

A DFT Study on Sc-Catalyzed Diastereoselective Cyclization of 2-picoline with 1,5-hexadiene: Mechanism and Origins of Regio- and Stereoselectivity

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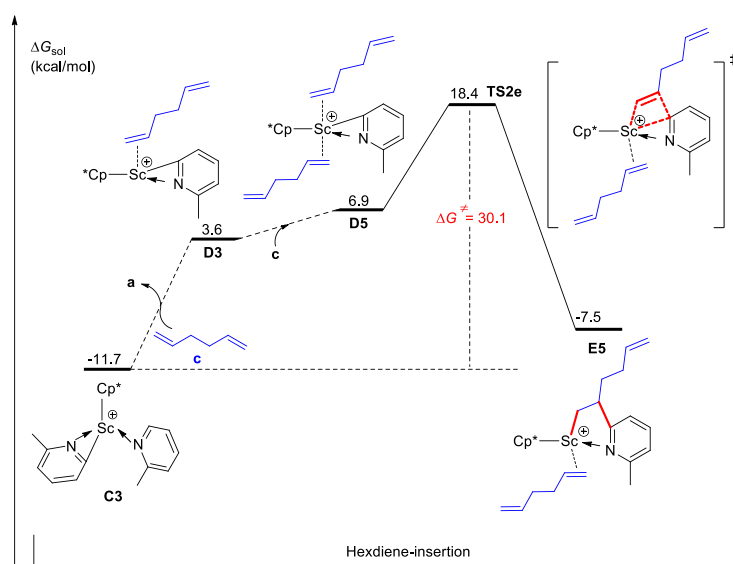


Figure S1. The computed energy profiles for 1,5-hexadiene insertion based on species **D1** with a coordinated 1,5-hexadiene.

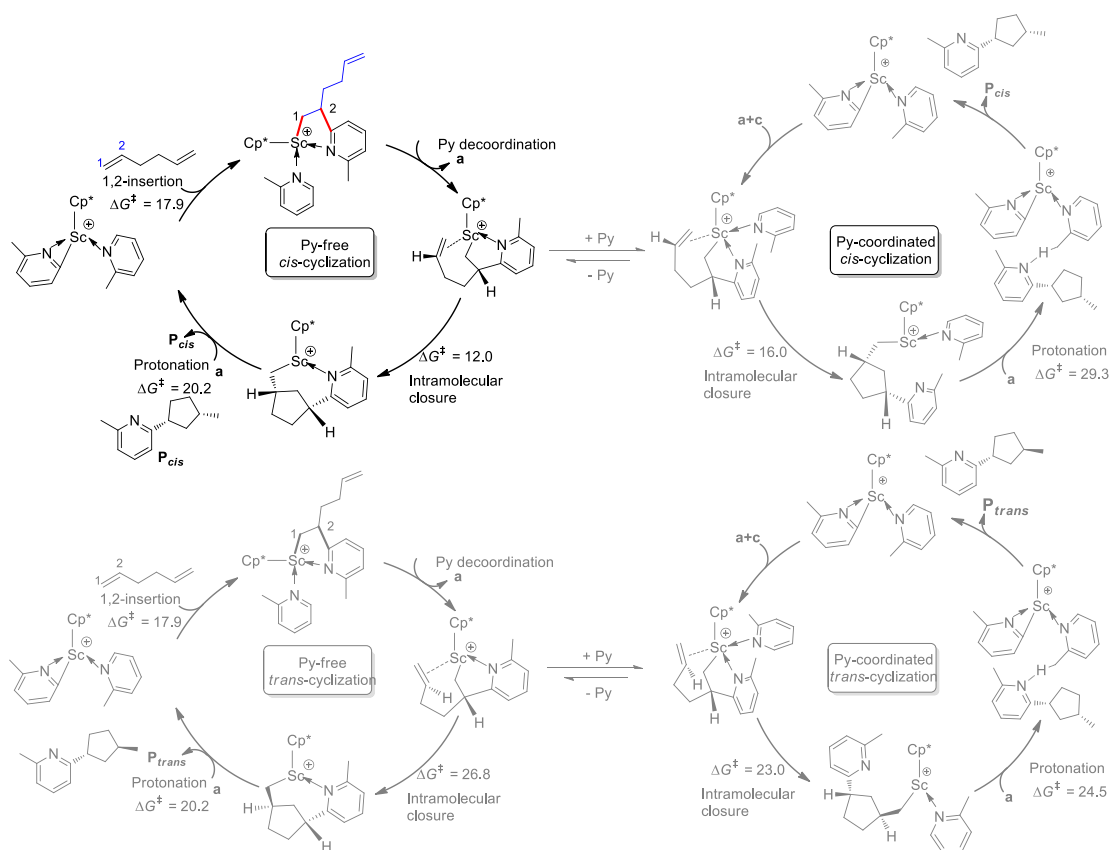


Figure S2. The computed energy profiles for *cis*-cyclization and *trans*-cyclization processes based on 1,5-hexadiene insertion intermediate.

Table S1 Computed free energy ΔG (kcal/mol) for all the species including solution-phase single point energies, the gas phase zero-point correction, thermal correction to enthalpy, thermal correction to Gibbs free energy

Structural name	SCF_D	Zero-point correction	Thermal correction to Enthalpy	Thermal correction to Gibbs Free Energy	ΔG (kcal/mol)	ΔG^a (kcal/mol)
1	-841.2740312	0.416149	0.441294	0.362838		
a	-287.455585	0.116808	0.123831	0.086328	0.0	0.0
c	-234.4746958	0.142728	0.15103	0.111134		
A1	-1128.775138	0.535794	0.568	0.475131	-12.3	-14.2
TS1a	-1128.73449	0.53184	0.563563	0.472149	11.4	9.5
B1	-1128.763656	0.535831	0.568549	0.473538	-6.1	-8.0
C1	-723.4147717	0.330278	0.352232	0.278763		
b	-405.3124902	0.202609	0.213438	0.168167	0.1	0.1
A2	-1128.775103	0.535153	0.567715	0.472516	-13.9	-15.8
TS1b	-1128.735015	0.532514	0.563544	0.474121	12.3	10.4
B2	-1128.764134	0.535569	0.567822	0.474446	-5.8	-7.7
C2	-723.415195	0.329696	0.351184	0.276601	-1.5	-1.5
A3	-1416.256088	0.65574	0.694787	0.587251	-12.0	-15.8
TS1c	-1416.212011	0.651059	0.68992	0.582483	12.7	8.9
B3	-1416.231362	0.652504	0.69415	0.571892	-6.1	-9.9
C3	-1010.912364	0.449343	0.478644	0.38839	-11.7	-13.6
A4	-1416.253937	0.655947	0.694922	0.587571	-10.5	-14.3
TS1d	-1416.201456	0.650776	0.689483	0.581885	18.9	15.1
B4	-1416.238509	0.652778	0.693612	0.575065	-8.6	-12.4
C4	-1010.915246	0.448695	0.477618	0.388736	-13.3	-15.2
D1	-1245.399795	0.594728	0.632364	0.524099	-4.2	-8.0
TS2a	-1245.38687	0.595136	0.631113	0.527752	6.2	22.4
E1	-1245.43191	0.596081	0.632507	0.528025	-21.9	-25.7
D2	-1245.395505	0.594462	0.632373	0.522404	-2.6	-6.4
TS2b	-1245.383536	0.594619	0.630988	0.527038	7.8	4.0
E2	-1245.431343	0.596808	0.63303	0.529326	-20.8	-24.6
D3	-957.9035714	0.474614	0.50551	0.409673	3.6	1.7
TS2c	-957.8856285	0.47474	0.504046	0.413916	17.6	15.7
E3	-957.9347774	0.475991	0.505554	0.414583	-12.9	-14.8
D4	-957.9033762	0.474637	0.505314	0.411799	5.1	3.2
TS2d	-957.8833209	0.474469	0.503892	0.414416	19.3	17.4
E4	-957.9330353	0.476528	0.505866	0.417174	-10.1	-12.0
F1	-1245.433461	0.596015	0.632675	0.527001	-23.5	-27.3
TS3a	-1245.395868	0.592558	0.62844	0.524956	-1.2	-5.0
G1	-1245.431665	0.597224	0.633585	0.528484	-21.5	-25.3

P_{mono}	-521.9758354	0.263924	0.278817	0.221585	-25.1	-28.9
F2	-1532.903503	0.716223	0.759724	0.639103	-16.4	-22.1
TS3b	-1532.863641	0.712513	0.755382	0.637482	7.6	1.9
G2	-1532.920631	0.717048	0.760803	0.641232	-25.9	-31.6
H1	-1245.429658	0.598381	0.633322	0.535222	-16.0	-19.8
TS4a	-1245.414793	0.598521	0.632246	0.536366	-5.9	-9.7
J1	-1245.426077	0.598655	0.634009	0.530328	-16.8	-20.6
H2	-1245.430943	0.595822	0.632396	0.52607	-22.5	-26.3
TS4b	-1245.397317	0.595753	0.630937	0.529164	0.5	-3.3
J2	-1245.424945	0.598542	0.633941	0.530262	-16.2	-20.0
H3	-957.9484622	0.477874	0.506121	0.422053	-16.8	-18.7
TS4c	-957.9383673	0.478326	0.50537	0.422894	-9.9	-11.8
J3	-957.9536195	0.480157	0.507698	0.424301	-18.6	-20.5
H4	-957.9447328	0.477982	0.506368	0.421569	-14.7	-16.6
TS4d	-957.9143371	0.477899	0.50512	0.422523	4.9	3.0
J4	-957.945136	0.480947	0.508018	0.426561	-11.9	-13.8
K1_{cis}	-1245.444822	0.600277	0.634798	0.536848	-24.5	-28.3
TS5a_{cis}	-1245.41035	0.59692	0.630733	0.534622	-4.3	-8.1
L1_{cis}	-1245.463311	0.600758	0.635785	0.535425	-37.0	-40.8
P_{cis}	-522.0036133	0.267134	0.280754	0.226551	-39.4	-43.2
K2_{trans}	-1245.43409	0.600322	0.634829	0.535848	-18.4	-22.2
TS5b_{trans}	-1245.400686	0.59716	0.630875	0.534641	1.8	-2.0
L2_{trans}	-1245.461814	0.60023	0.635538	0.533679	-37.1	-40.9
P_{trans}	-522.0039091	0.267199	0.280718	0.225782	-40.1	-43.9
K3_{cis}	-1532.92197	0.717672	0.760763	0.639038	-28.1	-33.8
TS5c_{cis}	-1532.875212	0.71491	0.757079	0.638908	1.2	-4.5
L3_{cis}	-1532.92584	0.717206	0.761394	0.632521	-34.6	-40.3
K4_{trans}	-1532.924438	0.718172	0.760813	0.641965	-27.8	-33.5
TS5d_{trans}	-1532.884541	0.715102	0.756893	0.641036	-3.3	-9.0
L4_{trans}	-1532.925819	0.717227	0.761536	0.631308	-35.3	-41.0
D5	-1192.397097	0.619652	0.659	0.544843	6.9	3.1
TS2e	-1192.381107	0.619609	0.657611	0.547166	18.4	14.6
E5	-1192.422233	0.620704	0.659042	0.546993	-7.5	-11.3

ΔG^a : A free energy of solvation calculated was added to the thermodynamic corrections for Gibbs free energy and 1.9 kcal/mol (the standard state change from 1 atm (1 mol of an ideal gas) to 1 mol/L (1 mol/L in toluene solution) at 298.15 K) to get the final solution-phase Gibbs free energies for all the species.

DFT Optimized Cartesian Coordinates of All Structures

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

48 (the number of atoms involved in the molecule)

1, $E_{\text{SCRF}} = -841.2740312$ a.u.

Sc	0.272897000	0.423093000	-0.336293000
N	-1.579801000	1.760195000	-0.412293000
C	-0.791004000	-0.477306000	-2.028593000
H	-0.899003000	0.337294000	-2.753993000
H	-0.542706000	-1.407206000	-2.538193000
C	-1.852604000	-0.615804000	-1.025693000
C	-2.210703000	0.466396000	-0.155393000
C	-3.109203000	0.275197000	0.909107000
H	-3.397802000	1.111198000	1.538107000
C	-3.651305000	-0.976502000	1.154007000
H	-4.350905000	-1.111301000	1.973207000
C	-3.297307000	-2.057502000	0.335807000
H	-3.723308000	-3.039602000	0.520807000
C	-2.415506000	-1.879604000	-0.715493000
H	-2.157508000	-2.719104000	-1.355193000
C	-1.549200000	2.677095000	0.744407000
H	-2.546699000	3.058497000	0.996307000
H	-0.915198000	3.533194000	0.495507000
H	-1.142800000	2.175995000	1.630807000
C	-2.143900000	2.467496000	-1.586393000
H	-2.250001000	1.781596000	-2.426493000
H	-1.481099000	3.289895000	-1.871593000
H	-3.133799000	2.871897000	-1.340793000
C	2.630797000	0.617289000	-0.009593000
C	2.035097000	0.429790000	1.276207000
C	1.458195000	-0.879609000	1.305807000
C	1.719394000	-1.505010000	0.046907000
C	2.437096000	-0.581911000	-0.767493000
C	2.088698000	1.398990000	2.424707000
H	1.242198000	1.282791000	3.110007000
H	2.114300000	2.443190000	2.094107000
H	2.997198000	1.236489000	3.019307000
C	0.801094000	-1.530308000	2.491107000
H	1.537793000	-2.096409000	3.075907000
H	0.016893000	-2.234607000	2.195207000
H	0.351295000	-0.799308000	3.170907000
C	1.379992000	-2.920009000	-0.315593000
H	1.225492000	-3.042009000	-1.391893000
H	0.478692000	-3.271208000	0.196207000
H	2.197291000	-3.594110000	-0.027593000
C	2.976895000	-0.850511000	-2.141693000
H	3.986595000	-1.277513000	-2.081393000

H	3.052997000	0.060488000	-2.744393000
H	2.355494000	-1.561911000	-2.693393000
C	3.400899000	1.828188000	-0.460493000
H	4.469499000	1.708886000	-0.238693000
H	3.322299000	1.994788000	-1.540593000
H	3.076000000	2.743588000	0.046207000

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a, $E_{(\text{SCRF})} = -287.455585$ a.u.

C	0.875227000	0.007351000	-0.000860000
C	0.156539000	1.208643000	-0.000598000
C	-1.234775000	1.167678000	0.000216000
C	-1.868918000	-0.071614000	0.000605000
C	-1.068474000	-1.212537000	0.000080000
N	0.265495000	-1.187511000	-0.000704000
H	-1.813514000	2.088263000	0.000290000
H	0.684528000	2.158577000	-0.001123000
H	-2.951885000	-0.155504000	0.001000000
C	2.380035000	-0.012426000	0.000534000
H	2.801800000	0.996940000	-0.022390000
H	2.752680000	-0.526402000	0.893900000
H	2.753512000	-0.568475000	-0.866556000
H	-1.523392000	-2.203393000	-0.000057000

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Al, $E_{(\text{SCRF})} = -1128.775138$ a.u.

Sc	-0.041213000	0.042701000	-0.062586000
N	0.965980000	-1.906754000	0.731179000
C	0.786488000	-0.781504000	-1.931027000
H	0.209298000	-1.703532000	-2.089996000
H	0.892713000	-0.264817000	-2.887248000
C	2.094650000	-0.999655000	-1.273277000
C	2.204097000	-1.519929000	0.047054000
C	3.452001000	-1.650795000	0.671614000
H	3.526251000	-2.072920000	1.668057000
C	4.612531000	-1.253862000	0.022057000
H	5.573759000	-1.368170000	0.514014000
C	4.531226000	-0.717519000	-1.266351000
H	5.434061000	-0.411049000	-1.787489000
C	3.299572000	-0.592083000	-1.889410000
H	3.244805000	-0.198013000	-2.900861000
C	1.077275000	-1.934305000	2.202214000
H	1.708423000	-2.762490000	2.549837000
H	0.081737000	-2.074864000	2.630070000
H	1.496747000	-0.994458000	2.569852000
C	0.472143000	-3.224855000	0.267870000
H	0.420327000	-3.251532000	-0.820337000
H	-0.525618000	-3.406675000	0.677826000
H	1.149765000	-4.020707000	0.603856000
C	-1.109984000	2.131639000	0.748815000
C	0.044484000	1.892063000	1.557934000
C	1.196203000	1.993418000	0.720627000

C	0.752344000	2.291351000	-0.606131000
C	-0.669015000	2.375174000	-0.583789000
C	0.054888000	1.757271000	3.055560000
H	0.957356000	1.257587000	3.421610000
H	-0.810977000	1.207809000	3.442159000
H	0.032175000	2.747701000	3.529352000
C	2.629332000	1.967711000	1.169130000
H	2.983621000	2.988018000	1.368594000
H	3.291331000	1.535264000	0.413142000
H	2.767537000	1.397257000	2.092875000
C	1.634452000	2.630028000	-1.770018000
H	1.148484000	2.420090000	-2.727737000
H	2.576473000	2.075071000	-1.744283000
H	1.885573000	3.699280000	-1.761749000
C	-1.541941000	2.758866000	-1.742864000
H	-1.599685000	3.851370000	-1.838872000
H	-2.568238000	2.396328000	-1.624117000
H	-1.156399000	2.377715000	-2.694963000
C	-2.518761000	2.291218000	1.242926000
H	-2.752343000	3.353627000	1.392784000
H	-3.259163000	1.900188000	0.536450000
H	-2.678888000	1.796762000	2.205969000
C	-3.095047000	-1.147552000	0.558071000
C	-4.389132000	-1.524069000	0.191442000
C	-4.774593000	-1.476651000	-1.142797000
C	-3.850725000	-1.047400000	-2.093690000
C	-2.583278000	-0.689346000	-1.661903000
N	-2.201743000	-0.733436000	-0.367542000
H	-5.779383000	-1.767214000	-1.435842000
H	-5.084566000	-1.850571000	0.958731000
H	-4.101432000	-0.989358000	-3.147573000
H	-1.829949000	-0.351325000	-2.367984000
C	-2.655698000	-1.225511000	1.990981000
H	-3.478086000	-0.979238000	2.668978000
H	-2.326711000	-2.241973000	2.242002000
H	-1.834256000	-0.532789000	2.201507000

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TS1a, $E_{\text{(SCRF)}} = -1128.73449$ a.u., IF = $i1304.8009$ cm⁻¹

Sc	-0.067482000	0.045806000	-0.032742000
N	0.823871000	-2.024298000	0.539291000
C	0.867847000	-0.765231000	-2.089552000
H	0.587161000	-1.715374000	-2.563728000
H	1.053679000	-0.046894000	-2.893782000
C	2.099319000	-0.919716000	-1.248268000
C	2.098041000	-1.558071000	0.020718000
C	3.286759000	-1.698197000	0.752201000
H	3.280503000	-2.204155000	1.711898000
C	4.485649000	-1.211980000	0.250912000
H	5.400580000	-1.341099000	0.821523000
C	4.507973000	-0.566594000	-0.988417000

H	5.443341000	-0.189106000	-1.391625000
C	3.334228000	-0.420932000	-1.712385000
H	3.359165000	0.060182000	-2.686392000
C	0.762413000	-2.165378000	2.004076000
H	1.344671000	-3.024663000	2.362889000
H	-0.280674000	-2.319501000	2.293002000
H	1.138575000	-1.260799000	2.491297000
C	0.360058000	-3.278762000	-0.090096000
H	0.406207000	-3.202869000	-1.175802000
H	-0.674608000	-3.468398000	0.206417000
H	0.990002000	-4.119773000	0.229017000
C	-1.175572000	2.096388000	0.769940000
C	-0.088029000	1.810210000	1.650151000
C	1.126447000	1.948460000	0.911829000
C	0.784682000	2.308959000	-0.428120000
C	-0.636902000	2.402679000	-0.511858000
C	-0.202166000	1.553809000	3.127004000
H	0.670562000	1.027166000	3.526885000
H	-1.093120000	0.971099000	3.386794000
H	-0.275155000	2.501140000	3.677534000
C	2.518651000	1.895020000	1.472510000
H	2.865114000	2.905166000	1.729247000
H	3.236714000	1.476841000	0.760843000
H	2.575970000	1.299439000	2.389341000
C	1.748398000	2.728652000	-1.499117000
H	1.398263000	2.465753000	-2.503423000
H	2.735869000	2.281032000	-1.358314000
H	1.882151000	3.818732000	-1.485212000
C	-1.407600000	2.889833000	-1.703783000
H	-1.462941000	3.986698000	-1.704276000
H	-2.435309000	2.514708000	-1.712183000
H	-0.935910000	2.593737000	-2.646771000
C	-2.620849000	2.192822000	1.158528000
H	-2.876749000	3.223012000	1.439651000
H	-3.288340000	1.908251000	0.338827000
H	-2.859425000	1.559600000	2.018711000
C	-3.269280000	-1.286310000	0.444250000
C	-4.319378000	-1.412469000	-0.467946000
C	-4.126893000	-1.064249000	-1.804744000
C	-2.883271000	-0.593793000	-2.225431000
C	-1.872532000	-0.490047000	-1.273773000
N	-2.077059000	-0.834804000	0.009116000
H	-4.947777000	-1.157776000	-2.511187000
H	-5.283421000	-1.776914000	-0.126229000
H	-2.707709000	-0.315495000	-3.260433000
H	-0.528059000	-0.513183000	-1.764455000
C	-3.410427000	-1.659977000	1.889733000
H	-4.449842000	-1.584498000	2.220275000
H	-3.090129000	-2.696904000	2.055230000
H	-2.795324000	-1.014134000	2.523008000

B1, $E_{(\text{SCRF})} = -1128.763656$ a.u.

Sc	-0.323888000	0.096754000	-0.045394000
N	1.060922000	-1.682437000	0.612725000
C	1.645482000	-1.015093000	-2.235447000
H	1.711764000	-1.955626000	-2.798965000
H	1.817894000	-0.204563000	-2.949027000
C	2.673297000	-0.976144000	-1.128867000
C	2.419844000	-1.322617000	0.215046000
C	3.462844000	-1.309978000	1.148284000
H	3.281856000	-1.587727000	2.180371000
C	4.752942000	-0.948856000	0.772031000
H	5.546995000	-0.948047000	1.512869000
C	5.015317000	-0.595796000	-0.548494000
H	6.017193000	-0.310200000	-0.854895000
C	3.981106000	-0.613710000	-1.477872000
H	4.185675000	-0.345043000	-2.511715000
C	0.825429000	-1.661600000	2.071095000
H	1.357038000	-2.470554000	2.589309000
H	-0.245411000	-1.801223000	2.251381000
H	1.142306000	-0.705577000	2.498015000
C	0.679345000	-3.023321000	0.099582000
H	0.811952000	-3.073153000	-0.980579000
H	-0.371864000	-3.211703000	0.331485000
H	1.302570000	-3.796272000	0.567656000
C	-1.504419000	2.183157000	0.454172000
C	-0.458498000	2.042964000	1.414794000
C	0.791296000	2.126911000	0.725441000
C	0.510548000	2.304655000	-0.663289000
C	-0.908428000	2.339333000	-0.830887000
C	-0.640288000	1.962486000	2.904696000
H	0.213155000	1.492332000	3.404647000
H	-1.540766000	1.406370000	3.186984000
H	-0.741325000	2.967586000	3.335034000
C	2.152224000	2.190753000	1.358537000
H	2.426093000	3.233559000	1.568272000
H	2.932378000	1.775565000	0.713395000
H	2.194621000	1.657529000	2.314215000
C	1.525745000	2.579847000	-1.735555000
H	1.166198000	2.286514000	-2.727242000
H	2.476086000	2.068719000	-1.551370000
H	1.744972000	3.654876000	-1.784761000
C	-1.641361000	2.643332000	-2.105195000
H	-1.781660000	3.726581000	-2.219521000
H	-2.632925000	2.181902000	-2.124623000
H	-1.097990000	2.294235000	-2.988932000
C	-2.973106000	2.269096000	0.747717000
H	-3.295174000	3.318026000	0.788691000
H	-3.577865000	1.776224000	-0.020354000
H	-3.226650000	1.819448000	1.712424000

C	-3.297327000	-1.540430000	0.580996000
C	-4.241166000	-1.983873000	-0.340672000
C	-4.010021000	-1.814397000	-1.710392000
C	-2.841719000	-1.197779000	-2.148194000
C	-1.913978000	-0.759789000	-1.197359000
N	-2.171159000	-0.954326000	0.117968000
H	-4.752216000	-2.161408000	-2.425463000
H	-5.153467000	-2.456651000	0.010600000
H	-2.655730000	-1.052649000	-3.208661000
H	0.586202000	-0.957355000	-1.932836000
C	-3.464464000	-1.703455000	2.062733000
H	-4.506986000	-1.901302000	2.325291000
H	-2.867329000	-2.545777000	2.435938000
H	-3.138134000	-0.803320000	2.593373000
39			
C1, $E_{\text{(SCRF)}} = -723.4147717$ a.u.			
Sc	0.051781000	-0.452924000	-0.000940000
C	1.895364000	0.534652000	1.155084000
C	2.314560000	-0.761703000	0.714690000
C	2.315547000	-0.761586000	-0.713526000
C	1.896984000	0.534846000	-1.154280000
C	1.649904000	1.340789000	0.000296000
C	2.743162000	-1.899990000	1.598697000
H	2.567174000	-2.878215000	1.138367000
H	2.237645000	-1.889529000	2.570311000
H	3.819721000	-1.838431000	1.804231000
C	2.745391000	-1.899782000	-1.597051000
H	3.822601000	-1.839310000	-1.799464000
H	2.242638000	-1.888054000	-2.570071000
H	2.566993000	-2.878159000	-1.137943000
C	1.812214000	0.999456000	-2.580885000
H	1.028373000	1.750046000	-2.724488000
H	1.621776000	0.176691000	-3.277847000
H	2.759172000	1.461673000	-2.888655000
C	1.318288000	2.803130000	0.000262000
H	2.239316000	3.400778000	0.001621000
H	0.741176000	3.092182000	0.883091000
H	0.743478000	3.092717000	-0.883890000
C	1.808766000	0.999129000	2.581618000
H	2.754943000	1.462389000	2.890227000
H	1.023985000	1.748864000	2.724565000
H	1.618637000	0.176100000	3.278344000
C	-3.340981000	-0.966904000	-0.000452000
C	-4.339518000	0.002351000	-0.000103000
C	-4.001291000	1.360733000	0.000044000
C	-2.664754000	1.749358000	-0.000156000
C	-1.683945000	0.755653000	-0.000460000
N	-2.053170000	-0.551908000	-0.000577000
H	-4.791409000	2.107542000	0.000307000
H	-5.381091000	-0.303889000	0.000054000

H	-2.388800000	2.799412000	-0.000086000
C	-3.617323000	-2.439727000	-0.000797000
H	-4.690945000	-2.641897000	0.000944000
H	-3.183983000	-2.918757000	-0.887000000
H	-3.180842000	-2.919817000	0.883270000
23			
b, $E_{\text{(SCRF)}} = -405.3124902$ a.u.			
N	1.575225000	-0.057718000	-0.178263000
C	-0.057435000	2.325395000	-0.375033000
H	0.208725000	2.840816000	0.558335000
H	-0.772045000	2.968052000	-0.900140000
C	-0.647807000	0.962509000	-0.131404000
C	0.165401000	-0.192772000	-0.057796000
C	-0.443238000	-1.447481000	0.089001000
H	0.173670000	-2.339790000	0.141491000
C	-1.827468000	-1.572647000	0.180032000
H	-2.272561000	-2.558273000	0.293664000
C	-2.630275000	-0.437100000	0.133894000
H	-3.711773000	-0.520614000	0.202952000
C	-2.032705000	0.811784000	-0.024205000
H	-2.658195000	1.700166000	-0.092216000
C	2.296372000	-1.207098000	-0.687083000
H	2.405293000	-2.029831000	0.044461000
H	3.305894000	-0.890017000	-0.974461000
H	1.794073000	-1.598361000	-1.576545000
C	2.239749000	0.517167000	0.982484000
H	1.709329000	1.406505000	1.328418000
H	3.260078000	0.813144000	0.710708000
H	2.300562000	-0.193051000	1.827350000
H	0.854804000	2.246732000	-0.975516000
62			
A2, $E_{\text{(SCRF)}} = -1128.775103$ a.u.			
Sc	-0.038534000	0.098884000	-0.114372000
N	0.764616000	-1.984821000	0.588465000
C	0.870210000	-0.648160000	-1.971822000
H	0.242914000	-1.512284000	-2.230579000
H	1.075179000	-0.076919000	-2.879226000
C	2.105202000	-0.996812000	-1.236253000
C	2.075293000	-1.621270000	0.043093000
C	3.257436000	-1.872306000	0.753187000
H	3.225387000	-2.370348000	1.716409000
C	4.487897000	-1.497224000	0.231990000
H	5.396822000	-1.704517000	0.788743000
C	4.543979000	-0.862885000	-1.012810000
H	5.502624000	-0.572951000	-1.434193000
C	3.377980000	-0.617949000	-1.720395000
H	3.429662000	-0.144491000	-2.697240000
C	0.742897000	-2.138927000	2.054420000
H	1.304737000	-3.022992000	2.383152000
H	-0.292770000	-2.271047000	2.379947000

