

A Theoretical Investigation of the Mechanism of Hydrovinylation Reaction

Jorly Joseph,^{±‡} T. V. RajanBabu,^{+} and Eluvathingal D. Jemmis^{*‡,†}*

[±] School of Chemistry, University of Hyderabad, Central University (P. O.), Hyderabad-500046, India,

[‡]Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore-560012, India,

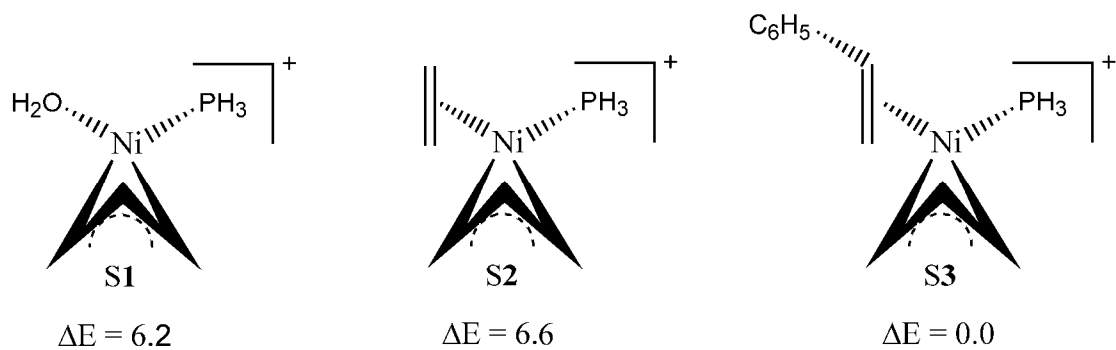
[†] Indian Institute of Science Education and Research, Thiruvananthapuram, 695016, India,

⁺ Department of Chemistry, The Ohio State University, Columbus, OH 43210.

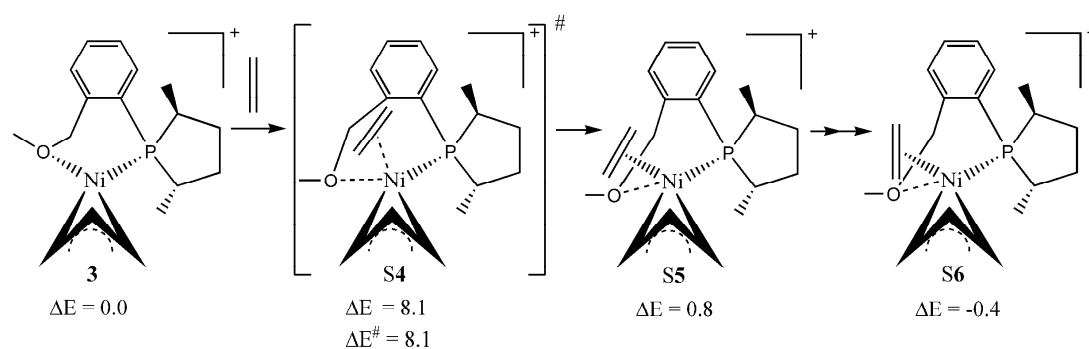
jemmis@iisertvm.ac.in, rajanbabu.1@osu.edu

Supporting Information

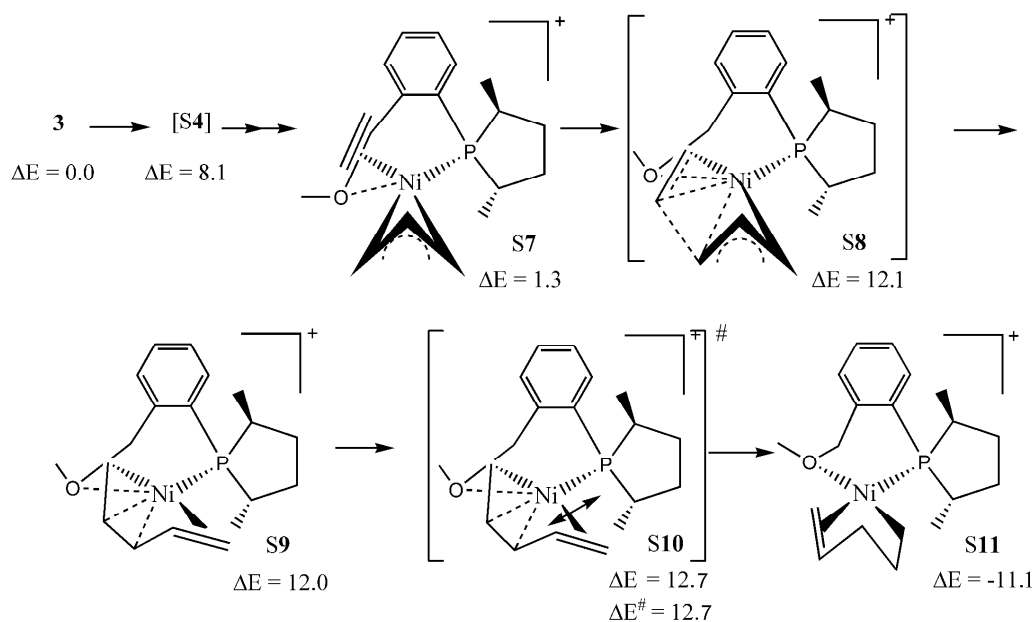
Scheme S1. Coordinating Ability of Olefins versus H₂O



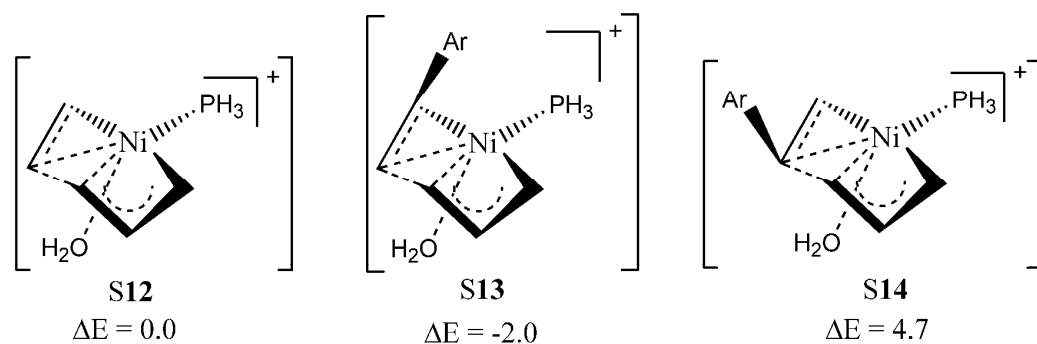
Scheme S2. Reaction Path for the Lowest Allyl Olefin Complex Formation



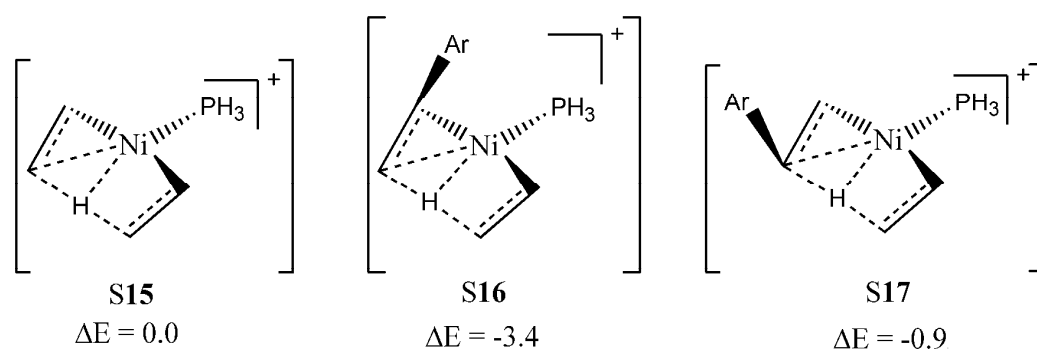
Scheme S3. Initiation from **3** (with fewer steps)



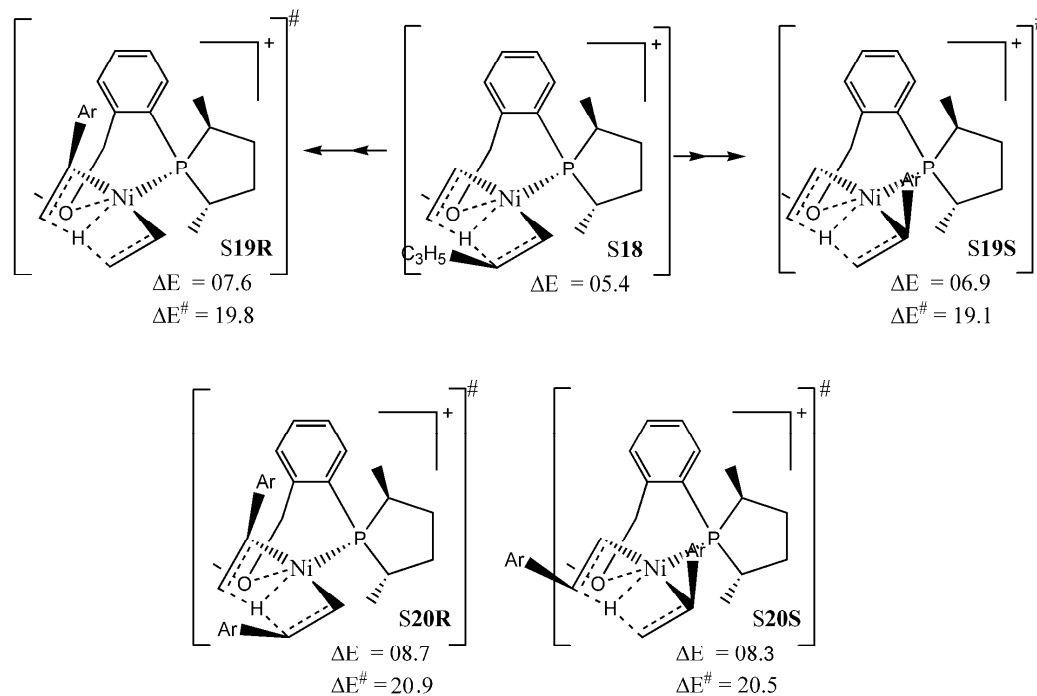
Scheme S4. Comparison of Styrene and Ethene for Initiation in Model Systems



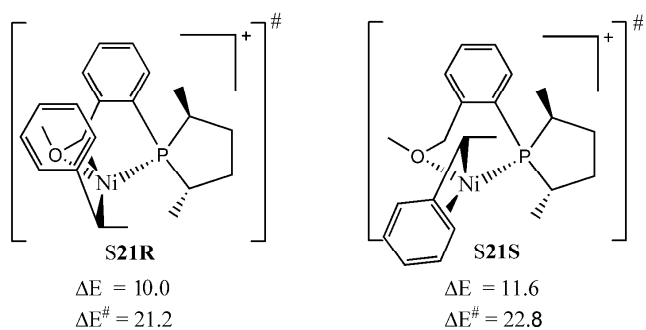
Scheme S5. Lowest β -H Transfer Transition States for Model Systems



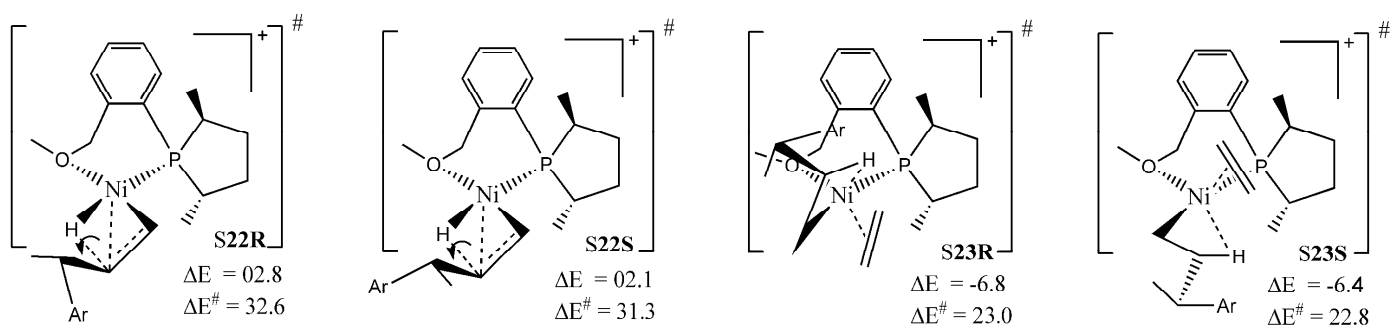
Scheme S6. Lowest Second H-Transfer Transition States (**S19R**, **S19S**, **S20R**, **S20S**)



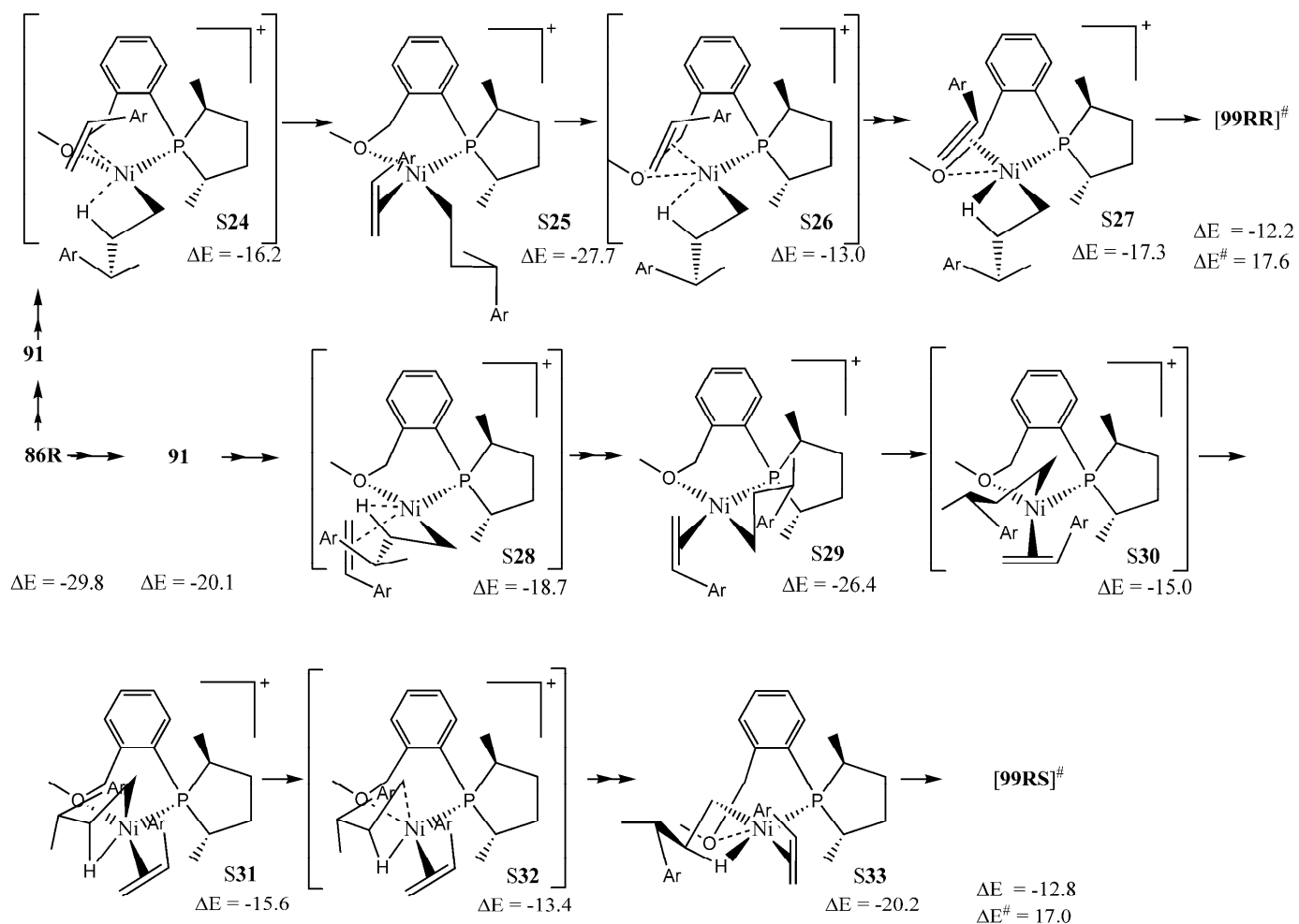
Scheme S7. Lowest Tetrahedral Transition States for Cis-Trans Interconversion of η^3 -Benzyl



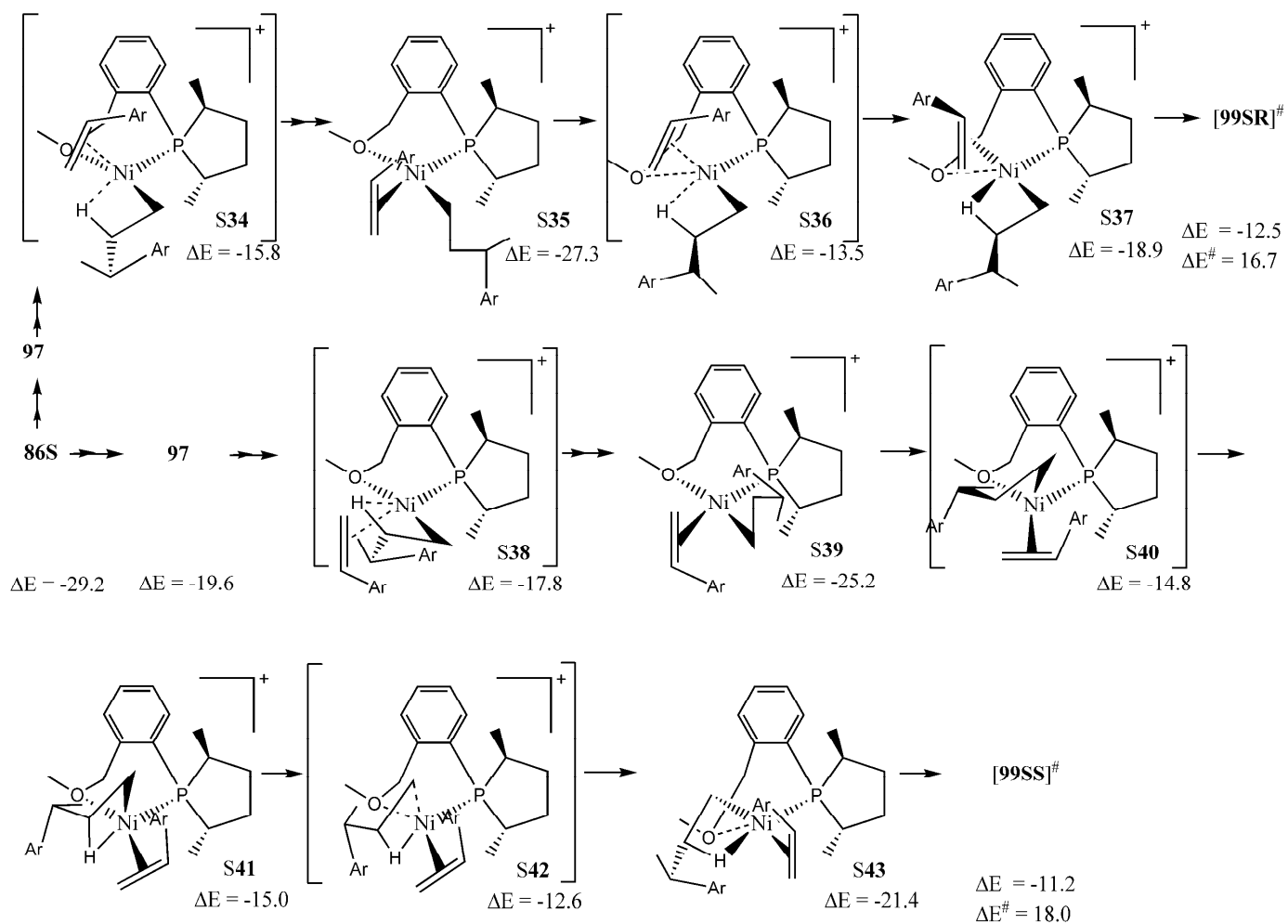
Scheme S8. Rate Determining Transition States for Product Elimination via β -hydride Pathway



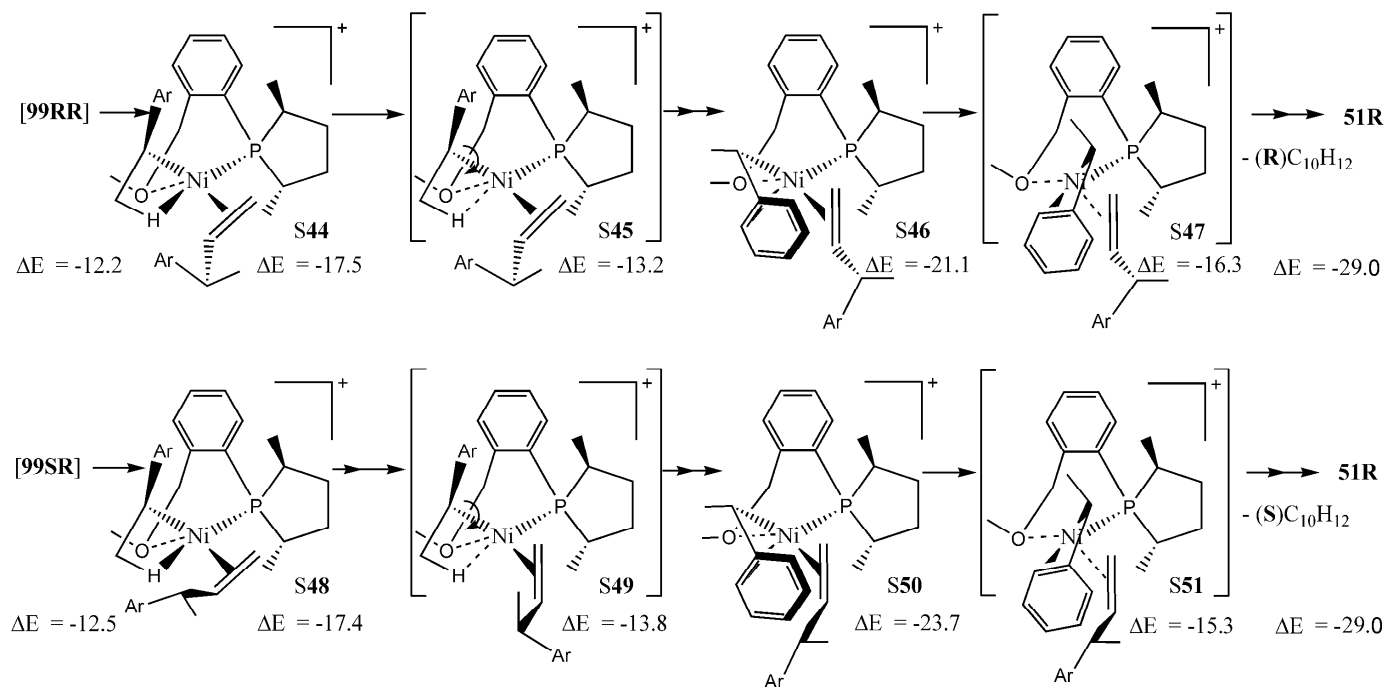
Scheme S9. Reaction Path to Reach the β -H-Transfer Transition States for (**R**) Product



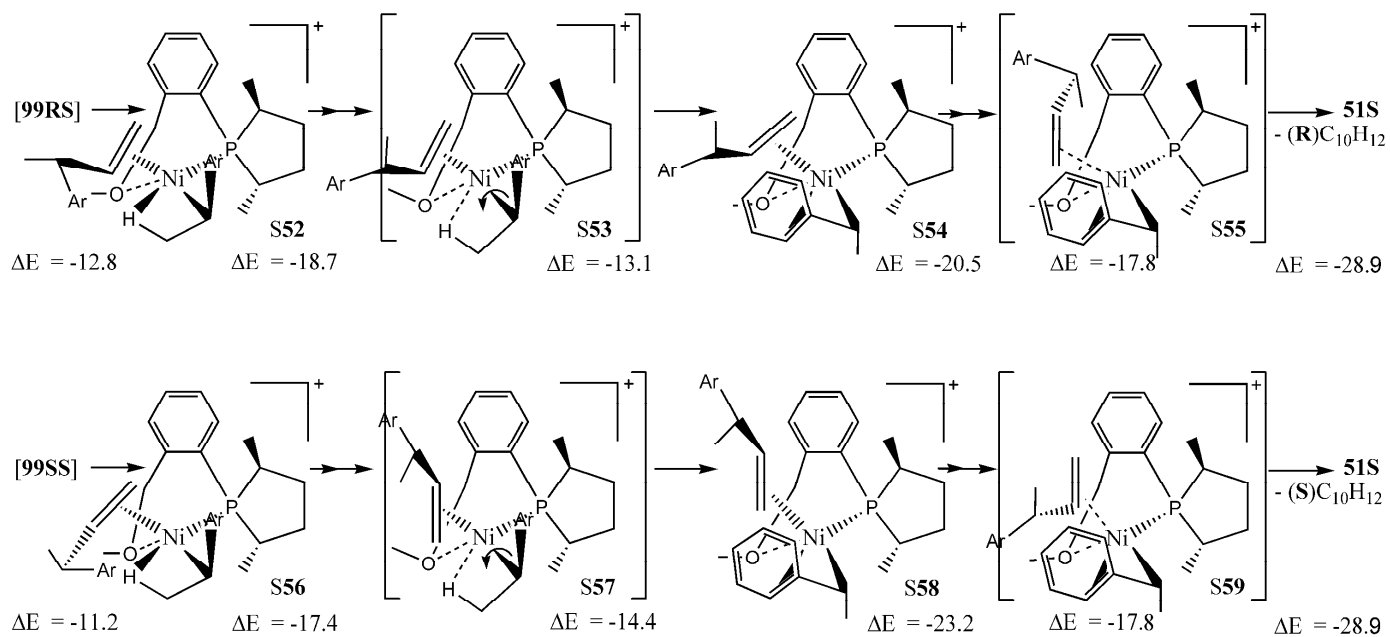
Scheme S10. Reaction Path to Reach the β -H-Transfer Transition States for (S) Product



Scheme S11. Reaction Path to Reach **(R)** η^3 -Benzylic from the β -H-Transfer Transition States



Scheme S12. Reaction Path to Reach **(S)** η^3 -Benzylic from the β -H-Transfer Transition States



Gaussian Reference

Gaussian 03, Revision B.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2003.

Gaussian 03, Revision B.05, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2003.

Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

Gaussian 03, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

Coordinates of Structures (in Å) and their Energies (E + ZPE, in Hartree).

H₂O				28	-1.608193000	0.218885000	0.301528000
E + ZPE = -76.387789				15	0.459774000	0.904826000	0.140416000
.....				6	0.737391000	2.172303000	-1.218948000
Ethene				1	0.956870000	1.631917000	-2.143353000
E + ZPE = -78.536227				6	1.930016000	3.079014000	-0.775111000
.....				1	2.735240000	3.061046000	-1.518442000
Styrene				1	1.577616000	4.116403000	-0.730076000
E + ZPE = -309.514550				6	2.458026000	2.656723000	0.613456000
.....				1	2.877591000	3.511514000	1.159305000
1,4.pentadiene				1	3.267297000	1.922821000	0.510152000
E + ZPE = -195.183875				6	1.304367000	2.013517000	1.401656000
.....				1	0.544457000	2.783501000	1.602301000
6	-2.375929000	-0.175981000	-0.148843000	6	1.735182000	1.391831000	2.729003000
6	-1.176768000	-0.177866000	0.433773000	1	2.451259000	0.576705000	2.574602000
1	-3.185533000	-0.809109000	0.204450000	1	0.881537000	1.000478000	3.291805000
1	-0.993196000	-0.838057000	1.282303000	1	2.225533000	2.145054000	3.358006000
1	-2.596261000	0.463932000	-1.001410000	6	-0.543147000	2.991831000	-1.455134000
6	-0.000010000	0.663904000	-0.000758000	1	-0.878018000	3.489419000	-0.536066000
1	-0.313885000	1.316544000	-0.828063000	1	-1.352586000	2.356899000	-1.822660000
1	0.313748000	1.319415000	0.824102000	1	-0.347506000	3.772577000	-2.200901000
6	1.176630000	-0.179206000	-0.432944000	6	1.683984000	-0.460098000	-0.151969000
1	0.992635000	-0.841460000	-1.279760000	6	2.659567000	-0.340611000	-1.152473000
6	2.376073000	-0.175634000	0.149076000	1	2.705411000	0.554947000	-1.761169000
1	2.596797000	0.466740000	0.999688000	6	3.587254000	-1.353490000	-1.401470000
1	3.185717000	-0.809313000	-0.203135000	1	4.326965000	-1.225290000	-2.187022000
.....				6	3.555865000	-2.519009000	-0.643255000
Product				1	4.270037000	-3.317463000	-0.824613000
E + ZPE = -388.079004				6	2.590160000	-2.655268000	0.353427000
.....				1	2.559211000	-3.566514000	0.946597000
1	1.758146000	-0.269689000	1.913402000	6	1.648763000	-1.652640000	0.613943000
6	1.267925000	-0.694327000	-0.176440000	6	0.633800000	-1.913872000	1.717981000
6	1.780803000	-1.112050000	1.213113000	1	0.571808000	-1.070239000	2.408741000
1	1.150180000	-1.905493000	1.626633000	1	0.962427000	-2.791663000	2.296226000
1	2.809581000	-1.485175000	1.158094000	8	-0.702212000	-2.112793000	1.272113000
1	1.306635000	-1.585863000	-0.821774000	6	-0.883790000	-3.278124000	0.475558000
6	-0.199218000	-0.268844000	-0.112534000	1	-0.581438000	-4.178543000	1.032488000
6	-0.563124000	0.999498000	0.360778000	1	-1.948785000	-3.330677000	0.243903000
6	-1.215115000	-1.153866000	-0.493955000	1	-0.324882000	-3.216718000	-0.464056000
1	0.214457000	1.703145000	0.647493000	6	-1.949105000	0.711207000	2.181123000
1	-0.950337000	-2.141353000	-0.867028000	1	-1.582548000	1.628512000	2.636907000
6	-1.904897000	1.369340000	0.454889000	6	-3.142511000	0.786688000	1.415553000
6	-2.559296000	-0.787924000	-0.402052000	6	-3.504492000	-0.345069000	0.672097000
1	-2.166949000	2.358327000	0.822505000	1	-3.350558000	-1.344830000	1.073417000
1	-3.331913000	-1.489831000	-0.705661000	1	-3.566988000	1.758956000	1.165797000
6	-2.908786000	0.476365000	0.073799000	1	-4.270501000	-0.261421000	-0.091322000
1	-3.954114000	0.765420000	0.143804000	1	-1.744868000	-0.190633000	2.758079000
6	3.198419000	0.965210000	-0.358981000	35	-1.606345000	-0.580720000	-1.878777000
6	2.113735000	0.365107000	-0.852102000			
1	1.766989000	0.647636000	-1.847064000	2'			
1	3.598914000	0.737534000	0.625001000	E + ZPE = -5159.572478			
1	3.735736000	1.714292000	-0.934501000			
.....				28	-1.621880000	0.186841000	0.285368000
2				15	0.434100000	0.909462000	0.140633000
E + ZPE = -5159.573447				6	0.664883000	2.178522000	-1.229407000
.....				1	0.912995000	1.638768000	-2.146880000
2				6	1.816282000	3.137767000	-0.789069000
E + ZPE = -5159.573447				1	2.618293000	3.158221000	-1.535819000

1	1.416760000	4.157832000	-0.739676000
6	2.367296000	2.737216000	0.595864000
1	2.760926000	3.606918000	1.137528000
1	3.200388000	2.030932000	0.488719000
6	1.241263000	2.056574000	1.392737000
1	0.452682000	2.796812000	1.593839000
6	1.706484000	1.464040000	2.722025000
1	2.450192000	0.674013000	2.568583000
1	0.874336000	1.047755000	3.299508000
1	2.175354000	2.241467000	3.337813000
6	-0.644492000	2.943767000	-1.489247000
1	-1.006101000	3.445520000	-0.582996000
1	-1.426161000	2.272058000	-1.852032000
1	-0.472369000	3.717256000	-2.248225000
6	1.700710000	-0.418536000	-0.149408000
6	2.654916000	-0.278603000	-1.167594000
1	2.662061000	0.612321000	-1.784533000
6	3.609358000	-1.264433000	-1.423693000
1	4.330781000	-1.121000000	-2.223476000
6	3.626836000	-2.422740000	-0.654335000
1	4.361243000	-3.201286000	-0.841422000
6	2.685404000	-2.577112000	0.362759000
1	2.695932000	-3.481749000	0.966610000
6	1.718327000	-1.601634000	0.632413000
6	0.744297000	-1.878441000	1.770287000
1	0.681878000	-1.027301000	2.451717000
1	1.119483000	-2.737875000	2.348489000
8	-0.599218000	-2.120629000	1.377110000
6	-0.785077000	-3.303902000	0.610328000
1	-0.435277000	-4.187211000	1.167612000
1	-1.858647000	-3.383952000	0.431657000
1	-0.272631000	-3.246581000	-0.355874000
6	-3.610923000	-0.086913000	0.458127000
1	-4.059705000	-1.038174000	0.191257000
6	-2.994025000	0.058704000	1.707665000
6	-2.155667000	1.187846000	1.899514000
1	-2.491956000	2.167876000	1.553837000
1	-2.873419000	-0.811337000	2.350649000
1	-1.558790000	1.227259000	2.808053000
1	-4.000760000	0.774538000	-0.081791000
35	-1.561081000	-0.709551000	-1.854675000

3
E + ZPE = -2587.621090

28	1.634207000	-0.685595000	-0.179177000
15	-0.036080000	0.751887000	-0.022276000
6	0.029829000	1.898183000	1.471476000
1	-0.982807000	1.909776000	1.889835000
6	0.325865000	3.286839000	0.860958000
1	0.049139000	4.078385000	1.566199000
1	1.404611000	3.387859000	0.679538000
6	-0.437294000	3.403332000	-0.465681000
1	-0.150001000	4.300650000	-1.025292000
1	-1.516199000	3.481674000	-0.275744000
6	-0.144640000	2.133919000	-1.296974000
1	0.878213000	2.211626000	-1.685894000
6	-1.093253000	1.890262000	-2.472952000
1	-2.130602000	1.777533000	-2.143472000
1	-0.819260000	0.994359000	-3.041578000
1	-1.051384000	2.740730000	-3.162320000
6	0.999543000	1.464245000	2.574049000
1	2.029425000	1.402762000	2.206027000

1	0.727416000	0.489396000	2.993931000
1	0.984196000	2.190148000	3.394763000
6	-1.671352000	-0.097319000	0.048729000
6	-2.820479000	0.589773000	0.472196000
1	-2.758049000	1.636778000	0.751347000
6	-4.064042000	-0.039661000	0.534266000
1	-4.936228000	0.519905000	0.858439000
6	-4.177581000	-1.383271000	0.184343000
1	-5.137738000	-1.887050000	0.238338000
6	-3.045724000	-2.082660000	-0.232586000
1	-3.135338000	-3.131456000	-0.504269000
6	-1.796196000	-1.458026000	-0.318577000
6	-0.639446000	-2.273508000	-0.848430000
1	-0.273963000	-1.899583000	-1.809318000
1	-0.941743000	-3.315883000	-0.990703000
8	0.538712000	-2.277742000	0.001555000
6	0.349367000	-2.902480000	1.288433000
1	-0.079072000	-3.898391000	1.140785000
1	1.337234000	-2.990085000	1.740801000
1	-0.308992000	-2.299571000	1.920917000
6	2.983685000	0.634960000	-0.660435000
1	3.073456000	1.605052000	-0.178330000
6	3.619016000	-0.479333000	-0.046956000
6	3.322776000	-1.742450000	-0.559261000
1	3.200650000	-1.896057000	-1.632363000
1	4.028670000	-0.385722000	0.958293000
1	3.595124000	-2.630200000	0.004279000
1	2.946495000	0.690827000	-1.751136000

3'
E + ZPE = -2587.620467

28	1.650244000	-0.654724000	-0.200927000
15	-0.053113000	0.753060000	-0.021920000
6	0.002315000	1.855224000	1.504867000
1	-1.024073000	1.886597000	1.888669000
6	0.349447000	3.247502000	0.932381000
1	0.108741000	4.028699000	1.662020000
1	1.429416000	3.311232000	0.742045000
6	-0.425198000	3.426063000	-0.380540000
1	-0.118518000	4.330999000	-0.916978000
1	-1.498469000	3.530625000	-0.171939000
6	-0.182796000	2.174612000	-1.254078000
1	0.826891000	2.245169000	-1.675564000
6	-1.171561000	1.978548000	-2.405257000
1	-2.201269000	1.882355000	-2.048147000
1	-0.935166000	1.088484000	-2.999088000
1	-1.129539000	2.842656000	-3.077440000
6	0.918737000	1.371099000	2.631266000
1	1.959041000	1.287183000	2.300767000
1	0.603738000	0.396432000	3.020936000
1	0.893102000	2.079746000	3.466599000
6	-1.674870000	-0.120930000	0.025593000
6	-2.839166000	0.552003000	0.430323000
1	-2.793244000	1.599912000	0.710144000
6	-4.075196000	-0.093292000	0.471882000
1	-4.959978000	0.454728000	0.781289000
6	-4.165410000	-1.438316000	0.119618000
1	-5.119959000	-1.954120000	0.156962000
6	-3.017956000	-2.123519000	-0.277584000
1	-3.089504000	-3.173506000	-0.550077000
6	-1.775229000	-1.482882000	-0.342904000
6	-0.598855000	-2.282153000	-0.853921000

1	-0.232855000	-1.909494000	-1.815091000
1	-0.881032000	-3.331151000	-0.989387000
8	0.570218000	-2.257146000	0.006689000
6	0.385209000	-2.879637000	1.294649000
1	-0.004830000	-3.891269000	1.148145000
1	1.369122000	-2.928429000	1.760858000
1	-0.303865000	-2.297726000	1.913980000
6	3.419896000	-1.634740000	-0.030141000
1	3.543363000	-2.654126000	-0.383884000
6	3.498184000	-0.576356000	-0.935000000
6	3.034164000	0.692090000	-0.484585000
1	3.352826000	1.051091000	0.495059000
1	3.583785000	-0.780787000	-2.001804000
1	2.924015000	1.481074000	-1.223990000
1	3.636087000	-1.474720000	1.027758000

5
E + ZPE = -5005.807538

28	1.605525000	0.093891000	-0.472560000
15	-0.447321000	0.697942000	0.041811000
6	-0.722050000	1.476967000	1.744273000
1	-1.422644000	0.818497000	2.269739000
6	-1.399469000	2.846002000	1.474867000
1	-2.031006000	3.136898000	2.322943000
1	-0.617856000	3.613310000	1.387017000
6	-2.185223000	2.785327000	0.158447000
1	-2.502010000	3.782947000	-0.172298000
1	-3.097595000	2.186344000	0.277267000
6	-1.261484000	2.125208000	-0.878040000
1	-0.430161000	2.817556000	-1.070595000
6	-1.922406000	1.764762000	-2.208181000
1	-2.760700000	1.076010000	-2.061644000
1	-1.214444000	1.288988000	-2.895758000
1	-2.308259000	2.666749000	-2.698716000
6	0.544888000	1.602322000	2.597956000
1	1.315880000	2.187854000	2.081764000
1	0.970023000	0.622667000	2.825240000
1	0.307837000	2.115806000	3.538469000
6	-1.655155000	-0.685960000	-0.107854000
6	-2.890102000	-0.720667000	0.558699000
1	-3.171356000	0.074314000	1.242105000
6	-3.777551000	-1.780089000	0.363518000
1	-4.726589000	-1.790660000	0.892955000
6	-3.445686000	-2.822677000	-0.502279000
1	-4.135024000	-3.649532000	-0.650456000
6	-2.220070000	-2.802522000	-1.168934000
1	-1.946599000	-3.616026000	-1.835251000
6	-1.332684000	-1.745528000	-0.970684000
1	-0.370090000	-1.753996000	-1.473263000
35	1.727283000	-1.518911000	1.163847000
6	1.761283000	1.103431000	-2.153312000
1	1.407055000	2.123239000	-2.282683000
6	3.040485000	0.913050000	-1.568445000
6	3.406849000	-0.395478000	-1.228817000
1	3.143660000	-1.234770000	-1.871700000
1	3.552652000	1.755489000	-1.103672000
1	4.257913000	-0.565166000	-0.578332000
1	1.429796000	0.422372000	-2.940533000

5'
E + ZPE = -5005.807841

28	1.602416000	0.063224000	-0.475886000
15	-0.441379000	0.694590000	0.035593000
6	-0.667233000	1.460892000	1.750850000
1	-1.420759000	0.847576000	2.258116000
6	-1.243067000	2.877509000	1.502067000
1	-1.828629000	3.212666000	2.366675000
1	-0.408384000	3.584125000	1.393791000
6	-2.065031000	2.874570000	0.206790000
1	-2.326561000	3.891917000	-0.111920000
1	-3.010652000	2.334873000	0.349200000
6	-1.211600000	2.164231000	-0.857287000
1	-0.353202000	2.812082000	-1.080136000
6	-1.932028000	1.837528000	-2.165231000
1	-2.798570000	1.191090000	-1.992851000
1	-1.270779000	1.325791000	-2.874173000
1	-2.286849000	2.757720000	-2.645294000
6	0.598791000	1.475069000	2.614783000
1	1.412204000	2.019527000	2.119020000
1	0.955072000	0.463014000	2.817844000
1	0.392219000	1.977644000	3.568285000
6	-1.694085000	-0.647348000	-0.115637000
6	-2.941847000	-0.628180000	0.527563000
1	-3.206999000	0.185516000	1.195580000
6	-3.862934000	-1.657319000	0.326711000
1	-4.822040000	-1.627785000	0.836968000
6	-3.551937000	-2.721345000	-0.521082000
1	-4.268199000	-3.524219000	-0.673688000
6	-2.313887000	-2.753813000	-1.163802000
1	-2.057333000	-3.584553000	-1.815397000
6	-1.392602000	-1.727273000	-0.959810000
1	-0.419437000	-1.773350000	-1.438472000
35	1.658939000	-1.660735000	1.048453000
6	3.563180000	-0.131456000	-0.906495000
1	4.016975000	-1.110268000	-1.015498000
6	2.851942000	0.427635000	-1.974080000
6	2.021337000	1.545931000	-1.697736000
1	2.408591000	2.357886000	-1.077307000
1	2.678038000	-0.163554000	-2.873206000
1	1.347249000	1.880063000	-2.483008000
1	4.004213000	0.499067000	-0.135086000

6
E + ZPE = -5005.778099

28	1.559137000	0.123817000	-0.451202000
15	-0.586271000	0.634590000	0.082397000
6	-0.868581000	1.415106000	1.779441000
1	-1.781161000	0.960451000	2.185010000
6	-1.154092000	2.902648000	1.480492000
1	-1.642227000	3.383633000	2.337110000
1	-0.203409000	3.430952000	1.319498000
6	-2.006411000	2.980545000	0.207434000
1	-2.122407000	4.012523000	-0.148086000
1	-3.017672000	2.600380000	0.409556000
6	-1.321942000	2.102163000	-0.858284000
1	-0.435107000	2.645227000	-1.215104000
6	-2.187909000	1.759378000	-2.071579000
1	-3.089343000	1.210985000	-1.780555000
1	-1.644635000	1.141344000	-2.795310000
1	-2.501192000	2.676705000	-2.585259000
6	0.271584000	1.185331000	2.775492000
1	1.214885000	1.605228000	2.407272000

1	0.441463000	0.120463000	2.958408000
1	0.039370000	1.668011000	3.733339000
6	-1.811612000	-0.733824000	-0.048278000
6	-3.136867000	-0.636304000	0.410091000
1	-3.487666000	0.275017000	0.886334000
6	-4.022781000	-1.703031000	0.263663000
1	-5.043970000	-1.609490000	0.623800000
6	-3.598176000	-2.888299000	-0.341571000
1	-4.287806000	-3.720964000	-0.451319000
6	-2.285042000	-3.000517000	-0.797035000
1	-1.942963000	-3.922421000	-1.259140000
6	-1.398784000	-1.931766000	-0.651021000
1	-0.371411000	-2.035601000	-0.986602000
35	2.263007000	-1.665931000	0.846147000
6	2.575710000	1.788854000	-0.733469000
1	3.222768000	2.069033000	0.096884000
6	2.984525000	0.756659000	-1.621369000
6	1.888059000	0.282381000	-2.390114000
1	1.196972000	0.995073000	-2.839385000
1	3.921071000	0.217960000	-1.521251000
1	1.971417000	-0.666749000	-2.917918000
1	1.929934000	2.588153000	-1.098072000

7
E + ZPE = -5159.548506

28	-1.458792000	-0.017491000	0.636599000
15	0.553154000	0.869320000	0.191469000
6	0.821281000	2.107144000	-1.212799000
1	1.182059000	1.515347000	-2.058091000
6	1.911356000	3.113170000	-0.724825000
1	2.651901000	3.299768000	-1.511909000
1	1.421141000	4.075046000	-0.528388000
6	2.579612000	2.627244000	0.573845000
1	3.044721000	3.459651000	1.118371000
1	3.378185000	1.905950000	0.358648000
6	1.498336000	1.941404000	1.422662000
1	0.754852000	2.697515000	1.717457000
6	2.020479000	1.252243000	2.682709000
1	2.719470000	0.444244000	2.437641000
1	1.205140000	0.833107000	3.283609000
1	2.555782000	1.970393000	3.316022000
6	-0.443458000	2.832557000	-1.690082000
1	-0.865559000	3.465360000	-0.901364000
1	-1.198605000	2.117152000	-2.024915000
1	-0.181819000	3.489805000	-2.529409000
6	1.760543000	-0.498118000	-0.185152000
6	2.780588000	-0.373051000	-1.139424000
1	2.895734000	0.548930000	-1.697276000
6	3.672992000	-1.414618000	-1.402145000
1	4.451053000	-1.279623000	-2.148539000
6	3.560972000	-2.617255000	-0.711173000
1	4.247029000	-3.435770000	-0.909841000
6	2.548550000	-2.764372000	0.236121000
1	2.447766000	-3.704367000	0.774186000
6	1.650944000	-1.726865000	0.508462000
6	0.572713000	-1.962910000	1.541823000
1	0.585767000	-1.209179000	2.331440000
1	0.709693000	-2.946381000	2.009029000
8	-0.759576000	-1.901779000	1.004779000
6	-1.097090000	-3.023696000	0.167529000
1	-0.886018000	-3.945071000	0.725024000
1	-2.159352000	-2.940856000	-0.050282000

1	-0.536270000	-2.991773000	-0.768105000
6	-2.323540000	1.702961000	1.019229000
1	-2.467626000	2.420966000	0.218136000
6	-3.265078000	0.636618000	1.125803000
6	-2.932489000	-0.377949000	2.022501000
1	-2.452631000	-0.148967000	2.973030000
1	-4.000177000	0.468965000	0.343946000
1	-3.463898000	-1.325589000	1.983484000
1	-1.912333000	2.128183000	1.936528000
35	-1.925737000	-0.485019000	-1.844114000

8
E + ZPE = -5321.729045

28	-0.887612000	-0.868636000	-0.912077000
15	1.036368000	-0.717008000	0.169250000
6	1.104072000	-1.383450000	1.934922000
1	1.114097000	-0.512916000	2.596460000
6	2.446655000	-2.162654000	2.050567000
1	2.890145000	-2.021802000	3.042392000
1	2.234840000	-3.235056000	1.951515000
6	3.404025000	-1.741671000	0.928129000
1	4.227955000	-2.456057000	0.812837000
1	3.858406000	-0.765371000	1.143215000
6	2.577540000	-1.652583000	-0.367840000
1	2.206207000	-2.659322000	-0.605969000
6	3.352017000	-1.121110000	-1.574288000
1	3.655948000	-0.077960000	-1.436029000
1	2.773283000	-1.198254000	-2.500947000
1	4.262998000	-1.713569000	-1.715887000
6	-0.103616000	-2.245920000	2.329778000
1	-0.228345000	-3.103703000	1.660082000
1	-1.027524000	-1.663354000	2.322088000
1	0.050095000	-2.641045000	3.341257000
6	1.551883000	1.060215000	0.241412000
6	2.104020000	1.643971000	1.389490000
1	2.275769000	1.049962000	2.280080000
6	2.460296000	2.994646000	1.421276000
1	2.894738000	3.414634000	2.323898000
6	2.264263000	3.791592000	0.297527000
1	2.538521000	4.842244000	0.311316000
6	1.716373000	3.225934000	-0.854510000
1	1.572311000	3.842888000	-1.738325000
6	1.358167000	1.875336000	-0.902310000
6	0.805208000	1.319170000	-2.197545000
1	1.359927000	0.439962000	-2.529037000
1	0.873573000	2.071990000	-2.991133000
8	-0.564742000	0.873891000	-2.105536000
6	-1.518836000	1.937624000	-2.238219000
1	-1.334614000	2.475257000	-3.175898000
1	-2.503421000	1.472951000	-2.269662000
1	-1.459983000	2.628664000	-1.391397000
6	-0.642408000	-2.769682000	-1.369042000
1	-0.170224000	-3.461102000	-0.675576000
6	-2.016085000	-2.466351000	-1.190352000
6	-2.518372000	-1.414844000	-1.972175000
1	-2.195828000	-1.304102000	-3.006727000
1	-2.546801000	-2.808392000	-0.304227000
1	-3.497665000	-1.006706000	-1.739423000
1	-0.226655000	-2.809650000	-2.377838000
35	-2.189642000	0.478356000	0.909275000
11	-3.927814000	1.563803000	2.466460000

