8.625460000	0.848831000	-1.391831000
H	-8.800354000	-0.282321000	-0.042404000
C	-4.552111000	-2.823014000	1.259820000
C	-3.191975000	-2.657693000	0.985616000
C	-2.809719000	-2.172562000	-0.254883000
C	-3.752405000	-1.886716000	-1.240649000
C	-5.110750000	-2.059976000	-0.995916000
C	-5.504651000	-2.519248000	0.281303000
H	-4.854022000	-3.186710000	2.233954000
H	-3.427914000	-1.529083000	-2.211296000
O	-1.440090000	-1.956845000	-0.523890000
C	-0.762484000	-3.109313000	-1.093118000
H	-1.224619000	-3.356411000	-2.052606000
H	0.277571000	-2.822747000	-1.216056000
H	-0.844644000	-3.951112000	-0.405079000
C	5.755014000	-2.751375000	-0.077327000
H	5.532207000	-3.587084000	0.596728000
H	5.747696000	-3.150855000	-1.098472000
H	6.766085000	-2.400568000	0.141066000
C	6.157769000	0.458457000	0.739201000
H	7.050305000	-0.165683000	0.656103000
H	6.264980000	1.299995000	0.044454000
H	6.129534000	0.878415000	1.751371000
O	0.028442000	5.813051000	0.149176000
C	0.890393000	6.643757000	-0.628569000
H	0.329779000	7.423628000	-1.152310000
H	1.582738000	7.116353000	0.072498000
H	1.460083000	6.057331000	-1.356085000

O	-6.846640000	-2.627626000	0.461114000
C	-7.331708000	-3.047004000	1.732098000
H	-7.018999000	-2.353367000	2.522029000
H	-8.418651000	-3.040921000	1.650444000
H	-6.987847000	-4.059811000	1.973757000
C	-1.191819000	5.644371000	-2.588682000
H	-1.626457000	6.493641000	-2.052143000
H	-0.268893000	5.993858000	-3.064161000
H	-1.884116000	5.361403000	-3.386219000
C	-6.150513000	-1.775444000	-2.043859000
H	-6.742376000	-2.671511000	-2.260797000
H	-6.854911000	-1.010594000	-1.702897000
H	-5.685925000	-1.433238000	-2.972977000
H	-2.441902000	-2.891655000	1.733676000

MeO⁺TS2'

Sc	0.072707000	0.589866000	-0.123115000
C	1.483854000	4.203978000	0.586930000
C	2.734914000	4.722095000	0.888010000
C	3.824951000	4.228027000	0.138776000
C	3.637513000	3.282388000	-0.870461000
H	4.498113000	2.938626000	-1.422332000
C	2.371511000	2.756516000	-1.192724000
C	3.539749000	1.161150000	-2.836788000
H	4.257525000	1.953463000	-3.079682000
H	3.350462000	0.646769000	-3.786760000
C	2.199180000	1.779093000	-2.374949000
H	1.855968000	2.411447000	-3.209155000
C	1.146652000	0.649779000	-2.191947000
H	1.348434000	-0.139831000	-2.923995000
H	0.136221000	1.003565000	-2.465436000

N	-1.689687000	-0.010251000	-0.203724000
N	-3.224901000	-1.822069000	0.139015000
N	-4.022128000	0.205716000	0.296159000
C	-2.862279000	-0.497167000	0.043996000
C	-4.594876000	-1.939538000	0.443460000
C	-5.091003000	-0.677855000	0.549532000
C	-2.306171000	-2.895755000	-0.087546000
C	-1.673934000	-3.490828000	1.019619000
C	-0.781161000	-4.536712000	0.769575000
H	-0.279942000	-5.024053000	1.598947000
C	-0.527790000	-4.964794000	-0.532344000
C	-1.152131000	-4.346180000	-1.610322000
H	-0.942642000	-4.685757000	-2.620075000
C	-2.056114000	-3.297085000	-1.409733000
C	-1.915797000	-2.978404000	2.432607000
H	-2.904302000	-2.506952000	2.453531000
C	-0.885801000	-1.888072000	2.788554000
H	-0.959426000	-1.049837000	2.089460000
H	0.134741000	-2.283416000	2.736938000
H	-1.060453000	-1.510113000	3.803116000
C	-1.917041000	-4.091890000	3.489155000
C	-2.715187000	-2.617521000	-2.598711000
H	-3.411383000	-1.864951000	-2.217398000
C	-3.528884000	-3.610570000	-3.444193000
H	-4.288362000	-4.118333000	-2.839570000
H	-2.888907000	-4.379650000	-3.890295000
H	-4.037345000	-3.086962000	-4.261187000
C	-1.664666000	-1.882363000	-3.448502000
C	-4.080462000	1.633365000	0.252870000
C	-4.601556000	2.250908000	-0.900437000

C	-4.195477000	4.398838000	0.160737000
C	-4.657260000	3.648645000	-0.919945000
H	-5.062720000	4.157361000	-1.787800000
C	-3.655671000	3.764081000	1.275987000
H	-3.295065000	4.358706000	2.110217000
C	-3.584875000	2.367691000	1.343141000
C	-2.991014000	1.684259000	2.563817000
H	-2.905925000	0.617652000	2.345428000
C	-3.908123000	1.835751000	3.788850000
H	-3.484508000	1.315723000	4.655332000
H	-4.899271000	1.414515000	3.590880000
H	-4.040642000	2.889637000	4.057733000
C	-1.575382000	2.201616000	2.868607000
C	-4.999431000	1.423613000	-2.114606000
H	-5.291293000	0.428681000	-1.764575000
C	-3.775494000	1.236352000	-3.033659000
H	-4.024524000	0.581737000	-3.876331000
H	-2.935399000	0.794380000	-2.489290000
H	-3.451911000	2.201642000	-3.442249000
C	-6.189156000	2.004045000	-2.889872000
H	-0.921416000	-4.528826000	3.623537000
H	-2.226435000	-3.687399000	4.458579000
H	-2.605987000	-4.899445000	3.220176000
H	-2.144382000	-1.346892000	-4.275203000
H	-1.120703000	-1.158116000	-2.835951000
H	-0.940471000	-2.583985000	-3.878025000
H	-7.047929000	2.183888000	-2.234255000
H	-5.936109000	2.949384000	-3.382254000
H	-6.498960000	1.305193000	-3.673610000
H	-1.096905000	1.580711000	3.633705000

H	-0.950904000	2.191615000	1.967843000
H	-1.590488000	3.233556000	3.237379000
H	-4.255228000	5.483039000	0.130217000
H	0.157450000	-5.788833000	-0.708357000
H	0.610204000	4.528153000	1.146407000
C	1.315218000	3.251535000	-0.420468000
O	0.014722000	2.706332000	-0.545879000
C	-0.953002000	3.458634000	-1.316980000
H	-1.888467000	2.907994000	-1.246054000
H	-1.061920000	4.453112000	-0.880983000
H	-0.612889000	3.528200000	-2.353888000
C	4.142199000	0.170001000	-1.835716000
H	4.070710000	0.576262000	-0.818284000
H	3.535129000	-0.738663000	-1.830135000
C	5.593333000	-0.235410000	-2.098419000
H	6.250683000	0.644265000	-2.023386000
H	5.698146000	-0.608353000	-3.127075000
C	6.048350000	-1.314267000	-1.109009000
H	5.902540000	-0.943268000	-0.082925000
H	5.388378000	-2.187584000	-1.204031000
C	7.499609000	-1.766886000	-1.280002000
H	8.171359000	-0.904396000	-1.167503000
H	7.646506000	-2.137535000	-2.303648000
C	7.886210000	-2.858284000	-0.278317000
H	8.921349000	-3.187755000	-0.417262000
H	7.786084000	-2.498130000	0.753414000
H	7.236054000	-3.735143000	-0.387421000
C	2.172366000	-2.372843000	-0.305897000
C	1.702561000	-1.103978000	0.037520000
C	2.182226000	-0.568394000	1.236946000

C	3.110983000	-1.196941000	2.050435000
C	3.622785000	-2.443714000	1.656146000
C	3.122155000	-3.030302000	0.480802000
H	1.854964000	-2.849490000	-1.229144000
H	3.473135000	-0.742647000	2.966693000
O	1.588038000	0.677974000	1.542360000
C	2.095409000	1.453248000	2.633190000
H	3.156996000	1.660357000	2.473685000
H	1.535201000	2.385583000	2.630211000
H	1.943371000	0.919794000	3.575829000
C	-6.452474000	-0.174379000	0.881363000
H	-7.127652000	-1.009563000	1.080359000
H	-6.434181000	0.467043000	1.770686000
H	-6.879741000	0.419003000	0.064493000
C	-5.240134000	-3.273576000	0.586841000
H	-6.302811000	-3.161152000	0.812772000
H	-5.147870000	-3.860625000	-0.334590000
H	-4.780877000	-3.860714000	1.390835000
O	5.035777000	4.737667000	0.482513000
C	6.188548000	4.301975000	-0.229585000
H	6.115657000	4.552843000	-1.294637000
H	7.029439000	4.835697000	0.213702000
H	6.340083000	3.220887000	-0.118497000
O	3.651262000	-4.214989000	0.015969000
C	3.152834000	-5.393510000	0.649280000
H	3.620415000	-6.237586000	0.139050000
H	3.414715000	-5.426004000	1.713621000
H	2.063881000	-5.456203000	0.546676000
C	2.952258000	5.744855000	1.967989000
H	3.648342000	5.374498000	2.729069000

H	3.398924000	6.657899000	1.559254000
H	2.009263000	6.008625000	2.454998000
H	1.460276000	-0.325193000	-1.067622000
C	4.712978000	-3.109988000	2.452899000
H	4.309702000	-3.843173000	3.162707000
H	5.402047000	-3.638824000	1.788872000
H	5.279634000	-2.374387000	3.031075000

Sc-3-INT1

Sc	-0.841032000	-1.838471000	-0.238806000
C	-3.327298000	-4.485836000	-1.115776000
C	-3.496454000	-5.614601000	-0.323352000
H	-3.776946000	-6.559815000	-0.775443000
C	-3.288583000	-5.521855000	1.061597000
C	-2.930611000	-4.318564000	1.653486000
H	-2.780999000	-4.263512000	2.727738000
C	-2.786219000	-3.130785000	0.896787000
C	-2.277330000	-1.856369000	1.442012000
H	-2.899437000	-0.986343000	1.198634000
H	-2.078591000	-1.883065000	2.513299000
N	0.148064000	-0.313855000	-0.507710000
N	2.173115000	0.963473000	-0.706797000
N	0.275059000	2.082107000	-0.674631000
C	0.809666000	0.816931000	-0.597377000
C	2.467551000	2.304832000	-0.928616000
C	1.300089000	2.992829000	-0.908527000
H	-3.413671000	-6.404215000	1.681681000
H	-3.456561000	-4.520186000	-2.193197000
C	-2.976509000	-3.285569000	-0.499679000
O	-2.680537000	-2.151876000	-1.316329000
C	-3.813595000	-1.347385000	-1.733745000

H	-3.401447000	-0.493092000	-2.270621000
H	-4.448708000	-1.945229000	-2.390087000
H	-4.370879000	-1.021436000	-0.852447000
H	1.121390000	4.042409000	-1.052247000
H	3.468787000	2.659118000	-1.091623000
C	-1.178640000	2.298189000	-0.601083000
H	-1.598344000	1.555089000	-1.291581000
C	-1.645653000	3.694232000	-1.057751000
C	-1.738386000	2.003799000	0.809838000
H	-1.208324000	3.925062000	-2.037090000
C	-1.305639000	4.805090000	-0.038350000
C	-3.184998000	3.618026000	-1.184467000
H	-1.345916000	1.041745000	1.150297000
C	-1.343452000	3.112913000	1.799575000
C	-3.271746000	1.932721000	0.684571000
H	-1.710154000	5.754425000	-0.410180000
H	-0.226787000	4.950180000	0.072390000
C	-1.913764000	4.464407000	1.332393000
H	-3.465265000	2.860683000	-1.929148000
H	-3.566335000	4.579047000	-1.548909000
C	-3.815168000	3.283371000	0.183292000
H	-0.250472000	3.171314000	1.884810000
H	-1.726350000	2.860774000	2.796163000
H	-3.554163000	1.129572000	-0.011313000
H	-3.713004000	1.683543000	1.657541000
H	-1.647655000	5.246098000	2.053100000
C	-3.445353000	4.375606000	1.204243000
H	-4.905001000	3.227638000	0.077119000
H	-3.894751000	4.145124000	2.178565000
H	-3.851261000	5.343544000	0.884487000

C	3.068185000	-0.205287000	-0.712470000
H	2.623867000	-0.889750000	-1.446555000
C	3.095805000	-0.927692000	0.654917000
C	4.512270000	0.103227000	-1.154537000
H	2.064261000	-1.077488000	0.992394000
C	3.866818000	-0.103009000	1.699224000
C	3.787860000	-2.287123000	0.438774000
H	4.493972000	0.657358000	-2.101136000
C	5.308834000	0.884330000	-0.085288000
C	5.206269000	-1.260841000	-1.371524000
H	3.841540000	-0.625372000	2.663550000
H	3.377156000	0.867869000	1.849778000
C	5.321393000	0.099549000	1.237264000
H	3.227644000	-2.884999000	-0.296095000
H	3.794410000	-2.853786000	1.378223000
C	5.229856000	-2.059629000	-0.052497000
H	4.894335000	1.881681000	0.092190000
H	6.332199000	1.032197000	-0.451166000
H	4.685857000	-1.829750000	-2.153011000
H	6.229707000	-1.092950000	-1.726769000
H	5.871690000	0.670026000	1.994225000
C	6.000070000	-1.265002000	1.018816000
H	5.718166000	-3.026327000	-0.221524000
H	7.040859000	-1.119294000	0.703664000
H	6.025882000	-1.830094000	1.959326000