H	1.166012000	-1.254755000	2.538215000
C	0.239812000	-3.228176000	-0.023425000
H	0.294984000	-3.170058000	-1.110380000
H	-0.802207000	-3.372583000	0.276996000
H	0.833576000	-4.090445000	0.307503000
C	-1.050686000	2.214285000	0.694254000
C	-0.058976000	1.810170000	1.641952000
C	1.214537000	1.868343000	0.999641000
C	1.007843000	2.303208000	-0.346743000
C	-0.388563000	2.514779000	-0.530900000
C	-0.301976000	1.552946000	3.103474000
H	0.453998000	0.896621000	3.546994000
H	-1.285981000	1.110398000	3.295682000
H	-0.269105000	2.493449000	3.669554000
C	2.551286000	1.672141000	1.656299000
H	2.963352000	2.638021000	1.977993000
H	3.281952000	1.213757000	0.983137000
H	2.485184000	1.043248000	2.549920000
C	2.081341000	2.648696000	-1.334358000
H	1.758070000	2.486075000	-2.367592000
H	2.989636000	2.062061000	-1.172762000
H	2.356372000	3.708319000	-1.244343000
C	-1.023121000	3.079415000	-1.769094000
H	-0.943841000	4.174715000	-1.776502000
H	-2.088907000	2.839098000	-1.836056000
H	-0.537199000	2.720962000	-2.683284000
C	-2.502155000	2.451151000	0.993561000
H	-2.655165000	3.471411000	1.369622000
H	-3.132853000	2.339556000	0.105835000
H	-2.888153000	1.770979000	1.760210000
C	-3.026520000	-0.771618000	-1.252194000
C	-4.315609000	-1.302280000	-1.128116000
C	-4.794278000	-1.695238000	0.113953000
C	-3.973556000	-1.538076000	1.230980000
C	-2.712209000	-1.001066000	1.038527000
N	-2.231771000	-0.633118000	-0.167393000
H	-5.794104000	-2.107869000	0.213759000
H	-4.933421000	-1.398675000	-2.015795000
H	-4.304623000	-1.814171000	2.226576000
H	-2.052645000	-0.836837000	1.888167000
C	-2.504978000	-0.359477000	-2.597134000
H	-2.152937000	-1.232299000	-3.160922000
H	-3.296173000	0.110937000	-3.188964000
H	-1.669605000	0.340630000	-2.518787000
62			
TS1b, $E_{\text{(SCRF)}} = -1128.735015$ a.u., $\text{IF} = i1211.7546$ cm ⁻¹			
Sc	-0.136294000	0.189595000	-0.208797000
N	0.377030000	-2.021599000	0.397403000
C	1.001116000	-0.726792000	-2.152797000
H	0.677526000	-1.600096000	-2.736197000

H	1.414708000	-0.006688000	-2.866797000
C	2.053820000	-1.107081000	-1.154597000
C	1.770627000	-1.771984000	0.065903000
C	2.809731000	-2.147673000	0.929903000
H	2.591937000	-2.671375000	1.854003000
C	4.131528000	-1.872259000	0.609003000
H	4.924932000	-2.184451000	1.281703000
C	4.431821000	-1.202456000	-0.579397000
H	5.463719000	-0.988545000	-0.842497000
C	3.406717000	-0.824667000	-1.433197000
H	3.643712000	-0.324465000	-2.368297000
C	0.126433000	-2.268102000	1.828203000
H	0.539843000	-3.230797000	2.156603000
H	-0.953167000	-2.296814000	1.989403000
H	0.562424000	-1.471297000	2.437003000
C	-0.208658000	-3.137105000	-0.380797000
H	-0.039459000	-2.993504000	-1.446897000
H	-1.285157000	-3.177817000	-0.194797000
H	0.247251000	-4.089401000	-0.078897000
C	-0.906217000	2.435287000	0.509303000
C	-0.151012000	1.857695000	1.576703000
C	1.199890000	1.720110000	1.141403000
C	1.276984000	2.203011000	-0.201997000
C	-0.021119000	2.650597000	-0.583897000
C	-0.657709000	1.594990000	2.966203000
H	-0.121200000	0.779695000	3.463903000
H	-1.725806000	1.355978000	2.979603000
H	-0.527818000	2.484491000	3.597003000
C	2.365394000	1.323622000	2.001203000
H	2.786684000	2.207127000	2.499603000
H	3.170299000	0.861830000	1.423403000
H	2.080801000	0.622119000	2.792403000
C	2.529183000	2.435724000	-0.994097000
H	2.384084000	2.259123000	-2.065897000
H	3.352189000	1.801232000	-0.657497000
H	2.855872000	3.478927000	-0.885897000
C	-0.338727000	3.365293000	-1.865497000
H	0.031962000	4.398097000	-1.827097000
H	-1.415528000	3.424981000	-2.051397000
H	0.126978000	2.892598000	-2.737897000
C	-2.340122000	2.870871000	0.582703000
H	-2.407833000	3.921771000	0.893803000
H	-2.852821000	2.791667000	-0.381897000
H	-2.912416000	2.282966000	1.306103000
C	-2.645086000	-0.551032000	-1.112297000
C	-3.772178000	-1.314243000	-1.451397000
C	-4.568172000	-1.832752000	-0.439697000
C	-4.229175000	-1.592148000	0.897203000
C	-3.072482000	-0.877435000	1.163103000
N	-2.284488000	-0.393328000	0.186903000

H	-5.459666000	-2.404061000	-0.683697000
H	-4.026876000	-1.458046000	-2.497097000
H	-4.844871000	-1.958455000	1.711903000
H	-2.753384000	-0.681333000	2.183303000
C	-1.733893000	0.128178000	-2.051997000
H	-1.867490000	-0.195623000	-3.088397000
H	-1.872705000	1.213277000	-2.019197000
H	-0.326489000	-0.278007000	-2.059797000
62			
B2, $E_{\text{(SCRF)}} = -1128.764134$ a.u.			
Sc	-0.512642000	0.232571000	-0.179143000
N	0.849061000	-1.596202000	0.476755000
C	1.890557000	-0.996512000	-2.277534000
H	1.866736000	-1.954697000	-2.814013000
H	2.292364000	-0.256214000	-2.975949000
C	2.753899000	-1.072909000	-1.043381000
C	2.278397000	-1.345386000	0.256899000
C	3.180121000	-1.395061000	1.327735000
H	2.837675000	-1.610606000	2.332634000
C	4.541882000	-1.180889000	1.131435000
H	5.217768000	-1.226590000	1.980296000
C	5.023719000	-0.922111000	-0.147107000
H	6.083591000	-0.757732000	-0.316814000
C	4.129483000	-0.869850000	-1.210069000
H	4.500659000	-0.659105000	-2.210330000
C	0.469983000	-1.664011000	1.905429000
H	0.923678000	-2.527632000	2.409020000
H	-0.615558000	-1.783760000	1.972383000
H	0.768707000	-0.752359000	2.427865000
C	0.441306000	-2.883499000	-0.149601000
H	0.638351000	-2.872728000	-1.220151000
H	-0.629148000	-3.041951000	0.007365000
H	0.998069000	-3.712625000	0.305391000
C	-1.411577000	2.508854000	-0.120560000
C	-0.985697000	2.191205000	1.203725000
C	0.433969000	2.046617000	1.189017000
C	0.881427000	2.253022000	-0.150032000
C	-0.261624000	2.536239000	-0.961234000
C	-1.868919000	2.161680000	2.417953000
H	-1.506594000	1.469686000	3.186919000
H	-2.896690000	1.880854000	2.167003000
H	-1.915516000	3.154162000	2.885761000
C	1.321679000	1.900522000	2.391949000
H	1.678348000	2.885793000	2.720885000
H	2.211643000	1.294921000	2.188528000
H	0.794274000	1.461359000	3.245754000
C	2.314194000	2.369332000	-0.582817000
H	2.453885000	2.108645000	-1.636326000
H	2.983041000	1.738940000	0.009342000
H	2.656153000	3.406720000	-0.465405000

C	-0.226082000	2.928237000	-2.410095000
H	-0.080588000	4.011610000	-2.513630000
H	-1.154753000	2.676648000	-2.931139000
H	0.593697000	2.441897000	-2.948493000
C	-2.818795000	2.843344000	-0.520333000
H	-3.081012000	3.854964000	-0.183833000
H	-2.952657000	2.826156000	-1.605753000
H	-3.552105000	2.157936000	-0.081917000
C	-2.554547000	-1.155136000	-1.047711000
C	-3.301440000	-2.318237000	-1.321361000
C	-4.026834000	-2.916328000	-0.304345000
C	-3.999396000	-2.373235000	0.990415000
C	-3.198319000	-1.270650000	1.219391000
N	-2.473115000	-0.695534000	0.238816000
H	-4.635770000	-3.792197000	-0.512515000
H	-3.336578000	-2.699431000	-2.337296000
H	-4.580901000	-2.805799000	1.797525000
H	-3.114922000	-0.822384000	2.206364000
C	-1.744394000	-0.366380000	-1.977048000
H	-1.516182000	-0.866148000	-2.919930000
H	-2.213523000	0.603377000	-2.181015000
H	0.839759000	-0.726690000	-2.099850000

39

C2, $E_{\text{(SCRF)}} = -723.415195$ a.u.

Sc	-0.025015000	0.143940000	-0.324951000
C	2.281063000	0.047798000	-0.930444000
C	2.093053000	1.207205000	-0.113816000
C	1.710232000	0.765020000	1.190519000
C	1.680551000	-0.665958000	1.181952000
C	2.038584000	-1.110873000	-0.123977000
C	2.314910000	2.632642000	-0.537199000
H	1.694236000	3.338482000	0.025189000
H	2.119972000	2.788164000	-1.603734000
H	3.359001000	2.923434000	-0.362662000
C	1.461911000	1.644643000	2.384858000
H	2.391663000	1.791887000	2.949498000
H	0.737279000	1.209663000	3.081629000
H	1.102873000	2.640605000	2.104283000
C	1.394328000	-1.545681000	2.364031000
H	0.970069000	-2.508652000	2.065237000
H	0.702814000	-1.079949000	3.074109000
H	2.320036000	-1.756007000	2.915331000
C	2.234680000	-2.534694000	-0.551372000
H	3.279545000	-2.836349000	-0.401199000
H	2.006704000	-2.685273000	-1.611127000
H	1.610906000	-3.223294000	0.024834000
C	2.744117000	0.040469000	-2.360743000
H	3.839858000	-0.007479000	-2.406307000
H	2.366927000	-0.825255000	-2.915172000
H	2.445999000	0.944339000	-2.902742000

C	-2.387897000	-0.805668000	-0.388841000
C	-3.611869000	-1.156150000	0.209466000
C	-4.587264000	-0.187041000	0.378598000
C	-4.342077000	1.135947000	-0.021080000
C	-3.102121000	1.444604000	-0.544420000
N	-2.140688000	0.509254000	-0.707507000
H	-5.550178000	-0.454910000	0.804996000
H	-3.791271000	-2.190405000	0.485274000
H	-5.098336000	1.906407000	0.082985000
H	-2.847633000	2.456255000	-0.849443000
C	-1.232645000	-1.674388000	-0.627848000
H	-1.260807000	-2.646877000	-0.139100000
H	-1.026853000	-1.799552000	-1.703482000
76			
A3, $E_{\text{(SCRF)}} = -1416.256088$ a.u.			
Sc	-0.345052000	0.241645000	-0.290517000
N	0.712318000	-2.200242000	0.460666000
C	0.520506000	-0.876751000	-2.017398000
H	-0.285231000	-1.621371000	-2.119382000
H	0.622075000	-0.395525000	-2.993095000
C	1.798787000	-1.512275000	-1.609973000
C	1.920734000	-2.137623000	-0.348791000
C	3.140254000	-2.663772000	0.077795000
H	3.224097000	-3.153255000	1.043371000
C	4.274848000	-2.560043000	-0.727705000
H	5.220725000	-2.968911000	-0.383976000
C	4.179163000	-1.940948000	-1.972068000
H	5.053263000	-1.863763000	-2.613506000
C	2.956394000	-1.431291000	-2.402704000
H	2.884198000	-0.959651000	-3.380591000
C	-0.075855000	-3.381272000	0.051322000
H	-0.264315000	-3.356175000	-1.022876000
H	-1.028256000	-3.399063000	0.588839000
H	0.472451000	-4.307721000	0.276909000
C	-1.723799000	2.336439000	0.058364000
C	-0.410207000	2.781145000	-0.263162000
C	-0.118209000	2.361903000	-1.593422000
C	-1.273026000	1.704575000	-2.114042000
C	-2.264402000	1.693647000	-1.096419000
C	0.419724000	3.725212000	0.555175000
H	1.492747000	3.603433000	0.379137000
H	0.244275000	3.617772000	1.629988000
H	0.169520000	4.762911000	0.296182000
C	1.101532000	2.724811000	-2.389813000
H	1.940890000	3.011871000	-1.749035000
H	0.896270000	3.581900000	-3.045390000
H	1.436829000	1.903720000	-3.032861000
C	-1.478515000	1.327370000	-3.551469000
H	-2.110665000	0.442064000	-3.679428000
H	-0.532681000	1.131295000	-4.063367000

H	-1.969810000	2.148565000	-4.091129000
C	-3.715355000	1.357309000	-1.275147000
H	-4.294637000	2.279291000	-1.422830000
H	-4.148080000	0.851468000	-0.405338000
H	-3.892109000	0.733257000	-2.155385000
C	-2.534486000	2.727550000	1.261526000
H	-3.209175000	3.558910000	1.014260000
H	-3.169413000	1.912392000	1.627745000
H	-1.912419000	3.072219000	2.093723000
C	-3.122553000	-1.743265000	-0.192133000
C	-4.170809000	-2.378591000	0.484997000
C	-4.316420000	-2.228921000	1.856895000
C	-3.401784000	-1.427309000	2.537476000
C	-2.392096000	-0.826269000	1.802730000
N	-2.233108000	-0.970735000	0.472784000
H	-5.129317000	-2.719699000	2.384342000
H	-4.868172000	-2.987891000	-0.082000000
H	-3.469576000	-1.263330000	3.607937000
H	-1.672846000	-0.185326000	2.302764000
C	-2.972568000	-1.939015000	-1.670624000
H	-2.431761000	-2.868454000	-1.886039000
H	-3.952775000	-2.018322000	-2.149908000
H	-2.425455000	-1.116325000	-2.132794000
C	0.966887000	-2.317028000	1.901234000
H	0.016499000	-2.216672000	2.436121000
H	1.391128000	-3.294059000	2.176646000
H	1.655889000	-1.536058000	2.227230000
C	1.634913000	1.196511000	2.375639000
C	2.863810000	1.592646000	2.907135000
C	3.987708000	1.664073000	2.091736000
C	3.850915000	1.342300000	0.745777000
C	2.600394000	0.953284000	0.286184000
N	1.507263000	0.865930000	1.069356000
H	4.946573000	1.972105000	2.498867000
H	2.926597000	1.848112000	3.960402000
H	4.688005000	1.382112000	0.057319000
C	0.424600000	1.121921000	3.258488000
H	0.582670000	1.675511000	4.187846000
H	-0.450528000	1.549319000	2.759251000
H	0.199776000	0.084122000	3.533604000
H	2.467023000	0.692056000	-0.757959000

76

TS1c, $E_{(\text{SCRF})} = -1416.212011$ a.u., IF = $i1304.0366$ cm⁻¹

Sc	0.464627000	-0.328035000	-0.303316000
N	-1.576147000	1.863925000	0.483998000
C	-1.336629000	0.205094000	-1.788003000
H	-0.615189000	1.013331000	-2.010615000
H	-1.410192000	-0.407019000	-2.689196000
C	-2.668381000	0.762678000	-1.403648000
C	-2.795286000	1.516663000	-0.222551000

C	-4.053515000	1.948205000	0.203981000
H	-4.151822000	2.540723000	1.109192000
C	-5.197002000	1.624179000	-0.524129000
H	-6.170540000	1.960755000	-0.178779000
C	-5.082918000	0.878388000	-1.695390000
H	-5.968092000	0.626459000	-2.272975000
C	-3.828455000	0.454033000	-2.126043000
H	-3.740261000	-0.133370000	-3.037493000
C	-1.130224000	3.191227000	0.033804000
H	-1.007268000	3.192513000	-1.052340000
H	-0.176918000	3.443809000	0.507710000
H	-1.863548000	3.972112000	0.290040000
C	2.405433000	-1.852103000	-0.235555000
C	1.273145000	-2.674238000	-0.489894000
C	0.747004000	-2.318251000	-1.763748000
C	1.576414000	-1.295236000	-2.316718000
C	2.607484000	-1.013643000	-1.374849000
C	0.802727000	-3.823213000	0.349619000
H	-0.277456000	-3.978543000	0.266189000
H	1.039345000	-3.688039000	1.409264000
H	1.288990000	-4.753758000	0.027299000
C	-0.359142000	-3.040824000	-2.475181000
H	-1.213330000	-3.246185000	-1.820436000
H	-0.003284000	-4.009076000	-2.851926000
H	-0.725924000	-2.479226000	-3.338851000
C	1.486877000	-0.773389000	-3.722661000
H	2.098520000	0.121867000	-3.870669000
H	0.461944000	-0.527583000	-4.020608000
H	1.852751000	-1.525478000	-4.434014000
C	3.840628000	-0.191513000	-1.609326000
H	4.674661000	-0.844021000	-1.901227000
H	4.162348000	0.350388000	-0.713686000
H	3.713871000	0.535742000	-2.415930000
C	3.353662000	-1.971966000	0.922111000
H	4.238553000	-2.558766000	0.640141000
H	3.720336000	-0.998369000	1.267744000
H	2.894896000	-2.482835000	1.774002000
C	2.275005000	2.536291000	-0.388291000
C	3.106324000	3.500735000	0.191640000
C	3.432686000	3.424803000	1.538804000
C	2.918542000	2.370445000	2.291406000
C	2.103089000	1.449219000	1.652821000
N	1.778069000	1.515209000	0.345274000
H	4.078644000	4.170598000	1.993236000
H	3.491303000	4.306031000	-0.426864000
H	3.144973000	2.259002000	3.346687000
H	1.685452000	0.610678000	2.200929000
C	1.903534000	2.648226000	-1.837299000
H	1.114494000	3.396054000	-1.977946000
H	2.761591000	2.971184000	-2.434631000

H	1.546704000	1.698606000	-2.242605000
C	-1.724823000	1.877349000	1.941590000
H	-0.733162000	1.968181000	2.397797000
H	-2.332844000	2.720684000	2.304547000
H	-2.186288000	0.946489000	2.277105000
C	-0.556496000	-1.540859000	2.837152000
C	-1.718184000	-2.227429000	3.190589000
C	-2.709333000	-2.459042000	2.236195000
C	-2.526155000	-2.006374000	0.932114000
C	-1.344724000	-1.330543000	0.633326000
N	-0.407983000	-1.104151000	1.568387000
H	-3.615501000	-2.991236000	2.514421000
H	-1.841823000	-2.577400000	4.210975000
H	-3.283348000	-2.161683000	0.169876000
C	0.524346000	-1.250032000	3.836498000
H	0.412485000	-1.871277000	4.728984000
H	1.516319000	-1.435653000	3.413071000
H	0.484056000	-0.202150000	4.160969000
H	-1.333983000	-0.682983000	-0.643547000

76

B3, $E_{\text{(SCRF)}} = -1416.231362$ a.u.

Sc	1.672025000	-0.194693000	-0.021296000
N	-4.009903000	1.672135000	-0.001361000
C	-3.663320000	0.429873000	-2.622573000
H	-4.446908000	0.913468000	-3.221134000
H	-3.137578000	-0.258605000	-3.292781000
C	-4.227116000	-0.308480000	-1.437483000
C	-4.386642000	0.306743000	-0.172374000
C	-4.884315000	-0.454307000	0.895379000
H	-5.022224000	0.007082000	1.868095000
C	-5.230977000	-1.793931000	0.731795000
H	-5.630189000	-2.352099000	1.575105000
C	-5.087815000	-2.400486000	-0.512669000
H	-5.362345000	-3.441728000	-0.657784000
C	-4.586807000	-1.652691000	-1.577139000
H	-4.462848000	-2.124282000	-2.550211000
C	-4.908013000	2.627220000	-0.650220000
H	-5.102891000	2.337034000	-1.683434000
H	-4.442310000	3.619486000	-0.656298000
H	-5.876956000	2.703939000	-0.128613000
C	3.972786000	-0.348324000	-0.808145000
C	3.460727000	-1.678404000	-0.711586000
C	2.414894000	-1.818675000	-1.673664000
C	2.275954000	-0.574652000	-2.356191000
C	3.241874000	0.336193000	-1.825569000
C	4.007350000	-2.781008000	0.149663000
H	3.224409000	-3.474475000	0.472553000
H	4.506244000	-2.397309000	1.045608000
H	4.752481000	-3.369243000	-0.402200000
C	1.677516000	-3.086316000	-1.991820000

H	1.519038000	-3.704910000	-1.103146000
H	2.245771000	-3.690866000	-2.711659000
H	0.697357000	-2.887616000	-2.434732000
C	1.347625000	-0.317467000	-3.509795000
H	1.199743000	0.751813000	-3.691952000
H	0.362573000	-0.772979000	-3.359636000
H	1.757890000	-0.741355000	-4.435792000
C	3.525490000	1.722743000	-2.329904000
H	4.280552000	1.698810000	-3.126710000
H	3.912084000	2.379141000	-1.543224000
H	2.635693000	2.201676000	-2.751629000
C	5.143944000	0.202291000	-0.044449000
H	6.084353000	-0.015726000	-0.567801000
H	5.091246000	1.290671000	0.066891000
H	5.234593000	-0.236877000	0.955658000
C	0.629215000	2.832711000	0.182500000
C	0.529077000	4.132806000	0.684763000
C	1.365189000	4.543452000	1.715705000
C	2.300001000	3.645180000	2.231269000
C	2.351781000	2.374456000	1.683739000
N	1.541352000	1.971537000	0.684380000
H	1.293419000	5.552637000	2.111175000
H	-0.204288000	4.811639000	0.260566000
H	2.975361000	3.922556000	3.033528000
H	3.070853000	1.643670000	2.048317000
C	-0.281259000	2.341601000	-0.904139000
H	-1.231495000	1.970076000	-0.496294000
H	-0.521130000	3.147270000	-1.604646000
H	0.173271000	1.533273000	-1.491553000
C	-3.729874000	2.088234000	1.362744000
H	-3.252644000	3.075019000	1.337846000
H	-4.630362000	2.179713000	1.995606000
H	-3.043224000	1.381292000	1.838605000
C	0.716669000	-2.102312000	2.666797000
C	-0.483817000	-2.777744000	2.855620000
C	-1.482801000	-2.710466000	1.876614000
C	-1.275729000	-1.976202000	0.713997000
C	-0.054543000	-1.313228000	0.546874000
N	0.884080000	-1.398172000	1.525083000
H	-2.423498000	-3.233034000	2.030509000
H	-0.639168000	-3.351164000	3.764713000
H	-2.050816000	-1.913174000	-0.043944000
C	1.829905000	-2.104925000	3.671634000
H	1.607805000	-2.771346000	4.508958000
H	2.769355000	-2.431884000	3.212403000
H	1.991426000	-1.098107000	4.076402000
H	-2.967676000	1.213266000	-2.305102000
53			
C3, $E_{(\text{SCRF})} = -1010.912364$ a.u.			
Sc	0.096023000	0.164218000	-0.102949000

C	-0.214648000	2.186502000	1.218592000
C	1.191719000	1.977166000	1.072644000
C	1.517232000	2.125584000	-0.309713000
C	0.312603000	2.410080000	-1.017945000
C	-0.759197000	2.456585000	-0.072124000
C	2.175250000	1.785040000	2.192004000
H	3.049499000	1.206982000	1.876931000
H	1.729635000	1.276597000	3.053754000
H	2.543838000	2.754821000	2.551699000
C	2.897453000	2.091849000	-0.896884000
H	3.558403000	1.408221000	-0.355335000
H	3.356720000	3.088568000	-0.854709000
H	2.888389000	1.780691000	-1.945406000
C	0.216390000	2.715343000	-2.486029000
H	-0.791590000	2.549042000	-2.879320000
H	0.910785000	2.111964000	-3.080000000
H	0.460864000	3.768372000	-2.677722000
C	-2.181198000	2.849356000	-0.356491000
H	-2.322436000	3.926348000	-0.195923000
H	-2.895173000	2.333722000	0.294552000
H	-2.469977000	2.647800000	-1.393286000
C	-0.967865000	2.229111000	2.518080000
H	-0.945315000	3.241159000	2.943727000
H	-2.023403000	1.963006000	2.396293000
H	-0.534461000	1.564544000	3.274335000
C	-2.666995000	-1.170715000	-1.000272000
C	-3.869258000	-1.867093000	-0.873638000
C	-4.353289000	-2.186233000	0.390949000
C	-3.622439000	-1.803227000	1.514593000
C	-2.435183000	-1.115954000	1.317757000
N	-1.963156000	-0.803845000	0.095309000
H	-5.288186000	-2.728635000	0.498984000
H	-4.415808000	-2.153990000	-1.766381000
H	-3.960547000	-2.031728000	2.519662000
H	-1.832613000	-0.797951000	2.165839000
C	-2.107574000	-0.777292000	-2.336427000
H	-1.033133000	-1.000748000	-2.404917000
H	-2.603139000	-1.312877000	-3.149999000
H	-2.250248000	0.296071000	-2.515944000
C	2.334979000	-2.265019000	0.828732000
C	3.182208000	-3.014537000	0.019650000
C	3.168563000	-2.825633000	-1.367434000
C	2.310110000	-1.889929000	-1.934811000
C	1.470781000	-1.145802000	-1.097878000
N	1.515819000	-1.364399000	0.241517000
H	3.835045000	-3.413824000	-1.993870000
H	3.849684000	-3.742543000	0.470662000
H	2.294131000	-1.734727000	-3.009993000
C	2.274643000	-2.416511000	2.319160000
H	3.046590000	-3.100434000	2.680687000

H	2.411273000	-1.449318000	2.815215000
H	1.300333000	-2.814012000	2.629516000
76			
A4, $E_{(\text{SCRF})} = -1416.253937$ a.u.			
Sc	-0.321810000	0.223821000	-0.301432000
N	0.765405000	-2.092771000	0.753177000
C	0.402367000	-1.173375000	-1.896923000
H	-0.383094000	-1.945456000	-1.909635000
H	0.470290000	-0.798293000	-2.921764000
C	1.702019000	-1.764397000	-1.479994000
C	1.907504000	-2.182788000	-0.147204000
C	3.147476000	-2.677510000	0.264740000
H	3.301013000	-3.006500000	1.287643000
C	4.211864000	-2.756152000	-0.633690000
H	5.171777000	-3.140918000	-0.300909000
C	4.027380000	-2.353729000	-1.955501000
H	4.845541000	-2.421157000	-2.667704000
C	2.788261000	-1.869038000	-2.364676000
H	2.646688000	-1.558252000	-3.397483000
C	-0.080388000	-3.292970000	0.572811000
H	-0.392061000	-3.389677000	-0.467787000
H	-0.969131000	-3.220184000	1.206071000
H	0.476282000	-4.200582000	0.848574000
C	-1.375511000	2.519945000	-0.167010000
C	-0.176589000	2.680382000	-0.924498000
C	-0.317196000	1.948554000	-2.133778000
C	-1.610949000	1.343890000	-2.135282000
C	-2.273533000	1.721959000	-0.932433000
C	0.910234000	3.664125000	-0.608437000
H	1.857475000	3.413135000	-1.094380000
H	1.095140000	3.754617000	0.466610000
H	0.626379000	4.663017000	-0.967513000
C	0.609728000	2.006292000	-3.311683000
H	1.648156000	2.195158000	-3.022127000
H	0.314955000	2.824538000	-3.983326000
H	0.591285000	1.087162000	-3.904365000
C	-2.226944000	0.640526000	-3.310247000
H	-3.138925000	0.100036000	-3.037682000
H	-1.540751000	-0.073102000	-3.779556000
H	-2.511553000	1.364819000	-4.085343000
C	-3.729991000	1.530330000	-0.628873000
H	-4.301907000	2.404206000	-0.968981000
H	-3.927789000	1.417852000	0.442181000
H	-4.152749000	0.657938000	-1.135350000
C	-1.729791000	3.315479000	1.057907000
H	-2.021279000	4.337763000	0.779579000
H	-2.580739000	2.889560000	1.599731000
H	-0.893620000	3.412395000	1.759412000
C	-2.902555000	-1.039068000	1.662761000
C	-4.013143000	-1.865967000	1.852469000

C	-4.511704000	-2.622273000	0.798541000
C	-3.889358000	-2.516893000	-0.441060000
C	-2.790340000	-1.677790000	-0.554563000
N	-2.278318000	-0.960937000	0.464986000
H	-5.374308000	-3.267120000	0.939731000
H	-4.483332000	-1.903143000	2.830200000
H	-4.242490000	-3.065760000	-1.307877000
H	-2.296037000	-1.563441000	-1.512923000
C	-2.393169000	-0.200295000	2.796842000
H	-3.078661000	-0.233984000	3.647382000
H	-1.417448000	-0.551194000	3.150429000
H	-2.294237000	0.845969000	2.489190000
C	1.144902000	-2.037275000	2.170935000
H	0.253500000	-1.832069000	2.770566000
H	1.562164000	-2.989839000	2.529406000
H	1.880071000	-1.249523000	2.339960000
C	2.680898000	1.282030000	0.857438000
C	3.531599000	1.782688000	1.852177000
C	3.045053000	2.064541000	3.119551000
C	1.691314000	1.846990000	3.375329000
C	0.910109000	1.345132000	2.348348000
N	1.373925000	1.051636000	1.117012000
H	3.702291000	2.456471000	3.890557000
H	4.576188000	1.952487000	1.609078000
H	1.249160000	2.063622000	4.342232000
C	3.224656000	0.996260000	-0.506182000
H	3.743497000	0.031106000	-0.523553000
H	2.434690000	0.957621000	-1.258574000
H	3.947464000	1.765762000	-0.796380000
H	-0.148176000	1.171607000	2.511634000

76

TS1d, $E_{(\text{SCRF})} = -1416.201456$ a.u., IF = $i1208.4013$ cm⁻¹

Sc	0.668587000	-0.326084000	-0.294026000
N	-2.398020000	1.131402000	0.832414000
C	-1.215627000	0.418435000	-1.667448000
H	-0.797280000	1.378376000	-1.337612000
H	-0.948245000	0.266830000	-2.716726000
C	-2.697665000	0.397596000	-1.482428000
C	-3.269572000	0.672067000	-0.221902000
C	-4.647384000	0.525018000	-0.038083000
H	-5.092511000	0.744944000	0.927858000
C	-5.467749000	0.101476000	-1.082732000
H	-6.536112000	-0.009903000	-0.919370000
C	-4.912813000	-0.164152000	-2.331609000
H	-5.542648000	-0.488067000	-3.155522000
C	-3.540935000	-0.016425000	-2.521529000
H	-3.107047000	-0.233106000	-3.495532000
C	-2.269594000	2.591756000	0.781763000
H	-1.949091000	2.910027000	-0.213699000
H	-1.526105000	2.924710000	1.513824000

H	-3.225116000	3.095075000	1.004806000
C	2.955735000	-1.231703000	-0.444176000
C	2.130983000	-2.100880000	-1.215255000
C	1.635476000	-1.363595000	-2.327202000
C	2.171280000	-0.042330000	-2.255563000
C	2.997073000	0.035134000	-1.094435000
C	1.969963000	-3.574750000	-0.981554000
H	1.212206000	-4.013057000	-1.637797000
H	1.699775000	-3.814157000	0.053260000
H	2.911582000	-4.096792000	-1.196283000
C	0.840898000	-1.918758000	-3.473397000
H	0.038000000	-2.590065000	-3.149987000
H	1.490273000	-2.495665000	-4.145265000
H	0.385224000	-1.125823000	-4.073504000
C	2.053676000	0.989935000	-3.341923000
H	2.510211000	1.941151000	-3.053160000
H	1.016803000	1.188684000	-3.639287000
H	2.578755000	0.652731000	-4.244837000
C	3.921299000	1.156648000	-0.720689000
H	4.930644000	0.958262000	-1.105186000
H	4.011911000	1.278846000	0.363971000
H	3.604741000	2.118147000	-1.134037000
C	3.791904000	-1.643489000	0.731635000
H	4.793295000	-1.953803000	0.403097000
H	3.939882000	-0.827707000	1.448951000
H	3.354224000	-2.493070000	1.264370000
C	1.288864000	2.356033000	1.781717000
C	1.480664000	3.710631000	2.067600000
C	1.449334000	4.652988000	1.047028000
C	1.232852000	4.209605000	-0.253779000
C	1.054297000	2.850000000	-0.462278000
N	1.066271000	1.925366000	0.518200000
H	1.595122000	5.707633000	1.262316000
H	1.654765000	4.013338000	3.095358000
H	1.204194000	4.894096000	-1.095143000
H	0.902183000	2.480777000	-1.471000000
C	1.350070000	1.338711000	2.878303000
H	1.406406000	1.818028000	3.858779000
H	0.471974000	0.686946000	2.865931000
H	2.241789000	0.710427000	2.766022000
C	-2.801261000	0.720031000	2.174364000
H	-1.999093000	0.969658000	2.877436000
H	-3.714755000	1.222147000	2.534054000
H	-2.963985000	-0.360147000	2.200988000
C	-0.783950000	-2.266581000	1.110934000
C	-1.585243000	-2.967335000	2.026150000
C	-1.118640000	-3.178250000	3.314495000
C	0.138978000	-2.681858000	3.678671000
C	0.850444000	-1.946660000	2.746997000
N	0.390973000	-1.712161000	1.502496000

H	-1.711679000	-3.744851000	4.027388000
H	-2.537970000	-3.371112000	1.697365000
H	0.552421000	-2.855805000	4.666552000
C	-1.075393000	-2.079267000	-0.321161000
H	-2.135535000	-2.217938000	-0.552177000
H	-1.057505000	-0.814216000	-0.982676000
H	-0.503650000	-2.795640000	-0.918409000
H	1.819255000	-1.524598000	2.992577000

76

B4, $E_{(\text{SCRF})} = -1416.238509$ a.u.