9

E + ZPE = -5321.719654

28	1.090346000	-0.417475000	0.948598000
15	-0.953187000	-0.836195000	-0.082063000
6	-0.979396000	-1.839638000	-1.687335000
1	-1.184294000	-1.138405000	-2.501225000
6	-2.145133000	-2.862643000	-1.551309000
1	-2.651325000	-3.002554000	-2.513008000
1	-1.720956000	-3.837193000	-1.276492000
6	-3.114863000	-2.417255000	-0.450718000
1	-3.775367000	-3.236270000	-0.140347000
1	-3.762450000	-1.603674000	-0.802963000
6	-2.266030000	-1.919133000	0.731280000
1	-1.693517000	-2.772599000	1.125509000
6	-3.077345000	-1.305976000	1.873484000
1	-3.602438000	-0.399014000	1.554871000
1	-2.452697000	-1.060478000	2.739219000
1	-3.833962000	-2.021302000	2.216017000
6	0.356169000	-2.529797000	-1.998514000
1	0.669910000	-3.188958000	-1.180983000
1	1.151558000	-1.801127000	-2.171401000
1	0.249095000	-3.148206000	-2.898021000
6	-1.829249000	0.755237000	-0.456773000
6	-2.566929000	0.964365000	-1.630486000
1	-2.675067000	0.168584000	-2.358893000
6	-3.191471000	2.185963000	-1.894470000
1	-3.759185000	2.312323000	-2.811831000
6	-3.089384000	3.229792000	-0.980307000
1	-3.571699000	4.183196000	-1.174296000
6	-2.363008000	3.038662000	0.195685000
1	-2.290807000	3.848490000	0.918003000
6	-1.731617000	1.821928000	0.473044000
6	-0.991939000	1.681296000	1.787669000
1	-1.307952000	0.793680000	2.336949000
1	-1.186649000	2.553739000	2.422405000
8	0.437875000	1.533333000	1.648525000
6	1.104195000	2.764705000	1.339783000
1	0.850025000	3.513962000	2.099188000
1	2.173876000	2.560717000	1.370110000
1	0.824779000	3.128236000	0.346079000
6	2.395669000	-1.893497000	1.161840000
1	3.336138000	-1.829845000	0.621465000
6	2.227440000	-1.156171000	2.357247000
6	0.867844000	-1.121982000	2.774516000
1	0.290450000	-2.045582000	2.758996000
1	2.986922000	-0.488148000	2.754979000
1	0.567285000	-0.414207000	3.543548000
1	1.869437000	-2.838981000	1.036114000
35	2.207365000	0.555992000	-1.002630000
11	4.534227000	0.717664000	-2.155250000

10

E + ZPE = -2587.583186

28	1.744348000	-0.584488000	-0.112673000
15	-0.075382000	0.797494000	-0.008314000
6	-0.095022000	1.950655000	1.485308000
1	-1.130899000	1.974170000	1.841848000
6	0.248793000	3.330938000	0.884026000
1	-0.034068000	4.128697000	1.580044000
1	1.334826000	3.409887000	0.734759000

6	-0.472305000	3.456397000	-0.463696000
1	-0.163103000	4.352803000	-1.013146000
1	-1.555847000	3.539921000	-0.304581000
6	-0.163452000	2.185851000	-1.285495000
1	0.869119000	2.263338000	-1.652468000
6	-1.085605000	1.940952000	-2.481723000
1	-2.129504000	1.828007000	-2.173659000
1	-0.800764000	1.043644000	-3.042541000
1	-1.029753000	2.790387000	-3.171567000
6	0.803600000	1.516829000	2.646005000
1	1.853950000	1.454732000	2.341192000
1	0.502976000	0.544272000	3.052198000
1	0.739791000	2.244119000	3.463197000
6	-1.686866000	-0.102841000	0.017938000
6	-2.867771000	0.560791000	0.386846000
1	-2.844016000	1.618146000	0.631893000
6	-4.092967000	-0.104624000	0.441654000
1	-4.989596000	0.437577000	0.726431000
6	-4.156091000	-1.461156000	0.133278000
1	-5.101240000	-1.993344000	0.180172000
6	-2.993775000	-2.135077000	-0.241152000
1	-3.047124000	-3.191435000	-0.492396000
6	-1.759364000	-1.478965000	-0.314129000
6	-0.568982000	-2.272885000	-0.812262000
1	-0.133423000	-1.818757000	-1.709378000
1	-0.879960000	-3.287554000	-1.085644000
8	0.531138000	-2.371255000	0.121270000
6	0.295077000	-3.263169000	1.222960000
1	0.090490000	-4.272322000	0.848130000
1	1.208858000	-3.277127000	1.819502000
1	-0.544452000	-2.916866000	1.835037000
6	3.515187000	-0.155245000	0.613027000
1	3.720047000	-0.540989000	1.612225000
6	3.600880000	-1.024829000	-0.499607000
6	2.937126000	-0.480030000	-1.633959000
1	3.102245000	0.560260000	-1.913190000
1	3.868948000	-2.074636000	-0.416674000
1	2.680774000	-1.136214000	-2.466551000
1	3.700828000	0.911014000	0.490457000

11

E + ZPE = -2666.141612

28	-1.670084000	-0.175958000	0.101001000
15	0.355374000	0.844550000	0.021430000
6	0.796946000	2.220653000	-1.188531000
1	1.274980000	1.745449000	-2.050552000
6	1.801723000	3.161144000	-0.440896000
1	2.707893000	3.311530000	-1.036952000
1	1.333170000	4.146580000	-0.339559000
6	2.142581000	2.616131000	0.959219000
1	2.427556000	3.426292000	1.640521000
1	2.996212000	1.929272000	0.914414000
6	0.917848000	1.859519000	1.501402000
1	0.098363000	2.577770000	1.653161000
6	1.169967000	1.115415000	2.812653000
1	1.930630000	0.336216000	2.693566000
1	0.256985000	0.657327000	3.209915000
1	1.534381000	1.815377000	3.572649000
6	-0.412338000	3.017617000	-1.702574000
1	-0.944061000	3.515014000	-0.884848000
1	-1.130972000	2.401668000	-2.250524000
1	-0.061422000	3.800165000	-2.384660000

6	1.682805000	-0.431033000	-0.196544000
6	2.834900000	-0.202646000	-0.963013000
1	2.993503000	0.753965000	-1.447665000
6	3.814441000	-1.187511000	-1.115041000
1	4.698345000	-0.977267000	-1.709844000
6	3.657406000	-2.427480000	-0.502561000
1	4.414385000	-3.197604000	-0.614539000
6	2.512834000	-2.675892000	0.256039000
1	2.386210000	-3.643413000	0.735856000
6	1.525607000	-1.698592000	0.417282000
6	0.306686000	-2.026709000	1.243638000
1	0.130206000	-1.302908000	2.040334000
1	0.404843000	-3.014669000	1.704790000
8	-0.918582000	-2.018906000	0.460254000
6	-1.123730000	-3.236094000	-0.278880000
1	-1.115787000	-4.081735000	0.416525000
1	-2.102388000	-3.170537000	-0.751528000
1	-0.345078000	-3.373132000	-1.036286000
6	-2.660193000	1.492677000	0.400095000
1	-2.904857000	2.145082000	-0.433796000
6	-3.528121000	0.389805000	0.668077000
6	-3.069443000	-0.534500000	1.597448000
1	-2.498361000	-0.214360000	2.467148000
6	-1.452939000	-0.594751000	-2.407332000
6	-2.766579000	-0.717136000	-2.143518000
1	-3.447689000	0.115217000	-2.296304000
1	-3.226960000	-1.671814000	-1.905575000
1	-0.776010000	-1.442577000	-2.375516000
1	-1.041252000	0.331122000	-2.793216000
1	-4.344012000	0.137131000	-0.003055000
1	-3.548255000	-1.505798000	1.682323000
1	-2.222568000	2.016764000	1.249907000

12
E + ZPE = -2666.150363

28	-1.725321000	-0.408474000	0.011257000
15	0.307120000	0.843341000	-0.067692000
6	0.532616000	2.243879000	-1.329867000
1	1.471434000	2.037622000	-1.851899000
6	0.718412000	3.525623000	-0.482389000
1	1.250682000	4.287664000	-1.062491000
1	-0.266656000	3.946746000	-0.237076000
6	1.454824000	3.157571000	0.806155000
1	1.482810000	3.991518000	1.517256000
1	2.496895000	2.888652000	0.587188000
6	0.727460000	1.947235000	1.419186000
1	-0.246337000	2.299535000	1.791408000
6	1.484397000	1.288634000	2.575508000
1	2.450146000	0.891308000	2.248991000
1	0.921304000	0.471827000	3.040072000
1	1.676061000	2.031572000	3.357846000
6	-0.559951000	2.386178000	-2.392478000
1	-1.551330000	2.520888000	-1.946539000
1	-0.593643000	1.524412000	-3.064562000
1	-0.353573000	3.270980000	-3.005620000
6	1.781609000	-0.268928000	-0.226796000
6	2.965738000	0.127199000	-0.865772000
1	3.051175000	1.113537000	-1.306984000
6	4.074088000	-0.719500000	-0.940839000
1	4.976560000	-0.378809000	-1.439499000
6	4.018941000	-1.989240000	-0.373744000
1	4.874268000	-2.655694000	-0.427507000

6	2.850079000	-2.400314000	0.266858000
1	2.804807000	-3.390340000	0.714148000
6	1.733990000	-1.561175000	0.352600000
6	0.515240000	-2.068040000	1.087170000
1	0.212105000	-1.407124000	1.898652000
1	0.713398000	-3.056907000	1.514393000
8	-0.663020000	-2.182539000	0.243027000
6	-0.523853000	-3.261176000	-0.704772000
1	-0.344510000	-4.191390000	-0.156073000
1	-1.455377000	-3.349293000	-1.258525000
1	0.305387000	-3.071023000	-1.392676000
6	-2.902168000	1.119804000	0.371645000
1	-3.662399000	1.357373000	-0.367989000
6	-3.183978000	0.113135000	1.355341000
6	-2.143843000	-0.259635000	2.184218000
1	-1.389677000	0.457835000	2.487771000
6	-2.133206000	-0.688147000	-1.983890000
6	-3.129454000	-1.278988000	-1.220412000
1	-4.094655000	-0.791480000	-1.122288000
1	-3.145041000	-2.342536000	-1.000649000
1	-1.325052000	-1.273651000	-2.414170000
1	-2.329694000	0.255986000	-2.477245000
1	-4.079339000	-0.497877000	1.287567000
1	-2.221570000	-1.159569000	2.787653000
1	-2.307475000	1.981004000	0.668474000

13
E + ZPE = -2666.146562

28	1.560003000	-0.736443000	0.159077000
15	-0.088061000	0.948628000	-0.036145000
6	0.111850000	2.463498000	1.051909000
1	-0.882043000	2.925731000	1.126721000
6	0.966839000	3.363625000	0.137369000
1	1.066254000	4.364566000	0.571947000
1	1.984941000	2.955602000	0.054608000
6	0.278272000	3.407227000	-1.232036000
1	0.932997000	3.822412000	-2.005278000
1	-0.592547000	4.070687000	-1.166369000
6	-0.211858000	1.983859000	-1.634453000
1	0.496414000	1.544041000	-2.343355000
6	-1.593703000	2.031298000	-2.299493000
1	-2.355507000	2.422907000	-1.617602000
1	-1.934044000	1.053951000	-2.653321000
1	-1.549831000	2.697733000	-3.168843000
6	0.680952000	2.281369000	2.458467000
1	1.684527000	1.842017000	2.438127000
1	0.041675000	1.653635000	3.087267000
1	0.761981000	3.258158000	2.948460000
6	-1.738335000	0.192195000	0.247199000
6	-2.633498000	0.671050000	1.210640000
1	-2.386887000	1.545394000	1.804763000
6	-3.862477000	0.038873000	1.423054000
1	-4.545595000	0.428989000	2.171642000
6	-4.208823000	-1.080483000	0.671075000
1	-5.164765000	-1.571403000	0.825779000
6	-3.318164000	-1.571913000	-0.286707000
1	-3.591852000	-2.442192000	-0.878420000
6	-2.082061000	-0.957890000	-0.504314000
6	-1.130936000	-1.525257000	-1.536494000
1	-0.705896000	-0.744504000	-2.171449000
1	-1.652939000	-2.231893000	-2.191630000
8	0.013496000	-2.192878000	-0.955612000

6	-0.259496000	-3.557383000	-0.610004000
1	-0.731962000	-4.070399000	-1.455621000
1	0.697349000	-4.039583000	-0.406121000
1	-0.911216000	-3.630970000	0.268980000
6	3.524450000	-0.288393000	0.363398000
1	4.118590000	-0.742049000	1.149385000
6	3.271842000	-0.984034000	-0.836330000
6	2.331696000	-0.346105000	-1.670393000
1	2.394540000	0.731316000	-1.792996000
6	0.827903000	-1.160231000	2.052033000
6	1.759924000	-2.111915000	1.688664000
1	2.758141000	-2.099005000	2.111038000
1	1.453774000	-3.065233000	1.271723000
1	-0.235718000	-1.353535000	1.950490000
1	1.099191000	-0.382158000	2.756829000
1	3.564835000	-2.021884000	-0.969588000
1	1.892293000	-0.885468000	-2.504866000
1	3.539883000	0.800817000	0.359129000

14
E + ZPE = -2666.155749

28	1.452312000	-0.895867000	0.371536000
15	0.178464000	0.901418000	-0.093953000
6	0.713187000	2.469610000	0.784427000
1	-0.119288000	3.175994000	0.662940000
6	1.874808000	2.912889000	-0.129977000
1	2.160458000	3.943422000	0.105968000
1	2.752899000	2.292990000	0.092628000
6	1.466419000	2.767048000	-1.613827000
1	2.329560000	2.476667000	-2.220191000
1	1.125997000	3.731809000	-2.003096000
6	0.303610000	1.734701000	-1.781420000
1	0.577310000	0.979917000	-2.522536000
6	-0.995771000	2.417726000	-2.238041000
1	-1.330369000	3.177926000	-1.523617000
1	-1.819195000	1.713227000	-2.381791000
1	-0.816839000	2.921120000	-3.194852000
6	1.121143000	2.422529000	2.258320000
1	1.955682000	1.732764000	2.425508000
1	0.300360000	2.135902000	2.923391000
1	1.454568000	3.418564000	2.570414000
6	-1.591288000	0.539171000	0.239354000
6	-2.247407000	1.181565000	1.298692000
1	-1.727266000	1.923019000	1.896120000
6	-3.583074000	0.899733000	1.596615000
1	-4.072409000	1.415144000	2.417568000
6	-4.280136000	-0.030361000	0.831501000
1	-5.320676000	-0.251632000	1.048748000
6	-3.635079000	-0.676524000	-0.225854000
1	-4.186878000	-1.391113000	-0.831593000
6	-2.295853000	-0.418730000	-0.535573000
6	-1.651884000	-1.168660000	-1.690952000
1	-1.062322000	-0.499772000	-2.322043000
1	-2.433991000	-1.606257000	-2.325361000
8	-0.740330000	-2.191657000	-1.276675000
6	-1.378803000	-3.425157000	-0.957511000
1	-1.930683000	-3.813436000	-1.824123000
1	-0.589691000	-4.132650000	-0.693867000
1	-2.071527000	-3.325396000	-0.110755000
6	3.042239000	-2.189129000	0.544044000
1	2.954492000	-3.187545000	0.961124000
6	2.727958000	-1.963478000	-0.796764000

6	2.631653000	-0.621863000	-1.225919000
1	3.369306000	0.102314000	-0.876440000
6	0.312445000	-2.025101000	1.722281000
6	0.911989000	-0.983723000	2.382892000
1	0.328922000	-0.108992000	2.647046000
1	1.841625000	-1.117184000	2.931420000
1	0.728893000	-3.026636000	1.729033000
1	-0.717836000	-1.939073000	1.394808000
1	2.252838000	-2.749278000	-1.381043000
1	2.232154000	-0.419547000	-2.213942000
1	3.737911000	-1.529482000	1.064490000

15
E + ZPE = -2666.147792

28	1.650089000	-0.152177000	-0.152147000
15	-0.347207000	0.850710000	-0.045402000
6	-0.701675000	2.210047000	1.214818000
1	-1.302889000	1.752023000	2.005753000
6	-1.535518000	3.293362000	0.459756000
1	-2.353919000	3.657171000	1.089820000
1	-0.883588000	4.154286000	0.267844000
6	-2.049200000	2.748916000	-0.881433000
1	-2.330225000	3.562527000	-1.560279000
1	-2.945519000	2.132089000	-0.739681000
6	-0.930368000	1.890911000	-1.499509000
1	-0.076232000	2.546639000	-1.722777000
6	-1.331336000	1.155495000	-2.778975000
1	-2.120854000	0.419681000	-2.593081000
1	-0.480854000	0.648511000	-3.248020000
1	-1.717548000	1.874119000	-3.510190000
6	0.541134000	2.825919000	1.876006000
1	1.199308000	3.298217000	1.140764000
1	1.130321000	2.097723000	2.440718000
1	0.223697000	3.605626000	2.577642000
6	-1.671305000	-0.424399000	0.181266000
6	-2.807431000	-0.206763000	0.973719000
1	-2.959934000	0.744599000	1.470692000
6	-3.781907000	-1.195213000	1.135080000
1	-4.654083000	-0.993134000	1.749627000
6	-3.633950000	-2.428251000	0.506961000
1	-4.385743000	-3.202133000	0.627643000
6	-2.507812000	-2.663548000	-0.283059000
1	-2.392626000	-3.623294000	-0.780901000
6	-1.527108000	-1.682078000	-0.457235000
6	-0.345424000	-1.986235000	-1.346425000
1	-0.222666000	-1.245797000	-2.138183000
1	-0.461623000	-2.965634000	-1.821203000
8	0.922339000	-1.979280000	-0.636261000
6	1.222575000	-3.230427000	0.006462000
1	1.251935000	-4.024671000	-0.746627000
1	2.205552000	-3.128527000	0.464076000
1	0.473179000	-3.470858000	0.767737000
6	3.560880000	-0.665794000	-0.698716000
1	3.719308000	-1.572964000	-1.275562000
6	3.087027000	0.485345000	-1.341390000
6	2.628801000	1.521493000	-0.480669000
1	3.210924000	1.773119000	0.405865000
6	1.150825000	-0.845069000	2.487545000
6	2.480015000	-0.760457000	2.334325000
1	3.016583000	0.167261000	2.514575000
1	3.088220000	-1.636665000	2.130361000
1	0.619007000	-1.786381000	2.390928000

1	0.556570000	0.006505000	2.801861000
1	2.830798000	0.477655000	-2.399410000
1	2.128314000	2.377962000	-0.924474000
1	4.172166000	-0.570657000	0.194551000

S1

E + ZPE = -2044.711735

28	-0.134518000	0.169889000	-0.025422000
6	-2.113854000	0.204073000	0.213164000
1	-2.213161000	0.254341000	1.299185000
15	2.003580000	-0.386456000	-0.011781000
1	3.000864000	0.615502000	-0.036161000
1	2.488191000	-1.199009000	-1.055506000
1	2.455672000	-1.119560000	1.102132000
6	-1.701938000	-0.986520000	-0.403140000
6	-0.662352000	-1.699154000	0.243912000
1	-0.689176000	-1.821870000	1.328896000
8	0.043276000	2.093158000	0.038363000
1	0.814072000	2.605244000	-0.255833000
1	-0.735958000	2.665573000	-0.046976000
1	-1.927720000	-1.171941000	-1.452269000
1	-0.200093000	-2.528951000	-0.285347000
1	-2.757226000	0.884962000	-0.340112000

S2

E + ZPE = -2046.859485

28	0.130812000	0.044763000	-0.028039000
6	2.117734000	-0.003392000	-0.329920000
1	2.129600000	-0.045743000	-1.421414000
15	-2.022401000	-0.545013000	0.005459000
1	-3.006660000	0.465785000	0.041858000
1	-2.480580000	-1.353858000	1.063748000
1	-2.491294000	-1.291648000	-1.093177000
6	1.727705000	-1.128370000	0.410248000
6	0.666441000	-1.897514000	-0.106198000
1	0.617019000	-2.090196000	-1.180499000
6	-0.099081000	2.029901000	-0.597286000
6	0.082115000	1.966067000	0.762667000
1	-0.764751000	2.006289000	1.445379000
1	1.051798000	2.160732000	1.211775000
1	0.729290000	2.271534000	-1.258408000
1	-1.091142000	2.153918000	-1.025532000
1	1.994413000	-1.205879000	1.463371000
1	0.215363000	-2.668507000	0.512387000
1	2.800742000	0.719266000	0.106654000

S3

E + ZPE = -2277.848315

28	1.340581000	0.031097000	0.126426000
6	2.610840000	-1.520344000	0.305181000
1	3.431073000	-1.029711000	0.832478000
15	0.668494000	2.096691000	-0.377706000
1	-0.083900000	2.856500000	0.540871000
1	-0.119926000	2.282583000	-1.529919000
1	1.696274000	3.022130000	-0.648002000
6	2.377147000	-1.239152000	-1.049104000
6	2.572833000	0.092429000	-1.467774000
1	3.430686000	0.651051000	-1.089380000

6	0.578511000	-0.046280000	2.034103000
6	-0.192391000	-0.893019000	1.253639000
1	0.073264000	-1.947750000	1.236949000
1	1.340457000	-0.473263000	2.680563000
1	0.213529000	0.930484000	2.338655000
1	1.781094000	-1.920501000	-1.654187000
1	2.239701000	0.390891000	-2.458379000
1	2.320103000	-2.483412000	0.714160000
6	-1.453327000	-0.578035000	0.574416000
6	-2.215959000	0.571307000	0.872078000
1	-1.902542000	1.241666000	1.667293000
6	-1.936578000	-1.475668000	-0.399862000
1	-1.375659000	-2.382286000	-0.615274000
6	-3.125541000	-1.220055000	-1.077442000
6	-3.408661000	0.819104000	0.199795000
6	-3.861532000	-0.069916000	-0.781627000
1	-3.998945000	1.694684000	0.452836000
1	-3.485111000	-1.921387000	-1.824012000
1	-4.795842000	0.125007000	-1.299401000

S4

E + ZPE = -2666.144361

28	1.653064000	-0.194131000	-0.128190000
15	-0.305962000	0.869859000	-0.052438000
6	-0.543538000	2.245184000	1.223911000
1	-1.216179000	1.852241000	1.992136000
6	-1.234076000	3.416623000	0.463605000
1	-1.959647000	3.918360000	1.112511000
1	-0.470660000	4.163260000	0.210367000
6	-1.877440000	2.904398000	-0.830918000
1	-2.122622000	3.728781000	-1.510579000
1	-2.816220000	2.375336000	-0.622093000
6	-0.874996000	1.940008000	-1.491687000
1	0.017415000	2.516054000	-1.771731000
6	-1.409562000	1.228622000	-2.735569000
1	-2.241094000	0.558253000	-2.494817000
1	-0.632002000	0.653055000	-3.249342000
1	-1.780723000	1.971796000	-3.449886000
6	0.744562000	2.701941000	1.924219000
1	1.498595000	3.045240000	1.208048000
1	1.191761000	1.916355000	2.539878000
1	0.516298000	3.545070000	2.586064000
6	-1.678046000	-0.351132000	0.195420000
6	-2.786795000	-0.081483000	1.010132000
1	-2.881757000	0.873075000	1.515338000
6	-3.806980000	-1.020381000	1.185339000
1	-4.655519000	-0.778957000	1.818453000
6	-3.733654000	-2.254147000	0.546308000
1	-4.520989000	-2.990266000	0.676523000
6	-2.637400000	-2.538837000	-0.269345000
1	-2.582910000	-3.497953000	-0.778544000
6	-1.610119000	-1.608907000	-0.456653000
6	-0.463594000	-1.969386000	-1.373513000
1	-0.309226000	-1.216733000	-2.149104000
1	-0.659057000	-2.923487000	-1.874140000
8	0.807322000	-2.062794000	-0.685614000
6	1.064632000	-3.366705000	-0.142736000
1	1.077537000	-4.106227000	-0.950998000
1	2.046784000	-3.331914000	0.328546000
1	0.304554000	-3.645412000	0.595965000
6	2.463918000	1.281740000	-1.151021000
1	2.312231000	2.321688000	-0.873518000

6	3.473943000	0.549835000	-0.478735000
6	3.506525000	-0.828254000	-0.715308000
1	3.275532000	-1.220470000	-1.704359000
6	0.989381000	-1.016822000	2.357505000
6	2.317231000	-0.842593000	2.267978000
1	2.786688000	0.103374000	2.522919000
1	2.987297000	-1.674288000	2.072453000
1	0.524214000	-1.984176000	2.202142000
1	0.327896000	-0.216338000	2.672011000
1	3.997111000	0.983176000	0.370958000
1	4.142612000	-1.461643000	-0.104125000
1	2.263204000	1.074671000	-2.203860000

S5
E + ZPE = -2666.156054

28	-1.763531000	-0.052314000	-0.210032000
15	0.250136000	0.879761000	0.027090000
6	0.514366000	2.331570000	-1.146621000
1	0.991295000	1.955234000	-2.056555000
6	1.448180000	3.342496000	-0.407031000
1	2.310582000	3.600036000	-1.030155000
1	0.890959000	4.272743000	-0.249105000
6	1.893990000	2.779584000	0.953903000
1	2.140311000	3.584242000	1.656020000
1	2.797909000	2.167864000	0.847492000
6	0.757817000	1.908295000	1.520872000
1	-0.110976000	2.554904000	1.710945000
6	1.141796000	1.184035000	2.811693000
1	1.970826000	0.487666000	2.648071000
1	0.305627000	0.633126000	3.252762000
1	1.472387000	1.917285000	3.555627000
6	-0.820003000	2.989975000	-1.540676000
1	-1.382504000	3.317286000	-0.658225000
1	-1.464680000	2.328491000	-2.128026000
1	-0.621727000	3.879299000	-2.149179000
6	1.642849000	-0.314061000	-0.221486000
6	2.711240000	0.013683000	-1.069723000
1	2.738168000	0.972961000	-1.574037000
6	3.769107000	-0.872657000	-1.285299000
1	4.582070000	-0.588542000	-1.946688000
6	3.775429000	-2.108966000	-0.648116000
1	4.592753000	-2.806228000	-0.805124000
6	2.720505000	-2.447243000	0.200979000
1	2.731405000	-3.408809000	0.708208000
6	1.648650000	-1.576701000	0.426685000
6	0.541495000	-2.028417000	1.362706000
1	0.281951000	-1.243536000	2.074965000
1	0.880608000	-2.896843000	1.942613000
8	-0.687817000	-2.350470000	0.699063000
6	-0.673548000	-3.627483000	0.062284000
1	-0.478699000	-4.423405000	0.793212000
1	-1.665406000	-3.778521000	-0.369536000
1	0.081049000	-3.679991000	-0.733059000
6	-2.189163000	0.361803000	1.704048000
1	-1.846501000	1.257363000	2.209778000
6	-3.355921000	0.441401000	0.921247000
6	-3.698493000	-0.688759000	0.168824000
1	-3.500902000	-1.683436000	0.564022000
6	-1.024515000	-0.604353000	-2.062921000
6	-2.387083000	-0.823401000	-2.049941000
1	-3.066695000	-0.116111000	-2.518309000
1	-2.777154000	-1.827896000	-1.922000000

1	-0.334100000	-1.428107000	-1.915692000
1	-0.622571000	0.253762000	-2.592127000
1	-3.804524000	1.407240000	0.694799000
1	-4.513611000	-0.626861000	-0.543507000
1	-1.948679000	-0.573877000	2.206318000

S6
E + ZPE = -2666.157962

28	1.715112000	-0.016372000	-0.233393000
15	-0.368388000	-0.866619000	0.030088000
6	-0.859664000	-2.283043000	-1.098690000
1	-1.078432000	-1.893363000	-2.098379000
6	-2.125243000	-2.931018000	-0.452236000
1	-3.021136000	-2.698659000	-1.035263000
1	-2.011710000	-4.019394000	-0.487479000
6	-2.299736000	-2.451513000	1.010457000
1	-2.603193000	-3.274109000	1.667355000
1	-3.092318000	-1.696544000	1.069191000
6	-0.988479000	-1.824501000	1.527323000
1	-0.235898000	-2.616209000	1.645588000
6	-1.161724000	-1.117033000	2.870663000
1	-1.873272000	-0.287230000	2.802549000
1	-0.215506000	-0.742068000	3.273358000
1	-1.562583000	-1.827148000	3.602615000
6	0.281605000	-3.314659000	-1.208455000
1	0.536704000	-3.739852000	-0.231473000
1	1.195633000	-2.901413000	-1.642549000
1	-0.043833000	-4.143787000	-1.845926000
6	-1.576754000	0.504785000	-0.235432000
6	-2.620808000	0.393173000	-1.164838000
1	-2.757858000	-0.522002000	-1.729818000
6	-3.512391000	1.447040000	-1.381890000
1	-4.315880000	1.331456000	-2.103127000
6	-3.370105000	2.634026000	-0.669610000
1	-4.061191000	3.456505000	-0.826824000
6	-2.326224000	2.763845000	0.248545000
1	-2.214233000	3.691500000	0.804513000
6	-1.419225000	1.723642000	0.473473000
6	-0.286710000	1.941313000	1.457624000
1	-0.195066000	1.114973000	2.161942000
1	-0.464696000	2.852755000	2.040648000
8	1.008095000	2.034514000	0.828490000
6	1.258187000	3.331608000	0.274055000
1	1.168737000	4.096633000	1.054638000
1	2.281118000	3.330263000	-0.104680000
1	0.563814000	3.561003000	-0.542404000
6	2.359985000	-0.773293000	1.545390000
1	2.046764000	-1.745260000	1.912530000
6	3.421213000	-0.700088000	0.624515000
6	3.661423000	0.540117000	0.015683000
1	3.543746000	1.455037000	0.592442000
6	1.477322000	1.014135000	-2.025113000
6	1.883436000	-0.274699000	-2.286051000
1	1.167472000	-1.014643000	-2.626850000
1	2.923745000	-0.510057000	-2.492386000
1	2.193136000	1.830002000	-2.012722000
1	0.434422000	1.298928000	-2.130512000
1	3.823996000	-1.611316000	0.185904000
1	4.351191000	0.602248000	-0.821256000
1	2.177595000	0.060342000	2.221676000

16

E + ZPE = -2666.153267

28	1.556817000	-0.754490000	0.295732000
15	0.076593000	0.909963000	-0.025291000
6	0.404696000	2.454285000	0.976699000
1	-0.524751000	3.038691000	0.943146000
6	1.444159000	3.165049000	0.086545000
1	1.600131000	4.190414000	0.439068000
1	2.411490000	2.656480000	0.178669000
6	0.943406000	3.147327000	-1.369914000
1	1.776605000	3.244025000	-2.073341000
1	0.295469000	4.014747000	-1.536127000
6	0.109789000	1.857067000	-1.669873000
1	0.625791000	1.232454000	-2.404479000
6	-1.273878000	2.212356000	-2.235546000
1	-1.863382000	2.802428000	-1.525858000
1	-1.863441000	1.333603000	-2.508242000
1	-1.140222000	2.816749000	-3.140049000
6	0.851535000	2.297926000	2.430572000
1	1.781088000	1.721764000	2.505827000
1	0.093350000	1.811696000	3.052733000
1	1.043561000	3.285966000	2.863240000
6	-1.663560000	0.364163000	0.221082000
6	-2.457056000	0.957996000	1.211817000
1	-2.057449000	1.750200000	1.836051000
6	-3.778195000	0.550977000	1.415525000
1	-4.375586000	1.028104000	2.186604000
6	-4.322181000	-0.456082000	0.623915000
1	-5.350181000	-0.774133000	0.768576000
6	-3.536560000	-1.058661000	-0.361155000
1	-3.964711000	-1.840855000	-0.983198000
6	-2.208542000	-0.675058000	-0.573107000
6	-1.391710000	-1.395840000	-1.629894000
1	-0.800514000	-0.696806000	-2.227805000
1	-2.060767000	-1.930434000	-2.317762000
8	-0.434967000	-2.310699000	-1.083920000
6	-1.008914000	-3.540911000	-0.648127000
1	-1.547079000	-4.032557000	-1.469956000
1	-0.182964000	-4.183703000	-0.335886000
1	-1.697805000	-3.397648000	0.194579000
6	3.164053000	-2.027796000	0.002110000
1	3.053520000	-3.106351000	-0.022406000
6	2.852725000	-1.279255000	-1.144247000
6	2.833471000	0.116647000	-0.993503000
1	3.547288000	0.591724000	-0.318913000
6	0.507029000	-1.167504000	2.026370000
6	1.438816000	-2.171148000	1.862643000
1	2.356949000	-2.168518000	2.441675000
1	1.145741000	-3.133457000	1.456235000
1	2.375271000	-1.751460000	-2.000194000
1	2.527144000	0.733983000	-1.828923000
1	3.925684000	-1.661056000	0.687655000
1	-0.530569000	-1.345343000	1.767899000
1	0.685807000	-0.378068000	2.749949000

17

E + ZPE = -2666.138669

28	1.542274000	-0.436658000	0.158644000
15	-0.103986000	0.961943000	-0.017664000
6	0.060891000	2.485767000	1.048342000
1	-0.939085000	2.938531000	1.094374000

6	0.932457000	3.378405000	0.141605000
1	0.993230000	4.391753000	0.553495000
1	1.959079000	2.988765000	0.112808000
6	0.300069000	3.378743000	-1.257487000
1	0.992050000	3.760599000	-2.014806000
1	-0.564936000	4.052613000	-1.252785000
6	-0.194354000	1.948633000	-1.638693000
1	0.519215000	1.479952000	-2.322472000
6	-1.570595000	1.989929000	-2.316008000
1	-2.336757000	2.396514000	-1.647702000
1	-1.910774000	1.008519000	-2.656825000
1	-1.514986000	2.642659000	-3.194863000
6	0.602547000	2.308777000	2.466009000
1	1.617157000	1.896134000	2.455326000
1	-0.026641000	1.650365000	3.073405000
1	0.645577000	3.281791000	2.967600000
6	-1.729897000	0.154909000	0.261217000
6	-2.595930000	0.631199000	1.254261000
1	-2.317330000	1.484241000	1.864048000
6	-3.835137000	0.026387000	1.479133000
1	-4.491190000	0.414652000	2.252367000
6	-4.224576000	-1.062074000	0.704354000
1	-5.189890000	-1.532982000	0.863541000
6	-3.364756000	-1.548131000	-0.282972000
1	-3.673160000	-2.395038000	-0.891076000
6	-2.114102000	-0.967194000	-0.514206000
6	-1.205867000	-1.575065000	-1.568773000
1	-0.708214000	-0.806160000	-2.166078000
1	-1.798080000	-2.191736000	-2.258655000
8	-0.140515000	-2.362344000	-1.021713000
6	-0.565329000	-3.644222000	-0.562585000
1	-1.061781000	-4.200930000	-1.369023000
1	0.331873000	-4.190002000	-0.262880000
1	-1.248240000	-3.567526000	0.292899000
6	3.373004000	-1.600998000	0.334529000
1	3.815510000	-2.592520000	0.248936000
6	2.987581000	-1.069411000	-1.002998000
6	2.940162000	0.289020000	-1.233984000
1	3.492244000	0.991564000	-0.611945000
6	1.034754000	-1.080035000	1.838828000
6	2.118698000	-2.046485000	1.505276000
1	2.812014000	-2.203831000	2.332211000
1	1.746041000	-3.000459000	1.137672000
1	2.660445000	-1.773845000	-1.765173000
1	2.655892000	0.657915000	-2.214473000
1	4.060998000	-0.939897000	0.865251000
1	0.034492000	-1.506965000	1.891041000
1	1.247767000	-0.427550000	2.685320000

18

E + ZPE = -2666.138444

28	1.540264000	-0.382115000	0.134703000
15	-0.146576000	0.960843000	-0.013300000
6	-0.032579000	2.485241000	1.058722000
1	-1.049025000	2.898581000	1.112495000
6	0.796915000	3.416761000	0.151729000
1	0.820320000	4.429428000	0.569113000
1	1.837962000	3.068294000	0.112555000
6	0.153762000	3.398381000	-1.241611000
1	0.816017000	3.826193000	-2.000988000
1	-0.747837000	4.022440000	-1.221219000
6	-0.261789000	1.947556000	-1.633584000

1	0.489319000	1.517040000	-2.302596000
6	-1.624833000	1.921221000	-2.337458000
1	-2.423089000	2.287070000	-1.683406000
1	-1.908749000	0.925101000	-2.686710000
1	-1.585491000	2.577996000	-3.214206000
6	0.523248000	2.321831000	2.472336000
1	1.556548000	1.959254000	2.452809000
1	-0.070428000	1.627505000	3.075452000
1	0.521231000	3.291089000	2.982929000
6	-1.744594000	0.099385000	0.263280000
6	-2.630534000	0.548626000	1.251528000
1	-2.383586000	1.411407000	1.861359000
6	-3.849698000	-0.096878000	1.472548000
1	-4.521819000	0.271116000	2.241884000
6	-4.198932000	-1.199825000	0.699131000
1	-5.148630000	-1.702427000	0.855277000
6	-3.318352000	-1.659940000	-0.282344000
1	-3.594480000	-2.519274000	-0.888573000
6	-2.087119000	-1.037657000	-0.509735000
6	-1.153707000	-1.618615000	-1.557254000
1	-0.685956000	-0.836753000	-2.161929000
1	-1.719545000	-2.265498000	-2.241434000
8	-0.059193000	-2.358260000	-1.000460000
6	-0.437261000	-3.649600000	-0.525801000
1	-0.914619000	-4.232136000	-1.325378000
1	0.478978000	-4.159928000	-0.221613000
1	-1.121248000	-3.587219000	0.329858000
6	3.443128000	-1.484391000	0.375472000
1	3.991094000	-2.423434000	0.283129000
6	3.033467000	-0.997590000	-0.986086000
6	2.964640000	0.345676000	-1.271476000
1	3.475056000	1.087178000	-0.659778000
6	1.128729000	-1.021933000	1.828742000
6	2.239495000	-1.978059000	1.476094000
1	2.888098000	-2.162556000	2.335494000
1	1.864647000	-2.928722000	1.098721000
1	2.742487000	-1.737934000	-1.728946000
1	2.681817000	0.672483000	-2.267480000
1	4.079733000	-0.758958000	0.888315000
1	0.151516000	-1.488228000	1.949164000
1	1.360564000	-0.357589000	2.661821000

19
E + ZPE = -2666.137577

28	1.486468000	-0.229163000	0.017201000
15	-0.326409000	0.938065000	0.004389000
6	-0.450284000	2.465600000	1.067404000
1	-1.517718000	2.725402000	1.092808000
6	0.253941000	3.503255000	0.170756000
1	0.133364000	4.509484000	0.586995000
1	1.333288000	3.299288000	0.142809000
6	-0.365056000	3.394083000	-1.228320000
1	0.230959000	3.919667000	-1.981161000
1	-1.352201000	3.872081000	-1.215811000
6	-0.546421000	1.898082000	-1.625155000
1	0.284265000	1.589838000	-2.268952000
6	-1.865912000	1.664730000	-2.372792000
1	-2.731264000	1.900890000	-1.745036000
1	-1.983019000	0.638384000	-2.730892000
1	-1.900135000	2.323157000	-3.248535000
6	0.082078000	2.403753000	2.498681000
1	1.168646000	2.273097000	2.514003000

1	-0.369729000	1.593558000	3.079840000
1	-0.141118000	3.345236000	3.012490000
6	-1.790790000	-0.136339000	0.261877000
6	-2.765464000	0.179465000	1.217214000
1	-2.678337000	1.079890000	1.816147000
6	-3.870394000	-0.652078000	1.417581000
1	-4.615772000	-0.386392000	2.161159000
6	-4.013678000	-1.809925000	0.658664000
1	-4.873557000	-2.457275000	0.801431000
6	-3.041911000	-2.138581000	-0.289417000
1	-3.157201000	-3.042117000	-0.883168000
6	-1.923117000	-1.326692000	-0.495805000
6	-0.877402000	-1.752268000	-1.507896000
1	-0.559755000	-0.919485000	-2.141240000
1	-1.286768000	-2.526450000	-2.169027000
8	0.336011000	-2.241611000	-0.908399000
6	0.210733000	-3.576375000	-0.407652000
1	-0.167615000	-4.242886000	-1.193116000
1	1.209741000	-3.907615000	-0.120104000
1	-0.457380000	-3.623379000	0.460504000
6	3.718944000	-1.005489000	0.487139000
1	4.489125000	-1.781115000	0.427175000
6	3.233610000	-0.685864000	-0.915041000
6	3.007450000	0.605604000	-1.311188000
1	3.364819000	1.450688000	-0.727288000
6	1.443385000	-0.659400000	1.816522000
6	2.629314000	-1.575389000	1.518644000
1	3.197535000	-1.731715000	2.443662000
1	2.299628000	-2.560815000	1.181682000
1	3.099183000	-1.511155000	-1.612054000
1	2.714157000	0.825103000	-2.334593000
1	4.179605000	-0.116794000	0.930979000
1	0.560865000	-1.192972000	2.176051000
1	1.699170000	0.155843000	2.495673000

20
E + ZPE = -2666.175497

28	1.431618000	-0.455233000	-0.211370000
15	-0.436238000	0.756590000	-0.024957000
6	-0.582032000	1.974045000	1.410754000
1	-1.591133000	1.823810000	1.810343000
6	-0.520588000	3.368318000	0.741726000
1	-0.973681000	4.120554000	1.397336000
1	0.527372000	3.663321000	0.600919000
6	-1.227479000	3.293384000	-0.618917000
1	-1.056783000	4.197662000	-1.214120000
1	-2.313180000	3.210096000	-0.479802000
6	-0.698742000	2.050648000	-1.370189000
1	0.316288000	2.271448000	-1.721205000
6	-1.537980000	1.604714000	-2.569388000
1	-2.559331000	1.340382000	-2.279230000
1	-1.094787000	0.741094000	-3.078071000
1	-1.596995000	2.419777000	-3.299088000
6	0.412385000	1.773684000	2.558569000
1	1.447775000	1.913941000	2.233620000
1	0.324003000	0.777130000	3.005786000
1	0.214654000	2.504483000	3.350869000
6	-1.969938000	-0.273421000	0.049449000
6	-3.203468000	0.331150000	0.348522000
1	-3.255698000	1.397809000	0.539681000
6	-4.386277000	-0.405794000	0.397985000
1	-5.323369000	0.093587000	0.624697000

6	-4.356054000	-1.778232000	0.161233000
1	-5.267869000	-2.365730000	0.206668000
6	-3.140760000	-2.396945000	-0.125942000
1	-3.115663000	-3.469293000	-0.302670000
6	-1.949675000	-1.665044000	-0.198763000
6	-0.693351000	-2.416125000	-0.575913000
1	-0.345850000	-2.155567000	-1.580594000
1	-0.879176000	-3.495520000	-0.557167000
8	0.442298000	-2.145100000	0.278478000
6	0.260203000	-2.539267000	1.652478000
1	0.011987000	-3.604586000	1.690910000
1	1.210892000	-2.366408000	2.158371000
1	-0.532362000	-1.954468000	2.128850000
6	4.392695000	-0.419617000	0.034415000
1	5.110783000	-0.742899000	0.794071000
6	3.319726000	-1.466535000	-0.170087000
6	2.685145000	-1.641545000	-1.374504000
1	3.008304000	-1.090062000	-2.254134000
6	2.476316000	1.118490000	-0.453427000
6	3.706192000	0.900136000	0.431365000
1	4.405123000	1.744802000	0.353560000
1	3.410079000	0.850036000	1.488020000
1	3.167466000	-2.203209000	0.618812000
1	2.078277000	-2.523086000	-1.561513000
1	4.947889000	-0.279067000	-0.900241000
1	1.970606000	2.047581000	-0.174525000
1	2.756369000	1.218582000	-1.511444000

S7

E + ZPE = -2666.155243

28	1.564660000	-0.717078000	0.289076000
15	0.037973000	0.899722000	-0.042586000
6	0.390695000	2.439398000	0.959901000
1	-0.525146000	3.045059000	0.927103000
6	1.445716000	3.110752000	0.055611000
1	1.654181000	4.126226000	0.409305000
1	2.390696000	2.555469000	0.131317000
6	0.923420000	3.117367000	-1.394150000
1	1.751167000	3.167981000	-2.108959000
1	0.319882000	4.016992000	-1.555632000
6	0.022467000	1.868634000	-1.671884000
1	0.471092000	1.243575000	-2.447481000
6	-1.379335000	2.281854000	-2.146332000
1	-1.905135000	2.880683000	-1.395040000
1	-2.013022000	1.425697000	-2.391779000
1	-1.281044000	2.894574000	-3.049739000
6	0.848384000	2.287652000	2.410969000
1	1.748606000	1.666756000	2.487947000
1	0.075195000	1.855930000	3.054744000
1	1.095412000	3.273222000	2.820955000
6	-1.682662000	0.317188000	0.233555000
6	-2.468126000	0.887700000	1.243148000
1	-2.074346000	1.690632000	1.858092000
6	-3.772661000	0.444115000	1.476800000
1	-4.365137000	0.902909000	2.262663000
6	-4.306209000	-0.576366000	0.695652000
1	-5.320907000	-0.924041000	0.864104000
6	-3.528653000	-1.153457000	-0.311497000
1	-3.951145000	-1.944340000	-0.926399000
6	-2.217919000	-0.731810000	-0.554980000
6	-1.414170000	-1.409088000	-1.651651000
1	-0.905076000	-0.676284000	-2.284219000

1	-2.085110000	-1.987353000	-2.300903000
8	-0.371679000	-2.261198000	-1.160740000
6	-0.842838000	-3.528749000	-0.708262000
1	-1.338371000	-4.074129000	-1.522662000
1	0.032630000	-4.095973000	-0.384007000
1	-1.542428000	-3.430671000	0.132303000
6	2.361957000	-0.288214000	-1.493682000
1	2.493974000	0.724655000	-1.857353000
6	3.354571000	-0.815786000	-0.648324000
6	3.106876000	-2.059682000	-0.058228000
1	2.556012000	-2.823407000	-0.605225000
6	0.445016000	-1.174905000	1.961022000
6	1.647693000	-1.842277000	2.055838000
1	2.459352000	-1.449323000	2.663664000
1	1.698033000	-2.904931000	1.843292000
1	4.133772000	-0.169451000	-0.247334000
1	3.786894000	-2.433652000	0.698835000
1	1.803829000	-0.950838000	-2.155089000
1	-0.447750000	-1.699544000	1.638116000
1	0.271933000	-0.280454000	2.548929000

S8

E + ZPE = -2666.138068

28	1.555646000	-0.363703000	0.163470000
15	-0.143625000	0.961888000	-0.037598000
6	-0.018528000	2.507035000	1.004497000
1	-1.030991000	2.930540000	1.054882000
6	0.814772000	3.408330000	0.069882000
1	0.860850000	4.427754000	0.468488000
1	1.849983000	3.041231000	0.022650000
6	0.153652000	3.374813000	-1.314835000
1	0.815960000	3.771774000	-2.090648000
1	-0.733744000	4.018802000	-1.297466000
6	-0.296698000	1.924105000	-1.668407000
1	0.421152000	1.474403000	-2.359802000
6	-1.685325000	1.906698000	-2.321912000
1	-2.454036000	2.295966000	-1.646246000
1	-1.996460000	0.908923000	-2.642335000
1	-1.668547000	2.547400000	-3.211226000
6	0.546662000	2.378166000	2.418312000
1	1.558648000	1.958068000	2.407946000
1	-0.078453000	1.750227000	3.061238000
1	0.604198000	3.368976000	2.882306000
6	-1.728742000	0.088968000	0.275437000
6	-2.597634000	0.544011000	1.275703000
1	-2.348477000	1.422255000	1.862238000
6	-3.801296000	-0.114698000	1.539240000
1	-4.459967000	0.258184000	2.317810000
6	-4.152175000	-1.237448000	0.796066000
1	-5.089413000	-1.751809000	0.985606000
6	-3.290144000	-1.701230000	-0.200151000
1	-3.569660000	-2.574116000	-0.785090000
6	-2.074734000	-1.065371000	-0.470964000
6	-1.169901000	-1.644912000	-1.545207000
1	-0.742433000	-0.860435000	-2.176084000
1	-1.749777000	-2.310785000	-2.198798000
8	-0.037241000	-2.354767000	-1.028571000
6	-0.357196000	-3.643738000	-0.509852000
1	-0.817930000	-4.271904000	-1.284303000
1	0.583831000	-4.101792000	-0.196556000
1	-1.034978000	-3.582215000	0.351054000
6	2.444482000	-0.391399000	-1.753454000

1	2.477479000	0.472689000	-2.409507000
6	3.320882000	-0.466817000	-0.694625000
6	3.312804000	-1.630198000	0.237866000
1	2.964380000	-2.547657000	-0.239398000
1	1.039279000	-1.037570000	1.825718000
6	2.458152000	-1.493776000	1.782871000
1	3.120432000	-0.876214000	2.390023000
1	2.574395000	-2.544577000	2.052074000
1	3.997227000	0.359795000	-0.479843000
1	4.301066000	-1.795005000	0.665176000
1	1.929528000	-1.270013000	-2.135468000
1	0.285636000	-1.820523000	1.743808000
1	0.814439000	-0.336247000	2.625734000