Sc-3-INT2

Sc	-0.472100000	-0.080705000	-0.041502000
C	-2.283183000	-1.863795000	-3.238077000
C	-3.640769000	-1.754599000	-3.545143000
H	-4.146109000	-2.557109000	-4.072045000

C	-4.339618000	-0.605996000	-3.155970000
C	-3.694881000	0.433658000	-2.487769000
H	-4.252036000	1.320963000	-2.204790000
C	-2.320854000	0.371803000	-2.174587000
C	-1.576451000	1.376210000	-1.375310000
H	-0.725646000	1.790711000	-1.934642000
H	-2.209878000	2.205938000	-1.057765000
C	-3.380262000	1.097095000	2.312079000
H	-3.770080000	1.793114000	3.070884000
H	-3.511105000	0.087082000	2.718100000
H	-5.397450000	-0.515485000	-3.385378000
H	-1.711163000	-2.748840000	-3.501013000
C	-1.668619000	-0.818814000	-2.560805000
O	-0.332771000	-0.968132000	-2.101002000
C	0.696996000	-0.612077000	-3.053295000
H	1.641833000	-0.680772000	-2.515966000
H	0.668829000	-1.314229000	-3.890058000
H	0.536730000	0.408353000	-3.411523000
C	-4.204327000	1.258710000	1.027740000
H	-4.046479000	2.262120000	0.609775000
H	-3.836794000	0.553253000	0.275549000
C	-5.698832000	1.019867000	1.254672000
H	-6.105828000	1.811583000	1.898912000
H	-5.831792000	0.079104000	1.804969000
C	-6.493846000	0.951980000	-0.051385000
H	-6.374357000	1.894893000	-0.605288000
H	-6.062233000	0.169320000	-0.692047000
C	-7.984561000	0.668759000	0.152640000
H	-8.422469000	1.457267000	0.779280000
H	-8.099010000	-0.267228000	0.718229000

C	-8.754622000	0.569802000	-1.166010000
H	-9.816316000	0.362574000	-0.996577000
H	-8.683710000	1.504191000	-1.735367000
H	-8.354741000	-0.233924000	-1.797208000
C	-3.728913000	-2.945609000	2.963643000
C	-2.451654000	-2.779150000	2.411034000
C	-2.398784000	-2.370936000	1.073996000
C	-3.532605000	-2.155737000	0.296583000
C	-4.788099000	-2.342652000	0.872864000
C	-4.883066000	-2.733382000	2.209315000
H	-3.812396000	-3.252160000	4.002652000
H	-3.430646000	-1.850007000	-0.738375000
H	-5.681313000	-2.175992000	0.280147000
H	-5.857420000	-2.874295000	2.666516000
O	-1.134135000	-2.146134000	0.479247000
C	-0.543835000	-3.328496000	-0.116264000
H	-1.177218000	-3.670551000	-0.937639000
H	0.436320000	-3.036317000	-0.488727000
H	-0.447278000	-4.103837000	0.646405000
C	-1.207603000	-3.059641000	3.216352000
H	-0.952406000	-4.126525000	3.184188000
H	-0.343183000	-2.505358000	2.841747000
H	-1.357643000	-2.799142000	4.268239000
C	-1.918991000	1.394817000	2.147758000
H	-1.672626000	2.339536000	1.659617000
C	-0.916942000	0.625864000	2.613260000
H	-1.126042000	-0.301645000	3.140451000
H	0.122312000	0.937116000	2.556717000
N	1.349589000	0.253163000	0.211509000
N	3.708453000	-0.233217000	0.318724000

N	3.087017000	1.867336000	0.592550000
C	2.597857000	0.597752000	0.349150000
C	4.851927000	0.523144000	0.568636000
C	4.468130000	1.810179000	0.744020000
H	5.061883000	2.674280000	0.978958000
H	5.836958000	0.096117000	0.601451000
C	2.167514000	3.007149000	0.705901000
H	1.345971000	2.627385000	1.324408000
C	1.567828000	3.410248000	-0.659556000
C	2.744800000	4.254149000	1.403264000
H	1.229601000	2.503554000	-1.167316000
C	2.606521000	4.146447000	-1.521713000
C	0.368581000	4.331768000	-0.373389000
H	3.220377000	3.959295000	2.347043000
C	3.740504000	5.037649000	0.519068000
C	1.538904000	5.178435000	1.694270000
H	2.162432000	4.391000000	-2.494882000
H	3.466637000	3.492759000	-1.719087000
C	3.068669000	5.430082000	-0.807523000
H	-0.381416000	3.791717000	0.221337000
H	-0.118027000	4.614117000	-1.315051000
C	0.852442000	5.588217000	0.374147000
H	4.648665000	4.464652000	0.308585000
H	4.059890000	5.934538000	1.064107000
H	0.823341000	4.668495000	2.353051000
H	1.885875000	6.070550000	2.229158000
H	3.789909000	5.963899000	-1.437299000
C	1.859169000	6.337934000	-0.518604000
H	-0.001937000	6.238397000	0.596925000
H	2.192713000	7.258055000	-0.022192000

H	1.376636000	6.636518000	-1.458114000
C	3.559182000	-1.664798000	0.057553000
H	2.473007000	-1.768672000	-0.016225000
C	4.035149000	-2.589841000	1.198547000
C	4.168962000	-2.131505000	-1.282144000
H	3.639985000	-2.211510000	2.149139000
C	5.570724000	-2.698483000	1.262312000
C	3.456375000	-3.990812000	0.902981000
H	3.873228000	-1.428101000	-2.071070000
C	5.704557000	-2.229013000	-1.211639000
C	3.591314000	-3.532070000	-1.574305000
H	5.845653000	-3.400301000	2.059611000
H	6.023745000	-1.739474000	1.534256000
C	6.116106000	-3.201258000	-0.088489000
H	2.358381000	-3.949105000	0.887857000
H	3.737704000	-4.682863000	1.706039000
C	3.992201000	-4.505651000	-0.448164000
H	6.151165000	-1.240931000	-1.055775000
H	6.086046000	-2.588699000	-2.175386000
H	2.496240000	-3.477626000	-1.661603000
H	3.968844000	-3.895822000	-2.537758000
H	7.209413000	-3.264510000	-0.041801000
C	5.529124000	-4.594959000	-0.383310000
H	3.572382000	-5.497470000	-0.654891000
H	5.923330000	-4.977101000	-1.333477000
H	5.831325000	-5.303554000	0.398145000
Sc-3-INT3			
Sc	0.457839000	-0.629428000	0.103383000
C	2.521857000	-2.338160000	-2.805897000
C	3.719133000	-3.031943000	-2.965947000

H	4.419541000	-2.737939000	-3.740850000
C	3.998238000	-4.112515000	-2.126484000
C	3.088223000	-4.489945000	-1.141587000
H	3.311809000	-5.338928000	-0.502763000
C	1.881112000	-3.800970000	-0.938722000
C	0.951921000	-4.204017000	0.183917000
H	-0.093526000	-4.084556000	-0.124227000
H	1.104605000	-5.276419000	0.346170000
C	2.615002000	-3.272518000	1.939898000
H	3.188804000	-4.168368000	1.667704000
H	2.684773000	-3.198897000	3.032600000
C	1.134075000	-3.479752000	1.561372000
H	0.741323000	-4.209364000	2.285822000
C	0.302433000	-2.186312000	1.667757000
H	0.422052000	-1.776509000	2.685254000
H	-0.764509000	-2.463911000	1.608025000
H	4.923486000	-4.667429000	-2.245184000
H	2.263589000	-1.503096000	-3.449584000
C	1.638616000	-2.729761000	-1.803226000
O	0.474146000	-1.945008000	-1.616686000
C	-0.648150000	-2.266359000	-2.479042000
H	-1.433988000	-1.561746000	-2.213227000
H	-0.343585000	-2.146825000	-3.521573000
H	-0.963857000	-3.294652000	-2.290756000
C	3.303874000	-2.038093000	1.338293000
H	3.015712000	-1.904774000	0.286097000
H	2.978830000	-1.137422000	1.875333000
C	4.832038000	-2.113682000	1.390343000
H	5.159330000	-3.001508000	0.831813000
H	5.153259000	-2.267326000	2.430034000

C	5.513679000	-0.870220000	0.818363000
H	5.163789000	-0.711613000	-0.213067000
H	5.195884000	0.014855000	1.385834000
C	7.042548000	-0.953181000	0.821997000
H	7.358885000	-1.830080000	0.240370000
H	7.392719000	-1.126691000	1.848603000
C	7.709473000	0.304484000	0.260488000
H	8.800769000	0.214158000	0.259411000
H	7.388874000	0.493856000	-0.771855000
H	7.445499000	1.186629000	0.855280000
C	3.574686000	2.551621000	2.200714000
C	2.637399000	1.827460000	1.457211000
C	2.923222000	1.612212000	0.104039000
C	4.073654000	2.103160000	-0.502544000
C	4.984401000	2.831230000	0.263168000
C	4.738625000	3.051234000	1.616979000
H	3.374607000	2.735255000	3.252420000
H	4.275639000	1.911587000	-1.549702000
H	5.887320000	3.212141000	-0.201875000
H	5.445590000	3.615239000	2.216441000
O	1.983391000	0.862805000	-0.626757000
C	1.812511000	1.209740000	-2.019621000
H	2.607166000	0.761296000	-2.619046000
H	0.841429000	0.811686000	-2.317234000
H	1.814729000	2.296292000	-2.123860000
C	1.367645000	1.312341000	2.082207000
H	1.175197000	1.798717000	3.041713000
H	0.485855000	1.511000000	1.456402000
H	1.418312000	0.236180000	2.309164000
N	-1.190977000	0.219271000	-0.155919000

N	-3.586981000	0.105660000	0.073105000
N	-2.692942000	2.091517000	-0.304269000
C	-2.379150000	0.752831000	-0.129408000
C	-4.619989000	1.038599000	0.023549000
C	-4.072022000	2.256535000	-0.197920000
H	-4.552769000	3.212353000	-0.290737000
H	-5.652610000	0.768863000	0.143670000
C	-1.628692000	3.084061000	-0.471350000
H	-0.764814000	2.457752000	-0.710113000
C	-1.298632000	3.853141000	0.826998000
C	-1.817787000	4.082526000	-1.633494000
H	-1.235363000	3.134615000	1.653453000
C	-2.369400000	4.916075000	1.133876000
C	0.065065000	4.540431000	0.612533000
H	-2.105128000	3.531163000	-2.537105000
C	-2.854627000	5.181068000	-1.323772000
C	-0.449155000	4.770203000	-1.843990000
H	-2.104143000	5.440202000	2.060486000
H	-3.341406000	4.441247000	1.313500000
C	-2.461803000	5.921211000	-0.031384000
H	0.841941000	3.789917000	0.414477000
H	0.362459000	5.071927000	1.525023000
C	-0.034122000	5.527595000	-0.565875000
H	-3.866220000	4.771765000	-1.245302000
H	-2.881535000	5.886511000	-2.163733000
H	0.312931000	4.022578000	-2.104742000
H	-0.514294000	5.465777000	-2.689339000
H	-3.217341000	6.681141000	0.199315000
C	-1.093109000	6.597060000	-0.237798000
H	0.939381000	6.006230000	-0.726339000

H	-1.155352000	7.329425000	-1.052649000
H	-0.802095000	7.146436000	0.666565000
C	-3.630687000	-1.340794000	0.307195000
H	-2.570916000	-1.593865000	0.382010000
C	-4.225070000	-2.149605000	-0.865559000
C	-4.301659000	-1.771146000	1.630124000
H	-3.786814000	-1.787749000	-1.804848000
C	-5.759337000	-2.029270000	-0.922062000
C	-3.840218000	-3.625542000	-0.631431000
H	-3.908907000	-1.151000000	2.444671000
C	-5.838845000	-1.675907000	1.573572000
C	-3.915996000	-3.249850000	1.858559000
H	-6.137890000	-2.632201000	-1.757012000
H	-6.059570000	-0.995477000	-1.128871000
C	-6.373142000	-2.523716000	0.402935000
H	-2.746089000	-3.730332000	-0.605645000
H	-4.205151000	-4.241529000	-1.462845000
C	-4.446006000	-4.115805000	0.698222000
H	-6.173405000	-0.637049000	1.487847000
H	-6.251381000	-2.047445000	2.519899000
H	-2.825628000	-3.348056000	1.940880000
H	-4.340775000	-3.595616000	2.808726000
H	-7.464874000	-2.436365000	0.354909000
C	-5.980120000	-3.996280000	0.627305000
H	-4.162826000	-5.161983000	0.864401000
H	-6.429119000	-4.367230000	1.557257000
H	-6.369112000	-4.619230000	-0.188401000
Sc-3-INT4			
Sc	0.713208000	0.239547000	1.189021000
C	0.431065000	3.529681000	-1.304657000

C	-0.406003000	3.971496000	-2.326185000
H	-0.665877000	5.022716000	-2.393851000
C	-0.919504000	3.051637000	-3.243026000
C	-0.575916000	1.706395000	-3.144615000
H	-0.984105000	0.993302000	-3.855104000
C	0.292976000	1.231917000	-2.149501000
C	0.648601000	-0.235940000	-2.119097000
H	1.183402000	-0.506325000	-1.201444000
H	-0.281236000	-0.812638000	-2.106704000
C	2.863942000	0.002663000	-3.394489000
H	2.687935000	1.085399000	-3.460733000
H	3.346388000	-0.280566000	-4.339055000
C	1.503669000	-0.712377000	-3.314632000
H	0.954231000	-0.451439000	-4.229743000
C	1.634976000	-2.239660000	-3.267044000
H	2.257695000	-2.608101000	-4.089191000
H	0.653178000	-2.720319000	-3.346956000
H	-1.587810000	3.383489000	-4.031083000
H	0.809686000	4.224333000	-0.562396000
C	0.766835000	2.179661000	-1.236788000
O	1.574098000	1.733881000	-0.158108000
C	2.868383000	2.382754000	-0.009751000
H	3.442463000	1.776212000	0.689403000
H	3.359500000	2.410720000	-0.982719000
H	2.734769000	3.391155000	0.385783000
C	3.839911000	-0.274515000	-2.244662000
H	3.370633000	-0.037879000	-1.279702000
H	4.081121000	-1.344223000	-2.203479000
C	5.140675000	0.523615000	-2.385638000
H	4.904423000	1.591246000	-2.515264000