Sc	-1.800671000	-0.149786000	-0.105892000
N	5.105821000	0.791163000	0.243440000
C	4.458404000	-1.878924000	1.271158000
H	4.465304000	-1.034588000	1.968052000
H	5.440892000	-2.364212000	1.341000000
C	4.142764000	-1.437551000	-0.134830000
C	4.462578000	-0.143163000	-0.616712000
C	4.091447000	0.203212000	-1.925983000
H	4.338720000	1.186415000	-2.313177000
C	3.438384000	-0.701860000	-2.760201000
H	3.185467000	-0.408924000	-3.776173000
C	3.145292000	-1.982634000	-2.300887000
H	2.658675000	-2.706454000	-2.948981000
C	3.497507000	-2.330136000	-0.997374000
H	3.270356000	-3.329411000	-0.629858000
C	6.488743000	0.458857000	0.591686000
H	6.576850000	-0.584212000	0.894713000
H	6.812347000	1.086540000	1.429066000
H	7.174485000	0.628043000	-0.254850000
C	-3.606723000	-1.586082000	0.687639000
C	-3.230045000	-2.051090000	-0.608142000
C	-1.893749000	-2.547840000	-0.530864000
C	-1.446970000	-2.389365000	0.814853000
C	-2.506101000	-1.803526000	1.570993000
C	-4.120045000	-2.094117000	-1.816596000
H	-3.552578000	-2.043128000	-2.751270000
H	-4.845516000	-1.274642000	-1.825881000
H	-4.691145000	-3.031811000	-1.840276000
C	-1.138764000	-3.243027000	-1.625987000
H	-1.474028000	-2.930639000	-2.619597000
H	-1.286582000	-4.329492000	-1.564300000
H	-0.061756000	-3.056342000	-1.567959000
C	-0.137174000	-2.871721000	1.368137000
H	0.157769000	-2.320581000	2.266985000
H	0.677194000	-2.790084000	0.640049000
H	-0.206068000	-3.931008000	1.650691000
C	-2.499033000	-1.600014000	3.059731000
H	-2.635988000	-2.558532000	3.577165000
H	-3.311857000	-0.946517000	3.391467000
H	-1.556368000	-1.175084000	3.422994000

C	-4.964020000	-1.062296000	1.065552000
H	-5.643362000	-1.887404000	1.316931000
H	-4.930725000	-0.404177000	1.940838000
H	-5.432171000	-0.504942000	0.247152000
C	-0.714456000	1.771779000	2.281719000
C	0.263016000	2.378850000	3.069401000
C	1.607340000	2.107414000	2.833264000
C	1.957630000	1.229172000	1.809403000
C	0.934648000	0.650584000	1.072109000
N	-0.370068000	0.906794000	1.300639000
H	2.374261000	2.577902000	3.442274000
H	-0.036423000	3.062172000	3.858052000
H	2.994585000	0.994947000	1.578996000
H	1.160578000	-0.042509000	0.264410000
C	-2.172511000	2.082177000	2.457178000
H	-2.378884000	2.468227000	3.458950000
H	-2.494316000	2.844548000	1.736445000
H	-2.795945000	1.190936000	2.315421000
C	5.010809000	2.191050000	-0.138919000
H	5.359747000	2.805375000	0.698260000
H	5.626060000	2.452341000	-1.017375000
H	3.971178000	2.458006000	-0.353126000
C	-1.663987000	1.540843000	-2.019635000
C	-1.266809000	2.800242000	-2.517643000
C	-2.074313000	3.902304000	-2.303513000
C	-3.268393000	3.769831000	-1.573935000
C	-3.574032000	2.532248000	-1.043313000
N	-2.785691000	1.453482000	-1.231860000
H	-1.798325000	4.867524000	-2.720111000
H	-0.360072000	2.872670000	-3.110130000
H	-3.932796000	4.613204000	-1.419108000
C	-0.958809000	0.273531000	-2.144964000
H	0.058768000	0.328831000	-2.530420000
H	3.723658000	-2.612322000	1.620013000
H	-1.546101000	-0.471393000	-2.693876000
H	-4.467987000	2.373668000	-0.445205000

53

C4, $E_{\text{(SCRF)}} = -1010.915246$ a.u.

Sc	-0.362730000	0.208585000	-0.186691000
C	-2.278717000	0.043413000	1.310803000
C	-2.720862000	0.693197000	0.119515000
C	-2.631670000	-0.241770000	-0.957032000
C	-2.131746000	-1.468505000	-0.427740000
C	-1.918860000	-1.296543000	0.973480000
C	-3.271691000	2.087080000	0.032603000
H	-3.101098000	2.539706000	-0.949281000
H	-2.834030000	2.751892000	0.783824000
H	-4.357327000	2.082430000	0.197732000
C	-3.118375000	-0.020596000	-2.359758000
H	-3.031492000	1.025770000	-2.668156000

H	-4.178542000	-0.293446000	-2.444648000
H	-2.570053000	-0.624921000	-3.089319000
C	-1.980875000	-2.760237000	-1.178111000
H	-1.172133000	-3.380979000	-0.777459000
H	-1.789926000	-2.600809000	-2.244626000
H	-2.901693000	-3.354733000	-1.108693000
C	-1.532256000	-2.389259000	1.929564000
H	-2.386960000	-3.052115000	2.117868000
H	-1.221377000	-1.996570000	2.902623000
H	-0.721662000	-3.019461000	1.545624000
C	-2.289725000	0.646025000	2.687574000
H	-3.279693000	0.540205000	3.150370000
H	-1.573999000	0.163368000	3.361818000
H	-2.061955000	1.717229000	2.669538000
C	2.147862000	-1.564794000	0.914215000
C	3.189827000	-2.485352000	0.799107000
C	3.424297000	-3.117037000	-0.418181000
C	2.608699000	-2.815485000	-1.507217000
C	1.587115000	-1.896799000	-1.323349000
N	1.353219000	-1.286942000	-0.144202000
H	4.233391000	-3.835249000	-0.515635000
H	3.810875000	-2.698369000	1.663480000
H	2.754968000	-3.281058000	-2.475977000
H	0.925378000	-1.627033000	-2.143522000
C	1.886219000	-0.821701000	2.191361000
H	2.345072000	-1.325296000	3.046071000
H	2.304008000	0.191803000	2.141591000
H	0.811462000	-0.742071000	2.395645000
C	0.983705000	2.193277000	-1.087094000
C	2.208461000	2.824491000	-1.388190000
C	2.892091000	3.495370000	-0.389839000
C	2.378397000	3.524928000	0.917622000
C	1.213001000	2.830789000	1.176591000
N	0.546728000	2.159887000	0.213749000
H	3.815126000	4.020294000	-0.621572000
H	2.568318000	2.821209000	-2.412395000
H	2.880868000	4.069010000	1.710214000
C	0.118294000	1.449655000	-1.997292000
H	0.549478000	1.229909000	-2.974325000
H	-0.859185000	1.933191000	-2.112379000
H	0.780742000	2.794308000	2.173490000

16

C, $E_{\text{(SCRF)}} = -234.4746958$ a.u.

C	2.992614000	-0.203066000	-0.149808000
H	3.029910000	-1.289669000	-0.208937000
H	3.915591000	0.327875000	-0.369191000
C	1.872784000	0.440808000	0.180424000
H	1.884143000	1.531943000	0.225138000
C	0.557664000	-0.211675000	0.489135000
H	0.240914000	0.054070000	1.508292000

H	0.671374000	-1.303667000	0.469633000
C	-0.557623000	0.211775000	-0.489012000
H	-0.240917000	-0.053954000	-1.508184000
H	-0.671295000	1.303772000	-0.469526000
C	-1.872712000	-0.440764000	-0.180300000
C	-2.992734000	0.202950000	0.149590000
H	-1.883848000	-1.531922000	-0.224753000
H	-3.915610000	-0.328186000	0.368899000
H	-3.030214000	1.289570000	0.208457000
69			
D1, $E_{\text{(SCRF)}} = -1245.399795$ a.u.			
Sc	0.300240000	-0.078458000	0.205277000
C	0.029596000	-1.419870000	2.275852000
C	1.392641000	-0.998445000	2.233203000
C	1.415248000	0.425287000	2.330241000
C	0.074020000	0.881452000	2.468204000
C	-0.784626000	-0.251942000	2.414041000
C	2.617158000	-1.865105000	2.316847000
H	3.368577000	-1.621700000	1.555950000
H	2.377270000	-2.927678000	2.226195000
H	3.102350000	-1.732332000	3.292640000
C	2.660986000	1.255653000	2.440850000
H	3.074896000	1.198785000	3.456973000
H	2.466440000	2.312052000	2.235430000
H	3.450764000	0.917114000	1.759917000
C	-0.360226000	2.289368000	2.742562000
H	-1.349198000	2.501738000	2.325501000
H	0.338043000	3.024105000	2.330994000
H	-0.417196000	2.467464000	3.824714000
C	-2.266635000	-0.227073000	2.647712000
H	-2.485826000	-0.187696000	3.723345000
H	-2.762279000	-1.119166000	2.254946000
H	-2.740526000	0.646811000	2.189588000
C	-0.463132000	-2.835148000	2.393062000
H	-0.548144000	-3.124100000	3.449142000
H	-1.456141000	-2.968788000	1.951035000
H	0.209406000	-3.560223000	1.922748000
C	0.670639000	3.263397000	-0.742893000
C	-0.330205000	4.169249000	-1.084790000
C	-1.661760000	3.749047000	-1.131245000
C	-1.980456000	2.430118000	-0.824078000
C	-0.952776000	1.546702000	-0.475466000
N	0.324242000	1.986275000	-0.462958000
H	-2.440922000	4.459716000	-1.397143000
H	-0.067209000	5.198765000	-1.310254000
H	-3.015078000	2.098129000	-0.845041000
C	2.118094000	3.663218000	-0.700316000
H	2.232415000	4.672442000	-0.292371000
H	2.702732000	2.974360000	-0.085853000
H	2.554172000	3.678908000	-1.708139000

C	-1.028662000	-1.994968000	-1.222266000
H	-1.112592000	-2.801691000	-0.496228000
H	-0.169003000	-2.009752000	-1.888705000
C	-2.049897000	-1.143380000	-1.446730000
H	-1.952082000	-0.416569000	-2.253705000
C	-3.374139000	-1.170795000	-0.755823000
H	-3.553424000	-0.208605000	-0.260483000
H	-3.379767000	-1.942815000	0.022822000
C	-4.525062000	-1.428544000	-1.756153000
H	-4.341893000	-2.386641000	-2.263145000
H	-4.520737000	-0.651857000	-2.531612000
C	-5.861490000	-1.459869000	-1.072825000
C	-6.856392000	-0.605203000	-1.309270000
H	-6.001547000	-2.249898000	-0.333068000
H	-7.806249000	-0.677835000	-0.786729000
H	-6.765930000	0.191781000	-2.045481000
C	2.658586000	-2.016657000	-1.375907000
C	3.775837000	-2.212000000	-2.194021000
C	4.339566000	-1.143557000	-2.877097000
C	3.763542000	0.115893000	-2.730167000
C	2.663133000	0.241613000	-1.897679000
N	2.110972000	-0.787621000	-1.217022000
H	5.206808000	-1.290544000	-3.514493000
H	4.189683000	-3.211455000	-2.289255000
H	4.155249000	0.986208000	-3.246099000
C	2.033017000	-3.198390000	-0.696762000
H	1.472375000	-3.804693000	-1.419374000
H	2.799260000	-3.845990000	-0.260229000
H	1.349170000	-2.894582000	0.097383000
H	2.184970000	1.202956000	-1.757392000

69

TS2a, $E_{(\text{SCRF})} = -1245.38687$ a.u., IF = $i263.2388$ cm⁻¹

Sc	0.301818000	-0.095436000	0.079238000
C	-0.068910000	-1.362273000	2.169528000
C	1.334095000	-1.116030000	2.092736000
C	1.542379000	0.292606000	2.188803000
C	0.273678000	0.917338000	2.337452000
C	-0.724893000	-0.101998000	2.322146000
C	2.425719000	-2.146093000	2.135173000
H	3.248710000	-1.922302000	1.446856000
H	2.056056000	-3.148861000	1.904131000
H	2.859527000	-2.194006000	3.142870000
C	2.883382000	0.963713000	2.262431000
H	3.271072000	0.944862000	3.290022000
H	2.837542000	2.016615000	1.964050000
H	3.630486000	0.467418000	1.633336000
C	0.015914000	2.369485000	2.612360000
H	-0.895303000	2.728495000	2.122155000
H	0.844324000	3.006633000	2.287485000
H	-0.112245000	2.539332000	3.689890000

C	-2.173598000	0.119054000	2.649707000
H	-2.298740000	0.258637000	3.732036000
H	-2.799100000	-0.730856000	2.365147000
H	-2.580289000	1.011135000	2.161945000
C	-0.721406000	-2.712092000	2.266922000
H	-0.743140000	-3.059297000	3.308565000
H	-1.757789000	-2.695826000	1.915542000
H	-0.191276000	-3.476180000	1.688085000
C	0.090294000	3.208011000	-0.889521000
C	-0.990739000	4.074646000	-0.984096000
C	-2.288253000	3.570137000	-0.879135000
C	-2.485542000	2.207137000	-0.707347000
C	-1.371275000	1.364659000	-0.618317000
N	-0.131463000	1.881066000	-0.708139000
H	-3.139328000	4.244076000	-0.936756000
H	-0.818023000	5.135786000	-1.133303000
H	-3.494732000	1.814824000	-0.655623000
C	1.501866000	3.703116000	-0.992096000
H	1.529439000	4.795302000	-1.017769000
H	2.102467000	3.373979000	-0.136721000
H	1.980560000	3.337888000	-1.908658000
C	-0.854797000	-1.509275000	-1.285452000
H	-1.045420000	-2.440680000	-0.753798000
H	-0.214666000	-1.594421000	-2.163918000
C	-1.895597000	-0.550342000	-1.317997000
H	-2.018323000	-0.002340000	-2.253338000
C	-3.192779000	-0.899991000	-0.623001000
H	-3.711659000	-0.035631000	-0.203816000
H	-2.976036000	-1.568847000	0.217578000
C	-4.147906000	-1.610128000	-1.607344000
H	-3.633024000	-2.483639000	-2.031953000
H	-4.378806000	-0.939193000	-2.445252000
C	-5.419938000	-2.040925000	-0.936295000
C	-6.633699000	-1.581547000	-1.240119000
H	-5.314550000	-2.783066000	-0.142890000
H	-7.522251000	-1.930814000	-0.721393000
H	-6.788121000	-0.848245000	-2.029901000
C	2.778085000	-1.868772000	-1.435152000
C	4.001910000	-1.973188000	-2.105568000
C	4.758046000	-0.839809000	-2.370167000
C	4.275687000	0.396067000	-1.945147000
C	3.056871000	0.427228000	-1.287103000
N	2.307451000	-0.664733000	-1.033846000
H	5.707903000	-0.918755000	-2.891192000
H	4.350407000	-2.954781000	-2.412275000
H	4.828334000	1.314340000	-2.114019000
C	1.974469000	-3.106877000	-1.168130000
H	1.397772000	-3.395544000	-2.055403000
H	2.634089000	-3.944802000	-0.923472000
H	1.274366000	-2.963826000	-0.343973000

H	2.651303000	1.369282000	-0.935998000
69			
El, $E_{\text{(SCRF)}} = -1245.43191$ a.u.			
Sc	0.405957000	-0.281099000	0.068800000
C	0.447827000	-2.760122000	0.128753000
C	1.693811000	-2.321467000	0.664632000
C	1.428943000	-1.623826000	1.882179000
C	0.017500000	-1.626796000	2.095683000
C	-0.585328000	-2.330073000	1.008916000
C	3.063350000	-2.677691000	0.162912000
H	3.791364000	-1.878889000	0.340784000
H	3.069861000	-2.903298000	-0.907878000
H	3.439170000	-3.572438000	0.677143000
C	2.491002000	-1.147848000	2.833893000
H	2.982697000	-2.003758000	3.314758000
H	2.083306000	-0.529714000	3.639431000
H	3.283883000	-0.574463000	2.337085000
C	-0.714992000	-1.138270000	3.314507000
H	-1.637720000	-0.602776000	3.063236000
H	-0.101544000	-0.470614000	3.926284000
H	-1.000289000	-1.982759000	3.955340000
C	-2.025462000	-2.735304000	0.910027000
H	-2.153399000	-3.768040000	1.263183000
H	-2.396817000	-2.698480000	-0.118751000
H	-2.673553000	-2.106080000	1.527185000
C	0.239443000	-3.655634000	-1.057991000
H	0.007712000	-4.677359000	-0.728965000
H	-0.595013000	-3.326244000	-1.687392000
H	1.130641000	-3.724427000	-1.689352000
C	-0.261180000	2.615342000	1.525434000
C	-0.772018000	3.909554000	1.526711000
C	-1.696977000	4.277382000	0.554621000
C	-2.109746000	3.330229000	-0.371479000
C	-1.582538000	2.037905000	-0.326345000
N	-0.640000000	1.703246000	0.595899000
H	-2.097544000	5.287098000	0.529476000
H	-0.444279000	4.615331000	2.283961000
H	-2.846910000	3.574144000	-1.130246000
C	0.713025000	2.196775000	2.589827000
H	0.233888000	2.228055000	3.575411000
H	1.070926000	1.172783000	2.445511000
H	1.576165000	2.870699000	2.634763000
C	-1.052511000	-0.109276000	-1.561739000
H	-1.524460000	-1.002709000	-1.985280000
H	-0.402085000	0.287763000	-2.364841000
C	-2.109512000	0.961897000	-1.249727000
H	-2.428372000	1.477387000	-2.170500000
C	-3.401348000	0.393165000	-0.610107000
H	-4.022780000	1.223501000	-0.249551000
H	-3.128771000	-0.196876000	0.275296000

C	-4.250927000	-0.455198000	-1.567666000
H	-3.658017000	-1.304555000	-1.935518000
H	-4.516953000	0.145134000	-2.447919000
C	-5.498420000	-0.968797000	-0.908399000
C	-6.741256000	-0.662308000	-1.279831000
H	-5.349058000	-1.637518000	-0.058417000
H	-7.607800000	-1.065195000	-0.762500000
H	-6.940992000	-0.003758000	-2.123376000
C	2.847093000	0.155885000	-2.119905000
C	4.025086000	0.731670000	-2.606748000
C	4.709584000	1.671833000	-1.849061000
C	4.204107000	2.021603000	-0.597644000
C	3.035567000	1.411092000	-0.174714000
N	2.359390000	0.501388000	-0.906461000
H	5.624704000	2.121381000	-2.223653000
H	4.394352000	0.431583000	-3.582644000
H	4.703049000	2.745122000	0.038324000
C	2.095616000	-0.841235000	-2.949773000
H	1.450202000	-0.332063000	-3.676141000
H	2.787294000	-1.473161000	-3.514909000
H	1.459730000	-1.489077000	-2.340789000
H	2.618157000	1.652000000	0.798792000

69

D2, $E_{\text{(SCRF)}} = -1245.395505$ a.u.

Sc	-0.527638000	-0.337333000	-0.010027000
C	0.151137000	-2.714851000	0.201237000
C	0.350917000	-2.118474000	1.483933000
C	-0.927883000	-1.728298000	1.984925000
C	-1.909225000	-2.090447000	1.014141000
C	-1.243935000	-2.703858000	-0.085531000
C	1.652922000	-2.137754000	2.235445000
H	1.911738000	-3.167546000	2.515382000
H	1.604717000	-1.565379000	3.166348000
H	2.494725000	-1.753221000	1.648091000
C	-1.242951000	-1.197839000	3.355885000
H	-1.763281000	-1.961336000	3.948509000
H	-1.898309000	-0.318178000	3.333933000
H	-0.340405000	-0.928157000	3.910351000
C	-3.394888000	-2.004516000	1.199888000
H	-3.918720000	-1.790569000	0.263014000
H	-3.670515000	-1.232129000	1.924245000
H	-3.789033000	-2.956537000	1.580307000
C	-1.908581000	-3.377291000	-1.249675000
H	-2.114736000	-4.430986000	-1.017065000
H	-1.284534000	-3.360278000	-2.148516000
H	-2.862752000	-2.906789000	-1.503242000
C	1.196001000	-3.450065000	-0.586817000
H	1.252585000	-4.495957000	-0.255134000
H	0.970344000	-3.474032000	-1.658096000
H	2.196187000	-3.024524000	-0.458412000

C	-3.581452000	1.173568000	-0.594645000
C	-4.293095000	1.240005000	-1.789928000
C	-3.779160000	0.630346000	-2.939949000
C	-2.557828000	-0.035406000	-2.888924000
C	-1.866585000	-0.080473000	-1.672266000
N	-2.401903000	0.517542000	-0.587435000
H	-4.339142000	0.685184000	-3.870741000
H	-5.242094000	1.766994000	-1.822015000
H	-2.148090000	-0.508129000	-3.777450000
C	-4.059311000	1.804412000	0.679026000
H	-4.336118000	1.038418000	1.412539000
H	-3.271103000	2.418914000	1.127935000
H	-4.934487000	2.435952000	0.505714000
C	1.548819000	-0.206935000	-1.951468000
H	1.630055000	-1.277574000	-2.124904000
H	0.755784000	0.312909000	-2.485750000
C	2.481370000	0.463922000	-1.250850000
H	2.388886000	1.548392000	-1.171366000
C	3.712524000	-0.120195000	-0.634956000
H	3.701384000	-1.213392000	-0.704754000
H	3.752357000	0.141872000	0.432640000
C	4.994415000	0.418970000	-1.313182000
H	4.982293000	1.518361000	-1.270420000
H	4.986753000	0.141539000	-2.373874000
C	6.236889000	-0.102081000	-0.651346000
C	7.140146000	-0.884186000	-1.241603000
H	6.384303000	0.192408000	0.389463000
H	8.024508000	-1.231775000	-0.714657000
H	7.036549000	-1.197769000	-2.278804000
C	0.741466000	2.432070000	1.623779000
C	1.054291000	3.793444000	1.695254000
C	0.750012000	4.635589000	0.634059000
C	0.132741000	4.094070000	-0.491881000
C	-0.151216000	2.737713000	-0.493763000
N	0.141361000	1.908983000	0.531310000
H	0.991751000	5.693600000	0.682140000
H	1.536519000	4.178853000	2.588289000
H	-0.125213000	4.703778000	-1.351443000
C	1.043830000	1.523326000	2.774875000
H	0.170424000	1.431491000	3.431576000
H	1.309269000	0.520620000	2.430776000
H	1.869135000	1.911181000	3.378298000
H	-0.635761000	2.283539000	-1.353441000

69

TS2b, $E_{\text{(SCRF)}} = -1245.383536$ a.u., $\text{IF} = i254.7922$ cm^{-1}

Sc	-0.179693000	-0.082515000	0.063163000
C	0.406033000	-1.382437000	2.076091000
C	0.882765000	-0.057201000	2.317853000
C	-0.249726000	0.807741000	2.383017000
C	-1.422090000	0.015896000	2.198430000

C	-1.018862000	-1.337783000	2.029737000
C	2.283036000	0.306162000	2.721083000
H	2.375580000	0.270961000	3.815072000
H	2.569513000	1.318241000	2.415291000
H	3.025990000	-0.385245000	2.316561000
C	-0.256498000	2.244776000	2.817689000
H	-0.585714000	2.321955000	3.862717000
H	-0.940131000	2.863422000	2.225096000
H	0.737904000	2.696420000	2.767320000
C	-2.826847000	0.532248000	2.318596000
H	-3.561728000	-0.188958000	1.949321000
H	-2.974684000	1.474808000	1.777453000
H	-3.078615000	0.731052000	3.369105000
C	-1.921157000	-2.533311000	1.963004000
H	-2.040358000	-2.975776000	2.961012000
H	-1.524132000	-3.317471000	1.310691000
H	-2.923012000	-2.277500000	1.605918000
C	1.234444000	-2.635059000	2.059918000
H	1.289158000	-3.077585000	3.063760000
H	0.812365000	-3.397395000	1.396387000
H	2.263837000	-2.447707000	1.739329000
C	-2.929269000	-1.706310000	-1.353613000
C	-3.033281000	-3.032687000	-1.761267000
C	-1.888171000	-3.830215000	-1.841075000
C	-0.648285000	-3.280551000	-1.543892000
C	-0.594637000	-1.942355000	-1.144138000
N	-1.708527000	-1.200010000	-1.050491000
H	-1.973833000	-4.873410000	-2.134802000
H	-4.008384000	-3.441631000	-2.007125000
H	0.257222000	-3.876038000	-1.621875000
C	-4.131613000	-0.813978000	-1.263940000
H	-5.053245000	-1.401241000	-1.236516000
H	-4.098524000	-0.187227000	-0.367772000
H	-4.193402000	-0.154219000	-2.139307000
C	1.194184000	-1.137779000	-1.858795000
H	1.675193000	-2.108097000	-1.752020000
H	0.656453000	-1.008497000	-2.797059000
C	1.803819000	-0.025580000	-1.262697000
H	1.611687000	0.929861000	-1.757965000
C	3.154517000	-0.158700000	-0.590025000
H	3.205823000	-1.103463000	-0.034206000
H	3.311927000	0.638959000	0.145408000
C	4.320862000	-0.122980000	-1.604009000
H	4.249121000	0.808360000	-2.186521000
H	4.208109000	-0.948292000	-2.318861000
C	5.661191000	-0.201226000	-0.934259000
C	6.531534000	-1.200355000	-1.082276000
H	5.916034000	0.630173000	-0.273888000
H	7.488589000	-1.205918000	-0.567670000
H	6.326390000	-2.046304000	-1.736347000

C	0.037792000	3.214347000	-0.599112000
C	-0.454727000	4.445860000	-1.042504000
C	-1.730835000	4.537015000	-1.580929000
C	-2.501583000	3.379602000	-1.667268000
C	-1.953893000	2.193191000	-1.206784000
N	-0.716042000	2.093017000	-0.677709000
H	-2.117499000	5.491446000	-1.926619000
H	0.176085000	5.325834000	-0.959531000
H	-3.504844000	3.391719000	-2.080127000
C	1.431724000	3.124300000	-0.054500000
H	1.655917000	3.987420000	0.579559000
H	1.580136000	2.215544000	0.532384000
H	2.165167000	3.122734000	-0.870475000
H	-2.517130000	1.269073000	-1.258733000

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E2, $E_{\text{(SCRF)}} = -1245.431343$ a.u.