S9

E + ZPE = -2666.138099

28	1.550365000	-0.314522000	0.144197000
15	-0.177919000	0.963808000	-0.036175000
6	-0.097452000	2.511288000	1.006970000
1	-1.123121000	2.900650000	1.063972000
6	0.697170000	3.443960000	0.069606000
1	0.708364000	4.463543000	0.470311000
1	1.744789000	3.115167000	0.013678000
6	0.026665000	3.387831000	-1.309175000
1	0.658087000	3.827185000	-2.087944000
1	-0.895277000	3.981079000	-1.277071000
6	-0.344244000	1.918202000	-1.670997000
1	0.414587000	1.504074000	-2.341056000
6	-1.712738000	1.831206000	-2.359642000
1	-2.516709000	2.181382000	-1.704004000
1	-1.965188000	0.819158000	-2.686727000
1	-1.705739000	2.471655000	-3.249261000
6	0.479348000	2.397057000	2.417166000
1	1.504374000	2.010366000	2.399757000
1	-0.121394000	1.746723000	3.061054000
1	0.506558000	3.387860000	2.883933000
6	-1.738440000	0.047128000	0.275719000
6	-2.627135000	0.486915000	1.265642000
1	-2.407056000	1.376721000	1.846301000
6	-3.813722000	-0.202583000	1.527234000
1	-4.488013000	0.159153000	2.297639000
6	-4.127873000	-1.341663000	0.792553000
1	-5.051860000	-1.880097000	0.980279000
6	-3.245483000	-1.791090000	-0.192254000
1	-3.495675000	-2.677623000	-0.769919000
6	-2.046093000	-1.124467000	-0.460599000
6	-1.117193000	-1.692809000	-1.520089000
1	-0.703514000	-0.905159000	-2.156175000
1	-1.674465000	-2.380473000	-2.170768000
8	0.027975000	-2.368623000	-0.985498000
6	-0.265845000	-3.655386000	-0.445631000
1	-0.710602000	-4.306036000	-1.210771000
0	0.683889000	-4.087509000	-0.122079000
1	-0.947362000	-3.593521000	0.412154000
6	2.471084000	-0.403933000	-1.785119000
1	2.484552000	0.434254000	-2.474912000
6	3.323741000	-0.408428000	-0.708697000
6	3.362332000	-1.552873000	0.265026000
1	3.014876000	-2.483214000	-0.189884000
6	1.121569000	-0.986706000	1.819373000
6	2.579423000	-1.367155000	1.770432000
1	3.202232000	-0.671402000	2.335757000

1	2.740650000	-2.379413000	2.148957000
1	3.977341000	0.442722000	-0.520207000
1	4.382222000	-1.699860000	0.623531000
1	1.975300000	-1.308533000	-2.129113000
1	0.421392000	-1.821589000	1.765377000
1	0.870839000	-0.307752000	2.631194000

S10

E + ZPE = -2666.137107

28	-1.388744000	-0.474742000	0.023189000
15	0.220500000	0.940596000	0.016418000
6	0.136366000	2.479947000	-1.042988000
1	1.167513000	2.846671000	-1.136022000
6	-0.604427000	3.449202000	-0.098963000
1	-0.592878000	4.463064000	-0.513882000
1	-1.659749000	3.153925000	-0.011119000
6	0.098087000	3.384265000	1.261430000
1	-0.470612000	3.898102000	2.043342000
1	1.067268000	3.893391000	1.186156000
6	0.341681000	1.901413000	1.655534000
1	-0.501447000	1.547780000	2.259469000
6	1.637161000	1.715195000	2.453945000
1	2.516350000	1.995428000	1.864927000
1	1.780485000	0.688823000	2.803176000
1	1.609037000	2.360461000	3.339637000
6	-0.482170000	2.366645000	-2.435318000
1	-1.513427000	2.001614000	-2.386798000
1	0.089037000	1.703908000	-3.092999000
1	-0.503304000	3.355931000	-2.905798000
6	1.793149000	0.033997000	-0.267533000
6	2.750015000	0.510447000	-1.173023000
1	2.580871000	1.433925000	-1.716564000
6	3.940867000	-0.185159000	-1.396371000
1	4.668584000	0.206023000	-2.100947000
6	4.189507000	-1.369877000	-0.710269000
1	5.114874000	-1.914672000	-0.870532000
6	3.237621000	-1.859403000	0.186899000
1	3.434462000	-2.784943000	0.722504000
6	2.034796000	-1.185050000	0.416644000
6	1.036126000	-1.793305000	1.384941000
1	0.649023000	-1.054089000	2.091453000
1	1.520457000	-2.585594000	1.969283000
8	-0.137872000	-2.334688000	0.750988000
6	0.100101000	-3.567044000	0.062737000
1	0.502173000	-4.314868000	0.757321000
1	-0.864886000	-3.912845000	-0.313128000
1	0.795840000	-3.435976000	-0.774047000
6	-2.567485000	-0.638926000	1.881716000
1	-2.397280000	0.044489000	2.708648000
6	-3.228137000	-0.219667000	0.756410000
6	-3.577197000	-1.180460000	-0.368712000
1	-3.418361000	-2.218775000	-0.053510000
6	-1.320912000	-0.910896000	-1.787014000
6	-2.848392000	-0.893507000	-1.772544000
1	-3.216486000	0.072928000	-2.130319000
1	-3.241792000	-1.665402000	-2.445726000
1	-3.605832000	0.799061000	0.679453000
1	-4.645724000	-1.085015000	-0.589029000
1	-2.401268000	-1.692622000	2.088262000
1	-0.883372000	-1.910535000	-1.876932000
1	-0.899774000	-0.255745000	-2.544879000

S11

E + ZPE = -2666.174981

28	1.474786000	-0.457722000	0.222614000
15	-0.407505000	0.757743000	0.116792000
6	-0.693898000	1.940800000	1.556440000
1	-1.733945000	1.786736000	1.864675000
6	-0.568007000	3.349492000	0.927471000
1	-1.089602000	4.086879000	1.547912000
1	0.488215000	3.647444000	0.903968000
6	-1.128974000	3.303685000	-0.500912000
1	-0.904375000	4.222337000	-1.054944000
1	-2.222850000	3.210847000	-0.477634000
6	-0.518277000	2.080514000	-1.222580000
1	0.525486000	2.311824000	-1.463492000
6	-1.227874000	1.668074000	-2.514428000
1	-2.276577000	1.409408000	-2.341472000
1	-0.740479000	0.810853000	-2.992472000
1	-1.200990000	2.499265000	-3.227690000
6	0.204533000	1.707182000	2.775586000
1	1.264703000	1.813471000	2.524669000
1	0.052018000	0.712632000	3.209783000
1	-0.028336000	2.442244000	3.554344000
6	-1.939290000	-0.261014000	-0.046947000
1	-3.203172000	0.302070000	0.194686000
6	-3.289820000	1.336190000	0.511338000
6	-4.373790000	-0.437902000	0.024172000
1	-5.336856000	0.026404000	0.213506000
6	-4.299772000	-1.767268000	-0.385571000
1	-5.203600000	-2.354531000	-0.515398000
6	-3.052468000	-2.345595000	-0.617587000
1	-2.993550000	-3.386683000	-0.924977000
6	-1.872459000	-1.609972000	-0.464125000
6	-0.559897000	-2.301065000	-0.749763000
1	-0.050806000	-1.886582000	-1.625464000
1	-0.723086000	-3.368763000	-0.931681000
8	0.404586000	-2.174154000	0.323793000
6	-0.037919000	-2.745198000	1.573157000
1	-0.301962000	-3.795579000	1.415493000
1	0.799180000	-2.677264000	2.267664000
1	-0.898182000	-2.198887000	1.969760000
6	3.136870000	-1.594888000	0.792168000
1	2.705107000	-2.487989000	1.232394000
6	3.178118000	-1.438346000	-0.572094000
6	4.043976000	-0.397999000	-1.253372000
1	4.958828000	-0.251021000	-0.668151000
6	2.526986000	1.120543000	0.010772000
6	3.259081000	0.926882000	-1.318115000
1	2.540843000	0.887565000	-2.148869000
1	3.931095000	1.768493000	-1.534786000
1	3.237284000	1.164532000	0.848303000
1	1.981423000	2.067140000	0.026954000
1	2.708445000	-2.196053000	-1.200238000
1	4.345334000	-0.739283000	-2.248270000
1	3.796341000	-1.018317000	1.435618000

S12

E + ZPE = -2123.241496

28	0.062901000	0.046007000	-0.051731000
6	-2.037343000	0.418894000	-0.544335000
1	-2.015015000	0.825319000	-1.557442000

15	2.178023000	0.128540000	-0.334816000
1	2.927081000	-1.065508000	-0.310531000
1	2.937788000	0.888412000	0.579879000
1	2.649485000	0.680041000	-1.542859000
6	-1.349439000	1.315724000	0.437863000
6	-0.311420000	2.136375000	0.053781000
1	-0.165317000	2.419727000	-0.986651000
6	-0.133604000	-1.579666000	-0.944757000
6	-1.569182000	-1.251784000	-0.677582000
1	-1.963178000	-1.740949000	0.212450000
1	-2.200955000	-1.478798000	-1.537703000
1	0.149733000	-1.591567000	-1.999166000
1	-1.663043000	1.271318000	1.478918000
1	0.172042000	2.777019000	0.786285000
1	-3.073512000	0.257458000	-0.246362000
8	-0.013453000	-0.973021000	2.100240000
1	-0.109985000	-0.551874000	2.969994000
1	0.188604000	-1.903540000	2.291678000
1	0.248238000	-2.456444000	-0.419529000

S13

E + ZPE = -2354.223058

28	-1.204878000	0.058230000	-0.120448000
6	-1.554125000	-2.071399000	0.132535000
1	-0.873814000	-2.565919000	-0.562384000
15	-0.571423000	1.938138000	-0.945526000
1	0.095316000	2.864303000	-0.117357000
1	-1.546522000	2.795463000	-1.498598000
1	0.337533000	1.885417000	-2.020188000
6	-2.586106000	-1.256075000	-0.568032000
6	-2.311179000	-0.634973000	-1.769786000
1	-1.509149000	-0.981927000	-2.419200000
6	0.245225000	-0.089571000	1.090703000
6	-0.529265000	-1.337134000	1.375037000
1	-1.183057000	-1.234684000	2.239172000
1	0.121489000	-2.202837000	1.494195000
1	0.139374000	0.661305000	1.876542000
1	-3.543153000	-1.104823000	-0.073040000
1	-3.077558000	-0.036799000	-2.255084000
1	-2.018239000	-2.816337000	0.777936000
6	1.628665000	-0.156098000	0.565509000
6	2.537508000	0.867141000	0.895298000
1	2.222197000	1.667019000	1.562064000
6	2.073909000	-1.192099000	-0.278280000
1	1.403749000	-2.004092000	-0.549181000
6	3.378876000	-1.206469000	-0.764628000
6	3.843337000	0.852906000	0.409071000
6	4.268246000	-0.183456000	-0.424440000
1	4.531483000	1.645168000	0.688683000
1	3.704834000	-2.019536000	-1.406606000
1	5.286479000	-0.199042000	-0.800981000
8	-2.705276000	1.083247000	1.586230000
1	-3.660180000	1.244499000	1.515081000
1	-2.451201000	1.477703000	2.436608000

S14

E + ZPE = -2354.212289

28	1.595190000	-0.051491000	0.001550000
6	-0.093952000	-0.822085000	1.267755000
1	-0.380614000	0.043051000	1.868879000

15	2.868860000	1.567947000	-0.543333000
1	2.917400000	2.004171000	-1.884203000
1	4.253459000	1.432185000	-0.303122000
1	2.653105000	2.809046000	0.090438000
6	1.328372000	-1.237230000	1.554457000
6	2.254215000	-0.347069000	2.044590000
1	1.951939000	0.594694000	2.496866000
6	0.209705000	0.519212000	-1.095465000
6	-0.592233000	-0.510299000	-0.318627000
1	-0.531418000	-1.476724000	-0.822433000
1	0.327135000	0.282910000	-2.156160000
1	1.603094000	-2.275876000	1.378872000
1	3.264681000	-0.676535000	2.271288000
1	-0.768895000	-1.645878000	1.512047000
8	2.079039000	-1.824026000	-1.342739000
1	2.653121000	-2.581843000	-1.145069000
1	2.004141000	-1.799410000	-2.310651000
1	-0.137133000	1.546583000	-0.971447000
6	-2.059412000	-0.122583000	-0.174486000
6	-3.039270000	-1.002285000	-0.647341000
1	-2.746193000	-1.938793000	-1.116158000
6	-2.456544000	1.081126000	0.422461000
1	-1.713306000	1.783818000	0.794240000
6	-3.808977000	1.396735000	0.545101000
6	-4.393842000	-0.685915000	-0.525225000
6	-4.781594000	0.513402000	0.071314000
1	-5.142513000	-1.378688000	-0.898073000
1	-4.102767000	2.333204000	1.010065000
1	-5.834594000	0.760776000	0.165911000

21
E + ZPE = -2897.110649

28	0.509648000	1.284751000	0.568456000
15	-0.691599000	-0.513991000	0.800725000
6	0.090661000	-2.183698000	1.126579000
1	0.348434000	-2.654125000	0.174324000
6	-0.972836000	-3.017174000	1.911492000
1	-1.361445000	-3.831483000	1.292212000
1	-0.475854000	-3.491209000	2.764336000
6	-2.132548000	-2.116361000	2.400668000
1	-2.467584000	-2.404290000	3.403568000
1	-3.001147000	-2.219853000	1.739690000
6	-1.687730000	-0.640870000	2.398380000
1	-0.926963000	-0.494052000	3.177669000
6	-2.839338000	0.331566000	2.648817000
1	-3.603086000	0.262881000	1.866791000
1	-2.503847000	1.371799000	2.723742000
1	-3.325205000	0.082548000	3.599009000
6	1.386356000	-2.016282000	1.940862000
1	1.207686000	-1.494425000	2.888226000
1	2.155944000	-1.476821000	1.385249000
1	1.785288000	-3.006635000	2.186784000
6	-1.911858000	-0.709443000	-0.568323000
6	-2.129867000	-1.955219000	-1.174373000
1	-1.588013000	-2.830614000	-0.833560000
6	-3.049986000	-2.103877000	-2.214939000
1	-3.202812000	-3.081176000	-2.663125000
6	-3.771948000	-1.001871000	-2.663626000
1	-4.495904000	-1.107393000	-3.465930000
6	-3.558250000	0.245654000	-2.074600000
1	-4.124861000	1.105577000	-2.423621000
6	-2.631980000	0.417678000	-1.040582000

6	-2.422987000	1.811212000	-0.477706000
1	-2.382271000	1.807987000	0.611701000
1	-3.257006000	2.461142000	-0.771863000
8	-1.187122000	2.420952000	-0.890610000
6	-1.225028000	2.881707000	-2.244614000
1	-2.068419000	3.569235000	-2.387488000
1	-0.296772000	3.422921000	-2.431527000
1	-1.312912000	2.049663000	-2.953371000
6	2.429667000	2.882047000	0.506185000
1	2.820234000	3.884435000	0.301556000
6	1.256418000	2.971237000	1.455968000
6	1.102600000	2.054962000	2.467837000
1	1.914708000	1.392956000	2.760683000
6	1.511029000	0.829399000	-0.977444000
6	2.104900000	2.251624000	-0.919384000
1	3.054536000	2.253466000	-1.465517000
1	1.443666000	2.947886000	-1.437221000
1	0.562177000	3.802756000	1.344793000
1	0.294143000	2.158272000	3.188269000
1	3.232137000	2.309606000	0.980418000
1	0.751372000	0.754824000	-1.759876000
6	2.442418000	-0.315534000	-1.066614000
6	3.734235000	-0.308316000	-0.504195000
1	4.092339000	0.566225000	0.029996000
6	2.039461000	-1.467737000	-1.772097000
1	1.055848000	-1.485364000	-2.236701000
6	2.883757000	-2.566675000	-1.904325000
6	4.581024000	-1.407106000	-0.635945000
6	4.158888000	-2.542082000	-1.332399000
1	5.575333000	-1.374898000	-0.200075000
1	2.555943000	-3.437021000	-2.465720000
1	4.822771000	-3.394655000	-1.439899000

22
E + ZPE = -2897.107365

28	-0.197262000	-0.652820000	-0.835407000
15	1.645972000	-0.712972000	0.281534000
6	1.762789000	-1.855844000	1.753139000
1	2.655402000	-1.539899000	2.310260000
6	2.103543000	-3.190434000	1.061244000
1	2.359559000	-3.951186000	1.806958000
1	1.224864000	-3.562563000	0.516012000
6	3.271823000	-2.920802000	0.105964000
1	3.437730000	-3.753827000	-0.584744000
1	4.190861000	-2.808893000	0.694416000
6	3.027635000	-1.600871000	-0.684024000
1	2.599412000	-1.839436000	-1.663599000
6	4.326151000	-0.810826000	-0.889987000
1	4.758694000	-0.491712000	0.063837000
1	4.194841000	0.078317000	-1.512621000
1	5.059158000	-1.454684000	-1.389776000
6	0.574853000	-1.926432000	2.711824000
1	-0.307326000	-2.349662000	2.221370000
1	0.304137000	-0.946495000	3.117695000
1	0.824874000	-2.578350000	3.556171000
6	2.227134000	0.966818000	0.738491000
6	2.597905000	1.270591000	2.054969000
1	2.553847000	0.511254000	2.828454000
6	3.034307000	2.551826000	2.401310000
1	3.319175000	2.764158000	3.427391000
6	3.109569000	3.544638000	1.428846000
1	3.456755000	4.540677000	1.686287000

6	2.732339000	3.254274000	0.115785000
1	2.793161000	4.030670000	-0.642972000
6	2.278701000	1.983058000	-0.247595000
6	1.830732000	1.740472000	-1.676467000
1	2.200435000	0.786396000	-2.061877000
1	2.220628000	2.530966000	-2.331035000
8	0.403518000	1.667574000	-1.823770000
6	-0.229846000	2.947293000	-1.763443000
1	0.210773000	3.627670000	-2.503966000
1	-1.282285000	2.796576000	-2.009690000
1	-0.146960000	3.395561000	-0.766052000
6	-2.423841000	-0.990355000	-1.628952000
1	-3.266746000	-0.699962000	-2.265210000
6	-1.195006000	-1.179215000	-2.503489000
6	-0.349362000	-2.242560000	-2.325300000
1	-0.624154000	-3.090757000	-1.702190000
6	-1.253305000	-0.018196000	0.542302000
6	-2.368538000	0.159466000	-0.498769000
1	-2.218601000	1.105227000	-1.025239000
1	-1.025342000	-0.465276000	-3.307586000
1	0.489710000	-2.399409000	-2.998265000
1	-2.686717000	-1.937463000	-1.148768000
1	-0.948270000	0.923187000	1.004759000
1	-1.508052000	-0.750797000	1.309612000
6	-3.737372000	0.227295000	0.174854000
6	-4.487864000	1.405925000	0.088149000
1	-4.087517000	2.261961000	-0.450205000
6	-4.269855000	-0.861590000	0.878883000
1	-3.704062000	-1.785835000	0.972376000
6	-5.529733000	-0.776202000	1.470534000
6	-5.748870000	1.492945000	0.680388000
6	-6.273674000	0.401441000	1.372377000
1	-6.319077000	2.413782000	0.598117000
1	-5.929978000	-1.630549000	2.008850000
1	-7.254621000	0.467015000	1.833555000

23
E + ZPE = -2666.176611

28	1.426523000	-0.495692000	-0.251744000
15	-0.438776000	0.757568000	-0.014275000
6	-0.517146000	1.791737000	1.566438000
1	-1.527234000	1.633599000	1.962239000
6	-0.402657000	3.252735000	1.072077000
1	-0.798960000	3.938913000	1.829027000
1	0.655376000	3.512157000	0.933142000
6	-1.146208000	3.377552000	-0.264550000
1	-0.950782000	4.340947000	-0.749138000
1	-2.230861000	3.321528000	-0.104790000
6	-0.682814000	2.218783000	-1.175529000
1	0.333899000	2.450787000	-1.511670000
6	-1.550938000	1.963788000	-2.410066000
1	-2.580132000	1.705869000	-2.143388000
1	-1.148778000	1.155680000	-3.031315000
1	-1.582236000	2.867721000	-3.028377000
6	0.493435000	1.411681000	2.652976000
1	1.526062000	1.520763000	2.303673000
1	0.356091000	0.380469000	2.997058000
1	0.368614000	2.065360000	3.523679000
6	-1.988259000	-0.243107000	-0.026499000
6	-3.218121000	0.368525000	0.271004000
1	-3.255729000	1.426120000	0.511198000
6	-4.411604000	-0.352588000	0.260844000

1	-5.347217000	0.149364000	0.487960000
6	-4.394126000	-1.714114000	-0.034962000
1	-5.315282000	-2.288662000	-0.037542000
6	-3.180685000	-2.340670000	-0.314389000
1	-3.165944000	-3.405983000	-0.530470000
6	-1.978222000	-1.624509000	-0.324674000
6	-0.712484000	-2.375942000	-0.667902000
1	-0.306975000	-2.082553000	-1.641631000
1	-0.908651000	-3.453150000	-0.700428000
8	0.375555000	-2.146919000	0.258567000
6	0.116831000	-2.594778000	1.603240000
1	-0.128055000	-3.661506000	1.585299000
1	1.035152000	-2.438598000	2.169901000
1	-0.705193000	-2.031414000	2.054826000
6	4.182140000	-0.275071000	0.456295000
1	3.977950000	0.096632000	1.469339000
6	3.249845000	-1.422860000	0.151839000
6	2.814059000	-1.731818000	-1.118678000
1	3.194412000	-1.215781000	-1.995336000
6	2.434303000	1.059551000	-0.730565000
6	3.951353000	0.835171000	-0.571808000
1	4.404395000	0.554274000	-1.529371000
1	4.454764000	1.757219000	-0.259270000
1	3.078944000	-2.152734000	0.943389000
1	2.328839000	-2.685749000	-1.304958000
1	5.221752000	-0.632852000	0.466771000
1	2.120940000	1.891685000	-0.086451000
1	2.177172000	1.346690000	-1.759480000

24
E + ZPE = -2666.176850

28	1.485035000	-0.360712000	0.035480000
15	-0.483843000	0.769997000	0.058709000
6	-0.774739000	1.748404000	1.648946000
1	-1.804102000	1.518391000	1.949472000
6	-0.706017000	3.225702000	1.198835000
1	-1.198100000	3.868658000	1.937151000
1	0.344099000	3.544277000	1.149986000
6	-1.346908000	3.343397000	-0.189722000
1	-1.178290000	4.331469000	-0.632898000
1	-2.434631000	3.211748000	-0.120606000
6	-0.730848000	2.245634000	-1.084381000
1	0.291822000	2.556313000	-1.324818000
6	-1.467095000	1.973266000	-2.398244000
1	-2.496715000	1.643364000	-2.232796000
1	-0.960270000	1.209906000	-2.999315000
1	-1.501477000	2.891131000	-2.995519000
6	0.164127000	1.404226000	2.808715000
1	1.211494000	1.594408000	2.548027000
1	0.071376000	0.356379000	3.115231000
1	-0.077280000	2.022281000	3.680937000
6	-1.945105000	-0.337344000	-0.138331000
6	-3.243095000	0.173134000	0.029656000
1	-3.387101000	1.215673000	0.294629000
6	-4.368801000	-0.631625000	-0.145044000
1	-5.360182000	-0.207938000	-0.016294000
6	-4.213417000	-1.975395000	-0.479909000
1	-5.081865000	-2.613186000	-0.612784000
6	-2.931545000	-2.503148000	-0.628075000
1	-2.810319000	-3.555895000	-0.870916000
6	-1.794845000	-1.702520000	-0.470151000
6	-0.439803000	-2.343733000	-0.658029000

1	0.076518000	-1.972556000	-1.549529000
1	-0.543002000	-3.428971000	-0.764599000
8	0.478145000	-2.084721000	0.431552000
6	0.048401000	-2.626195000	1.696899000
1	-0.086238000	-3.707981000	1.597756000
1	0.839432000	-2.420515000	2.417431000
1	-0.886170000	-2.161992000	2.024660000
6	3.129336000	-1.099284000	0.981188000
1	2.789565000	-1.850864000	1.688083000
6	3.262603000	-1.423318000	-0.352129000
6	4.056931000	-0.579661000	-1.321332000
1	5.108911000	-0.898300000	-1.311882000
6	2.382871000	1.138804000	-0.729850000
6	3.881250000	0.891370000	-0.941591000
1	4.278404000	1.548249000	-1.725706000
1	4.451785000	1.124986000	-0.035088000
1	2.970410000	-2.424198000	-0.668971000
1	3.691567000	-0.752282000	-2.341735000
1	3.653475000	-0.253085000	1.416580000
1	2.199228000	2.077474000	-0.191371000
1	1.899337000	1.230516000	-1.716334000

25
E + ZPE = -2666.171227

28	1.419559000	-0.492322000	-0.242460000
15	-0.431795000	0.759498000	-0.018418000
6	-0.486632000	1.939520000	1.451897000
1	-1.479519000	1.805735000	1.896075000
6	-0.415923000	3.348997000	0.816574000
1	-0.820472000	4.095002000	1.509941000
1	0.632986000	3.619993000	0.638956000
6	-1.180367000	3.327470000	-0.514262000
1	-1.015110000	4.243902000	-1.092127000
1	-2.260793000	3.262213000	-0.330801000
6	-0.710636000	2.094735000	-1.319236000
1	0.294575000	2.302700000	-1.703899000
6	-1.606462000	1.701740000	-2.495925000
1	-2.623000000	1.457618000	-2.173016000
1	-1.206737000	0.839700000	-3.041911000
1	-1.670190000	2.536263000	-3.202856000
6	0.559483000	1.679853000	2.541165000
1	1.580640000	1.766770000	2.155468000
1	0.444775000	0.685647000	2.987577000
1	0.446611000	2.413745000	3.347152000
6	-1.982554000	-0.238063000	0.070570000
6	-3.193520000	0.370148000	0.442604000
1	-3.219959000	1.425799000	0.692341000
6	-4.386628000	-0.350648000	0.490254000
1	-5.307339000	0.149216000	0.775502000
6	-4.388234000	-1.707671000	0.175048000
1	-5.308934000	-2.281459000	0.216191000
6	-3.193759000	-2.329928000	-0.184692000
1	-3.193048000	-3.391138000	-0.420694000
6	-1.993057000	-1.614200000	-0.252721000
6	-0.751923000	-2.359655000	-0.687513000
1	-0.394129000	-2.034093000	-1.669503000
1	-0.957274000	-3.433928000	-0.746870000
8	0.385322000	-2.170930000	0.188848000
6	0.178874000	-2.639557000	1.536271000
1	-0.110739000	-3.694703000	1.509494000
1	1.131461000	-2.534005000	2.056036000
1	-0.593763000	-2.053512000	2.042468000

6	4.270311000	-0.486208000	0.411165000
1	4.419672000	-0.560823000	1.492850000
6	3.235423000	-1.504127000	-0.011058000
6	2.768713000	-1.632113000	-1.299649000
1	3.182533000	-1.037696000	-2.109381000
6	2.461562000	1.052799000	-0.326002000
6	3.852322000	0.962441000	0.031384000
1	4.604157000	1.420770000	-0.622044000
1	3.850436000	1.564510000	0.945737000
1	3.025021000	-2.314891000	0.685986000
1	2.220420000	-2.522064000	-1.598454000
1	5.233137000	-0.753535000	-0.043164000
1	1.988856000	1.990609000	-0.326407000
1	2.530484000	1.098445000	-1.729499000

26
E + ZPE = -2666.170280

28	1.462549000	-0.492245000	0.239207000
15	-0.398746000	0.762104000	0.104104000
6	-0.699100000	1.967792000	1.523441000
1	-1.752289000	1.841090000	1.797384000
6	-0.520796000	3.366439000	0.885483000
1	-1.040140000	4.122646000	1.484864000
1	0.542820000	3.637776000	0.887289000
6	-1.044823000	3.320527000	-0.556791000
1	-0.781119000	4.226994000	-1.113676000
1	-2.141105000	3.257099000	-0.562556000
6	-0.446939000	2.074620000	-1.249336000
1	0.608960000	2.277889000	-1.463762000
6	-1.133724000	1.665388000	-2.554285000
1	-2.191876000	1.432503000	-2.403088000
1	-0.655454000	0.792317000	-3.012382000
1	-1.071533000	2.488363000	-3.274820000
6	0.148971000	1.728137000	2.776644000
1	1.218824000	1.823150000	2.567771000
1	-0.031462000	0.737032000	3.207966000
1	-0.106156000	2.468514000	3.543255000
6	-1.945951000	-0.233097000	-0.067819000
6	-3.202975000	0.362750000	0.128990000
1	-3.274804000	1.409535000	0.404906000
6	-4.385341000	-0.359802000	-0.033344000
1	-5.341737000	0.130961000	0.119572000
6	-4.331336000	-1.706028000	-0.387142000
1	-5.244376000	-2.280678000	-0.508632000
6	-3.092184000	-2.316502000	-0.575109000
1	-3.049320000	-3.369582000	-0.841532000
6	-1.899677000	-1.598580000	-0.432115000
6	-0.601143000	-2.327365000	-0.688297000
1	-0.085773000	-1.957279000	-1.580036000
1	-0.787099000	-3.397603000	-0.828621000
8	0.371570000	-2.179905000	0.373881000
6	-0.056390000	-2.707510000	1.646038000
1	-0.329411000	-3.760541000	1.525690000
1	0.793659000	-2.623449000	2.323423000
1	-0.907516000	-2.143634000	2.038709000
6	3.153870000	-1.602465000	0.704390000
1	2.811929000	-2.497841000	1.216247000
6	3.034558000	-1.507635000	-0.664299000
6	3.760805000	-0.496928000	-1.522936000
1	4.821098000	-0.778019000	-1.576297000
6	2.573956000	1.053588000	0.163230000
6	3.579949000	0.955003000	-1.002494000

1	3.232554000	1.573552000	-1.836615000
1	4.542878000	1.382403000	-0.698380000
1	2.562685000	-2.341204000	-1.185322000
1	3.381728000	-0.574868000	-2.547351000
1	3.855062000	-0.982598000	1.254733000
1	3.083838000	1.059362000	1.137034000
1	2.042034000	2.006646000	0.108326000

27
E + ZPE = -2666.153030

28	-1.348720000	-0.191081000	-0.263680000
15	0.505365000	0.792092000	-0.008932000
6	0.993612000	2.060284000	-1.311727000
1	2.055240000	1.877065000	-1.514177000
6	0.867316000	3.412903000	-0.575352000
1	1.430208000	4.188605000	-1.106534000
1	-0.183227000	3.733136000	-0.566025000
6	1.367008000	3.222076000	0.864470000
1	1.160384000	4.099446000	1.487637000
1	2.456215000	3.080714000	0.870341000
6	0.669978000	1.972604000	1.447081000
1	-0.368696000	2.241776000	1.674543000
6	1.307428000	1.386623000	2.708121000
1	2.341049000	1.071830000	2.535137000
1	0.748021000	0.520618000	3.079747000
1	1.314981000	2.139633000	3.503835000
6	0.239813000	1.974264000	-2.641322000
1	-0.835089000	2.139016000	-2.514097000
1	0.381070000	1.001117000	-3.124938000
1	0.612896000	2.739575000	-3.331325000
6	1.899191000	-0.418864000	0.058073000
6	3.226630000	0.036002000	-0.012255000
1	3.433837000	1.098044000	-0.095319000
6	4.305666000	-0.846590000	0.032658000
1	5.319786000	-0.461727000	-0.016289000
6	4.073613000	-2.216218000	0.134055000
1	4.903703000	-2.915495000	0.158656000
6	2.763004000	-2.686796000	0.196937000
1	2.583096000	-3.756240000	0.272796000
6	1.671378000	-1.810452000	0.174531000
6	0.293891000	-2.416341000	0.333483000
1	-0.163313000	-2.145100000	1.288100000
1	0.353340000	-3.508548000	0.285624000
8	-0.675380000	-1.984062000	-0.656248000
6	-0.376213000	-2.406778000	-2.004113000
1	-0.252299000	-3.493803000	-2.017613000
1	-1.233031000	-2.127406000	-2.618074000
1	0.531476000	-1.920703000	-2.373620000
6	-4.374330000	-0.327954000	0.338724000
1	-5.231883000	-0.796132000	-0.157023000
6	-3.507541000	-1.385172000	0.975743000
6	-2.851409000	-1.248409000	2.137000000
1	-2.947806000	-0.354212000	2.748644000
6	-2.425353000	1.301652000	-0.059407000
6	-3.533517000	0.457811000	-0.685806000
1	-4.155426000	1.045784000	-1.372304000
1	-3.066817000	-0.301731000	-1.376732000
1	-3.413856000	-2.323674000	0.427833000
1	-2.245002000	-2.051903000	2.547000000
1	-4.767732000	0.362192000	1.093043000
1	-2.193519000	2.188071000	-0.655670000
1	-2.641869000	1.607587000	0.968465000

28
E + ZPE = -2666.157551

28	-1.235448000	-0.209149000	-0.584193000
15	0.568328000	0.791698000	-0.052393000
6	1.166016000	2.088278000	-1.276880000
1	2.245174000	1.927576000	-1.382639000
6	0.940254000	3.423541000	-0.531229000
1	1.542536000	4.217983000	-0.985737000
1	-0.111349000	3.725382000	-0.628356000
6	1.284746000	3.211103000	0.949649000
1	1.005517000	4.076036000	1.561841000
1	2.367861000	3.074419000	1.070972000
6	0.538287000	1.947809000	1.431745000
1	-0.522696000	2.202766000	1.539039000
6	1.031595000	1.351934000	2.751264000
1	2.082715000	1.052441000	2.696948000
1	0.443301000	0.475976000	3.046770000
1	0.936349000	2.095754000	3.549949000
6	0.529762000	2.016520000	-2.667611000
1	-0.557979000	2.132249000	-2.619596000
1	0.751173000	1.067697000	-3.168971000
1	0.923301000	2.820200000	-3.300130000
6	1.950900000	-0.407908000	0.172839000
6	3.281064000	0.039336000	0.219576000
1	3.503213000	1.097730000	1.128144000
6	4.342978000	-0.848525000	0.394484000
1	5.360424000	-0.471464000	0.433945000
6	4.090678000	-2.213219000	0.513047000
1	4.908812000	-2.915405000	0.640433000
6	2.776338000	-2.675829000	0.461030000
1	2.581407000	-3.741458000	0.551538000
6	1.700165000	-1.794840000	0.304353000
6	0.305914000	-2.380886000	0.331869000
1	-0.266948000	-2.044180000	1.200518000
1	0.353905000	-3.474010000	0.366194000
8	-0.522987000	-2.013116000	-0.803415000
6	-0.075026000	-2.542494000	-2.069962000
1	0.010383000	-3.630439000	-1.990831000
1	-0.839517000	-2.285665000	-2.803995000
1	0.887777000	-2.108893000	-2.355324000
6	-4.427546000	-0.412628000	0.092800000
1	-5.094435000	-1.085066000	-0.462626000
6	-3.850795000	-1.143236000	1.275805000
6	-3.897172000	-0.719445000	2.541265000
1	-4.382848000	0.215106000	2.814261000
6	-2.424348000	1.184897000	-0.336138000
6	-3.350021000	0.124836000	-0.873538000
1	-3.777344000	0.415040000	-1.838571000
1	-2.734411000	-0.803807000	-1.186286000
1	-3.383864000	-2.106408000	1.056304000
1	-3.480394000	-1.304706000	3.356248000
1	-5.034101000	0.435860000	0.427819000
1	-2.349163000	2.076084000	-0.962221000
1	-2.599999000	1.453375000	0.708766000

29
E + ZPE = -2666.147229

28	1.001761000	-0.337083000	-0.088078000
15	-0.782404000	0.754937000	0.008821000

6	-0.989529000	1.877716000	1.498852000
1	-2.018194000	1.728043000	1.846775000
6	-0.877980000	3.296977000	0.897658000
1	-1.299554000	4.035655000	1.588311000
1	0.180273000	3.556777000	0.759545000
6	-1.597344000	3.299150000	-0.459814000
1	-1.431001000	4.232658000	-1.008814000
1	-2.681896000	3.207278000	-0.312302000
6	-1.074525000	2.095773000	-1.276418000
1	-0.065650000	2.340038000	-1.629378000
6	-1.928017000	1.687605000	-2.478078000
1	-2.942742000	1.404527000	-2.181714000
1	-1.486073000	0.845211000	-3.022172000
1	-2.004648000	2.526629000	-3.178146000
6	-0.042647000	1.595529000	2.668340000
1	1.006683000	1.694358000	2.371536000
1	-0.191272000	0.589378000	3.076231000
1	-0.228770000	2.308445000	3.479394000
6	-2.223936000	-0.398624000	0.002785000
6	-3.497362000	0.068615000	0.366066000
1	-3.638315000	1.108865000	0.641646000
6	-4.609624000	-0.773708000	0.373932000
1	-5.581922000	-0.380137000	0.654346000
6	-4.463058000	-2.114563000	0.027955000
1	-5.318098000	-2.783383000	0.040036000
6	-3.205000000	-2.597168000	-0.331050000
1	-3.092462000	-3.644097000	-0.601183000
6	-2.084020000	-1.759672000	-0.362101000
6	-0.780290000	-2.359563000	-0.841653000
1	-0.448648000	-1.919656000	-1.786384000
1	-0.890629000	-3.437556000	-0.995314000
8	0.341015000	-2.154733000	0.061488000
6	0.227939000	-2.854163000	1.321612000
1	0.103996000	-3.923104000	1.125031000
1	1.162107000	-2.684822000	1.857781000
1	-0.619551000	-2.474302000	1.899344000
6	6.659675000	-0.797818000	0.410976000
1	7.367281000	-1.621835000	0.398990000
6	5.714673000	-0.671985000	-0.521452000
6	4.708439000	0.443386000	-0.570526000
1	4.935594000	1.197990000	0.190592000
6	2.182386000	1.034806000	-0.415431000
6	3.249289000	-0.060210000	-0.344924000
1	3.246614000	-0.556069000	0.642721000
1	3.063409000	-0.839158000	-1.108042000
1	2.329678000	1.808549000	0.344795000
1	2.133117000	1.503318000	-1.404822000
1	5.642536000	-1.417390000	-1.315012000
1	4.738471000	0.945678000	-1.546221000
1	6.773878000	-0.072261000	1.214022000

.....
30
E + ZPE = -2666.156756

28	1.062310000	-0.622940000	-0.548581000
15	-0.511283000	0.743534000	-0.097792000
6	-0.254052000	1.805288000	1.432205000
1	-1.212311000	1.797677000	1.965024000
6	-0.022983000	3.220988000	0.857372000
1	-0.183990000	3.976353000	1.634562000
1	1.020940000	3.318244000	0.529327000
6	-0.965738000	3.411741000	-0.339643000
1	-0.749167000	4.335673000	-0.887568000

1	-2.005485000	3.486272000	0.006395000
6	-0.802946000	2.187689000	-1.267875000
1	0.154979000	2.292809000	-1.790551000
6	-1.906613000	1.996531000	-2.309653000
1	-2.887539000	1.856358000	-1.845631000
1	-1.711545000	1.133659000	-2.956364000
1	-1.963319000	2.882083000	-2.952064000
6	0.837030000	1.318876000	2.390030000
1	1.814606000	1.260071000	1.900141000
1	0.602593000	0.331151000	2.802982000
1	0.925935000	2.011929000	3.234464000
6	-2.107315000	-0.148013000	0.146989000
6	-3.214513000	0.528057000	0.685416000
1	-3.136192000	1.578974000	0.946322000
6	-4.434295000	-0.117004000	0.889441000
1	-5.274472000	0.434682000	1.300137000
6	-4.563621000	-1.466785000	0.570253000
1	-5.504429000	-1.983407000	0.733324000
6	-3.471504000	-2.156401000	0.045388000
1	-3.573391000	-3.210811000	-0.198733000
6	-2.247190000	-1.517030000	-0.183013000
6	-1.143927000	-2.332097000	-0.820624000
1	-0.902972000	-1.984333000	-1.829651000
1	-1.441996000	-3.382865000	-0.893331000
8	0.126277000	-2.284106000	-0.116431000
6	0.104546000	-2.870423000	1.202131000
1	-0.247510000	-3.903679000	1.127319000
1	1.132165000	-2.856095000	1.566436000
1	-0.544557000	-2.298129000	1.871093000
6	4.843980000	0.374664000	1.536206000
1	4.762336000	0.438306000	2.617622000
6	4.313799000	-0.640095000	0.850118000
6	4.411540000	-0.823076000	-0.639576000
1	5.068953000	-0.059987000	-1.070703000
6	2.297138000	0.556442000	-1.257600000
6	3.053473000	-0.739985000	-1.372042000
1	2.425310000	-1.598547000	-0.916314000
1	3.145303000	-1.071350000	-2.411126000
1	2.753103000	1.289244000	-0.587154000
1	2.029457000	1.010332000	-2.213878000
1	3.783413000	-1.425887000	1.393959000
1	4.866939000	-1.798077000	-0.859847000
1	5.406335000	1.165281000	1.043872000

.....
31
E + ZPE = -2666.151430

28	1.286457000	-0.263936000	-0.355920000
15	-0.520584000	0.788270000	-0.004266000
6	-0.621489000	1.912646000	1.504885000
1	-1.545748000	1.637357000	2.024502000
6	-0.786139000	3.331577000	0.909771000
1	-1.226423000	4.005776000	1.652762000
1	0.203634000	3.736943000	0.659298000
6	-1.638215000	3.235535000	-0.363276000
1	-1.650820000	4.181675000	-0.916323000
1	-2.681603000	3.004280000	-0.110993000
6	-1.041289000	2.112058000	-1.235998000
1	-0.093839000	2.479360000	-1.646462000
6	-1.919324000	1.633843000	-2.393202000
1	-2.875297000	1.234001000	-2.042274000
1	-1.422585000	0.857631000	-2.986732000
1	-2.133616000	2.472070000	-3.065225000

6	0.539739000	1.784119000	2.493288000
1	1.497506000	2.012127000	2.015082000
1	0.602034000	0.778270000	2.922326000
1	0.401778000	2.488877000	3.321117000
6	-1.936272000	-0.396546000	0.122175000
6	-3.160262000	0.016461000	0.673399000
1	-3.279967000	1.029544000	1.042420000
6	-4.254561000	-0.845881000	0.752458000
1	-5.188247000	-0.492829000	1.179795000
6	-4.140821000	-2.153059000	0.286640000
1	-4.982211000	-2.836202000	0.349692000
6	-2.930851000	-0.586530000	-0.256303000
1	-2.839556000	-3.605797000	-0.614763000
6	-1.830538000	-1.724449000	-0.356196000
6	-0.575637000	-2.266039000	-1.002321000
1	-0.338635000	-1.760187000	-1.942296000
1	-0.688517000	-3.333770000	-1.215719000
8	0.618389000	-2.101647000	-0.189103000
6	0.593242000	-2.870148000	1.033809000
1	0.439768000	-3.925083000	0.787261000
1	1.564735000	-2.737309000	1.506351000
1	-0.202706000	-2.518103000	1.696149000
6	3.513613000	-0.520015000	1.808918000
1	3.094657000	-1.120811000	2.612208000
6	3.828863000	-1.046053000	0.617784000
6	4.407085000	-0.280473000	-0.544230000
1	4.910831000	0.629137000	-0.199059000
6	2.304404000	1.151333000	-0.976041000
6	3.274006000	0.097706000	-1.516348000
1	2.707764000	-0.846101000	-1.745544000
1	3.658133000	0.385999000	-2.502951000
1	2.758093000	1.818601000	-0.236833000
1	1.874036000	1.750071000	-1.783683000
1	3.660797000	-2.111007000	0.446899000
1	5.154007000	-0.893993000	-1.060388000
1	3.709516000	0.524151000	2.040665000

32
E + ZPE = -2666.122971

28	-1.362494000	-0.033197000	0.211569000
15	0.830239000	-0.737217000	-0.002479000
6	1.395389000	-1.869679000	1.392969000
1	2.381792000	-1.501278000	1.695861000
6	1.577862000	-3.244811000	0.709600000
1	2.221952000	-3.888114000	1.319573000
1	0.606398000	-3.752042000	0.634408000
6	2.157323000	-3.013971000	-0.692566000
1	2.164651000	-3.933319000	-1.289092000
1	3.199858000	-2.676291000	-0.619440000
6	1.307657000	-1.925931000	-1.387006000
1	0.356652000	-2.383699000	-1.691777000
6	1.947740000	-1.287795000	-2.622181000
1	2.897858000	-0.801724000	-2.381051000
1	1.292580000	-0.540424000	-3.084071000
1	2.146863000	-2.058650000	-3.374790000
6	0.497322000	-1.887222000	2.634126000
1	-0.511383000	-2.243804000	2.403558000
1	0.413682000	-0.895231000	3.092439000
1	0.920417000	-2.559299000	3.389244000
6	2.018629000	0.671029000	-0.035050000
6	3.381083000	0.486487000	0.248591000
1	3.761780000	-0.502411000	0.482857000

6	4.279695000	1.553758000	0.225158000
1	5.329363000	1.379197000	0.441287000
6	3.825156000	2.836366000	-0.073368000
1	4.514223000	3.675216000	-0.086215000
6	2.474098000	3.038667000	-0.353517000
1	2.119527000	4.039325000	-0.587718000
6	1.566138000	1.974147000	-0.349003000
6	0.132036000	2.259088000	-0.724874000
1	-0.169898000	1.737794000	-1.637799000
1	-0.017166000	3.330579000	-0.891661000
8	-0.837645000	1.837766000	0.268427000
6	-0.847890000	2.618278000	1.483165000
1	-0.897487000	3.679290000	1.221275000
1	-1.745457000	2.327498000	2.028174000
1	0.046674000	2.418553000	2.080487000
6	-2.893302000	-0.964114000	-0.700121000
6	-2.106823000	-1.855101000	0.048803000
1	-1.402329000	-2.513528000	-0.450021000
1	-2.604810000	0.443480000	0.751196000
1	-2.604199000	-0.794982000	-1.743698000
1	-2.512067000	-2.247552000	0.980821000
6	-4.362868000	-0.701202000	-0.437590000
1	-4.896955000	-1.460456000	-1.034708000
1	-4.603799000	-0.900287000	0.612214000
6	-4.844760000	0.665815000	-0.842854000
1	-4.667485000	0.947969000	-1.881918000
6	-5.476209000	1.514806000	-0.031177000
1	-5.691882000	1.263598000	1.005421000
1	-5.821576000	2.484546000	-0.377637000

33
E + ZPE = -2666.125436

28	-1.451332000	-0.046615000	0.664095000
15	0.658147000	-0.748182000	-0.029480000
6	1.460602000	-1.876314000	1.256572000
1	2.491149000	-1.515931000	1.355588000
6	1.495896000	-3.262905000	0.575800000
1	2.232159000	-3.908452000	1.067832000
1	0.521561000	-3.759545000	0.686701000
6	1.811646000	-3.059221000	-0.912084000
1	1.692604000	-3.985592000	-1.485522000
1	2.855978000	-2.743872000	-1.036649000
6	0.866213000	-1.964224000	-1.453098000
1	-0.131767000	-2.415100000	-1.557065000
6	1.262091000	-1.357221000	-2.801160000
1	2.242349000	-0.873656000	-2.754722000
1	0.535966000	-0.610847000	-3.142612000
1	1.310483000	-2.143181000	-3.562793000
6	0.815251000	-1.859463000	2.646598000
1	-0.223412000	-2.206445000	2.625822000
1	0.831650000	-0.857891000	3.091579000
1	1.367685000	-2.522108000	3.322357000
6	1.845397000	0.644333000	-0.234117000
6	3.221941000	0.399826000	-0.369536000
1	3.595230000	-0.619566000	-0.374501000
6	4.136395000	1.444122000	-0.505323000
1	5.193793000	1.224794000	-0.618288000
6	3.687015000	2.763057000	-0.489072000
1	4.390333000	3.584759000	-0.583111000
6	2.325314000	3.024383000	-0.342006000
1	1.976850000	4.053997000	-0.324057000
6	1.395339000	1.984890000	-0.225762000

6	-0.067879000	2.348830000	-0.138811000
1	-0.630645000	2.025837000	-1.019374000
1	-0.190500000	3.433046000	-0.051823000
8	-0.767249000	1.744133000	0.979403000
6	-0.498980000	2.324571000	2.272317000
1	-0.627832000	3.409125000	2.207115000
1	-1.233943000	1.905000000	2.958832000
1	0.516707000	2.084548000	2.601549000
6	-2.686914000	-1.111736000	-0.513551000
6	-2.371308000	-1.825250000	0.638508000
1	-1.622417000	-2.612451000	0.595457000
1	-2.629664000	0.378175000	1.403032000
1	-2.098017000	-1.310783000	-1.411696000
1	-3.092298000	-1.913978000	1.446523000
6	-4.010230000	-0.437625000	-0.787620000
1	-4.614379000	-1.176844000	-1.341185000
1	-4.537985000	-0.227929000	0.147519000
6	-3.881957000	0.812645000	-1.623344000
1	-3.448836000	0.679485000	-2.616229000
6	-4.279798000	2.026355000	-1.237877000
1	-4.737101000	2.196242000	-0.265518000
1	-4.188827000	2.889740000	-1.891050000

34
E + ZPE = -2666.153938

28	1.565848000	-0.205228000	0.148636000
15	-0.602877000	0.789915000	-0.006018000
6	-1.061659000	1.988778000	1.377356000
1	-2.140697000	1.874711000	1.531712000
6	-0.816566000	3.373246000	0.743764000
1	-1.290747000	4.157349000	1.345095000
1	0.259924000	3.593825000	0.724277000
6	-1.371562000	3.328154000	-0.686172000
1	-1.119264000	4.230660000	-1.254385000
1	-2.467885000	3.268075000	-0.656755000
6	-0.801826000	2.073007000	-1.385713000
1	0.232966000	2.292002000	-1.681210000
6	-1.572504000	1.614789000	-2.625518000
1	-2.608087000	1.353150000	-2.387568000
1	-1.106588000	0.743223000	-3.098991000
1	-1.592295000	2.421034000	-3.367355000
6	-0.370343000	1.749782000	2.722029000
1	0.716542000	1.865034000	2.654343000
1	-0.586332000	0.750481000	3.117184000
1	-0.727807000	2.474924000	3.461796000
6	-1.992849000	-0.423564000	-0.073073000
6	-3.321154000	0.004916000	0.087482000
1	-3.539239000	1.061280000	0.210393000
6	-4.386606000	-0.894812000	0.085672000
1	-5.402373000	-0.530112000	0.204970000
6	-4.137598000	-2.256919000	-0.064272000
1	-4.955304000	-2.971074000	-0.055049000
6	-2.826190000	-2.700793000	-0.228073000
1	-2.636181000	-3.763777000	-0.354140000
6	-1.747620000	-1.807230000	-0.251128000
6	-0.385121000	-2.391517000	-0.570437000
1	-0.024168000	-2.046588000	-1.542817000
1	-0.453880000	-3.483770000	-0.614231000
8	0.686423000	-2.062815000	0.348004000
6	0.512996000	-2.600624000	1.671607000
1	0.347066000	-3.680859000	1.606898000
1	1.440462000	-2.409235000	2.213668000