H	5.649755000	0.221306000	-3.311023000
C	6.092099000	0.360086000	-1.198617000
H	5.587507000	0.697618000	-0.282678000
H	6.307973000	-0.708007000	-1.047571000
C	7.409360000	1.124866000	-1.358613000
H	7.191789000	2.184192000	-1.554975000
H	7.937375000	0.753471000	-2.246871000
C	8.318228000	1.007866000	-0.132959000
H	9.263874000	1.539327000	-0.281424000
H	7.836248000	1.433417000	0.756510000
H	8.555746000	-0.040258000	0.085474000
C	4.414432000	-0.405879000	2.048670000
C	3.027415000	-0.499400000	2.312640000
C	2.511860000	0.520920000	3.149398000
C	3.280644000	1.531139000	3.719939000
C	4.646971000	1.561513000	3.457613000
C	5.203328000	0.589548000	2.613619000
H	4.864119000	-1.147945000	1.396351000
H	2.803894000	2.277262000	4.348475000
H	5.270101000	2.333271000	3.896674000
H	6.267183000	0.609302000	2.397859000
O	1.095189000	0.566881000	3.304565000
C	0.561096000	-0.083326000	4.486131000
H	0.908540000	0.451772000	5.372171000
H	-0.524264000	-0.026156000	4.401896000
H	0.894051000	-1.123970000	4.513417000
C	2.117353000	-1.444030000	1.640564000
H	2.627573000	-2.126263000	0.960468000
H	1.488995000	-2.017804000	2.333804000
H	2.090050000	-2.573996000	-2.327381000

N	-1.027501000	-0.200859000	0.713765000
N	-3.019121000	0.329717000	-0.526555000
N	-2.305150000	-1.757709000	-0.597291000
C	-2.047064000	-0.520137000	-0.034923000
C	-3.802588000	-0.358189000	-1.448800000
C	-3.365584000	-1.639387000	-1.492091000
H	-3.723868000	-2.464445000	-2.079863000
H	-4.604601000	0.108917000	-1.990777000
C	-1.416422000	-2.905012000	-0.352413000
H	-0.404471000	-2.517876000	-0.519198000
C	-1.644454000	-4.091187000	-1.308970000
C	-1.484669000	-3.401533000	1.108688000
H	-1.641283000	-3.731406000	-2.346437000
C	-2.953812000	-4.854528000	-1.007063000
C	-0.461447000	-5.062813000	-1.099124000
H	-1.377263000	-2.538010000	1.771567000
C	-2.815427000	-4.122831000	1.379773000
C	-0.306369000	-4.372854000	1.314350000
H	-3.030271000	-5.705835000	-1.694859000
H	-3.840915000	-4.236127000	-1.175607000
C	-2.949902000	-5.344224000	0.451095000
H	0.485401000	-4.560511000	-1.336423000
H	-0.559220000	-5.907329000	-1.791891000
C	-0.446427000	-5.570224000	0.357123000
H	-3.657101000	-3.435064000	1.224965000
H	-2.850882000	-4.438456000	2.430015000
H	0.642925000	-3.852900000	1.135039000
H	-0.292304000	-4.721841000	2.354757000
H	-3.891059000	-5.865576000	0.661489000
C	-1.765024000	-6.303821000	0.663734000

H	0.400020000	-6.253632000	0.494001000
H	-1.756755000	-6.672065000	1.697687000
H	-1.871650000	-7.180184000	0.011674000
C	-3.017926000	1.769244000	-0.213167000
H	-2.026236000	2.129298000	-0.508923000
C	-3.197381000	2.032694000	1.299366000
C	-4.078333000	2.568691000	-0.996050000
H	-2.475034000	1.420894000	1.845221000
C	-4.627152000	1.687141000	1.747599000
C	-2.912254000	3.526346000	1.543923000
H	-3.972715000	2.361180000	-2.068420000
C	-5.514393000	2.257754000	-0.518583000
C	-3.798760000	4.066259000	-0.742271000
H	-4.719802000	1.853328000	2.828329000
H	-4.830972000	0.623291000	1.569754000
C	-5.641597000	2.558374000	0.985170000
H	-1.886015000	3.768477000	1.230866000
H	-2.982515000	3.745177000	2.616930000
C	-3.923225000	4.383067000	0.760284000
H	-5.790012000	1.214060000	-0.701110000
H	-6.218053000	2.874471000	-1.091609000
H	-2.796621000	4.325449000	-1.101925000
H	-4.514557000	4.668304000	-1.315342000
H	-6.658363000	2.319725000	1.318452000
C	-5.347335000	4.047873000	1.241114000
H	-3.715491000	5.446996000	0.926606000
H	-6.079614000	4.671482000	0.712479000
H	-5.445952000	4.273963000	2.310709000
Sc-3-TS1			
Sc	-0.451840000	-0.447109000	0.143761000

C	-4.004726000	2.301578000	0.011011000
C	-4.826338000	2.831607000	1.010537000
H	-5.747851000	3.332919000	0.733843000
C	-4.457540000	2.710576000	2.349025000
C	-3.271460000	2.061286000	2.689920000
H	-2.979653000	1.981914000	3.733293000
C	-2.422346000	1.513315000	1.715808000
C	-1.168103000	0.804123000	2.073823000
H	-0.295420000	1.219242000	1.529730000
H	-0.927984000	0.981420000	3.119142000
C	-2.736319000	-1.405334000	2.748137000
H	-3.108606000	-0.546793000	3.315066000
H	-2.888040000	-2.283114000	3.392056000
C	-1.244505000	-1.273529000	2.524550000
H	-0.679491000	-1.052948000	3.425824000
C	-0.588682000	-2.142444000	1.591009000
H	-1.214019000	-2.889932000	1.101420000
H	0.404434000	-2.494954000	1.862054000
H	-5.088577000	3.125522000	3.128287000
H	-4.295347000	2.386777000	-1.029343000
C	-2.833097000	1.655975000	0.380235000
O	-1.979675000	1.057021000	-0.564536000
C	-2.032801000	1.539307000	-1.918353000
H	-1.153247000	1.140347000	-2.421279000
H	-2.939517000	1.183927000	-2.414470000
H	-2.000926000	2.631163000	-1.920112000
C	-3.558445000	-1.563749000	1.459221000
H	-3.116010000	-0.952251000	0.659735000
H	-3.514638000	-2.597167000	1.095476000
C	-5.014464000	-1.119715000	1.618983000

H	-5.027750000	-0.104924000	2.034500000
H	-5.518491000	-1.762916000	2.353450000
C	-5.792719000	-1.125631000	0.302458000
H	-5.225660000	-0.551639000	-0.446595000
H	-5.858221000	-2.151182000	-0.085655000
C	-7.196576000	-0.528396000	0.422890000
H	-7.114675000	0.497037000	0.809143000
H	-7.770046000	-1.092480000	1.170660000
C	-7.952489000	-0.519780000	-0.907427000
H	-8.951572000	-0.084469000	-0.800946000
H	-7.413388000	0.065292000	-1.663646000
H	-8.073769000	-1.536829000	-1.300041000
C	-2.533792000	-4.804538000	-1.515385000
C	-1.485685000	-3.874689000	-1.493429000
C	-1.816626000	-2.553312000	-1.815218000
C	-3.105660000	-2.158584000	-2.154696000
C	-4.125037000	-3.108431000	-2.179618000
C	-3.834766000	-4.433794000	-1.854758000
H	-2.317624000	-5.838087000	-1.259664000
H	-3.302409000	-1.117697000	-2.386538000
H	-5.134879000	-2.811090000	-2.440599000
H	-4.622199000	-5.180722000	-1.863134000
O	-0.821160000	-1.551793000	-1.750846000
C	0.040931000	-1.472090000	-2.913775000
H	-0.561094000	-1.208447000	-3.787591000
H	0.778765000	-0.704433000	-2.685398000
H	0.533862000	-2.433005000	-3.073191000
C	-0.078715000	-4.293402000	-1.149461000
H	0.496389000	-3.471043000	-0.718159000
H	-0.086297000	-5.115155000	-0.427913000

H	0.457445000	-4.648662000	-2.038891000
N	1.307589000	0.090879000	-0.227387000
N	2.835201000	1.830331000	-0.874265000
N	3.675311000	-0.185054000	-0.554546000
C	2.498260000	0.538706000	-0.499602000
C	4.184166000	1.874741000	-1.212384000
C	4.698309000	0.635664000	-1.022013000
H	5.697260000	0.278230000	-1.192071000
H	4.665537000	2.766688000	-1.569201000
C	3.684468000	-1.624004000	-0.255606000
H	2.843824000	-2.031639000	-0.831965000
C	3.405923000	-1.911073000	1.237773000
C	4.969252000	-2.358043000	-0.686298000
H	2.526706000	-1.336108000	1.540217000
C	4.617791000	-1.528579000	2.103650000
C	3.120756000	-3.418790000	1.370372000
H	5.195765000	-2.118274000	-1.733039000
C	6.178835000	-2.023937000	0.215911000
C	4.677387000	-3.870412000	-0.554799000
H	4.381601000	-1.710793000	3.159594000
H	4.829339000	-0.455794000	2.004900000
C	5.847960000	-2.353245000	1.681206000
H	2.242835000	-3.689755000	0.769195000
H	2.880291000	-3.660220000	2.413581000
C	4.350822000	-4.222404000	0.911102000
H	6.471875000	-0.972403000	0.140909000
H	7.040513000	-2.613072000	-0.121913000
H	3.839936000	-4.151347000	-1.207669000
H	5.551670000	-4.439510000	-0.892900000
H	6.703369000	-2.091616000	2.314978000

C	5.546699000	-3.857446000	1.810080000
H	4.141710000	-5.296075000	0.988397000
H	6.429595000	-4.441937000	1.521333000
H	5.320951000	-4.110916000	2.853868000
C	1.803284000	2.868802000	-0.904462000
H	0.923290000	2.343561000	-1.294405000
C	2.083037000	4.071520000	-1.826078000
C	1.442753000	3.374661000	0.510443000
H	2.395623000	3.710802000	-2.814064000
C	3.133831000	5.047773000	-1.253024000
C	0.744011000	4.837180000	-1.946689000
H	1.328138000	2.507626000	1.168339000
C	2.539145000	4.303159000	1.058906000
C	0.110689000	4.137487000	0.395185000
H	3.229151000	5.899852000	-1.937476000
H	4.127135000	4.594148000	-1.187126000
C	2.696907000	5.529370000	0.140756000
H	-0.022676000	4.186431000	-2.390042000
H	0.869915000	5.688253000	-2.626558000
C	0.287270000	5.334406000	-0.558418000
H	3.490380000	3.760386000	1.134009000
H	2.272641000	4.619584000	2.074991000
H	-0.675250000	3.464442000	0.028555000
H	-0.210698000	4.486158000	1.384231000
H	3.460452000	6.200783000	0.550291000
C	1.356263000	6.277910000	0.024501000
H	-0.664662000	5.869488000	-0.659739000
H	1.037542000	6.639776000	1.010345000
H	1.474196000	7.159254000	-0.618610000

Sc-3-TS2

Sc	0.499052000	0.232773000	0.262968000
C	2.939370000	-2.658889000	1.488161000
C	4.292556000	-2.878994000	1.737348000
H	4.791694000	-3.741011000	1.307054000
C	4.991389000	-1.988599000	2.555191000
C	4.342772000	-0.888189000	3.111390000
H	4.894094000	-0.209130000	3.754345000
C	2.989164000	-0.621239000	2.855828000
C	2.317264000	0.603041000	3.436008000
H	1.274547000	0.378579000	3.689638000
H	2.820375000	0.816234000	4.385037000
C	3.730158000	2.239411000	2.017239000
H	4.485681000	2.029536000	2.785847000
H	3.794785000	3.318524000	1.830149000
C	2.340598000	1.926942000	2.607794000
H	2.153345000	2.694975000	3.371511000
C	1.198908000	2.073931000	1.576765000
H	1.090934000	3.144961000	1.359647000
H	0.234478000	1.819902000	2.060235000
H	6.043056000	-2.155551000	2.764860000
H	2.359605000	-3.342627000	0.876719000
C	2.323459000	-1.542626000	2.044785000
O	0.963429000	-1.307497000	1.732209000
C	0.006436000	-2.005771000	2.571855000
H	-0.975686000	-1.685482000	2.229625000
H	0.135554000	-3.082791000	2.443310000
H	0.171835000	-1.726547000	3.615018000
C	4.081665000	1.482363000	0.726308000
H	3.563433000	0.515344000	0.703255000
H	3.710934000	2.036671000	-0.141008000

C	5.576113000	1.208943000	0.540482000
H	5.977475000	0.752978000	1.455594000
H	6.114516000	2.157834000	0.408649000
C	5.845104000	0.282640000	-0.646329000
H	5.291557000	-0.656288000	-0.492815000
H	5.432621000	0.730363000	-1.558170000
C	7.324700000	-0.039808000	-0.865348000
H	7.737755000	-0.498262000	0.044366000
H	7.882941000	0.894293000	-1.015643000
C	7.550572000	-0.970134000	-2.059620000
H	8.613202000	-1.191189000	-2.205227000
H	7.026110000	-1.923947000	-1.920196000
H	7.171155000	-0.518682000	-2.984187000
C	3.146763000	1.858166000	-3.031338000
C	2.260620000	1.155530000	-2.203681000
C	2.339348000	-0.243875000	-2.251593000
C	3.209218000	-0.930889000	-3.086233000
C	4.066088000	-0.196098000	-3.910701000
C	4.037974000	1.196615000	-3.876894000
H	3.115160000	2.944007000	-3.019784000
H	3.244549000	-2.013641000	-3.098556000
H	4.755913000	-0.719499000	-4.564189000
H	4.704540000	1.770311000	-4.512920000
O	1.466656000	-0.911764000	-1.360281000
C	1.139969000	-2.284226000	-1.636717000
H	2.012319000	-2.920614000	-1.471949000
H	0.345807000	-2.555359000	-0.941497000
H	0.785330000	-2.377611000	-2.666141000
C	1.268061000	1.831276000	-1.315302000
H	1.364358000	2.917773000	-1.390391000