Sc	0.301191000	-0.005153000	0.221923000
C	-0.286314000	0.484549000	2.558720000
C	-0.326102000	-0.933142000	2.431300000
C	0.998536000	-1.386862000	2.158992000
C	1.861741000	-0.250586000	2.142828000
C	1.067910000	0.908467000	2.388377000
C	-1.507183000	-1.807309000	2.736501000
H	-1.491368000	-2.102376000	3.794485000
H	-1.513758000	-2.735015000	2.153920000
H	-2.456192000	-1.297312000	2.556950000
C	1.452380000	-2.817415000	2.100997000
H	1.820016000	-3.144407000	3.083066000
H	2.270502000	-2.968823000	1.388383000
H	0.640233000	-3.498283000	1.827352000
C	3.361045000	-0.325432000	2.071257000
H	3.822677000	0.650481000	1.892248000
H	3.714698000	-1.015478000	1.295610000
H	3.768710000	-0.693564000	3.022202000
C	1.560925000	2.307768000	2.627096000
H	1.570435000	2.529385000	3.702364000
H	0.926791000	3.064430000	2.152083000
H	2.582826000	2.456512000	2.266343000
C	-1.422734000	1.369264000	2.978810000
H	-1.476211000	1.433206000	4.074289000
H	-1.306178000	2.393413000	2.608656000
H	-2.389925000	0.994289000	2.631657000
C	1.556359000	2.812111000	-1.084376000
C	1.448802000	4.045026000	-1.720608000
C	0.191535000	4.527732000	-2.068098000
C	-0.926550000	3.767363000	-1.757002000
C	-0.771279000	2.544409000	-1.102724000
N	0.461434000	2.070920000	-0.783768000
H	0.087725000	5.484611000	-2.572064000
H	2.347147000	4.612895000	-1.942052000

H	-1.925298000	4.110765000	-2.007550000
C	2.911952000	2.269263000	-0.738451000
H	3.565643000	3.062780000	-0.363260000
H	2.854094000	1.498521000	0.035917000
H	3.401512000	1.846861000	-1.625262000
C	-1.973859000	1.736108000	-0.698869000
H	-2.312786000	2.119604000	0.277534000
H	-2.786172000	1.987535000	-1.397854000
C	-1.734699000	0.225305000	-0.581123000
H	-1.439456000	-0.126276000	-1.600949000
C	-3.015123000	-0.506359000	-0.175590000
H	-3.408099000	-0.060670000	0.749284000
H	-2.794739000	-1.551651000	0.078905000
C	-4.150852000	-0.506051000	-1.222255000
H	-3.759528000	-0.929409000	-2.161643000
H	-4.462889000	0.520824000	-1.449779000
C	-5.343993000	-1.297027000	-0.771745000
C	-6.558966000	-0.795043000	-0.549334000
H	-5.174761000	-2.363072000	-0.604130000
H	-7.383017000	-1.417752000	-0.211416000
H	-6.779255000	0.259723000	-0.705841000
C	0.773071000	-2.741114000	-1.558514000
C	1.464119000	-3.616199000	-2.400816000
C	2.743505000	-3.299013000	-2.839187000
C	3.319157000	-2.102768000	-2.415988000
C	2.579932000	-1.284275000	-1.577589000
N	1.334303000	-1.577881000	-1.153512000
H	3.285232000	-3.975454000	-3.494025000
H	0.988174000	-4.543518000	-2.703916000
H	4.318496000	-1.810381000	-2.720582000
C	-0.615613000	-3.056728000	-1.095751000
H	-0.802474000	-4.133649000	-1.121280000
H	-0.786238000	-2.708129000	-0.072028000
H	-1.360116000	-2.574188000	-1.740137000
H	3.002170000	-0.351742000	-1.218062000

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D3, $E_{\text{(SCRF)}} = -957.9035714$ a.u.

Sc	0.435540000	-0.213951000	-0.229713000
C	1.174237000	-2.333188000	0.709732000
C	1.858459000	-2.173958000	-0.531906000
C	2.705957000	-1.025597000	-0.422977000
C	2.558050000	-0.490195000	0.890262000
C	1.597413000	-1.285048000	1.587228000
C	1.827151000	-3.117043000	-1.700917000
H	1.905928000	-2.598585000	-2.663200000
H	0.920052000	-3.728823000	-1.720996000
H	2.675090000	-3.812626000	-1.649905000
C	3.668676000	-0.555939000	-1.477440000
H	4.586199000	-1.158624000	-1.456623000
H	3.968304000	0.485354000	-1.326906000

H	3.258631000	-0.643775000	-2.490381000
C	3.326316000	0.659185000	1.472469000
H	2.733860000	1.220693000	2.200950000
H	3.663076000	1.362444000	0.705086000
H	4.221583000	0.294125000	1.992534000
C	1.203352000	-1.131223000	3.028238000
H	1.849581000	-1.742823000	3.671667000
H	0.172532000	-1.450657000	3.213348000
H	1.293282000	-0.094806000	3.365249000
C	0.250977000	-3.458667000	1.082446000
H	0.810665000	-4.266008000	1.572813000
H	-0.526005000	-3.143424000	1.787540000
H	-0.242736000	-3.902529000	0.211637000
C	0.679697000	3.154939000	-0.819228000
C	0.250900000	4.198261000	-0.005778000
C	-0.382468000	3.920308000	1.212163000
C	-0.581153000	2.602930000	1.611600000
C	-0.139702000	1.571784000	0.775147000
N	0.463999000	1.886961000	-0.400466000
H	-0.713097000	4.742868000	1.841903000
H	0.412277000	5.224831000	-0.320435000
H	-1.068353000	2.376430000	2.555649000
C	1.362229000	3.362808000	-2.137412000
H	1.519718000	4.424825000	-2.340481000
H	2.336832000	2.862060000	-2.154124000
H	0.764360000	2.946369000	-2.957274000
C	-1.219190000	-1.271364000	-2.007002000
H	-1.177173000	-2.319692000	-1.713882000
H	-0.617305000	-0.979703000	-2.869245000
C	-2.101171000	-0.418761000	-1.443225000
H	-2.155502000	0.603026000	-1.827669000
C	-3.071214000	-0.759809000	-0.357145000
H	-2.931117000	-0.075848000	0.491944000
H	-2.899482000	-1.781724000	0.004305000
C	-4.535576000	-0.616562000	-0.845371000
H	-4.681533000	-1.283409000	-1.706428000
H	-4.705688000	0.408258000	-1.198192000
C	-5.515499000	-0.953731000	0.240716000
C	-6.377578000	-0.088840000	0.774478000
H	-5.501217000	-1.985215000	0.595994000
H	-7.072787000	-0.386554000	1.554447000
H	-6.433479000	0.946055000	0.441454000

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TS2c, $E_{(\text{SCRF})} = -957.8856285$ a.u., $\text{IF} = i274.4601 \text{ cm}^{-1}$

Sc	0.536068000	-0.159641000	-0.319951000
C	1.060222000	-2.428454000	0.409989000
C	1.929023000	-2.130118000	-0.677763000
C	2.791996000	-1.058539000	-0.274251000
C	2.450826000	-0.696198000	1.061631000
C	1.360763000	-1.525040000	1.476410000

C	2.013297000	-2.878072000	-1.977404000
H	2.375413000	-2.246761000	-2.795609000
H	1.045968000	-3.290655000	-2.280381000
H	2.712034000	-3.720817000	-1.893379000
C	3.931973000	-0.514480000	-1.089185000
H	4.805708000	-1.174986000	-1.015358000
H	4.250077000	0.475166000	-0.748805000
H	3.686256000	-0.437451000	-2.154522000
C	3.162639000	0.293828000	1.939135000
H	2.473578000	0.892569000	2.545638000
H	3.787918000	0.981806000	1.362923000
H	3.827955000	-0.228226000	2.639150000
C	0.737960000	-1.533703000	2.845822000
H	1.294092000	-2.199367000	3.519089000
H	-0.296277000	-1.893542000	2.829130000
H	0.739157000	-0.541348000	3.309735000
C	0.071811000	-3.556250000	0.470605000
H	0.526709000	-4.435305000	0.945817000
H	-0.817579000	-3.306317000	1.059772000
H	-0.260030000	-3.868630000	-0.524090000
C	1.018533000	3.209422000	-0.284299000
C	0.206545000	4.244917000	0.164142000
C	-1.124371000	3.984624000	0.501811000
C	-1.645409000	2.704495000	0.351792000
C	-0.798334000	1.687737000	-0.095749000
N	0.491800000	1.964325000	-0.378864000
H	-1.755171000	4.790011000	0.869093000
H	0.612601000	5.247733000	0.250421000
H	-2.690511000	2.513317000	0.571424000
C	2.452875000	3.399749000	-0.667847000
H	2.728983000	4.456588000	-0.647903000
H	3.113226000	2.863815000	0.023149000
H	2.641035000	3.012589000	-1.675196000
C	-1.097816000	-0.788669000	-1.711566000
H	-1.326963000	-1.829167000	-1.482245000
H	-0.770801000	-0.609640000	-2.738845000
C	-1.894443000	0.207208000	-1.074754000
H	-2.222523000	1.043421000	-1.693190000
C	-2.899297000	-0.254388000	-0.039815000
H	-3.159207000	0.534818000	0.670324000
H	-2.467533000	-1.076165000	0.550058000
C	-4.197228000	-0.747908000	-0.717180000
H	-3.946816000	-1.549405000	-1.425660000
H	-4.634966000	0.069670000	-1.304382000
C	-5.194358000	-1.242418000	0.290746000
C	-6.383721000	-0.685593000	0.517693000
H	-4.898427000	-2.121564000	0.865960000
H	-7.069322000	-1.088084000	1.258193000
H	-6.725543000	0.185190000	-0.039078000

E3, $E_{\text{(SCRF)}} = -957.9347774$ a.u.

Sc	0.582608000	0.194950000	-0.096149000
C	2.011068000	-1.790816000	-0.252341000
C	2.519838000	-0.820535000	-1.159110000
C	2.956666000	0.311926000	-0.396677000
C	2.725983000	0.031048000	0.984410000
C	2.117752000	-1.259965000	1.071206000
C	2.669133000	-0.988758000	-2.642076000
H	2.632162000	-0.031892000	-3.172603000
H	1.889136000	-1.630563000	-3.061575000
H	3.636388000	-1.450186000	-2.880965000
C	3.641331000	1.527564000	-0.958663000
H	4.707636000	1.325275000	-1.123289000
H	3.584856000	2.387630000	-0.283347000
H	3.227686000	1.832216000	-1.926806000
C	3.131257000	0.884589000	2.153172000
H	2.421633000	0.822530000	2.986323000
H	3.241720000	1.939161000	1.882617000
H	4.102518000	0.555622000	2.545310000
C	1.764580000	-1.980708000	2.343122000
H	2.627203000	-2.547334000	2.717586000
H	0.952943000	-2.701435000	2.198816000
H	1.466827000	-1.295668000	3.144989000
C	1.533216000	-3.166155000	-0.610766000
H	2.365404000	-3.881311000	-0.569761000
H	0.765399000	-3.534364000	0.077429000
H	1.123048000	-3.206176000	-1.623818000
C	-0.967101000	3.037301000	0.555079000
C	-2.045079000	3.903048000	0.410603000
C	-3.180194000	3.470978000	-0.273484000
C	-3.217822000	2.181752000	-0.790977000
C	-2.115830000	1.346301000	-0.618085000
N	-1.011991000	1.784034000	0.040829000
H	-4.027259000	4.139057000	-0.402206000
H	-1.990980000	4.904571000	0.824430000
H	-4.087291000	1.818082000	-1.329322000
C	0.286421000	3.440358000	1.277066000
H	0.236664000	4.481111000	1.605834000
H	0.448160000	2.822462000	2.169392000
H	1.169013000	3.346094000	0.630746000
C	-0.716980000	-0.435273000	-1.716784000
H	-0.704073000	-1.470050000	-2.073289000
H	-0.526806000	0.202962000	-2.596205000
C	-2.090357000	-0.086968000	-1.102909000
H	-2.903696000	-0.193753000	-1.836797000
C	-2.442106000	-1.014075000	0.090519000
H	-3.294680000	-0.602736000	0.646213000
H	-1.604975000	-1.022407000	0.823440000
C	-2.763277000	-2.460789000	-0.308977000
H	-1.911987000	-2.890410000	-0.854505000

H	-3.612052000	-2.452853000	-1.004878000
C	-3.088873000	-3.320353000	0.879034000
C	-4.271258000	-3.892371000	1.104241000
H	-2.281780000	-3.471706000	1.599371000
H	-4.450207000	-4.506640000	1.982338000
H	-5.103644000	-3.778061000	0.412255000
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D4, $E_{\text{(SCRF)}} = -957.9033762$ a.u.			
Sc	-0.141121000	-0.278437000	-0.351062000
C	-1.626930000	-2.063389000	0.299212000
C	-0.474062000	-2.694353000	-0.260625000
C	0.644404000	-2.398737000	0.575131000
C	0.179665000	-1.588582000	1.660396000
C	-1.222633000	-1.390919000	1.493755000
C	-0.487453000	-3.617024000	-1.445727000
H	-0.849749000	-4.609994000	-1.148886000
H	0.508796000	-3.760535000	-1.874942000
H	-1.152412000	-3.265345000	-2.242474000
C	2.033038000	-2.954773000	0.433486000
H	2.131306000	-3.888503000	1.002755000
H	2.798383000	-2.271658000	0.817523000
H	2.284963000	-3.191480000	-0.605222000
C	1.004618000	-1.128792000	2.829953000
H	0.630585000	-0.194844000	3.261792000
H	2.056945000	-0.976477000	2.567459000
H	0.984425000	-1.879268000	3.631184000
C	-2.140922000	-0.680782000	2.444890000
H	-2.625909000	-1.400780000	3.116990000
H	-2.936046000	-0.139909000	1.922071000
H	-1.607301000	0.036910000	3.075035000
C	-3.035905000	-2.222722000	-0.192124000
H	-3.478380000	-3.145762000	0.205782000
H	-3.673759000	-1.392640000	0.123335000
H	-3.087251000	-2.283374000	-1.283761000
C	-1.350348000	2.829533000	0.484824000
C	-2.463369000	3.478811000	-0.038622000
C	-3.218322000	2.868760000	-1.048169000
C	-2.860707000	1.611526000	-1.523932000
C	-1.738422000	0.980970000	-0.976769000
N	-1.027665000	1.611906000	-0.009030000
H	-4.087449000	3.383701000	-1.450555000
H	-2.741718000	4.456900000	0.341995000
H	-3.443119000	1.125468000	-2.301263000
C	-0.484693000	3.417820000	1.557823000
H	-0.940038000	4.312900000	1.988810000
H	-0.314120000	2.694790000	2.362659000
H	0.496218000	3.701543000	1.156869000
C	1.066678000	-0.720041000	-2.732912000
H	1.623706000	-1.651991000	-2.657539000
H	0.089259000	-0.765787000	-3.214379000

C	1.606036000	0.456508000	-2.359548000
H	1.023878000	1.369219000	-2.520567000
C	2.956426000	0.629853000	-1.732017000
H	3.528464000	1.366958000	-2.310066000
H	3.514668000	-0.312997000	-1.764771000
C	2.850173000	1.130516000	-0.276168000
H	2.284512000	0.381229000	0.320294000
H	2.284401000	2.070285000	-0.239925000
C	4.189680000	1.316525000	0.377915000
C	4.635187000	2.475790000	0.860959000
H	4.823054000	0.430384000	0.431875000
H	5.619196000	2.560485000	1.313067000
H	4.038853000	3.385415000	0.819980000

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TS2d, $E_{(\text{SCRF})} = -957.8833209$ a.u., IF = $i292.7684$ cm⁻¹

Sc	-0.086242000	-0.051884000	-0.347636000
C	-0.228181000	1.417182000	1.564358000
C	1.079224000	1.606099000	1.008003000
C	0.924086000	2.166802000	-0.292317000
C	-0.476055000	2.345822000	-0.533008000
C	-1.183421000	1.905872000	0.622185000
C	2.367608000	1.425174000	1.756046000
H	2.587180000	2.326214000	2.344286000
H	3.220442000	1.262027000	1.091764000
H	2.326287000	0.591259000	2.464232000
C	2.015780000	2.634254000	-1.213457000
H	2.087312000	3.729617000	-1.191492000
H	1.840161000	2.354870000	-2.259665000
H	2.995023000	2.244287000	-0.924569000
C	-1.057064000	3.001484000	-1.754313000
H	-2.127670000	2.803781000	-1.860580000
H	-0.562405000	2.683684000	-2.680277000
H	-0.939525000	4.091738000	-1.697872000
C	-2.661396000	2.006064000	0.857248000
H	-2.897583000	2.919687000	1.418192000
H	-3.044921000	1.162914000	1.441247000
H	-3.226735000	2.050101000	-0.078151000
C	-0.524298000	0.966477000	2.966829000
H	-0.477496000	1.815072000	3.662108000
H	-1.524328000	0.531401000	3.054572000
H	0.194805000	0.221985000	3.324440000
C	-3.301994000	-1.001675000	-1.045601000
C	-4.181765000	-1.702372000	-0.223544000
C	-3.710172000	-2.324363000	0.937853000
C	-2.355105000	-2.284045000	1.248503000
C	-1.511648000	-1.570576000	0.395091000
N	-1.996995000	-0.943721000	-0.695596000
H	-4.406899000	-2.844878000	1.590042000
H	-5.233302000	-1.755695000	-0.487562000
H	-1.964065000	-2.792875000	2.124963000

C	-3.724265000	-0.333253000	-2.317222000
H	-4.810187000	-0.223623000	-2.368514000
H	-3.266616000	0.656378000	-2.412809000
H	-3.405339000	-0.926729000	-3.183427000
C	0.287790000	-2.558736000	0.087816000
H	0.407392000	-2.865956000	1.126349000
H	-0.332252000	-3.229094000	-0.503777000
C	1.350031000	-1.881635000	-0.540403000
H	1.372145000	-1.976431000	-1.635400000
C	2.725111000	-1.783304000	0.111250000
H	3.101667000	-2.798976000	0.301063000
H	2.669906000	-1.299778000	1.095939000
C	3.748732000	-1.056524000	-0.771001000
H	3.387815000	-0.034414000	-0.969960000
H	3.808224000	-1.558059000	-1.746409000
C	5.114803000	-1.006191000	-0.151133000
C	6.211862000	-1.540282000	-0.687423000
H	5.187959000	-0.500872000	0.813831000
H	7.176916000	-1.479100000	-0.192118000
H	6.188166000	-2.056568000	-1.645479000

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E4, $E_{\text{(SCRF)}} = -957.9330353$ a.u.

Sc	-0.105597000	0.279576000	-0.452214000
C	-0.135834000	1.663718000	1.520406000
C	1.186827000	1.751081000	0.986723000
C	1.096295000	2.384504000	-0.289820000
C	-0.274007000	2.718456000	-0.527309000
C	-1.036015000	2.279929000	0.595697000
C	2.449807000	1.410286000	1.718614000
H	2.814449000	2.289823000	2.266088000
H	3.252083000	1.094429000	1.046200000
H	2.296514000	0.615489000	2.453708000
C	2.251159000	2.751073000	-1.179559000
H	2.615303000	3.758569000	-0.938606000
H	1.976981000	2.762597000	-2.240540000
H	3.099233000	2.069820000	-1.060140000
C	-0.784798000	3.478260000	-1.720067000
H	-1.864135000	3.362008000	-1.859082000
H	-0.293754000	3.178352000	-2.653663000
H	-0.594202000	4.552754000	-1.601172000
C	-2.493054000	2.538301000	0.859189000
H	-2.604801000	3.329566000	1.611605000
H	-3.018459000	1.657772000	1.246516000
H	-3.022364000	2.878692000	-0.035336000
C	-0.508647000	1.148193000	2.880469000
H	-0.474295000	1.959529000	3.619805000
H	-1.524756000	0.740249000	2.903860000
H	0.176741000	0.370192000	3.230916000
C	-3.081649000	-1.033660000	-0.897330000
C	-4.059370000	-1.981018000	-0.618801000

C	-3.738021000	-3.074478000	0.184108000
C	-2.445187000	-3.206597000	0.675252000
C	-1.497839000	-2.227944000	0.377067000
N	-1.833511000	-1.153708000	-0.381481000
H	-4.489852000	-3.825389000	0.410480000
H	-5.054840000	-1.867743000	-1.035817000
H	-2.159640000	-4.060708000	1.281171000
C	-3.334382000	0.117852000	-1.825823000
H	-4.396986000	0.369965000	-1.873346000
H	-2.795441000	1.019614000	-1.511036000
H	-3.013892000	-0.134901000	-2.845624000
C	-0.069377000	-2.321395000	0.858762000
H	-0.023472000	-1.947630000	1.895134000
H	0.185454000	-3.390826000	0.936939000
C	0.943791000	-1.565264000	-0.023450000
H	0.772716000	-1.940815000	-1.066474000
C	2.386946000	-1.890093000	0.339641000
H	2.523456000	-2.977125000	0.464491000
H	2.639712000	-1.446040000	1.312356000
C	3.389722000	-1.406301000	-0.717206000
H	3.242487000	-0.323428000	-0.872396000
H	3.170212000	-1.890635000	-1.679341000
C	4.819236000	-1.667353000	-0.341965000
C	5.666874000	-2.419396000	-1.043615000
H	5.162201000	-1.205154000	0.585821000
H	6.691290000	-2.580017000	-0.719054000
H	5.369305000	-2.903074000	-1.972510000

69

F1, $E_{\text{(SCRF)}} = -1245.433461$ a.u.

Sc	-0.726663000	-0.148947000	0.235924000
C	-1.616798000	-0.329355000	2.516713000
C	-1.948886000	0.980246000	2.066395000
C	-2.872458000	0.860386000	0.988271000
C	-3.120910000	-0.529167000	0.773544000
C	-2.333548000	-1.266227000	1.710493000
C	-1.492506000	2.261589000	2.701465000
H	-1.530099000	3.105802000	2.004996000
H	-0.471864000	2.187747000	3.092395000
H	-2.138572000	2.524129000	3.549889000
C	-3.594942000	1.990204000	0.312585000
H	-4.505379000	2.254462000	0.867256000
H	-3.909791000	1.733114000	-0.704577000
H	-2.984572000	2.897137000	0.252337000
C	-4.203841000	-1.080960000	-0.112955000
H	-4.123439000	-2.164103000	-0.242669000
H	-4.225867000	-0.625355000	-1.110569000
H	-5.188166000	-0.891677000	0.335285000
C	-2.358448000	-2.752843000	1.933694000
H	-3.043728000	-3.010456000	2.752093000
H	-1.373759000	-3.146778000	2.209080000

H	-2.698371000	-3.302335000	1.050334000
C	-0.807730000	-0.661360000	3.734640000
H	-1.447125000	-0.663132000	4.627740000
H	-0.348330000	-1.652502000	3.667745000
H	-0.007311000	0.063530000	3.910181000
C	-0.037006000	-2.801388000	-1.631430000
C	0.802675000	-3.796340000	-2.128119000
C	2.167996000	-3.701507000	-1.897780000
C	2.665930000	-2.613682000	-1.187198000
C	1.791738000	-1.638908000	-0.710430000
N	0.449979000	-1.753509000	-0.929281000
H	2.842774000	-4.469675000	-2.265621000
H	0.381141000	-4.631335000	-2.679107000
H	3.728473000	-2.529512000	-0.997589000
C	-1.514843000	-2.867009000	-1.886140000
H	-2.076685000	-2.213575000	-1.211999000
H	-1.748655000	-2.570487000	-2.916280000
H	-1.891080000	-3.885996000	-1.751691000
C	1.236932000	-0.142033000	1.200481000
H	1.309070000	-0.959568000	1.934551000
H	1.499035000	0.777244000	1.741916000
C	2.240099000	-0.406437000	0.060079000
H	2.176009000	0.427882000	-0.664464000
C	3.718534000	-0.474097000	0.494386000
H	4.358794000	-0.647459000	-0.381141000
H	3.857594000	-1.330825000	1.169488000
C	4.224266000	0.802882000	1.179226000
H	3.648633000	0.975668000	2.099151000
H	4.049185000	1.668034000	0.523641000
C	5.684508000	0.719780000	1.519646000
C	6.632457000	1.514623000	1.023624000
H	5.964141000	-0.063708000	2.226362000
H	7.675708000	1.406141000	1.307445000
H	6.400693000	2.311246000	0.318404000
C	-0.928296000	1.879526000	-2.345551000
C	-0.721534000	3.068208000	-3.046064000
C	-0.013001000	4.107619000	-2.452338000
C	0.479730000	3.935766000	-1.160939000
C	0.235073000	2.729983000	-0.520701000
N	-0.454248000	1.720947000	-1.089224000
H	0.151657000	5.037171000	-2.989722000
H	-1.116482000	3.169710000	-4.052032000
H	1.039250000	4.715534000	-0.655143000
C	-1.654494000	0.720725000	-2.961644000
H	-2.190784000	1.020853000	-3.865355000
H	-0.948252000	-0.070864000	-3.241338000
H	-2.388896000	0.296996000	-2.265908000
H	0.600670000	2.551406000	0.486323000

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TS3a, $E_{\text{(SCRF)}} = -1245.395868$ a.u., $\text{IF} = i1298.5981 \text{ cm}^{-1}$

Sc	-0.688474000	-0.296341000	-0.223865000
C	-0.896648000	-2.695095000	-0.753376000
C	-1.586508000	-2.487536000	0.477120000
C	-2.708638000	-1.647793000	0.216400000
C	-2.703920000	-1.320726000	-1.170661000
C	-1.575969000	-1.964547000	-1.772960000
C	-1.264860000	-3.152215000	1.784060000
H	-1.641441000	-2.580333000	2.637735000
H	-0.187096000	-3.288534000	1.923437000
H	-1.723350000	-4.148651000	1.835739000
C	-3.771274000	-1.269354000	1.205335000
H	-4.544385000	-2.047156000	1.260663000
H	-4.274823000	-0.337052000	0.930768000
H	-3.368702000	-1.143997000	2.215839000
C	-3.788652000	-0.568148000	-1.888705000
H	-3.451071000	-0.161426000	-2.846777000
H	-4.185588000	0.262532000	-1.294277000
H	-4.635962000	-1.231648000	-2.106395000
C	-1.252742000	-2.031993000	-3.240361000
H	-1.547422000	-3.005180000	-3.654653000
H	-0.181961000	-1.913285000	-3.444766000
H	-1.789334000	-1.272280000	-3.816539000
C	0.236776000	-3.652331000	-0.978753000
H	-0.151924000	-4.646655000	-1.236688000
H	0.886699000	-3.343529000	-1.805214000
H	0.860425000	-3.775010000	-0.087921000
C	0.267743000	2.101399000	-2.131821000
C	1.001240000	3.224529000	-2.489025000
C	2.238724000	3.441536000	-1.885668000
C	2.713834000	2.520333000	-0.965419000
C	1.949098000	1.390848000	-0.653016000
N	0.735582000	1.208464000	-1.223730000
H	2.824521000	4.322115000	-2.134411000
H	0.604645000	3.920440000	-3.221282000
H	3.672513000	2.672506000	-0.481842000
C	-1.076151000	1.812632000	-2.733540000
H	-1.841810000	1.662165000	-1.959735000
H	-1.417017000	2.638100000	-3.363698000
H	-1.038908000	0.910960000	-3.355783000
C	1.466142000	-0.803563000	0.504392000
H	1.470281000	-1.414446000	-0.415463000
H	1.805342000	-1.485750000	1.291285000
C	2.449911000	0.354716000	0.337970000
H	2.545194000	0.876836000	1.305295000
C	3.871570000	-0.125519000	-0.054413000
H	4.526656000	0.737719000	-0.221071000
H	3.810876000	-0.655700000	-1.015656000
C	4.542438000	-1.024429000	0.994166000
H	3.953292000	-1.943000000	1.124978000
H	4.554685000	-0.511726000	1.966003000

C	5.944298000	-1.392583000	0.600038000
C	7.040080000	-1.062579000	1.283196000
H	6.045163000	-1.969279000	-0.321194000
H	8.031217000	-1.357153000	0.949244000
H	6.988029000	-0.492790000	2.209437000
C	-2.237044000	2.197468000	1.663632000
C	-2.214745000	2.421833000	3.040436000
C	-1.423877000	1.620775000	3.865636000
C	-0.652429000	0.603410000	3.307884000
C	-0.711020000	0.423984000	1.927764000
N	-1.481251000	1.205750000	1.150328000
H	-1.414241000	1.794604000	4.938625000
H	-2.818965000	3.219346000	3.461769000
H	-0.024656000	-0.031160000	3.926613000
C	-3.057332000	3.024532000	0.720890000
H	-3.728333000	3.696329000	1.261692000
H	-2.410179000	3.636546000	0.081014000
H	-3.662153000	2.386745000	0.067564000
H	0.337159000	-0.295070000	1.343440000

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G1, $E_{\text{(SCRF)}} = -1245.431665$ a.u.