1	-0.332167000	-2.127224000	2.182252000
6	2.811987000	1.225446000	0.532298000
1	2.444424000	1.832240000	1.358335000
6	3.432331000	-0.015547000	0.812080000
6	4.432130000	-0.653514000	-0.135057000
1	5.435580000	-0.231781000	0.012247000
6	2.406827000	-0.743275000	-1.484142000
6	3.898882000	-0.442773000	-1.553151000
1	4.391177000	-1.100381000	-2.280974000
1	4.079892000	0.583248000	-1.889837000
1	3.483826000	-0.329810000	1.857756000
1	4.505909000	-1.726483000	0.080847000
1	3.097058000	1.808427000	-0.340739000
1	1.810196000	-0.250918000	-2.263853000
1	2.224671000	-1.822781000	-1.482756000

35
E + ZPE = -2666.161678

28	-1.544990000	-0.364365000	0.163292000
15	0.559916000	0.767593000	0.003796000
6	0.867759000	2.114783000	-1.290404000
1	1.835279000	1.873901000	-1.741139000
6	1.010977000	3.423346000	-0.476222000
1	1.579215000	4.165913000	-1.047692000
1	0.016213000	3.856676000	-0.302090000
6	1.672898000	3.098691000	0.868477000
1	1.643994000	3.953667000	1.554006000
1	2.731442000	2.846293000	0.722788000
6	0.931235000	1.891638000	1.478487000
1	-0.057467000	2.232196000	1.814256000
6	1.639360000	1.228066000	2.661753000
1	2.625314000	0.845672000	2.380854000
1	1.056330000	0.398121000	3.077446000
1	1.780330000	1.959760000	3.465005000
6	-0.159787000	2.197169000	-2.423535000
1	-1.147507000	2.494551000	-2.056831000
1	-0.259437000	1.246917000	-2.959615000
1	0.153621000	2.953131000	-3.152290000
6	2.003855000	-0.384209000	-0.124617000
6	3.268124000	0.064451000	-0.540362000
1	3.423054000	1.106445000	-0.797168000
6	4.360551000	-0.799791000	-0.624545000
1	5.325253000	-0.417512000	-0.944348000
6	4.206686000	-2.145364000	-0.301182000
1	5.046812000	-2.829349000	-0.371472000
6	2.958933000	-2.610862000	0.110949000
1	2.836585000	-3.661287000	0.362917000
6	1.860088000	-1.750576000	0.215369000
6	0.563821000	-2.332449000	0.727359000
1	0.278202000	-1.925471000	1.702324000
1	0.650788000	-3.418741000	0.835190000
8	-0.584458000	-2.072079000	-0.118907000
6	-0.493991000	-2.620770000	-1.448290000
1	-0.186992000	-3.669110000	-1.382529000
1	-1.492960000	-2.557240000	-1.880477000
1	0.222008000	-2.058324000	-2.055017000
6	-2.501497000	1.362514000	0.447270000
1	-1.842126000	2.212543000	0.302039000
6	-3.068293000	0.737550000	-0.662846000
6	-4.376647000	-0.024299000	-0.605903000
1	-5.215130000	0.679033000	-0.713332000
6	-3.003474000	-1.455242000	0.780103000

6	-4.386362000	-0.811590000	0.700965000
1	-5.186079000	-1.561969000	0.717422000
1	-4.572491000	-0.147565000	1.552708000
1	-2.732199000	1.054149000	-1.650857000
1	-4.435014000	-0.712372000	-1.458135000
1	-2.995455000	1.337168000	1.416411000
1	-2.695170000	-1.724123000	1.803548000
1	-2.975179000	-2.366438000	0.171250000

36

E + ZPE = -2666.132287

28	-1.428347000	-0.631709000	-0.139451000
15	0.373074000	0.782308000	-0.074669000
6	0.553141000	1.934992000	-1.560316000
1	1.593651000	1.843490000	-1.889689000
6	0.345540000	3.350637000	-0.975787000
1	0.762159000	4.107268000	-1.650147000
1	-0.730375000	3.560236000	-0.892825000
6	0.989840000	3.398396000	0.415635000
1	0.742184000	4.322967000	0.949871000
1	2.084069000	3.369184000	0.328178000
6	0.495182000	2.167622000	1.204270000
1	-0.548943000	2.353541000	1.490305000
6	1.290277000	1.842216000	2.470852000
1	2.343364000	1.646554000	2.247770000
1	0.889085000	0.965936000	2.992785000
1	1.246121000	2.687675000	3.166353000
6	-0.347973000	1.616540000	-2.756511000
1	-1.409841000	1.715563000	-2.504343000
1	-0.178917000	0.605180000	-3.142924000
1	-0.143063000	2.317449000	-3.573713000
6	1.958995000	-0.162187000	0.003000000
6	3.182766000	0.448685000	-0.316277000
1	3.210298000	1.491353000	-0.615316000
6	4.387835000	-0.250999000	-0.249475000
1	5.317761000	0.252178000	-0.496728000
6	4.390159000	-1.590919000	0.131215000
1	5.320311000	-2.148848000	0.178364000
6	3.184534000	-2.215496000	0.446833000
1	3.185493000	-3.262242000	0.740610000
6	1.970499000	-1.519745000	0.400879000
6	0.720964000	-2.264111000	0.811332000
1	0.265432000	-1.848967000	1.713661000
1	0.955294000	-3.315551000	1.008131000
8	-0.344591000	-2.238970000	-0.174353000
6	-0.005074000	-2.895577000	-1.413602000
1	0.394620000	-3.889592000	-1.190385000
1	-0.927424000	-2.989936000	-1.982897000
1	0.732344000	-2.311776000	-1.972092000
6	-4.134198000	0.404380000	0.513401000
1	-4.925631000	-0.283522000	0.829180000
6	-3.010244000	0.467977000	1.524477000
6	-2.502856000	-0.587485000	2.191757000
1	-2.968007000	-1.568427000	2.169352000
6	-3.001461000	-1.501045000	-0.723995000
6	-3.498800000	-0.094183000	-0.796638000
1	-4.071395000	0.138310000	-1.703407000
1	-2.563929000	0.567331000	-0.951541000
1	-2.566306000	1.448342000	1.689455000
1	-1.683338000	-0.456941000	2.894005000
1	-4.585643000	1.391818000	0.380592000
1	-3.515531000	-2.156627000	-0.022024000

1	-2.884265000	-1.985139000	-1.697401000
---	--------------	--------------	--------------

37

E + ZPE = -2666.145240

28	-1.238181000	-0.525060000	-0.580338000
15	0.513649000	0.801562000	-0.111245000
6	0.919132000	2.093403000	-1.420412000
1	1.996305000	2.027370000	-1.607410000
6	0.618008000	3.442431000	-0.725441000
1	1.139944000	4.259183000	-1.236209000
1	-0.456989000	3.659789000	-0.798000000
6	1.022756000	3.328608000	0.749932000
1	0.699083000	4.198791000	1.332385000
1	2.116171000	3.275365000	0.839722000
6	0.392168000	2.036356000	1.310092000
1	-0.688061000	2.205990000	1.419913000
6	0.952500000	1.564588000	2.652920000
1	2.025763000	1.359693000	2.591502000
1	0.453606000	0.656180000	3.009294000
1	0.801860000	2.340433000	3.411610000
6	0.189266000	1.897533000	-2.753554000
1	-0.899261000	1.940003000	-2.629623000
1	0.443355000	0.940534000	-3.222625000
1	0.469529000	2.691025000	-3.455518000
6	2.038725000	-0.200562000	0.145049000
6	3.320523000	0.353075000	0.006180000
1	3.438311000	1.400484000	-0.251895000
6	4.469139000	-0.414097000	0.206697000
1	5.448097000	0.043262000	0.099480000
6	4.353167000	-1.761261000	0.541128000
1	5.239979000	-2.369084000	0.691991000
6	3.086605000	-2.328819000	0.678714000
1	2.997309000	-3.380883000	0.940802000
6	1.926875000	-1.567402000	0.496917000
6	0.593641000	-2.240824000	0.723337000
1	0.026519000	-1.784361000	1.538641000
1	0.735958000	-3.298460000	0.966255000
8	-0.312155000	-2.182597000	-0.413590000
6	0.130353000	-2.913812000	-1.577237000
1	0.398327000	-3.929889000	-1.272840000
1	-0.714474000	-2.943780000	-2.263754000
1	0.989013000	-2.422341000	-2.043814000
6	-4.129385000	0.535150000	0.281488000
1	-5.113658000	0.099654000	0.078436000
6	-3.627023000	0.086614000	1.627118000
6	-4.210897000	-0.832089000	2.398990000
1	-5.126599000	-1.335489000	2.096433000
6	-2.895966000	-1.280890000	-1.081547000
6	-3.201714000	0.138515000	-0.886124000
1	-3.453642000	0.661239000	-1.813723000
1	-2.171314000	0.744492000	-0.622490000
1	-2.723206000	0.584326000	1.986450000
1	-3.810146000	-1.099249000	3.372696000
1	-4.254472000	1.626366000	0.278531000
1	-3.298358000	-1.978945000	-0.348167000
1	-2.934605000	-1.652566000	-2.106685000

38

E + ZPE = -2666.137162

28	0.980422000	-1.022272000	-0.216646000
----	-------------	--------------	--------------

15	-0.333393000	0.703100000	-0.036729000
6	0.082896000	1.865728000	1.374983000
1	-0.869940000	2.184136000	1.812307000
6	0.728073000	3.075122000	0.661149000
1	0.727997000	3.948330000	1.323133000
1	1.776344000	2.844070000	0.430817000
6	-0.049364000	3.332963000	-0.636536000
1	0.437628000	4.088889000	-1.262807000
1	-1.054777000	3.711119000	-0.405930000
6	-0.158123000	1.994260000	-1.400352000
1	0.819878000	1.773201000	-1.844026000
6	-1.220178000	1.956140000	-2.500157000
1	-2.224542000	2.133544000	-2.103412000
1	-1.228916000	0.996202000	-3.028671000
1	-1.010442000	2.735053000	-3.241586000
6	0.943024000	1.246083000	2.480029000
1	1.890502000	0.873346000	2.078124000
1	0.428440000	0.418232000	2.980990000
1	1.172161000	1.998824000	3.242733000
6	-2.114621000	0.257872000	0.114781000
6	-3.053396000	1.174427000	0.613619000
1	-2.738506000	2.165622000	0.923461000
6	-4.406360000	0.846862000	0.710503000
1	-5.111764000	1.578109000	1.093468000
6	-4.843430000	-0.416095000	0.317268000
1	-5.892565000	-0.684078000	0.395636000
6	-3.922312000	-1.340554000	-0.174724000
1	-4.263816000	-2.326853000	-0.478744000
6	-2.566023000	-1.018774000	-0.294043000
6	-1.640925000	-2.055813000	-0.888557000
1	-1.222480000	-1.740568000	-1.849024000
1	-2.177366000	-2.996706000	-1.048880000
8	-0.473407000	-2.352253000	-0.077612000
6	-0.770058000	-2.897547000	1.222981000
1	-1.443774000	-3.752164000	1.109279000
1	0.177520000	-3.232763000	1.646759000
1	-1.227763000	-2.144041000	1.870545000
6	4.153257000	-0.928415000	-0.343532000
1	4.075931000	-0.735923000	-1.419217000
6	4.435134000	0.346245000	0.404517000
6	4.617945000	1.537300000	-0.168394000
1	4.560387000	1.668729000	-1.247127000
6	2.232408000	-2.567541000	-0.678309000
6	2.951062000	-1.718955000	0.134860000
1	2.910385000	-1.875179000	1.215795000
1	1.874359000	0.093551000	-0.321405000
1	4.529508000	0.254205000	1.487767000
1	4.861696000	2.419896000	0.416235000
1	5.011369000	-1.608805000	-0.209622000
1	2.430911000	-2.589054000	-1.749712000
1	1.723915000	-3.439638000	-0.279493000

39
E + ZPE = -2666.143530

28	-1.100531000	-0.131740000	0.557746000
15	0.815025000	0.808287000	0.058824000
6	0.730855000	2.005729000	-1.382579000
1	1.650864000	1.865385000	-1.961979000
6	0.785462000	3.389056000	-0.696968000
1	1.055591000	4.160776000	-1.426247000
1	-0.209946000	3.646625000	-0.311027000
6	1.789885000	3.308873000	0.459271000

1	1.777210000	4.213789000	1.077023000
1	2.810824000	3.206193000	0.066428000
6	1.432616000	2.072760000	1.315756000
1	0.538675000	2.309932000	1.904386000
6	2.535832000	1.596599000	2.262432000
1	3.442089000	1.307887000	1.720991000
1	2.216000000	0.741289000	2.868259000
1	2.801025000	2.404953000	2.952749000
6	-0.469777000	1.801976000	-2.310606000
1	-1.412682000	1.892857000	-1.760431000
1	-0.446953000	0.820620000	-2.797713000
1	-0.466893000	2.561094000	-3.100674000
6	2.148926000	-0.414278000	-0.266276000
6	3.326511000	-0.047828000	-0.935673000
1	3.464582000	0.972806000	-1.278846000
6	4.345853000	-0.972657000	-1.165549000
1	5.250093000	-0.662166000	-1.680201000
6	4.196154000	-2.288923000	-0.734362000
1	4.980271000	-3.018157000	-0.913310000
6	3.027195000	-2.670465000	-0.075460000
1	2.911400000	-3.699704000	0.254867000
6	2.002462000	-1.751352000	0.174892000
6	0.785392000	-2.234382000	0.934673000
1	0.672685000	-1.737740000	1.903058000
1	0.859007000	-3.311058000	1.118907000
8	-0.479480000	-1.989816000	0.261177000
6	-0.603814000	-2.660526000	-1.010895000
1	-0.462645000	-3.735403000	-0.862125000
1	-1.613874000	-2.470167000	-1.372477000
1	0.130784000	-2.282247000	-1.727484000
6	-3.997396000	0.400145000	-0.091248000
1	-3.927951000	1.320726000	0.502140000
6	-5.427992000	-0.089655000	-0.138004000
6	-6.119339000	-0.297009000	-1.258580000
1	-5.691092000	-0.112668000	-2.241981000
6	-2.625353000	-0.635519000	1.808970000
6	-3.109742000	-0.661712000	0.519447000
1	-3.124604000	-1.621700000	0.002510000
1	-1.449735000	1.246396000	0.773172000
1	-5.890578000	-0.283136000	0.829574000
1	-7.147976000	-0.644750000	-1.235875000
1	-3.666467000	0.641711000	-1.109921000
1	-2.850417000	0.197672000	2.470051000
1	-2.296339000	-1.553869000	2.292082000

40R
E + ZPE = -2975.660383

28	-0.963201000	-0.952028000	-0.007538000
15	0.847122000	-0.163466000	0.998221000
6	0.525777000	1.378821000	2.016716000
1	0.614356000	2.250856000	1.363977000
6	1.598417000	1.391360000	3.153819000
1	2.238139000	2.275974000	3.074207000
1	1.078653000	1.473718000	4.114490000
6	2.448731000	0.102687000	3.127310000
1	2.755938000	-0.192776000	4.136896000
1	3.369500000	0.261842000	2.554183000
6	1.643191000	-1.033401000	2.466927000
1	0.796060000	-1.288147000	3.117987000
6	2.479682000	-2.289890000	2.224715000
1	3.307043000	-2.095985000	1.533977000
1	1.889074000	-3.124807000	1.834864000

1	2.917132000	-2.622038000	3.172892000
6	-0.902216000	1.371195000	2.593200000
1	-1.084275000	0.490383000	3.220073000
1	-1.663727000	1.408279000	1.809778000
1	-1.037993000	2.253911000	3.227976000
6	2.269189000	0.191074000	-0.132664000
6	2.922101000	1.432829000	-0.071610000
1	2.587660000	2.194861000	0.623043000
6	4.018922000	1.719973000	-0.886537000
1	4.503993000	2.688909000	-0.814058000
6	4.492012000	0.757608000	-1.773648000
1	5.352643000	0.963153000	-2.402996000
6	3.855106000	-0.481383000	-1.842096000
1	4.235511000	-1.239396000	-2.522259000
6	2.741021000	-0.783632000	-1.048713000
6	2.075304000	-2.135874000	-1.238029000
1	1.659978000	-2.512987000	-0.302228000
1	2.817699000	-2.867870000	-1.586381000
8	0.969828000	-2.104688000	-2.143573000
6	1.340926000	-2.091412000	-3.519016000
1	1.971965000	-2.957572000	-3.763042000
1	0.415614000	-2.153985000	-4.096250000
1	1.872152000	-1.171155000	-3.794028000
6	-3.694467000	-2.201582000	0.891068000
1	-3.714561000	-1.311683000	1.531543000
6	-4.680694000	-2.056165000	-0.237727000
6	-5.504094000	-1.018278000	-0.397099000
1	-5.515250000	-0.184167000	0.302478000
6	-1.186235000	-2.313993000	1.373329000
6	-2.257855000	-2.501998000	0.460451000
1	-2.157390000	-3.348694000	-0.222996000
1	-2.160319000	-1.513253000	-0.733212000
1	-4.723797000	-2.886170000	-0.944831000
1	-6.219068000	-0.976234000	-1.213646000
1	-3.995350000	-3.049670000	1.526270000
1	-1.417765000	-1.898646000	2.352919000
1	-0.369208000	-3.031937000	1.371513000
6	-0.864546000	0.506788000	-1.426379000
6	-1.776863000	-0.503747000	-1.826672000
1	0.134521000	0.430007000	-1.845481000
1	-1.421832000	-1.245694000	-2.537826000
1	-2.827699000	-0.242290000	-1.930702000
6	-1.293218000	1.884014000	-1.092773000
6	-2.594052000	2.197373000	-0.655714000
1	-3.334381000	1.410655000	-0.531690000
6	-0.373130000	2.935880000	-1.248205000
1	0.630842000	2.715365000	-1.601931000
6	-0.739658000	4.255603000	-0.985517000
6	-2.958718000	3.515224000	-0.389910000
6	-2.033287000	4.549940000	-0.551878000
1	-3.969695000	3.737325000	-0.060465000
1	-0.017664000	5.054517000	-1.128771000
1	-2.322412000	5.577007000	-0.350029000

40S

E + ZPE = -2975.661373

28	-0.445622000	0.962562000	-0.101844000
15	0.769117000	-0.816768000	0.387782000
6	0.377059000	-1.550241000	2.078740000
1	1.096822000	-1.136823000	2.791497000
6	0.555982000	-3.095586000	1.940725000
1	1.155517000	-3.491318000	2.767112000

1	-0.432592000	-3.562215000	2.020758000
6	1.170118000	-3.455527000	0.578121000
1	0.935185000	-4.489120000	0.298066000
1	2.263859000	-3.378121000	0.606421000
6	0.613464000	-2.479075000	-0.474977000
1	-0.469293000	-2.637757000	-0.557945000
6	1.254688000	-2.643299000	-1.853173000
1	2.328207000	-2.429021000	-1.828966000
1	0.792745000	-2.004700000	-2.613453000
1	1.134955000	-3.679501000	-2.189272000
6	-1.035007000	-1.196462000	2.573587000
1	-1.806523000	-1.526074000	1.870245000
1	-1.166654000	-0.123181000	2.739877000
1	-1.219154000	-1.701948000	3.528581000
6	2.589682000	-0.462829000	0.341500000
6	3.420116000	-0.896875000	1.386337000
1	3.004221000	-1.426550000	2.235731000
6	4.798823000	-0.675074000	1.364892000
1	5.412059000	-1.024763000	2.190037000
6	5.376512000	-0.018438000	0.283420000
1	6.448145000	0.153088000	0.249476000
6	4.564576000	0.413520000	-0.765538000
1	5.016532000	0.913497000	-1.618700000
6	3.178854000	0.213316000	-0.758361000
6	2.380307000	0.751735000	-1.932957000
1	1.586044000	0.063816000	-2.228641000
1	3.044166000	0.876406000	-2.799824000
8	1.714259000	1.988521000	-1.660954000
6	2.579528000	3.120794000	-1.651993000
1	3.109586000	3.215356000	-2.609902000
1	1.947809000	4.000650000	-1.510247000
1	3.315714000	3.069251000	-0.839541000
6	-1.538702000	0.046740000	-1.531736000
6	-1.708275000	1.455519000	-1.615617000
1	-2.697381000	1.863673000	-1.416552000
1	-1.185133000	2.243305000	-0.391134000
1	-0.853032000	-0.392294000	-2.252826000
6	0.501905000	1.883219000	1.360281000
6	-0.422270000	2.819573000	0.827039000
1	0.305932000	1.483504000	2.353093000
1	1.553288000	1.990492000	1.112385000
1	0.007231000	3.588521000	0.181191000
1	-1.138721000	1.994221000	-2.370875000
6	-2.639877000	-0.850275000	-1.104461000
6	-3.594584000	-0.470474000	-0.143164000
1	-3.533596000	0.506985000	0.329354000
6	-2.764572000	-2.117785000	-1.699077000
1	-2.052933000	-2.420927000	-2.463581000
6	-3.809018000	-2.975017000	-1.352769000
6	-4.635726000	-1.328173000	0.205891000
6	-4.746153000	-2.585066000	-0.395221000
1	-5.365033000	-1.014559000	0.947339000
1	-3.893515000	-3.943604000	-1.836923000
1	-5.560281000	-3.250375000	-0.123852000
6	-1.612493000	3.291372000	1.663557000
1	-1.197876000	4.004832000	2.392469000
1	-2.018755000	2.455844000	2.246054000
6	-2.708859000	3.965158000	0.881009000
1	-2.399923000	4.796341000	0.244781000
6	-4.000748000	3.637885000	0.944491000
1	-4.357859000	2.835995000	1.588225000
1	-4.755163000	4.176873000	0.378797000

S15

E + ZPE = -2008.734676

28	-0.234533000	0.013316000	-0.000005000
15	1.921104000	-0.180560000	0.000001000
1	2.603832000	0.401565000	1.085231000
1	2.603864000	0.401716000	-1.085127000
1	2.512563000	-1.458403000	-0.000082000
6	0.028883000	1.964203000	0.000001000
6	-1.363997000	1.702782000	0.000004000
1	-1.726737000	0.178869000	-0.000025000
1	-1.924049000	1.888309000	-0.915817000
1	0.489591000	2.325355000	0.917693000
1	0.489587000	2.325358000	-0.917692000
6	-0.407892000	-1.939167000	0.000002000
6	-1.711686000	-1.387652000	0.000006000
1	-0.024557000	-2.383292000	0.917058000
1	-2.298486000	-1.444942000	0.916023000
1	-2.298496000	-1.444963000	-0.916004000
1	-0.024566000	-2.383302000	-0.917054000
1	-1.924027000	1.888289000	0.915843000

S16

E + ZPE = -2239.718500

28	-1.432410000	-0.116450000	0.156164000
15	-0.990832000	1.976830000	-0.219081000
1	-2.064360000	2.887755000	-0.178169000
1	-0.453702000	2.273271000	-1.486546000
1	-0.062971000	2.661219000	0.590866000
6	-2.817979000	-0.001645000	-1.230984000
6	-2.871415000	-1.297050000	-0.653397000
1	-1.846939000	-1.512005000	0.510771000
1	-2.495314000	-2.138370000	-1.234252000
1	-3.614799000	0.701925000	-0.998356000
1	-2.387348000	0.108374000	-2.224999000
6	0.172195000	-0.266738000	1.354982000
6	-0.658694000	-1.405901000	1.525370000
1	0.117841000	0.482509000	2.143421000
1	-1.250953000	-1.458955000	2.437102000
1	-0.287603000	-2.370303000	1.181142000
6	1.424811000	-0.261191000	0.572268000
6	1.682820000	-1.193238000	-0.452865000
1	0.961773000	-1.974161000	-0.682655000
6	2.392229000	0.723606000	0.845870000
1	2.218417000	1.438162000	1.647298000
6	3.587343000	0.766581000	0.130398000
6	2.875094000	-1.144308000	-1.169804000
6	3.830066000	-0.164544000	-0.881296000
1	3.063467000	-1.874033000	-1.951430000
1	4.330494000	1.521927000	0.367149000
1	4.761092000	-0.132618000	-1.438886000
1	-3.717955000	-1.539980000	-0.012083000

S17

E + ZPE = -2239.714462

28	1.353133000	0.244666000	0.169420000
15	2.988313000	-1.100129000	-0.280426000
1	4.255991000	-0.706437000	0.191687000
1	3.287228000	-1.342598000	-1.635848000
1	2.962082000	-2.426166000	0.193894000

6	2.208649000	1.575255000	-1.024555000
6	1.056709000	2.154929000	-0.453160000
1	0.239288000	1.162539000	0.562583000
1	0.169248000	2.280096000	-1.071894000
1	3.186779000	1.896523000	-0.671521000
1	2.175707000	1.254341000	-2.064080000
6	0.547060000	-1.100545000	1.325114000
6	-0.405365000	-0.041007000	1.271902000
1	1.121230000	-1.222001000	2.242933000
1	-0.470354000	0.562691000	2.179508000
1	1.182571000	2.910454000	0.321069000
1	0.309909000	-2.033235000	0.817892000
6	-1.683703000	-0.130588000	0.508306000
6	-2.794554000	0.588603000	0.972391000
1	-2.707640000	1.195984000	1.870297000
6	-1.810384000	-0.905851000	-0.656052000
1	-0.963206000	-1.470538000	-1.039145000
6	-3.029719000	-0.975876000	-1.325713000
6	-4.016696000	0.511172000	0.305295000
6	-4.136005000	-0.269452000	-0.845234000
1	-4.872833000	1.060544000	0.684629000
1	-3.118339000	-1.582899000	-2.221606000
1	-5.086052000	-0.327856000	-1.367536000

S18

E + ZPE = -2744.684866

28	-1.241007000	-0.284661000	-0.089089000
15	0.623159000	0.878159000	0.034831000
6	0.629243000	2.344091000	-1.143275000
1	1.063515000	2.018650000	-2.093338000
6	1.505040000	3.451824000	-0.473549000
1	2.310613000	3.767693000	-1.144119000
1	0.876581000	4.334052000	-0.308486000
6	2.068944000	2.964349000	0.875370000
1	2.244393000	3.802501000	1.559239000
1	3.035752000	2.465854000	0.735047000
6	1.074632000	1.966498000	1.499304000
1	0.142776000	2.500782000	1.732479000
6	1.604775000	1.304443000	2.771569000
1	2.497950000	0.703609000	2.570099000
1	0.858247000	0.669971000	3.258391000
1	1.888171000	2.078661000	3.493254000
6	-0.797931000	2.849877000	-1.419151000
1	-1.309885000	3.136042000	-0.492717000
1	-1.416020000	2.106373000	-1.931056000
1	-0.753026000	3.740216000	-2.056092000
6	2.133430000	-0.134341000	-0.300577000
6	3.105610000	0.324537000	-1.202205000
1	2.984420000	1.278543000	-1.703077000
6	4.254349000	-0.421342000	-1.476131000
1	4.989660000	-0.038445000	-2.177406000
6	4.450595000	-1.645120000	-0.844559000
1	5.341184000	-2.232947000	-1.045149000
6	3.491865000	-2.113090000	0.055221000
1	3.649861000	-3.064685000	0.556814000
6	2.330759000	-1.385688000	0.339071000
6	1.336205000	-1.980234000	1.321894000
1	0.999422000	-1.236916000	2.046417000
1	1.817496000	-2.790208000	1.886174000
8	0.139507000	-2.472289000	0.708093000
6	0.305277000	-3.736538000	0.068808000
1	0.643510000	-4.494439000	0.788113000

1	-0.674069000	-4.029046000	-0.316197000
1	1.022257000	-3.685416000	-0.760673000
6	-4.155648000	0.265218000	0.920899000
1	-3.923515000	1.277191000	0.568085000
6	-5.117307000	-0.409501000	-0.021566000
6	-5.628196000	0.154662000	-1.117469000
1	-5.375196000	1.172350000	-1.409674000
6	-1.739834000	0.150442000	1.751100000
6	-2.860711000	-0.506080000	1.180792000
1	-3.002228000	-1.547256000	1.478831000
1	-2.574257000	-0.952362000	-0.292905000
1	-5.421278000	-1.421824000	0.249706000
1	-6.340744000	-0.367922000	-1.749069000
1	-4.634367000	0.380432000	1.905500000
1	-1.820149000	1.217619000	1.949961000
1	-1.122525000	-0.398924000	2.457128000
6	-0.702050000	-0.749098000	-1.934454000
6	-2.004303000	-1.258201000	-1.709740000
1	0.141900000	-1.431773000	-1.926318000
1	-2.125342000	-2.332130000	-1.574441000
1	-2.848083000	-0.775208000	-2.198451000
1	-0.590729000	0.105076000	-2.596905000

S19R

E + ZPE = -2859.012133

28	0.394423000	1.732303000	0.299573000
15	-0.473134000	-0.183334000	0.996538000
6	0.766731000	-1.352943000	1.777392000
1	1.244888000	-1.934413000	0.985045000
6	-0.042248000	-2.258963000	2.760756000
1	-0.018292000	-3.303427000	2.434721000
1	0.452529000	-2.230821000	3.737378000
6	-1.502918000	-1.768859000	2.894266000
1	-1.879747000	-1.912809000	3.913069000
1	-2.161646000	-2.344532000	2.233758000
6	-1.592001000	-0.279422000	2.506710000
1	-1.064495000	0.314862000	3.264465000
6	-3.034397000	0.216988000	2.401284000
1	-3.587055000	-0.313000000	1.618536000
1	-3.102465000	1.292134000	2.207193000
1	-3.551501000	0.030150000	3.349146000
6	1.867738000	-0.569769000	2.516334000
1	1.453709000	0.071747000	3.302827000
1	2.462870000	0.045781000	1.837276000
1	2.547623000	-1.278648000	3.001654000
6	-1.397371000	-1.117210000	-0.307090000
6	-1.129325000	-2.479920000	-0.513388000
1	-0.365366000	-2.981486000	0.069198000
6	-1.838308000	-3.226675000	-1.456609000
1	-1.609814000	-4.279765000	-1.591196000
6	-2.842744000	-2.620305000	-2.205073000
1	-3.411834000	-3.193304000	-2.930883000
6	-3.118497000	-1.266805000	-2.010736000
1	-3.912651000	-0.796402000	-2.584981000
6	-2.405855000	-0.493804000	-1.085464000
6	-2.728275000	0.987575000	-0.994113000
1	-2.609453000	1.361603000	0.023745000
1	-3.773701000	1.158520000	-1.287455000
8	-1.865882000	1.805528000	-1.788554000
6	-2.182925000	1.812004000	-3.177898000
1	-3.220651000	2.134506000	-3.341499000
1	-1.510700000	2.530886000	-3.651910000

1	-2.035918000	0.826665000	-3.638599000
6	-0.204368000	2.638410000	1.924670000
6	0.382959000	3.617872000	1.080648000
1	1.353276000	4.026148000	1.361822000
1	0.913379000	3.046045000	-0.241555000
1	0.345809000	2.316072000	2.805890000
1	-1.284886000	2.636596000	2.040743000
6	1.207143000	0.820140000	-1.323113000
6	1.277116000	2.232134000	-1.473411000
1	0.378114000	0.337457000	-1.833117000
1	0.538568000	2.701712000	-2.118239000
1	2.264112000	2.691891000	-1.506369000
6	2.411720000	-0.024371000	-1.157096000
6	3.613656000	0.454900000	-0.603757000
1	3.684776000	1.482197000	-0.253864000
6	2.368380000	-1.358956000	-1.597595000
1	1.453428000	-1.742564000	-2.042058000
6	3.488726000	-2.183617000	-1.499163000
6	4.731567000	-0.369593000	-0.502010000
6	4.673824000	-1.692711000	-0.948585000
1	5.651311000	0.021696000	-0.077004000
1	3.438615000	-3.206586000	-1.861059000
1	5.548328000	-2.332045000	-0.873743000
1	-0.272913000	4.327843000	0.577628000

S19S

E + ZPE = -2859.013259

28	0.322084000	-1.353757000	0.526333000
15	-0.379505000	0.722573000	0.251951000
6	0.119204000	1.882600000	1.648760000
1	-0.690347000	1.887516000	2.384798000
6	0.300793000	3.295408000	1.006414000
1	-0.269580000	4.049107000	1.558934000
1	1.355993000	3.576972000	1.094917000
6	-0.094910000	3.277965000	-0.480937000
1	0.420499000	4.069178000	-1.037695000
1	-1.170063000	3.457429000	-0.602077000
6	0.259419000	1.898259000	-1.067415000
1	1.349143000	1.771984000	-1.032662000
6	-0.224499000	1.713839000	-2.506105000
1	-1.316083000	1.766149000	-2.576350000
1	0.104461000	0.766400000	-2.945841000
1	0.182144000	2.516127000	-3.132076000
6	1.405352000	1.430567000	2.361474000
1	2.247194000	1.350231000	1.666351000
1	1.294020000	0.466456000	2.866692000
1	1.673038000	2.171942000	3.122825000
6	-2.223670000	0.808069000	0.085473000
6	-2.957718000	1.741701000	0.833147000
1	-2.456437000	2.413230000	1.520615000
6	-4.345232000	1.845863000	0.712022000
1	-4.882265000	2.580072000	1.305066000
6	-5.026605000	1.016680000	-0.172680000
1	-6.104204000	1.092311000	-0.282058000
6	-4.309859000	0.085783000	-0.925203000
1	-4.838946000	-0.555509000	-1.625903000
6	-2.920787000	-0.043190000	-0.810416000
6	-2.234146000	-1.109475000	-1.645433000
1	-1.297031000	-0.744338000	-2.069550000
1	-2.884077000	-1.395186000	-2.483916000
8	-1.871322000	-2.278481000	-0.902944000
6	-2.972909000	-3.129712000	-0.594768000

1	-3.485714000	-3.451211000	-1.511546000
1	-2.562982000	-4.009749000	-0.094136000
1	-3.697712000	-2.639666000	0.067689000
6	1.673890000	-1.283809000	-0.965329000
6	1.448254000	-2.635082000	-0.577832000
1	2.288042000	-3.180657000	-0.148638000
1	0.689442000	-2.803322000	0.742780000
1	1.170782000	-0.964807000	-1.874881000
6	-0.820659000	-1.418272000	2.133730000
6	-0.179339000	-2.677386000	2.000117000
1	-0.490005000	-0.752784000	2.925682000
1	-1.874326000	-1.340197000	1.882862000
1	-0.782832000	-3.531534000	1.696399000
1	0.624408000	-2.923448000	2.693467000
1	0.784591000	-3.236614000	-1.195736000
6	2.963878000	-0.602410000	-0.702557000
6	3.727811000	-0.847945000	0.453272000
1	3.366647000	-1.539541000	1.211113000
6	3.470039000	0.300253000	-1.653891000
1	2.907084000	0.486230000	-2.565549000
6	4.700977000	0.928193000	-1.464830000
6	4.955947000	-0.218547000	0.644284000
6	5.446874000	0.673358000	-0.313196000
1	5.532081000	-0.424855000	1.541615000
1	5.079470000	1.609776000	-2.220996000
1	6.405748000	1.160484000	-0.163853000

S20R

E + ZPE = -3089.988602

28	-0.677144000	-0.670861000	-0.241021000
15	1.086698000	-0.220279000	1.016159000
6	0.957344000	1.368751000	2.007222000
1	1.319920000	2.192602000	1.387303000
6	1.837166000	1.167906000	3.283636000
1	2.647500000	1.903105000	3.316250000
1	1.212446000	1.359162000	4.162908000
6	2.402912000	-0.267433000	3.347213000
1	2.505588000	-0.609616000	4.383258000
1	3.404683000	-0.305326000	2.903837000
6	1.477288000	-1.218691000	2.564279000
1	0.513860000	-1.283150000	3.088134000
6	2.058287000	-2.624935000	2.415901000
1	3.001402000	-2.614516000	1.859447000
1	1.370956000	-3.319169000	1.922063000
1	2.270236000	-3.035868000	3.409356000
6	-0.504945000	1.676400000	2.376424000
1	-0.959055000	0.863036000	2.955182000
1	-1.118797000	1.868044000	1.492647000
1	-0.536011000	2.575281000	3.002377000
6	2.694306000	-0.176380000	0.097399000
6	3.567569000	0.910340000	0.267984000
1	3.294717000	1.736454000	0.914335000
6	4.808066000	0.956883000	-0.370934000
1	5.461009000	1.810772000	-0.216394000
6	5.205484000	-0.098404000	-1.186495000
1	6.174241000	-0.082564000	-1.676681000
6	4.348868000	-1.184526000	-1.364254000
1	4.665427000	-2.016380000	-1.988469000
6	3.090387000	-1.241552000	-0.751558000
6	2.200160000	-2.431419000	-1.066673000
1	1.563192000	-2.693470000	-0.220316000
1	2.822034000	-3.308880000	-1.294507000

8	1.293944000	-2.191051000	-2.145462000
6	1.883642000	-2.278225000	-3.439152000
1	2.357472000	-3.258583000	-3.589259000
1	1.073659000	-2.162088000	-4.162882000
1	2.628452000	-1.489755000	-3.606987000
6	-1.389572000	-1.886479000	1.095806000
6	-2.323283000	-1.938781000	0.014553000
1	-1.815031000	-1.101004000	-1.135370000
1	-1.700610000	-1.404474000	2.019556000
1	-0.746328000	-2.751152000	1.241700000
6	-0.126728000	0.724034000	-1.625803000
6	-1.123643000	-0.128966000	-2.158624000
1	0.895885000	0.478841000	-1.899095000
1	-0.798514000	-0.922704000	-2.826079000
1	-2.099431000	0.296194000	-2.388874000
1	-2.259493000	-2.840124000	-0.598946000
6	-3.707462000	-1.377833000	0.106279000
6	-4.015247000	-0.251342000	0.885772000
1	-3.235500000	0.255245000	1.448806000
6	-4.734327000	-1.999952000	-0.617668000
1	-4.509721000	-2.870483000	-1.229599000
6	-6.044896000	-1.527620000	-0.543172000
6	-5.323826000	0.222983000	0.955724000
6	-6.343041000	-0.414840000	0.243551000
1	-5.549229000	1.090538000	1.569217000
1	-6.830497000	-2.030401000	-1.099344000
1	-7.362269000	-0.044846000	0.301985000
6	-0.365496000	2.153298000	-1.324493000
6	0.725849000	3.039551000	-1.349523000
1	1.716929000	2.655247000	-1.578012000
6	-1.642322000	2.676144000	-1.044608000
1	-2.509133000	2.020499000	-1.009016000
6	-1.818081000	4.038246000	-0.811789000
6	0.548672000	4.403866000	-1.118352000
6	-0.724295000	4.907738000	-0.847433000
1	1.403122000	5.072887000	-1.159679000
1	-2.812327000	4.423761000	-0.605055000
1	-0.865778000	5.969885000	-0.671173000

S20S

E + ZPE = -3089.989333

28	0.394619000	-0.424140000	-0.449955000
15	-1.328613000	0.645778000	0.417210000
6	-1.032381000	1.374755000	2.126274000
1	-1.336916000	0.628501000	2.866074000
6	-1.920104000	2.657859000	2.221761000
1	-2.548491000	2.629558000	3.117954000
1	-1.257143000	3.522959000	2.335003000
6	-2.774196000	2.834994000	0.952592000
1	-3.018516000	3.890187000	0.783474000
1	-3.728659000	2.303546000	1.047126000
6	-1.998968000	2.268917000	-0.252253000
1	-1.101811000	2.881082000	-0.412106000
6	-2.828064000	2.236617000	-1.537094000
1	-3.704153000	1.587895000	-1.434098000
1	-2.252680000	1.902439000	-2.407016000
1	-3.192431000	3.245448000	-1.761933000
6	0.448459000	1.706268000	2.369870000
1	0.835470000	2.411215000	1.627474000
1	1.081681000	0.815359000	2.347318000
1	0.557578000	2.168240000	3.357620000
6	-2.825550000	-0.443128000	0.538172000

6	-3.580493000	-0.470999000	1.721184000
1	-3.285051000	0.126517000	2.575692000
6	-4.733008000	-1.251226000	1.834769000
1	-5.293799000	-1.248995000	2.764673000
6	-5.160037000	-2.014974000	0.753441000
1	-6.060194000	-2.618036000	0.824357000
6	-4.422426000	-1.994237000	-0.430296000
1	-4.762425000	-2.579468000	-1.281150000
6	-3.255533000	-1.231454000	-0.560519000
6	-2.500515000	-1.313367000	-1.875722000
1	-2.086536000	-0.345103000	-2.163052000
1	-3.187438000	-1.627077000	-2.674159000
8	-1.375402000	-2.197385000	-1.839974000
6	-1.723544000	-3.578654000	-1.879814000
1	-2.326813000	-3.804732000	-2.770135000
1	-0.787515000	-4.139036000	-1.937381000
1	-2.276116000	-3.890096000	-0.984183000
6	0.861002000	1.013268000	-1.797289000
1	1.436847000	-0.223236000	-2.184196000
1	2.523238000	-0.305232000	-2.177695000
1	1.413308000	-1.347278000	-1.068734000
1	-0.039904000	1.308069000	-2.329709000
6	0.251820000	-1.734034000	1.002418000
6	1.276193000	-2.236866000	0.143227000
1	-0.711239000	-2.234750000	0.972734000
1	0.956641000	-3.057300000	-0.501045000
1	0.940933000	-0.798038000	-2.963773000
1	0.533457000	-1.363717000	1.984536000
6	2.721100000	-2.323537000	0.523942000
6	3.305271000	-1.509066000	1.506544000
1	2.707382000	-0.771233000	2.033817000
6	3.526895000	-3.263186000	-0.136459000
1	3.089493000	-3.902508000	-0.900179000
6	4.875825000	-3.403285000	0.188955000
6	4.654170000	-1.646376000	1.829888000
6	5.443603000	-2.593987000	1.173269000
1	5.088876000	-1.015414000	2.599752000
1	5.479832000	-4.145318000	-0.324716000
1	6.493332000	-2.700749000	1.429783000
6	1.668202000	2.141542000	-1.277527000
6	2.841006000	1.949428000	-0.523092000
1	3.181177000	0.945426000	-0.281000000
6	1.269205000	3.459217000	-1.563183000
1	0.381972000	3.628927000	-2.168808000
6	2.016920000	4.549172000	-1.118271000
6	3.586075000	3.038696000	-0.077226000
6	3.176783000	4.342602000	-0.370052000
1	4.490521000	2.869672000	0.500109000
1	1.697500000	5.557816000	-1.363762000
1	3.761189000	5.189225000	-0.022376000

41
E + ZPE = -2975.665116

28	-1.058367000	-0.541827000	-0.076569000
15	0.853214000	-0.628534000	0.897363000
6	1.606561000	0.827673000	1.809262000
1	2.225844000	1.377140000	1.093668000
6	2.470833000	0.217128000	2.964865000
1	3.502146000	0.581577000	2.912468000
1	2.065081000	0.577473000	3.916601000
6	2.430508000	-1.326010000	2.945857000
1	2.571343000	-1.737611000	3.951975000

1	3.240093000	-1.730781000	2.326806000
6	1.078878000	-1.776227000	2.365120000
1	0.280483000	-1.476367000	3.058443000
6	0.967657000	-3.278198000	2.105262000
1	1.696840000	-3.614828000	1.360113000
1	-0.035897000	-3.563342000	1.769230000
1	1.166110000	-3.831324000	3.029981000
6	0.548382000	1.796964000	2.357611000
1	-0.136870000	1.295891000	3.049873000
1	-0.037778000	2.263517000	1.563597000
1	1.050196000	2.596085000	2.914872000
6	2.127727000	-1.184344000	-0.323987000
6	3.444098000	-0.701717000	-0.300585000
1	3.747403000	0.026079000	0.443718000
6	4.397490000	-1.149914000	-1.218444000
1	5.411464000	-0.763881000	-1.171308000
6	4.047107000	-2.089868000	-2.183635000
1	4.782238000	-2.445138000	-2.899259000
6	2.736923000	-2.568396000	-2.230889000
1	2.458486000	-3.297079000	-2.988428000
6	1.773454000	-2.129559000	-1.317531000
6	0.364526000	-2.660309000	-1.431210000
1	0.000615000	-3.098805000	-0.501228000
1	0.299700000	-3.424820000	-2.212167000
8	-0.597125000	-1.612823000	-1.746776000
6	-0.525570000	-1.205979000	-3.127374000
1	-0.646969000	-2.086672000	-3.766175000
1	-1.348390000	-0.517281000	-3.309109000
1	0.431705000	-0.720809000	-3.341530000
6	-4.513672000	-0.446756000	0.659114000
1	-4.450686000	0.604298000	0.344270000
6	-5.443134000	-1.203823000	-0.249530000
6	-6.525256000	-1.870545000	0.152053000
1	-6.822775000	-1.901413000	1.198256000
6	-2.054211000	-0.245902000	1.467905000
6	-3.088465000	-1.040929000	0.702408000
1	-3.127434000	-2.081227000	1.039830000
1	-2.766400000	-1.127028000	-0.387072000
1	-5.187605000	-1.194973000	-1.311469000
1	-7.162677000	-2.401950000	-0.548727000
1	-4.907073000	-0.443463000	1.682163000
1	-2.328413000	0.795386000	1.660760000
1	-1.734822000	-0.720628000	2.396802000
6	-0.913069000	1.975794000	-1.720047000
6	-2.106463000	1.423813000	-1.408758000
1	-0.345444000	1.543023000	-2.543246000
1	-2.568885000	0.686921000	-2.058184000
1	-2.745029000	1.846531000	-0.639353000
6	-0.279829000	3.145110000	-1.099973000
6	1.081927000	3.394444000	-1.351979000
1	1.637705000	2.714048000	-1.993587000
6	-0.990268000	4.056680000	-0.295690000
1	-2.053254000	3.914666000	-0.124059000
6	-0.351157000	5.163898000	0.255013000
6	1.722714000	4.500210000	-0.796160000
6	1.007822000	5.386819000	0.011810000
1	2.773967000	4.678037000	-1.003875000
1	-0.916014000	5.863722000	0.863967000
1	1.501003000	6.256433000	0.436164000

42
E + ZPE = -2975.687892

28	0.485035000	-0.362991000	-0.695998000
15	-1.277149000	0.119534000	0.669306000
6	-1.071347000	-0.563753000	2.420815000
1	-2.024686000	-1.051064000	2.658231000
6	-0.923465000	0.694930000	3.304570000
1	-1.143514000	0.450822000	4.350043000
1	0.117331000	1.044228000	3.272106000
6	-1.854717000	1.782868000	2.757103000
1	-1.674206000	2.752129000	3.236012000
1	-2.902000000	1.523235000	2.960164000
6	-1.617923000	1.888884000	1.233940000
1	-0.661820000	2.401341000	1.086020000
6	-2.692067000	2.657215000	0.459564000
1	-3.680018000	2.199083000	0.560422000
1	-2.457920000	2.723803000	-0.608482000
1	-2.756083000	3.680890000	0.844935000
6	0.057194000	-1.583655000	2.594391000
1	1.031342000	-1.159258000	2.327084000
1	-0.105405000	-2.479211000	1.983840000
1	0.110016000	-1.907565000	3.640287000
6	-2.885104000	-0.551608000	0.055578000
6	-4.027348000	-0.502832000	0.872032000
1	-3.960237000	-0.100270000	1.877423000
6	-5.266308000	-0.955775000	0.419000000
1	-6.132589000	-0.899041000	1.071213000
6	-5.383756000	-1.480396000	-0.866593000
1	-6.342014000	-1.839545000	-1.229153000
6	-4.255307000	-1.559041000	-1.681264000
1	-4.341105000	-1.988939000	-2.676147000
6	-3.010051000	-1.097054000	-1.241281000
6	-1.827494000	-1.227593000	-2.171045000
1	-1.459744000	-0.257317000	-2.520091000
1	-2.099422000	-1.816083000	-3.054480000
8	-0.683826000	-1.853855000	-1.542643000
6	-0.930661000	-3.209935000	-1.123048000
1	-1.223898000	-3.809201000	-1.991241000
1	0.003156000	-3.595423000	-0.714211000
1	-1.714648000	-3.249502000	-0.361529000
6	1.756545000	3.700455000	-0.501327000
1	2.842938000	3.532780000	-0.461997000
6	1.452708000	4.878791000	-1.386096000
6	0.800649000	5.976469000	-1.001484000
1	0.446582000	6.104270000	0.019925000
6	1.416719000	1.191737000	-0.112794000
6	1.079644000	2.397216000	-0.994657000
1	-0.003400000	2.571836000	-1.042618000
1	1.393950000	2.215293000	-2.030868000
1	1.796117000	4.799748000	-2.419025000
1	0.608221000	6.797855000	-1.685921000
1	1.436780000	3.915739000	0.526957000
1	2.491014000	0.988161000	-0.138428000
1	1.183887000	1.414483000	0.936698000
6	2.199793000	-1.526130000	-1.225187000
6	1.821603000	-0.645410000	-2.222701000
1	1.717842000	-2.502219000	-1.219615000
1	1.179452000	-0.987568000	-3.029715000
1	2.407052000	0.243425000	-2.431729000
6	3.392423000	-1.463257000	-0.368391000
6	3.491382000	-2.351171000	0.719384000
1	2.683395000	-3.054445000	0.908879000
6	4.464372000	-0.585244000	-0.616300000
1	4.436968000	0.075059000	-1.477789000
6	5.583911000	-0.583078000	0.211182000
6	4.609519000	-2.346499000	1.549157000

6	5.657672000	-1.457938000	1.298959000
1	4.668953000	-3.039976000	2.382767000
1	6.407670000	0.092294000	0.000012000
1	6.535386000	-1.457433000	1.938470000