H	0.237696000	1.614486000	-1.655223000
H	1.408791000	1.907235000	0.137117000
N	-1.367104000	0.089538000	0.199187000
N	-3.525477000	-0.977679000	0.063615000
N	-3.488045000	1.208143000	0.373238000
C	-2.670540000	0.107540000	0.199801000
C	-4.843198000	-0.538561000	0.186547000
C	-4.817791000	0.800815000	0.379268000
H	-5.631746000	1.482519000	0.541822000
H	-5.685637000	-1.202513000	0.134809000
C	-2.907457000	2.548146000	0.529302000
H	-2.051462000	2.388462000	1.194290000
C	-3.825737000	3.597986000	1.186153000
C	-2.364654000	3.104160000	-0.806614000
H	-4.256549000	3.183010000	2.105898000
C	-4.943639000	4.107750000	0.248973000
C	-2.916649000	4.801545000	1.532209000
H	-1.779434000	2.319564000	-1.294882000
C	-3.514637000	3.549727000	-1.725640000
C	-1.463970000	4.306247000	-0.468544000
H	-5.504672000	4.892039000	0.772117000
H	-5.668314000	3.327157000	-0.000315000
C	-4.330052000	4.665795000	-1.046016000
H	-2.125640000	4.489677000	2.226920000
H	-3.509356000	5.568505000	2.044904000
C	-2.296370000	5.387306000	0.245758000
H	-4.163662000	2.696045000	-1.961407000
H	-3.100840000	3.906052000	-2.677243000
H	-0.631567000	3.982648000	0.169646000
H	-1.025869000	4.713525000	-1.388474000

H	-5.131872000	4.996629000	-1.716361000
C	-3.415578000	5.855659000	-0.702469000
H	-1.652564000	6.235120000	0.508406000
H	-2.979389000	6.275727000	-1.617897000
H	-4.002544000	6.653875000	-0.230667000
C	-3.002927000	-2.320618000	-0.188451000
H	-1.926215000	-2.138117000	-0.249493000
C	-3.446862000	-2.944053000	-1.530874000
C	-3.242645000	-3.328817000	0.956567000
H	-3.322107000	-2.198120000	-2.324882000
C	-4.903977000	-3.443762000	-1.489583000
C	-2.524124000	-4.154845000	-1.789935000
H	-2.982928000	-2.853281000	1.910832000
C	-4.702299000	-3.819787000	0.996965000
C	-2.317161000	-4.535365000	0.692093000
H	-5.146316000	-3.912838000	-2.451297000
H	-5.604482000	-2.610411000	-1.375214000
C	-5.074640000	-4.468212000	-0.350814000
H	-1.478426000	-3.825108000	-1.861219000
H	-2.778787000	-4.612573000	-2.753414000
C	-2.681797000	-5.187380000	-0.656362000
H	-5.383456000	-2.996481000	1.237136000
H	-4.811638000	-4.552618000	1.806173000
H	-1.266121000	-4.210029000	0.681108000
H	-2.417693000	-5.266078000	1.503996000
H	-6.115759000	-4.809277000	-0.317295000
C	-4.144392000	-5.668952000	-0.607360000
H	-2.017509000	-6.039971000	-0.841871000
H	-4.267132000	-6.417872000	0.185320000
H	-4.410185000	-6.156299000	-1.553791000

Sc-4-INT1

Sc	0.477581000	1.516315000	-0.250701000
C	3.434857000	3.478091000	-1.512370000
C	3.739144000	4.746535000	-1.032090000
H	4.212731000	5.474985000	-1.681462000
C	3.416179000	5.078193000	0.292307000
C	2.811662000	4.154743000	1.134876000
H	2.575950000	4.425818000	2.159828000
C	2.519299000	2.838865000	0.706089000
C	1.767735000	1.848865000	1.507635000
H	2.263329000	0.873206000	1.584990000
H	1.494420000	2.205760000	2.500887000
N	-0.538856000	-0.011951000	-0.202490000
N	-2.480223000	-1.373826000	0.171229000
N	-0.533695000	-2.375702000	0.231687000
C	-1.129647000	-1.148417000	0.040636000
C	-2.713536000	-2.724072000	0.435896000
C	-1.510634000	-3.344571000	0.473679000
H	3.646238000	6.070912000	0.666911000
H	3.646719000	3.188530000	-2.536971000
C	2.835711000	2.564707000	-0.647673000
O	2.401758000	1.308703000	-1.165327000
C	3.372309000	0.224617000	-1.149869000
H	2.840798000	-0.666806000	-1.477005000
H	4.184804000	0.475595000	-1.834205000
H	3.746773000	0.088275000	-0.134026000
H	-1.245779000	-4.373218000	0.657298000
H	-3.713121000	-3.101393000	0.578811000
C	0.882832000	-2.583184000	0.218968000
C	1.480020000	-3.110959000	-0.933991000

C	1.623011000	-2.251418000	1.363051000
C	2.862124000	-3.323201000	-0.913760000
C	3.003314000	-2.468654000	1.331152000
C	3.638268000	-3.014770000	0.209440000
H	3.342125000	-3.741804000	-1.794909000
H	3.593200000	-2.225206000	2.211464000
C	-3.466423000	-0.339186000	0.066574000
C	-4.169359000	-0.194357000	-1.136713000
C	-3.670023000	0.508913000	1.163583000
C	-5.115903000	0.829610000	-1.216990000
C	-4.623439000	1.521618000	1.033788000
C	-5.360899000	1.692542000	-0.143115000
H	-5.673885000	0.957660000	-2.141106000
H	-4.802168000	2.186140000	1.875559000
C	0.655372000	-3.425247000	-2.156841000
H	1.293647000	-3.735023000	-2.988098000
H	-0.061019000	-4.232405000	-1.966028000
H	0.072271000	-2.553562000	-2.476043000
C	0.943732000	-1.688473000	2.585173000
H	0.489930000	-0.714973000	2.369447000
H	0.141991000	-2.348772000	2.934169000
H	1.657203000	-1.559910000	3.403042000
C	5.121646000	-3.289298000	0.220972000
H	5.657297000	-2.580371000	0.860156000
H	5.327210000	-4.294712000	0.609163000
H	5.548506000	-3.237419000	-0.785455000
C	-3.895619000	-1.103365000	-2.308546000
H	-2.831271000	-1.101843000	-2.571830000
H	-4.167308000	-2.142653000	-2.090156000
H	-4.464916000	-0.787391000	-3.186221000

C	-2.876059000	0.337036000	2.434071000
H	-2.926152000	-0.692653000	2.805014000
H	-1.815318000	0.565081000	2.270317000
H	-3.249822000	0.998733000	3.219632000
C	-6.417622000	2.764229000	-0.242600000
H	-6.517540000	3.134942000	-1.267477000
H	-7.397533000	2.373014000	0.058934000
H	-6.191456000	3.613246000	0.409719000

Sc-4-INT2

Sc	0.019461000	-0.192820000	0.085534000
C	-2.074293000	-2.785924000	2.456406000
C	-3.368147000	-3.242263000	2.199551000
H	-4.016072000	-3.533231000	3.019691000
C	-3.819772000	-3.306483000	0.876246000
C	-2.989682000	-2.944015000	-0.182734000
H	-3.356077000	-3.010490000	-1.202217000
C	-1.668533000	-2.497667000	0.031043000
C	-0.751575000	-1.997760000	-1.022669000
H	0.186961000	-2.570364000	-1.051225000
H	-1.204832000	-2.025103000	-2.015260000
C	-2.762624000	1.383795000	-2.231942000
H	-3.065966000	1.840267000	-3.186883000
H	-3.044275000	2.090885000	-1.442909000
H	-4.827893000	-3.652424000	0.667060000
H	-1.695418000	-2.693456000	3.470078000
C	-1.272496000	-2.417929000	1.383550000
O	-0.012837000	-1.810884000	1.628907000
C	1.088653000	-2.735199000	1.825807000
H	1.973135000	-2.121687000	1.977177000
H	0.879488000	-3.350623000	2.704022000

H	1.216762000	-3.359504000	0.940174000
C	-3.523985000	0.063683000	-2.053673000
H	-3.208874000	-0.651643000	-2.825629000
H	-3.245807000	-0.382065000	-1.093321000
C	-5.042560000	0.244943000	-2.103819000
H	-5.343597000	0.566348000	-3.110682000
H	-5.328884000	1.058086000	-1.424045000
C	-5.803431000	-1.024433000	-1.713780000
H	-5.535354000	-1.840697000	-2.400810000
H	-5.470324000	-1.348211000	-0.717337000
C	-7.324256000	-0.848933000	-1.703102000
H	-7.662464000	-0.539345000	-2.701117000
H	-7.586546000	-0.024602000	-1.024299000
C	-8.063975000	-2.119389000	-1.278282000
H	-9.148728000	-1.970316000	-1.272887000
H	-7.844731000	-2.949987000	-1.959736000
H	-7.765369000	-2.431069000	-0.269304000
C	-3.862145000	3.269457000	1.223900000
C	-2.535332000	2.855440000	1.405737000
C	-2.321820000	1.477303000	1.516499000
C	-3.350659000	0.541275000	1.472461000
C	-4.660123000	0.987135000	1.301323000
C	-4.912763000	2.353637000	1.173598000
H	-4.067432000	4.331756000	1.123991000
H	-3.127662000	-0.514667000	1.571849000
H	-5.471138000	0.267780000	1.260839000
H	-5.929227000	2.708010000	1.033850000
O	-0.996751000	0.999476000	1.661653000
C	-0.524352000	0.960735000	3.031888000
H	-1.114315000	0.234870000	3.595629000

H	0.521408000	0.657821000	2.993634000
H	-0.613937000	1.956735000	3.469553000
C	-1.412113000	3.856166000	1.501359000
H	-1.334658000	4.261348000	2.518775000
H	-0.443640000	3.420969000	1.248125000
H	-1.589405000	4.704645000	0.833556000
C	-1.271553000	1.224448000	-2.268434000
H	-0.890120000	0.462128000	-2.949535000
C	-0.391019000	1.980013000	-1.586888000
H	-0.722209000	2.780089000	-0.930037000
H	0.680444000	1.886175000	-1.727208000
N	1.870554000	0.081163000	-0.032751000
N	4.091541000	-0.712733000	-0.536561000
N	3.798349000	1.458545000	-0.422264000
C	3.122745000	0.251929000	-0.301377000
C	5.323838000	-0.105887000	-0.795015000
C	5.142116000	1.232574000	-0.728823000
H	5.832640000	2.049279000	-0.863839000
H	6.202827000	-0.691824000	-1.009296000
C	3.148128000	2.724915000	-0.300187000
C	2.835238000	3.444392000	-1.462260000
C	2.799889000	3.185614000	0.977067000
C	2.157358000	4.658124000	-1.318770000
C	2.122584000	4.403385000	1.071565000
C	1.794305000	5.154205000	-0.062708000
H	1.900519000	5.224645000	-2.210399000
H	1.849920000	4.778571000	2.055128000
C	3.833830000	-2.117480000	-0.485487000
C	3.100299000	-2.712404000	-1.522737000
C	4.300772000	-2.853087000	0.613236000

C	2.824421000	-4.078972000	-1.427366000
C	4.016525000	-4.220918000	0.655694000
C	3.278988000	-4.851243000	-0.352018000
H	2.253525000	-4.554896000	-2.220747000
H	4.371752000	-4.805491000	1.500778000
C	3.192755000	2.908562000	-2.826319000
H	2.705825000	3.491769000	-3.611997000
H	4.273601000	2.943958000	-3.005705000
H	2.891108000	1.860635000	-2.937026000
C	3.141536000	2.380606000	2.204072000
H	2.646190000	1.403279000	2.173637000
H	4.218983000	2.191553000	2.270909000
H	2.832904000	2.903549000	3.113493000
C	1.084621000	6.479007000	0.066728000
H	0.511764000	6.537925000	0.997475000
H	1.802061000	7.309148000	0.072606000
H	0.400026000	6.650002000	-0.770474000
C	2.629492000	-1.903562000	-2.703634000
H	1.856483000	-1.188247000	-2.401127000
H	3.451862000	-1.328188000	-3.143222000
H	2.212719000	-2.552623000	-3.477980000
C	5.057073000	-2.182530000	1.733199000
H	6.057220000	-1.863395000	1.418137000
H	4.537740000	-1.282511000	2.082887000
H	5.178566000	-2.862389000	2.580495000
C	3.002723000	-6.333150000	-0.297546000
H	2.030904000	-6.575750000	-0.738985000
H	3.763007000	-6.892403000	-0.857269000
H	3.015418000	-6.706056000	0.731138000