Sc	0.701673000	-0.322415000	0.045785000
C	0.202010000	-2.622026000	0.808573000
C	0.933476000	-2.726084000	-0.416339000
C	2.245726000	-2.222026000	-0.189121000
C	2.320383000	-1.776433000	1.163491000
C	1.057916000	-2.035279000	1.783601000
C	0.452072000	-3.363830000	-1.687793000
H	0.857748000	-2.865016000	-2.573957000
H	-0.639524000	-3.351547000	-1.769712000
H	0.762800000	-4.415791000	-1.736720000
C	3.385734000	-2.257175000	-1.162213000
H	4.006636000	-3.146936000	-0.991999000
H	4.039176000	-1.383866000	-1.067455000
H	3.036397000	-2.297053000	-2.197508000
C	3.564466000	-1.296687000	1.855619000
H	3.347390000	-0.613333000	2.684010000
H	4.242084000	-0.783871000	1.166034000
H	4.121131000	-2.142360000	2.281180000
C	0.742476000	-1.922317000	3.247843000
H	0.815487000	-2.907749000	3.727554000
H	-0.273993000	-1.557099000	3.437206000
H	1.444257000	-1.267138000	3.772458000
C	-1.153341000	-3.203800000	1.097947000
H	-1.049894000	-4.185979000	1.578470000
H	-1.742830000	-2.579979000	1.780095000
H	-1.743725000	-3.361859000	0.189937000
C	-0.328394000	2.102111000	1.757716000
C	-0.873217000	3.353640000	2.017368000
C	-1.979872000	3.777323000	1.286017000

C	-2.525402000	2.919625000	0.344451000
C	-1.949545000	1.663651000	0.129429000
N	-0.842403000	1.279218000	0.805711000
H	-2.413143000	4.758589000	1.457861000
H	-0.432254000	3.984817000	2.782143000
H	-3.399318000	3.209225000	-0.230880000
C	0.831758000	1.586863000	2.557372000
H	1.628690000	1.170843000	1.924614000
H	1.291057000	2.384835000	3.146543000
H	0.501765000	0.806683000	3.251247000
C	-1.740084000	-0.449354000	-1.264266000
H	-1.547279000	-1.132575000	-0.422577000
H	-2.225891000	-1.063307000	-2.027019000
C	-2.627018000	0.710696000	-0.834105000
H	-2.882805000	1.294081000	-1.730230000
C	-3.956888000	0.219296000	-0.207675000
H	-4.523148000	1.085552000	0.154244000
H	-3.728224000	-0.388201000	0.680158000
C	-4.855751000	-0.574049000	-1.168771000
H	-4.341616000	-1.490893000	-1.490913000
H	-5.042319000	0.020082000	-2.073571000
C	-6.163501000	-0.945294000	-0.529226000
C	-7.358720000	-0.527518000	-0.944985000
H	-6.100960000	-1.601542000	0.340616000
H	-8.274145000	-0.827918000	-0.442725000
H	-7.469667000	0.122789000	-1.810993000
C	3.164956000	1.969262000	-0.831686000
C	3.584725000	2.314296000	-2.112885000
C	2.983303000	1.721325000	-3.228154000
C	1.971371000	0.784121000	-3.052148000
C	1.578050000	0.455501000	-1.750221000
N	2.175753000	1.056674000	-0.699172000
H	3.315236000	1.996842000	-4.226456000
H	4.378355000	3.044836000	-2.237729000
H	1.497524000	0.312980000	-3.909050000
C	3.754332000	2.585271000	0.402471000
H	4.642043000	3.175878000	0.162063000
H	3.031875000	3.252444000	0.888495000
H	4.040051000	1.817601000	1.129221000
H	-0.803677000	-0.101239000	-1.735756000

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$P_{\text{mono}}, E_{(\text{SCRF})} = -521.9758354 \text{ a.u.}$

C	2.615415000	0.815976000	-0.118425000
C	3.341743000	-0.142360000	-0.833293000
C	2.763308000	-1.387256000	-1.061007000
C	1.485422000	-1.636782000	-0.571811000
C	0.825650000	-0.624973000	0.133950000
N	1.385220000	0.571999000	0.351377000
H	3.302866000	-2.153391000	-1.612969000
H	4.338349000	0.087096000	-1.200456000

H	1.002842000	-2.597401000	-0.731168000
C	3.177607000	2.182404000	0.168308000
H	3.241858000	2.348638000	1.249792000
H	4.174517000	2.312751000	-0.263483000
H	2.517068000	2.958190000	-0.234939000
C	-0.573622000	-0.632357000	2.208864000
H	-0.266907000	0.388762000	2.458142000
H	-1.563535000	-0.818249000	2.638937000
C	-0.573035000	-0.824989000	0.687193000
H	-0.873121000	-1.859798000	0.466146000
C	-1.552131000	0.119800000	-0.037669000
H	-1.440853000	-0.021110000	-1.121164000
H	-1.250111000	1.154599000	0.170809000
C	-3.029187000	-0.084897000	0.329947000
H	-3.169508000	0.108416000	1.403100000
H	-3.316164000	-1.131582000	0.157936000
C	-3.936849000	0.821134000	-0.449578000
C	-4.899801000	0.420246000	-1.280117000
H	-3.764943000	1.891451000	-0.317162000
H	-5.520698000	1.129024000	-1.822447000
H	-5.106508000	-0.635718000	-1.447251000
H	0.131193000	-1.321355000	2.688370000

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F2, $E_{\text{(SCRF)}} = -1532.903503$ a.u.

Sc	-0.479386000	-0.102950000	-0.569004000
C	-0.407269000	-1.137448000	-2.847089000
C	-1.438744000	-1.829259000	-2.150353000
C	-2.518908000	-0.921981000	-1.940247000
C	-2.139646000	0.341821000	-2.481882000
C	-0.828586000	0.212391000	-3.028063000
C	-1.462674000	-3.307768000	-1.892014000
H	-2.127395000	-3.574978000	-1.064775000
H	-0.468473000	-3.699379000	-1.653817000
H	-1.817874000	-3.850669000	-2.778615000
C	-3.931052000	-1.317707000	-1.607422000
H	-4.504128000	-1.442444000	-2.536905000
H	-4.469575000	-0.575258000	-1.009239000
H	-3.982018000	-2.273755000	-1.079548000
C	-3.091947000	1.464892000	-2.786102000
H	-2.570376000	2.388566000	-3.051288000
H	-3.785758000	1.692364000	-1.969281000
H	-3.711440000	1.193111000	-3.652330000
C	-0.107232000	1.264518000	-3.820491000
H	-0.447839000	1.268471000	-4.864954000
H	0.973681000	1.095820000	-3.838186000
H	-0.273562000	2.271882000	-3.423887000
C	0.782967000	-1.788530000	-3.485851000
H	0.503630000	-2.193434000	-4.468024000
H	1.607832000	-1.090047000	-3.650184000
H	1.169325000	-2.624243000	-2.893468000

C	0.085898000	3.288649000	-0.173876000
C	0.814055000	4.431694000	0.158979000
C	2.150348000	4.305009000	0.504047000
C	2.726468000	3.040148000	0.493720000
C	1.960987000	1.930455000	0.135236000
N	0.646511000	2.060971000	-0.188264000
H	2.740503000	5.177648000	0.770582000
H	0.325743000	5.401612000	0.141559000
H	3.771546000	2.919388000	0.750507000
C	-1.363795000	3.427673000	-0.527665000
H	-1.496380000	4.138516000	-1.351065000
H	-1.795069000	2.474551000	-0.835018000
H	-1.937331000	3.811181000	0.323948000
C	1.700879000	-0.255726000	-0.950003000
H	1.821389000	0.264978000	-1.912271000
H	2.109336000	-1.258542000	-1.120085000
C	2.531149000	0.522990000	0.073568000
H	2.399664000	0.078994000	1.080803000
C	4.055532000	0.510442000	-0.182907000
H	4.576947000	1.090607000	0.589377000
H	4.259743000	1.004229000	-1.143689000
C	4.677322000	-0.892879000	-0.181420000
H	4.231300000	-1.491951000	-0.987447000
H	4.441428000	-1.400125000	0.765617000
C	6.166817000	-0.850993000	-0.366954000
C	7.062702000	-1.279669000	0.522004000
H	6.515772000	-0.424974000	-1.309434000
H	8.130827000	-1.220948000	0.331130000
H	6.762374000	-1.713128000	1.474783000
C	-2.536918000	1.316467000	2.001773000
C	-2.710705000	1.825468000	3.295122000
C	-1.667620000	1.777396000	4.208229000
C	-0.457894000	1.212908000	3.806122000
C	-0.359915000	0.736505000	2.508785000
N	-1.362143000	0.781603000	1.609380000
H	-1.793749000	2.168365000	5.213954000
H	-3.671482000	2.250846000	3.570590000
H	0.391479000	1.143282000	4.477684000
C	-3.683116000	1.336861000	1.036360000
H	-4.505358000	0.709059000	1.400190000
H	-4.083175000	2.349555000	0.915815000
H	-3.375338000	0.964410000	0.058254000
H	0.569904000	0.289999000	2.168368000
C	-1.346928000	-2.656744000	1.642676000
C	-1.130550000	-3.782780000	2.444575000
C	0.138357000	-4.332197000	2.555098000
C	1.176075000	-3.732383000	1.847796000
C	0.887988000	-2.622100000	1.068158000
N	-0.340563000	-2.075149000	0.949597000
H	0.312645000	-5.207831000	3.174040000

H	-1.972153000	-4.218399000	2.975296000
H	2.191193000	-4.113825000	1.887467000
C	-2.727626000	-2.078771000	1.569254000
H	-2.956921000	-1.515698000	2.481883000
H	-2.836449000	-1.408742000	0.716795000
H	-3.474885000	-2.874375000	1.483213000
H	1.672412000	-2.140822000	0.500774000
83			
TS3b, $E_{(\text{SCRF})} = -1532.863641$ a.u., $\text{IF} = i1265.3075 \text{ cm}^{-1}$			
Sc	-0.506880000	-0.264707000	-0.501834000
C	-0.468364000	-1.547716000	-2.678886000
C	-1.437776000	-2.175763000	-1.848873000
C	-2.512342000	-1.262055000	-1.653508000
C	-2.208917000	-0.065506000	-2.368907000
C	-0.926717000	-0.231430000	-2.976864000
C	-1.446122000	-3.619503000	-1.443322000
H	-1.917203000	-3.774658000	-0.466995000
H	-0.437406000	-4.039901000	-1.395575000
H	-2.011641000	-4.217547000	-2.171144000
C	-3.844660000	-1.633339000	-1.070781000
H	-4.452721000	-2.157036000	-1.821874000
H	-4.427415000	-0.764817000	-0.749692000
H	-3.746543000	-2.311527000	-0.217516000
C	-3.213678000	0.987948000	-2.747744000
H	-2.742680000	1.880937000	-3.166495000
H	-3.858302000	1.304317000	-1.922150000
H	-3.877353000	0.587784000	-3.526414000
C	-0.271798000	0.723095000	-3.933345000
H	-0.556753000	0.495731000	-4.969652000
H	0.821261000	0.672280000	-3.886064000
H	-0.557133000	1.762229000	-3.742833000
C	0.695191000	-2.243605000	-3.320787000
H	0.349848000	-2.810766000	-4.195616000
H	1.458622000	-1.545895000	-3.675554000
H	1.181773000	-2.957720000	-2.648794000
C	0.308625000	3.079910000	-0.874005000
C	1.115233000	4.219071000	-0.932676000
C	2.472384000	4.102407000	-0.685045000
C	2.989582000	2.847911000	-0.379783000
C	2.143458000	1.741718000	-0.343733000
N	0.812690000	1.858413000	-0.599837000
H	3.122998000	4.971555000	-0.729063000
H	0.666881000	5.178433000	-1.173413000
H	4.047984000	2.732289000	-0.184154000
C	-1.163159000	3.231466000	-1.108968000
H	-1.354321000	3.791056000	-2.031110000
H	-1.662378000	2.265817000	-1.184242000
H	-1.623866000	3.793678000	-0.288279000
C	1.872369000	-0.622611000	-0.943625000
H	1.783743000	-0.193865000	-1.945922000

H	2.435700000	-1.554932000	-1.077305000
C	2.637438000	0.341372000	-0.032940000
H	2.364522000	0.130529000	1.021429000
C	4.170717000	0.196734000	-0.088431000
H	4.638633000	0.955634000	0.551195000
H	4.518593000	0.384150000	-1.114039000
C	4.688285000	-1.165854000	0.396735000
H	4.291406000	-1.966821000	-0.243425000
H	4.319096000	-1.356992000	1.414250000
C	6.188687000	-1.233529000	0.385508000
C	6.954290000	-1.402717000	1.463251000
H	6.662633000	-1.125423000	-0.591741000
H	8.038014000	-1.440418000	1.393733000
H	6.526672000	-1.517331000	2.458077000
C	-2.447403000	1.804106000	1.841254000
C	-2.602072000	2.481769000	3.057962000
C	-1.525819000	2.611127000	3.923689000
C	-0.305663000	2.049784000	3.551307000
C	-0.231167000	1.403885000	2.326489000
N	-1.263319000	1.276479000	1.472645000
H	-1.635233000	3.133080000	4.870195000
H	-3.573112000	2.896956000	3.312373000
H	0.569784000	2.110630000	4.189629000
C	-3.617989000	1.655961000	0.917597000
H	-4.518084000	1.360692000	1.467093000
H	-3.846523000	2.601909000	0.411595000
H	-3.410118000	0.902209000	0.157189000
H	0.709595000	0.962890000	2.010350000
C	-1.658768000	-2.187098000	2.250715000
C	-1.078753000	-3.286349000	2.888126000
C	0.160656000	-3.765866000	2.466242000
C	0.811198000	-3.140158000	1.405768000
C	0.174637000	-2.059254000	0.798692000
N	-1.013396000	-1.610297000	1.216593000
H	0.609929000	-4.621041000	2.964892000
H	-1.600777000	-3.759843000	3.714396000
H	1.780724000	-3.485010000	1.057768000
C	-2.964012000	-1.607681000	2.706844000
H	-2.791186000	-0.769955000	3.393871000
H	-3.543313000	-1.229944000	1.861552000
H	-3.561690000	-2.353469000	3.238480000
H	0.954583000	-1.402546000	-0.144026000

83

G2, $E_{(\text{SCRF})} = -1532.920631$ a.u.

Sc	-0.890902000	0.104718000	-0.162214000
C	-1.751835000	1.594584000	-1.967331000
C	-2.362510000	0.326054000	-2.166453000
C	-3.216859000	0.070070000	-1.056810000
C	-3.157495000	1.197359000	-0.181375000
C	-2.249070000	2.141933000	-0.749530000

C	-2.260053000	-0.518791000	-3.399775000
H	-2.278473000	-1.589928000	-3.174110000
H	-1.342840000	-0.315026000	-3.958866000
H	-3.104776000	-0.314563000	-4.071727000
C	-4.182259000	-1.075406000	-0.961939000
H	-5.133866000	-0.818401000	-1.447362000
H	-4.423126000	-1.345526000	0.071964000
H	-3.800619000	-1.969715000	-1.463193000
C	-4.125178000	1.478378000	0.934263000
H	-3.692214000	2.073153000	1.745905000
H	-4.532480000	0.562041000	1.371013000
H	-4.980238000	2.051528000	0.550555000
C	-2.058488000	3.560845000	-0.299463000
H	-2.736128000	4.224776000	-0.853597000
H	-1.041545000	3.925549000	-0.474566000
H	-2.285868000	3.695968000	0.761948000
C	-0.855975000	2.297300000	-2.943388000
H	-1.446992000	2.817267000	-3.709626000
H	-0.233495000	3.052910000	-2.454161000
H	-0.193725000	1.599947000	-3.466179000
C	0.391354000	2.597968000	1.683259000
C	1.031077000	3.790299000	2.016774000
C	2.134064000	4.202863000	1.281830000
C	2.588899000	3.379712000	0.264018000
C	1.925525000	2.182740000	-0.021262000
N	0.802250000	1.815302000	0.651104000
H	2.638710000	5.137405000	1.510862000
H	0.656267000	4.383477000	2.844946000
H	3.470512000	3.648975000	-0.307454000
C	-0.759602000	2.140633000	2.531015000
H	-1.210303000	2.985201000	3.059487000
H	-1.546593000	1.660962000	1.941440000
H	-0.417565000	1.420511000	3.282784000
C	2.942508000	1.885969000	-2.338053000
H	3.788905000	2.572317000	-2.218260000
H	3.245489000	1.129610000	-3.068752000
C	2.546845000	1.222296000	-1.012725000
H	1.802605000	0.444492000	-1.221571000
C	3.761599000	0.556842000	-0.318595000
H	3.458208000	0.191849000	0.671812000
H	4.525913000	1.323939000	-0.128042000
C	4.391903000	-0.610141000	-1.093825000
H	4.793190000	-0.240931000	-2.048139000
H	3.622923000	-1.354667000	-1.337009000
C	5.496966000	-1.262125000	-0.313614000
C	5.506622000	-2.536458000	0.078930000
H	6.342563000	-0.621465000	-0.056564000
H	6.337601000	-2.955112000	0.640399000
H	4.692181000	-3.216794000	-0.166240000
C	-1.165948000	-1.457126000	2.913591000

C	-0.629974000	-2.213252000	3.959742000
C	0.738866000	-2.450156000	4.017199000
C	1.550812000	-1.924976000	3.015398000
C	0.948182000	-1.181091000	2.010997000
N	-0.373451000	-0.940415000	1.949945000
H	1.162582000	-3.038309000	4.826394000
H	-1.293878000	-2.612675000	4.720287000
H	2.623818000	-2.085479000	3.002453000
C	-2.636141000	-1.181330000	2.833385000
H	-3.202275000	-1.849504000	3.487611000
H	-2.858166000	-0.151524000	3.137421000
H	-3.000346000	-1.311487000	1.809646000
H	1.547253000	-0.756676000	1.210657000
C	-0.859066000	-3.302642000	-0.900822000
C	-0.105347000	-3.967322000	-1.865849000
C	0.791773000	-3.247450000	-2.660229000
C	0.933421000	-1.875967000	-2.474450000
C	0.156317000	-1.239542000	-1.498592000
N	-0.707207000	-1.968646000	-0.766746000
H	1.374376000	-3.766003000	-3.418374000
H	-0.220058000	-5.039735000	-1.993365000
H	1.631659000	-1.308490000	-3.083992000
C	-1.803538000	-4.018772000	0.019118000
H	-1.377253000	-4.089856000	1.027571000
H	-2.755733000	-3.486375000	0.100927000
H	-2.003415000	-5.035259000	-0.330488000
H	2.110649000	2.449050000	-2.770728000

69

H1, $E_{(\text{SCRF})} = -1245.429658$ a.u.

Sc	-0.508841000	-0.312799000	-0.078812000
C	-2.609289000	-0.167766000	1.300440000
C	-2.626946000	0.968581000	0.441791000
C	-2.747432000	0.503579000	-0.901864000
C	-2.846278000	-0.920674000	-0.861794000
C	-2.762300000	-1.332938000	0.495770000
C	-2.745677000	2.390280000	0.907720000
H	-2.455819000	3.111870000	0.138785000
H	-2.139320000	2.594055000	1.796646000
H	-3.787231000	2.610928000	1.177316000
C	-3.030330000	1.340515000	-2.120462000
H	-4.091309000	1.270914000	-2.395356000
H	-2.461167000	1.025479000	-3.005163000
H	-2.823611000	2.400910000	-1.949515000
C	-3.293939000	-1.785276000	-2.005897000
H	-2.878928000	-2.798329000	-1.972236000
H	-3.049641000	-1.351355000	-2.981626000
H	-4.386800000	-1.896358000	-1.981488000
C	-3.044157000	-2.714551000	1.005403000
H	-4.127633000	-2.863165000	1.112139000
H	-2.601968000	-2.894426000	1.989447000

H	-2.688257000	-3.499832000	0.329673000
C	-2.647837000	-0.135845000	2.800725000
H	-3.685729000	-0.156408000	3.159779000
H	-2.136030000	-0.993427000	3.247972000
H	-2.193256000	0.773509000	3.207816000
C	2.814089000	0.193055000	-1.124907000
C	4.193845000	0.219936000	-0.913693000
C	4.734857000	-0.471425000	0.162699000
C	3.882296000	-1.216005000	0.967827000
C	2.512148000	-1.221025000	0.701080000
N	1.978061000	-0.479300000	-0.301936000
H	5.804269000	-0.450408000	0.354044000
H	4.828408000	0.776887000	-1.596862000
H	4.265441000	-1.806761000	1.794589000
C	2.253125000	0.899983000	-2.327656000
H	2.831697000	0.639389000	-3.221054000
H	1.213606000	0.622398000	-2.518577000
H	2.303194000	1.988385000	-2.217462000
C	0.173592000	-1.567326000	1.577747000
H	-0.503312000	-2.347166000	1.941843000
H	0.167176000	-0.792511000	2.366283000
C	1.584576000	-2.137823000	1.460089000
H	2.026596000	-2.293316000	2.457065000
C	1.594268000	-3.537104000	0.791355000
H	0.830963000	-4.147820000	1.290556000
H	2.556928000	-4.025843000	0.986023000
C	1.371408000	-3.560182000	-0.727355000
H	1.357419000	-4.615234000	-1.040949000
H	2.221369000	-3.102289000	-1.246651000
C	0.097924000	-2.948715000	-1.220664000
C	0.026836000	-2.043270000	-2.215445000
H	-0.825069000	-3.330533000	-0.783419000
H	-0.920632000	-1.747569000	-2.656244000
H	0.932802000	-1.692943000	-2.704317000
C	0.802393000	2.612053000	1.121504000
C	1.148888000	3.964003000	1.029201000
C	0.886790000	4.678395000	-0.132974000
C	0.271259000	4.018168000	-1.193066000
C	-0.044339000	2.677405000	-1.029899000
N	0.211622000	1.970950000	0.086271000
H	1.150501000	5.729584000	-0.207196000
H	1.619292000	4.446513000	1.880093000
H	0.033011000	4.524179000	-2.122966000
C	1.067701000	1.849138000	2.383578000
H	1.751764000	1.013284000	2.204853000
H	1.513709000	2.495578000	3.143284000
H	0.139203000	1.437969000	2.794378000
H	-0.538588000	2.140087000	-1.834308000

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TS4a, $E_{\text{(SCRF)}} = -1245.414793$ a.u., $\text{IF} = i263.5419 \text{ cm}^{-1}$

Sc	-0.603859000	-0.329495000	-0.180824000
C	-2.442685000	-0.359247000	1.520762000
C	-2.632595000	0.831935000	0.763148000
C	-2.958629000	0.454476000	-0.574096000
C	-3.010730000	-0.968318000	-0.629100000
C	-2.690870000	-1.471855000	0.660413000
C	-2.696649000	2.220371000	1.328036000
H	-2.460612000	2.988009000	0.584667000
H	-2.018135000	2.359776000	2.176153000
H	-3.709503000	2.432542000	1.696013000
C	-3.407710000	1.372499000	-1.676331000
H	-4.502920000	1.368575000	-1.757722000
H	-3.020670000	1.076187000	-2.659404000
H	-3.111305000	2.410164000	-1.496443000
C	-3.553350000	-1.782086000	-1.766011000
H	-3.044506000	-2.745870000	-1.881329000
H	-3.491865000	-1.253305000	-2.722544000
H	-4.615605000	-2.005641000	-1.597054000
C	-2.866080000	-2.896028000	1.096458000
H	-3.929150000	-3.107363000	1.275476000
H	-2.342442000	-3.113454000	2.032583000
H	-2.527481000	-3.616806000	0.343093000
C	-2.250308000	-0.437848000	3.010049000
H	-3.216748000	-0.554873000	3.518745000
H	-1.630596000	-1.289948000	3.311622000
H	-1.790643000	0.467943000	3.418971000
C	3.092318000	0.501070000	-0.727890000
C	4.397429000	0.586318000	-0.234134000
C	4.823874000	-0.309384000	0.737776000
C	3.949680000	-1.311118000	1.141977000
C	2.662339000	-1.347675000	0.603657000
N	2.212286000	-0.414771000	-0.265254000
H	5.829453000	-0.250159000	1.145206000
H	5.069053000	1.344123000	-0.627306000
H	4.257695000	-2.071660000	1.853511000
C	2.678594000	1.415085000	-1.846865000
H	3.468560000	1.453231000	-2.604871000
H	1.766138000	1.061143000	-2.328846000
H	2.517237000	2.442159000	-1.501206000
C	0.294607000	-2.164352000	0.798426000
H	-0.320178000	-3.003500000	1.126549000
H	0.063898000	-1.342713000	1.531920000
C	1.758349000	-2.518110000	0.895681000
H	2.004669000	-2.909885000	1.892945000
C	1.988276000	-3.641347000	-0.138119000
H	1.447223000	-4.534636000	0.199983000
H	3.045866000	-3.914459000	-0.221342000
C	1.432721000	-3.150057000	-1.469736000
H	1.345887000	-3.983078000	-2.180663000
H	2.114256000	-2.423347000	-1.923598000

C	0.059172000	-2.530114000	-1.352479000
C	-0.301579000	-1.417991000	-2.151438000
H	-0.738655000	-3.237303000	-1.127706000
H	-1.263279000	-1.431398000	-2.654837000
H	0.505990000	-0.931477000	-2.702174000
C	0.641296000	2.564266000	0.915031000
C	0.899087000	3.936297000	0.837179000
C	0.552137000	4.646412000	-0.306286000
C	-0.049147000	3.964521000	-1.362926000
C	-0.271702000	2.603779000	-1.216911000
N	0.058496000	1.909923000	-0.112349000
H	0.742903000	5.713916000	-0.370748000
H	1.364759000	4.437160000	1.680385000
H	-0.340961000	4.470109000	-2.277473000
C	1.018333000	1.776006000	2.134442000
H	1.968872000	1.251286000	1.981610000
H	1.133993000	2.427875000	3.004595000
H	0.255230000	1.027884000	2.377071000
H	-0.737944000	2.037107000	-2.019578000

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J1, $E_{(\text{SCRF})} = -1245.426077$ a.u.

Sc	-1.193487000	-0.264983000	-0.219744000
C	-2.286981000	-0.894188000	1.886710000
C	-3.097079000	0.108898000	1.276760000
C	-3.603261000	-0.424379000	0.050860000
C	-3.123463000	-1.759460000	-0.088326000
C	-2.300189000	-2.045353000	1.041490000
C	-3.466066000	1.437336000	1.872625000
H	-3.627609000	2.204534000	1.108454000
H	-2.701454000	1.812524000	2.560590000
H	-4.398276000	1.356243000	2.446901000
C	-4.561606000	0.259668000	-0.881619000
H	-5.596799000	-0.024481000	-0.650518000
H	-4.383057000	-0.011694000	-1.927883000
H	-4.508412000	1.350420000	-0.801313000
C	-3.535049000	-2.740852000	-1.143800000
H	-2.731156000	-3.439020000	-1.399613000
H	-3.845963000	-2.242430000	-2.066151000
H	-4.385545000	-3.342503000	-0.795895000
C	-1.692292000	-3.380829000	1.366897000
H	-2.417916000	-4.015148000	1.893360000
H	-0.818148000	-3.292926000	2.021362000
H	-1.387948000	-3.928664000	0.468894000
C	-1.649615000	-0.825904000	3.246851000
H	-2.261753000	-1.361532000	3.984402000
H	-0.654209000	-1.285264000	3.273860000
H	-1.552698000	0.202457000	3.608754000
C	4.412483000	0.999948000	0.216113000
C	5.535662000	0.549047000	0.917014000
C	5.610167000	-0.791032000	1.280410000

C	4.570816000	-1.645366000	0.925401000
C	3.484452000	-1.120651000	0.221312000
N	3.403095000	0.175475000	-0.107695000
H	6.467369000	-1.165909000	1.833246000
H	6.332806000	1.241163000	1.172220000
H	4.600802000	-2.699787000	1.185734000
C	4.303525000	2.429240000	-0.239681000
H	4.831341000	3.111481000	0.433780000
H	4.746243000	2.544447000	-1.237476000
H	3.255984000	2.734532000	-0.313883000
C	0.998920000	-1.346829000	-0.352867000
H	0.451329000	-1.559050000	0.593209000
H	1.212869000	-0.259939000	-0.431432000
C	2.379069000	-2.040454000	-0.264785000
H	2.317033000	-2.885506000	0.429193000
C	2.640467000	-2.586840000	-1.706988000
H	2.556317000	-3.679286000	-1.701975000
H	3.647586000	-2.341787000	-2.056347000
C	1.548762000	-1.972031000	-2.583269000
H	1.332572000	-2.557756000	-3.482354000
H	1.838265000	-0.963791000	-2.907731000
C	0.314213000	-1.863709000	-1.671041000
C	-0.845708000	-1.004487000	-2.200903000
H	-0.051691000	-2.879338000	-1.462285000
H	-1.534680000	-1.580598000	-2.820943000
H	-0.436011000	-0.179689000	-2.810389000
C	-0.192446000	2.770130000	0.431394000
C	-0.097249000	4.145607000	0.215994000
C	-0.717968000	4.718158000	-0.889667000
C	-1.426071000	3.901220000	-1.769126000
C	-1.484414000	2.543560000	-1.495664000
N	-0.889843000	1.986570000	-0.421947000
H	-0.649491000	5.788285000	-1.063358000
H	0.462457000	4.757168000	0.916625000
H	-1.923037000	4.302148000	-2.646034000
C	0.493499000	2.096231000	1.582707000
H	1.398274000	1.575501000	1.241278000
H	0.794881000	2.818655000	2.345600000
H	-0.164122000	1.362551000	2.065384000
H	-2.021155000	1.864244000	-2.153967000

69

H2, $E_{\text{(SCRF)}} = -1245.430943$ a.u.