43

E + ZPE = -2975.662217

28	-0.812219000	-0.594051000	-0.062755000
15	1.050178000	0.060498000	0.866142000
6	1.263542000	1.849954000	1.379472000
1	1.455247000	2.453817000	0.488353000
6	2.475711000	1.870939000	2.364863000
1	3.345022000	2.348133000	1.902562000
1	2.207687000	2.492578000	3.225438000
6	2.837267000	0.437669000	2.830005000
1	3.091535000	0.416424000	3.895541000
1	3.719419000	0.073028000	2.290984000
6	1.659203000	-0.516451000	2.2591633000
1	0.828347000	-0.250698000	3.219546000
6	2.008468000	-1.986035000	2.780071000
1	2.821212000	-2.316115000	2.124294000
1	1.147701000	-2.648685000	2.638278000
1	2.350944000	-2.120796000	3.812243000
6	-0.008677000	2.396189000	2.050906000
1	-0.275971000	1.825159000	2.946919000
1	-0.864514000	2.404063000	1.374156000
1	0.174817000	3.428397000	2.368473000
6	2.413013000	-0.325132000	-0.325304000
6	3.331983000	0.659906000	-0.717097000
1	3.266353000	1.663969000	-0.314389000
6	4.360422000	0.373515000	-1.617907000
1	5.063240000	1.153133000	-1.896394000
6	4.484412000	-0.908300000	-2.146186000
1	5.284521000	-1.142084000	-2.841929000
6	3.567537000	-1.893907000	-1.777665000
1	3.662173000	-2.895445000	-2.190124000
6	2.527343000	-1.623413000	-0.882702000
6	1.529272000	-2.715797000	-0.566503000
1	1.319861000	-2.782732000	-0.500015000
1	1.915860000	-3.689357000	-0.890614000
8	0.244873000	-2.487943000	-1.179252000
6	0.186403000	-2.944714000	-2.535653000
1	0.515533000	-3.988967000	-2.595481000
1	-0.856031000	-2.892801000	-2.852686000
1	0.807533000	-2.328754000	-3.197367000
6	-3.973315000	-1.596160000	0.858095000
1	-4.200730000	-0.607556000	0.432181000
6	-4.637917000	-2.676068000	0.048985000
6	-5.491268000	-3.575411000	0.538507000
1	-5.780050000	-3.579147000	1.587590000
6	-1.695743000	-0.630125000	1.595650000
6	-2.438971000	-1.755229000	0.934178000
1	-2.166357000	-2.724491000	1.362332000
1	-2.096950000	-1.847845000	-0.151717000
1	-4.381875000	-2.707021000	-1.012173000
1	-5.943185000	-4.336505000	-0.090935000
1	-4.367268000	-1.594971000	1.880856000
1	-2.266292000	0.290300000	1.753747000
1	-1.161424000	-0.914001000	2.501018000
6	-0.926068000	0.929061000	-1.697818000
6	-1.775499000	-0.132372000	-1.912280000
1	0.075515000	0.861976000	-2.123055000

1	-1.474966000	-0.938241000	-2.570376000
1	-2.846754000	-0.024533000	-1.762816000
6	-1.327325000	2.292826000	-1.300803000
6	-0.424787000	3.347742000	-1.519907000
1	0.548664000	3.133472000	-1.955911000
6	-2.592731000	2.598925000	-0.766377000
1	-3.318663000	1.809166000	-0.592672000
6	-2.936607000	3.912645000	-0.459871000
6	-0.770240000	4.664604000	-1.217342000
6	-2.026756000	4.951109000	-0.682547000
1	-0.061942000	5.465947000	-1.406857000
1	-3.919363000	4.129657000	-0.051386000
1	-2.300424000	5.975218000	-0.447037000

44

E + ZPE = -2975.672191

28	-0.454082000	-0.366220000	0.246160000
15	1.406733000	0.676726000	0.612595000
6	1.277343000	2.545175000	0.529672000
1	1.231121000	2.868682000	-0.515253000
6	2.545949000	3.102840000	1.241722000
1	3.249228000	3.517560000	0.513653000
1	2.243891000	3.935462000	1.885568000
6	3.233564000	1.991728000	2.073861000
1	3.562095000	2.366901000	3.049194000
1	4.133633000	1.637921000	1.557369000
6	2.284123000	0.789626000	2.271668000
1	1.475924000	1.070329000	2.960178000
6	3.017079000	-0.421554000	2.848960000
1	3.802019000	-0.778939000	2.173915000
1	2.346476000	-1.252971000	3.083907000
1	3.504651000	-0.129310000	3.785861000
6	-0.006617000	3.013787000	1.241999000
1	-0.002445000	2.741122000	2.302838000
1	-0.913408000	2.599458000	0.794544000
1	-0.070969000	4.106335000	1.189371000
6	2.668564000	0.125424000	-0.621490000
6	3.295584000	1.067608000	-1.451255000
1	3.063423000	2.122302000	-1.357133000
6	4.238229000	0.681163000	-2.406542000
1	4.711363000	1.433295000	-3.030699000
6	4.569936000	-0.662803000	-2.545385000
1	5.306594000	-0.975547000	-3.279213000
6	3.947398000	-1.610989000	-1.731759000
1	4.212118000	-2.660238000	-1.836638000
6	2.991760000	-1.248888000	-0.776027000
6	2.336338000	-2.353293000	0.038560000
1	2.235584000	-2.068928000	1.085002000
1	2.962095000	-3.255478000	0.000819000
8	1.006673000	-2.676249000	-0.379863000
6	0.952495000	-3.487755000	-1.549927000
1	1.500823000	-4.427138000	-1.395972000
1	-0.100177000	-3.716859000	-1.728029000
1	1.364666000	-2.973149000	-2.427660000
6	-3.088989000	-1.695728000	2.053373000
1	-3.451109000	-0.660965000	2.063204000
6	-4.097529000	-2.603813000	1.402982000
6	-5.304819000	-2.229834000	0.977439000
1	-5.648719000	-1.201799000	1.065761000
6	-0.610800000	-0.950730000	2.032732000
6	-1.693764000	-1.764410000	1.398502000
1	-1.371498000	-2.798807000	1.248182000

1	-1.862068000	-1.405184000	0.312929000
1	-3.802210000	-3.650690000	1.313456000
1	-6.002848000	-2.942282000	0.546726000
1	-2.956020000	-1.995725000	3.102250000
1	-0.951711000	-0.178358000	2.728108000
1	0.213814000	-1.525452000	2.450930000
6	-1.164697000	0.735115000	-1.478116000
6	-0.664365000	-0.501547000	-1.821652000
1	-0.483897000	1.580821000	-1.554131000
1	0.349829000	-0.586520000	-2.195512000
1	-1.321535000	-1.335495000	-2.053194000
6	-2.581894000	1.124561000	-1.353415000
6	-3.643691000	0.202458000	-1.415623000
1	-3.446478000	-0.860517000	-1.519113000
6	-2.892240000	2.492389000	-1.234008000
1	-2.086822000	3.222075000	-1.210197000
6	-4.214201000	2.928202000	-1.182352000
6	-4.964251000	0.638738000	-1.365322000
6	-5.255399000	2.001219000	-1.247153000
1	-5.769774000	-0.086569000	-1.427395000
1	-4.430634000	3.989202000	-1.101115000
1	-6.287731000	2.336576000	-1.213674000

45

E + ZPE = -2975.671214

28	-0.304539000	0.821381000	-0.432077000
15	1.013502000	-0.432267000	0.758189000
6	1.719148000	0.195604000	2.395111000
1	2.737638000	-0.206448000	2.436042000
6	0.880590000	-0.529579000	3.468125000
1	1.382788000	-0.480322000	4.441206000
1	-0.090703000	-0.031591000	3.587685000
6	0.675662000	-1.977302000	3.002640000
1	-0.049667000	-2.508854000	3.629073000
1	1.621459000	-2.530403000	3.079247000
6	0.202667000	-1.955605000	1.531402000
1	-0.864498000	-1.703851000	1.513980000
6	0.400416000	-3.275005000	0.782195000
1	1.447010000	-3.593438000	0.851290000
1	0.076428000	-3.205797000	-0.261373000
1	-0.190861000	-4.063817000	1.260701000
6	1.815466000	1.710899000	2.567571000
1	0.828760000	2.179614000	2.599989000
1	2.390701000	2.179589000	1.761386000
1	2.321996000	1.946122000	3.510641000
6	2.511721000	-0.991058000	-0.181702000
6	3.500675000	-1.735175000	0.486859000
1	3.368529000	-1.997507000	1.531445000
6	4.659894000	-2.165512000	-0.156201000
1	5.397203000	-2.744977000	0.391189000
6	4.866331000	-1.841179000	-1.495051000
1	5.770752000	-2.155905000	-2.006597000
6	3.901987000	-1.100374000	-2.174128000
1	4.064003000	-0.844796000	-3.218421000
6	2.720756000	-0.683790000	-1.546012000
6	1.703294000	0.017461000	-2.420588000
1	0.867585000	-0.643686000	-2.664116000
1	2.169325000	0.321178000	-3.364371000
8	1.086022000	1.185622000	-1.838408000
6	1.995625000	2.288235000	-1.642157000
1	2.497240000	2.509049000	-2.589613000
1	1.395871000	3.146057000	-1.336200000

1	2.737731000	2.048915000	-0.874407000
6	-1.315083000	3.752630000	1.130911000
1	-0.357797000	3.608388000	1.642648000
6	-1.266253000	5.018819000	0.318790000
6	-0.189021000	5.795137000	0.185482000
1	0.745084000	5.570988000	0.698082000
6	-1.543498000	1.157096000	0.936208000
6	-1.648472000	2.516411000	0.275097000
1	-0.943865000	2.552446000	-0.617582000
1	-2.624393000	2.649271000	-0.205342000
1	-1.171075000	1.198978000	1.961649000
1	-2.449305000	0.549799000	0.894062000
6	-1.918019000	-0.715105000	-1.832479000
6	-1.801410000	0.579123000	-2.234765000
1	-1.159724000	-1.424541000	-2.164011000
1	-2.603969000	1.292068000	-2.076209000
1	-1.057907000	0.864009000	-2.970687000
6	-3.036097000	-1.333165000	-1.110257000
6	-2.995445000	-2.717255000	-0.860090000
1	-2.135441000	-3.292973000	-1.192979000
6	-4.177793000	-0.616726000	-0.700047000
1	-4.257709000	0.446556000	-0.906079000
6	-5.227057000	-1.261172000	-0.051646000
6	-4.047234000	-3.363678000	-0.214192000
6	-5.165294000	-2.636030000	0.196313000
1	-3.997889000	-4.434379000	-0.038959000
1	-6.101416000	-0.693073000	0.252228000
1	-5.988970000	-3.136428000	0.696804000
1	-2.084837000	3.832217000	1.911231000
1	-0.206382000	6.700087000	-0.415036000
1	-2.188680000	5.295580000	-0.194183000

46
E + ZPE = -2975.683701

28	0.417662000	-0.032107000	-0.897884000
15	-1.201449000	-0.554966000	0.605908000
6	-1.363480000	-2.287121000	1.353414000
1	-2.440116000	-2.483127000	1.363729000
6	-0.886813000	-2.128827000	2.815981000
1	-1.285747000	-2.942761000	3.432312000
1	0.207277000	-2.207634000	2.858866000
6	-1.330390000	-0.752555000	3.328120000
1	-0.870282000	-0.510229000	4.293050000
1	-2.416847000	-0.737678000	3.485882000
6	-0.941627000	0.302621000	2.269820000
1	0.143829000	0.454576000	2.317980000
6	-1.628559000	1.659644000	2.431647000
1	-2.717040000	1.577923000	2.353863000
1	-1.285018000	2.381445000	1.682598000
1	-1.393024000	2.075297000	3.417740000
6	-0.701712000	-3.437645000	0.592150000
1	0.387433000	-3.362479000	0.604609000
1	-1.033974000	-3.485668000	-0.450945000
1	-0.970890000	-4.389541000	1.063971000
6	-2.925387000	-0.134483000	0.057522000
6	-4.027901000	-0.564672000	0.817933000
1	-3.875549000	-1.131914000	1.729340000
6	-5.339514000	-0.272622000	0.445337000
1	-6.163377000	-0.617299000	1.062963000
6	-5.583011000	0.452862000	-0.717953000
1	-6.599225000	0.675520000	-1.028394000
6	-4.505644000	0.889850000	-1.485239000

1	-4.691966000	1.458746000	-2.392848000
6	-3.183475000	0.623495000	-1.108039000
6	-2.096464000	1.244288000	-1.954570000
1	-1.615007000	2.076759000	-1.432865000
1	-2.521798000	1.638345000	-2.884155000
8	-1.011110000	0.360358000	-2.305830000
6	-1.395179000	-0.729495000	-3.166073000
1	-1.883448000	-0.330024000	-4.060776000
1	-0.476898000	-1.244801000	-3.451331000
1	-2.071208000	-1.418413000	-2.650111000
6	1.780781000	-0.772549000	0.214253000
6	2.429549000	-1.942779000	-0.536670000
1	1.669751000	-2.621274000	-0.950883000
1	3.012417000	-1.593337000	-1.394468000
1	1.381633000	-1.141160000	1.166158000
1	2.518413000	-0.005486000	0.468114000
6	1.379630000	1.784823000	-1.443877000
6	1.804848000	0.723187000	-2.225286000
1	2.799243000	0.312106000	-2.101128000
1	0.491512000	2.318977000	-1.780664000
1	1.344539000	0.554150000	-3.194907000
6	2.140319000	2.515809000	-0.421282000
6	1.475896000	3.495999000	0.339833000
1	0.420653000	3.688191000	0.157031000
6	3.515645000	2.313710000	-0.198255000
1	4.064544000	1.598055000	-0.802506000
6	4.192279000	3.052650000	0.767958000
6	2.151615000	4.232994000	1.308792000
6	3.512522000	4.008982000	1.528461000
1	1.622706000	4.987503000	1.883536000
1	5.255574000	2.893087000	0.920372000
1	4.045650000	4.587456000	2.277131000
6	3.375876000	-2.771004000	0.370994000
1	4.143970000	-2.108854000	0.789827000
1	2.798313000	-3.160238000	1.223218000
6	4.025763000	-3.909177000	-0.367692000
1	3.350082000	-4.672851000	-0.757217000
6	5.336226000	-4.031462000	-0.581404000
1	6.048038000	-3.296983000	-0.209529000
1	5.751172000	-4.874877000	-1.126049000

47
E + ZPE = -2975.667073

28	-0.248244000	0.297051000	-0.979995000
15	1.432817000	-0.884878000	0.254709000
6	1.047604000	-1.808254000	1.859869000
1	1.900580000	-1.646368000	2.525561000
6	1.062846000	-3.296223000	1.451785000
1	1.163860000	-3.927679000	2.341745000
1	0.107383000	-3.561183000	0.980025000
6	2.212186000	-3.500297000	0.466067000
1	2.212121000	-4.506482000	0.030965000
1	3.174377000	-3.373483000	0.980668000
6	2.083052000	-2.438478000	-0.646671000
1	1.254468000	-2.736825000	-1.304375000
6	3.352720000	-2.297368000	-1.490103000
1	4.185561000	-1.894999000	-0.905378000
1	3.211858000	-1.662550000	-2.370498000
1	3.650775000	-3.286119000	-1.857311000
6	-0.222984000	-1.386494000	2.600325000
1	-1.118626000	-1.576383000	2.000724000
1	-0.207818000	-0.328607000	2.879120000

1	-0.314782000	-1.969482000	3.523892000
6	2.892869000	0.213094000	0.562600000
6	3.628963000	0.192890000	1.754859000
1	3.376897000	-0.499337000	2.549588000
6	4.710573000	1.053436000	1.959820000
1	5.261378000	1.008214000	2.894592000
6	5.079427000	1.956848000	0.968344000
1	5.920512000	2.627042000	1.116990000
6	4.355153000	1.994991000	-0.223906000
1	4.642578000	2.696452000	-1.003404000
6	3.267735000	1.143713000	-0.441610000
6	2.530554000	1.243170000	-1.757337000
1	2.409145000	0.269572000	-2.238008000
1	3.078898000	1.883198000	-2.457243000
8	1.184139000	1.761039000	-1.630054000
6	1.137667000	3.186235000	-1.445422000
1	1.683022000	3.679901000	-2.257546000
1	0.089194000	3.477384000	-1.485856000
1	1.571021000	3.471575000	-0.480983000
6	-1.174031000	1.161535000	0.444352000
6	-2.168084000	2.267818000	0.157741000
1	-1.768622000	3.008009000	-0.546290000
1	-3.083762000	1.866706000	-0.284498000
1	-0.310065000	1.551255000	1.003463000
1	-1.643048000	0.354313000	1.011053000
6	-1.656900000	-0.871471000	-1.760339000
6	-1.612944000	0.399563000	-2.376783000
1	-2.426392000	1.105307000	-2.256240000
1	-1.010936000	-1.644884000	-2.192794000
1	-1.055606000	0.520734000	-3.307169000
6	-2.779285000	-1.449299000	-0.993298000
6	-2.631907000	-2.733331000	-0.437189000
1	-1.702387000	-3.276530000	-0.593721000
6	-4.009606000	-0.791154000	-0.823049000
1	-4.179743000	0.173668000	-1.289651000
6	-5.040691000	-1.384550000	-0.097246000
6	-3.662166000	-3.329204000	0.286333000
6	-4.870004000	-2.651212000	0.466054000
1	-3.528207000	-4.324764000	0.699545000
1	-5.986786000	-0.862846000	0.014150000
1	-5.678531000	-3.114080000	1.023955000
6	-2.558588000	3.003437000	1.471274000
1	-2.962344000	2.278651000	2.188678000
1	-1.649733000	3.428087000	1.922012000
6	-3.565745000	4.093772000	1.222434000
1	-3.233568000	4.913438000	0.583297000
6	-4.804819000	4.110947000	1.714267000
1	-5.176818000	3.316374000	2.358179000
1	-5.491965000	4.925454000	1.503399000

48
E + ZPE = -2975.667438

28	-0.313569000	0.397615000	-0.868054000
15	1.476860000	-0.755532000	0.271320000
6	1.249376000	-1.611303000	1.944591000
1	2.028918000	-1.216260000	2.602748000
6	1.525718000	-3.113219000	1.675438000
1	1.874259000	-3.603336000	2.591357000
1	0.584207000	-3.603475000	1.393726000
6	2.532039000	-3.246642000	0.528635000
1	2.617696000	-4.282561000	0.179336000
1	3.534033000	-2.937635000	0.854498000

6	2.053037000	-2.328685000	-0.612010000
1	1.129954000	-2.757956000	-1.027418000
6	3.059498000	-2.140339000	-1.748679000
1	3.980407000	-1.664459000	-1.397573000
1	2.653689000	-1.535836000	-2.568546000
1	3.326966000	-3.115474000	-2.170818000
6	-0.104226000	-1.365926000	2.618434000
1	-0.934161000	-1.711965000	1.993386000
1	-0.262740000	-0.308522000	2.850644000
1	-0.147362000	-1.921019000	3.562598000
6	3.001830000	0.289522000	0.404660000
6	3.985138000	0.063857000	1.379460000
1	3.870710000	-0.737483000	-2.100845000
6	5.140024000	0.846361000	1.447764000
1	5.882220000	0.642687000	2.213859000
6	5.335387000	1.877322000	0.533585000
1	6.228948000	2.492379000	0.577819000
6	4.369718000	2.115363000	-0.444560000
1	4.522159000	2.917927000	-1.162027000
6	3.208878000	1.339083000	-0.526121000
6	2.220946000	1.652582000	-1.627665000
1	2.002976000	0.775610000	-2.247939000
1	2.625670000	2.421701000	-2.295242000
8	0.932836000	2.100766000	-1.150255000
6	0.969997000	3.391762000	-0.519728000
1	1.386094000	4.127323000	-1.217005000
1	-0.058714000	3.658701000	-0.283973000
1	1.571668000	3.365955000	0.394508000
6	-1.441991000	1.128247000	0.479441000
6	-2.487154000	2.173008000	0.151404000
1	-2.087861000	2.954887000	-0.507433000
1	-3.337287000	1.725270000	-0.370467000
1	-0.657129000	1.545811000	1.127296000
1	-1.890351000	0.253866000	0.959136000
6	-1.523838000	-0.914349000	-1.749794000
6	-1.601156000	0.373493000	-2.329347000
1	-2.496464000	0.976923000	-2.240132000
1	-0.786294000	-1.600353000	-2.179199000
1	-1.013857000	0.589587000	-3.224520000
6	-2.605579000	-1.627198000	-1.036437000
6	-2.339267000	-2.891807000	-0.480234000
1	-1.347917000	-3.325802000	-0.593604000
6	-3.907198000	-1.110974000	-0.915508000
1	-4.161735000	-0.163686000	-1.379800000
6	-4.897443000	-1.824023000	-0.242289000
6	-3.328051000	-3.606262000	0.192341000
6	-4.611624000	-3.070370000	0.319326000
1	-3.101764000	-4.584440000	0.606864000
1	-5.899734000	-1.411803000	-0.170234000
1	-5.387275000	-3.627119000	0.836620000
6	-3.024217000	2.841787000	1.448235000
1	-3.430025000	2.070848000	2.114473000
1	-2.182913000	3.311146000	1.979508000
6	-4.081764000	3.870342000	1.149849000
1	-3.760037000	4.727167000	0.555704000
6	-5.351749000	3.792149000	1.547712000
1	-5.715438000	2.957331000	2.143634000
1	-6.075157000	4.565029000	1.304094000

49
E + ZPE = -2975.663274

28	-0.279007000	0.305759000	-0.677839000
----	--------------	-------------	--------------

15	1.349589000	-0.808401000	0.317014000
6	1.245636000	-1.803262000	1.929085000
1	1.977934000	-1.362446000	2.609792000
6	1.692082000	-3.244462000	1.554141000
1	2.206870000	-3.710268000	2.401293000
1	0.796022000	-3.848029000	1.359034000
6	2.558421000	-3.216444000	0.292738000
1	2.700014000	-4.220722000	-0.123770000
1	3.557134000	-2.815092000	0.507454000
6	1.839892000	-2.312041000	-0.723110000
1	0.881767000	-2.788590000	-0.974064000
6	2.619293000	-2.059524000	-2.014350000
1	3.539606000	-1.495166000	-1.832797000
1	2.024097000	-1.523436000	-2.761975000
1	2.902546000	-3.018490000	-2.462276000
6	-0.106876000	-1.797971000	2.650611000
1	-0.932218000	-2.076106000	1.986658000
1	-0.331394000	-0.828871000	3.102112000
1	-0.073761000	-2.534674000	3.461684000
6	2.899581000	0.207485000	0.400880000
6	3.866967000	-0.009796000	1.394336000
1	3.717519000	-0.766392000	2.154978000
6	5.056510000	0.720779000	1.432301000
1	5.782722000	0.521823000	2.214654000
6	5.305020000	1.691075000	0.467461000
1	6.226290000	2.265219000	0.484944000
6	4.354584000	1.922053000	-0.527003000
1	4.546716000	2.679560000	-1.282721000
6	3.156707000	1.201389000	-0.579935000
6	2.187159000	1.530812000	-1.696479000
1	1.898682000	0.642544000	-2.266447000
1	2.657094000	2.225978000	-2.402819000
8	0.947879000	2.100176000	-1.243210000
6	1.097778000	3.417471000	-0.695083000
1	1.561146000	4.076446000	-1.439071000
1	0.097868000	3.783603000	-0.465364000
1	1.707361000	3.405795000	0.214830000
6	-0.927938000	1.014527000	0.958231000
6	-2.012992000	1.953204000	0.461477000
1	-1.651142000	2.609335000	-0.340794000
1	-2.853765000	1.383261000	0.055554000
1	-0.137381000	1.543127000	1.503149000
1	-1.345977000	0.229188000	1.587140000
6	-1.554970000	-0.953898000	-1.757708000
6	-1.365792000	0.246949000	-2.430095000
1	-2.130393000	1.017795000	-2.458055000
1	-0.878853000	-1.771894000	-2.012392000
1	-0.618401000	0.315039000	-3.219010000
6	-2.784486000	-1.403556000	-1.068832000
6	-2.758746000	-2.601991000	-0.333340000
1	-1.835917000	-3.176495000	-0.282447000
6	-3.999990000	-0.703095000	-1.156674000
1	-4.066604000	0.196635000	-1.761015000
6	-5.141285000	-1.174645000	-0.510465000
6	-3.899106000	-3.074848000	0.312277000
6	-5.094798000	-2.357666000	0.230598000
1	-3.858558000	-4.006529000	0.869185000
1	-6.073445000	-0.624394000	-0.599423000
1	-5.987702000	-2.726430000	0.726524000
6	-2.553549000	2.853989000	1.612550000
1	-2.934677000	2.218552000	2.420452000
1	-1.715868000	3.432604000	2.027511000
6	-3.635183000	3.783053000	1.133411000
1	-3.335270000	4.521125000	0.387514000

6	-4.901847000	3.753634000	1.548810000
1	-5.244427000	3.037377000	2.292938000
1	-5.642750000	4.453049000	1.172006000

50

E + ZPE = -2975.674495

28	-0.413856000	-0.306619000	0.196617000
15	1.366744000	0.886088000	-0.148272000
6	1.307442000	2.013830000	-1.645822000
1	1.653668000	1.445828000	-2.514302000
6	2.255798000	3.216820000	-1.331450000
1	3.072879000	3.269060000	-2.057880000
1	1.684542000	4.144321000	-1.446218000
6	2.813909000	3.122191000	0.106323000
1	2.970317000	4.117155000	0.538202000
1	3.790045000	2.623386000	0.107738000
6	1.844433000	2.309004000	0.987029000
1	0.915667000	2.884324000	1.112309000
6	2.419039000	1.982735000	2.366047000
1	3.312160000	1.353778000	2.289237000
1	1.695131000	1.484330000	3.018659000
1	2.714967000	2.910869000	2.867619000
6	-0.122820000	2.499545000	-1.935059000
1	-0.525065000	3.076098000	-1.094098000
1	-0.813187000	1.678464000	-2.146898000
1	-0.111389000	3.163656000	-2.806411000
6	2.897946000	-0.141297000	-0.306296000
6	3.807060000	0.110728000	-1.345889000
1	3.618423000	0.901254000	-2.062658000
6	4.979383000	-0.634749000	-1.487247000
1	5.662765000	-0.411770000	-2.301120000
6	5.265731000	-1.651247000	-0.582025000
1	6.176390000	-2.234889000	-0.676891000
6	4.368995000	-1.916461000	0.453373000
1	4.593151000	-2.708472000	1.163645000
6	3.185012000	-1.186796000	0.608410000
6	2.253702000	-1.572534000	1.742723000
1	1.893380000	-0.694886000	2.281971000
1	2.793646000	-2.200289000	2.464401000
8	1.072694000	-2.255094000	1.308956000
6	1.304417000	-3.613501000	0.940995000
1	1.764299000	-4.165951000	1.771528000
1	0.329745000	-4.054334000	0.723335000
1	1.948912000	-3.694773000	0.056513000
6	-1.627936000	0.919681000	1.438826000
6	-1.024915000	-0.087668000	2.163119000
1	-1.566947000	-0.982301000	2.457588000
1	-1.727793000	-1.439318000	-0.045939000
1	-1.117784000	1.879665000	1.385104000
6	-0.107101000	-1.149831000	-1.479664000
6	-1.330160000	-1.887741000	-1.035649000
1	-0.240523000	-0.541120000	-2.376031000
1	0.805827000	-1.741260000	-1.532644000
1	-1.092588000	-2.910550000	-0.729116000
1	-0.129419000	0.116329000	2.739912000
6	-3.035688000	0.966668000	0.996228000
6	-4.011404000	0.086562000	1.499593000
1	-3.736562000	-0.676493000	2.221513000
6	-3.438814000	1.974026000	0.099916000
1	-2.701651000	2.676654000	-0.279452000
6	-4.770791000	2.095909000	-0.288628000
6	-5.344004000	0.214953000	1.118512000

6	-5.728303000	1.216833000	0.222378000
1	-6.087776000	-0.459953000	1.531348000
1	-5.064246000	2.884069000	-0.975731000
1	-6.770824000	1.320266000	-0.064099000
6	-2.530891000	-1.863256000	-2.004241000
1	-2.154210000	-2.208864000	-2.977185000
1	-2.876835000	-0.832360000	-2.144732000
6	-3.667628000	-2.748519000	-1.571589000
1	-3.411951000	-3.796312000	-1.404150000
6	-4.931429000	-2.353787000	-1.418316000
1	-5.233772000	-1.323075000	-1.586572000
1	-5.714037000	-3.050351000	-1.130917000

51R

E + ZPE = -2780.505922

28	-1.075713000	-0.151504000	0.147004000
15	1.031581000	-0.678798000	-0.007654000
6	1.753071000	-1.695202000	1.410721000
1	2.682366000	-1.186733000	1.692651000
6	2.111194000	-3.056024000	0.768609000
1	2.864561000	-3.573069000	1.373512000
1	1.222548000	-3.700612000	0.753954000
6	2.594829000	-2.812308000	-0.668281000
1	2.685120000	-3.749233000	-1.229866000
1	3.592451000	-2.354094000	-0.663224000
6	1.581020000	-1.870897000	-1.354382000
1	0.675426000	-2.454174000	-1.560709000
6	2.050031000	-1.231217000	-2.662657000
1	2.943079000	-0.615549000	-2.519231000
1	1.272162000	-0.599682000	-3.106712000
1	2.295289000	-2.012558000	-3.390432000
6	0.864266000	-1.797893000	2.653507000
1	-0.101856000	-2.258233000	2.421979000
1	0.677285000	-0.815983000	3.102523000
1	1.353071000	-2.416944000	3.414475000
6	2.098644000	0.827010000	-0.110598000
6	3.496467000	0.705175000	-0.034465000
1	3.950569000	-0.274022000	0.077093000
6	4.332485000	1.819069000	-0.104432000
1	5.409275000	1.690027000	-0.050588000
6	3.778866000	3.090672000	-0.236517000
1	4.417379000	3.967561000	-0.282311000
6	2.393751000	3.232390000	-0.297355000
1	1.962194000	4.225945000	-0.389349000
6	1.543706000	2.120859000	-0.247337000
6	0.058375000	2.373999000	-0.377129000
1	-0.342943000	2.002437000	-1.324568000
1	-0.146503000	3.448715000	-0.329716000
8	-0.753504000	1.728035000	0.633677000
6	-0.537842000	2.208510000	1.973709000
1	-0.658729000	3.296184000	1.988514000
1	-1.302481000	1.745337000	2.597207000
1	0.460761000	1.938289000	2.330518000
1	-2.322034000	-2.817339000	1.256591000
6	-1.973549000	-2.996804000	0.234642000
6	-1.861177000	-1.726731000	-0.592391000
1	-2.687102000	-3.687440000	-0.233988000
1	-1.013913000	-3.519961000	0.299924000
1	-1.536313000	-1.939478000	-1.615039000
6	-2.908441000	-0.708784000	-0.535564000
6	-3.178137000	-0.160210000	0.752611000
6	-3.406512000	-0.015651000	-1.676743000

1	-2.970198000	-0.746076000	1.646499000
1	-3.185193000	-0.407847000	-2.665913000
6	-4.007106000	0.976739000	0.880676000
6	-4.199288000	1.106534000	-1.528938000
1	-4.265055000	1.342882000	1.870275000
1	-4.602972000	1.601128000	-2.407811000
6	-4.503052000	1.609092000	-0.244594000
1	-5.143584000	2.480360000	-0.145517000

51S

E + ZPE = -2780.505789

28	1.029671000	-0.113681000	-0.411349000
15	-0.930824000	0.719039000	0.056404000
6	-1.039637000	1.580253000	1.734940000
1	-1.959569000	1.205569000	2.197907000
6	-1.241217000	3.070064000	1.380621000
1	-1.650314000	3.613399000	2.239865000
1	-0.269851000	3.528159000	1.148684000
6	-2.158988000	3.152166000	0.153610000
1	-2.215945000	4.170993000	-0.246360000
1	-3.182888000	2.863270000	0.425025000
6	-1.598707000	2.187800000	-0.914424000
1	-0.696610000	2.651812000	-1.328912000
6	-2.546667000	1.857466000	-2.068982000
1	-3.460596000	1.368444000	-1.718898000
1	-2.075401000	1.201193000	-2.809451000
1	-2.836588000	2.779951000	-2.584182000
6	0.125011000	1.305074000	2.688481000
1	1.082525000	1.618135000	2.260141000
1	0.199863000	0.242286000	2.944025000
1	-0.018994000	1.857433000	3.624201000
6	-2.247922000	-0.576018000	0.096954000
6	-3.513827000	-0.281961000	0.630736000
1	-3.724974000	0.710508000	1.015685000
6	-4.528394000	-1.238081000	0.672974000
1	-5.498902000	-0.977025000	1.084070000
6	-4.287707000	-2.523248000	0.192100000
1	-5.065807000	-3.279532000	0.228213000
6	-3.033970000	-2.836422000	-0.330374000
1	-2.844388000	-3.840998000	-0.700195000
6	-2.013844000	-1.880041000	-0.396638000
6	-0.709099000	-2.289725000	-1.040391000
1	-0.539413000	-1.770649000	-1.988683000
1	-0.708253000	-3.365346000	-1.245808000
8	0.470058000	-1.992803000	-0.252999000
6	0.584625000	-2.747134000	0.970092000
1	0.498283000	-3.814169000	0.741740000
1	1.575611000	-2.535826000	1.371859000
1	-0.192150000	-2.453491000	1.682816000
1	2.117271000	1.044030000	-3.002887000
6	1.847613000	1.877699000	-2.347998000
6	1.913360000	1.523364000	-0.868503000
1	0.851405000	2.217784000	-2.648073000
1	2.547596000	2.695953000	-2.562088000
1	1.744066000	2.393021000	-0.229043000
6	2.948004000	0.630976000	-0.367443000
6	3.026785000	-0.649878000	-0.992430000
6	3.633220000	0.818487000	0.869813000
1	2.719087000	-0.777166000	-2.029170000
1	3.571726000	1.786196000	1.360140000
6	3.832602000	-1.666808000	-0.422254000
6	4.403791000	-0.190397000	1.408265000

1	3.937162000	-2.615336000	-0.940934000
1	4.951953000	-0.016460000	2.329869000
6	4.502565000	-1.446842000	0.764686000
1	5.129637000	-2.223005000	1.193122000

52

E + ZPE = -2975.668509

28	-0.960822000	-0.997322000	-0.117050000
15	0.775045000	-0.185209000	0.992785000
6	0.348189000	1.294857000	2.065082000
1	0.397685000	2.197536000	1.451218000
6	1.393344000	1.321092000	3.226349000
1	1.991196000	2.237247000	3.190669000
1	0.849688000	1.345769000	4.176959000
6	2.305774000	0.076475000	3.175997000
1	2.601873000	-0.241969000	4.181951000
1	3.231144000	0.301118000	2.633396000
6	1.574319000	-1.073677000	2.455538000
1	0.728913000	-1.392971000	3.078976000
6	2.483473000	-2.275746000	2.197312000
1	3.313080000	-2.017809000	1.531174000
1	1.950620000	-3.132214000	1.772942000
1	2.918436000	-2.608991000	3.146323000
6	-1.087888000	1.175983000	2.608646000
1	-1.226627000	0.260235000	3.195593000
1	-1.834532000	1.199493000	1.810652000
1	-1.290811000	2.021226000	3.275677000
6	2.223933000	0.268912000	-0.065255000
6	2.819849000	1.532875000	0.067291000
1	2.420748000	2.253893000	0.771474000
6	3.937565000	1.893516000	-0.688094000
1	4.378196000	2.877984000	-0.561434000
6	4.487651000	0.983476000	-1.586004000
1	5.365261000	1.245987000	-2.169041000
6	3.906603000	-0.276964000	-1.725602000
1	4.347627000	-0.993680000	-2.413903000
6	2.773441000	-0.652602000	-0.992963000
6	2.175047000	-2.024638000	-1.255489000
1	1.734912000	-2.447721000	-0.351313000
1	2.963728000	-2.713779000	-1.589557000
8	1.111194000	-2.014193000	-2.209685000
6	1.542975000	-1.942433000	-3.565106000
1	2.224976000	-2.770630000	-3.803892000
1	0.648839000	-2.031410000	-4.186440000
1	2.041779000	-0.990700000	-3.789195000
6	-3.582970000	-2.310372000	0.817470000
1	-3.581628000	-1.511014000	1.568373000
6	-4.516634000	-1.967793000	-0.314907000
6	-5.322172000	-0.904473000	-0.340133000
1	-5.349300000	-0.187175000	0.478277000
6	-1.090512000	-2.513396000	1.269488000
6	-2.160630000	-2.658815000	0.412886000
1	-2.061286000	-3.365238000	-0.413171000
1	-2.081436000	-1.336968000	-1.292066000
1	-4.546504000	-2.680325000	-1.141118000
1	-6.007867000	-0.727157000	-1.163725000
1	-3.970547000	-3.208295000	1.327538000
1	-1.253455000	-2.111705000	2.266602000
1	-0.207704000	-3.135525000	1.152435000
6	-0.791593000	0.471035000	-1.382568000
6	-1.720017000	-0.498572000	-2.018319000
1	0.201070000	0.462337000	-1.824686000

1	-1.266951000	-1.065300000	-2.830718000
1	-2.685546000	-0.077035000	-2.299429000
6	-1.275936000	1.833774000	-1.060396000
6	-2.598496000	2.091019000	-0.649416000
1	-3.310203000	1.272869000	-0.560807000
6	-0.395092000	2.924759000	-1.178067000
1	0.623162000	2.749971000	-1.515306000
6	-0.817843000	4.223715000	-0.898982000
6	-3.020139000	3.388770000	-0.368095000
6	-2.131411000	4.460454000	-0.488713000
1	-4.046470000	3.566463000	-0.059632000
1	-0.125111000	5.052732000	-1.013301000
1	-2.464126000	5.472069000	-0.276086000

53

E + ZPE = -2975.664586

28	0.888806000	0.258850000	0.035489000
15	-0.957875000	-0.666541000	0.741043000
6	-0.890730000	-2.510229000	1.071780000
1	-0.935123000	-3.058248000	0.125905000
6	-2.117860000	-2.824969000	1.977304000
1	-2.925100000	-3.277992000	1.395036000
1	-1.819419000	-3.569544000	2.722453000
6	-2.624523000	-1.529719000	2.665869000
1	-2.818391000	-1.691568000	3.732001000
1	-3.574055000	-1.211707000	2.220486000
6	-1.598071000	-0.388245000	2.496871000
1	-0.719211000	-0.615139000	3.114579000
6	-2.149698000	0.966832000	2.935273000
1	-3.032248000	1.253415000	2.354702000
1	-1.407286000	1.768836000	2.868681000
1	-2.459729000	0.902554000	3.984579000
6	0.429773000	-2.879848000	-1.776723000
1	0.534303000	-2.376041000	2.743546000
1	1.308154000	-2.645665000	1.172063000
1	0.438471000	-3.957629000	1.974426000
6	-2.394906000	-0.365940000	-0.389332000
6	-3.050422000	-1.463540000	-0.972658000
1	-2.720355000	-2.474102000	-0.763412000
6	-4.145229000	-1.295307000	-1.821181000
1	-4.629948000	-2.165743000	-2.253190000
6	-4.619563000	-0.015003000	-2.090231000
1	-5.484611000	0.130145000	-2.730285000
6	-3.975323000	1.084300000	-1.524215000
1	-4.354637000	2.083474000	-1.722351000
6	-2.852884000	0.941657000	-0.697573000
6	-2.170636000	2.210020000	-0.212647000
1	-1.651162000	2.049327000	0.730796000
1	-2.923906000	2.993639000	-0.043877000
8	-1.162885000	2.694965000	-1.098358000
6	-1.650742000	3.424301000	-2.218361000
1	-2.297852000	4.253049000	-1.896861000
1	-0.776822000	3.834310000	-2.729493000
1	-2.207829000	2.787218000	-2.918050000
6	2.785982000	2.655342000	0.428776000
1	2.492186000	3.108491000	-0.524860000
6	3.286311000	3.741130000	1.356038000
6	3.237463000	5.044901000	1.083843000
1	2.832050000	5.421879000	0.147035000
6	1.759853000	0.779986000	1.825258000
6	1.618016000	1.931958000	1.080801000
1	0.739696000	2.556431000	1.243351000

1	1.272889000	1.413205000	-1.468350000
1	3.696312000	3.397658000	2.305555000
1	3.611904000	5.786424000	1.783539000
1	3.596385000	1.941448000	0.226033000
1	2.722450000	0.271179000	1.872711000
1	1.066179000	0.534479000	2.622017000
6	0.844148000	-0.737655000	-1.589812000
6	0.962405000	0.631881000	-2.214357000
1	-0.024296000	-1.309791000	-1.907848000
1	0.012903000	0.977771000	-2.616142000
1	1.747544000	0.677757000	-2.977491000
6	2.073759000	-1.523892000	-1.406158000
6	3.329573000	-0.893266000	-1.254170000
1	3.426677000	0.179801000	-1.392604000
6	2.027386000	-2.933976000	-1.337405000
1	1.076254000	-3.439456000	-1.485320000
6	3.178212000	-3.677387000	-1.112939000
6	4.481478000	-1.643332000	-1.006675000
6	4.409819000	-3.033281000	-0.932441000
1	5.438242000	-1.140530000	-0.899937000
1	3.124070000	-4.761749000	-1.084064000
1	5.308414000	-3.617332000	-0.758097000

54
E + ZPE = -2975.686751

28	1.023987000	-0.401562000	0.007959000
15	-1.072253000	-0.761606000	0.628869000
6	-1.439923000	-2.594325000	0.841677000
1	-1.757336000	-2.998379000	-0.124437000
6	-2.571104000	-2.710440000	1.911077000
1	-3.472534000	-3.156098000	1.478938000
1	-2.234524000	-3.397794000	2.694402000
6	-2.891418000	-1.330923000	2.523480000
1	-3.172502000	-1.418857000	3.579034000
1	-3.745921000	-0.875047000	2.009933000
6	-1.680201000	-0.386237000	2.379192000
1	-0.864167000	-0.740221000	3.026113000
6	-2.043181000	1.050912000	2.764134000
1	-2.809538000	1.460229000	2.097521000
1	-1.188316000	1.733539000	2.768991000
1	-2.457858000	1.054887000	3.778589000
6	-0.187032000	-3.369213000	1.288217000
1	0.196299000	-3.000568000	2.246685000
1	0.624864000	-3.320783000	0.558062000
1	-0.445986000	-4.424480000	1.429663000
6	-2.390768000	-0.067832000	-0.469692000
6	-3.424094000	-0.897391000	-0.934490000
1	-3.448725000	-1.947141000	-0.666723000
6	-4.449681000	-0.402774000	-1.742171000
1	-5.233716000	-1.071294000	-2.085058000
6	-4.467889000	0.944741000	-2.088751000
1	-5.267185000	1.345508000	-2.704784000
6	-3.450652000	1.781391000	-1.629925000
1	-3.473098000	2.837788000	-1.885596000
6	-2.399740000	1.301573000	-0.838499000
6	-1.311853000	2.282004000	-0.436760000
1	-0.912406000	2.054441000	0.552171000
1	-1.732696000	3.296943000	-0.394549000
8	-0.174304000	2.273600000	-1.302997000
6	-0.369886000	2.972650000	-2.528836000
1	-0.675914000	4.011774000	-2.342155000
1	0.591319000	2.974892000	-3.047716000

1	-1.119736000	2.485750000	-3.164668000
6	2.245242000	2.224870000	1.124327000
1	1.644147000	2.710805000	0.346648000
6	2.418152000	3.166307000	2.295372000
6	1.836148000	4.361719000	2.396073000
1	1.192046000	4.755016000	1.611910000
6	2.188187000	-0.272598000	1.718702000
6	1.575932000	0.949794000	1.595031000
1	0.655344000	1.112972000	2.147596000
1	0.459554000	0.291956000	-3.042274000
1	3.061130000	2.808665000	3.099664000
1	1.995923000	5.002093000	3.258742000
1	3.222711000	1.984794000	0.689548000
1	3.226299000	-0.410790000	1.426484000
1	1.774044000	-1.037608000	2.372321000
6	0.705102000	-1.390554000	-1.665060000
6	0.056539000	-0.704356000	-2.854557000
1	0.309929000	-2.398417000	-1.519376000
1	-1.023492000	-0.607776000	-2.723031000
1	0.228896000	-1.310641000	-3.754130000
6	2.145735000	-1.314601000	-1.475321000
6	2.734085000	-0.019366000	-1.433963000
1	2.180765000	0.841854000	-1.800468000
6	2.959929000	-2.431450000	-1.119629000
1	2.519252000	-3.424664000	-1.125470000
6	4.300871000	-2.265784000	-0.837790000
6	4.112570000	0.126196000	-1.167509000
6	4.887060000	-0.980391000	-0.868700000
1	4.565413000	1.112021000	-1.215054000
1	4.916057000	-3.131350000	-0.609649000
1	5.949461000	-0.868532000	-0.673580000

55
E + ZPE = -2975.667221

28	0.342728000	-0.671999000	0.009098000
15	-1.357658000	0.469345000	0.793142000
6	-2.067106000	0.249065000	2.507394000
1	-3.027482000	0.783919000	2.496273000
6	-1.066608000	1.080462000	3.333172000
1	-1.435125000	1.213600000	4.356228000
1	-0.124193000	0.522392000	3.415599000
6	-0.848846000	2.438609000	2.635661000
1	0.138232000	2.846990000	2.873934000
1	-1.581548000	3.160032000	3.012943000
6	-1.040792000	2.314547000	1.086729000
1	-0.113945000	2.579853000	0.569784000
6	-2.162388000	3.240910000	0.590045000
1	-3.122968000	2.997144000	1.056775000
1	-2.303170000	3.201211000	-0.493426000
1	-1.918685000	4.275876000	0.856671000
6	-2.290133000	-1.157242000	3.066499000
1	-1.339550000	-1.661335000	3.265618000
1	-2.881711000	-1.792958000	2.400555000
1	-2.825665000	-1.088527000	4.020030000
6	-2.697956000	0.310894000	-0.445803000
6	-3.966129000	-0.162204000	-0.082729000
1	-4.196181000	-0.364925000	0.957874000
6	-4.957809000	-0.379821000	-1.041987000
1	-5.935033000	-0.740513000	-0.735208000
6	-4.685832000	-0.135264000	-2.384725000
1	-5.445925000	-0.306595000	-3.140752000
6	-3.424973000	0.332852000	-2.758489000

1	-3.219528000	0.529475000	-3.807553000
6	-2.421646000	0.563564000	-1.811264000
6	-1.123675000	1.165024000	-2.299916000
1	-0.964825000	2.170157000	-1.883753000
1	-1.174277000	1.270121000	-3.389389000
8	0.043629000	0.367719000	-1.985160000
6	1.154401000	0.783353000	-2.791136000
1	1.392817000	1.839183000	-2.611150000
1	2.005977000	0.166425000	-2.509847000
1	0.924777000	0.639078000	-3.853920000
6	2.258968000	0.681681000	1.132447000
6	2.691728000	1.597361000	0.246399000
1	2.179163000	2.558284000	0.180965000
1	-1.068121000	-2.915556000	-1.512686000
1	2.814099000	-0.236577000	1.304513000
1	1.490519000	0.932207000	1.855719000
6	-0.325366000	-2.408849000	0.490710000
6	-1.349964000	-3.006693000	-0.459667000
1	-0.604640000	-2.557257000	1.531949000
1	-2.333049000	-2.541757000	-0.342707000
1	-1.462027000	-4.077819000	-0.241736000
6	1.098042000	-2.591119000	0.260826000
6	1.599767000	-2.181148000	-1.006202000
1	0.935792000	-2.122952000	-1.864758000
6	2.028459000	-2.948967000	1.280067000
1	1.648641000	-3.259546000	2.249763000
6	3.383227000	-2.952188000	1.024433000
6	2.996877000	-2.187032000	-1.241171000
6	3.875951000	-2.562194000	-0.243724000
1	3.374523000	-1.939613000	-2.229485000
1	4.079004000	-3.270229000	1.795692000
1	4.944261000	-2.589675000	-0.437320000
6	3.937798000	1.476561000	-0.594670000
1	4.294290000	0.439067000	-0.568649000
1	3.726067000	1.731239000	-1.640669000
6	5.011154000	2.410827000	-0.075482000
1	5.365919000	2.204301000	0.933872000
6	5.512492000	3.440485000	-0.757232000
1	5.181484000	3.678843000	-1.766211000
1	6.283695000	4.079642000	-0.337233000

56
E + ZPE = -2975.670920

28	-0.442834000	0.982333000	-0.123247000
15	0.740164000	-0.806961000	0.381723000
6	0.341308000	-1.532551000	2.076724000
1	1.063266000	-1.123593000	2.789986000
6	0.508769000	-3.079210000	1.945347000
1	1.098236000	-3.476825000	2.778076000
1	-0.484258000	-3.537451000	2.018414000
6	1.130422000	-3.447520000	0.588919000
1	0.892323000	-4.481085000	0.311499000
1	2.224270000	-3.375375000	0.624009000
6	0.583540000	-2.473422000	-0.471308000
1	-0.498900000	-2.629315000	-0.557387000
6	1.231322000	-2.651101000	-1.844891000
1	2.305700000	-2.441782000	-1.816348000
1	0.776605000	-2.017080000	-2.612961000
1	1.108846000	-3.689679000	-2.172618000
6	-1.069452000	-1.166627000	2.566206000
1	-1.840417000	-1.492589000	1.860893000
1	-1.194614000	-0.091625000	2.727202000