Sc-4-INT3

Sc	-0.121286000	-0.435021000	0.280043000
C	1.048967000	-2.973713000	-2.480566000
C	2.058579000	-3.915511000	-2.669084000
H	2.663249000	-3.892868000	-3.569898000
C	2.271535000	-4.891053000	-1.693257000
C	1.480206000	-4.921805000	-0.546675000
H	1.647986000	-5.692399000	0.199711000
C	0.467834000	-3.976917000	-0.314832000
C	-0.327985000	-4.011951000	0.970485000
H	-1.377070000	-3.759502000	0.779384000
H	-0.319253000	-5.051971000	1.314321000
C	1.699937000	-3.175120000	2.339205000
H	2.039591000	-4.209700000	2.194587000
H	1.931557000	-2.932688000	3.384229000
C	0.169931000	-3.115768000	2.151589000
H	-0.256540000	-3.609918000	3.038088000
C	-0.386392000	-1.679392000	2.084402000
H	-0.111244000	-1.152707000	3.013804000
H	-1.488318000	-1.746321000	2.115140000
H	3.049754000	-5.635273000	-1.829986000
H	0.842621000	-2.210390000	-3.224121000
C	0.286576000	-3.018080000	-1.316594000
O	-0.662496000	-1.985865000	-1.123882000
C	-2.004699000	-2.250336000	-1.619753000
H	-2.595018000	-1.377327000	-1.355273000
H	-1.957889000	-2.394265000	-2.701867000
H	-2.402565000	-3.140632000	-1.130603000
C	2.532854000	-2.247651000	1.441955000
H	2.125356000	-2.223126000	0.421889000
H	2.485428000	-1.222402000	1.829335000

C	4.003641000	-2.660350000	1.341250000
H	4.057972000	-3.671640000	0.915025000
H	4.432768000	-2.727256000	2.350810000
C	4.835498000	-1.699701000	0.490762000
H	4.378523000	-1.616349000	-0.507170000
H	4.791550000	-0.693549000	0.928967000
C	6.299257000	-2.121410000	0.338308000
H	6.343652000	-3.120525000	-0.116731000
H	6.752722000	-2.220008000	1.333955000
C	7.117008000	-1.136638000	-0.500461000
H	8.156488000	-1.464446000	-0.605940000
H	6.695717000	-1.032204000	-1.508444000
H	7.122850000	-0.141528000	-0.040493000
C	3.822533000	2.233926000	1.537069000
C	2.685574000	1.612056000	1.013601000
C	2.753731000	1.158092000	-0.307925000
C	3.886667000	1.329325000	-1.095079000
C	5.004852000	1.959594000	-0.546799000
C	4.976628000	2.406875000	0.772607000
H	3.791326000	2.596861000	2.560360000
H	3.919300000	0.961772000	-2.113462000
H	5.895669000	2.085854000	-1.152934000
H	5.844084000	2.895940000	1.203492000
O	1.614984000	0.503145000	-0.809703000
C	1.359987000	0.639723000	-2.225567000
H	2.020278000	-0.020637000	-2.791075000
H	0.320514000	0.348430000	-2.379501000
H	1.496020000	1.682458000	-2.514201000
C	1.432236000	1.448181000	1.828342000
H	1.453807000	2.080152000	2.719069000

H	0.540923000	1.755257000	1.264258000
H	1.306953000	0.420733000	2.201883000
N	-1.556359000	0.759090000	0.058387000
N	-3.873785000	1.410436000	0.129702000
N	-2.383915000	3.012458000	-0.029179000
C	-2.507128000	1.633663000	0.057236000
C	-4.564080000	2.624345000	0.084001000
C	-3.645101000	3.613311000	-0.011745000
H	-3.758997000	4.684043000	-0.064970000
H	-5.640001000	2.660744000	0.139721000
C	-1.112642000	3.650697000	-0.164846000
C	-0.477012000	4.158360000	0.973832000
C	-0.510876000	3.684696000	-1.431817000
C	0.800848000	4.707047000	0.821300000
C	0.766865000	4.235750000	-1.535537000
C	1.443038000	4.743845000	-0.418570000
H	1.311116000	5.102231000	1.695918000
H	1.244707000	4.282416000	-2.511978000
C	-4.430409000	0.095515000	0.185997000
C	-4.332031000	-0.626710000	1.384491000
C	-4.994590000	-0.454639000	-0.973646000
C	-4.799398000	-1.942803000	1.392848000
C	-5.466636000	-1.769425000	-0.911710000
C	-5.372697000	-2.529811000	0.258533000
H	-4.726873000	-2.519051000	2.311920000
H	-5.909460000	-2.211625000	-1.800932000
C	-1.137254000	4.069257000	2.326142000
H	-0.483244000	4.466251000	3.106945000
H	-2.077838000	4.630108000	2.357545000
H	-1.381792000	3.029922000	2.576818000

C	-1.232309000	3.129268000	-2.633208000
H	-1.439567000	2.060302000	-2.504729000
H	-2.198222000	3.623941000	-2.783998000
H	-0.640385000	3.262471000	-3.543125000
C	2.840097000	5.293094000	-0.556504000
H	3.560260000	4.483033000	-0.720190000
H	2.916148000	5.978423000	-1.407633000
H	3.148125000	5.833426000	0.342931000
C	-3.742841000	0.006536000	2.618156000
H	-2.683649000	0.240119000	2.468521000
H	-4.254599000	0.944372000	2.862193000
H	-3.827083000	-0.662938000	3.477856000
C	-5.054337000	0.334837000	-2.257949000
H	-5.755297000	1.174526000	-2.188946000
H	-4.076676000	0.763287000	-2.508622000
H	-5.376752000	-0.298629000	-3.088480000
C	-5.906405000	-3.940082000	0.308965000
H	-5.309459000	-4.571034000	0.975323000
H	-6.936635000	-3.954139000	0.686381000
H	-5.917421000	-4.401489000	-0.683367000

Sc-4-INT4

Sc	-0.121286000	-0.435021000	0.280043000
C	1.048967000	-2.973713000	-2.480566000
C	2.058579000	-3.915511000	-2.669084000
H	2.663249000	-3.892868000	-3.569898000
C	2.271535000	-4.891053000	-1.693257000
C	1.480206000	-4.921805000	-0.546675000
H	1.647986000	-5.692399000	0.199711000
C	0.467834000	-3.976917000	-0.314832000
C	-0.327985000	-4.011951000	0.970485000

H	-1.377070000	-3.759502000	0.779384000
H	-0.319253000	-5.051971000	1.314321000
C	1.699937000	-3.175120000	2.339205000
H	2.039591000	-4.209700000	2.194587000
H	1.931557000	-2.932688000	3.384229000
C	0.169931000	-3.115768000	2.151589000
H	-0.256540000	-3.609918000	3.038088000
C	-0.386392000	-1.679392000	2.084402000
H	-0.111244000	-1.152707000	3.013804000
H	-1.488318000	-1.746321000	2.115140000
H	3.049754000	-5.635273000	-1.829986000
H	0.842621000	-2.210390000	-3.224121000
C	0.286576000	-3.018080000	-1.316594000
O	-0.662496000	-1.985865000	-1.123882000
C	-2.004699000	-2.250336000	-1.619753000
H	-2.595018000	-1.377327000	-1.355273000
H	-1.957889000	-2.394265000	-2.701867000
H	-2.402565000	-3.140632000	-1.130603000
C	2.532854000	-2.247651000	1.441955000
H	2.125356000	-2.223126000	0.421889000
H	2.485428000	-1.222402000	1.829335000
C	4.003641000	-2.660350000	1.341250000
H	4.057972000	-3.671640000	0.915025000
H	4.432768000	-2.727256000	2.350810000
C	4.835498000	-1.699701000	0.490762000
H	4.378523000	-1.616349000	-0.507170000
H	4.791550000	-0.693549000	0.928967000
C	6.299257000	-2.121410000	0.338308000
H	6.343652000	-3.120525000	-0.116731000
H	6.752722000	-2.220008000	1.333955000

C	7.117008000	-1.136638000	-0.500461000
H	8.156488000	-1.464446000	-0.605940000
H	6.695717000	-1.032204000	-1.508444000
H	7.122850000	-0.141528000	-0.040493000
C	3.822533000	2.233926000	1.537069000
C	2.685574000	1.612056000	1.013601000
C	2.753731000	1.158092000	-0.307925000
C	3.886667000	1.329325000	-1.095079000
C	5.004852000	1.959594000	-0.546799000
C	4.976628000	2.406875000	0.772607000
H	3.791326000	2.596861000	2.560360000
H	3.919300000	0.961772000	-2.113462000
H	5.895669000	2.085854000	-1.152934000
H	5.844084000	2.895940000	1.203492000
O	1.614984000	0.503145000	-0.809703000
C	1.359987000	0.639723000	-2.225567000
H	2.020278000	-0.020637000	-2.791075000
H	0.320514000	0.348430000	-2.379501000
H	1.496020000	1.682458000	-2.514201000
C	1.432236000	1.448181000	1.828342000
H	1.453807000	2.080152000	2.719069000
H	0.540923000	1.755257000	1.264258000
H	1.306953000	0.420733000	2.201883000
N	-1.556359000	0.759090000	0.058387000
N	-3.873785000	1.410436000	0.129702000
N	-2.383915000	3.012458000	-0.029179000
C	-2.507128000	1.633663000	0.057236000
C	-4.564080000	2.624345000	0.084001000
C	-3.645101000	3.613311000	-0.011745000
H	-3.758997000	4.684043000	-0.064970000

H	-5.640001000	2.660744000	0.139721000
C	-1.112642000	3.650697000	-0.164846000
C	-0.477012000	4.158360000	0.973832000
C	-0.510876000	3.684696000	-1.431817000
C	0.800848000	4.707047000	0.821300000
C	0.766865000	4.235750000	-1.535537000
C	1.443038000	4.743845000	-0.418570000
H	1.311116000	5.102231000	1.695918000
H	1.244707000	4.282416000	-2.511978000
C	-4.430409000	0.095515000	0.185997000
C	-4.332031000	-0.626710000	1.384491000
C	-4.994590000	-0.454639000	-0.973646000
C	-4.799398000	-1.942803000	1.392848000
C	-5.466636000	-1.769425000	-0.911710000
C	-5.372697000	-2.529811000	0.258533000
H	-4.726873000	-2.519051000	2.311920000
H	-5.909460000	-2.211625000	-1.800932000
C	-1.137254000	4.069257000	2.326142000
H	-0.483244000	4.466251000	3.106945000
H	-2.077838000	4.630108000	2.357545000
H	-1.381792000	3.029922000	2.576818000
C	-1.232309000	3.129268000	-2.633208000
H	-1.439567000	2.060302000	-2.504729000
H	-2.198222000	3.623941000	-2.783998000
H	-0.640385000	3.262471000	-3.543125000
C	2.840097000	5.293094000	-0.556504000
H	3.560260000	4.483033000	-0.720190000
H	2.916148000	5.978423000	-1.407633000
H	3.148125000	5.833426000	0.342931000
C	-3.742841000	0.006536000	2.618156000

H	-2.683649000	0.240119000	2.468521000
H	-4.254599000	0.944372000	2.862193000
H	-3.827083000	-0.662938000	3.477856000
C	-5.054337000	0.334837000	-2.257949000
H	-5.755297000	1.174526000	-2.188946000
H	-4.076676000	0.763287000	-2.508622000
H	-5.376752000	-0.298629000	-3.088480000
C	-5.906405000	-3.940082000	0.308965000
H	-5.309459000	-4.571034000	0.975323000
H	-6.936635000	-3.954139000	0.686381000
H	-5.917421000	-4.401489000	-0.683367000

Sc-4-TS1

Sc	-0.121286000	-0.435021000	0.280043000
C	1.048967000	-2.973713000	-2.480566000
C	2.058579000	-3.915511000	-2.669084000
H	2.663249000	-3.892868000	-3.569898000
C	2.271535000	-4.891053000	-1.693257000
C	1.480206000	-4.921805000	-0.546675000
H	1.647986000	-5.692399000	0.199711000
C	0.467834000	-3.976917000	-0.314832000
C	-0.327985000	-4.011951000	0.970485000
H	-1.377070000	-3.759502000	0.779384000
H	-0.319253000	-5.051971000	1.314321000
C	1.699937000	-3.175120000	2.339205000
H	2.039591000	-4.209700000	2.194587000
H	1.931557000	-2.932688000	3.384229000
C	0.169931000	-3.115768000	2.151589000
H	-0.256540000	-3.609918000	3.038088000
C	-0.386392000	-1.679392000	2.084402000
H	-0.111244000	-1.152707000	3.013804000

H	-1.488318000	-1.746321000	2.115140000
H	3.049754000	-5.635273000	-1.829986000
H	0.842621000	-2.210390000	-3.224121000
C	0.286576000	-3.018080000	-1.316594000
O	-0.662496000	-1.985865000	-1.123882000
C	-2.004699000	-2.250336000	-1.619753000
H	-2.595018000	-1.377327000	-1.355273000
H	-1.957889000	-2.394265000	-2.701867000
H	-2.402565000	-3.140632000	-1.130603000
C	2.532854000	-2.247651000	1.441955000
H	2.125356000	-2.223126000	0.421889000
H	2.485428000	-1.222402000	1.829335000
C	4.003641000	-2.660350000	1.341250000
H	4.057972000	-3.671640000	0.915025000
H	4.432768000	-2.727256000	2.350810000
C	4.835498000	-1.699701000	0.490762000
H	4.378523000	-1.616349000	-0.507170000
H	4.791550000	-0.693549000	0.928967000
C	6.299257000	-2.121410000	0.338308000
H	6.343652000	-3.120525000	-0.116731000
H	6.752722000	-2.220008000	1.333955000
C	7.117008000	-1.136638000	-0.500461000
H	8.156488000	-1.464446000	-0.605940000
H	6.695717000	-1.032204000	-1.508444000
H	7.122850000	-0.141528000	-0.040493000
C	3.822533000	2.233926000	1.537069000
C	2.685574000	1.612056000	1.013601000
C	2.753731000	1.158092000	-0.307925000
C	3.886667000	1.329325000	-1.095079000
C	5.004852000	1.959594000	-0.546799000