Sc	0.464919000	-0.412710000	0.015635000
C	1.720028000	-2.371894000	-0.871347000
C	2.626902000	-1.641303000	-0.047113000
C	2.144948000	-1.696974000	1.296004000
C	0.934653000	-2.454671000	1.298504000
C	0.674969000	-2.868706000	-0.043104000
C	3.949961000	-1.066534000	-0.465236000
H	4.210914000	-0.167178000	0.103058000

H	3.973623000	-0.804787000	-1.527934000
H	4.756309000	-1.793670000	-0.300541000
C	2.893887000	-1.192865000	2.498073000
H	3.700607000	-1.888078000	2.766531000
H	2.255162000	-1.101208000	3.382492000
H	3.368401000	-0.219815000	2.323203000
C	0.156291000	-2.916190000	2.499757000
H	-0.927943000	-2.831686000	2.360119000
H	0.421665000	-2.361144000	3.403999000
H	0.366195000	-3.974211000	2.704788000
C	-0.418797000	-3.802134000	-0.468971000
H	-0.107347000	-4.846592000	-0.330887000
H	-0.674951000	-3.678487000	-1.525306000
H	-1.333772000	-3.662473000	0.116682000
C	1.898235000	-2.702239000	-2.325377000
H	2.283185000	-3.723990000	-2.441693000
H	0.957098000	-2.648987000	-2.882880000
H	2.617995000	-2.039945000	-2.816525000
C	-1.459853000	1.158760000	2.175920000
C	-2.426394000	2.091494000	2.534545000
C	-3.251250000	2.618660000	1.546525000
C	-3.110163000	2.176532000	0.239139000
C	-2.143747000	1.217368000	-0.074899000
N	-1.310804000	0.749663000	0.893058000
H	-4.001711000	3.363718000	1.796445000
H	-2.521686000	2.399817000	3.571101000
H	-3.749216000	2.573163000	-0.540307000
C	-0.569620000	0.555064000	3.224469000
H	-0.241479000	1.305758000	3.950526000
H	-1.107336000	-0.223107000	3.779413000
H	0.320029000	0.079723000	2.797005000
C	-1.062070000	-0.551571000	-1.527499000
H	-1.676604000	-1.392832000	-1.167492000
H	-0.785974000	-0.794157000	-2.562127000
C	-1.911587000	0.727993000	-1.498554000
H	-1.324316000	1.538940000	-1.967570000
C	2.130761000	1.974952000	-1.543893000
C	2.863539000	3.163233000	-1.615843000
C	3.153980000	3.875538000	-0.459032000
C	2.705760000	3.382806000	0.765513000
C	1.987902000	2.198069000	0.765280000
N	1.700343000	1.502031000	-0.352305000
H	3.724615000	4.798413000	-0.509938000
H	3.202013000	3.518177000	-2.584286000
H	2.909692000	3.897990000	1.698162000
C	1.782569000	1.206867000	-2.783368000
H	0.778240000	1.472145000	-3.135330000
H	2.485044000	1.429453000	-3.591102000
H	1.792320000	0.127303000	-2.607126000
H	1.628600000	1.777425000	1.701660000

C	-3.195960000	0.637650000	-2.365481000
H	-2.855737000	0.553260000	-3.405314000
H	-3.759993000	1.579457000	-2.323746000
C	-4.144247000	-0.541108000	-2.091595000
H	-3.618537000	-1.488750000	-2.256312000
H	-4.933296000	-0.495125000	-2.857048000
C	-4.794795000	-0.552843000	-0.739157000
C	-4.758815000	-1.572097000	0.122513000
H	-5.374481000	0.334265000	-0.476766000
H	-5.288667000	-1.539360000	1.071075000
H	-4.221260000	-2.491519000	-0.104281000

69

TS4b, $E_{(\text{SCRF})} = -1245.397317$ a.u., $\text{IF} = i179.2473$ cm⁻¹

Sc	-1.047231000	-0.278760000	-0.150748000
C	-2.653414000	-0.567961000	1.666471000
C	-2.885823000	0.746298000	1.157095000
C	-3.373712000	0.619810000	-0.178177000
C	-3.452136000	-0.767848000	-0.492797000
C	-3.002011000	-1.502742000	0.646176000
C	-2.803941000	2.028257000	1.935015000
H	-2.453012000	2.867527000	1.324981000
H	-2.141637000	1.946008000	2.802344000
H	-3.794015000	2.305729000	2.320406000
C	-3.870646000	1.742846000	-1.041658000
H	-4.940623000	1.919955000	-0.867636000
H	-3.758476000	1.526236000	-2.110015000
H	-3.357543000	2.686858000	-0.830142000
C	-4.102285000	-1.355398000	-1.710590000
H	-3.736904000	-2.363674000	-1.930359000
H	-3.951692000	-0.740883000	-2.604131000
H	-5.186719000	-1.438309000	-1.557847000
C	-3.038326000	-2.998224000	0.788894000
H	-4.048547000	-3.337554000	1.053795000
H	-2.368676000	-3.353764000	1.578812000
H	-2.763969000	-3.514262000	-0.138309000
C	-2.251635000	-0.916713000	3.072723000
H	-3.139649000	-1.086322000	3.695865000
H	-1.649586000	-1.830186000	3.120419000
H	-1.678039000	-0.117480000	3.554241000
C	4.164555000	0.269331000	-0.427269000
C	5.114479000	0.196362000	0.597450000
C	4.972119000	-0.778882000	1.578617000
C	3.893402000	-1.655909000	1.507151000
C	2.986415000	-1.522397000	0.451557000
N	3.119547000	-0.571371000	-0.484419000
H	5.697504000	-0.861334000	2.383842000
H	5.952721000	0.886706000	0.615092000
H	3.760634000	-2.437840000	2.249640000
C	4.275645000	1.284066000	-1.532120000
H	5.115557000	1.965869000	-1.373083000

H	4.420543000	0.782614000	-2.496098000
H	3.356307000	1.874967000	-1.611673000
C	0.474831000	-1.754897000	0.417927000
H	-0.324065000	-2.490636000	0.628806000
H	0.490562000	-1.056457000	1.292349000
C	1.812688000	-2.478424000	0.318840000
H	1.896412000	-3.184068000	1.155968000
C	0.662320000	2.413817000	0.721402000
C	1.164771000	3.705484000	0.545446000
C	0.865099000	4.421060000	-0.607517000
C	0.052693000	3.829260000	-1.572210000
C	-0.417165000	2.547943000	-1.331884000
N	-0.124865000	1.842717000	-0.220001000
H	1.252930000	5.425882000	-0.748538000
H	1.787941000	4.140272000	1.320546000
H	-0.218857000	4.345354000	-2.486944000
C	0.998147000	1.622486000	1.949796000
H	1.800124000	0.904432000	1.740351000
H	1.341564000	2.277374000	2.754835000
H	0.128546000	1.069187000	2.321730000
H	-1.068148000	2.063357000	-2.054100000
C	1.866569000	-3.302519000	-1.005250000
H	1.873446000	-4.374792000	-0.785236000
H	2.805196000	-3.084653000	-1.525073000
C	0.690345000	-2.968477000	-1.924458000
H	-0.209388000	-3.540285000	-1.662821000
H	0.938478000	-3.254199000	-2.957014000
C	0.388092000	-1.499992000	-1.932993000
C	-0.807933000	-0.947752000	-2.376189000
H	1.273502000	-0.862519000	-1.875225000
H	-0.786774000	0.037352000	-2.845752000
H	-1.625411000	-1.595240000	-2.686070000

69

J2, $E_{\text{(SCRF)}} = -1245.424945$ a.u.

Sc	1.206378000	-0.389500000	0.209542000
C	1.728445000	-1.357431000	-1.979254000
C	2.688355000	-0.327466000	-1.748799000
C	3.471188000	-0.704472000	-0.615293000
C	3.015642000	-1.976250000	-0.157589000
C	1.932035000	-2.374934000	-0.996138000
C	2.947417000	0.869322000	-2.618936000
H	3.165307000	1.772773000	-2.038331000
H	2.105189000	1.091924000	-3.281214000
H	3.816714000	0.689490000	-3.264929000
C	4.658207000	0.045171000	-0.082216000
H	5.581268000	-0.299638000	-0.567278000
H	4.793462000	-0.105705000	0.994345000
H	4.585850000	1.121900000	-0.268316000
C	3.662463000	-2.812800000	0.905084000
H	2.954248000	-3.502715000	1.373330000

H	4.101703000	-2.202791000	1.700214000
H	4.470576000	-3.419615000	0.474910000
C	1.217793000	-3.695269000	-0.925002000
H	1.794277000	-4.473362000	-1.442684000
H	0.233455000	-3.661745000	-1.403913000
H	1.079739000	-4.037249000	0.106717000
C	0.755078000	-1.426526000	-3.123323000
H	1.190280000	-1.976224000	-3.968277000
H	-0.172204000	-1.944017000	-2.854333000
H	0.481114000	-0.435289000	-3.499704000
C	-4.429228000	1.064827000	-0.883547000
C	-5.611476000	0.413968000	-1.248856000
C	-5.786548000	-0.918949000	-0.894139000
C	-4.784608000	-1.559014000	-0.172838000
C	-3.637913000	-0.836771000	0.167029000
N	-3.460065000	0.441391000	-0.192777000
H	-6.692683000	-1.450316000	-1.172365000
H	-6.376343000	0.947568000	-1.805160000
H	-4.890270000	-2.596739000	0.131062000
C	-4.186710000	2.499715000	-1.264166000
H	-5.119301000	3.008854000	-1.523252000
H	-3.711468000	3.040769000	-0.439941000
H	-3.523716000	2.564790000	-2.136742000
C	-1.127208000	-0.991266000	0.772264000
H	-0.608459000	-1.798494000	0.210930000
H	-1.201594000	-0.091619000	0.131091000
C	-2.578709000	-1.474504000	1.041065000
H	-2.616088000	-2.559453000	0.885590000
C	0.648124000	2.793817000	-0.221972000
C	0.785017000	4.154225000	0.058311000
C	1.615085000	4.568169000	1.094708000
C	2.300882000	3.609490000	1.838716000
C	2.124657000	2.275709000	1.506148000
N	1.322682000	1.870396000	0.500606000
H	1.726832000	5.625270000	1.318457000
H	0.238787000	4.878205000	-0.538086000
H	2.959165000	3.884633000	2.655809000
C	-0.267116000	2.296567000	-1.300437000
H	-1.224509000	1.957783000	-0.880399000
H	-0.486202000	3.083430000	-2.027168000
H	0.182613000	1.459627000	-1.849087000
H	2.637099000	1.490707000	2.056815000
C	-2.789019000	-1.209168000	2.549541000
H	-3.569493000	-1.851288000	2.970045000
H	-3.098130000	-0.166777000	2.699108000
C	-1.406536000	-1.444451000	3.148131000
H	-1.168099000	-2.516809000	3.161808000
H	-1.297609000	-1.070143000	4.171100000
C	-0.453440000	-0.718654000	2.178160000
C	1.034276000	-1.099114000	2.234651000

H	-0.566450000	0.359337000	2.374624000
H	1.548692000	-0.618150000	3.074662000
H	1.147084000	-2.185567000	2.347568000
55			
H3, $E_{(\text{SCRF})} = -957.9484622$ a.u.			
Sc	-0.392634000	-0.152620000	-0.107708000
C	-2.216405000	0.167543000	1.492168000
C	-1.978566000	1.423971000	0.847664000
C	-2.346808000	1.288260000	-0.525051000
C	-2.789581000	-0.053686000	-0.730744000
C	-2.708993000	-0.743534000	0.516975000
C	-1.567036000	2.687194000	1.553547000
H	-2.414225000	3.109887000	2.109187000
H	-1.228098000	3.461655000	0.858653000
H	-0.764550000	2.520227000	2.281297000
C	-2.428098000	2.380940000	-1.554778000
H	-3.475806000	2.658562000	-1.729025000
H	-2.017764000	2.084480000	-2.528100000
H	-1.911422000	3.291263000	-1.237512000
C	-3.444477000	-0.562819000	-1.983376000
H	-3.012843000	-0.127590000	-2.891743000
H	-4.511117000	-0.301567000	-1.986195000
H	-3.392795000	-1.653458000	-2.070004000
C	-3.165349000	-2.149484000	0.778466000
H	-4.225651000	-2.165961000	1.063458000
H	-2.605372000	-2.616631000	1.594405000
H	-3.065103000	-2.789982000	-0.104474000
C	-2.117812000	-0.084504000	2.967728000
H	-3.063789000	0.177338000	3.460073000
H	-1.914901000	-1.134870000	3.195960000
H	-1.335694000	0.518239000	3.441561000
C	2.235019000	1.787333000	-0.544037000
C	3.548005000	2.193591000	-0.336542000
C	4.405329000	1.376708000	0.398258000
C	3.931029000	0.169536000	0.892659000
C	2.606391000	-0.200745000	0.654299000
N	1.772890000	0.614622000	-0.041519000
H	5.431446000	1.683075000	0.581813000
H	3.889256000	3.140492000	-0.742112000
H	4.572802000	-0.489714000	1.469047000
C	1.276542000	2.611294000	-1.352981000
H	1.105955000	2.161539000	-2.340275000
H	0.306881000	2.706722000	-0.851157000
H	1.660606000	3.620754000	-1.519662000
C	0.550152000	-1.473981000	1.346520000
H	0.156283000	-2.464680000	1.603888000
H	0.354217000	-0.836049000	2.230005000
C	2.064875000	-1.531227000	1.131322000
H	2.585000000	-1.756658000	2.075976000
C	2.482968000	-2.662671000	0.162190000

H	2.083851000	-3.603185000	0.563305000
H	3.574781000	-2.765409000	0.160898000
C	2.024803000	-2.487242000	-1.290659000
H	2.376077000	-3.364092000	-1.856632000
H	2.504511000	-1.616503000	-1.754616000
C	0.545886000	-2.426306000	-1.497162000
C	-0.093511000	-1.527994000	-2.280608000
H	-0.038584000	-3.224733000	-1.036782000
H	-1.144793000	-1.641302000	-2.530298000
H	0.469744000	-0.772250000	-2.833596000

55

TS4c, $E_{(\text{SCRF})} = -957.9383673$ a.u., IF = $i268.1511$ cm⁻¹

Sc	-0.415967000	-0.143716000	-0.214348000
C	-2.092664000	0.235710000	1.532561000
C	-1.978994000	1.452014000	0.792998000
C	-2.448229000	1.200779000	-0.533860000
C	-2.852534000	-0.166334000	-0.609645000
C	-2.623357000	-0.765092000	0.664763000
C	-1.597469000	2.781625000	1.383669000
H	-2.417626000	3.174811000	1.998605000
H	-1.393241000	3.535623000	0.617347000
H	-0.717211000	2.720043000	2.034418000
C	-2.645597000	2.210974000	-1.629631000
H	-3.704334000	2.492131000	-1.702368000
H	-2.355055000	1.825211000	-2.613899000
H	-2.086285000	3.134713000	-1.453804000
C	-3.577237000	-0.791824000	-1.764674000
H	-3.215930000	-0.428347000	-2.732498000
H	-4.648908000	-0.557248000	-1.713977000
H	-3.493963000	-1.883355000	-1.763818000
C	-2.991622000	-2.169424000	1.051035000
H	-4.040100000	-2.222189000	1.372498000
H	-2.385137000	-2.543050000	1.882436000
H	-2.879907000	-2.870348000	0.216616000
C	-1.839567000	0.096186000	3.007546000
H	-2.710371000	0.446371000	3.577648000
H	-1.666000000	-0.943316000	3.302942000
H	-0.982166000	0.689518000	3.346098000
C	2.147995000	1.838812000	-0.546044000
C	3.435151000	2.314972000	-0.325144000
C	4.340546000	1.526596000	0.382136000
C	3.942364000	0.273459000	0.827439000
C	2.641130000	-0.162461000	0.574957000
N	1.755398000	0.627114000	-0.078368000
H	5.346957000	1.886546000	0.576520000
H	3.720325000	3.291453000	-0.702826000
H	4.627413000	-0.371069000	1.369749000
C	1.144356000	2.618128000	-1.344473000
H	1.012040000	2.177094000	-2.341503000
H	0.166052000	2.644811000	-0.849324000

H	1.463058000	3.653703000	-1.487009000
C	0.697393000	-1.716081000	0.954687000
H	0.391808000	-2.674800000	1.378049000
H	0.208069000	-0.955559000	1.620944000
C	2.202517000	-1.550207000	0.986140000
H	2.604554000	-1.744368000	1.991007000
C	2.762977000	-2.617196000	0.020604000
H	2.588197000	-3.604188000	0.466778000
H	3.843464000	-2.516368000	-0.127187000
C	2.004528000	-2.481522000	-1.295131000
H	2.185381000	-3.354329000	-1.936230000
H	2.366355000	-1.609268000	-1.854747000
C	0.507882000	-2.364480000	-1.104739000
C	-0.255727000	-1.538658000	-1.970107000
H	0.018263000	-3.266102000	-0.741630000
H	-1.237803000	-1.881900000	-2.283098000
H	0.296575000	-0.973853000	-2.728379000

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J3, $E_{\text{(SCRF)}} = -957.9536195$ a.u.

Sc	-0.477265000	-0.085500000	-0.344291000
C	-1.983493000	0.188254000	1.553382000
C	-2.043244000	1.397906000	0.801489000
C	-2.604567000	1.088725000	-0.477708000
C	-2.916615000	-0.305548000	-0.502821000
C	-2.527703000	-0.862279000	0.747317000
C	-1.707469000	2.762702000	1.335372000
H	-2.515105000	3.125823000	1.984482000
H	-1.588371000	3.505712000	0.540591000
H	-0.792425000	2.768373000	1.939095000
C	-2.963192000	2.063287000	-1.565605000
H	-4.042254000	2.264546000	-1.556132000
H	-2.724996000	1.682741000	-2.566072000
H	-2.462055000	3.028756000	-1.445569000
C	-3.648497000	-1.011007000	-1.604674000
H	-3.339498000	-0.665051000	-2.596529000
H	-4.729321000	-0.834415000	-1.521798000
H	-3.495296000	-2.093190000	-1.569515000
C	-2.744251000	-2.285731000	1.171813000
H	-3.772767000	-2.429819000	1.527466000
H	-2.082149000	-2.579674000	1.992436000
H	-2.588551000	-2.988977000	0.347046000
C	-1.552876000	0.085302000	2.990004000
H	-2.375929000	0.369072000	3.659138000
H	-1.259788000	-0.932808000	3.265797000
H	-0.713218000	0.750637000	3.221959000
C	1.918342000	1.919479000	-0.619776000
C	3.114970000	2.570305000	-0.352495000
C	4.090440000	1.910427000	0.394135000
C	3.853466000	0.611738000	0.820595000
C	2.635105000	-0.003192000	0.519419000

N	1.675744000	0.665084000	-0.159613000
H	5.029472000	2.403866000	0.628328000
H	3.279722000	3.576197000	-0.724763000
H	4.603938000	0.062882000	1.381172000
C	0.847535000	2.538971000	-1.472030000
H	0.814996000	2.065851000	-2.462835000
H	-0.149736000	2.459262000	-1.013687000
H	1.024611000	3.606072000	-1.628356000
C	0.979611000	-1.967738000	0.757866000
H	0.875834000	-2.845234000	1.403257000
H	0.234868000	-1.291291000	1.238009000
C	2.418694000	-1.450585000	0.892658000
H	2.795421000	-1.593587000	1.912044000
C	3.163143000	-2.377992000	-0.103467000
H	3.263317000	-3.369067000	0.355921000
H	4.170020000	-2.024884000	-0.347867000
C	2.225804000	-2.424828000	-1.309780000
H	2.424526000	-3.274419000	-1.969914000
H	2.358762000	-1.517029000	-1.913785000
C	0.783800000	-2.469806000	-0.753526000
C	-0.257658000	-1.759574000	-1.654995000
H	0.476002000	-3.514903000	-0.646622000
H	-1.112088000	-2.405331000	-1.870186000
H	0.196329000	-1.483078000	-2.618750000

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H4, $E_{(\text{SCRF})} = -957.9447328$ a.u.

Sc	-0.369484000	-0.133109000	-0.065980000
C	-2.229031000	0.182444000	1.483839000
C	-1.992867000	1.434282000	0.828823000
C	-2.327096000	1.277982000	-0.549417000
C	-2.751757000	-0.071778000	-0.748493000
C	-2.693502000	-0.744415000	0.510197000
C	-1.612228000	2.708749000	1.531761000
H	-2.468693000	3.107078000	2.091078000
H	-1.300101000	3.492327000	0.834693000
H	-0.802334000	2.565907000	2.256813000
C	-2.387076000	2.353556000	-1.598012000
H	-3.431187000	2.617484000	-1.810786000
H	-1.942742000	2.045512000	-2.552823000
H	-1.888594000	3.273690000	-1.280337000
C	-3.375295000	-0.600434000	-2.009020000
H	-2.914367000	-0.187789000	-2.913059000
H	-4.439083000	-0.330731000	-2.045956000
H	-3.328800000	-1.692294000	-2.074541000
C	-3.143855000	-2.150043000	0.782313000
H	-4.208460000	-2.169676000	1.050460000
H	-2.593691000	-2.602560000	1.612881000
H	-3.025969000	-2.802031000	-0.089835000
C	-2.150487000	-0.050755000	2.963455000
H	-3.102857000	0.216201000	3.440700000

H	-1.948649000	-1.097886000	3.206095000
H	-1.374154000	0.557987000	3.438918000
C	2.258462000	1.807246000	-0.478591000
C	3.591318000	2.161945000	-0.307998000
C	4.446329000	1.291190000	0.365611000
C	3.949022000	0.084952000	0.838141000
C	2.603387000	-0.233486000	0.640135000
N	1.776583000	0.634348000	0.004524000
H	5.488596000	1.556410000	0.520057000
H	3.950048000	3.110504000	-0.694157000
H	4.588876000	-0.613866000	1.368366000
C	1.299447000	2.687880000	-1.224401000
H	1.709095000	3.690759000	-1.368344000
H	1.081963000	2.279287000	-2.220287000
H	0.350744000	2.791123000	-0.686382000
C	0.535131000	-1.459190000	1.415654000
H	0.107256000	-2.455884000	1.586867000
H	0.409443000	-0.912745000	2.365223000
C	2.038632000	-1.559491000	1.114930000
H	2.602705000	-1.797062000	2.030272000
C	2.401558000	-2.705138000	0.125536000
H	2.460987000	-3.635153000	0.702189000
H	3.407913000	-2.535305000	-0.278948000
C	1.420293000	-2.967756000	-1.028362000
H	0.493430000	-3.416255000	-0.652808000
H	1.882009000	-3.726194000	-1.680067000
C	1.092565000	-1.798065000	-1.901244000
C	-0.148218000	-1.480160000	-2.325342000
H	1.933521000	-1.195112000	-2.249256000
H	-0.318817000	-0.686711000	-3.051828000
H	-1.003413000	-2.109269000	-2.078385000

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TS4d, $E_{\text{(SCRF)}} = -957.9143371$ a.u., IF = $i346.1277$ cm⁻¹

Sc	-0.462972000	-0.119235000	-0.265905000
C	-2.096265000	0.195107000	1.523068000
C	-2.005240000	1.436533000	0.819513000
C	-2.493844000	1.222013000	-0.505335000
C	-2.887806000	-0.148216000	-0.618362000
C	-2.640893000	-0.779493000	0.637435000
C	-1.635425000	2.750053000	1.452021000
H	-2.428403000	3.077219000	2.137009000
H	-1.512778000	3.547174000	0.712920000
H	-0.712601000	2.694711000	2.041534000
C	-2.701675000	2.261122000	-1.571980000
H	-3.760488000	2.545815000	-1.626735000
H	-2.424158000	1.901106000	-2.570065000
H	-2.137147000	3.178241000	-1.378884000
C	-3.609287000	-0.748937000	-1.788644000
H	-3.246808000	-0.361998000	-2.746906000
H	-4.681820000	-0.518807000	-1.735100000

H	-3.515915000	-1.838229000	-1.813813000
C	-2.990182000	-2.196038000	0.990729000
H	-4.034085000	-2.264807000	1.323849000
H	-2.370660000	-2.583432000	1.805976000
H	-2.882358000	-2.874107000	0.137979000
C	-1.815208000	0.012011000	2.987948000
H	-2.692854000	0.298571000	3.582557000
H	-1.587210000	-1.028160000	3.241123000
H	-0.981791000	0.633134000	3.335435000
C	2.169263000	1.935008000	-0.492197000
C	3.481469000	2.384950000	-0.368593000
C	4.436608000	1.546281000	0.196922000
C	4.056363000	0.276431000	0.614457000
C	2.730427000	-0.126808000	0.469011000
N	1.796726000	0.706966000	-0.061716000
H	5.464867000	1.878701000	0.307979000
H	3.745008000	3.378214000	-0.717485000
H	4.777088000	-0.405140000	1.056363000
C	1.118062000	2.772812000	-1.160924000
H	1.394457000	3.830444000	-1.173700000
H	0.979963000	2.463601000	-2.206211000
H	0.152558000	2.695369000	-0.647028000
C	0.786720000	-1.580873000	0.864636000
H	0.377024000	-2.536840000	1.199164000
H	0.354393000	-0.801529000	1.546756000
C	2.287946000	-1.510937000	0.918441000
H	2.669285000	-1.648275000	1.939887000
C	2.807756000	-2.697600000	0.037949000
H	3.148598000	-3.514105000	0.680844000
H	3.670268000	-2.386262000	-0.561688000
C	1.655175000	-3.165561000	-0.876276000
H	1.046097000	-3.950700000	-0.415220000
H	2.047875000	-3.583178000	-1.812222000
C	0.836024000	-1.949081000	-1.220809000
C	-0.428020000	-1.780850000	-1.835720000
H	1.532093000	-1.154004000	-1.517212000
H	-0.450738000	-1.185656000	-2.753941000
H	-1.166259000	-2.579461000	-1.796899000

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J4, $E_{\text{(SCRF)}} = -957.945136$ a.u.

Sc	-0.569664000	-0.232489000	-0.481050000
C	-1.816082000	0.306005000	1.535248000
C	-1.828652000	1.482408000	0.727841000
C	-2.551063000	1.179832000	-0.467459000
C	-3.005384000	-0.174614000	-0.382241000
C	-2.559377000	-0.709780000	0.856578000
C	-1.323168000	2.824742000	1.175897000
H	-1.958902000	3.216469000	1.980389000
H	-1.341769000	3.565627000	0.371954000
H	-0.301409000	2.783680000	1.571503000

C	-2.917546000	2.134735000	-1.571056000
H	-3.976064000	2.414651000	-1.495993000
H	-2.781085000	1.702649000	-2.570360000
H	-2.340682000	3.063403000	-1.528685000
C	-3.888587000	-0.860594000	-1.381809000
H	-3.731825000	-0.483341000	-2.397692000
H	-4.946708000	-0.693977000	-1.139116000
H	-3.721823000	-1.940987000	-1.401190000
C	-2.903530000	-2.059128000	1.411428000
H	-3.788427000	-1.989738000	2.057901000
H	-2.097114000	-2.479915000	2.022268000
H	-3.134458000	-2.778680000	0.621600000
C	-1.277125000	0.229609000	2.936376000
H	-2.012157000	0.624215000	3.650634000
H	-1.061402000	-0.798785000	3.244123000
H	-0.363414000	0.821023000	3.062951000
C	1.922236000	1.931251000	-0.626052000
C	3.117994000	2.586419000	-0.341071000
C	4.102578000	1.916140000	0.376055000
C	3.878886000	0.596698000	0.750429000
C	2.664148000	-0.014147000	0.440807000
N	1.677919000	0.671070000	-0.195425000
H	5.039195000	2.408534000	0.621638000
H	3.272365000	3.602254000	-0.690614000
H	4.640558000	0.030611000	1.278093000
C	0.890194000	2.563817000	-1.513237000
H	0.955758000	3.655021000	-1.501099000
H	1.036279000	2.241213000	-2.553197000
H	-0.132265000	2.303292000	-1.210369000
C	1.006171000	-1.890298000	0.672062000
H	0.805442000	-2.843461000	1.175116000
H	0.345371000	-1.179300000	1.215007000
C	2.467828000	-1.485053000	0.772176000
H	2.878116000	-1.659753000	1.771979000
C	3.155549000	-2.442443000	-0.274455000
H	3.759052000	-3.194978000	0.240696000
H	3.835409000	-1.881953000	-0.924387000
C	2.004710000	-3.090847000	-1.091526000
H	1.752122000	-4.087453000	-0.712054000
H	2.246306000	-3.193011000	-2.153362000
C	0.821279000	-2.133676000	-0.856017000
C	-0.620400000	-2.282090000	-1.265389000
H	1.202793000	-1.215461000	-1.370714000
H	-0.746442000	-2.414210000	-2.347605000
H	-1.159270000	-3.066764000	-0.726901000
69			
K1 _{cis} , E _(SCRF) = -1245.444822 a.u.			
Sc	0.206767000	0.289699000	0.169300000
C	2.056960000	1.892461000	0.674625000
C	1.160866000	2.576688000	-0.200580000

C	-0.078220000	2.743980000	0.486744000
C	0.057213000	2.162195000	1.782833000
C	1.381629000	1.653962000	1.904848000
C	1.580810000	3.219106000	-1.494013000
H	2.230463000	4.081224000	-1.291968000
H	0.733225000	3.595221000	-2.073633000
H	2.156297000	2.544349000	-2.139894000
C	-1.251253000	3.580172000	0.055464000
H	-1.309766000	4.489011000	0.668257000
H	-2.212355000	3.064233000	0.163683000
H	-1.162992000	3.906136000	-0.983972000
C	-0.971771000	2.241554000	2.872050000
H	-1.992383000	2.233445000	2.474108000
H	-0.859051000	3.175012000	3.440280000
H	-0.887072000	1.416895000	3.585805000
C	2.017362000	1.144147000	3.164329000
H	2.569561000	1.952483000	3.662230000
H	2.737561000	0.338337000	2.983091000
H	1.277597000	0.774821000	3.879506000
C	3.520164000	1.683787000	0.414673000
H	4.085011000	2.595771000	0.651664000
H	3.940618000	0.882961000	1.030903000
H	3.728225000	1.441803000	-0.633097000
C	-2.365579000	0.802673000	-1.789733000
C	-3.719640000	1.092133000	-1.917426000
C	-4.649091000	0.288040000	-1.265281000
C	-4.190387000	-0.823250000	-0.577811000
C	-2.816930000	-1.079751000	-0.484334000
N	-1.907518000	-0.217001000	-1.010352000
H	-5.712598000	0.499205000	-1.334580000
H	-4.034640000	1.925508000	-2.537299000
H	-4.886589000	-1.523390000	-0.126392000
C	-1.368628000	1.547892000	-2.625704000
H	-0.404665000	1.675055000	-2.125135000
H	-1.187769000	0.993386000	-3.555541000
H	-1.737715000	2.538487000	-2.901676000
C	-0.919607000	-2.756739000	0.129137000
H	-0.798689000	-3.824931000	-0.089783000
H	-0.347589000	-2.228123000	-0.643317000
C	-2.416847000	-2.418910000	0.105890000
H	-2.934075000	-3.140424000	-0.540679000
C	-2.898346000	-2.636448000	1.582141000
H	-3.711264000	-3.366658000	1.636531000
H	-3.287125000	-1.701805000	2.000684000
C	-1.648284000	-3.104872000	2.351528000
H	-1.575607000	-4.200389000	2.320294000
H	-1.669181000	-2.805037000	3.404319000
C	-0.478291000	-2.472750000	1.574274000
C	-0.320600000	-0.973769000	1.866474000
H	0.465589000	-2.987973000	1.795322000

H	0.215388000	-0.837102000	2.812733000
H	-1.318826000	-0.525214000	2.049375000
C	2.256913000	-1.308563000	-1.965578000
C	3.321972000	-2.165114000	-2.248039000
C	4.060188000	-2.723244000	-1.209561000
C	3.714804000	-2.411761000	0.102744000
C	2.647817000	-1.550946000	0.312169000
N	1.929891000	-1.004952000	-0.688733000
H	4.889776000	-3.391470000	-1.422288000
H	3.562263000	-2.390488000	-3.282240000
H	4.255627000	-2.822793000	0.948619000
C	1.432995000	-0.702232000	-3.061788000
H	1.745935000	-1.072047000	-4.041256000
H	0.371467000	-0.945522000	-2.934142000
H	1.532990000	0.389316000	-3.070472000
H	2.336332000	-1.281950000	1.317804000

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TS5acis, $E_{\text{(SCRF)}} = -1245.41035$ a.u., IF = $i1268.5138$ cm⁻¹

Sc	0.311595000	0.177263000	0.184496000
C	2.285521000	1.380506000	1.095368000
C	1.551236000	2.308491000	0.304071000
C	0.284591000	2.519912000	0.936307000
C	0.249850000	1.725668000	2.120036000
C	1.487262000	1.024118000	2.219466000
C	2.137114000	3.095446000	-0.835059000
H	2.850680000	3.836446000	-0.450900000
H	1.379699000	3.650432000	-1.395383000
H	2.689424000	2.467083000	-1.543445000
C	-0.739188000	3.557881000	0.571970000
H	-0.593632000	4.462812000	1.177175000
H	-1.765251000	3.218484000	0.750119000
H	-0.667532000	3.864131000	-0.475138000
C	-0.843464000	1.759362000	3.148644000
H	-1.835733000	1.877191000	2.698224000
H	-0.702932000	2.609412000	3.829800000
H	-0.862764000	0.855660000	3.764609000
C	1.961264000	0.202597000	3.381824000
H	2.646661000	0.790803000	4.006048000
H	2.506607000	-0.693564000	3.065738000
H	1.138492000	-0.116517000	4.027358000
C	3.718004000	0.997822000	0.869042000
H	4.389756000	1.776251000	1.255681000
H	3.978358000	0.064719000	1.376801000
H	3.949431000	0.874133000	-0.194541000
C	-1.948611000	1.280718000	-1.814594000
C	-3.185477000	1.853396000	-2.090685000
C	-4.339175000	1.223828000	-1.635273000
C	-4.212006000	0.003170000	-0.992480000
C	-2.943606000	-0.533416000	-0.739502000
N	-1.817981000	0.149789000	-1.069455000

H	-5.318937000	1.653599000	-1.824294000
H	-3.237461000	2.767120000	-2.674159000
H	-5.090279000	-0.563791000	-0.698798000
C	-0.714217000	1.838132000	-2.459021000
H	0.186295000	1.738414000	-1.844848000
H	-0.524101000	1.298524000	-3.394958000
H	-0.831877000	2.896163000	-2.706089000
C	-1.541366000	-2.673985000	-0.208948000
H	-1.696352000	-3.692427000	-0.583419000
H	-0.816294000	-2.208758000	-0.887445000
C	-2.900997000	-1.944175000	-0.185232000
H	-3.596323000	-2.493470000	-0.831808000
C	-3.414042000	-2.067743000	1.289409000
H	-4.440089000	-2.444975000	1.331246000
H	-3.423018000	-1.086741000	1.777937000
C	-2.415554000	-3.012143000	1.978897000
H	-2.710849000	-4.057108000	1.817877000
H	-2.360142000	-2.848673000	3.060496000
C	-1.087775000	-2.728287000	1.256799000
C	-0.463391000	-1.405347000	1.703891000
H	-0.364630000	-3.539241000	1.413382000
H	-0.051336000	-1.489604000	2.714639000
H	-1.253761000	-0.633372000	1.785569000
C	2.385199000	-1.182233000	-2.296113000
C	3.332260000	-2.202407000	-2.205325000
C	3.511267000	-2.885547000	-1.001387000
C	2.736099000	-2.547507000	0.104709000
C	1.808734000	-1.518430000	-0.041254000
N	1.648756000	-0.871761000	-1.208209000
H	4.251673000	-3.678639000	-0.934768000
H	3.925351000	-2.459069000	-3.077598000
H	2.846196000	-3.069447000	1.050699000
C	2.138402000	-0.427112000	-3.566765000
H	2.848246000	-0.720146000	-4.344025000
H	1.126493000	-0.624336000	-3.939644000
H	2.229682000	0.652424000	-3.407580000
H	0.813741000	-1.458942000	0.921901000

69

L1cis, $E_{(\text{SCRF})} = -1245.463311$ a.u.