1	-1.260243000	-1.666632000	3.522745000
6	2.566006000	-0.469610000	0.333684000
6	3.391309000	-0.907075000	1.381231000
1	2.969496000	-1.427123000	2.233640000
6	4.772711000	-0.701998000	1.358384000
1	5.381790000	-1.054904000	-2.185241000
6	5.357999000	-0.057179000	0.273983000
1	6.431488000	0.102097000	0.239422000
6	4.550898000	0.380350000	-0.776521000
1	5.008301000	0.873032000	-1.631004000
6	3.163125000	0.195525000	-0.768873000
6	2.369876000	0.739932000	-1.944143000
1	1.582942000	0.049833000	-2.253032000
1	3.039152000	0.879231000	-2.804333000
8	1.693851000	1.969682000	-1.661953000
6	2.550457000	3.109172000	-1.648774000
1	3.069286000	3.218577000	-2.611034000
1	1.913586000	3.982180000	-1.489560000
1	3.295679000	3.053382000	-0.844864000
6	-1.439734000	0.064459000	-1.492216000
6	-1.679322000	1.514980000	-1.745225000
1	-2.733951000	1.793701000	-1.755907000
1	-1.304480000	2.196333000	-0.881720000
1	-0.808337000	-0.399848000	-2.248074000
6	0.608183000	1.886457000	1.445415000
6	-0.312408000	2.797979000	0.980124000
1	0.437738000	1.385178000	2.394866000
1	1.638846000	1.931672000	1.111865000
1	0.027656000	3.527803000	0.244087000
1	-1.144750000	1.903457000	-2.612645000
6	-2.590541000	-0.790862000	-1.105007000
6	-3.565436000	-0.360224000	-0.184475000
1	-3.495423000	0.630548000	0.258540000
6	-2.740873000	-2.067064000	-1.677177000
1	-2.020609000	-2.406954000	-2.417701000
6	-3.819059000	-2.885515000	-1.341494000
6	-4.640661000	-1.179025000	0.154557000
6	-4.770190000	-2.446912000	-0.418988000
1	-5.383697000	-0.825370000	0.863800000
1	-3.920876000	-3.860910000	-1.808477000
1	-5.611921000	-3.081234000	-0.157628000
6	-1.561578000	3.184158000	1.752893000
1	-1.233616000	3.950668000	2.475252000
1	-1.924543000	2.340036000	2.351287000
6	-2.679318000	3.762834000	0.923909000
1	-2.395549000	4.555843000	0.229571000
6	-3.962781000	3.413362000	1.024161000
1	-4.296720000	2.652527000	1.727302000
1	-4.733654000	3.895055000	0.429640000

57
E + ZPE = -2975.666132

28	-0.641966000	0.551272000	-0.653689000
15	0.663438000	-0.775706000	0.502698000
6	0.071868000	-1.060719000	2.264930000
1	0.349724000	-0.198019000	2.878812000
6	0.775482000	-2.363972000	2.757007000
1	1.532021000	-2.135656000	3.513611000
1	0.027303000	-2.992690000	3.250717000
6	1.420289000	-3.122882000	1.571189000
1	1.274658000	-4.205039000	1.663042000
1	2.503231000	-2.954374000	1.559146000

6	0.836775000	-2.628805000	0.230516000	15	-1.156141000	0.881344000	0.260650000
1	-0.203645000	-2.968038000	0.142340000	6	-0.971807000	1.802863000	1.896477000
6	1.633141000	-3.146327000	-0.968247000	1	-1.036987000	1.078688000	2.714426000
1	2.666256000	-2.783623000	-0.949918000	6	-2.132198000	2.843682000	1.966719000
1	1.186796000	-2.873352000	-1.929474000	1	-2.794435000	2.631098000	2.811896000
1	1.672126000	-4.240936000	-0.930779000	1	-1.698310000	3.831129000	2.157776000
6	-1.459277000	-1.210754000	2.320083000	6	-2.929339000	2.864168000	0.646576000
1	-1.810314000	-2.053458000	1.717120000	1	-3.293388000	3.872057000	0.416965000
1	-1.984923000	-0.317143000	1.976814000	1	-3.815415000	2.223566000	0.724473000
1	-1.762056000	-1.398892000	3.356317000	6	-2.052218000	2.349462000	-0.513562000
6	2.403440000	-0.141692000	0.622363000	1	-1.256520000	3.080288000	-0.712315000
6	2.974830000	0.070016000	1.888684000	6	-2.876774000	2.140110000	-1.784938000
1	2.399203000	-0.110347000	2.788366000	1	-3.646464000	1.374557000	-1.639609000
6	4.293872000	0.502178000	2.034529000	1	-2.269648000	1.864062000	-2.649409000
1	4.702715000	0.654153000	3.029009000	1	-3.390527000	3.074411000	-2.038186000
6	5.079051000	0.715599000	0.905979000	6	0.398728000	2.498088000	1.988950000
1	6.113043000	1.032315000	1.003819000	1	0.546809000	3.206631000	1.165725000
6	4.525332000	0.512672000	-0.357400000	1	1.232653000	1.790678000	1.979748000
1	5.142710000	0.664022000	-1.239168000	1	0.454448000	3.067783000	2.923417000
6	3.194488000	0.109451000	-0.528682000	6	-2.496663000	-0.379526000	0.501377000
6	2.672490000	0.002104000	-1.951276000	6	-3.189694000	-0.440719000	1.720743000
1	1.879072000	-0.741354000	-2.030446000	1	-2.947281000	0.243260000	2.525773000
1	3.488128000	-0.311767000	-2.619229000	6	-4.211522000	-1.368024000	1.933842000
8	2.090551000	1.210152000	-2.442632000	1	-4.728529000	-1.388252000	2.888617000
6	3.027507000	2.203920000	-2.844165000	6	-4.568639000	-2.249475000	0.918236000
1	3.730920000	1.804217000	-3.588772000	1	-5.369646000	-2.967370000	1.066810000
1	2.449975000	3.011583000	-3.299541000	6	-3.891819000	-2.197321000	-0.300195000
1	3.595048000	2.604293000	-1.994306000	1	-4.181391000	-2.872457000	-1.101606000
6	-1.187268000	-0.694361000	-1.977886000	6	-2.851642000	-1.287897000	-0.528077000
6	-1.039844000	0.483568000	-2.905048000	6	-2.141346000	-1.334102000	-1.868864000
1	-1.910420000	0.632258000	-3.552991000	1	-1.832377000	-0.337043000	-2.181358000
1	-0.976436000	1.447257000	-2.326734000	1	-2.824381000	-1.724386000	-2.636497000
1	-0.601938000	-1.571334000	-2.238223000	8	-0.938463000	-2.109221000	-1.860937000
6	0.183436000	2.354467000	0.007214000	6	-1.148349000	-3.514996000	-1.961179000
6	-1.169259000	2.413732000	0.239411000	1	-1.715378000	-3.762645000	-2.869672000
1	0.880764000	2.196364000	0.826103000	1	-0.160436000	-3.976853000	-2.020720000
1	0.630836000	2.718645000	-0.913147000	1	-1.679671000	-3.915263000	-1.087773000
1	-1.806428000	2.841025000	-0.537583000	6	0.959173000	1.267635000	-1.832262000
1	-0.122888000	0.443175000	-3.491315000	6	0.440587000	0.759301000	-3.172488000
6	-2.518047000	-0.979703000	-1.414316000	1	1.105737000	1.097076000	-3.977885000
6	-3.481354000	0.043083000	-1.255015000	1	0.375552000	-0.331204000	-3.227579000
1	-3.301802000	1.034599000	-1.659757000	1	0.705092000	2.313347000	-1.655196000
6	-2.854624000	-2.279465000	-0.973661000	6	0.405086000	-1.442658000	1.076116000
1	-2.148495000	-3.090876000	-1.131363000	6	1.771612000	-1.377326000	0.974530000
6	-4.086086000	-2.540554000	-0.387830000	1	-0.086729000	-1.058606000	1.966719000
6	-4.711480000	-0.220250000	-0.648183000	1	-0.174414000	-2.136605000	0.476634000
6	-5.015855000	-1.507328000	-0.208416000	1	2.265028000	-2.043953000	0.273496000
1	-5.441221000	0.577631000	-0.545313000	1	-0.551793000	1.158316000	-3.389661000
1	-4.333770000	-3.552166000	-0.079266000	6	2.332998000	0.960971000	-1.461427000
1	-5.979365000	-1.715261000	0.246964000	6	2.811269000	-0.358323000	-1.664445000
6	-1.800721000	2.388377000	1.615371000	1	2.226586000	-1.063958000	-2.247443000
1	-1.115828000	1.902606000	2.323408000	6	3.191048000	1.897383000	-0.808512000
1	-2.734673000	1.814937000	1.609128000	1	2.827365000	2.906345000	-0.633401000
6	-2.090804000	3.803563000	2.066548000	6	4.480231000	1.547986000	-0.465237000
1	-1.220417000	4.449404000	2.180591000	6	4.128920000	-0.701282000	-1.305276000
6	-3.311143000	4.282497000	2.306884000	6	4.956796000	0.242069000	-0.720271000
1	-4.202129000	3.666781000	2.201085000	1	4.499146000	-1.701003000	-1.511922000
1	-3.466143000	5.307336000	2.631298000	1	5.139361000	2.282210000	-0.011348000
				1	5.981825000	-0.013995000	-0.468494000
				6	2.670199000	-0.809366000	2.051970000
				1	2.080825000	-0.162326000	2.715633000
				1	3.471145000	-0.200541000	1.619482000
				6	3.281466000	-1.937394000	2.854888000
				1	2.575677000	-2.568000000	3.395391000

58
E + ZPE = -2975.679280

28 0.814329000 0.068413000 -0.324708000

6	4.587114000	-2.196180000	2.922145000
1	5.320652000	-1.590170000	2.394267000
1	4.975123000	-3.017609000	3.517403000

59
E + ZPE = -2975.670344

28	-0.525095000	-0.505616000	-0.459231000
15	1.412671000	-0.595332000	0.553587000
6	1.360766000	-0.694541000	2.441699000
1	1.591606000	0.305393000	2.822125000
6	2.474946000	-1.700636000	2.857744000
1	2.985946000	-1.357403000	3.763589000
1	1.999692000	-2.656793000	3.109921000
6	3.453782000	-1.922439000	1.698511000
1	4.048410000	-2.831850000	1.844541000
1	4.164503000	-1.090181000	1.619213000
6	2.632216000	-2.021476000	0.399104000
1	2.009511000	-2.924564000	0.455377000
6	3.498974000	-2.082111000	-0.860528000
1	4.096648000	-1.172756000	-0.980769000
1	2.911005000	-2.231960000	-1.771322000
1	4.194555000	-2.925401000	-0.784148000
6	-0.007219000	-1.109843000	3.001727000
1	-0.317297000	-2.087939000	2.618101000
1	-0.794744000	-0.389935000	2.764962000
1	0.056195000	-1.191568000	4.093075000
6	2.427359000	0.895310000	0.113144000
6	3.195103000	1.578481000	1.066751000
1	3.217844000	1.242624000	2.097423000
6	3.959319000	2.696730000	0.722598000
1	4.546014000	3.201466000	1.484384000
6	3.968175000	3.153335000	-0.591440000
1	4.558978000	4.020580000	-0.870194000
6	3.211438000	2.483093000	-1.553983000
1	3.226336000	2.831400000	-2.583911000
6	2.440342000	1.363061000	-1.226431000
6	1.649130000	0.683777000	-2.325607000
1	1.814108000	-0.395404000	-2.334668000
1	1.952052000	1.072928000	-3.304426000
8	0.220894000	0.841563000	-2.180043000
6	-0.283075000	2.051014000	-2.760343000
1	-0.067378000	2.072836000	-3.835282000
1	-1.363832000	2.048224000	-2.609005000
1	0.150995000	2.938768000	-2.284721000
6	-0.746475000	-2.401851000	-0.541961000
6	-0.095894000	-3.156060000	-1.693377000
1	-0.574610000	-4.138998000	-1.801134000
1	-0.193485000	-2.642660000	-2.654892000
1	-0.627387000	-2.937615000	0.403675000
6	-0.749714000	1.807528000	0.728021000
6	-2.087832000	1.698531000	0.643304000
1	-0.243079000	1.722923000	1.685831000
1	-0.146258000	2.146719000	-0.103602000
1	-2.579606000	1.883813000	-0.310287000
1	0.967735000	-3.334708000	-1.517585000
6	-2.088836000	-1.860986000	-0.720670000
6	-2.270935000	-0.953073000	-1.799786000
1	-1.561629000	-0.924801000	-2.621352000
6	-3.161476000	-2.052074000	0.195632000
1	-3.026798000	-2.739944000	1.025956000
6	-4.375268000	-1.426858000	-0.006489000
6	-3.514893000	-0.303400000	-1.971233000

6	-4.555441000	-0.539711000	-1.091879000
1	-3.664774000	0.347156000	-2.828482000
1	-5.204153000	-1.626869000	0.666979000
1	-5.519816000	-0.064425000	-1.245111000
6	-3.013638000	1.476532000	1.812110000
1	-2.426225000	1.222473000	2.704725000
1	-3.687088000	0.637784000	1.606839000
6	-3.832499000	2.723242000	2.074151000
1	-3.266089000	3.608842000	2.361435000
6	-5.159024000	2.793163000	1.965405000
1	-5.759204000	1.930993000	1.681541000
1	-5.699226000	3.713162000	2.169172000

60R
E + ZPE = -2859.022997

28	0.930362000	-0.559745000	0.608481000
15	-0.600153000	0.965364000	0.223506000
6	-0.603979000	2.353161000	1.481724000
1	-1.590777000	2.829844000	1.412233000
6	0.413280000	3.324174000	0.851182000
1	0.420696000	4.273468000	1.398577000
1	1.426543000	2.905315000	0.921777000
6	0.001409000	3.516608000	-0.612150000
1	0.783789000	4.013630000	-1.195761000
1	-0.882931000	4.164980000	-0.649338000
6	-0.356684000	2.143811000	-1.249425000
1	0.515442000	1.760901000	-1.783508000
6	-1.530876000	2.261080000	-2.229060000
1	-2.448595000	2.581220000	-1.725013000
1	-1.746927000	1.327511000	-2.755581000
1	-1.287796000	3.014979000	-2.987266000
6	-0.317841000	2.006474000	2.941988000
1	0.663921000	1.533969000	3.056988000
1	-1.072112000	1.335616000	3.365239000
1	-0.317490000	2.922863000	3.542860000
6	-2.292051000	0.245332000	0.095755000
6	-3.313968000	0.680731000	0.950746000
1	-3.119919000	1.445436000	1.695108000
6	-4.603041000	0.148632000	0.868499000
1	-5.376293000	0.504872000	1.542588000
6	-4.890296000	-0.824865000	-0.083222000
1	-5.891853000	-1.236053000	-0.165874000
6	-3.878632000	-1.271213000	-0.935290000
1	-4.105252000	-2.026580000	-1.683858000
6	-2.576309000	-0.766311000	-0.855890000
6	-1.517269000	-1.347633000	-1.776104000
1	-0.817361000	-0.580225000	-2.115993000
1	-1.996058000	-1.777744000	-2.667260000
8	-0.693086000	-2.339075000	-1.153334000
6	-1.334407000	-3.599419000	-0.978744000
1	-1.689181000	-3.995010000	-1.940883000
1	-0.584437000	-4.281254000	-0.571455000
1	-2.180813000	-3.536458000	-0.283416000
1	2.662963000	-3.378045000	-0.315222000
6	3.204927000	-3.015931000	0.563906000
6	2.704165000	-1.648646000	1.021191000
1	4.264301000	-2.939812000	0.294569000
1	3.113399000	-3.764469000	1.356457000
1	3.204639000	-1.332678000	1.936601000
6	2.839488000	-0.571321000	-0.002199000
6	2.199283000	-0.703821000	-1.263149000
6	3.621319000	0.590306000	0.245691000

1	1.684731000	-1.623279000	-1.530957000
1	4.097806000	0.709718000	1.215284000
6	2.445627000	0.248042000	-2.274075000
6	3.834583000	1.522257000	-0.755678000
1	2.016742000	0.098420000	-3.260888000
1	4.469905000	2.382308000	-0.565289000
6	3.258690000	1.343839000	-2.028385000
1	3.462783000	2.060770000	-2.818220000
6	-0.072039000	-1.309425000	2.036005000
6	1.024460000	-2.242949000	1.882303000
1	1.601899000	-2.466393000	2.775731000
1	0.811847000	-3.135056000	1.298684000
1	-1.052453000	-1.640326000	1.700330000
1	-0.103335000	-0.744916000	2.965962000

60S

E + ZPE = -2859.022732

28	0.909461000	-0.626993000	0.419162000
15	-0.624544000	0.920421000	0.229926000
6	-0.504471000	2.232233000	1.557376000
1	-1.462530000	2.769995000	1.545463000
6	0.560539000	3.155568000	0.932246000
1	0.658224000	4.074583000	1.520981000
1	1.540308000	2.658718000	0.955807000
6	0.132026000	3.455854000	-0.512252000
1	0.975924000	3.812008000	-1.111801000
1	-0.612458000	4.260455000	-0.503175000
6	-0.511749000	2.195315000	-1.170386000
1	0.171208000	1.781750000	-1.914040000
6	-1.843485000	2.532817000	-1.855170000
1	-2.587606000	2.897769000	-1.139271000
1	-2.280338000	1.680995000	-2.383469000
1	-1.674067000	3.327507000	-2.591271000
6	-0.184721000	1.806755000	2.990330000
1	0.769108000	1.270359000	3.048187000
1	-0.963131000	1.170196000	3.423084000
1	-0.100515000	2.696194000	3.624930000
6	-2.322184000	0.212683000	0.197220000
6	-3.247072000	0.554996000	1.192545000
1	-2.974386000	1.249527000	1.980192000
6	-4.536608000	0.017184000	1.195539000
1	-5.235785000	0.298579000	1.977349000
6	-4.919773000	-0.866436000	0.191329000
1	-5.922883000	-1.281876000	0.177196000
6	-4.004529000	-1.215884000	-0.803787000
1	-4.308516000	-1.898413000	-1.593791000
6	-2.703439000	-0.702588000	-0.815148000
6	-1.747721000	-1.157658000	-1.904150000
1	-1.135142000	-0.328460000	-2.269143000
1	-2.318336000	-1.545750000	-2.759545000
8	-0.805133000	-2.146039000	-1.472837000
6	-1.361668000	-3.449964000	-1.333331000
1	-1.797387000	-3.793205000	-2.282069000
1	-0.540387000	-4.116025000	-1.059118000
1	-2.132478000	-3.485511000	-0.552856000
6	2.532845000	-2.025975000	0.415014000
6	2.800520000	-0.747857000	-0.293288000
6	2.053809000	-0.481313000	-1.474192000
6	3.748427000	0.221864000	0.145822000
1	1.443686000	-1.264835000	-1.918748000
1	4.316661000	0.048460000	1.053372000
6	2.363830000	0.657130000	-2.254457000

6	3.992260000	1.353598000	-0.608642000
1	1.873115000	0.792145000	-3.214164000
1	4.740485000	2.067951000	-0.277613000
6	3.311498000	1.567917000	-1.826381000
1	3.556594000	2.432464000	-2.436166000
6	-0.079115000	-1.471951000	1.792550000
6	1.185014000	-2.179317000	1.849707000
1	1.824885000	-1.924907000	2.691345000
1	1.140630000	-3.251576000	1.672599000
1	-0.936736000	-2.013757000	1.397587000
1	-0.324708000	-0.855729000	2.654069000
1	2.153610000	-2.772034000	-0.285329000
6	3.698073000	-2.596442000	1.215061000
1	4.033254000	-1.929527000	2.014822000
1	3.434649000	-3.555428000	1.669291000
1	4.545531000	-2.765987000	0.541231000

S21R

E + ZPE = -2780.472098

28	-1.147324000	-0.004591000	0.154164000
15	0.964315000	0.770965000	-0.062438000
6	1.157012000	1.739792000	-1.669827000
1	2.135263000	1.476524000	-2.087840000
6	1.202562000	3.209091000	-1.201276000
1	1.596460000	3.851649000	-1.996967000
1	0.184354000	3.561456000	-0.983026000
6	2.060416000	3.269828000	0.068940000
1	2.027625000	4.258786000	0.540291000
1	3.111764000	3.073045000	-0.180577000
6	1.544584000	2.189580000	1.045100000
1	0.612437000	2.556172000	1.493633000
6	2.510699000	1.818572000	2.171889000
1	3.450972000	1.413973000	1.785398000
1	2.081483000	1.074721000	2.852614000
1	2.747455000	2.709311000	2.764685000
6	0.082283000	1.431681000	-2.715942000
1	-0.923995000	1.622301000	-2.323796000
1	0.129055000	0.388525000	-3.050048000
1	0.217077000	2.062640000	-3.601876000
6	2.269210000	-0.534463000	-0.114092000
6	3.558086000	-0.220807000	-0.576271000
1	3.794293000	0.795241000	-0.877241000
6	4.561409000	-1.186155000	-0.657022000
1	5.549430000	-0.910698000	-1.013482000
6	4.285366000	-2.499087000	-0.283070000
1	5.053380000	-3.263742000	-0.349162000
6	3.011738000	-2.827614000	0.179475000
1	2.801149000	-3.851534000	0.478065000
6	1.997805000	-1.867063000	0.282374000
6	0.677894000	-2.306652000	0.888125000
1	0.461545000	-1.748034000	1.803003000
1	0.732900000	-3.368324000	1.156788000
8	-0.483848000	-2.108429000	0.059480000
6	-0.544702000	-2.969935000	-1.085653000
1	-0.490700000	-4.018676000	-0.770520000
1	-1.508970000	-2.785873000	-1.562961000
1	0.269467000	-2.756352000	-1.787493000
1	-1.867562000	2.073611000	2.364752000
6	-1.671715000	1.100917000	2.824635000
6	-1.916672000	-0.061135000	1.895055000
1	-2.334981000	1.013368000	3.696778000
1	-0.643618000	1.097450000	3.203055000

1	-1.730813000	-1.027307000	2.372494000
6	-2.982607000	-0.085592000	0.908656000
6	-3.764031000	-1.238282000	0.585837000
6	-2.955046000	1.023821000	-0.004586000
1	-3.778591000	-2.073461000	1.280541000
1	-2.650775000	2.009732000	0.335303000
6	-4.498625000	-1.277919000	-0.578356000
6	-3.722299000	0.943514000	-1.198292000
1	-5.112884000	-2.144065000	-0.805427000
1	-3.748712000	1.794348000	-1.872956000
6	-4.460529000	-0.188812000	-1.486160000
1	-5.050405000	-0.232970000	-2.397114000

S21S

E + ZPE = -2780.469466

28	1.171588000	-0.212531000	-0.141187000
15	-1.029709000	-0.743711000	0.102383000
6	-1.911087000	-1.832086000	-1.165419000
1	-2.909095000	-1.388982000	-1.270179000
6	-2.063732000	-3.186519000	-0.442734000
1	-2.807737000	-3.807644000	-0.954487000
1	-1.113107000	-3.737152000	-0.474432000
6	-2.455128000	-2.898557000	1.013028000
1	-2.443731000	-3.805364000	1.628465000
1	-3.478799000	-2.502511000	1.052714000
6	-1.464311000	-1.853465000	1.569466000
1	-0.514557000	-2.369775000	1.766609000
6	-1.898450000	-1.150332000	2.857283000
1	-2.838823000	-0.605821000	2.730875000
1	-1.143530000	-0.436909000	3.206671000
1	-2.045508000	-1.890597000	3.651753000
6	-1.271865000	-1.903452000	-2.552252000
1	-0.261774000	-2.323690000	-2.514628000
1	-1.213068000	-0.916045000	-3.022671000
1	-1.872417000	-2.544044000	-3.208141000
6	-2.047830000	0.797032000	0.162821000
6	-3.439562000	0.724338000	0.334930000
1	-3.921041000	-0.241894000	0.452458000
6	-4.231682000	1.872138000	0.360981000
1	-5.304842000	1.785217000	0.502233000
6	-3.639561000	3.123103000	0.201479000
1	-4.245127000	4.024181000	0.213807000
6	-2.260076000	3.212440000	0.018857000
1	-1.800868000	4.189331000	-0.110671000
6	-1.450100000	2.070353000	0.002872000
6	0.043431000	2.266792000	-0.158955000
1	0.595753000	1.873633000	0.709904000
1	0.277921000	3.336929000	-0.209195000
8	0.633384000	1.606420000	-1.291767000
6	0.185465000	2.080277000	-2.568076000
1	0.414140000	3.147365000	-2.675251000
1	0.737030000	1.513232000	-3.319205000
1	-0.890641000	1.920536000	-2.695646000
1	2.374735000	-3.100203000	-0.076587000
6	2.418397000	-2.704938000	-1.094892000
6	2.470876000	-1.198535000	-1.150246000
1	1.566739000	-3.102509000	-1.655798000
1	3.326120000	-3.111213000	-1.563823000
1	2.532593000	-0.808898000	-2.171089000
6	3.138307000	-0.392865000	-0.152771000
6	2.676052000	-0.643787000	1.189759000
6	3.907792000	0.784780000	-0.422737000

1	2.409256000	-1.649957000	1.501874000
1	4.252540000	0.965088000	-1.437081000
6	3.022570000	0.287050000	2.212081000
6	4.223942000	1.654105000	0.593684000
1	2.728320000	0.082964000	3.237568000
1	4.833100000	2.529868000	0.391354000
6	3.762768000	1.412835000	1.916820000
1	4.033211000	2.105776000	2.708371000

61

E + ZPE = -2859.024163

28	-0.973968000	-0.190760000	0.657009000
15	0.949543000	0.723313000	-0.056995000
6	1.050020000	1.683637000	-1.691851000
1	1.969273000	1.322131000	-2.166388000
6	1.277125000	3.151829000	-1.275529000
1	1.688103000	3.721891000	-2.116819000
1	0.321130000	3.621624000	-1.015476000
6	2.217131000	3.170786000	-0.064402000
1	2.258585000	4.162027000	0.401837000
1	3.241735000	2.935008000	-0.379879000
6	1.729777000	2.120449000	0.961173000
1	0.870741000	2.547383000	1.491014000
6	2.784764000	1.740732000	2.005272000
1	3.665101000	1.275612000	1.553555000
1	2.395219000	1.055637000	2.763485000
1	3.118334000	2.646146000	2.525282000
6	-0.098452000	1.477557000	-2.678590000
1	-1.059618000	1.782574000	-2.258004000
1	-0.188081000	0.431875000	-2.990135000
1	0.077339000	2.074243000	-3.581258000
6	2.264818000	-0.574685000	-0.290261000
6	3.539049000	-0.156401000	-0.721540000
1	3.732053000	0.896877000	-0.892127000
6	4.581476000	-1.053934000	-0.938800000
1	5.551093000	-0.686949000	-1.261628000
6	4.366600000	-2.417492000	-0.749668000
1	5.163229000	-3.133416000	-0.927266000
6	3.109520000	-2.856755000	-0.346311000
1	2.934285000	-3.921935000	-0.215582000
6	2.059226000	-1.960431000	-0.100425000
6	0.773723000	-2.576888000	0.410612000
1	0.700927000	-2.504514000	1.496813000
1	0.746082000	-3.641733000	0.154100000
8	-0.435038000	-1.975178000	-0.087313000
6	-0.667960000	-2.253515000	-1.483814000
1	-0.728030000	-3.337654000	-1.623283000
1	-1.618568000	-1.794489000	-1.746887000
1	0.141159000	-1.844384000	-2.096284000
1	-1.565157000	2.992662000	-0.177539000
6	-1.890430000	2.783669000	0.844856000
6	-2.089251000	1.309818000	1.121479000
1	-2.830978000	3.329558000	1.004774000
1	-1.155961000	3.222436000	1.527026000
1	-2.319285000	1.152742000	2.179786000
6	-2.952897000	0.524921000	0.236632000
6	-3.280374000	-0.795122000	0.646440000
6	-3.368063000	0.933894000	-1.063701000
1	-3.204436000	-1.073814000	1.688536000
1	-3.185257000	1.954002000	-1.383772000
6	-3.958826000	-1.673030000	-0.223015000
6	-4.051895000	0.069668000	-1.896620000

1	-4.227455000	-2.666309000	0.124879000
1	-4.389573000	0.414394000	-2.869872000
6	-4.336056000	-1.250665000	-1.486677000
1	-4.885164000	-1.915652000	-2.146862000
6	-0.037332000	-0.409190000	2.983033000
6	-1.101177000	-1.225710000	3.082982000
1	-0.104852000	0.641449000	3.246632000
1	0.961935000	-0.790278000	2.795590000
1	-2.060272000	-0.855276000	3.430457000
1	-1.028456000	-2.299706000	2.934827000

62
E + ZPE = -2859.031917

28	-0.943042000	-0.340311000	0.911969000
15	0.948233000	0.731032000	-0.085720000
6	1.107107000	1.737958000	-1.691236000
1	2.094202000	1.473380000	-2.086632000
6	1.174047000	3.202840000	-1.216991000
1	1.549272000	3.845335000	-2.022193000
1	0.168231000	3.568400000	-0.968463000
6	2.078194000	3.252114000	0.021051000
1	2.037940000	4.228152000	0.518433000
1	3.123654000	3.098517000	-0.276799000
6	1.635318000	2.136581000	0.995724000
1	0.743702000	2.496004000	1.519868000
6	2.675962000	1.770254000	2.058178000
1	3.597410000	1.377399000	1.620521000
1	2.297065000	1.026126000	2.765895000
1	2.937076000	2.665892000	2.633868000
6	0.084986000	1.465034000	-2.793722000
1	-0.934955000	1.695363000	-2.478705000
1	0.108139000	0.420618000	-3.122661000
1	0.311729000	2.086245000	-3.668107000
6	2.323097000	-0.516211000	-0.287863000
6	3.594830000	-0.029128000	-0.652558000
1	3.748569000	1.037914000	-0.768935000
6	4.682824000	-0.869738000	-0.869443000
1	5.645995000	-0.447695000	-1.140034000
6	4.520551000	-2.248151000	-0.747974000
1	5.352026000	-2.922505000	-0.928644000
6	3.272015000	-2.755019000	-0.404285000
1	3.140957000	-3.831242000	-0.319511000
6	2.173946000	-1.916788000	-0.156298000
6	0.922824000	-2.630984000	0.319061000
1	0.885196000	-2.663811000	1.411042000
1	0.936572000	-3.669526000	-0.030830000
8	-0.324442000	-2.045714000	-0.083274000
6	-0.622827000	-2.237591000	-1.479472000
1	-0.661075000	-3.311391000	-1.690604000
1	-1.599690000	-1.791724000	-1.662819000
1	0.137260000	-1.763770000	-2.108431000
1	-1.409205000	2.820086000	0.438015000
6	-1.935937000	2.490279000	1.337143000
6	-2.229213000	1.005947000	1.361277000
1	-2.876380000	3.056183000	1.395681000
1	-1.337225000	2.781796000	2.205643000
1	-2.665238000	0.738274000	2.325455000
6	-2.977277000	0.397428000	0.235558000
6	-3.637667000	-0.845574000	0.414262000
6	-3.089214000	1.015954000	-1.034552000
1	-3.649497000	-1.311081000	1.392742000
1	-2.656206000	1.997971000	-1.187139000

6	-4.332693000	-1.453470000	-0.631826000
6	-3.793989000	0.416148000	-2.070226000
1	-4.838065000	-2.399738000	-0.463518000
1	-3.881690000	0.921888000	-3.027312000
6	-4.409276000	-0.827948000	-1.876516000
1	-4.965353000	-1.290958000	-2.686545000
6	-0.202658000	-0.582104000	2.778163000
6	-1.293688000	-1.429647000	2.610557000
1	-0.308268000	0.338503000	3.346558000
1	0.817216000	-0.955630000	2.715780000
1	-2.242679000	-1.192768000	3.081778000
1	-1.157070000	-2.482393000	2.375394000

63
E + ZPE = -2859.021107

28	-0.746866000	-0.683793000	-0.932939000
15	1.454684000	-0.618792000	0.164398000
6	1.617523000	-1.070846000	2.002872000
1	2.379016000	-0.380898000	2.385408000
6	2.221036000	-2.489259000	1.989488000
1	2.627783000	-2.739104000	2.976309000
1	1.436454000	-3.228303000	1.773220000
6	3.295043000	-2.530705000	0.895477000
1	3.664187000	-3.548078000	0.721694000
1	4.162609000	-1.929619000	1.198464000
6	2.673431000	-1.956388000	-0.395496000
1	2.008135000	-2.729019000	-0.804443000
6	3.673647000	-1.566215000	-1.486717000
1	4.354196000	-0.776182000	-1.156132000
1	3.173601000	-1.213103000	-2.396060000
1	4.279571000	-2.436830000	-1.762190000
6	0.367326000	-0.912542000	2.867731000
1	-0.424873000	-1.608725000	2.573543000
1	-0.036176000	0.104789000	2.825000000
1	0.611866000	-1.125323000	3.914808000
6	2.289335000	1.030695000	0.070965000
6	3.570461000	1.194689000	0.626475000
1	4.073609000	0.349609000	1.085510000
6	4.226665000	2.424412000	0.604127000
1	5.219218000	2.515454000	1.035032000
6	3.598681000	3.529918000	0.034398000
1	4.091924000	4.497073000	0.019697000
6	2.324089000	3.388360000	-0.510863000
1	1.832555000	4.253197000	-0.949529000
6	1.661398000	2.154326000	-0.513848000
6	0.316378000	2.087202000	-1.207666000
1	0.385121000	1.506614000	-2.129646000
1	-0.005629000	3.096645000	-1.490053000
8	-0.736361000	1.473532000	-0.442360000
6	-1.169385000	2.299476000	0.652216000
1	-1.569155000	3.243140000	0.264015000
1	-1.953811000	1.756407000	1.173072000
1	-0.335201000	2.505882000	1.331911000
1	-1.398930000	-2.453351000	0.956354000
6	-2.125299000	-2.666166000	0.160813000
6	-2.507110000	-1.433939000	-0.649425000
1	-3.012886000	-3.078296000	0.659321000
1	-1.705108000	-3.453218000	-0.468060000
1	-2.966212000	-1.718387000	-1.596131000
6	-3.310635000	-0.393815000	0.031221000
6	-4.043740000	0.536363000	-0.737911000
6	-3.422649000	-0.323371000	1.435789000

1	-3.981605000	0.492742000	-1.822533000
1	-2.893101000	-1.035709000	2.060210000
6	-4.856176000	1.487915000	-0.133295000
6	-4.248554000	0.623655000	2.042420000
1	-5.420370000	2.185309000	-0.745557000
1	-4.340231000	0.643730000	3.124586000
6	-4.964948000	1.533104000	1.261870000
1	-5.612744000	2.265607000	1.734370000
6	-0.361501000	-1.882977000	-2.444857000
6	-0.995682000	-0.709238000	-2.888441000
1	-0.914669000	-2.818008000	-2.418026000
1	0.710914000	-2.006102000	-2.575918000
1	-2.029725000	-0.718671000	-3.219010000
1	-0.403475000	0.092659000	-3.328103000

64
E + ZPE = -2859.029111

28	0.617716000	-1.154175000	-0.015670000
15	-1.682128000	-0.394283000	0.109959000
6	-2.872334000	-1.068941000	-1.202858000
1	-3.438356000	-0.199150000	-1.558444000
6	-3.833213000	-1.993006000	-0.420545000
1	-4.755820000	-2.149293000	-0.990983000
1	-3.372385000	-2.983066000	-0.294362000
6	-4.102215000	-1.368697000	0.953824000
1	-4.634497000	-2.059598000	1.617889000
1	-4.738914000	-0.480772000	0.850356000
6	-2.738077000	-0.980340000	1.562015000
1	-2.251768000	-1.917625000	1.866739000
6	-2.794186000	-0.058010000	2.782390000
1	-3.262808000	0.901793000	2.547569000
1	-1.796393000	0.149156000	3.186142000
1	-3.380042000	-0.531781000	3.577887000
6	-2.208563000	-1.743367000	-2.407615000
1	-1.587565000	-2.595807000	-2.108516000
1	-1.581002000	-1.046565000	-2.972713000
1	-2.974152000	-2.121230000	-3.094858000
6	-1.834429000	1.441431000	0.000826000
6	-3.097173000	2.057398000	0.025977000
1	-3.993939000	1.450772000	0.099404000
6	-3.233390000	3.443558000	-0.039258000
1	-4.222143000	3.891399000	-0.010424000
6	-2.098119000	4.244715000	-0.147888000
1	-2.190598000	5.324889000	-0.206764000
6	-0.839032000	3.649039000	-0.201089000
1	0.044598000	4.273385000	-0.307471000
6	-0.688195000	2.259686000	-0.120237000
6	0.716602000	1.701521000	-0.162422000
1	1.052400000	1.335259000	0.812666000
1	1.429897000	2.470806000	-0.475030000
8	0.862118000	0.570213000	-1.057730000
6	0.664232000	0.900181000	-2.445541000
1	1.449920000	1.592920000	-2.763847000
1	0.736500000	-0.026727000	-3.012348000
1	-0.318564000	1.355420000	-2.598725000
1	2.390396000	-1.264722000	-2.495159000
6	2.624359000	-2.055337000	-1.777244000
6	2.494362000	-1.622349000	-0.318994000
1	3.655745000	-2.371840000	-1.985979000
1	1.976312000	-2.909707000	-2.003263000
1	2.715502000	-2.485449000	0.314609000
6	3.341060000	-0.475584000	0.131477000

6	3.632495000	-0.316521000	1.502442000
6	3.883961000	0.472463000	-0.757754000
1	3.264392000	-1.049496000	2.216231000
1	3.716879000	0.369240000	-1.825170000
6	4.409217000	0.743338000	1.966069000
6	4.670087000	1.528447000	-0.298690000
1	4.622249000	0.831488000	3.027680000
1	5.093896000	2.231568000	-1.010778000
6	4.929764000	1.675741000	1.066100000
1	5.544807000	2.497112000	1.421736000
6	0.174191000	-3.041842000	0.492515000
6	0.549812000	-2.312069000	1.613668000
1	0.868650000	-3.731720000	0.021007000
1	-0.875245000	-3.232917000	0.281493000
1	1.536309000	-2.433253000	2.047023000
1	-0.192621000	-1.903800000	2.294602000

65
E + ZPE = -2859.028496

28	0.720626000	-1.202822000	-0.109239000
15	-1.589253000	-0.404382000	0.191856000
6	-2.913852000	-1.132339000	-0.959070000
1	-3.526969000	-0.271352000	-1.251219000
6	-3.767302000	-2.035130000	-0.042001000
1	-4.733234000	-2.248672000	-0.513948000
1	-3.267636000	-3.003822000	0.102465000
6	-3.928659000	-1.325963000	1.308169000
1	-4.385039000	-1.979307000	2.060796000
1	-4.592762000	-0.458565000	1.202646000
6	-2.525697000	-0.875310000	1.767854000
1	-2.006345000	-1.780341000	2.108957000
6	-2.490826000	0.139963000	2.912838000
1	-2.993349000	1.074595000	2.648673000
1	-1.464303000	0.384227000	3.208685000
1	-2.997346000	-0.276069000	3.790946000
6	-2.426126000	-1.814394000	-2.240298000
1	-1.784146000	-2.677894000	-2.038681000
1	-1.873396000	-1.125070000	-2.886168000
1	-3.286353000	-2.176503000	-2.814901000
6	-1.768562000	1.418258000	-0.055095000
6	-3.028745000	2.030432000	0.061371000
1	-3.900989000	1.432857000	0.304690000
6	-3.195491000	3.401322000	-0.128967000
1	-4.180738000	3.845443000	-0.023598000
6	-2.096443000	4.190720000	-0.462491000
1	-2.213529000	5.258050000	-0.623445000
6	-0.844213000	3.596873000	-0.606156000
1	0.010004000	4.209924000	-0.882715000
6	-0.660484000	2.224331000	-0.397115000
6	0.745239000	1.684433000	-0.516289000
1	1.174921000	1.438461000	0.458375000
1	1.402466000	2.428844000	-0.976528000
8	0.852948000	0.462022000	-1.289972000
6	0.508451000	0.620914000	-2.678658000
1	1.194717000	1.339213000	-3.139692000
1	0.621717000	-0.353713000	-3.151946000
1	-0.521607000	0.973768000	-2.784801000
1	2.695408000	-1.012258000	-2.526925000
6	2.942892000	-1.842455000	-1.860956000
6	2.614881000	-1.569489000	-0.399259000
1	4.018348000	-2.035979000	-1.977098000
1	2.418306000	-2.731661000	-2.227484000

1	2.859678000	-2.461855000	0.181634000
6	3.242435000	-0.375441000	0.239778000
6	3.215996000	-0.231213000	1.645087000
6	3.871667000	0.643662000	-0.504131000
1	2.779066000	-1.014967000	2.257869000
1	3.940313000	0.558449000	-1.583559000
6	3.773023000	0.882534000	2.273581000
6	4.441750000	1.748735000	0.123703000
1	3.743420000	0.960520000	3.356648000
1	4.942265000	2.506481000	-0.473072000
6	4.386219000	1.880619000	1.514528000
1	4.831852000	2.743184000	2.001062000
6	0.321963000	-3.156189000	0.020129000
6	0.612399000	-2.639234000	1.279024000
1	1.060411000	-3.735065000	-0.527310000
1	-0.709357000	-3.329067000	-0.276345000
1	1.578208000	-2.819759000	1.738849000
1	-0.179409000	-2.407340000	1.984306000

66

E + ZPE = -2859.038148

28	0.970822000	-0.499118000	0.963854000
15	-0.923038000	0.841819000	0.255972000
6	-1.644428000	2.230383000	1.285204000
1	-2.591612000	2.496354000	0.798430000
6	-0.675076000	3.383454000	0.961232000
1	-1.043352000	4.325116000	1.384094000
1	0.314788000	3.202602000	1.401468000
6	-0.587520000	3.446789000	-0.571871000
1	0.228118000	4.095136000	-0.909192000
1	-1.518405000	3.880080000	-0.959021000
6	-0.418495000	2.014525000	-1.159268000
1	0.645132000	1.822694000	-1.326827000
6	-1.159505000	1.827354000	-2.487000000
1	-2.239479000	1.967141000	-2.372759000
1	-0.994630000	0.836707000	-2.923271000
1	-0.801788000	2.568447000	-3.211723000
6	-1.940092000	1.953142000	2.760961000
1	-1.046769000	1.702067000	3.337780000
1	-2.654515000	1.130536000	2.876135000
1	-2.386767000	2.841413000	3.221799000
6	-2.345226000	-0.192088000	-0.309004000
6	-3.677123000	0.155782000	-0.041153000
1	-3.911429000	1.062512000	0.504579000
6	-4.737262000	-0.647698000	-0.467907000
1	-5.758226000	-0.349231000	-0.249204000
6	-4.482699000	-1.821376000	-1.171529000
1	-5.300788000	-2.449777000	-1.510021000
6	-3.162291000	-2.192635000	-1.428346000
1	-2.958489000	-3.115527000	-1.965991000
6	-2.092919000	-1.398877000	-1.004140000
6	-0.684411000	-1.860355000	-1.284727000
1	-0.103185000	-1.120457000	-1.839422000
1	-0.693572000	-2.789477000	-1.866616000
8	0.088003000	-2.098122000	-0.079323000
6	-0.425593000	-3.194519000	0.703083000
1	-0.515475000	-4.083732000	0.069241000
1	0.293787000	-3.383988000	1.497451000
1	-1.401848000	-2.947120000	1.130191000
6	1.383793000	0.479302000	2.654524000
6	0.769866000	-0.752367000	2.917951000
1	-0.289952000	-0.801817000	3.162505000

1	2.326178000	-3.217853000	-0.047821000
1	0.823511000	1.404879000	2.712820000
1	2.448317000	0.601824000	2.831885000
6	2.743988000	-1.266352000	0.874747000
6	2.941777000	-2.763579000	0.730497000
1	3.346133000	-0.896417000	1.705632000
1	3.992840000	-2.972068000	0.487586000
1	2.729021000	-3.276531000	1.674702000
6	2.872256000	-0.392152000	-0.310617000
6	3.315097000	0.947371000	-0.157258000
1	3.576247000	1.307321000	0.833450000
6	2.590105000	-0.838415000	-1.625583000
1	2.287378000	-1.867686000	-1.783850000
6	2.752463000	0.003361000	-2.722956000
6	3.476484000	1.786742000	-1.255606000
6	3.196846000	1.317060000	-2.542847000
1	3.841720000	2.799456000	-1.112312000
1	2.554611000	-0.370456000	-3.723473000
1	3.338130000	1.966141000	-3.402159000
1	1.362694000	-1.584412000	3.290680000

67

E + ZPE = -2859.034363

28	1.003998000	-0.565375000	0.900200000
15	-0.682173000	0.947496000	0.213272000
6	-1.065200000	2.436840000	1.288023000
1	-2.045327000	2.800539000	0.951022000
6	-0.003852000	3.435339000	0.791903000
1	-0.183323000	4.428644000	1.218898000
1	0.988635000	3.117049000	1.138215000
6	-0.071905000	3.460890000	-0.741184000
1	0.835672000	3.890665000	-1.177903000
1	-0.903311000	4.107041000	-1.046411000
6	-0.325581000	2.029242000	-1.310470000
1	0.598102000	1.643089000	-1.749416000
6	-1.413883000	2.056189000	-2.392906000
1	-2.376452000	2.388111000	-1.989947000
1	-1.571765000	1.087987000	-2.874822000
1	-1.118886000	2.766238000	-3.174749000
6	-1.096261000	2.271985000	2.808301000
1	-0.094520000	2.091397000	3.211457000
1	-1.752970000	1.458014000	3.133591000
1	-1.465098000	3.194432000	3.270653000
6	-2.264321000	0.060456000	-0.109018000
6	-3.437720000	0.401321000	0.578070000
1	-3.432972000	1.200771000	1.311260000
6	-4.639713000	-0.267795000	0.332044000
1	-5.535284000	0.017686000	0.875874000
6	-4.685307000	-1.285463000	-0.616069000
1	-5.616882000	-1.803108000	-0.823793000
6	-3.520282000	-1.640709000	-1.299025000
1	-3.554888000	-2.435316000	-2.040593000
6	-2.304667000	-0.995368000	-1.052725000
6	-1.060247000	-1.469334000	-1.779131000
1	-0.450927000	-0.638114000	-2.140568000
1	-1.344373000	-2.075263000	-2.650293000
8	-0.176151000	-2.228653000	-0.941969000
6	-0.667272000	-3.542820000	-0.674002000
1	-0.840453000	-4.084904000	-1.613551000
1	0.100454000	-4.064058000	-0.101362000
1	-1.599559000	-3.520071000	-0.097170000
1	3.815458000	-3.314664000	0.547669000

6	2.766409000	-3.020798000	0.690260000
6	2.675827000	-1.539825000	0.977808000
1	2.388769000	-3.607983000	1.534058000
1	2.214181000	-3.316864000	-0.204883000
1	3.181417000	-1.275604000	1.908617000
6	2.895453000	-0.548546000	-0.069150000
6	3.018710000	0.809756000	0.334374000
6	2.872900000	-0.826991000	-1.465188000
1	3.119501000	1.041418000	1.392152000
1	2.753983000	-1.850323000	-1.802866000
6	3.216817000	1.825537000	-0.610042000
6	3.067847000	0.187224000	-2.389500000
1	3.374560000	2.847077000	-0.277490000
1	3.096982000	-0.048838000	-3.449269000
6	3.255831000	1.514736000	-1.965210000
1	3.439578000	2.294878000	-2.698286000
6	0.653520000	-0.849877000	2.878128000
6	-0.090203000	-1.739858000	2.117814000
1	0.196243000	0.042569000	3.288022000
1	1.555934000	-1.175566000	3.390165000
1	-1.144825000	-1.561209000	1.926810000
1	0.229801000	-2.771205000	2.007374000

68
E + ZPE = -2859.034096

28	0.869260000	-0.839722000	0.582004000
15	-0.506101000	0.997665000	0.094123000
6	-0.302236000	2.529135000	1.164434000
1	-1.203301000	3.135309000	0.996714000
6	0.875682000	3.205841000	0.436615000
1	1.048269000	4.207441000	0.846511000
1	1.792897000	2.628871000	0.615098000
6	0.550833000	3.260839000	-1.063959000
1	1.463413000	3.348252000	-1.661208000
1	-0.048437000	4.154567000	-1.270119000
6	-0.273381000	2.006337000	-1.499988000
1	0.319037000	1.392730000	-2.182494000
6	-1.572236000	2.425339000	-2.204954000
1	-2.219129000	3.013024000	-1.544571000
1	-2.158416000	1.580477000	-2.574438000
1	-1.321486000	3.055355000	-3.066529000
6	-0.067546000	2.395138000	2.669543000
1	0.848312000	1.836225000	2.887735000
1	-0.901415000	1.913460000	3.191105000
1	0.048836000	3.394133000	3.104934000
6	-2.259510000	0.445588000	0.125401000
6	-3.151801000	0.939064000	1.086473000
1	-2.828079000	1.690343000	1.799741000
6	-4.473967000	0.489242000	1.141230000
1	-5.148485000	0.889202000	1.892456000
6	-4.921180000	-0.459322000	0.226308000
1	-5.948745000	-0.808952000	0.254438000
6	-4.039270000	-0.959261000	-0.734841000
1	-4.393726000	-1.690861000	-1.457068000
6	-2.708437000	-0.534246000	-0.796897000
6	-1.792658000	-1.134567000	-1.850057000
1	-1.178034000	-0.372609000	-2.334099000
1	-2.394885000	-1.612902000	-2.633846000
8	-0.854207000	-2.087298000	-1.328134000
6	-1.434182000	-3.373538000	-1.111833000
1	-1.850142000	-3.769693000	-2.047872000
1	-0.634498000	-4.032135000	-0.771418000