C	4.976628000	2.406875000	0.772607000
H	3.791326000	2.596861000	2.560360000
H	3.919300000	0.961772000	-2.113462000
H	5.895669000	2.085854000	-1.152934000
H	5.844084000	2.895940000	1.203492000
O	1.614984000	0.503145000	-0.809703000
C	1.359987000	0.639723000	-2.225567000
H	2.020278000	-0.020637000	-2.791075000
H	0.320514000	0.348430000	-2.379501000
H	1.496020000	1.682458000	-2.514201000
C	1.432236000	1.448181000	1.828342000
H	1.453807000	2.080152000	2.719069000
H	0.540923000	1.755257000	1.264258000
H	1.306953000	0.420733000	2.201883000
N	-1.556359000	0.759090000	0.058387000
N	-3.873785000	1.410436000	0.129702000
N	-2.383915000	3.012458000	-0.029179000
C	-2.507128000	1.633663000	0.057236000
C	-4.564080000	2.624345000	0.084001000
C	-3.645101000	3.613311000	-0.011745000
H	-3.758997000	4.684043000	-0.064970000
H	-5.640001000	2.660744000	0.139721000
C	-1.112642000	3.650697000	-0.164846000
C	-0.477012000	4.158360000	0.973832000
C	-0.510876000	3.684696000	-1.431817000
C	0.800848000	4.707047000	0.821300000
C	0.766865000	4.235750000	-1.535537000
C	1.443038000	4.743845000	-0.418570000
H	1.311116000	5.102231000	1.695918000
H	1.244707000	4.282416000	-2.511978000

C	-4.430409000	0.095515000	0.185997000
C	-4.332031000	-0.626710000	1.384491000
C	-4.994590000	-0.454639000	-0.973646000
C	-4.799398000	-1.942803000	1.392848000
C	-5.466636000	-1.769425000	-0.911710000
C	-5.372697000	-2.529811000	0.258533000
H	-4.726873000	-2.519051000	2.311920000
H	-5.909460000	-2.211625000	-1.800932000
C	-1.137254000	4.069257000	2.326142000
H	-0.483244000	4.466251000	3.106945000
H	-2.077838000	4.630108000	2.357545000
H	-1.381792000	3.029922000	2.576818000
C	-1.232309000	3.129268000	-2.633208000
H	-1.439567000	2.060302000	-2.504729000
H	-2.198222000	3.623941000	-2.783998000
H	-0.640385000	3.262471000	-3.543125000
C	2.840097000	5.293094000	-0.556504000
H	3.560260000	4.483033000	-0.720190000
H	2.916148000	5.978423000	-1.407633000
H	3.148125000	5.833426000	0.342931000
C	-3.742841000	0.006536000	2.618156000
H	-2.683649000	0.240119000	2.468521000
H	-4.254599000	0.944372000	2.862193000
H	-3.827083000	-0.662938000	3.477856000
C	-5.054337000	0.334837000	-2.257949000
H	-5.755297000	1.174526000	-2.188946000
H	-4.076676000	0.763287000	-2.508622000
H	-5.376752000	-0.298629000	-3.088480000
C	-5.906405000	-3.940082000	0.308965000
H	-5.309459000	-4.571034000	0.975323000

H	-6.936635000	-3.954139000	0.686381000
H	-5.917421000	-4.401489000	-0.683367000
Sc-4-TS2			
Sc	-0.064047000	-0.201180000	0.339640000
C	1.472732000	-2.696121000	-2.311523000
C	2.610013000	-3.479845000	-2.498510000
H	3.174767000	-3.407525000	-3.422234000
C	3.003843000	-4.364628000	-1.492823000
C	2.270491000	-4.457550000	-0.311405000
H	2.582283000	-5.155267000	0.459773000
C	1.138430000	-3.661981000	-0.080015000
C	0.388129000	-3.743688000	1.230884000
H	-0.687337000	-3.616247000	1.062110000
H	0.518211000	-4.765817000	1.601886000
C	2.343805000	-2.709787000	2.569738000
H	2.754653000	-3.723301000	2.472319000
H	2.560834000	-2.402826000	3.600383000
C	0.813500000	-2.786841000	2.390869000
H	0.425742000	-3.297684000	3.283259000
C	0.131846000	-1.398756000	2.370677000
H	0.147962000	-1.003919000	3.395813000
H	-0.948796000	-1.523616000	2.165268000
H	3.881825000	-4.987477000	-1.631149000
H	1.125383000	-2.011404000	-3.078557000
C	0.768735000	-2.801323000	-1.116321000
O	-0.339828000	-1.946720000	-0.922229000
C	-1.617319000	-2.447757000	-1.412449000
H	-2.354624000	-1.696697000	-1.140977000
H	-1.552762000	-2.576391000	-2.495492000
H	-1.839330000	-3.400694000	-0.928675000

C	3.069248000	-1.761684000	1.601402000
H	2.521300000	-1.702243000	0.651481000
H	3.068547000	-0.747380000	2.009433000
C	4.510138000	-2.157758000	1.273144000
H	4.534809000	-3.205708000	0.945482000
H	5.126359000	-2.103221000	2.181429000
C	5.106256000	-1.268452000	0.180208000
H	4.474623000	-1.344649000	-0.718257000
H	5.056136000	-0.219528000	0.497556000
C	6.549199000	-1.614678000	-0.192626000
H	6.601544000	-2.662925000	-0.518986000
H	7.183334000	-1.541990000	0.701421000
C	7.104389000	-0.704121000	-1.290537000
H	8.138924000	-0.959266000	-1.543271000
H	6.506580000	-0.783520000	-2.207389000
H	7.083807000	0.345821000	-0.974612000
C	3.618035000	2.154552000	1.529834000
C	2.476615000	1.592342000	0.942921000
C	2.502441000	1.444720000	-0.451915000
C	3.562551000	1.861522000	-1.243307000
C	4.679305000	2.431588000	-0.623446000
C	4.709156000	2.568234000	0.763053000
H	3.635399000	2.281357000	2.608624000
H	3.548552000	1.734683000	-2.318988000
H	5.520001000	2.752325000	-1.229517000
H	5.576003000	3.004435000	1.249253000
O	1.364518000	0.808920000	-0.995228000
C	1.113525000	0.953745000	-2.403795000
H	1.855049000	0.392041000	-2.976770000
H	0.117646000	0.546358000	-2.577925000

H	1.132996000	2.012379000	-2.667234000
C	1.277762000	1.178853000	1.730214000
H	1.455816000	1.332454000	2.798651000
H	0.426619000	1.836332000	1.483238000
H	0.869934000	-0.195493000	2.001291000
N	-1.766990000	0.564111000	0.175794000
N	-4.143029000	0.930597000	0.115717000
N	-2.851238000	2.703050000	0.061834000
C	-2.814036000	1.320565000	0.128024000
C	-4.971271000	2.053412000	0.032849000
C	-4.173631000	3.147390000	0.001001000
H	-4.413262000	4.197611000	-0.043753000
H	-6.045172000	1.960203000	0.026306000
C	-1.649126000	3.472807000	-0.024467000
C	-1.031013000	3.904270000	1.155811000
C	-1.076179000	3.682122000	-1.285841000
C	0.198318000	4.559654000	1.048625000
C	0.153512000	4.342485000	-1.345088000
C	0.812612000	4.776299000	-0.189321000
H	0.696887000	4.893460000	1.954938000
H	0.607615000	4.527495000	-2.316117000
C	-4.527179000	-0.445591000	0.068215000
C	-4.412819000	-1.220787000	1.231353000
C	-4.925650000	-0.996204000	-1.158822000
C	-4.707939000	-2.583062000	1.139983000
C	-5.224044000	-2.361482000	-1.198235000
C	-5.120784000	-3.170334000	-0.061507000
H	-4.625471000	-3.198582000	2.032517000
H	-5.537387000	-2.803965000	-2.140713000
C	-1.657250000	3.617812000	2.496691000

H	-1.050359000	4.029688000	3.306918000
H	-2.663551000	4.043714000	2.573891000
H	-1.755805000	2.537166000	2.657647000
C	-1.765449000	3.184676000	-2.531274000
H	-1.894527000	2.095728000	-2.500744000
H	-2.766015000	3.617269000	-2.640356000
H	-1.190677000	3.438923000	-3.426173000
C	2.169008000	5.428592000	-0.270539000
H	2.335383000	5.886116000	-1.250464000
H	2.284527000	6.204851000	0.492348000
H	2.962106000	4.688766000	-0.109480000
C	-3.975243000	-0.599285000	2.532354000
H	-2.944042000	-0.235874000	2.462171000
H	-4.602762000	0.260201000	2.793107000
H	-4.032390000	-1.323320000	3.349315000
C	-4.989747000	-0.150029000	-2.405964000
H	-5.794860000	0.591751000	-2.356302000
H	-4.058268000	0.408634000	-2.555906000
H	-5.164982000	-0.771624000	-3.287886000
C	-5.475194000	-4.635474000	-0.121695000
H	-4.884585000	-5.221190000	0.589872000
H	-6.532148000	-4.791058000	0.128605000
H	-5.315085000	-5.047032000	-1.123146000

styrene-INT2

Sc	-0.738218000	-0.495763000	-0.194311000
C	-2.557605000	-4.219094000	-0.342638000
C	-3.779096000	-4.493877000	-0.960357000
H	-4.392069000	-5.317817000	-0.610523000
C	-4.210553000	-3.683916000	-2.016491000
C	-3.423815000	-2.629001000	-2.476995000

H	-3.765969000	-2.022605000	-3.310715000
C	-2.170170000	-2.339886000	-1.901855000
C	-1.291657000	-1.202107000	-2.270509000
H	-0.301543000	-1.555611000	-2.589522000
H	-1.706980000	-0.601956000	-3.083716000
C	-1.652101000	1.922723000	-0.652909000
H	-0.767582000	2.282466000	-0.139520000
C	-2.867045000	2.002243000	-0.068101000
H	-2.912140000	2.372031000	0.955509000
N	1.071031000	-0.005015000	0.010670000
N	2.672951000	1.788557000	-0.092686000
N	3.475544000	-0.213653000	0.227374000
C	2.281013000	0.466646000	0.043857000
C	4.070781000	1.918176000	0.004574000
C	4.570884000	0.673609000	0.204664000
C	1.781479000	2.870228000	-0.368779000
C	1.299813000	3.638322000	0.707644000
C	0.441672000	4.702993000	0.414390000
H	0.049108000	5.314401000	1.220270000
C	0.086311000	4.991639000	-0.902094000
C	0.584826000	4.221880000	-1.949115000
H	0.304781000	4.460769000	-2.970505000
C	1.447357000	3.146787000	-1.705484000
C	1.655786000	3.286359000	2.144158000
H	2.556678000	2.665141000	2.123074000
C	0.532782000	2.437591000	2.767613000
H	0.365523000	1.530909000	2.177322000
H	-0.402798000	3.008508000	2.804676000
H	0.789112000	2.141016000	3.791174000
C	1.963889000	4.518522000	3.006373000

C	1.994655000	2.323820000	-2.861466000
H	2.657311000	1.558064000	-2.448029000
C	2.828992000	3.191402000	-3.818919000
H	3.646453000	3.695113000	-3.292099000
H	2.216274000	3.962831000	-4.297994000
H	3.264543000	2.572261000	-4.610641000
C	0.866836000	1.596854000	-3.611642000
C	3.605704000	-1.632599000	0.342224000
C	3.825855000	-2.384704000	-0.826156000
C	3.844267000	-4.378661000	0.561104000
C	3.932136000	-3.773444000	-0.691048000
H	4.096703000	-4.387265000	-1.570274000
C	3.678498000	-3.604882000	1.708390000
H	3.650115000	-4.088401000	2.679174000
C	3.574103000	-2.212035000	1.623732000
C	3.438337000	-1.347722000	2.869354000
H	3.778654000	-0.340476000	2.606915000
C	4.309578000	-1.838662000	4.034227000
H	4.277856000	-1.114222000	4.854810000
H	5.353780000	-1.963623000	3.729155000
H	3.958632000	-2.796542000	4.433437000
C	1.964655000	-1.228067000	3.290762000
C	3.934934000	-1.710776000	-2.186862000
H	4.223630000	-0.668340000	-2.015891000
C	2.570644000	-1.688621000	-2.896614000
H	2.640496000	-1.151143000	-3.848690000
H	1.820034000	-1.194458000	-2.275437000
H	2.228941000	-2.708141000	-3.113401000
C	5.013060000	-2.341161000	-3.079881000
H	1.076742000	5.141850000	3.162346000

H	2.319643000	4.205969000	3.993798000
H	2.736668000	5.144172000	2.547403000
H	1.276528000	1.000964000	-4.434272000
H	0.328498000	0.920228000	-2.942924000
H	0.148802000	2.306217000	-4.038965000
H	5.979207000	-2.395876000	-2.567002000
H	4.741854000	-3.353951000	-3.397115000
H	5.141367000	-1.741658000	-3.987128000
H	1.859761000	-0.567023000	4.158759000
H	1.368717000	-0.820411000	2.469486000
H	1.565310000	-2.212380000	3.566067000
H	3.930346000	-5.458120000	0.646020000
H	-0.580457000	5.822753000	-1.111826000
H	-5.165451000	-3.885694000	-2.492932000
H	-2.209343000	-4.803225000	0.504117000
C	-1.799576000	-3.154924000	-0.812758000
O	-0.639169000	-2.742580000	-0.113490000
C	0.540881000	-3.561671000	-0.291277000
H	1.330408000	-3.080532000	0.278088000
H	0.342173000	-4.566226000	0.089454000
H	0.805338000	-3.602283000	-1.349412000
C	-5.193174000	0.487266000	2.877658000
C	-3.810810000	0.289503000	2.769326000
C	-3.381990000	-0.603396000	1.781971000
C	-4.256465000	-1.265881000	0.928592000
C	-5.625551000	-1.045073000	1.059247000
C	-6.092575000	-0.173266000	2.041499000
H	-5.563172000	1.176414000	3.632126000
H	-3.872328000	-1.941702000	0.176348000
H	-6.314480000	-1.544601000	0.386922000