Sc	0.539356000	0.232390000	-0.174762000
C	2.560731000	1.619581000	0.058864000
C	2.459885000	1.249800000	-1.314302000
C	1.288578000	1.870460000	-1.854437000
C	0.666970000	2.610121000	-0.806968000
C	1.447808000	2.448282000	0.378639000
C	3.500171000	0.488382000	-2.086388000
H	4.303401000	1.160507000	-2.416177000
H	3.093597000	0.016215000	-2.986343000
H	3.970773000	-0.294436000	-1.482171000
C	0.885633000	1.930302000	-3.302117000

H	1.128046000	2.914960000	-3.723353000
H	-0.189921000	1.779969000	-3.455455000
H	1.419494000	1.193829000	-3.910149000
C	-0.484996000	3.556867000	-0.983221000
H	-1.182087000	3.225851000	-1.760591000
H	-0.118297000	4.546745000	-1.287305000
H	-1.052049000	3.700144000	-0.058296000
C	1.217900000	3.148195000	1.686543000
H	1.711341000	4.129390000	1.692864000
H	1.617664000	2.577546000	2.529879000
H	0.154584000	3.325787000	1.880584000
C	3.689895000	1.275810000	0.983055000
H	4.457535000	2.060723000	0.962827000
H	3.353143000	1.175819000	2.019434000
H	4.179676000	0.338479000	0.702549000
C	-0.728473000	-1.988379000	-2.126443000
C	-1.583273000	-2.975625000	-2.608065000
C	-2.809289000	-3.171666000	-1.982944000
C	-3.145485000	-2.382280000	-0.889728000
C	-2.255550000	-1.403606000	-0.447481000
N	-1.067087000	-1.211508000	-1.070844000
H	-3.493736000	-3.936129000	-2.340031000
H	-1.284512000	-3.578771000	-3.459295000
H	-4.089154000	-2.525156000	-0.376608000
C	0.606882000	-1.737335000	-2.761550000
H	0.605195000	-0.792058000	-3.315071000
H	1.407705000	-1.697768000	-2.010827000
H	0.867202000	-2.531745000	-3.465864000
C	-2.153722000	0.940571000	0.606885000
H	-1.188093000	1.147308000	1.105811000
H	-2.079987000	1.228563000	-0.450567000
C	-2.544269000	-0.554794000	0.765543000
H	-1.931854000	-0.969964000	1.581702000
C	-4.002801000	-0.529172000	1.254884000
H	-4.282531000	-1.437300000	1.798760000
H	-4.690091000	-0.423892000	0.405720000
C	-4.048905000	0.726792000	2.125008000
H	-3.549958000	0.531614000	3.083050000
H	-5.069674000	1.052582000	2.349355000
C	-3.262192000	1.777233000	1.316357000
C	-4.152059000	2.521501000	0.317925000
H	-2.807476000	2.514804000	1.987681000
H	-4.929826000	3.087456000	0.842050000
H	-4.651744000	1.832614000	-0.374322000
C	2.253951000	-2.376767000	1.323764000
C	2.349633000	-2.666671000	2.681691000
C	1.688994000	-1.859730000	3.614267000
C	0.939268000	-0.770684000	3.181654000
C	0.864573000	-0.505879000	1.809538000
N	1.515663000	-1.312120000	0.941544000

H	1.769595000	-2.089509000	4.674209000
H	2.938561000	-3.518488000	3.008270000
H	0.424354000	-0.134434000	3.896430000
C	2.920696000	-3.206185000	0.266986000
H	3.578678000	-3.958227000	0.709689000
H	2.175313000	-3.730150000	-0.343885000
H	3.519031000	-2.580592000	-0.404430000
H	-3.573736000	3.232183000	-0.282766000

30

Pcis, $E_{(\text{SCRF})} = -522.0036133$ a.u.

C	-2.463849000	0.850069000	-0.027230000
C	-3.391916000	-0.174464000	-0.243487000
C	-2.934184000	-1.486268000	-0.315882000
C	-1.573077000	-1.734648000	-0.172538000
C	-0.709324000	-0.654576000	0.040490000
N	-1.154804000	0.606522000	0.110993000
H	-3.630561000	-2.305105000	-0.481279000
H	-4.448263000	0.056267000	-0.350415000
H	-1.180326000	-2.746700000	-0.223411000
C	-2.886452000	2.291812000	0.065958000
H	-2.367250000	2.890715000	-0.690712000
H	-3.965149000	2.410634000	-0.073987000
H	-2.613827000	2.706239000	1.043316000
C	1.613834000	-0.163845000	-0.903655000
H	1.548260000	-0.673005000	-1.872916000
H	1.244360000	0.862335000	-1.036271000
C	0.780232000	-0.851634000	0.191441000
H	0.989595000	-1.929646000	0.154459000
C	1.364759000	-0.266903000	1.504165000
H	1.355968000	-1.012382000	2.307027000
H	0.737008000	0.568827000	1.828599000
C	2.792542000	0.224029000	1.159190000
H	3.558466000	-0.206707000	1.814294000
H	2.855401000	1.313686000	1.277124000
C	3.030676000	-0.145396000	-0.320393000
C	4.008714000	0.771179000	-1.046384000
H	3.422092000	-1.173988000	-0.360448000
H	4.995882000	0.761171000	-0.568228000
H	3.646954000	1.807512000	-1.042260000
H	4.143291000	0.468364000	-2.091903000

69

K2trans, $E_{(\text{SCRF})} = -1245.43409$ a.u.

Sc	-0.519091000	0.350990000	-0.206894000
C	-2.336166000	1.630608000	0.838867000
C	-1.299677000	1.548122000	1.819780000
C	-0.173883000	2.269074000	1.326138000
C	-0.516280000	2.790345000	0.041478000
C	-1.861875000	2.418504000	-0.247675000
C	-1.506743000	0.987960000	3.199864000
H	-2.295746000	1.549226000	3.716955000

H	-0.608398000	1.062612000	3.817453000
H	-1.824437000	-0.062515000	3.196362000
C	1.097589000	2.596386000	2.058530000
H	1.999956000	2.269139000	1.528111000
H	1.118983000	2.146728000	3.053725000
H	1.184392000	3.681471000	2.195437000
C	0.342260000	3.713281000	-0.774882000
H	1.407881000	3.572360000	-0.565990000
H	0.108008000	4.762202000	-0.548026000
H	0.191771000	3.578726000	-1.850870000
C	-2.697176000	2.931741000	-1.381871000
H	-3.332322000	3.759339000	-1.038610000
H	-3.361949000	2.168294000	-1.800560000
H	-2.083954000	3.317640000	-2.200308000
C	-3.750222000	1.172161000	1.049807000
H	-4.297367000	1.897679000	1.667503000
H	-4.301071000	1.083185000	0.108520000
H	-3.806832000	0.207301000	1.565333000
C	2.648282000	-0.741995000	1.824831000
C	3.995832000	-0.825290000	2.176948000
C	4.951643000	-0.978800000	1.181239000
C	4.521979000	-1.068839000	-0.134334000
C	3.158668000	-0.968911000	-0.426375000
N	2.231007000	-0.773098000	0.537921000
H	6.007413000	-1.047040000	1.428486000
H	4.280251000	-0.782679000	3.224022000
H	5.229577000	-1.224229000	-0.943699000
C	1.614490000	-0.687826000	2.909607000
H	1.425936000	-1.694955000	3.303216000
H	1.948471000	-0.073117000	3.750685000
H	0.668802000	-0.287294000	2.540789000
C	1.224866000	-1.135301000	-2.054731000
H	0.932607000	-1.645950000	-2.980796000
H	0.703974000	-1.664868000	-1.242506000
C	2.736530000	-1.134149000	-1.876161000
H	3.173840000	-2.080185000	-2.216482000
C	3.224417000	0.039577000	-2.798496000
H	3.780840000	-0.345019000	-3.658117000
H	3.904488000	0.701081000	-2.251776000
C	1.948134000	0.791044000	-3.241330000
H	1.623240000	0.470133000	-4.237962000
H	2.079295000	1.876694000	-3.273616000
C	0.883481000	0.353029000	-2.220932000
C	-0.590502000	0.614322000	-2.379416000
H	1.254091000	0.872150000	-1.280022000
H	-0.814413000	1.595351000	-2.802345000
H	-1.065258000	-0.163871000	-2.989833000
C	-1.822738000	-2.702746000	0.466252000
C	-2.767011000	-3.711805000	0.262823000
C	-3.834771000	-3.502697000	-0.601682000

C	-3.937824000	-2.277232000	-1.255340000
C	-2.963996000	-1.321595000	-1.012913000
N	-1.924920000	-1.515173000	-0.173715000
H	-4.571681000	-4.283914000	-0.765257000
H	-2.653880000	-4.656124000	0.786072000
H	-4.748913000	-2.063178000	-1.943249000
C	-0.680805000	-2.902694000	1.416479000
H	-0.497168000	-3.966637000	1.589001000
H	0.244995000	-2.454848000	1.039473000
H	-0.904845000	-2.446726000	2.388753000
H	-2.993295000	-0.358698000	-1.513571000

69

TS5btrans, $E_{(\text{SCRF})} = -1245.400686$ a.u., IF = $i1225.8134$ cm⁻¹

Sc	0.494939000	-0.316588000	-0.113067000
C	2.324567000	-1.188357000	1.287642000
C	1.337955000	-0.662983000	2.173744000
C	0.159909000	-1.460646000	2.040419000
C	0.428049000	-2.479171000	1.076297000
C	1.770186000	-2.319557000	0.624251000
C	1.635038000	0.372299000	3.222767000
H	2.375419000	-0.020312000	3.931905000
H	0.750569000	0.641292000	3.804482000
H	2.057514000	1.294619000	2.806822000
C	-1.080729000	-1.400901000	2.885930000
H	-2.002587000	-1.420766000	2.293838000
H	-1.108363000	-0.504094000	3.508891000
H	-1.117077000	-2.263150000	3.564389000
C	-0.489634000	-3.620778000	0.744570000
H	-1.541756000	-3.358399000	0.897089000
H	-0.280093000	-4.484045000	1.390570000
H	-0.376247000	-3.964169000	-0.288995000
C	2.544594000	-3.278454000	-0.230843000
H	3.214998000	-3.881912000	0.395181000
H	3.168902000	-2.772397000	-0.975166000
H	1.893134000	-3.978863000	-0.761021000
C	3.761087000	-0.757779000	1.250266000
H	4.316169000	-1.211235000	2.083075000
H	4.258309000	-1.064755000	0.325896000
H	3.871507000	0.327522000	1.345197000
C	-2.357509000	1.548407000	1.392075000
C	-3.664396000	1.772708000	1.828178000
C	-4.726506000	1.427624000	1.003461000
C	-4.441945000	0.910124000	-0.252210000
C	-3.113404000	0.704852000	-0.631088000
N	-2.079611000	0.969460000	0.201629000
H	-5.753245000	1.587928000	1.320498000
H	-3.834255000	2.227876000	2.799334000
H	-5.238159000	0.676498000	-0.953204000
C	-1.216974000	2.041609000	2.230056000
H	-1.124117000	3.129568000	2.123242000

H	-1.377447000	1.839301000	3.293106000
H	-0.268343000	1.597069000	1.924549000
C	-1.361212000	0.191495000	-2.377107000
H	-1.188880000	0.259097000	-3.458546000
H	-0.800834000	1.020906000	-1.922140000
C	-2.847666000	0.240179000	-2.053060000
H	-3.369515000	0.949861000	-2.705547000
C	-3.349320000	-1.218082000	-2.343185000
H	-4.003141000	-1.240753000	-3.219642000
H	-3.935751000	-1.599048000	-1.500593000
C	-2.076648000	-2.066764000	-2.566549000
H	-1.858524000	-2.182991000	-3.634805000
H	-2.148494000	-3.069220000	-2.134953000
C	-0.960211000	-1.221044000	-1.928886000
C	0.497734000	-1.524392000	-2.147831000
H	-1.219711000	-1.317418000	-0.833324000
H	0.758462000	-2.570090000	-1.982419000
H	0.787761000	-1.249805000	-3.170045000
C	2.000238000	2.834610000	-0.582839000
C	3.154803000	3.164316000	-1.293162000
C	3.849122000	2.179323000	-1.997369000
C	3.376548000	0.870031000	-1.996429000
C	2.221545000	0.596798000	-1.266931000
N	1.566960000	1.555730000	-0.589892000
H	4.748686000	2.441018000	-2.548657000
H	3.503833000	4.192297000	-1.295374000
H	3.883515000	0.086240000	-2.551533000
C	1.218016000	3.852383000	0.189431000
H	1.538739000	4.866788000	-0.060444000
H	0.148696000	3.760475000	-0.024303000
H	1.355673000	3.712767000	1.268184000
H	1.550072000	-0.532783000	-1.652897000

69

L2trans, $E_{\text{(SCRF)}} = -1245.461814$ a.u.

Sc	-0.609690000	-0.079865000	0.151917000
C	-2.348769000	0.090900000	1.876378000
C	-2.384367000	-1.241986000	1.371262000
C	-1.158599000	-1.883379000	1.732921000
C	-0.363766000	-0.939729000	2.444933000
C	-1.098468000	0.283080000	2.530934000
C	-3.576397000	-1.897443000	0.733312000
H	-4.210819000	-2.369467000	1.495286000
H	-3.299174000	-2.682855000	0.021949000
H	-4.202526000	-1.174242000	0.201863000
C	-0.824450000	-3.339814000	1.573959000
H	0.165838000	-3.508835000	1.133512000
H	-1.562068000	-3.862688000	0.957857000
H	-0.825078000	-3.839154000	2.551617000
C	0.935620000	-1.256737000	3.128453000
H	1.536696000	-1.975889000	2.561035000

H	0.750184000	-1.706711000	4.113283000
H	1.546866000	-0.365137000	3.302894000
C	-0.693730000	1.514570000	3.289175000
H	-1.156881000	1.524598000	4.284684000
H	-1.002789000	2.432033000	2.778029000
H	0.388747000	1.568711000	3.444212000
C	-3.473460000	1.081175000	1.826480000
H	-4.164154000	0.922217000	2.665442000
H	-3.110512000	2.110733000	1.892292000
H	-4.058850000	0.996149000	0.905378000
C	0.712317000	-2.309771000	-1.673114000
C	1.609229000	-3.214854000	-2.231377000
C	2.966032000	-3.080027000	-1.959969000
C	3.387484000	-2.022229000	-1.167156000
C	2.451147000	-1.123843000	-0.649186000
N	1.125708000	-1.287627000	-0.881404000
H	3.685150000	-3.782328000	-2.372086000
H	1.240174000	-4.014907000	-2.865271000
H	4.440529000	-1.879137000	-0.949422000
C	-0.761361000	-2.454085000	-1.917363000
H	-0.952037000	-2.915758000	-2.890649000
H	-1.224466000	-3.094871000	-1.158817000
H	-1.278806000	-1.486526000	-1.921456000
C	4.204998000	0.750906000	-0.340547000
H	5.076658000	0.462227000	0.257560000
H	4.421800000	0.469874000	-1.376365000
C	2.921959000	0.036443000	0.194137000
H	3.159411000	-0.374560000	1.185750000
C	1.906353000	1.168953000	0.394965000
H	1.178523000	0.964516000	1.200745000
H	1.375200000	1.389433000	-0.543169000
C	2.768599000	2.381573000	0.756259000
H	3.128608000	2.289656000	1.790436000
H	2.226559000	3.329071000	0.677144000
C	3.943653000	2.273398000	-0.225520000
C	5.171956000	3.086326000	0.167048000
H	3.586949000	2.630617000	-1.202420000
H	4.934935000	4.153761000	0.236526000
H	5.561594000	2.764104000	1.140782000
C	-2.729939000	1.197751000	-2.296263000
C	-3.010302000	2.534602000	-2.559200000
C	-2.389586000	3.538669000	-1.807826000
C	-1.501670000	3.196255000	-0.794463000
C	-1.246609000	1.842100000	-0.549042000
N	-1.855141000	0.902333000	-1.306712000
H	-2.612018000	4.581910000	-2.019951000
H	-3.710631000	2.789773000	-3.348894000
H	-1.018214000	3.965939000	-0.199126000
C	-3.346150000	0.077067000	-3.080487000
H	-4.186339000	0.434065000	-3.681760000

H	-2.615548000	-0.369234000	-3.767046000
H	-3.710057000	-0.715587000	-2.418535000
H	5.975718000	2.973492000	-0.568966000

30

Ptrans, $E_{\text{(SCRF)}} = -522.0039091$ a.u.

C	-2.376531000	0.896451000	0.075563000
C	-3.370189000	-0.058881000	-0.165119000
C	-2.989818000	-1.380629000	-0.374569000
C	-1.638195000	-1.707421000	-0.338366000
C	-0.706200000	-0.693553000	-0.091343000
N	-1.076774000	0.577652000	0.110678000
H	-3.738284000	-2.146356000	-0.564994000
H	-4.416719000	0.232477000	-0.187264000
H	-1.304780000	-2.729128000	-0.499629000
C	-2.713765000	2.344937000	0.308063000
H	-3.793889000	2.519347000	0.294637000
H	-2.317180000	2.678088000	1.273666000
H	-2.249790000	2.972906000	-0.461265000
C	1.628655000	-0.098457000	-0.994116000
H	2.107459000	-0.733999000	-1.750617000
H	1.007732000	0.629086000	-1.525409000
C	0.776209000	-0.977701000	-0.028796000
H	0.927946000	-2.034450000	-0.281373000
C	1.377339000	-0.714116000	1.375155000
H	1.273600000	-1.577814000	2.041781000
H	0.844981000	0.128789000	1.832788000
C	2.825763000	-0.315124000	1.095218000
H	3.426180000	-1.201595000	0.840105000
H	3.311501000	0.174395000	1.948108000
C	2.700727000	0.599767000	-0.130007000
C	4.007893000	0.878551000	-0.862917000
H	2.280694000	1.555057000	0.217239000
H	4.735520000	1.376194000	-0.210158000
H	4.462969000	-0.054551000	-1.220501000
H	3.848144000	1.525044000	-1.734459000

83

K3cis, $E_{\text{(SCRF)}} = -1532.92197$ a.u.

Sc	-1.490097000	-0.309802000	0.084225000
C	-1.647295000	-2.238145000	1.626167000
C	-2.650620000	-1.318099000	2.060548000
C	-3.626225000	-1.216544000	1.024299000
C	-3.229313000	-2.074663000	-0.040763000
C	-2.013593000	-2.712714000	0.329905000
C	-2.805857000	-0.731167000	3.437682000
H	-3.009941000	0.346925000	3.434611000
H	-1.922580000	-0.896012000	4.062001000
H	-3.645590000	-1.207997000	3.959477000
C	-4.946460000	-0.510618000	1.132106000
H	-5.727457000	-1.212511000	1.454650000
H	-5.277466000	-0.088264000	0.177386000

H	-4.925862000	0.297385000	1.869972000
C	-4.022878000	-2.371541000	-1.279379000
H	-3.379175000	-2.608491000	-2.133724000
H	-4.674597000	-1.539148000	-1.564667000
H	-4.672194000	-3.243577000	-1.122195000
C	-1.365066000	-3.847333000	-0.403952000
H	-1.925269000	-4.776929000	-0.233278000
H	-0.341266000	-4.021894000	-0.062789000
H	-1.331669000	-3.684214000	-1.485900000
C	-0.495642000	-2.777258000	2.430114000
H	-0.676352000	-3.825306000	2.701356000
H	0.452967000	-2.750765000	1.880800000
H	-0.349920000	-2.234104000	3.368955000
C	5.865315000	1.134437000	-0.384633000
C	6.880582000	0.557972000	0.387272000
C	6.774485000	-0.783077000	0.739638000
C	5.664230000	-1.505807000	0.313585000
C	4.692686000	-0.856961000	-0.454319000
N	4.794721000	0.437599000	-0.787613000
H	7.548326000	-1.259765000	1.336228000
H	7.736381000	1.150899000	0.697585000
H	5.551627000	-2.556867000	0.565490000
C	5.938636000	2.571110000	-0.827856000
H	4.962571000	3.055371000	-0.721543000
H	6.681981000	3.136850000	-0.258235000
H	6.211448000	2.629552000	-1.888927000
C	2.138018000	-0.932403000	-0.593768000
H	1.887473000	-1.070140000	0.467071000
H	2.222718000	0.146113000	-0.782706000
C	3.475016000	-1.590160000	-0.966307000
H	3.486639000	-2.606833000	-0.550436000
C	3.408536000	-1.681601000	-2.516013000
H	3.892893000	-2.595278000	-2.875759000
H	3.952942000	-0.835731000	-2.947320000
C	1.908382000	-1.611374000	-2.888103000
H	1.586453000	-2.447853000	-3.518879000
H	1.701778000	-0.693969000	-3.454936000
C	1.125024000	-1.571928000	-1.551977000
C	-0.250979000	-0.901771000	-1.626082000
H	0.986155000	-2.612228000	-1.224821000
H	-0.881532000	-1.477518000	-2.328290000
H	-0.118857000	0.090422000	-2.110611000
C	-3.512817000	2.250793000	-0.506903000
C	-4.383730000	3.020635000	-1.280961000
C	-4.597301000	2.698486000	-2.616245000
C	-3.930667000	1.601533000	-3.157910000
C	-3.085219000	0.875254000	-2.333594000
N	-2.875197000	1.180667000	-1.036059000
H	-5.272731000	3.293487000	-3.224363000
H	-4.886316000	3.869834000	-0.828200000

H	-4.060196000	1.308965000	-4.194497000
C	-3.224359000	2.616074000	0.919298000
H	-3.027218000	1.730276000	1.530922000
H	-2.343599000	3.267168000	0.981982000
H	-4.064647000	3.155826000	1.364422000
H	-2.543761000	0.014978000	-2.715316000
C	0.587214000	2.253874000	0.675282000
C	1.509334000	2.978282000	1.435619000
C	1.797140000	2.598435000	2.739823000
C	1.142590000	1.490784000	3.272366000
C	0.232813000	0.822735000	2.469275000
N	-0.053223000	1.180087000	1.199195000
H	2.518070000	3.156530000	3.330342000
H	2.002780000	3.835076000	0.987773000
H	1.327265000	1.148851000	4.285199000
C	0.325762000	2.648512000	-0.747992000
H	-0.693860000	2.415416000	-1.063164000
H	0.492539000	3.720324000	-0.888317000
H	1.011308000	2.118727000	-1.420163000
H	-0.300776000	-0.040727000	2.848106000

83

TS5ccis, $E_{(\text{SCRF})} = -1532.875212$ a.u., $\text{IF} = i1247.5833 \text{ cm}^{-1}$

Sc	-1.309711000	-0.285528000	0.039069000
C	-0.949505000	-1.501051000	2.190754000
C	-2.154232000	-0.744977000	2.322779000
C	-3.109799000	-1.282638000	1.413218000
C	-2.498751000	-2.363498000	0.711730000
C	-1.168752000	-2.503189000	1.196177000
C	-2.447279000	0.318949000	3.342995000
H	-2.997540000	1.166221000	2.918752000
H	-1.540228000	0.717391000	3.806854000
H	-3.065129000	-0.087594000	4.154424000
C	-4.554734000	-0.890012000	1.335948000
H	-5.155895000	-1.509927000	2.014539000
H	-4.967800000	-1.020816000	0.330668000
H	-4.712768000	0.152040000	1.630451000
C	-3.184242000	-3.285373000	-0.253543000
H	-2.491024000	-3.695086000	-0.995390000
H	-3.990531000	-2.781172000	-0.795110000
H	-3.633031000	-4.136942000	0.275079000
C	-0.255695000	-3.668083000	0.951923000
H	-0.378757000	-4.408116000	1.755352000
H	0.801373000	-3.383628000	0.943110000
H	-0.477638000	-4.181612000	0.012531000
C	0.238744000	-1.485447000	3.113519000
H	0.248108000	-2.398487000	3.723349000
H	1.200354000	-1.450628000	2.587306000
H	0.210593000	-0.648350000	3.818265000
C	5.419108000	1.024295000	-0.256272000
C	6.361212000	0.515525000	0.644886000

C	6.221708000	-0.792919000	1.094926000
C	5.152322000	-1.554255000	0.632798000
C	4.256508000	-0.973572000	-0.269575000
N	4.388164000	0.289753000	-0.695770000
H	6.939596000	-1.215568000	1.793293000
H	7.187976000	1.135198000	0.980051000
H	5.017778000	-2.583120000	0.955673000
C	5.523115000	2.425030000	-0.795931000
H	4.579002000	2.961986000	-0.652856000
H	6.325798000	2.989374000	-0.312705000
H	5.720298000	2.404008000	-1.874245000
C	1.738916000	-1.050762000	-0.734740000
H	1.363867000	-1.057528000	0.301796000
H	1.871288000	-0.004770000	-1.039283000
C	3.098656000	-1.757613000	-0.843374000
H	3.036383000	-2.719381000	-0.316503000
C	3.230407000	-2.027622000	-2.367364000
H	3.752470000	-2.971363000	-2.554081000
H	3.829055000	-1.230801000	-2.819259000
C	1.792891000	-2.016164000	-2.937915000
H	1.542109000	-2.934326000	-3.480243000
H	1.673858000	-1.189030000	-3.649340000
C	0.845433000	-1.799744000	-1.730823000
C	-0.469437000	-1.107503000	-2.110372000
H	0.617434000	-2.783269000	-1.305442000
H	-0.953273000	-1.720597000	-2.887259000
H	-0.231583000	-0.156515000	-2.617059000
C	-3.834818000	2.004430000	-0.686311000
C	-4.852584000	1.950380000	-1.640177000
C	-4.930078000	0.865741000	-2.515214000
C	-3.986849000	-0.158309000	-2.437300000
C	-2.990961000	-0.049889000	-1.469546000
N	-2.931336000	1.005474000	-0.643584000
H	-5.724400000	0.826435000	-3.256399000
H	-5.579677000	2.755078000	-1.692826000
H	-4.020449000	-1.007109000	-3.113938000
C	-3.710536000	3.121519000	0.305401000
H	-2.660356000	3.327183000	0.530820000
H	-4.180391000	4.036412000	-0.065895000
H	-4.206088000	2.857018000	1.248157000
H	-1.817348000	-0.791846000	-1.693652000
C	0.320322000	2.656364000	-0.417078000
C	1.035397000	3.777303000	0.015263000
C	1.490300000	3.859876000	1.324906000
C	1.218788000	2.803889000	2.189694000
C	0.496802000	1.727241000	1.699091000
N	0.041158000	1.637532000	0.432740000
H	2.047198000	4.729356000	1.662517000
H	1.234109000	4.578047000	-0.690282000
H	1.554472000	2.807245000	3.221324000

C	-0.107819000	2.560399000	-1.850823000
H	-1.080178000	2.074937000	-1.956744000
H	-0.170088000	3.553809000	-2.303450000
H	0.625656000	1.984205000	-2.428175000
H	0.266078000	0.888473000	2.343762000

83

L3cis, $E_{(\text{SCRF})} = -1532.92584$ a.u.