1	-2.226870000	-3.341767000	-0.353673000
1	3.102067000	-3.970379000	-0.096683000
6	2.127708000	-3.473324000	0.005068000
6	2.314443000	-2.149160000	0.723718000
1	1.484717000	-4.152323000	0.574140000
1	1.707742000	-3.368100000	-0.998345000
1	2.688276000	-2.285115000	1.740425000
6	2.892592000	-1.011506000	0.040873000
6	3.840907000	-0.132633000	0.643804000
6	2.321059000	-0.629924000	-1.205659000
1	4.252067000	-0.392685000	1.615445000
1	1.675608000	-1.320053000	-1.745090000
6	4.290884000	0.984726000	-0.030547000
6	2.815889000	0.502722000	-1.889550000
1	5.054590000	1.614357000	0.416790000
1	2.452543000	0.724784000	-2.888408000
6	3.791852000	1.296228000	-1.315053000
1	4.189990000	2.150895000	-1.853939000
6	0.319110000	-1.022019000	2.540490000
6	-0.344697000	-1.963116000	1.776825000
1	-0.196838000	-0.124206000	2.856741000
1	1.194943000	-1.283318000	3.128109000
1	-1.369619000	-1.788383000	1.464463000
1	-0.014467000	-2.995826000	1.747429000

69
E + ZPE = -2859.026836

28	-0.951852000	-0.096257000	0.564844000
15	0.971985000	0.719068000	-0.152976000
6	1.132246000	1.528153000	-1.854897000
1	2.151491000	1.286535000	-2.180244000
6	1.095100000	3.037678000	-1.551400000
1	1.437962000	3.609489000	-2.421465000
1	0.066286000	3.362725000	-1.345111000
6	1.986864000	3.274882000	-0.325606000
1	1.893806000	4.296489000	0.059976000
1	3.040263000	3.140239000	-0.605921000
6	1.602617000	2.253026000	0.770601000
1	0.695956000	2.623497000	1.264390000
6	2.677474000	2.056431000	1.844395000
1	3.608311000	1.659019000	1.430768000
1	2.353229000	1.382613000	2.642800000
1	2.906974000	3.023585000	2.306418000
6	0.173173000	1.050317000	-2.942720000
1	-0.872859000	1.189019000	-2.661645000
1	0.321559000	-0.010099000	-3.172541000
1	0.351588000	1.611174000	-3.867500000
6	2.306726000	-0.568223000	-0.188274000
6	3.602533000	-0.167494000	-0.567741000
1	3.798645000	0.875631000	-0.793262000
6	4.658188000	-1.069966000	-0.664254000
1	5.645402000	-0.719240000	-0.949396000
6	4.432693000	-2.420362000	-0.404273000
1	5.239598000	-3.141783000	-0.488972000
6	3.155341000	-2.841828000	-0.047653000
1	2.978253000	-3.897702000	0.142694000
6	2.088525000	-1.939855000	0.080275000
6	0.789344000	-2.538852000	0.588431000
1	0.704349000	-2.422087000	1.670256000
1	0.776878000	-3.614443000	0.380999000
8	-0.422076000	-1.977906000	0.052497000
6	-0.686415000	-2.400145000	-1.301777000

1	-0.759831000	-3.492105000	-1.325430000
1	-1.637423000	-1.959597000	-1.594471000
1	0.112730000	-2.065823000	-1.970321000
1	-3.069259000	2.964180000	1.748996000
6	-2.301457000	2.196161000	1.913868000
6	-1.923067000	1.557274000	0.586408000
1	-2.708913000	1.487965000	2.640910000
1	-1.445151000	2.698046000	2.378062000
1	-1.545702000	2.316581000	-0.102552000
6	-2.850690000	0.632882000	-0.077187000
6	-3.308959000	-0.499154000	0.646003000
6	-3.198013000	0.725027000	-1.455668000
1	-3.271342000	-0.509100000	1.725830000
1	-2.902805000	1.611482000	-2.009418000
6	-4.053946000	-1.507781000	-0.000227000
6	-3.951194000	-0.257182000	-2.069023000
1	-4.420260000	-2.352254000	0.576297000
1	-4.238009000	-0.147220000	-3.111042000
6	-4.367619000	-1.394922000	-1.344149000
1	-4.964935000	-2.158590000	-1.833628000
6	-0.038326000	-0.173472000	2.883744000
6	-1.112535000	-0.967576000	3.043947000
1	-0.083511000	0.883600000	3.123027000
1	0.950461000	-0.573729000	2.681716000
1	-2.049814000	-0.569533000	3.417032000
1	-1.066856000	-2.046248000	2.924852000

70
E + ZPE = -2859.035325

28	-0.554338000	-0.935454000	0.021847000
15	1.044642000	0.754997000	-0.031089000
6	0.853594000	1.914538000	-1.510452000
1	1.859077000	2.040086000	-1.926680000
6	0.414427000	3.257096000	-0.882725000
1	0.601022000	4.080548000	-1.581355000
1	-0.667929000	3.241705000	-0.694344000
6	1.170274000	3.440163000	0.438514000
1	0.792755000	4.295613000	1.010309000
1	2.232558000	3.636183000	0.241208000
6	1.023994000	2.138785000	1.257919000
1	0.009024000	2.115677000	1.673130000
6	2.013823000	1.994925000	2.417072000
1	3.051459000	2.004881000	2.071007000
1	1.855442000	1.070104000	2.983410000
1	1.884858000	2.830150000	3.114538000
6	-0.060788000	1.407625000	-2.628515000
1	-1.079235000	1.226983000	-2.270484000
1	0.313859000	0.478556000	-3.072208000
1	-0.115892000	2.153476000	-3.429761000
6	2.787859000	0.144931000	-0.079820000
6	3.834082000	0.971173000	-0.520472000
1	3.628443000	1.976835000	-0.871863000
6	5.159828000	0.535129000	-0.506033000
1	5.948161000	1.198238000	-0.849396000
6	5.464661000	-0.745482000	-0.050474000
1	6.492341000	-1.095376000	-0.038569000
6	4.436752000	-1.581316000	0.384889000
1	4.671332000	-2.583774000	0.734341000
6	3.105653000	-1.151855000	0.382714000
6	2.037424000	-2.099746000	0.870913000
1	1.509793000	-1.719171000	1.750849000
1	2.474617000	-3.066549000	1.143442000

8	1.002584000	-2.335077000	-0.113050000
6	1.470337000	-3.067583000	-1.262212000
1	2.003929000	-3.963464000	-0.928480000
1	0.593167000	-3.368384000	-1.833927000
1	2.131002000	-2.449867000	-1.878113000
1	-0.544961000	-0.080105000	2.577379000
6	-1.592375000	-0.238402000	2.292937000
6	-1.885124000	0.206251000	0.853279000
1	-2.197968000	0.347074000	2.998109000
1	-1.829136000	-1.292031000	2.476965000
1	-1.526163000	1.227151000	0.703276000
6	-3.326636000	0.200756000	0.454785000
6	-4.298634000	-0.606300000	1.073782000
6	-3.760128000	1.076323000	-0.560017000
1	-4.019848000	-1.270386000	1.887126000
1	-3.035920000	1.734705000	-1.035897000
6	-5.638148000	-0.548473000	0.686983000
6	-5.094676000	1.133004000	-0.953240000
1	-6.368504000	-1.175794000	1.190028000
1	-5.398799000	1.822529000	-1.735677000
6	-6.041806000	0.315448000	-0.331496000
1	-7.084751000	0.360245000	-0.630493000
6	-1.716034000	-1.737254000	-1.422306000
6	-1.833872000	-2.514897000	-0.285637000
1	-1.045384000	-2.016505000	-2.233343000
1	-2.495450000	-1.031664000	-1.690226000
1	-1.244804000	-3.418760000	-0.158207000
1	-2.713847000	-2.429572000	0.340607000

71
E + ZPE = -2859.021446

28	0.552178000	-1.115404000	0.478031000
15	-0.891749000	0.709388000	0.344756000
6	-1.449085000	1.311798000	2.054174000
1	-2.480494000	1.648421000	1.893280000
6	-0.580480000	2.559707000	2.300823000
1	-0.985587000	3.148393000	3.132005000
1	0.438201000	2.261633000	2.585884000
6	-0.549926000	3.357495000	0.990876000
1	0.164746000	4.187374000	1.031882000
1	-1.537205000	3.799780000	0.801667000
6	-0.175348000	2.384687000	-0.149541000
1	0.904041000	2.202499000	-0.077935000
6	-0.483196000	2.889109000	-1.562018000
1	-1.550896000	3.073622000	-1.710778000
1	-0.161083000	2.179978000	-2.333095000
1	0.044859000	3.833007000	-1.740243000
6	-1.468940000	0.291023000	3.192680000
1	-0.464320000	-0.044932000	3.464802000
1	-2.073494000	-0.588599000	2.943965000
1	-1.909819000	0.744141000	4.087783000
6	-2.505172000	0.423185000	-0.511827000
6	-3.466590000	1.448494000	-0.539091000
1	-3.243424000	2.414043000	-0.095876000
6	-4.718282000	1.262856000	-1.124591000
1	-5.435237000	2.078298000	-1.136693000
6	-5.042964000	0.027997000	-1.681991000
1	-6.018474000	-0.135015000	-2.129882000
6	-4.106332000	-1.003725000	-1.654519000
1	-4.360386000	-1.967765000	-2.088140000
6	-2.837777000	-0.823980000	-1.089015000
6	-1.853803000	-1.967785000	-1.196165000

1	-1.032087000	-1.705275000	-1.867892000
1	-2.347224000	-2.850829000	-1.618147000
8	-1.220652000	-2.349251000	0.043253000
6	-2.055857000	-3.145248000	0.899072000
1	-2.337193000	-4.073543000	0.389224000
1	-1.468350000	-3.383134000	1.786731000
1	-2.957053000	-2.592850000	1.186694000
1	0.834292000	-2.707394000	-1.608680000
6	1.779986000	-2.159992000	-1.671991000
6	1.727502000	-0.764482000	-1.045029000
1	2.013043000	-2.048491000	-2.740513000
1	2.554529000	-2.792954000	-1.236993000
1	1.074674000	-0.113602000	-1.636502000
6	3.041094000	-0.091039000	-0.884991000
6	4.188198000	-0.753889000	-0.401718000
6	3.184834000	1.254360000	-1.278505000
1	4.128816000	-1.794576000	-0.097494000
1	2.332252000	1.777300000	-1.702882000
6	5.411556000	-0.097623000	-0.302805000
6	4.409585000	1.912520000	-1.186723000
1	6.279249000	-0.631944000	0.072948000
1	4.493499000	2.945224000	-1.512590000
6	5.527772000	1.240330000	-0.691768000
1	6.484425000	1.748864000	-0.618543000
6	1.864671000	-1.114480000	1.982472000
6	1.634026000	-2.420824000	1.553422000
1	1.351589000	-0.734858000	2.864143000
1	2.782274000	-0.594872000	1.731647000
1	0.932670000	-3.057853000	2.093269000
1	2.376781000	-2.962571000	0.977331000

72

E + ZPE = -2859.027808

28	0.750433000	-0.417682000	0.655705000
15	-1.270319000	0.772652000	0.210310000
6	-2.077522000	1.841572000	1.550119000
1	-3.150960000	1.637493000	1.475227000
6	-1.824465000	3.298225000	1.096627000
1	-2.547026000	3.972542000	1.570392000
1	-0.828916000	3.623838000	1.428685000
6	-1.903795000	3.354036000	-0.434312000
1	-1.563670000	4.320300000	-0.824674000
1	-2.942944000	3.229332000	-0.766028000
6	-1.035783000	2.208590000	-0.997776000
1	0.018779000	2.484574000	-0.866484000
6	-1.266889000	1.885052000	-2.475485000
1	-2.298665000	1.575553000	-2.668087000
1	-0.602656000	1.087854000	-2.829179000
1	-1.064188000	2.773019000	-3.084727000
6	-1.647196000	1.542032000	2.989416000
1	-0.585277000	1.750140000	3.153977000
1	-1.839791000	0.499054000	3.264502000
1	-2.212766000	2.172545000	3.684816000
6	-2.645462000	-0.277097000	-0.446201000
6	-3.939195000	0.251109000	-0.598265000
1	-4.138408000	1.285798000	-0.340098000
6	-4.993675000	-0.519405000	-1.087323000
1	-5.979000000	-0.076825000	-1.198303000
6	-4.776216000	-1.853162000	-1.424650000
1	-5.590270000	-2.468376000	-1.795503000
6	-3.501776000	-2.397165000	-1.276448000
1	-3.332405000	-3.438737000	-1.538063000

6	-2.429922000	-1.628205000	-0.806440000
6	-1.071670000	-2.295126000	-0.772083000
1	-0.409212000	-1.897254000	-1.547414000
1	-1.177664000	-3.370402000	-0.952697000
8	-0.331621000	-2.129353000	0.459216000
6	-0.973520000	-2.696803000	1.616926000
1	-1.232494000	-3.740311000	1.409974000
1	-0.248858000	-2.653300000	2.430359000
1	-1.875826000	-2.136167000	1.880453000
1	1.893913000	-3.231626000	1.205452000
6	2.746257000	-2.625218000	0.888024000
6	2.303124000	-1.444129000	0.036613000
1	3.412717000	-3.276072000	0.305830000
1	3.297440000	-2.331167000	1.786273000
1	1.693175000	-1.816483000	-0.804586000
6	3.371189000	-0.580926000	-0.521713000
6	4.588793000	-0.337241000	0.143359000
6	3.165793000	0.052331000	-1.766221000
1	4.798145000	-0.823680000	1.091318000
1	2.249830000	-0.149935000	-2.319427000
6	5.547471000	0.512604000	-0.404564000
6	4.122434000	0.902240000	-2.315401000
1	6.481372000	0.680644000	0.124094000
1	3.943724000	1.367822000	-3.280449000
6	5.317764000	1.139808000	-1.632339000
1	6.069857000	1.796918000	-2.058711000
6	1.659728000	1.254678000	1.298223000
6	1.791958000	0.220503000	2.226526000
1	0.937386000	2.047775000	1.464181000
1	2.492091000	1.527055000	0.658570000
1	1.124222000	0.159211000	3.086355000
1	2.739432000	-0.290826000	2.346180000

73

E + ZPE = -2859.027339

28	0.797558000	-0.532788000	0.732018000
15	-1.180201000	0.745638000	0.298573000
6	-2.038682000	1.729571000	1.673663000
1	-3.109644000	1.558364000	1.521302000
6	-1.730081000	3.209337000	1.348145000
1	-2.458995000	3.864556000	1.838778000
1	-0.744396000	3.480717000	1.750592000
6	-1.734155000	3.383163000	-0.175503000
1	-1.357382000	4.368187000	-0.474719000
1	-2.758523000	3.306875000	-0.563145000
6	-0.861118000	2.264772000	-0.782598000
1	0.190855000	2.506768000	-0.579859000
6	-1.026738000	2.058348000	-2.289527000
1	-2.051266000	1.776214000	-2.550928000
1	-0.353010000	1.282844000	-2.671406000
1	-0.788976000	2.987925000	-2.818760000
6	-1.705097000	1.315018000	3.109753000
1	-0.657009000	1.503694000	3.362106000
1	-1.918287000	0.255340000	3.288521000
1	-2.315766000	1.893236000	3.812444000
6	-2.542514000	-0.222332000	-0.499058000
6	-3.817215000	0.345360000	-0.669528000
1	-4.007540000	1.363332000	-0.345979000
6	-4.863763000	-0.362235000	-1.260147000
1	-5.833459000	0.110927000	-1.382194000
6	-4.658492000	-1.672755000	-1.684372000
1	-5.467021000	-2.240310000	-2.134776000

6	-3.402946000	-2.255085000	-1.521545000
1	-3.242477000	-3.278232000	-1.852466000
6	-2.337762000	-1.547825000	-0.949983000
6	-0.995507000	-2.246058000	-0.914590000
1	-0.291589000	-1.798711000	-1.623833000
1	-1.114764000	-3.298800000	-1.193361000
8	-0.306063000	-2.203918000	0.355289000
6	-0.993803000	-2.878914000	1.425171000
1	-1.242790000	-3.896880000	1.107879000
1	-0.303071000	-2.916243000	2.267787000
1	-1.907116000	-2.344228000	1.704777000
6	1.691649000	1.017503000	1.654016000
6	1.653852000	-0.108423000	2.478584000
1	2.307502000	-3.215627000	1.463859000
6	3.043081000	-2.573218000	0.968893000
6	2.365436000	-1.528824000	0.096667000
1	3.676389000	-3.221119000	0.347514000
1	3.690247000	-2.151824000	1.743691000
1	1.755230000	-2.053363000	-0.651508000
6	3.220663000	-0.541313000	-0.599353000
6	4.450948000	-0.084633000	-0.083154000
6	2.783346000	0.002303000	-1.827069000
1	4.831703000	-0.491864000	0.848560000
1	1.867893000	-0.375682000	-2.279757000
6	5.196787000	0.878178000	-0.756919000
6	3.526073000	0.971623000	-2.499534000
1	6.146760000	1.207179000	-0.345488000
1	3.172731000	1.363331000	-3.449137000
6	4.735535000	1.416242000	-1.963930000
1	5.324352000	2.163047000	-2.488085000
1	0.985159000	1.828158000	1.801988000
1	2.611560000	1.307276000	1.158525000
1	0.873881000	-0.216062000	3.232074000
1	2.551742000	-0.683015000	2.669103000

74

E + ZPE = -2859.038666

28	0.938441000	-0.656345000	0.795956000
15	-0.886163000	0.825597000	0.302494000
6	-1.448611000	2.185681000	1.461274000
1	-2.401022000	2.543787000	1.047912000
6	-0.414267000	3.283673000	1.150428000
1	-0.680763000	4.218160000	1.657261000
1	0.581399000	2.996861000	1.515558000
6	-0.412471000	3.451182000	-0.377447000
1	0.442539000	4.041589000	-0.723047000
1	-1.316203000	3.999897000	-0.670513000
6	-0.426340000	2.057404000	-1.075965000
1	0.593607000	1.797908000	-1.374240000
6	-1.317811000	2.034380000	-2.322537000
1	-2.362598000	2.253015000	-2.077712000
1	-1.291693000	1.070404000	-2.840701000
1	-0.974141000	2.797785000	-3.030662000
6	-1.678351000	1.845261000	2.935669000
1	-0.767680000	1.530191000	3.450628000
1	-2.422459000	1.050023000	3.053823000
1	-2.058565000	2.728841000	3.460793000
6	-2.397449000	-0.103568000	-0.203755000
6	-3.679301000	0.263110000	0.230591000
1	-3.818307000	1.126421000	0.871088000
6	-4.809486000	-0.465311000	-0.149137000
1	-5.789936000	-0.154379000	0.199168000

6	-4.676289000	-1.579865000	-0.972144000
1	-5.549827000	-2.149126000	-1.274827000
6	-3.405443000	-1.968447000	-1.398380000
1	-3.296188000	-2.843983000	-2.033888000
6	-2.266780000	-1.250266000	-1.023065000
6	-0.913759000	-1.723854000	-1.493645000
1	-0.357285000	-0.945374000	-2.021208000
1	-1.019282000	-2.580249000	-2.169563000
8	-0.037093000	-2.117419000	-0.407500000
6	-0.466474000	-3.322261000	0.253774000
1	-0.623710000	-4.111808000	-0.489452000
1	0.334285000	-3.614450000	0.932359000
1	-1.390259000	-3.154497000	0.816008000
6	1.450699000	0.046914000	2.589002000
6	0.662592000	-1.105080000	2.707323000
1	-0.395961000	-1.031004000	2.949501000
1	4.499335000	-2.436673000	1.046035000
1	1.027212000	1.031191000	2.752784000
1	2.515997000	-0.008900000	2.778924000
6	2.598658000	-1.602352000	0.506549000
6	3.704251000	-1.843146000	1.516767000
1	2.295767000	-2.550156000	0.054411000
1	4.174634000	-0.930530000	1.891226000
1	3.350014000	-2.419638000	2.378666000
6	2.779324000	-0.554762000	-0.523153000
6	3.325174000	0.717941000	-0.213905000
1	3.634075000	0.937838000	-0.802537000
6	2.422639000	-0.800619000	-1.873033000
1	2.034271000	-1.779223000	-2.138948000
6	2.619011000	0.159465000	-2.861421000
6	3.513022000	1.679854000	-1.203188000
6	3.166629000	1.403006000	-2.529351000
1	3.948826000	2.640311000	-0.944127000
1	2.366654000	-0.066142000	-3.893538000
1	3.332275000	2.148390000	-3.301823000
1	1.122822000	-2.053443000	2.973883000

75

E + ZPE = -2859.028590

28	1.067365000	-0.645521000	0.440391000
15	-0.663733000	0.851908000	0.220967000
6	-0.746072000	2.079665000	1.667746000
1	-1.544913000	1.750725000	2.338433000
6	-1.108361000	3.461779000	1.053753000
1	-1.789193000	4.008262000	1.715002000
1	-0.191644000	4.060476000	0.981598000
6	-1.690527000	3.276764000	-0.348627000
1	-1.691375000	4.217637000	-0.911835000
1	-2.731810000	2.933518000	-0.302354000
6	-0.829139000	2.224233000	-1.069367000
1	0.188820000	2.622493000	-1.167773000
6	-1.368119000	1.869807000	-2.456129000
1	-2.355321000	1.400250000	-2.399234000
1	-0.703249000	1.206348000	-3.017282000
1	-1.476004000	2.787359000	-3.045922000
6	0.549281000	2.160561000	2.490145000
1	1.423199000	2.353840000	1.857238000
1	0.736787000	1.255535000	3.073616000
1	0.470682000	2.990371000	3.202144000
6	-2.302246000	-0.021770000	0.134499000
6	-3.376150000	0.363984000	0.950188000
1	-3.273017000	1.191164000	1.642700000

6	-4.610855000	-0.287660000	0.894233000
1	-5.419962000	0.039269000	1.540527000
6	-4.796640000	-1.342875000	0.008143000
1	-5.751680000	-1.856333000	-0.047900000
6	-3.742082000	-1.732402000	-0.818494000
1	-3.890752000	-2.545732000	-1.524572000
6	-2.496540000	-1.096190000	-0.773790000
6	-1.418455000	-1.578421000	-1.727267000
1	-0.936707000	-0.739874000	-2.232515000
1	-1.869278000	-2.211308000	-2.503076000
8	-0.347748000	-2.294005000	-1.096686000
6	-0.688748000	-3.635366000	-0.749002000
1	-0.970420000	-4.207237000	-1.643030000
1	0.201940000	-4.085371000	-0.304839000
1	-1.514028000	-3.672170000	-0.026622000
6	1.298725000	-1.426503000	2.335440000
6	-0.045398000	-1.332011000	2.030559000
1	-0.656093000	-0.544535000	2.457835000
4	4.568365000	-2.784475000	0.309402000
1	1.798460000	-0.665327000	2.930542000
1	1.776038000	-2.395594000	2.339401000
6	2.677588000	-1.816312000	0.050215000
6	3.698339000	-2.509754000	0.921412000
1	2.168931000	-2.503981000	-0.628389000
1	4.060901000	-1.894353000	1.749948000
1	3.306519000	-3.441287000	1.341224000
6	2.938558000	-0.523466000	-0.508136000
6	3.949437000	0.378816000	-0.039305000
1	4.661454000	0.040362000	0.705856000
6	1.990864000	-0.051304000	-1.465094000
1	1.396122000	-0.779424000	-2.010890000
6	2.173049000	1.237189000	-2.041940000
6	4.059306000	1.637974000	-0.577198000
6	3.174746000	2.069883000	-1.600521000
1	4.853897000	2.299401000	-0.243938000
1	1.541271000	1.543036000	-2.869176000
1	3.319724000	3.044508000	-2.057105000
1	-0.599270000	-2.209290000	1.710231000

76

E + ZPE = -2859.031639

28	1.002726000	-0.817390000	0.576500000
15	-0.479810000	0.875954000	0.268686000
6	-0.231917000	2.143193000	1.640912000
1	-1.166687000	2.713560000	1.715505000
6	0.811888000	3.075659000	0.995228000
1	0.964926000	3.962067000	1.621062000
1	1.781679000	2.563622000	0.920319000
6	0.280796000	3.441702000	-0.391562000
1	1.038004000	3.944575000	-1.003091000
1	-0.555087000	4.143757000	-0.279003000
6	-0.226897000	2.162189000	-1.110423000
1	0.579432000	1.766737000	-1.729453000
6	-1.435435000	2.456487000	-2.007453000
1	-2.299915000	2.795358000	-1.427643000
1	-1.748958000	1.595226000	-2.603804000
1	-1.168825000	3.257708000	-2.707035000
6	0.166910000	1.657236000	3.035265000
1	1.072444000	1.040526000	3.006856000
1	-0.624797000	1.083871000	3.527766000
1	0.379846000	2.522466000	3.673189000
6	-2.253301000	0.369274000	0.211786000

6	-3.161963000	0.855973000	1.161947000
1	-2.831426000	1.530928000	1.944015000
6	-4.510064000	0.491466000	1.131195000
1	-5.191076000	0.885410000	1.879719000
6	-4.972740000	-0.363008000	0.135419000
1	-6.021188000	-0.641971000	0.091699000
6	-4.076289000	-0.859780000	-0.812115000
1	-4.439143000	-1.519177000	-1.596810000
6	-2.718093000	-0.523796000	-0.786058000
6	-1.797540000	-1.152982000	-1.817097000
1	-1.018020000	-0.454360000	-2.130918000
1	-2.375443000	-1.426501000	-2.711507000
8	-1.089241000	-2.299316000	-2.336883000
6	-1.870680000	-3.489943000	-1.289084000
1	-2.276004000	-3.733304000	-2.281383000
1	-1.200868000	-4.291820000	-0.971136000
1	-2.700134000	-3.408553000	-0.574703000
6	2.746513000	-1.809160000	0.619813000
6	2.838011000	-0.804624000	-0.415084000
6	1.903544000	-0.916382000	-1.484002000
6	3.707618000	0.329217000	-0.387208000
1	1.318040000	-1.826225000	-1.607074000
1	4.400324000	0.449282000	0.439327000
6	1.974998000	-0.020721000	-2.573709000
6	3.741131000	1.205117000	-1.452264000
1	1.331534000	-0.174823000	-3.435069000
1	4.450720000	2.027363000	-1.452724000
6	2.891267000	1.015459000	-2.566174000
1	2.968209000	1.683273000	-3.419369000
6	-0.389600000	-1.512226000	1.880079000
6	0.843774000	-2.020209000	2.253185000
1	1.386104000	-1.579595000	3.085315000
1	1.098092000	-3.050844000	2.031175000
1	-1.075305000	-2.106651000	-2.33782000
1	-0.853186000	-0.727954000	2.466443000
1	2.534299000	-2.805280000	0.228087000
6	3.743055000	-1.823867000	1.758317000
1	3.793379000	-0.868956000	2.292342000
1	3.505681000	-2.602555000	2.487454000
1	4.748187000	-2.042663000	1.373970000

77

E + ZPE = -2628.036837

28	1.613358000	-0.248551000	-0.443649000
15	-0.356429000	0.755151000	-0.014711000
6	-0.385625000	1.685994000	1.632064000
1	-1.314662000	1.374653000	2.123767000
6	-0.512503000	3.172571000	1.228968000
1	-0.887944000	3.762571000	2.072544000
1	0.481386000	3.570569000	0.981804000
6	-1.427807000	3.267384000	0.002314000
1	-1.423970000	4.274091000	-0.431049000
1	-2.466544000	3.051187000	0.282624000
6	-0.924875000	2.239318000	-1.033418000
1	0.000774000	2.641971000	-1.457855000
6	-1.884535000	1.936848000	-2.186439000
1	-2.835004000	1.527004000	-1.832810000
1	-1.454566000	1.223267000	-2.898752000
1	-2.100778000	2.859620000	-2.735997000
6	0.782342000	1.395565000	2.577566000
1	1.744943000	1.662741000	2.127139000
1	0.819839000	0.340630000	2.871012000

1	0.673845000	1.984263000	3.495675000
6	-1.790259000	-0.407251000	0.046304000
6	-3.038366000	0.022170000	0.527829000
1	-3.162149000	1.034615000	0.897668000
6	-4.144730000	-0.827276000	0.537390000
1	-5.098579000	-0.465655000	0.909434000
6	-4.018590000	-2.134935000	0.072527000
1	-4.872028000	-2.805945000	0.079647000
6	-2.781213000	-2.584342000	-0.386143000
1	-2.676442000	-3.610738000	-0.728743000
6	-1.668335000	-1.736947000	-0.411718000
6	-0.355808000	-2.287430000	-0.911538000
1	-0.045380000	-1.840654000	-1.860795000
1	-0.425125000	-3.370205000	-1.060904000
8	0.746926000	-2.033041000	-0.007768000
6	0.610013000	-2.666210000	1.280829000
1	0.397146000	-3.730130000	1.138512000
1	1.564582000	-2.551618000	1.793238000
1	-0.191471000	-2.200265000	1.861349000
6	3.403234000	-1.237855000	-0.153154000
6	3.815299000	-0.828443000	1.256547000
1	4.475525000	-1.594265000	1.685700000
1	4.374156000	0.114293000	1.258022000
1	4.289762000	-1.390341000	-0.765926000
1	2.867901000	-2.188958000	-0.197558000
6	2.190850000	1.327198000	-1.362077000
6	3.288721000	0.434090000	-1.464757000
1	3.437902000	-0.115479000	-2.390941000
1	2.319423000	2.224090000	-0.755829000
1	2.973244000	-0.705778000	1.946670000
1	1.571176000	1.476873000	-2.245456000
1	4.213155000	0.721389000	-0.975773000

78
E + ZPE = -2859.011273

28	-0.229910000	1.408646000	-0.436229000
15	0.618203000	-0.644404000	0.077267000
6	0.169343000	-1.266124000	1.807143000
1	1.110109000	-1.645039000	2.224389000
6	-0.771200000	-2.464100000	1.546695000
1	-0.818806000	-3.104225000	2.435197000
1	-1.787704000	-2.097961000	1.357512000
6	-0.256975000	-3.224224000	0.317365000
1	-0.977874000	-3.976440000	-0.022982000
1	0.668328000	-3.763507000	0.558118000
6	-0.005299000	-2.189768000	-0.802165000
1	-0.988743000	-1.892588000	-1.174843000
6	0.826665000	-2.685816000	-1.987240000
1	1.827562000	-3.006883000	-1.685474000
1	0.940625000	-1.915647000	-2.759053000
1	0.327240000	-3.543682000	-2.451627000
6	-0.400244000	-0.222157000	2.770230000
1	-1.343494000	0.192486000	2.400676000
1	0.300172000	0.602310000	2.945056000
1	-0.603782000	-0.686599000	3.741986000
6	2.466138000	-0.733761000	0.012352000
6	3.129985000	-1.893268000	0.448052000
1	2.563349000	-2.728074000	0.846631000
6	4.518253000	-2.007704000	0.376734000
1	5.001631000	-2.919070000	0.715590000
6	5.276818000	-0.951184000	-0.124032000
1	6.358476000	-1.027160000	-0.178249000

6	4.636938000	0.215819000	-0.537607000
1	5.227162000	1.050991000	-0.906626000
6	3.244031000	0.333739000	-0.482297000
6	2.610126000	1.624228000	-0.933380000
1	2.050750000	1.512796000	-1.867666000
1	3.370833000	2.396742000	-1.090373000
8	1.642530000	2.130153000	0.013754000
6	2.199642000	2.521054000	1.283860000
1	3.013402000	3.234172000	1.117569000
1	1.399162000	3.004568000	1.843880000
1	2.574149000	1.651408000	1.831793000
6	-0.793751000	3.389937000	-0.277941000
6	-1.439195000	3.525918000	1.096174000
1	-1.272229000	4.543148000	1.476090000
1	-2.523096000	3.378095000	1.051006000
1	-1.270135000	4.080712000	-0.971463000
1	0.261169000	3.667097000	-0.286602000
6	-1.752158000	0.630437000	-1.380934000
6	-1.797527000	2.042254000	-1.587350000
1	-2.689715000	2.550791000	-1.237623000
1	-1.041450000	2.832967000	1.847598000
1	-1.310566000	0.056757000	-2.197820000
1	-1.402336000	2.448838000	-2.516052000
6	-2.888440000	-0.069204000	-0.720577000
6	-3.477117000	0.382290000	0.473713000
1	-3.082088000	1.260473000	0.975209000
6	-3.437545000	-1.208815000	-1.335168000
1	-3.019907000	-1.561369000	-2.275702000
6	-4.534330000	-1.869957000	-0.781966000
6	-4.572950000	-0.277773000	1.028638000
6	-5.104580000	-1.409175000	0.405555000
1	-5.012412000	0.092611000	1.950532000
1	-4.946957000	-2.739976000	-1.284671000
1	-5.958391000	-1.921866000	0.838247000

79
E + ZPE = -2859.010267

28	0.455021000	-0.648809000	-0.259114000
15	-1.256826000	0.763329000	-0.004498000
6	-1.187569000	1.773138000	1.591228000
1	-2.200068000	1.736707000	2.010826000
6	-0.906495000	3.214657000	1.110974000
1	-1.168290000	3.934055000	1.895035000
1	0.168817000	3.333298000	0.917552000
6	-1.694555000	3.453660000	-0.182774000
1	-1.418082000	4.401433000	-0.658847000
1	-2.769388000	3.512626000	0.032711000
6	-1.402357000	2.271767000	-1.131721000
1	-0.389023000	2.414243000	-1.522024000
6	-2.350360000	2.133898000	-2.325284000
1	-3.388787000	1.993332000	-2.012236000
1	-2.075688000	1.289861000	-2.968338000
1	-2.304576000	3.041578000	-2.937309000
6	-0.207796000	1.261731000	2.649754000
1	0.821638000	1.243484000	2.274153000
1	-0.464637000	0.252741000	2.990936000
1	-0.228694000	1.917946000	3.527368000
6	-2.915837000	-0.047055000	-0.023308000
6	-4.067415000	0.670738000	0.338800000
1	-3.986632000	1.702179000	0.666166000
6	-5.334000000	0.089341000	0.277956000
1	-6.207875000	0.669742000	0.558222000

6	-5.469986000	-1.233041000	-0.140605000
1	-6.450572000	-1.696691000	-0.187882000
6	-4.334573000	-1.965010000	-0.485314000
1	-4.437755000	-3.002059000	-0.794885000
6	-3.061027000	-1.388169000	-0.438999000
6	-1.869161000	-2.231624000	-0.820181000
1	-1.382245000	-1.878320000	-1.734180000
1	-2.172826000	-3.271063000	-0.986419000
8	-0.827086000	-2.221976000	0.182907000
6	-1.226089000	-2.831822000	1.426736000
1	-1.655576000	-3.817933000	1.222882000
1	-0.327633000	-2.946586000	2.030282000
1	-1.959503000	-2.210170000	1.949236000
6	1.969621000	-2.025473000	0.096291000
6	2.146632000	-1.796400000	1.592254000
1	2.481109000	-2.727641000	2.070705000
1	2.919342000	-1.045732000	1.783975000
1	2.920944000	-2.334879000	-0.326404000
1	1.256133000	-2.812880000	-0.164542000
6	1.390567000	0.617980000	-1.294452000
6	2.420256000	-0.374865000	-1.215776000
1	2.474406000	-1.055018000	-2.062683000
1	1.605811000	1.589854000	-0.852314000
1	1.238737000	-1.474205000	2.114064000
1	0.874285000	0.699304000	-2.254020000
6	3.757793000	-0.046754000	-0.653459000
6	3.948701000	0.925588000	0.342112000
1	3.095396000	1.449990000	0.764062000
6	4.885869000	-0.704702000	-1.168519000
1	4.759779000	-1.456306000	-1.944855000
6	6.167244000	-0.391800000	-0.716845000
6	5.228199000	1.234457000	0.800150000
6	6.341969000	0.578037000	0.271164000
1	5.356367000	1.990079000	1.569816000
1	7.027269000	-0.903236000	-1.138864000
1	7.338528000	0.823142000	0.626123000

80
E + ZPE = -2628.024426

28	1.522899000	-0.792512000	-0.086671000
15	-0.248839000	0.746925000	0.025547000
6	-0.360856000	2.043111000	1.400445000
1	-1.417509000	2.081778000	1.687148000
6	0.001089000	3.371987000	0.699714000
1	-0.343018000	4.223868000	1.297146000
1	1.093359000	3.463099000	0.619329000
6	-0.623296000	3.359485000	-0.701687000
1	-0.281415000	4.204779000	-1.310085000
1	-1.715591000	3.445127000	-0.628525000
6	-0.246306000	2.021551000	-1.373002000
1	0.810692000	2.083307000	-1.667766000
6	-1.067155000	1.658533000	-2.612624000
1	-2.132291000	1.564982000	-2.380615000
1	-0.736164000	0.714786000	-3.061389000
1	-0.956469000	2.440119000	-3.372493000
6	0.454311000	1.748146000	2.663084000
1	1.529644000	1.711012000	2.459041000
1	0.160817000	0.800182000	3.127615000
1	0.292200000	2.539031000	3.404132000
6	-1.899454000	-0.086709000	0.012043000
6	-3.072706000	0.658519000	0.220537000
1	-3.014731000	1.731198000	0.373528000

6	-4.331464000	0.058697000	0.225669000
1	-5.218059000	0.665987000	0.380987000
6	-4.441340000	-1.317114000	0.037206000
1	-5.413668000	-1.799869000	0.050760000
6	-3.289123000	-2.074650000	-0.163735000
1	-3.375628000	-3.148697000	-0.308481000
6	-2.020866000	-1.481059000	-0.194422000
6	-0.851206000	-2.384858000	-0.515244000
1	-0.455514000	-2.196063000	-1.517873000
1	-1.165751000	-3.433170000	-0.475470000
8	0.296454000	-2.246462000	0.356172000
6	0.061923000	-2.617038000	1.728936000
1	-0.409673000	-3.604238000	1.755005000
1	1.039003000	-2.664128000	2.210447000
1	-0.577828000	-1.883686000	2.229770000
6	3.013546000	0.560876000	0.059930000
6	4.460272000	0.382984000	0.505067000
1	4.683695000	1.116688000	1.289575000
1	4.639074000	-0.608544000	0.934185000
1	2.848003000	1.507674000	-0.457148000
1	2.402632000	0.567836000	0.982760000
6	2.766701000	-2.013775000	-0.883112000
6	2.976101000	-0.737696000	-1.510203000
1	3.588739000	-2.426459000	-0.301196000
1	2.329602000	-0.453163000	-2.343945000
1	3.980776000	-0.365747000	-1.676997000
1	2.172320000	-2.769329000	-1.394302000
1	5.181517000	0.543879000	-0.302544000

81
E + ZPE = -2859.000385

28	-0.650405000	-0.781125000	0.255176000
15	1.666256000	-0.478461000	0.036763000
6	2.627655000	-1.172242000	1.510972000
1	3.322766000	-0.382368000	1.818436000
6	3.441921000	-2.346410000	0.921035000
1	4.280437000	-2.599293000	1.579745000
1	2.805341000	-3.240903000	0.864691000
6	3.907952000	-1.956256000	-0.486652000
1	4.348180000	-2.806451000	-1.020686000
1	4.686904000	-1.184757000	-0.428636000
6	2.683298000	-1.411477000	-1.252522000
1	2.054062000	-2.270540000	-1.519826000
6	3.004606000	-0.644554000	-2.537629000
1	3.634392000	0.228670000	-2.344096000
1	2.097251000	-0.298497000	-3.045421000
1	3.541819000	-1.298289000	-3.233796000
6	1.770758000	-1.560263000	2.720200000
1	1.039829000	-2.337153000	2.465908000
1	1.228005000	-0.702597000	3.133110000
1	2.407149000	-1.958558000	3.518897000
6	2.164535000	1.291951000	-0.086970000
6	3.499295000	1.691839000	0.086608000
1	4.260514000	0.957570000	0.330407000
6	3.881326000	3.026106000	-0.054723000
1	4.921797000	3.306682000	0.078790000
6	2.925105000	3.991823000	-0.363794000
1	3.211086000	5.033740000	-0.470593000
6	1.591931000	3.614707000	-0.520342000
1	0.842966000	4.370411000	-0.743673000
6	1.200369000	2.277309000	-0.395440000
6	-0.258710000	1.935850000	-0.583610000

1	-0.439403000	1.333106000	-1.477616000
1	-0.859699000	2.846839000	-0.670747000
8	-0.813373000	1.153830000	0.505420000
6	-0.777569000	1.824626000	1.781135000
1	-1.200704000	2.826991000	1.667806000
1	-1.394085000	1.243228000	2.463955000
1	0.247198000	1.891972000	2.157779000
6	-0.564960000	-2.736331000	-0.569457000
6	-0.674081000	-2.357872000	-2.045771000
1	-1.719578000	-2.298394000	-2.364140000
1	-0.200813000	-1.403703000	-2.299999000
1	-0.941553000	-3.751713000	-0.453741000
1	0.462555000	-2.830843000	-0.210476000
6	-2.431599000	-0.983702000	0.962833000
6	-2.087274000	-2.330070000	0.598229000
1	-2.308083000	-0.755858000	2.025057000
1	-2.759327000	-2.806210000	-0.110509000
1	-1.805567000	-2.996042000	1.410925000
1	-0.202253000	-3.133839000	-2.661939000
6	-3.544186000	-0.239991000	0.332115000
6	-3.968378000	-0.460796000	-0.991733000
1	-3.480189000	-1.214782000	-1.602632000
6	-4.216848000	0.743952000	1.079667000
1	-3.925209000	0.920270000	2.112707000
6	-5.273528000	1.470807000	0.534888000
6	-5.022679000	0.266931000	-1.539305000
6	-5.680145000	1.237781000	-0.779986000
1	-5.334567000	0.072408000	-2.561605000
1	-5.784958000	2.213475000	1.140757000
1	-6.504544000	1.800882000	-1.207075000

82
E + ZPE = -2858.998689

28	-0.733834000	0.835017000	-1.054100000
15	0.862839000	0.503810000	0.670902000
6	1.561619000	1.997271000	1.603396000
1	2.628063000	1.789090000	1.740535000
6	0.879329000	1.925812000	2.987017000
1	1.422806000	2.541168000	3.713228000
1	-0.137808000	2.337214000	2.921830000
6	0.820360000	0.451916000	3.407417000
1	0.219808000	0.307474000	4.313079000
1	1.830624000	0.087613000	3.637862000
6	0.229370000	-0.355840000	2.232408000
1	-0.853712000	-0.179782000	2.204350000
6	0.458133000	-1.866990000	2.303531000
1	1.523417000	-2.117930000	2.294884000
1	-0.026132000	-2.389422000	1.472119000
1	0.028420000	-2.260361000	3.231803000
6	1.447641000	3.353349000	0.900712000
1	0.406614000	3.660735000	0.758215000
1	1.941084000	3.350389000	-0.077775000
1	1.932309000	4.126779000	1.507468000
6	2.352552000	-0.426881000	0.090176000
6	3.508817000	-0.506536000	0.884262000
1	3.531626000	-0.040099000	1.863649000
6	4.646807000	-1.189659000	0.455520000
1	5.520635000	-1.237933000	1.098356000
6	4.656276000	-1.801365000	-0.795808000
1	5.539792000	-2.325598000	-1.146970000
6	3.518818000	-1.733869000	-1.598382000
1	3.523389000	-2.214403000	-2.573657000

6	2.362946000	-1.070158000	-1.169307000
6	1.149305000	-1.140855000	-2.066394000
1	0.348083000	-1.732335000	-1.615996000
1	1.414431000	-1.603944000	-3.023024000
8	0.526883000	0.133386000	-2.363875000
6	1.343628000	1.038492000	-3.131994000
1	1.716627000	0.516884000	-4.019109000
1	0.695985000	1.861615000	-3.433307000
1	2.183675000	1.408992000	-2.536385000
6	-1.990930000	2.052951000	0.019933000
6	-2.925490000	3.185416000	-0.386593000
1	-2.651600000	4.097211000	0.158526000
1	-2.849928000	3.415068000	-1.454632000
1	-2.117480000	1.755242000	1.061472000
1	-0.966370000	2.452240000	-0.098294000
6	-2.174153000	0.665569000	-2.277457000
6	-2.815910000	0.516037000	-0.984042000
1	-2.485380000	1.534284000	-2.856180000
1	-3.736900000	1.071252000	-0.832367000
1	-2.001939000	-0.211195000	-2.897978000
1	-3.974994000	2.972926000	-0.156052000
6	-2.889412000	-0.802610000	-0.268120000
6	-3.509095000	-0.854990000	0.992379000
1	-3.896129000	0.058927000	1.437189000
6	-2.443792000	-2.007715000	-0.836874000
1	-2.016837000	-2.017125000	-1.834859000
6	-2.598024000	-3.218820000	-0.159800000
6	-3.654877000	-2.061744000	1.674255000
6	-3.196034000	-3.250110000	1.101087000
1	-4.143032000	-2.076941000	2.644420000
1	-2.266325000	-4.141188000	-0.628167000
1	-3.320438000	-4.193576000	1.624084000

83
E + ZPE = -2744.680088

28	-0.789400000	-0.151568000	-1.009842000
15	1.115668000	-0.735059000	0.038877000
6	0.843059000	-1.502817000	1.747798000
1	1.552252000	-0.992086000	2.410261000
6	1.293523000	-2.971440000	-1.581875000
1	1.507745000	-3.414132000	2.561084000
1	0.474919000	-3.557339000	1.141384000
6	2.511677000	-3.003560000	0.651528000
1	2.777268000	-4.027139000	0.363437000
1	3.390178000	-2.582485000	1.156849000
6	2.159860000	-2.172151000	-0.600345000
1	1.455634000	-2.768019000	-1.189509000
6	3.339535000	-1.801221000	-1.502067000
1	4.087970000	-1.203083000	-0.974393000
1	3.017591000	-1.235360000	-2.383781000
1	3.830616000	-2.713301000	-1.859061000
6	-0.563126000	-1.347704000	2.331224000
1	-1.320061000	-1.824389000	1.698340000
1	-0.838567000	-0.295691000	2.464228000
1	-0.610884000	-1.823789000	3.317262000
6	2.279936000	0.672732000	0.309126000
6	3.412736000	0.513927000	1.124762000
1	3.597735000	-0.432545000	1.622030000
6	4.326620000	1.551422000	1.309281000
1	5.196806000	1.397522000	1.940222000
6	4.115679000	2.779702000	0.685518000
1	4.817459000	3.595995000	0.826353000

6	2.985062000	2.960830000	-0.109608000	1	2.403799000	4.081567000	-1.395443000
1	2.809007000	3.924846000	-0.580412000	6	2.119015000	2.059413000	-0.719303000
6	2.069592000	1.922464000	-0.312631000	6	0.926016000	1.857479000	-1.620484000
6	0.866695000	2.185164000	-1.184659000	1	1.113438000	1.121771000	-2.408188000
1	0.898225000	1.624423000	-2.123619000	1	0.645818000	2.799171000	-2.104419000
1	0.799213000	3.249413000	-1.434550000	8	-0.235919000	1.355533000	-0.917442000
8	-0.382218000	1.793013000	-0.566039000	6	-0.752547000	2.261738000	0.079853000
6	-0.698361000	2.524658000	0.634983000	1	-0.881112000	3.252044000	-0.367769000
1	-0.628743000	3.597884000	0.432453000	1	-1.725032000	1.878165000	0.388156000
1	-1.724128000	2.270367000	0.899865000	1	-0.075312000	2.325987000	0.936625000
1	-0.017802000	2.254073000	1.447599000	6	-2.262764000	-0.540164000	-1.183231000
6	-2.726864000	0.495767000	-1.312824000	6	-2.856536000	-0.865093000	0.193060000
6	-3.416927000	0.100207000	-0.010588000	1	-2.978477000	-1.952926000	0.287766000
1	-3.704170000	-0.958859000	-0.041060000	1	-2.938183000	-0.881568000	-1.965669000
1	-3.435491000	0.431448000	-2.137601000	1	-2.153895000	0.530695000	-1.368033000
1	-2.372015000	1.529704000	-1.329521000	6	0.104445000	-2.492789000	-1.401442000
6	-0.811860000	-1.847137000	-1.893508000	6	-1.163427000	-2.187574000	-1.963323000
6	-1.968650000	-1.183008000	-2.378479000	1	-1.228008000	-1.923585000	-3.016272000
1	-1.939077000	-0.714052000	-3.358933000	1	0.140455000	-3.232872000	-0.601710000
1	-0.957501000	-2.722336000	-1.260253000	1	-2.182506000	-0.564571000	1.004468000
1	-2.745963000	0.202342000	0.853569000	1	0.963369000	-2.526684000	-2.070817000
1	0.050499000	-1.920923000	-2.555597000	1	-2.015726000	-2.755136000	-1.606204000
1	-2.931119000	-1.618280000	-2.133595000	6	-4.195787000	-0.174422000	0.393310000
6	-4.692881000	0.941012000	0.249402000	6	-4.339751000	0.848032000	1.339650000
1	-5.387620000	0.808350000	-0.589040000	1	-3.493214000	1.124604000	1.965833000
1	-4.421078000	2.007412000	0.265211000	6	-5.311742000	-0.539174000	-0.373807000
6	-5.369803000	0.565919000	1.540689000	1	-5.229165000	-1.343141000	-1.102241000
1	-4.797452000	0.749591000	2.451759000	6	-6.535823000	0.105507000	-0.201807000
6	-6.586136000	0.028530000	1.633911000	6	-5.564078000	1.496578000	1.514434000
1	-7.195094000	-0.167811000	0.753695000	6	-6.664753000	1.128551000	0.740922000
1	-7.026621000	-0.225835000	2.593725000	1	-5.658247000	2.281562000	2.259585000
.....				1	-7.391811000	-0.194900000	-0.799415000
				1	-7.619343000	1.628488000	0.876176000
.....							