H	-7.157586000	0.006811000	2.147716000
O	-1.992769000	-0.865584000	1.651424000
C	-1.547663000	-1.884112000	2.586917000
H	-2.078559000	-2.814846000	2.377722000
H	-0.479134000	-2.012832000	2.437754000
H	-1.747593000	-1.546045000	3.605077000
C	-2.844950000	1.002884000	3.680290000
H	-1.878841000	1.164909000	3.197529000
H	-3.246594000	1.973919000	3.984887000
H	-2.661164000	0.431600000	4.599381000
C	5.965639000	0.184683000	0.387498000
H	6.667743000	1.020269000	0.345608000
H	6.093648000	-0.318226000	1.353442000
H	6.247163000	-0.534630000	-0.390421000
C	4.736029000	3.246114000	-0.100972000
H	5.819203000	3.135239000	-0.015271000
H	4.518050000	3.729685000	-1.059922000
H	4.400968000	3.929711000	0.688154000
H	-1.540028000	1.674022000	-1.705218000
C	-4.163572000	1.699389000	-0.673580000
C	-5.323426000	2.228718000	-0.088670000
C	-4.287323000	0.903446000	-1.825869000
C	-6.575316000	1.990406000	-0.651116000
H	-5.238401000	2.832862000	0.809672000
C	-5.538004000	0.646708000	-2.372729000
H	-3.401825000	0.468125000	-2.273699000
C	-6.686210000	1.194361000	-1.790582000
H	-7.463292000	2.416603000	-0.194358000
H	-5.622524000	0.019620000	-3.255265000
H	-7.662011000	0.998119000	-2.224729000

styrene-TS1

Sc	-0.937332000	-0.402889000	0.405787000
C	-4.108763000	0.015370000	3.324059000
C	-4.948941000	-0.996752000	3.801637000
H	-5.925609000	-0.739223000	4.197764000
C	-4.528230000	-2.325501000	3.762161000
C	-3.265827000	-2.649695000	3.263627000
H	-2.931413000	-3.683466000	3.263397000
C	-2.395565000	-1.659276000	2.779280000
C	-1.075989000	-1.965167000	2.191904000
H	-0.308853000	-1.212230000	2.442604000
H	-0.682402000	-2.915004000	2.539716000
C	-1.185274000	-2.971958000	0.275804000
H	-0.201535000	-3.417284000	0.372256000
C	-1.440493000	-2.233410000	-0.891777000
H	-0.635506000	-2.166793000	-1.617840000
N	0.896544000	-0.047514000	0.175714000
N	3.053257000	-0.927723000	-0.461255000
N	3.008432000	1.092406000	0.364200000
C	2.184035000	0.026810000	0.037936000
C	4.379262000	-0.455363000	-0.452420000
C	4.353601000	0.798029000	0.071063000
C	2.618060000	-2.199275000	-0.947671000
C	2.100909000	-2.278871000	-2.250889000
C	1.610055000	-3.517893000	-2.679389000
H	1.196948000	-3.614083000	-3.679048000
C	1.658299000	-4.631016000	-1.845434000
C	2.225407000	-4.535766000	-0.574627000
H	2.287136000	-5.421715000	0.047971000
C	2.722721000	-3.318038000	-0.099726000

C	2.115646000	-1.085937000	-3.195624000
H	2.554499000	-0.238305000	-2.661975000
C	0.702379000	-0.669445000	-3.628040000
H	0.104522000	-0.381431000	-2.759126000
H	0.185115000	-1.483396000	-4.148711000
H	0.747157000	0.186809000	-4.309550000
C	3.004571000	-1.371211000	-4.418768000
C	3.346272000	-3.194020000	1.285102000
H	4.070489000	-2.374199000	1.248959000
C	4.106627000	-4.454235000	1.719542000
H	4.833530000	-4.767469000	0.962742000
H	3.430606000	-5.295640000	1.907188000
H	4.646453000	-4.259771000	2.652057000
C	2.289859000	-2.801855000	2.330783000
C	2.483158000	2.350575000	0.787951000
C	2.092650000	2.500729000	2.129774000
C	1.287256000	4.721663000	1.561208000
C	1.481166000	3.705874000	2.495787000
H	1.176955000	3.860381000	3.526934000
C	1.723358000	4.562341000	0.246510000
H	1.589203000	5.373114000	-0.462003000
C	2.332397000	3.373009000	-0.169046000
C	2.788480000	3.181325000	-1.611110000
H	3.517676000	2.367191000	-1.624486000
C	3.485434000	4.425586000	-2.180872000
H	3.902249000	4.201018000	-3.168199000
H	4.302616000	4.759929000	-1.533025000
H	2.791079000	5.263784000	-2.304532000
C	1.626102000	2.739189000	-2.516848000
C	2.394986000	1.431103000	3.168429000

H	2.739862000	0.539022000	2.639107000
C	1.165283000	1.025728000	3.991692000
H	1.426847000	0.223066000	4.689380000
H	0.364186000	0.661108000	3.344670000
H	0.776570000	1.861370000	4.584888000
C	3.537014000	1.899985000	4.088844000
H	2.601253000	-2.189893000	-5.024632000
H	3.071359000	-0.483460000	-5.057381000
H	4.019088000	-1.651071000	-4.115805000
H	2.755843000	-2.647478000	3.310642000
H	1.775525000	-1.882839000	2.040490000
H	1.541074000	-3.595357000	2.436418000
H	4.432138000	2.157789000	3.513417000
H	3.243240000	2.787044000	4.661186000
H	3.803771000	1.111252000	4.800666000
H	1.995875000	2.508784000	-3.522112000
H	1.131379000	1.847998000	-2.121079000
H	0.880576000	3.537007000	-2.612571000
H	0.816531000	5.652614000	1.864133000
H	1.271984000	-5.584392000	-2.193451000
H	-5.177501000	-3.111759000	4.133958000
H	-4.431952000	1.050471000	3.344559000
C	-2.868472000	-0.335121000	2.812189000
O	-2.005401000	0.599157000	2.212273000
C	-2.002571000	1.938687000	2.741434000
H	-1.070227000	2.399738000	2.420230000
H	-2.855876000	2.501966000	2.354312000
H	-2.040078000	1.893476000	3.832082000
C	-4.611919000	2.377892000	-2.851887000
C	-3.314393000	2.034054000	-2.453084000

C	-3.140580000	1.680232000	-1.111549000
C	-4.197603000	1.619171000	-0.211165000
C	-5.479585000	1.958497000	-0.638730000
C	-5.682124000	2.355000000	-1.959805000
H	-4.779931000	2.656311000	-3.888782000
H	-4.017677000	1.289455000	0.804063000
H	-6.311396000	1.907298000	0.056668000
H	-6.675737000	2.627767000	-2.301482000
O	-1.836818000	1.410758000	-0.629527000
C	-1.092020000	2.638942000	-0.394851000
H	-1.657387000	3.278144000	0.285371000
H	-0.136316000	2.346919000	0.033708000
H	-0.933575000	3.153483000	-1.340770000
C	-2.174244000	2.033232000	-3.437764000
H	-1.394259000	1.327092000	-3.146720000
H	-2.532315000	1.755039000	-4.433187000
H	-1.711080000	3.024270000	-3.527584000
C	5.446950000	1.765161000	0.367006000
H	6.411683000	1.348072000	0.070014000
H	5.311780000	2.714636000	-0.163154000
H	5.494709000	1.996457000	1.437666000
C	5.501568000	-1.279929000	-0.980619000
H	6.442307000	-0.729584000	-0.909885000
H	5.616760000	-2.220239000	-0.429722000
H	5.339370000	-1.540561000	-2.033060000
H	-1.991627000	-3.535729000	0.736347000
C	-2.793059000	-1.868448000	-1.330459000
C	-3.012299000	-1.435797000	-2.654589000
C	-3.900876000	-1.905851000	-0.456328000
C	-4.284710000	-1.087158000	-3.091717000

H	-2.173511000	-1.400004000	-3.343687000
C	-5.173478000	-1.554207000	-0.902282000
H	-3.776681000	-2.231814000	0.571617000
C	-5.374721000	-1.144933000	-2.219375000
H	-4.429476000	-0.766884000	-4.119466000
H	-6.009697000	-1.597198000	-0.210267000
H	-6.364865000	-0.862789000	-2.561654000

styrene-INT3

Sc	1.013577000	-0.000705000	0.304450000
C	3.741507000	-2.912066000	1.013326000
C	4.984982000	-3.068921000	1.619798000
H	5.778396000	-3.596265000	1.099907000
C	5.197576000	-2.541863000	2.896071000
C	4.163964000	-1.887628000	3.560350000
H	4.326953000	-1.501135000	4.562812000
C	2.894766000	-1.724809000	2.981452000
C	1.799816000	-1.019689000	3.739864000
H	0.817725000	-1.368307000	3.404900000
H	1.891664000	-1.290522000	4.798394000
C	1.860472000	0.522292000	3.609199000
H	1.182091000	0.932458000	4.365431000
C	1.476943000	1.081745000	2.248850000
H	0.526567000	1.623677000	2.269009000
N	-0.840879000	-0.071114000	-0.062852000
N	-2.837588000	1.281009000	0.102330000
N	-3.079510000	-0.759015000	-0.630280000
C	-2.117176000	0.130762000	-0.180294000
C	-4.205764000	1.101970000	-0.176182000
C	-4.356801000	-0.167411000	-0.633892000
C	-2.246961000	2.437144000	0.699522000

C	-1.790065000	3.471257000	-0.137037000
C	-1.129464000	4.547690000	0.463381000
H	-0.752289000	5.358365000	-0.151316000
C	-0.951146000	4.594822000	1.845180000
C	-1.464161000	3.584902000	2.654884000
H	-1.350393000	3.652389000	3.732574000
C	-2.134136000	2.488479000	2.099472000
C	-1.996857000	3.408296000	-1.643380000
H	-2.804254000	2.694720000	-1.836007000
C	-0.742509000	2.862446000	-2.343779000
H	-0.471293000	1.886140000	-1.932221000
H	0.104477000	3.545197000	-2.208282000
H	-0.915852000	2.749471000	-3.419927000
C	-2.422501000	4.757283000	-2.240520000
C	-2.760193000	1.430935000	2.997563000
H	-3.230383000	0.678681000	2.357130000
C	-3.862829000	2.050503000	3.875124000
H	-4.618710000	2.561927000	3.270237000
H	-3.447807000	2.783659000	4.575420000
H	-4.363963000	1.273288000	4.462372000
C	-1.719569000	0.708015000	3.864109000
C	-2.767893000	-2.102955000	-0.993163000
C	-2.858179000	-3.104509000	-0.009973000
C	-1.941690000	-4.659585000	-1.636123000
C	-2.428689000	-4.390656000	-0.357487000
H	-2.479843000	-5.190355000	0.374805000
C	-1.924446000	-3.661159000	-2.609364000
H	-1.592915000	-3.899055000	-3.615703000
C	-2.360707000	-2.364849000	-2.312473000
C	-2.441041000	-1.288835000	-3.386780000

H	-3.002663000	-0.449168000	-2.966620000
C	-3.208597000	-1.783996000	-4.623314000
H	-3.344716000	-0.963503000	-5.335956000
H	-4.197231000	-2.168541000	-4.351319000
H	-2.670288000	-2.584807000	-5.142062000
C	-1.056423000	-0.749828000	-3.772400000
C	-3.409642000	-2.798023000	1.376642000
H	-3.934508000	-1.839962000	1.316393000
C	-2.287769000	-2.624520000	2.414038000
H	-2.707469000	-2.329245000	3.381458000
H	-1.578654000	-1.853338000	2.099244000
H	-1.743229000	-3.564513000	2.560966000
C	-4.429381000	-3.850008000	1.839115000
H	-1.622471000	5.502851000	-2.177896000
H	-2.672332000	4.636093000	-3.299916000
H	-3.300057000	5.162968000	-1.726241000
H	-2.206878000	-0.040122000	4.498607000
H	-0.981283000	0.200371000	3.240400000
H	-1.190710000	1.407412000	4.520984000
H	-5.226207000	-3.986565000	1.100383000
H	-3.960814000	-4.825235000	2.010615000
H	-4.888013000	-3.537792000	2.783256000
H	-1.151540000	0.057873000	-4.506511000
H	-0.539082000	-0.355866000	-2.894416000
H	-0.441132000	-1.538583000	-4.221701000
H	-1.607082000	-5.662477000	-1.885844000
H	-0.427918000	5.434064000	2.293507000
H	6.163243000	-2.656598000	3.378224000
H	3.555848000	-3.310940000	0.021565000
C	2.729991000	-2.231087000	1.689773000

O	1.495900000	-2.028460000	1.031877000
C	0.699931000	-3.221201000	0.816017000
H	-0.223723000	-2.889223000	0.349496000
H	1.237071000	-3.912211000	0.162621000
H	0.498788000	-3.691396000	1.779978000
C	4.645181000	1.105858000	-3.667169000
C	3.392822000	0.689801000	-3.199808000
C	3.386084000	-0.119428000	-2.059802000
C	4.544048000	-0.497985000	-1.396502000
C	5.777626000	-0.070092000	-1.886461000
C	5.826165000	0.729255000	-3.027175000
H	4.687288000	1.739885000	-4.548373000
H	4.478619000	-1.101954000	-0.499924000
H	6.690001000	-0.357961000	-1.373737000
H	6.781525000	1.066502000	-3.417149000
O	2.141357000	-0.581674000	-1.559495000
C	1.745026000	-1.845491000	-2.146926000
H	2.428425000	-2.630874000	-1.815392000
H	0.725392000	-2.048534000	-1.820467000
H	1.773582000	-1.763034000	-3.233938000
C	2.119549000	1.106191000	-3.885190000
H	1.391210000	1.491281000	-3.168237000
H	2.319217000	1.885917000	-4.624774000
H	1.641588000	0.270350000	-4.409770000
C	-5.554244000	-0.919889000	-1.099857000
H	-6.446726000	-0.293954000	-1.032137000
H	-5.445777000	-1.243740000	-2.142034000
H	-5.725852000	-1.820027000	-0.497708000
C	-5.188778000	2.201402000	0.028103000
H	-6.192537000	1.869260000	-0.246172000