Sc	-2.340688000	-0.129962000	-0.016953000
C	-3.557275000	-2.168795000	0.519970000
C	-4.349108000	-1.430501000	-0.411906000
C	-3.639466000	-1.380845000	-1.649915000
C	-2.407915000	-2.078986000	-1.479293000
C	-2.357176000	-2.573374000	-0.138979000
C	-5.743096000	-0.919703000	-0.184657000
H	-5.929849000	0.020327000	-0.713849000
H	-5.953994000	-0.754608000	0.876891000
H	-6.483169000	-1.645727000	-0.546523000
C	-4.156225000	-0.808250000	-2.936736000
H	-4.749418000	-1.557372000	-3.478509000
H	-3.344683000	-0.494195000	-3.599725000
H	-4.802962000	0.059010000	-2.771833000
C	-1.396185000	-2.326534000	-2.562462000
H	-0.420537000	-2.616318000	-2.160141000
H	-1.248287000	-1.447611000	-3.199863000
H	-1.723799000	-3.144573000	-3.217401000
C	-1.297768000	-3.465350000	0.443025000
H	-1.578830000	-4.521079000	0.332991000
H	-1.142592000	-3.285673000	1.512152000
H	-0.331296000	-3.343525000	-0.056332000
C	-3.963015000	-2.548221000	1.916300000
H	-4.535491000	-3.485335000	1.911397000
H	-3.098794000	-2.711958000	2.569008000
H	-4.604324000	-1.793606000	2.385877000
C	4.236969000	2.651132000	-0.103224000
C	5.408707000	3.411316000	-0.143210000
C	6.619721000	2.765805000	-0.367571000
C	6.619494000	1.388393000	-0.550920000
C	5.407174000	0.691960000	-0.497974000
N	4.240021000	1.318017000	-0.269220000
H	7.548504000	3.329128000	-0.404709000
H	5.366351000	4.487648000	-0.004661000
H	7.545083000	0.851410000	-0.737318000
C	2.900448000	3.310213000	0.114845000
H	2.401501000	2.906469000	1.003669000
H	3.002353000	4.391162000	0.246108000
H	2.239877000	3.132748000	-0.742102000
C	4.843299000	-1.635456000	0.459941000
H	5.525120000	-1.654764000	1.318194000
H	3.887023000	-1.213738000	0.800428000
C	5.380999000	-0.802684000	-0.714224000

H	6.414848000	-1.124869000	-0.895648000
C	4.510683000	-1.265105000	-1.911610000
H	5.085218000	-1.254874000	-2.843561000
H	3.677440000	-0.566995000	-2.044641000
C	3.998085000	-2.679140000	-1.541479000
H	4.254746000	-3.431372000	-2.294955000
H	2.901821000	-2.679394000	-1.463718000
C	4.610438000	-3.016025000	-0.164152000
C	3.776048000	-3.971245000	0.680555000
H	5.596904000	-3.474074000	-0.330242000
H	3.628897000	-4.930404000	0.170370000
H	2.783256000	-3.547323000	0.885799000
C	-4.057692000	2.829707000	0.281309000
C	-4.043452000	3.926467000	-0.573378000
C	-3.233145000	3.908961000	-1.714941000
C	-2.445019000	2.797509000	-1.993220000
C	-2.482340000	1.704737000	-1.119321000
N	-3.281118000	1.766519000	-0.023866000
H	-3.228311000	4.769156000	-2.380368000
H	-4.661637000	4.790463000	-0.348886000
H	-1.814361000	2.773805000	-2.877585000
C	-4.879890000	2.773555000	1.533871000
H	-4.234351000	2.760592000	2.420831000
H	-5.542947000	3.638626000	1.613841000
H	-5.492576000	1.865778000	1.556719000
H	4.255072000	-4.179972000	1.644301000
C	0.515152000	0.109032000	1.278910000
C	1.505930000	0.288934000	2.245518000
C	1.157912000	0.295262000	3.592382000
C	-0.178894000	0.125483000	3.952265000
C	-1.112386000	-0.040946000	2.941519000
N	-0.779954000	-0.050612000	1.636173000
H	1.920072000	0.433365000	4.354156000
H	2.533296000	0.427768000	1.922870000
H	-0.493846000	0.124539000	4.990409000
C	0.834291000	0.066250000	-0.186356000
H	0.163358000	0.719546000	-0.765732000
H	1.861969000	0.398890000	-0.374548000
H	0.739957000	-0.957525000	-0.571919000
H	-2.166641000	-0.173141000	3.173877000

83

K4trans, $E_{(\text{SCRF})} = -1532.924438$ a.u.

Sc	-1.163650000	-0.347784000	-0.070819000
C	-0.060529000	-2.233187000	1.102455000
C	-1.229488000	-1.915387000	1.863098000
C	-2.368705000	-2.228091000	1.061950000
C	-1.905373000	-2.730620000	-0.186913000
C	-0.485419000	-2.745201000	-0.161870000
C	-1.285082000	-1.553476000	3.323123000
H	-1.979946000	-0.733691000	3.543144000

H	-0.306505000	-1.265363000	3.717378000
H	-1.619896000	-2.415026000	3.915729000
C	-3.791262000	-2.258507000	1.538858000
H	-4.048581000	-3.266551000	1.891756000
H	-4.507086000	-2.009734000	0.748478000
H	-3.963979000	-1.578744000	2.378727000
C	-2.754353000	-3.295914000	-1.286639000
H	-2.301996000	-3.142262000	-2.272645000
H	-3.758961000	-2.860681000	-1.301912000
H	-2.880079000	-4.380175000	-1.160347000
C	0.383793000	-3.423612000	-1.177695000
H	0.245987000	-4.511935000	-1.119786000
H	1.443860000	-3.225270000	-1.004777000
H	0.152028000	-3.124946000	-2.205449000
C	1.360360000	-2.246701000	1.596562000
H	1.726848000	-3.279219000	1.664854000
H	2.054000000	-1.699706000	0.947432000
H	1.443641000	-1.817222000	2.598938000
C	5.228737000	-0.283796000	1.068433000
C	6.530415000	-0.621776000	0.685878000
C	6.855974000	-0.618137000	-0.665788000
C	5.876423000	-0.273298000	-1.590424000
C	4.596879000	0.054132000	-1.131914000
N	4.282728000	0.042143000	0.173362000
H	7.859707000	-0.876433000	-0.993253000
H	7.270533000	-0.879049000	1.437856000
H	6.095279000	-0.254443000	-2.654277000
C	4.832338000	-0.257449000	2.520035000
H	5.659109000	-0.558477000	3.169408000
H	4.518848000	0.751216000	2.814091000
H	3.988411000	-0.931157000	2.705066000
C	2.277158000	-0.512884000	-2.103925000
H	2.102543000	-0.894559000	-3.116998000
H	2.443376000	-1.377067000	-1.457052000
C	3.506921000	0.447813000	-2.103685000
H	3.946474000	0.446283000	-3.107183000
C	-4.270320000	0.856993000	0.249582000
C	-5.570877000	1.112833000	-0.193673000
C	-5.936744000	0.800174000	-1.497071000
C	-4.986726000	0.228296000	-2.341042000
C	-3.715180000	-0.000739000	-1.838682000
N	-3.351485000	0.303422000	-0.574578000
H	-6.946083000	0.995860000	-1.847889000
H	-6.286802000	1.555048000	0.492666000
H	-5.220456000	-0.038432000	-3.366392000
C	-3.859661000	1.226827000	1.645125000
H	-3.583579000	2.286881000	1.701551000
H	-4.681845000	1.065190000	2.348377000
H	-3.000497000	0.640799000	1.982930000
H	-2.941931000	-0.444555000	-2.458081000

C	2.922182000	1.854169000	-1.812388000
H	3.436612000	2.640515000	-2.374494000
H	3.044395000	2.076149000	-0.745496000
C	1.438482000	1.735230000	-2.152776000
H	1.284624000	1.774214000	-3.240415000
H	0.829176000	2.532098000	-1.711408000
C	1.058653000	0.327022000	-1.665488000
C	-0.335289000	-0.166803000	-2.082670000
H	1.139318000	0.370740000	-0.545997000
H	-0.857421000	0.627118000	-2.642997000
H	-0.283140000	-1.042287000	-2.738870000
C	0.243144000	2.297530000	1.507857000
C	0.486552000	3.659020000	1.714516000
C	-0.218782000	4.611536000	0.991498000
C	-1.163105000	4.180781000	0.061465000
C	-1.361802000	2.817115000	-0.085076000
N	-0.693131000	1.883131000	0.623272000
H	-0.032852000	5.670644000	1.145966000
H	1.237749000	3.956319000	2.439594000
H	-1.733535000	4.880816000	-0.539976000
C	1.047525000	1.260725000	2.225386000
H	1.399279000	1.632478000	3.192108000
H	0.458805000	0.356555000	2.400150000
H	1.930980000	0.979400000	1.634363000
H	-2.087581000	2.443529000	-0.800671000

83

TS5dtrans, $E_{\text{(SCRF)}} = -1532.884541$ a.u., IF = $i1271.0298$ cm⁻¹

Sc	-1.283665000	-0.347536000	-0.075574000
C	-0.276960000	-2.173775000	1.283979000
C	-1.369209000	-1.636840000	2.033703000
C	-2.570928000	-1.925123000	1.322576000
C	-2.228556000	-2.634854000	0.136488000
C	-0.812906000	-2.785685000	0.111587000
C	-1.330827000	-1.031376000	3.410581000
H	-1.750537000	-0.017821000	3.449200000
H	-0.314156000	-0.979840000	3.809558000
H	-1.915011000	-1.642258000	4.110140000
C	-3.956963000	-1.688898000	1.843237000
H	-4.291032000	-2.546586000	2.443163000
H	-4.687217000	-1.559511000	1.038586000
H	-4.008013000	-0.807183000	2.489491000
C	-3.191075000	-3.277912000	-0.818422000
H	-2.800993000	-3.308548000	-1.841209000
H	-4.152855000	-2.757535000	-0.846463000
H	-3.392692000	-4.315444000	-0.519536000
C	-0.040164000	-3.664348000	-0.826244000
H	0.060245000	-4.672761000	-0.401035000
H	0.972713000	-3.293961000	-1.010718000
H	-0.538363000	-3.778828000	-1.794019000
C	1.155635000	-2.316654000	1.720851000

H	1.427398000	-3.379205000	1.755733000
H	1.873566000	-1.824358000	1.054180000
H	1.315377000	-1.917509000	2.726615000
C	5.264456000	-0.348521000	1.031070000
C	6.588217000	-0.562920000	0.634296000
C	6.904206000	-0.498995000	-0.717865000
C	5.891813000	-0.224471000	-1.631159000
C	4.592519000	-0.021590000	-1.158734000
N	4.289133000	-0.084343000	0.147317000
H	7.924390000	-0.661899000	-1.055481000
H	7.351897000	-0.775049000	1.376685000
H	6.100577000	-0.168700000	-2.695749000
C	4.877256000	-0.391083000	2.484559000
H	5.700831000	-0.745115000	3.110820000
H	4.591953000	0.607665000	2.837182000
H	4.017413000	-1.051708000	2.637161000
C	2.294448000	-0.749015000	-2.069695000
H	2.163507000	-1.209054000	-3.056077000
H	2.493567000	-1.555600000	-1.358482000
C	3.461346000	0.283588000	-2.114553000
H	3.877668000	0.289851000	-3.127936000
C	-4.437815000	1.174310000	-0.072745000
C	-5.448685000	1.148372000	-1.037085000
C	-5.235805000	0.498328000	-2.252289000
C	-4.011915000	-0.122700000	-2.501450000
C	-3.043647000	-0.071500000	-1.502586000
N	-3.267573000	0.563699000	-0.341755000
H	-6.024515000	0.479515000	-3.000197000
H	-6.396880000	1.636488000	-0.830922000
H	-3.819281000	-0.630340000	-3.442036000
C	-4.602370000	1.871678000	1.245008000
H	-4.763396000	2.946743000	1.101051000
H	-5.472849000	1.486341000	1.787222000
H	-3.715443000	1.736146000	1.867967000
H	-1.736037000	-0.360809000	-1.896228000
C	2.793914000	1.656013000	-1.845431000
H	3.275917000	2.467142000	-2.400754000
H	2.877521000	1.892552000	-0.778029000
C	1.328345000	1.451654000	-2.223199000
H	1.212209000	1.453636000	-3.316465000
H	0.667431000	2.229850000	-1.827640000
C	1.011748000	0.039226000	-1.707222000
C	-0.297721000	-0.566880000	-2.226708000
H	1.021534000	0.103254000	-0.590342000
H	-0.520834000	-0.128843000	-3.209593000
H	-0.199097000	-1.644888000	-2.387267000
C	0.465882000	2.211945000	1.426094000
C	0.791394000	3.553141000	1.659104000
C	0.082503000	4.566081000	1.029886000
C	-0.953864000	4.213501000	0.168421000

C	-1.234194000	2.867638000	-0.003356000
N	-0.558380000	1.870360000	0.608286000
H	0.333101000	5.608522000	1.205146000
H	1.610647000	3.784803000	2.332686000
H	-1.538344000	4.960248000	-0.358894000
C	1.278779000	1.126132000	2.053276000
H	1.679174000	1.446538000	3.019810000
H	0.678147000	0.229773000	2.210573000
H	2.133002000	0.851174000	1.416343000
H	-2.040656000	2.562546000	-0.659956000

83

L4trans, $E_{\text{(SCRF)}} = -1532.925819$ a.u.

Sc	2.619203000	-0.141235000	0.080226000
C	2.490396000	-2.401307000	-0.845424000
C	3.102514000	-1.568391000	-1.834749000
C	4.352963000	-1.116966000	-1.319049000
C	4.512394000	-1.655334000	-0.006113000
C	3.361124000	-2.450619000	0.282641000
C	2.576026000	-1.305482000	-3.218204000
H	2.888044000	-0.328160000	-3.601574000
H	1.482417000	-1.347181000	-3.265793000
H	2.950872000	-2.057950000	-3.924438000
C	5.369950000	-0.286824000	-2.047152000
H	6.130610000	-0.927406000	-2.512615000
H	5.893283000	0.400740000	-1.374886000
H	4.919207000	0.308569000	-2.847096000
C	5.741288000	-1.535863000	0.847883000
H	5.512655000	-1.613749000	1.915484000
H	6.256807000	-0.584215000	0.690026000
H	6.453084000	-2.337892000	0.610634000
C	3.151696000	-3.280437000	1.517330000
H	3.586624000	-4.280679000	1.389399000
H	2.089922000	-3.423407000	1.745553000
H	3.631927000	-2.840701000	2.398547000
C	1.229370000	-3.200632000	-1.010062000
H	1.464281000	-4.231175000	-1.307801000
H	0.646702000	-3.262292000	-0.084500000
H	0.577933000	-2.791612000	-1.788749000
C	-4.577862000	2.687288000	-0.053412000
C	-5.647396000	3.433969000	-0.553874000
C	-6.760829000	2.763210000	-1.048145000
C	-6.771764000	1.374077000	-1.020484000
C	-5.665720000	0.692400000	-0.501501000
N	-4.587628000	1.344223000	-0.034101000
H	-7.608070000	3.315727000	-1.445912000
H	-5.603488000	4.519130000	-0.552580000
H	-7.626245000	0.816239000	-1.392681000
C	-3.354813000	3.370499000	0.499452000
H	-3.453950000	4.459061000	0.465662000
H	-3.182322000	3.076505000	1.541046000

H	-2.459624000	3.095003000	-0.071218000
C	-4.471031000	-1.525214000	-1.110401000
H	-4.745114000	-1.847630000	-2.121959000
H	-3.628798000	-0.833291000	-1.216328000
C	-5.669755000	-0.816044000	-0.423881000
H	-6.593018000	-1.164569000	-0.903682000
C	3.366201000	3.137181000	-0.674538000
C	4.166538000	4.018730000	0.043432000
C	4.763417000	3.601446000	1.239222000
C	4.559506000	2.307341000	1.705330000
C	3.750100000	1.440968000	0.962110000
N	3.184316000	1.888893000	-0.187570000
H	5.388923000	4.295937000	1.795230000
H	4.325647000	5.025805000	-0.330072000
H	5.022103000	1.971815000	2.629180000
C	2.690876000	3.504470000	-1.961980000
H	2.972318000	4.509613000	-2.285786000
H	2.959393000	2.800348000	-2.757606000
H	1.599650000	3.479307000	-1.853105000
H	-3.599029000	-4.857327000	-0.308089000
C	-5.665113000	-1.374088000	1.014287000
H	-6.635359000	-1.263191000	1.510680000
H	-4.922817000	-0.830103000	1.613452000
C	-5.234830000	-2.825991000	0.815706000
H	-6.069754000	-3.405824000	0.397000000
H	-4.931471000	-3.323497000	1.744211000
C	-4.093730000	-2.736919000	-0.213244000
C	-3.844677000	-4.029646000	-0.984188000
H	-3.175366000	-2.481978000	0.336791000
H	-4.735006000	-4.320734000	-1.555547000
H	-3.016312000	-3.923478000	-1.695541000
C	-0.520838000	0.094296000	0.689406000
C	-1.683101000	0.138218000	1.459356000
C	-1.608708000	-0.169504000	2.815974000
C	-0.379820000	-0.511389000	3.377758000
C	0.733106000	-0.531850000	2.551412000
N	0.669480000	-0.241496000	1.237732000
H	-2.504796000	-0.138940000	3.429655000
H	-2.628817000	0.422679000	0.995142000
H	-0.280391000	-0.753516000	4.430598000
C	-0.525159000	0.419360000	-0.777150000
H	0.160864000	1.247838000	-1.003915000
H	-0.227908000	-0.451497000	-1.375547000
H	-1.521455000	0.720751000	-1.109410000
H	1.715486000	-0.784179000	2.944479000
71			
D5, $E_{(\text{SCRF})} = -1192.397097$ a.u.			
Sc	-0.779977000	-0.233580000	-0.257245000
C	-2.310609000	0.603708000	-1.988024000
C	-2.094618000	-0.777591000	-2.275949000

C	-2.645038000	-1.538900000	-1.199050000
C	-3.184801000	-0.627919000	-0.244082000
C	-2.976066000	0.697924000	-0.729528000
C	-1.543390000	-1.338497000	-3.556456000
H	-1.093815000	-2.327269000	-3.417595000
H	-0.784751000	-0.690060000	-4.007312000
H	-2.341370000	-1.457647000	-4.301283000
C	-2.802661000	-3.032585000	-1.167149000
H	-3.761195000	-3.321590000	-1.617903000
H	-2.802043000	-3.433095000	-0.147777000
H	-2.021211000	-3.551026000	-1.731392000
C	-3.971690000	-0.991224000	0.981004000
H	-3.813224000	-0.281078000	1.798520000
H	-3.719004000	-1.989429000	1.351508000
H	-5.047236000	-0.995110000	0.759701000
C	-3.526073000	1.957548000	-0.127262000
H	-4.529044000	2.164890000	-0.524688000
H	-2.901851000	2.827648000	-0.352991000
H	-3.615441000	1.888418000	0.960490000
C	-2.059163000	1.760883000	-2.911632000
H	-3.003707000	2.099315000	-3.357532000
H	-1.627196000	2.627224000	-2.397561000
H	-1.399279000	1.492814000	-3.742084000
C	-0.822518000	-0.673707000	3.173063000
C	-0.797561000	0.304711000	4.160807000
C	-0.715504000	1.655985000	3.802025000
C	-0.658380000	2.016693000	2.460715000
C	-0.680509000	1.007598000	1.489690000
N	-0.754341000	-0.283077000	1.879201000
H	-0.703692000	2.416388000	4.579413000
H	-0.847637000	0.014245000	5.205896000
H	-0.608245000	3.063162000	2.173027000
C	-0.919029000	-2.139081000	3.477902000
H	-1.030057000	-2.313381000	4.551015000
H	-1.780616000	-2.586249000	2.969601000
H	-0.023384000	-2.675585000	3.141950000
C	1.103424000	0.689115000	-1.868043000
H	0.616543000	1.178945000	-2.706955000
H	1.346837000	-0.366945000	-1.991269000
C	1.549710000	1.398311000	-0.810658000
H	2.101007000	0.879159000	-0.022256000
C	1.472911000	2.885052000	-0.672915000
H	1.073823000	3.147898000	0.312547000
H	0.796269000	3.302108000	-1.428235000
C	2.876170000	3.523997000	-0.818625000
H	3.281535000	3.257668000	-1.804966000
H	3.555273000	3.099556000	-0.068025000
C	2.824315000	5.017111000	-0.670660000
C	3.430528000	5.703826000	0.297352000
H	2.242159000	5.552375000	-1.422528000

H	3.364734000	6.786825000	0.354630000
H	4.028889000	5.211369000	1.061994000
C	0.447561000	-2.634227000	-0.256479000
H	0.372184000	-3.046294000	-1.261332000
H	-0.429008000	-2.738062000	0.385791000
C	1.622062000	-2.200495000	0.238826000
H	1.655211000	-1.861541000	1.276710000
C	2.929535000	-2.224482000	-0.486303000
H	3.402884000	-1.233876000	-0.455353000
H	2.777897000	-2.484633000	-1.541535000
C	3.906430000	-3.237033000	0.162211000
H	3.439453000	-4.231636000	0.140927000
H	4.059743000	-2.977077000	1.217298000
C	5.226598000	-3.272496000	-0.551875000
C	6.392007000	-2.930042000	-0.003788000
H	5.200446000	-3.606447000	-1.590281000
H	7.321375000	-2.980002000	-0.564287000
H	6.464817000	-2.600367000	1.031169000

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TS2e, $E_{\text{(SCRF)}} = -1192.381107$ a.u., $\text{IF} = i271.4903 \text{ cm}^{-1}$

Sc	0.012212000	-0.597322000	-0.279120000
C	-1.330529000	-1.287641000	-2.218645000
C	-0.138306000	-2.069865000	-2.245431000
C	-0.144477000	-2.925665000	-1.100781000
C	-1.327872000	-2.653703000	-0.355936000
C	-2.063289000	-1.642523000	-1.045334000
C	0.852560000	-2.089296000	-3.375119000
H	1.780629000	-2.601203000	-3.102689000
H	1.113654000	-1.083074000	-3.724100000
H	0.440472000	-2.625806000	-4.239897000
C	0.828028000	-4.035720000	-0.819102000
H	0.471236000	-4.975224000	-1.261245000
H	0.952732000	-4.223428000	0.253286000
H	1.819349000	-3.846158000	-1.242472000
C	-1.814155000	-3.402807000	0.850761000
H	-2.348278000	-2.754961000	1.554044000
H	-0.997900000	-3.887459000	1.395422000
H	-2.513164000	-4.196457000	0.554608000
C	-3.457104000	-1.206867000	-0.693881000
H	-4.184071000	-1.960284000	-1.025595000
H	-3.732297000	-0.265967000	-1.177213000
H	-3.595066000	-1.080074000	0.384967000
C	-1.803621000	-0.405316000	-3.336768000
H	-2.354032000	-0.996083000	-4.081315000
H	-2.482199000	0.381468000	-2.993670000
H	-0.972960000	0.075697000	-3.863853000
C	0.068535000	-1.065496000	3.082463000
C	-0.776919000	-0.656257000	4.104693000
C	-1.766056000	0.294444000	3.836641000
C	-1.885719000	0.839045000	2.564191000

C	-1.019709000	0.396328000	1.557812000
N	-0.086961000	-0.526463000	1.848691000
H	-2.439638000	0.610846000	4.629036000
H	-0.667274000	-1.077978000	5.098794000
H	-2.637416000	1.596218000	2.373982000
C	1.158184000	-2.075020000	3.279963000
H	1.102170000	-2.527050000	4.273147000
H	1.090750000	-2.876127000	2.535985000
H	2.146735000	-1.610700000	3.179336000
C	0.065165000	1.529318000	-1.000120000
H	-0.356705000	1.577748000	-2.003014000
H	1.108806000	1.837227000	-0.932386000
C	-0.798462000	1.862529000	0.083969000
H	-0.345467000	2.430749000	0.898523000
C	-2.210800000	2.285052000	-0.258100000
H	-2.926823000	2.096238000	0.544138000
H	-2.554916000	1.710409000	-1.124968000
C	-2.248120000	3.791994000	-0.595060000
H	-1.538606000	3.990246000	-1.410646000
H	-1.905610000	4.371880000	0.272148000
C	-3.625267000	4.238758000	-0.992451000
C	-4.360618000	5.124731000	-0.321105000
H	-4.030932000	3.788642000	-1.900301000
H	-5.352352000	5.414354000	-0.657418000
H	-3.993703000	5.606771000	0.583515000
C	2.622343000	-1.112809000	-0.286948000
H	2.800718000	-1.307493000	-1.343358000
H	2.267609000	-1.949303000	0.316710000
C	3.017183000	0.038569000	0.290449000
H	2.878728000	0.152825000	1.367796000
C	3.727118000	1.159559000	-0.395442000
H	3.253983000	2.118202000	-0.144694000
H	3.676280000	1.037614000	-1.484298000
C	5.208811000	1.232643000	0.054414000
H	5.694131000	0.277995000	-0.192114000
H	5.258853000	1.345766000	1.144823000
C	5.934301000	2.366959000	-0.609634000
C	6.459112000	3.408938000	0.034331000
H	6.022338000	2.308361000	-1.695586000
H	6.979582000	4.202200000	-0.495040000
H	6.401035000	3.503075000	1.117329000

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E5, $E_{(\text{SCRF})} = -1192.422233$ a.u.

Sc	-0.114340000	0.817526000	0.056750000
C	0.772397000	2.272544000	-1.709210000
C	-0.426321000	2.890777000	-1.242360000
C	-0.224324000	3.289191000	0.114157000
C	1.098719000	2.905073000	0.489628000
C	1.712443000	2.281254000	-0.639544000
C	-1.617219000	3.201111000	-2.105285000

H	-2.486351000	3.515011000	-1.519013000
H	-1.918129000	2.352341000	-2.731342000
H	-1.386605000	4.027457000	-2.790275000
C	-1.172037000	4.105276000	0.947566000
H	-0.966563000	5.176703000	0.824105000
H	-1.084034000	3.891454000	2.018638000
H	-2.218213000	3.951415000	0.664179000
C	1.807162000	3.265484000	1.766518000
H	2.431168000	2.450659000	2.151548000
H	1.110455000	3.557191000	2.558294000
H	2.473258000	4.122636000	1.601862000
C	3.149650000	1.859204000	-0.717036000
H	3.782840000	2.716523000	-0.983334000
H	3.312659000	1.090492000	-1.477419000
H	3.522560000	1.475046000	0.238421000
C	1.028107000	1.841677000	-3.122658000
H	1.281209000	2.708997000	-3.747140000
H	1.862672000	1.138779000	-3.192030000
H	0.153608000	1.363781000	-3.577403000
C	0.120707000	-0.538075000	3.022054000
C	0.297822000	-1.591389000	3.911786000
C	0.704135000	-2.831404000	3.424272000
C	0.940960000	-2.978889000	2.065077000
C	0.777204000	-1.887110000	1.208869000
N	0.356254000	-0.689540000	1.694286000
H	0.836015000	-3.670841000	4.101426000
H	0.110120000	-1.439745000	4.970259000
H	1.263123000	-3.930871000	1.654267000
C	-0.372808000	0.795922000	3.506951000
H	0.137533000	1.090776000	4.429320000
H	-0.196925000	1.590962000	2.773566000
H	-1.446435000	0.762302000	3.731970000
C	0.404567000	-0.939064000	-1.119812000
H	0.896154000	-0.836446000	-2.091101000
H	-0.619607000	-1.296179000	-1.353035000
C	1.113842000	-2.001830000	-0.263921000
H	0.805627000	-3.017046000	-0.564924000
C	2.657150000	-1.967179000	-0.407581000
H	3.107706000	-2.612595000	0.357560000
H	3.011707000	-0.948640000	-0.199181000
C	3.166017000	-2.431002000	-1.780483000
H	2.752159000	-1.785296000	-2.568011000
H	2.797164000	-3.445558000	-1.981748000
C	4.665521000	-2.412199000	-1.860837000
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H	5.139791000	-1.436396000	-1.738216000
H	6.515733000	-3.409131000	-2.110513000
H	5.006719000	-4.476486000	-2.193549000
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H	-3.056881000	1.645829000	-0.251920000

H	-2.431600000	1.338350000	1.466236000
C	-2.908398000	-0.396390000	0.323717000
H	-2.641073000	-1.071175000	1.140115000
C	-3.535899000	-1.035173000	-0.872172000
H	-2.909914000	-1.860508000	-1.233666000
H	-3.632068000	-0.309063000	-1.688530000
C	-4.930772000	-1.611771000	-0.517529000
H	-5.563453000	-0.792090000	-0.149278000
H	-4.834042000	-2.335669000	0.301523000
C	-5.575430000	-2.267496000	-1.704330000
C	-5.881428000	-3.562298000	-1.778856000
H	-5.797461000	-1.614485000	-2.549707000
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