H	-5.213939000	2.530406000	1.072858000
H	-4.943613000	3.079526000	-0.581088000
H	2.864328000	0.851700000	3.906156000
C	2.434607000	1.743027000	1.387825000
C	1.933571000	2.411972000	0.229406000
C	3.845789000	1.582719000	1.464979000
C	2.797087000	2.965287000	-0.729501000
H	0.869792000	2.650132000	0.181926000
C	4.681671000	2.144968000	0.514109000
H	4.274095000	1.036195000	2.298923000
C	4.170634000	2.846206000	-0.590327000
H	2.376997000	3.503449000	-1.574347000
H	5.756819000	2.031120000	0.620834000
H	4.841934000	3.265729000	-1.330750000

styrene-TS1''

Sc	0.822089000	-0.002445000	0.323793000
C	3.218483000	3.612913000	-0.073846000
C	4.402335000	3.821780000	-0.786516000
H	5.040919000	4.661166000	-0.530780000
C	4.756199000	2.947419000	-1.813963000
C	3.923081000	1.882684000	-2.151160000
H	4.197983000	1.218602000	-2.962862000
C	2.719669000	1.647450000	-1.466249000
C	1.800610000	0.536602000	-1.833360000
H	0.739992000	0.840379000	-1.762429000
H	1.941527000	0.257995000	-2.872990000
C	2.293697000	-1.433664000	-1.359496000
H	1.743957000	-1.761691000	-2.236477000
C	1.790604000	-1.953938000	-0.108374000
H	2.547199000	-2.239317000	0.619915000

H	0.977649000	-2.674654000	-0.204169000
N	-1.054500000	-0.030245000	0.204350000
N	-2.951670000	-1.394088000	-0.358096000
N	-3.269301000	0.766325000	-0.295985000
C	-2.296603000	-0.200723000	-0.116539000
C	-4.304337000	-1.170245000	-0.666989000
C	-4.505773000	0.173874000	-0.631080000
C	-2.262174000	-2.645995000	-0.380277000
C	-2.007468000	-3.298415000	0.836245000
C	-1.260930000	-4.480970000	0.796032000
H	-1.047011000	-5.010624000	1.719647000
C	-0.793848000	-4.989914000	-0.413206000
C	-1.076607000	-4.331942000	-1.609067000
H	-0.714052000	-4.745436000	-2.544713000
C	-1.819181000	-3.147066000	-1.617970000
C	-2.527210000	-2.756382000	2.157713000
H	-3.062454000	-1.825223000	1.951472000
C	-1.375258000	-2.419311000	3.116118000
H	-0.673930000	-1.729568000	2.640019000
H	-0.822584000	-3.318789000	3.409671000
H	-1.760756000	-1.951767000	4.029741000
C	-3.524520000	-3.732020000	2.804667000
C	-2.103212000	-2.410583000	-2.919811000
H	-2.893862000	-1.679107000	-2.729128000
C	-2.602492000	-3.345384000	-4.031544000
H	-3.474542000	-3.922604000	-3.706397000
H	-1.830129000	-4.055850000	-4.345216000
H	-2.888361000	-2.762171000	-4.913379000
C	-0.865473000	-1.619398000	-3.374702000
C	-3.031891000	2.169605000	-0.149387000

C	-2.386728000	2.863714000	-1.190765000
C	-2.654896000	4.897551000	0.112918000
C	-2.217960000	4.244268000	-1.037598000
H	-1.739040000	4.816995000	-1.823918000
C	-3.259735000	4.181445000	1.143135000
H	-3.586661000	4.703804000	2.035295000
C	-3.462623000	2.800986000	1.032361000
C	-4.069757000	1.990427000	2.170693000
H	-4.626389000	1.156901000	1.731856000
C	-5.048857000	2.786210000	3.042286000
H	-5.543222000	2.115801000	3.752687000
H	-5.822172000	3.272539000	2.438386000
H	-4.540532000	3.559925000	3.628309000
C	-2.949654000	1.369048000	3.026240000
C	-1.890750000	2.132940000	-2.432240000
H	-1.523551000	1.157837000	-2.099405000
C	-0.720544000	2.845144000	-3.124696000
H	-0.303232000	2.197732000	-3.902838000
H	0.084554000	3.088458000	-2.423047000
H	-1.037182000	3.773214000	-3.613110000
C	-3.028377000	1.878713000	-3.438013000
H	-3.046056000	-4.685510000	3.054222000
H	-3.930191000	-3.308404000	3.730141000
H	-4.361806000	-3.946532000	2.131885000
H	-1.089249000	-1.028596000	-4.270334000
H	-0.535863000	-0.939137000	-2.585256000
H	-0.036758000	-2.296449000	-3.613746000
H	-3.815124000	1.254117000	-3.007647000
H	-3.477469000	2.823215000	-3.765230000
H	-2.640807000	1.363687000	-4.324337000

H	-3.370894000	0.737366000	3.816710000
H	-2.286643000	0.757187000	2.407517000
H	-2.353874000	2.157313000	3.503952000
H	-2.521227000	5.971395000	0.207974000
H	-0.213205000	-5.907589000	-0.426235000
H	5.678234000	3.100633000	-2.365458000
H	2.936915000	4.278086000	0.735406000
C	2.420720000	2.527729000	-0.411429000
O	1.278288000	2.186480000	0.325100000
C	0.492889000	3.225104000	0.944610000
H	-0.477721000	2.778602000	1.155267000
H	0.975595000	3.562679000	1.866487000
H	0.372913000	4.055677000	0.248210000
C	4.645113000	-1.492463000	3.328285000
C	3.259699000	-1.354141000	3.178568000
C	2.804303000	-0.115072000	2.713284000
C	3.655191000	0.946514000	2.425664000
C	5.030539000	0.780161000	2.591034000
C	5.522494000	-0.444608000	3.040427000
H	5.038596000	-2.443391000	3.675394000
H	3.248301000	1.881265000	2.060010000
H	5.703731000	1.598080000	2.356530000
H	6.590767000	-0.589206000	3.167441000
O	1.419772000	0.055768000	2.474351000
C	0.690167000	0.644989000	3.575931000
H	1.093787000	1.637647000	3.792922000
H	-0.348008000	0.710714000	3.259122000
H	0.779818000	0.001993000	4.454140000
C	2.309319000	-2.480031000	3.490408000
H	1.644910000	-2.688088000	2.647392000

H	2.861262000	-3.392362000	3.729480000
H	1.671104000	-2.242766000	4.349816000
C	-5.729701000	0.989631000	-0.871548000
H	-6.058835000	1.516703000	0.031520000
H	-5.560055000	1.748856000	-1.642827000
H	-6.549466000	0.348317000	-1.202996000
C	-5.231558000	-2.302297000	-0.942672000
H	-6.240268000	-1.931204000	-1.136604000
H	-4.911053000	-2.886394000	-1.812991000
H	-5.280488000	-2.991410000	-0.091211000
C	3.752976000	-1.311574000	-1.603387000
C	4.260332000	-1.518173000	-2.893418000
C	4.644398000	-0.968262000	-0.578475000
C	5.624874000	-1.392678000	-3.152804000
H	3.579374000	-1.785546000	-3.698402000
C	6.005742000	-0.833456000	-0.836583000
H	4.275712000	-0.798039000	0.425621000
C	6.502241000	-1.044233000	-2.124225000
H	6.002340000	-1.568680000	-4.155835000
H	6.677620000	-0.560881000	-0.028071000
H	7.564567000	-0.942252000	-2.324620000

styrene-INT3''

Sc	0.536946000	0.780120000	-0.225131000
C	2.765818000	2.861956000	-2.777521000
C	4.127475000	3.094487000	-2.957236000
H	4.486587000	4.101597000	-3.142597000
C	5.020954000	2.021287000	-2.889811000
C	4.554855000	0.726877000	-2.668758000
H	5.253733000	-0.101731000	-2.633069000
C	3.187338000	0.456226000	-2.493326000

C	2.683059000	-0.949383000	-2.284061000
H	1.631699000	-1.000138000	-2.582927000
H	3.231546000	-1.617046000	-2.957398000
C	2.787313000	-1.514443000	-0.827477000
H	2.175104000	-2.421537000	-0.854499000
C	2.167955000	-0.591713000	0.229102000
H	1.948654000	-1.182712000	1.128051000
N	-1.233013000	0.134606000	-0.140482000
N	-2.280062000	-1.746546000	0.944986000
N	-3.601263000	-0.248298000	0.063299000
C	-2.264681000	-0.552216000	0.243910000
C	-3.601037000	-2.164859000	1.190921000
C	-4.423803000	-1.228842000	0.648793000
C	-1.098015000	-2.488393000	1.262131000
C	-0.494034000	-2.302544000	2.518822000
C	0.680684000	-3.011326000	2.787166000
H	1.177363000	-2.887751000	3.743368000
C	1.226332000	-3.877147000	1.840911000
C	0.593893000	-4.063200000	0.615788000
H	1.018143000	-4.754190000	-0.106563000
C	-0.583774000	-3.375469000	0.302176000
C	-1.083138000	-1.334525000	3.534093000
H	-2.156915000	-1.254039000	3.332406000
C	-0.485413000	0.071998000	3.349451000
H	-0.709443000	0.451977000	2.346818000
H	0.602635000	0.055220000	3.486117000
H	-0.910206000	0.770912000	4.078409000
C	-0.921997000	-1.807438000	4.985510000
C	-1.267284000	-3.596145000	-1.038243000
H	-2.197238000	-3.019948000	-1.044567000

C	-1.638469000	-5.073362000	-1.248444000
H	-2.268865000	-5.445106000	-0.433657000
H	-0.748045000	-5.709527000	-1.296655000
H	-2.187402000	-5.197726000	-2.188281000
C	-0.397985000	-3.071682000	-2.191406000
C	-4.043345000	0.913601000	-0.642768000
C	-4.371621000	0.789690000	-2.005302000
C	-4.773620000	3.184930000	-2.043897000
C	-4.731616000	1.952336000	-2.693774000
H	-4.989754000	1.895276000	-3.746069000
C	-4.476580000	3.273371000	-0.686742000
H	-4.540038000	4.234372000	-0.184631000
C	-4.113021000	2.136060000	0.043468000
C	-3.823942000	2.235624000	1.532504000
H	-3.622410000	1.226912000	1.904973000
C	-5.036486000	2.781627000	2.304680000
H	-4.834648000	2.782240000	3.381477000
H	-5.927612000	2.171027000	2.124882000
H	-5.273019000	3.809624000	2.009014000
C	-2.567807000	3.077718000	1.800042000
C	-4.306803000	-0.557947000	-2.710296000
H	-4.387606000	-1.338103000	-1.946838000
C	-2.941218000	-0.742387000	-3.393331000
H	-2.874262000	-1.729505000	-3.864130000
H	-2.130988000	-0.651211000	-2.664781000
H	-2.797230000	0.013557000	-4.175388000
C	-5.456902000	-0.771119000	-3.704602000
H	0.124505000	-1.787386000	5.308641000
H	-1.481879000	-1.148541000	5.657532000
H	-1.295936000	-2.827974000	5.117737000

H	-0.908201000	-3.202757000	-3.151627000
H	-0.191908000	-2.006718000	-2.051994000
H	0.559115000	-3.602373000	-2.243367000
H	-6.430872000	-0.603556000	-3.232806000
H	-5.382048000	-0.101274000	-4.568132000
H	-5.434419000	-1.796929000	-4.087221000
H	-2.354389000	3.120185000	2.873848000
H	-1.706928000	2.633833000	1.292299000
H	-2.691741000	4.106499000	1.441651000
H	-5.058256000	4.076545000	-2.595229000
H	2.146074000	-4.410228000	2.061910000
H	6.084237000	2.192823000	-3.025406000
H	2.045261000	3.673583000	-2.811267000
C	2.328555000	1.560806000	-2.538242000
O	0.946897000	1.372036000	-2.270657000
C	0.063870000	1.356080000	-3.422510000
H	-0.947304000	1.287433000	-3.025754000
H	0.201463000	2.277958000	-3.991545000
H	0.296001000	0.486516000	-4.041948000
C	3.381165000	3.104461000	3.498732000
C	2.178009000	3.078021000	2.778370000
C	2.283066000	2.868935000	1.400934000
C	3.501454000	2.719442000	0.744969000
C	4.678602000	2.755519000	1.488806000
C	4.614568000	2.942796000	2.870535000
H	3.338988000	3.254236000	4.573927000
H	3.524024000	2.563298000	-0.326146000
H	5.633725000	2.631957000	0.988650000
H	5.525556000	2.964161000	3.460236000
O	1.096040000	2.756463000	0.622974000

C	0.568807000	4.017663000	0.143859000
H	1.324439000	4.509957000	-0.472680000
H	-0.320844000	3.786829000	-0.444019000
H	0.297887000	4.646259000	0.993978000
C	0.855589000	3.296195000	3.465548000
H	0.038163000	2.797015000	2.944894000
H	0.886994000	2.921575000	4.492156000
H	0.612682000	4.365569000	3.517877000
C	-5.908021000	-1.111440000	0.620364000
H	-6.366074000	-1.956649000	1.138815000
H	-6.245462000	-0.189620000	1.109063000
H	-6.294850000	-1.092934000	-0.405280000
C	-3.887812000	-3.426794000	1.927486000
H	-4.965684000	-3.574154000	2.025047000
H	-3.471225000	-4.297543000	1.407959000
H	-3.453369000	-3.414069000	2.934104000
H	2.910246000	0.160871000	0.547977000
C	4.211899000	-1.968859000	-0.534499000
C	4.592319000	-3.277600000	-0.860570000
C	5.181219000	-1.119140000	0.013705000
C	5.895685000	-3.727480000	-0.652165000
H	3.851384000	-3.953741000	-1.282970000
C	6.488933000	-1.560958000	0.218994000
H	4.915367000	-0.103972000	0.291101000
C	6.852393000	-2.866639000	-0.112545000
H	6.163077000	-4.749235000	-0.906850000
H	7.224637000	-0.884786000	0.646467000
H	7.868469000	-3.211921000	0.054055000