84
E + ZPE = -2859.005955

28	-0.224184000	-0.677799000	-0.892489000
15	1.770442000	-0.620923000	0.153615000
6	1.694430000	-1.145362000	1.969500000
1	2.251480000	-0.376743000	2.517757000
6	2.493877000	-2.466990000	2.021218000
1	2.816113000	-2.674683000	3.047791000
1	1.843289000	-3.299346000	1.719049000
6	3.677580000	-2.358105000	1.052295000
1	4.184427000	-3.320770000	0.919039000
1	4.428988000	-1.659840000	1.442733000
6	3.125635000	-1.854690000	-0.298333000
1	2.585424000	-2.691008000	-0.753831000
6	4.175157000	-1.363318000	-1.298198000
1	4.751881000	-0.521055000	-0.905445000
1	3.721810000	-1.049011000	-2.245408000
1	4.876682000	-2.174152000	-1.523558000
6	0.292240000	-1.245072000	2.574606000
1	-0.321874000	-1.988312000	2.054052000
1	-0.233629000	-0.284242000	2.550036000
1	0.361428000	-1.552133000	3.624390000
6	2.574953000	1.041461000	0.146095000
6	3.675749000	1.311851000	0.975716000
1	4.046647000	0.552520000	1.656031000
6	4.323559000	2.546964000	0.942855000
1	5.175866000	2.725805000	1.591399000
6	3.872110000	3.543895000	0.080127000
1	4.366087000	4.510214000	0.049869000
6	2.768509000	3.298295000	-0.735601000

85R
E + ZPE = -2937.575773

28	0.307712000	-0.968871000	-1.069942000
15	1.939920000	-0.561808000	0.429060000
6	1.358942000	-0.580261000	2.228876000
1	1.757914000	0.338620000	2.673816000
6	2.087378000	-1.791807000	2.856608000
1	2.122546000	-1.687688000	3.946848000
1	1.519247000	-2.708177000	2.645019000
6	3.486456000	-1.898097000	2.238770000
1	3.984406000	-2.833678000	2.518431000
1	4.127671000	-1.082857000	2.597226000
6	3.323132000	-1.817822000	0.706678000
1	2.892911000	-2.770302000	0.380375000
6	4.611601000	-1.579691000	-0.083676000
1	5.094222000	-0.638648000	0.195335000
1	4.429489000	-1.558644000	-1.164364000
1	5.320154000	-2.391713000	0.113739000
6	-0.157587000	-0.595234000	2.439420000
1	-0.622916000	-1.477669000	1.986386000
1	-0.641404000	0.296424000	2.027177000
1	-0.382153000	-0.619413000	3.511941000
6	2.791527000	1.060574000	0.189550000
6	3.624672000	1.591258000	1.187892000
1	3.747200000	1.070080000	2.131398000
6	4.319925000	2.785350000	0.994228000
1	4.961308000	3.168961000	1.781966000
6	4.186210000	3.478890000	-0.206926000

1	4.719549000	4.411042000	-0.366090000
6	3.348134000	2.975279000	-1.200953000
1	3.227740000	3.525047000	-2.131123000
6	2.655997000	1.773088000	-1.021599000
1	1.753826000	1.283717000	-2.127030000
1	2.108796000	0.354420000	-2.582079000
1	1.675129000	2.034344000	-2.920804000
8	0.415563000	0.980569000	-1.664768000
6	-0.296865000	2.131445000	-1.165251000
1	-0.267509000	2.925407000	-1.918090000
1	-1.328487000	1.824698000	-0.999933000
1	0.145658000	2.489020000	-0.230982000
6	-1.537685000	-0.971202000	-1.989504000
6	-2.450316000	-0.728843000	-0.791990000
1	-2.642562000	-1.676782000	-0.271468000
1	-2.027192000	-1.609853000	-2.720641000
1	-1.272614000	-0.061914000	-2.535843000
6	0.682050000	-2.841516000	-0.913905000
6	-0.397459000	-2.772735000	-1.830459000
1	-0.196790000	-2.873180000	-2.894057000
1	0.495217000	-3.293114000	0.060481000
1	-1.970242000	-0.077214000	-0.050719000
1	1.675838000	-3.044337000	-1.311631000
1	-1.342591000	-3.205766000	-1.521164000
6	-3.819016000	-0.084372000	-1.175145000
1	-3.605065000	0.781592000	-1.818220000
6	-4.712149000	-1.047782000	-1.977824000
1	-4.237186000	-1.360674000	-2.914208000
1	-4.946811000	-1.948876000	-1.399593000
1	-5.659499000	-0.563475000	-2.233517000
6	-4.522167000	0.443759000	0.068137000
6	-4.756137000	1.816687000	0.219453000
1	-4.449524000	2.501770000	-0.568913000
6	-4.944642000	-0.418572000	1.091233000
1	-4.787032000	-1.490699000	0.998711000
6	-5.580847000	0.078137000	2.228857000
6	-5.393997000	2.318466000	1.355840000
6	-5.807315000	1.449565000	2.365691000
1	-5.572962000	3.386349000	1.447342000
1	-5.906069000	-0.607301000	3.006803000
1	-6.307639000	1.835480000	3.249236000

85S

E + ZPE = -2937.577144

28	0.011550000	-0.134806000	-0.664094000
15	2.094642000	-0.733208000	-0.045553000
6	2.168025000	-1.596972000	1.636750000
1	2.985040000	-1.107920000	2.180382000
6	2.594179000	-3.044166000	1.303270000
1	2.998335000	-3.535342000	2.195527000
1	1.712412000	-3.622657000	0.994444000
6	3.609665000	-2.997699000	0.155655000
1	3.829674000	-3.998001000	-0.234710000
1	4.562959000	-2.581316000	0.505652000
6	3.011841000	-2.110751000	-0.956694000
1	2.215833000	-2.691438000	-1.434683000
6	3.992665000	-1.663947000	-2.043264000
1	4.817612000	-1.073487000	-1.634019000
1	3.499920000	-1.063574000	-2.816733000
1	4.421879000	-2.543936000	-2.535078000
6	0.898184000	-1.502732000	2.485777000
1	0.037815000	-1.955453000	1.980366000

1	0.644637000	-0.465836000	2.732281000
1	1.043156000	-2.036254000	3.432247000
6	3.278970000	0.679637000	0.064058000
6	4.536775000	0.517706000	0.668424000
1	4.812611000	-0.434878000	1.108534000
6	5.462009000	1.560855000	0.711404000
1	6.429207000	1.404335000	1.179468000
6	5.139109000	2.797330000	0.155648000
1	5.850061000	3.617235000	0.187392000
6	3.886877000	2.981367000	-0.428743000
1	3.625985000	3.951277000	-0.844876000
6	2.956192000	1.938582000	-0.487459000
6	1.615446000	2.203794000	-1.126425000
1	1.476415000	1.648583000	-2.058750000
1	1.501754000	3.269247000	-1.353494000
8	0.502504000	1.804436000	-0.291733000
6	0.400069000	2.544107000	0.941193000
1	0.404329000	3.616088000	0.720174000
1	-0.551045000	2.270922000	1.396882000
1	1.227146000	2.299869000	1.614250000
6	-1.945741000	0.490128000	-0.533048000
6	-2.350031000	0.034559000	0.865622000
1	-2.502861000	-1.053111000	0.878590000
1	-2.806504000	0.440068000	-1.196574000
1	-1.616156000	1.531318000	-0.582130000
6	-0.184776000	-1.812409000	-1.564779000
6	-1.414531000	-1.142921000	-1.793770000
1	-1.578097000	-0.643483000	-2.745680000
1	-0.198552000	-2.704741000	-0.938641000
1	-1.556154000	0.231602000	1.598593000
1	0.530992000	-1.861187000	-2.384586000
1	-2.312732000	-1.585355000	-1.377275000
6	-3.656903000	0.715664000	1.368114000
1	-3.503010000	1.802832000	1.314673000
6	-3.913441000	0.354227000	2.843085000
1	-3.074301000	0.665065000	3.477194000
1	-4.817657000	0.849624000	3.209834000
1	-4.050061000	-0.725256000	2.973420000
6	-4.848785000	0.381830000	0.480003000
6	-5.517771000	1.391210000	-0.224321000
1	-5.181405000	2.421608000	-0.129412000
6	-5.309730000	-0.937536000	0.346135000
1	-4.822063000	-1.742305000	0.892107000
6	-6.404230000	-1.235680000	-0.465870000
6	-6.615213000	1.097806000	-1.036898000
6	-7.061080000	-0.217900000	-1.161296000
1	-7.121841000	1.898542000	-1.568605000
1	-6.749174000	-2.262685000	-0.550095000
1	-7.915865000	-0.449337000	-1.790284000

86R

E + ZPE = -3168.586197

28	-0.707291000	-0.549035000	0.874782000
15	0.269811000	1.419368000	0.268662000
6	1.026490000	2.317163000	1.752566000
1	0.670236000	3.351429000	1.675028000
6	2.547511000	2.295273000	1.478408000
1	3.044677000	3.080853000	2.059059000
1	2.970613000	1.338364000	1.811275000
6	2.777354000	2.459279000	-0.028958000
1	3.818183000	2.253154000	-0.301441000
1	2.562117000	3.489458000	-0.341889000

6	1.844263000	1.466959000	-0.757618000
1	2.275457000	0.471264000	-0.622397000
6	1.676474000	1.706686000	-2.259572000
1	1.272245000	2.698999000	-2.479970000
1	1.015915000	0.964253000	-2.721727000
1	2.654210000	1.626212000	-2.747409000
6	0.635012000	1.765195000	3.126227000
1	0.935150000	0.717612000	3.239512000
1	-0.443550000	1.834435000	3.305594000
1	1.134099000	2.340004000	3.914859000
6	-0.904244000	2.625485000	-0.493920000
6	-0.492750000	3.944955000	-0.746448000
1	0.504193000	4.267229000	-0.464303000
6	-1.339861000	4.865732000	-1.362801000
1	-0.992044000	5.877223000	-1.549957000
6	-2.628542000	4.483111000	-1.730717000
1	-3.298417000	5.192842000	-2.206490000
6	-3.061193000	3.184921000	-1.465076000
1	-4.074208000	2.891820000	-1.729529000
6	-2.215752000	2.249492000	-0.858826000
6	-2.751002000	0.864011000	-0.588571000
1	-2.287409000	0.102129000	-1.221501000
1	-3.831287000	0.821810000	-0.763567000
8	-2.496791000	0.423813000	0.764991000
6	-3.154714000	1.219142000	1.767210000
1	-4.235558000	1.192936000	1.594398000
1	-2.925655000	0.771442000	2.733931000
1	-2.799547000	2.253415000	1.744390000
6	2.644238000	-2.870631000	-0.552122000
6	0.983566000	-1.446597000	0.827848000
6	1.291764000	-2.094645000	-0.527100000
1	0.504759000	-2.811776000	-0.793791000
1	1.298666000	-1.351903000	-1.336575000
1	2.646532000	-3.529187000	0.327384000
1	0.983375000	-2.224439000	1.602935000
1	1.794099000	-0.761465000	1.102306000
6	-1.695494000	-2.460215000	1.056805000
6	-1.520141000	-1.809228000	2.263256000
1	-0.914913000	-3.149186000	0.748535000
1	-0.711516000	-2.098350000	2.926944000
1	-2.351719000	-1.301778000	2.744179000
6	-2.926114000	-2.555671000	0.254210000
6	-2.841809000	-3.073202000	-1.052279000
1	-1.875297000	-3.385459000	-1.440904000
6	-4.192728000	-2.193098000	0.749946000
1	-4.293031000	-1.838214000	1.771049000
6	-5.329513000	-2.326817000	-0.042049000
6	-3.978947000	-3.200255000	-1.847920000
6	-5.226071000	-2.823884000	-1.345717000
1	-3.893927000	-3.604003000	-2.852481000
1	-6.302426000	-2.061725000	0.362032000
1	-6.116243000	-2.934247000	-1.958054000
6	3.846335000	-1.943653000	-0.420486000
6	4.317871000	-1.191393000	-1.508431000
1	3.837846000	-1.283172000	-2.479482000
6	4.513669000	-1.813716000	0.806238000
1	4.180046000	-2.402360000	1.658112000
6	5.610079000	-0.959917000	0.948359000
6	5.416027000	-0.339063000	-1.373424000
6	6.065652000	-0.217817000	-0.142548000
1	5.775157000	0.217268000	-2.235465000
1	6.116817000	-0.887781000	1.906983000
1	6.928116000	0.434823000	-0.040155000
6	2.720208000	-3.770537000	-1.798899000

1	3.672176000	-4.309423000	-1.836279000
1	1.911985000	-4.510624000	-1.787967000
1	2.625544000	-3.194288000	-2.726459000
.....			
86S			
E + ZPE = -3168.585274			
28	0.475342000	-0.780136000	-0.552147000
15	0.132308000	1.390827000	0.049158000
6	-1.179508000	2.313755000	-0.949128000
1	-0.718454000	3.274512000	-1.205601000
6	-2.329042000	2.563011000	0.056698000
1	-2.941219000	3.408828000	-0.276868000
1	-2.991500000	1.690263000	0.087235000
6	-1.727595000	2.809937000	1.447602000
1	-2.499137000	2.792286000	2.225809000
1	-1.257099000	3.800890000	1.493974000
6	-0.672342000	1.713270000	1.720854000
1	-1.207615000	0.782439000	1.936993000
6	0.284955000	1.998023000	2.880424000
1	0.867486000	2.909742000	2.718396000
1	0.987129000	1.171896000	3.041065000
1	-0.288181000	2.126728000	3.805431000
6	-1.615080000	1.629002000	-2.248450000
1	-2.073540000	0.653626000	-2.058159000
1	-0.775303000	1.489754000	-2.938823000
1	-2.360383000	2.247516000	-2.761451000
6	1.639249000	2.458453000	-0.023125000
6	1.520796000	3.850717000	0.131716000
1	0.544414000	4.301846000	0.273611000
6	2.638966000	4.683671000	0.117393000
1	2.514964000	5.754754000	0.245800000
6	3.907254000	4.136515000	-0.066892000
1	4.784850000	4.775429000	-0.087920000
6	4.041087000	2.760258000	-0.240444000
1	5.027949000	2.333070000	-0.400711000
6	2.927668000	1.912716000	-0.211133000
6	3.161448000	0.430004000	-0.373363000
1	3.006376000	-0.122111000	0.556688000
1	4.188224000	0.236954000	-0.701594000
8	2.267613000	-0.196945000	-1.322016000
6	2.397454000	0.297247000	-2.667530000
1	3.437579000	0.191312000	-2.992659000
1	1.751302000	-0.316346000	-3.295896000
1	2.094783000	1.346605000	-2.732592000
6	-3.475085000	-2.473473000	0.362091000
6	-1.246800000	-1.203448000	0.198884000
6	-2.122925000	-2.313608000	-0.388154000
1	-2.336933000	-2.111330000	-1.446824000
1	-1.623705000	-3.290095000	-0.354696000
1	-3.236801000	-2.627248000	1.424001000
1	-1.862547000	-0.299321000	0.198980000
1	-1.038003000	-1.419248000	1.261392000
6	1.113902000	-2.787762000	-0.258373000
6	0.751787000	-2.541609000	-1.569319000
1	0.350951000	-3.176208000	-0.410507000
1	-0.216210000	-2.858940000	-1.937471000
1	1.513672000	-2.376667000	-2.325262000
6	2.475933000	-2.852166000	0.297945000
6	2.635479000	-2.822780000	1.696741000
1	1.755121000	-2.750664000	2.331650000
6	3.622575000	-2.987041000	-0.506582000
1	3.521103000	-3.061395000	-1.584914000

6	4.886613000	-3.068678000	0.071769000
6	3.901673000	-2.893320000	2.274332000
6	5.031420000	-3.013812000	1.461943000
1	4.006103000	-2.869545000	3.355012000
1	5.761382000	-3.193075000	-0.560139000
1	6.018712000	-3.083890000	1.908983000
6	-4.357525000	-1.235159000	0.271056000
6	-4.836099000	-0.769189000	-0.964192000
1	-4.569759000	-1.292209000	-1.879904000
6	-4.743652000	-0.545642000	1.428647000
1	-4.397907000	-0.898364000	2.398223000
6	-5.582280000	0.570283000	1.360973000
6	-5.671744000	0.346014000	-1.038226000
6	-6.049285000	1.020808000	0.125504000
1	-6.039335000	0.680694000	-2.004723000
1	-5.879212000	1.078315000	2.274797000
1	-6.709599000	1.881694000	0.069399000
6	-4.216868000	-3.730800000	-0.132782000
1	-4.462217000	-3.658509000	-1.198651000
1	-3.602700000	-4.627580000	0.009855000
1	-5.154397000	-3.870615000	0.414660000

87
E + ZPE = -2859.051980

28	1.063580000	-0.663436000	-0.063619000
15	-1.142505000	-0.858969000	-0.128159000
6	-1.744806000	-2.141503000	-1.365833000
1	-2.690907000	-1.770371000	-1.766768000
6	-1.994727000	-3.385188000	-0.483784000
1	-2.607505000	-4.114313000	-1.025787000
1	-1.036722000	-3.880061000	-0.266794000
6	-2.656257000	-2.937474000	0.824389000
1	-2.705713000	-3.751506000	1.556711000
1	-3.689821000	-2.623278000	0.633839000
6	-1.844758000	-1.752461000	1.393359000
1	-0.961883000	-2.165498000	1.893730000
6	-2.596260000	-0.877338000	2.398983000
1	-3.487336000	-0.421490000	1.956705000
1	-1.969752000	-0.068043000	2.788728000
1	-2.919979000	-1.488508000	3.249277000
6	-0.820120000	-2.414851000	-2.553890000
1	0.170981000	-2.755298000	-2.231947000
1	-0.694594000	-1.529530000	-3.182845000
1	-1.254850000	-3.204510000	-3.177394000
6	-1.997050000	0.777795000	-0.270948000
6	-2.857093000	0.868061000	-1.380991000
1	-2.991558000	-0.004258000	-2.012414000
6	-3.551064000	2.035297000	-1.690793000
1	-4.202002000	2.064929000	-2.559625000
6	-3.406925000	3.151504000	-0.872509000
1	-3.945507000	4.069514000	-1.087487000
6	-2.556738000	3.082189000	0.228652000
1	-2.440031000	3.955155000	0.865006000
6	-1.834268000	1.924231000	0.547221000
6	-0.938693000	2.013036000	1.764531000
1	-0.984593000	1.058533000	2.308428000
1	-1.278827000	2.790182000	2.465983000
8	0.396327000	2.269367000	1.351552000
6	0.552539000	3.561644000	0.778055000
1	-0.158548000	4.277805000	1.213835000
1	1.571058000	3.885168000	1.001506000
1	0.408768000	3.543942000	-0.313305000

1	4.147263000	2.510346000	0.048990000
6	4.539264000	1.840480000	-0.724884000
6	3.517479000	0.773205000	-1.135397000
1	5.462250000	1.388412000	-0.347427000
1	4.798515000	2.460179000	-1.589088000
1	3.961807000	0.159158000	-1.929218000
6	3.096447000	-0.171454000	-0.018897000
6	2.580517000	0.334895000	1.203461000
6	3.011597000	-1.568248000	-0.273563000
1	2.672505000	1.390188000	1.435893000
1	3.426700000	-1.961522000	-1.196136000
6	1.896393000	-0.516944000	2.080729000
6	2.361999000	-2.429968000	0.625430000
1	1.459603000	-0.123770000	2.992792000
1	2.296195000	-3.492758000	0.418957000
6	1.764558000	-1.889421000	1.777022000
1	1.220294000	-2.536831000	2.455879000
6	1.106738000	0.270477000	-1.762856000
6	2.185155000	1.357996000	-1.669079000
1	2.340559000	1.828506000	-2.650903000
1	1.855116000	2.159949000	-0.995108000
1	0.149266000	0.701471000	-2.061523000
1	1.382406000	-0.481855000	-2.511622000

88
E + ZPE = -2859.041251

28	0.958602000	0.215207000	0.091078000
15	-1.187721000	0.796036000	0.142564000
6	-1.745138000	2.118552000	1.338049000
1	-2.843638000	2.105389000	1.304842000
6	-1.270973000	3.385693000	0.600381000
1	-1.653163000	4.283485000	1.098714000
1	-0.174416000	3.445755000	0.641874000
6	-1.764736000	3.296223000	-0.851455000
1	-1.224265000	3.988099000	-1.505461000
1	-2.819377000	3.593365000	-0.884158000
6	-1.653535000	1.832690000	-1.386542000
1	-0.811231000	1.758322000	-2.083416000
6	-2.937576000	1.407157000	-2.112431000
1	-3.801073000	1.421575000	-1.439163000
1	-2.875806000	0.408461000	-2.551967000
1	-3.137926000	2.113947000	-2.926108000
6	-1.290834000	2.038652000	2.795974000
1	-0.210459000	2.183412000	2.886467000
1	-1.545751000	1.083655000	3.265756000
1	-1.777595000	2.833062000	3.372489000
6	-2.317372000	-0.644711000	0.245463000
6	-3.311694000	-0.723909000	1.228802000
1	-3.448576000	0.085086000	1.938775000
6	-4.149286000	-1.839448000	1.314669000
1	-4.915385000	-1.879309000	2.083201000
6	-4.001851000	-2.888414000	0.412145000
1	-4.652217000	-3.756097000	0.467375000
6	-3.007151000	-2.822826000	-0.566933000
1	-2.894322000	-3.643188000	-1.271572000
6	-2.154116000	-1.720680000	-0.661751000
6	-1.075852000	-1.703180000	-1.727463000
1	-1.095942000	-0.780785000	-2.313654000
1	-1.223135000	-2.536514000	-2.426002000
8	0.259033000	-1.768790000	-1.195374000
6	0.617042000	-3.087492000	-0.770600000
1	0.461994000	-3.804872000	-1.586621000

1	1.676739000	-3.062566000	-0.515917000
1	0.034519000	-3.400505000	0.103839000
1	4.671030000	-2.229711000	1.027866000
6	4.785766000	-1.277744000	1.559053000
6	3.510765000	-0.428202000	1.503321000
1	5.641063000	-0.747936000	1.126921000
1	5.029359000	-1.517906000	2.598950000
1	3.668723000	0.457891000	2.133729000
6	3.139603000	0.081516000	0.112862000
6	3.372927000	-0.678003000	-1.067572000
6	2.623615000	1.400713000	-0.026020000
1	3.855321000	-1.646869000	-0.985539000
1	2.654228000	2.090246000	0.813137000
6	2.994679000	-0.206962000	-2.313590000
6	2.222597000	1.866083000	-1.304301000
1	3.168361000	-0.806569000	-3.201181000
1	1.835000000	2.875141000	-1.408139000
6	2.378467000	1.056993000	-2.426202000
1	2.071354000	1.422818000	-3.401821000
6	1.005313000	-0.333201000	1.902642000
6	2.274048000	-1.172165000	2.056071000
1	2.423981000	-1.417882000	3.118644000
1	2.171649000	-2.133136000	1.536177000
1	0.114522000	-0.902451000	2.190612000
1	1.060893000	0.556564000	2.538279000

89
E + ZPE = -2859.056653

28	0.840853000	-0.216149000	0.159230000
15	-1.262908000	-0.773227000	0.058016000
6	-1.830383000	-2.019231000	-1.243778000
1	-2.742953000	-1.585230000	-1.667337000
6	-2.217418000	-3.281331000	-0.435327000
1	-2.915654000	-3.898282000	-1.012482000
1	-1.325061000	-3.896365000	-0.261748000
6	-2.819450000	-2.844500000	0.908706000
1	-2.926096000	-3.690744000	1.596983000
1	-3.826870000	-2.435022000	0.759940000
6	-1.899141000	-1.766619000	1.526021000
1	-1.002613000	-2.267637000	1.908668000
6	-2.519192000	-0.952311000	2.663411000
1	-3.407915000	-0.403605000	2.337466000
1	-1.808556000	-0.229818000	3.080933000
1	-2.819217000	-1.623978000	3.475399000
6	-0.855593000	-2.274404000	-2.396901000
1	0.089928000	-2.700023000	-2.048522000
1	-0.633974000	-1.356213000	-2.952096000
1	-1.297553000	-2.984994000	-3.104677000
6	-2.404020000	0.671342000	-0.146656000
6	-3.775369000	0.448710000	-0.365346000
1	-4.160879000	-0.563564000	-0.420657000
6	-4.675388000	1.504207000	-0.505230000
1	-5.728922000	1.296414000	-0.666038000
6	-4.215055000	2.817837000	-0.444169000
1	-4.903050000	3.649307000	-0.562728000
6	-2.857783000	3.057874000	-0.241691000
1	-2.494724000	4.082106000	-0.205923000
6	-1.948225000	2.006193000	-0.078468000
6	-0.507785000	2.368592000	0.199853000
1	-0.238571000	2.194790000	1.244664000
1	-0.336277000	3.429344000	-0.014427000
8	0.452331000	1.601797000	-0.555282000

6	0.395778000	1.824489000	-1.976029000
1	0.528289000	2.892740000	-2.175694000
1	1.221065000	1.265517000	-2.415200000
1	-0.558873000	1.485168000	-2.390111000
1	4.649769000	-1.309520000	-1.878418000
6	4.904454000	-1.529659000	-0.834799000
6	3.701060000	-1.357848000	0.100052000
1	5.742854000	-0.888260000	-0.544309000
1	5.250106000	-2.567874000	-0.800274000
1	4.019631000	-1.673073000	1.103682000
6	3.222332000	0.089899000	0.257605000
6	3.623573000	1.116275000	-0.628755000
6	2.580114000	0.480651000	1.461937000
1	4.140039000	0.856858000	-1.547207000
1	2.440582000	-0.253953000	2.249087000
6	3.450779000	2.456981000	-0.305103000
6	2.449543000	1.844374000	1.800455000
1	3.808268000	3.222854000	-0.988172000
1	2.048687000	2.113384000	2.774203000
6	2.880244000	2.828056000	0.922466000
1	2.808922000	3.877247000	1.194957000
6	1.283405000	-2.021814000	0.534123000
6	2.533263000	-2.272903000	-0.308858000
1	2.845712000	-3.324910000	-0.228032000
1	2.313960000	-2.111997000	-1.375506000
1	0.517623000	-2.754428000	0.262824000
1	1.484970000	-2.179199000	1.603201000

90
E + ZPE = -2859.049102

28	0.670952000	-0.448479000	-0.306761000
15	-1.376548000	-0.758527000	0.093075000
6	-2.273853000	-2.023936000	-0.976177000
1	-3.238485000	-1.562293000	-1.216515000
6	-2.530972000	-3.206348000	-0.015032000
1	-3.325091000	-3.850316000	-0.409487000
1	-1.628394000	-3.827018000	0.062273000
6	-2.888318000	-2.632630000	1.364815000
1	-2.925791000	-3.413478000	2.132798000
1	-3.884809000	-2.171737000	1.335487000
6	-1.827521000	-1.570121000	1.729476000
1	-0.907674000	-2.095659000	2.013298000
6	-2.208412000	-0.614109000	2.861353000
1	-3.111451000	-0.041985000	2.627566000
1	-1.404187000	0.098618000	3.076852000
1	-2.399902000	-1.182866000	3.777932000
6	-1.588871000	-2.394693000	-2.293846000
1	-0.606856000	-2.850726000	-2.132590000
1	-1.457699000	-1.520450000	-2.941425000
1	-2.203593000	-3.117846000	-2.841812000
6	-2.350748000	0.801620000	-0.079653000
6	-3.754925000	0.752203000	-0.057655000
1	-4.263910000	-0.196724000	0.078028000
6	-4.529109000	1.903668000	-0.196654000
1	-5.612186000	1.832355000	-0.167767000
6	-3.906071000	3.136086000	-0.379301000
1	-4.496395000	4.038928000	-0.502284000
6	-2.514170000	3.202887000	-0.410329000
1	-2.028752000	4.164871000	-0.555115000
6	-1.724322000	2.058164000	-0.248065000
6	-0.224864000	2.251177000	-0.194476000
1	0.174767000	2.076650000	0.806415000

1	0.036620000	3.274210000	-0.483174000
8	0.532189000	1.349626000	-1.039954000
6	0.366373000	1.580054000	-2.453120000
1	0.630906000	2.617773000	-2.677849000
1	1.055146000	0.907422000	-2.964843000
1	-0.663505000	1.379511000	-2.764116000
1	4.888174000	-1.148040000	-1.759531000
6	4.971638000	-1.592480000	-0.760703000
6	3.689034000	-1.411712000	0.063677000
1	5.834692000	-1.141535000	-0.261144000
1	5.180242000	-2.658590000	-0.897642000
1	3.802436000	-1.997854000	0.985241000
6	3.413019000	0.032484000	0.477578000
6	3.861326000	1.125807000	-0.283774000
6	2.731028000	0.306698000	1.679241000
1	4.411099000	0.955135000	-1.204364000
1	2.430056000	-0.515533000	2.322688000
6	3.653466000	2.437341000	0.144491000
6	2.533370000	1.621373000	2.117537000
1	4.034811000	3.262435000	-0.451001000
1	2.048038000	1.801607000	3.073198000
6	2.996994000	2.691269000	1.351675000
1	2.868596000	3.711926000	1.701137000
6	1.201633000	-2.160093000	0.158889000
6	2.466189000	-1.985404000	-0.688482000
1	2.726759000	-2.927169000	-1.190645000
1	2.257963000	-1.294985000	-1.544889000
1	0.593641000	-2.994657000	-0.201420000
1	1.417291000	-2.329493000	1.218736000

91
E + ZPE = -2859.056252

28	-0.508828000	0.413020000	-0.923591000
15	1.306916000	0.790419000	0.123545000
6	2.330910000	2.236357000	-0.505502000
1	3.371963000	1.893271000	-0.499492000
6	2.163267000	3.304395000	0.598582000
1	2.950758000	4.061899000	0.516764000
1	1.205099000	3.824911000	0.466079000
6	2.185448000	2.591605000	1.958559000
1	1.924460000	3.269149000	2.779301000
1	3.194982000	2.213451000	2.169771000
6	1.184986000	1.415794000	1.894324000
1	0.172202000	1.831153000	1.951845000
6	1.336807000	0.357749000	2.988569000
1	2.318558000	-0.124797000	2.958363000
1	0.570641000	-0.421316000	2.907746000
1	1.225062000	0.827623000	3.972029000
6	1.992893000	2.713140000	-1.920488000
1	0.949805000	3.035805000	-2.000315000
1	2.165386000	1.928080000	-2.665282000
1	2.627590000	3.564987000	-2.189671000
6	2.412760000	-0.684936000	0.099723000
6	3.762114000	-0.564179000	0.469613000
1	4.156047000	0.397329000	0.783558000
6	4.622994000	-1.661692000	0.458541000
1	5.659565000	-1.537589000	0.757003000
6	4.147091000	-2.908519000	0.059703000
1	4.808975000	-3.768786000	0.035883000
6	2.811225000	-3.045801000	-0.315156000
1	2.441498000	-4.019627000	-0.626392000
6	1.931165000	-1.957437000	-0.289811000

6	0.482000000	-2.223212000	-0.633621000
1	-0.182883000	-2.084261000	0.223153000
1	0.361177000	-3.252380000	-0.987432000
8	-0.067278000	-1.344161000	-1.650859000
6	0.504227000	-1.515076000	-2.964762000
1	0.396859000	-2.561474000	-3.266404000
1	-0.066772000	-0.877243000	-3.640440000
1	1.560003000	-1.228480000	-2.973464000
1	-4.282573000	-0.586941000	-2.353350000
6	-4.710775000	0.287637000	-1.849109000
6	-3.776565000	0.837283000	-0.758832000
1	-5.671198000	-0.013806000	-1.420673000
1	-4.904249000	1.049026000	-2.612888000
1	-4.239462000	1.743195000	-0.347766000
6	-3.564730000	-0.133197000	0.395467000
6	-3.179994000	-1.465651000	0.171018000
6	-3.740388000	0.289145000	1.720282000
1	-3.073518000	-1.838399000	-0.844986000
1	-4.060857000	1.309980000	1.916347000
6	-2.972933000	-2.342174000	1.239054000
6	-3.529309000	-0.582621000	2.791143000
1	-2.704169000	-3.377093000	1.042732000
1	-3.681667000	-0.233071000	3.808434000
6	-3.140806000	-1.901582000	2.554229000
1	-2.989859000	-2.585983000	3.384048000
6	-1.433097000	1.938301000	-0.429107000
6	-2.428209000	1.304598000	-1.364617000
1	-2.587566000	1.917322000	-2.258409000
1	-1.969168000	0.352695000	-1.835601000
1	-1.061300000	2.910597000	-0.758556000
1	-1.750202000	1.973644000	0.615514000

92
E + ZPE= -3168.567945

28	-0.415321000	-0.188354000	-0.125895000
15	1.297972000	-1.456395000	-0.394107000
6	0.984836000	-3.315914000	-0.536124000
1	1.762014000	-3.781699000	0.080402000
6	1.282544000	-3.644172000	-2.015353000
1	1.466718000	-4.717836000	-2.136641000
1	0.408504000	-3.402716000	-2.634888000
6	2.486563000	-2.802639000	-2.459245000
1	2.643823000	-2.855169000	-3.542660000
1	3.403997000	-3.183225000	-1.990647000
6	2.245182000	-1.341036000	-2.020736000
1	1.509580000	-0.896773000	-2.703497000
6	3.495814000	-0.459701000	-2.008761000
1	4.264162000	-0.855143000	-1.337395000
1	3.271892000	0.565669000	-1.697496000
1	3.925032000	-0.416209000	-3.016430000
6	-0.370357000	-3.819141000	-0.034144000
1	-1.199642000	-3.417423000	-0.624146000
1	-0.540424000	-3.559971000	1.016771000
1	-0.411742000	-4.911774000	-0.111170000
6	2.506573000	-1.313093000	1.001469000
6	3.593591000	-2.201534000	1.072245000
1	3.730397000	-2.952476000	0.300895000
6	4.521753000	-2.143796000	2.110921000
1	5.354365000	-2.840539000	2.130462000
6	4.368560000	-1.195919000	3.120185000
1	5.075404000	-1.147269000	3.942897000
6	3.293141000	-0.311441000	3.070936000

1	3.172505000	0.425969000	3.860710000
6	2.367378000	-0.342918000	2.020336000
6	1.300771000	0.729561000	2.011977000
1	1.479452000	1.465739000	1.225832000
1	1.293926000	1.257448000	2.971826000
8	-0.045014000	0.253871000	1.767284000
6	-0.569215000	-0.591482000	2.811169000
1	-0.476333000	-0.073319000	3.770703000
1	-1.622806000	-0.757851000	2.585033000
1	-0.031975000	-1.543901000	2.846988000
1	-5.267229000	-0.343036000	-2.904390000
6	-4.385290000	-0.844647000	-2.494858000
6	-3.785833000	-1.021951000	-1.339691000
1	-3.658033000	-0.975607000	-3.303830000
1	-4.696045000	-1.839317000	-2.155751000
1	-3.491448000	0.952657000	-1.752646000
6	-4.786670000	0.236850000	-0.222696000
6	-5.362754000	-0.819290000	0.500480000
6	-5.147854000	1.547535000	0.115995000
1	-5.114761000	-1.848615000	0.251071000
1	-4.725227000	2.380912000	-0.441958000
6	-6.269973000	-0.570445000	1.530495000
6	-6.057282000	1.800983000	1.145181000
1	-6.710271000	-1.402356000	2.073478000
1	-6.329158000	2.825372000	1.384506000
6	-6.620081000	0.741716000	1.857024000
1	-7.331049000	0.935105000	2.655147000
6	-1.283021000	-0.699828000	-1.703472000
6	-2.503486000	-0.714256000	-0.807895000
1	-2.257777000	-0.172690000	0.161044000
1	-2.744874000	-1.730313000	-0.480078000
1	-1.056585000	-1.661275000	-2.165027000
1	-1.295672000	0.077882000	-2.475225000
6	0.045172000	2.527625000	-1.196363000
6	-0.981058000	2.295956000	-0.346272000
1	-0.074050000	2.205546000	-2.230496000
1	-1.940027000	1.972182000	-0.731610000
1	-0.971588000	2.634157000	0.685639000
6	1.305277000	3.230008000	-0.922663000
1	1.537799000	3.949462000	0.266481000
6	0.761756000	4.009090000	1.024386000
6	2.306851000	3.236919000	-1.911363000
1	2.131156000	2.714439000	-2.848879000
6	3.509086000	3.913482000	-1.712366000
6	2.738895000	4.624376000	0.465481000
6	3.730672000	4.605175000	-0.520342000
1	2.896576000	5.183893000	1.383111000
1	4.266954000	3.909654000	-2.490264000
1	4.662513000	5.140993000	-0.365574000

93
E + ZPE = -2859.052608

28	1.158916000	0.183264000	-0.189907000
15	-0.869775000	0.980649000	0.067568000
6	-0.920477000	2.403009000	1.284840000
1	-1.972089000	2.543082000	1.567596000
6	-0.530797000	3.582007000	0.371867000
1	-0.664196000	4.532819000	0.899748000
1	0.533948000	3.512385000	0.109387000
6	-1.414039000	3.503449000	-0.879885000
1	-1.050619000	4.157726000	-1.679251000
1	-2.421353000	3.852081000	-0.621719000

6	-1.517582000	2.031649000	-1.381777000
1	-0.812150000	1.872983000	-2.204138000
6	-2.931546000	1.704619000	-1.878842000
1	-3.668334000	1.781004000	-1.072698000
1	-3.012276000	0.705357000	-2.313956000
1	-3.211722000	2.425406000	-2.655947000
6	-0.066430000	2.277867000	2.546958000
1	0.985282000	2.094613000	2.301219000
1	-0.403996000	1.467247000	3.200359000
1	-0.119569000	3.208756000	3.122607000
6	-2.156038000	-0.253755000	0.526773000
6	-2.859950000	-0.095590000	1.730579000
1	-2.638532000	0.733757000	2.392602000
6	-3.861003000	-0.991838000	2.109114000
1	-4.388007000	-0.845738000	3.047214000
6	-4.187555000	-2.055016000	1.272775000
1	-4.978768000	-2.747264000	1.544553000
6	-3.493008000	-2.222988000	0.074520000
1	-3.761050000	-3.043408000	-0.586330000
6	-2.463295000	-1.355647000	-0.309572000
6	-1.714357000	-1.660851000	-1.596238000
1	-1.326018000	-0.748449000	-2.056309000
1	-2.401274000	-2.126898000	-2.318648000
8	-0.571096000	-2.495398000	-1.416992000
6	-0.869099000	-3.873631000	-1.227244000
1	-1.479403000	-4.264352000	-2.054668000
1	0.087434000	-4.401207000	-1.213173000
1	-1.390773000	-4.057541000	-0.279413000
6	3.386550000	-1.488786000	1.023110000
6	3.094886000	-0.599487000	-0.177366000
6	2.439846000	-1.137832000	-1.316754000
6	3.279490000	0.809111000	-0.089559000
1	2.304770000	-2.210122000	-1.398795000
1	3.814716000	1.232467000	0.753426000
6	1.879930000	-0.290772000	-2.286392000
6	2.718176000	1.653542000	-1.054432000
1	1.339338000	-0.711681000	-3.126616000
1	2.830269000	2.729417000	-0.970758000
6	1.982257000	1.103449000	-2.126777000
1	1.512507000	1.764957000	-2.846956000
6	0.934447000	-0.922184000	1.387044000
6	2.301288000	-1.107735000	2.059864000
1	2.603945000	-0.178335000	2.561013000
1	2.239698000	-1.873216000	2.847317000
1	0.547208000	-1.867051000	0.989067000
1	0.203869000	-0.543440000	2.105119000
1	3.209140000	-2.524849000	0.707421000
6	4.818289000	-1.386832000	1.563882000
1	5.053692000	-0.374582000	1.912086000
1	4.944752000	-2.061904000	2.416204000
1	5.555410000	-1.664362000	0.803312000

94
E + ZPE = -2859.039486

28	0.976027000	0.003697000	-0.042253000
15	-1.049062000	0.879621000	-0.008288000
6	-1.276342000	2.430173000	1.006398000
1	-2.359354000	2.602339000	1.077054000
6	-0.697860000	3.482931000	0.039839000
1	-0.885380000	4.493309000	0.419719000
1	0.393409000	3.366244000	-0.020423000
6	-1.352020000	3.267872000	-1.332775000

1	-0.799659000	3.776804000	-2.129337000
1	-2.356047000	3.708049000	-1.316596000
6	-1.489868000	1.744429000	-1.644881000
1	-0.723605000	1.446841000	-2.369382000
1	-2.873915000	1.412511000	-2.218898000
1	-3.669471000	1.650697000	-1.505208000
1	-2.983884000	0.362099000	-2.499807000
1	-3.042137000	2.014861000	-3.119231000
6	-0.668105000	2.477448000	2.408476000
1	0.415411000	2.323988000	2.382232000
1	-1.101109000	1.728388000	3.079070000
1	-0.852906000	3.461620000	2.853482000
6	-2.360369000	-0.336673000	0.393602000
6	-3.264508000	-0.106436000	1.438402000
1	-3.216718000	0.812284000	2.013933000
6	-4.246480000	-1.047133000	1.760828000
1	-4.937797000	-0.846856000	2.573901000
6	-4.336135000	-2.230701000	1.034777000
1	-5.099283000	-2.965354000	1.273181000
6	-3.434543000	-2.472946000	-0.004753000
1	-3.507973000	-3.397512000	-0.572294000
6	-2.439204000	-1.549812000	-0.335135000
6	-1.473509000	-1.873857000	-1.460654000
1	-1.402344000	-1.055714000	-2.182354000
1	-1.821057000	-2.760430000	-2.006794000
8	-0.125171000	-2.089176000	-1.017094000
6	0.063287000	-3.371130000	-0.416270000
1	-0.192693000	-4.168302000	-1.126486000
1	1.120650000	-3.449643000	-0.158477000
1	-0.543290000	-3.487897000	0.490060000
6	3.419364000	-0.726194000	1.516317000
6	3.084757000	-0.402182000	0.065126000
6	3.168030000	-1.393671000	-0.949457000
6	2.778488000	0.934226000	-0.320390000
1	3.483480000	-2.395840000	-0.670098000
1	2.909827000	1.757062000	0.376078000
6	2.832296000	-1.116236000	-2.266831000
6	2.404680000	1.201836000	-1.658919000
1	2.879328000	-1.893652000	-3.021961000
1	2.155986000	2.216998000	-1.953085000
6	2.404382000	0.179579000	-2.610339000
1	2.111241000	0.398676000	-3.633068000
6	0.903556000	-0.561546000	1.764714000
6	2.253040000	-0.229154000	2.398530000
1	2.343815000	0.854819000	2.552621000
1	2.321839000	-0.677238000	3.400847000
1	0.756076000	-1.647857000	1.679226000
1	0.074248000	-0.162292000	2.351445000
1	3.455501000	-1.821231000	1.598343000
6	4.782901000	-0.170463000	1.956648000
1	4.809920000	0.923142000	1.885309000
1	4.986849000	-0.441687000	2.997870000
1	5.594136000	-0.568352000	1.338246000

95

E + ZPE = -2859.056074

28	0.859402000	-0.199350000	0.016606000
15	-1.241060000	-0.775062000	0.029014000
6	-1.886449000	-1.937943000	-1.313006000
1	-2.837926000	-1.496856000	-1.630432000
6	-2.187489000	-3.261845000	-0.571635000
1	-2.910612000	-3.856331000	-1.141712000

1	-1.272370000	-3.863990000	-0.501113000
6	-2.704819000	-2.931573000	0.836782000
1	-2.748181000	-3.824395000	1.470993000
1	-3.727914000	-2.537187000	0.783599000
6	-1.766688000	-1.875049000	1.464923000
1	-0.838585000	-2.378996000	1.757517000
6	-2.326886000	-1.152434000	2.692241000
1	-3.245982000	-0.604739000	2.463617000
1	-1.604533000	-0.442641000	3.111168000
1	-2.559015000	-1.883894000	3.474293000
6	-0.999889000	-2.085511000	-2.552281000
1	-0.021075000	-2.507788000	-2.307219000
1	-0.842044000	-1.125324000	-3.055943000
1	-1.479278000	-2.757400000	-3.273316000
6	-2.403399000	0.665337000	-0.004853000
6	-3.785858000	0.435108000	-0.124889000
1	-4.164779000	-0.579064000	-0.193603000
6	-4.703701000	1.483962000	-0.149612000
1	-5.764685000	1.270061000	-0.236344000
6	-4.251582000	2.799512000	-0.070259000
1	-4.954028000	3.626779000	-0.101031000
6	-2.884974000	3.047588000	0.036784000
1	-2.529754000	4.073964000	0.087295000
6	-1.955252000	2.001589000	0.084844000
6	-0.501904000	2.373382000	0.271607000
1	-0.156296000	2.165352000	1.287237000
1	-0.359263000	3.443785000	0.085996000
8	0.411749000	1.650097000	-0.578223000
6	0.251185000	1.927648000	-1.981565000
1	0.364711000	3.003667000	-2.148312000
1	1.043818000	1.391375000	-2.501909000
1	-0.729831000	1.598259000	-2.338435000
1	5.417396000	-1.169019000	1.001045000
6	4.603532000	-1.854248000	0.742342000
6	3.713594000	-1.270266000	-0.371559000
1	4.039609000	-2.066037000	1.657144000
1	5.048207000	-2.796146000	0.404473000
1	4.338861000	-1.183533000	-1.268266000
6	3.229885000	0.140320000	-0.033326000
6	3.591873000	1.220309000	-0.872567000
6	2.657999000	0.452439000	1.227537000
1	4.055006000	1.004708000	-1.832541000
1	2.557470000	-0.321212000	1.980550000
6	3.445798000	2.538644000	-0.461905000
6	2.554367000	1.795812000	1.652496000
1	3.770967000	3.345016000	-1.113678000
1	2.204973000	2.006551000	2.659899000
6	2.940494000	2.831557000	0.815513000
1	2.885219000	3.861771000	1.155753000
6	1.349655000	-2.018105000	0.253956000
6	2.523774000	-2.191561000	-0.711426000
1	2.857380000	-3.240005000	-0.727849000
1	2.191450000	-1.974701000	-1.736793000
1	0.575952000	-2.748989000	-0.000058000
1	1.634193000	-2.234101000	1.292728000

96

E + ZPE = -2859.048749

28	0.693024000	-0.379693000	-0.429160000
15	-1.325751000	-0.768395000	0.067787000
6	-2.255791000	-1.995470000	-1.017890000
1	-3.247747000	-1.553024000	-1.165081000

6	-2.413707000	-3.242288000	-0.119314000
1	-3.212823000	-3.887273000	-0.501930000
1	-1.490308000	-3.836305000	-0.138408000
6	-2.697645000	-2.764664000	1.313296000
1	-2.662920000	-3.590629000	2.032647000
1	-3.706867000	-2.335709000	1.374277000
6	-1.647325000	-1.690938000	1.675032000
1	-0.695002000	-2.201458000	1.864176000
6	-1.979511000	-0.818636000	2.886812000
1	-2.911631000	-0.262800000	2.747417000
1	-1.183002000	-0.094869000	3.094171000
1	-2.094228000	-1.447297000	3.776706000
6	-1.650038000	-2.256646000	-2.398727000
1	-0.642748000	-2.679094000	-2.331508000
1	-1.595379000	-1.338790000	-2.994902000
1	-2.273093000	-2.969073000	-2.951245000
6	-2.349319000	0.769861000	0.041145000
6	-3.747794000	0.677051000	0.146914000
1	-4.221520000	-0.292248000	0.264925000
6	-4.560653000	1.809522000	0.113925000
1	-5.637411000	1.703671000	0.205446000
6	-3.984653000	3.067852000	-0.044802000
1	-4.606110000	3.957126000	-0.086419000
6	-2.599890000	3.178405000	-0.157233000
1	-2.151132000	4.160701000	-0.282571000
6	-1.769799000	2.052049000	-0.101101000
6	-0.276449000	2.292811000	-0.123426000
1	0.183941000	2.090510000	0.845266000
1	-0.064902000	3.335715000	-0.380717000
8	0.461710000	1.455676000	-1.047196000
6	0.208877000	1.742309000	-2.437236000
1	0.429096000	2.796834000	-2.629232000
1	0.886346000	1.115137000	-3.017241000
1	-0.830690000	1.522641000	-2.699523000
1	5.340946000	-1.765631000	0.964132000
6	4.413475000	-2.195253000	0.572804000
6	3.743075000	-1.224207000	-0.412853000
1	3.774381000	-2.436722000	1.428144000
1	4.662179000	-3.135960000	0.069315000
1	4.454350000	-1.056781000	-1.231302000
6	3.440104000	0.144614000	0.186620000
6	3.899087000	1.306504000	-0.457016000
6	2.743297000	0.296810000	1.401706000
1	4.456078000	1.212146000	-1.386591000
1	2.443000000	-0.576775000	1.970671000
6	3.690819000	2.570960000	0.092477000
6	2.548527000	1.565945000	1.963767000
1	4.078841000	3.449749000	-0.415159000
1	2.054429000	1.654166000	2.927992000
6	3.019726000	2.704665000	1.311543000
1	2.887315000	3.685983000	1.758501000
6	1.292096000	-2.113358000	-0.135888000
6	2.472035000	-1.817107000	-1.065663000
1	2.727245000	-2.700800000	-1.666629000
1	2.142779000	-1.078617000	-1.841468000
1	0.680297000	-2.932665000	-0.523257000
1	1.582942000	-2.364713000	0.887303000

97
E + ZPE = -2859.055438

28	0.526829000	-0.451695000	-0.962873000
15	-1.258441000	-0.824610000	0.140199000

6	-2.281011000	-2.298185000	-0.425270000
1	-3.324537000	-1.962571000	-0.417346000
6	-2.090208000	-3.328676000	0.710628000
1	-2.876886000	-4.090150000	0.668515000
1	-1.133171000	-3.850758000	0.576636000
6	-2.086901000	-2.572917000	2.047035000
1	-1.808452000	-3.223887000	2.883501000
1	-3.092125000	-2.188697000	2.267179000
6	-1.089422000	-1.399681000	1.924100000
1	-0.075381000	-1.814124000	1.965782000
6	-1.211822000	-0.310537000	2.991119000
1	-2.194083000	0.171521000	2.973482000
1	-0.448322000	0.465440000	2.866682000
1	-1.073923000	-0.751914000	3.984495000
6	-1.954423000	-2.820416000	-1.826763000
1	-0.908406000	-3.133799000	-1.906848000
1	-2.144398000	-2.064387000	-2.596797000
1	-2.582076000	-3.688424000	-2.058225000
6	-2.379125000	0.639371000	0.108166000
6	-3.716475000	0.516114000	0.518584000
1	-4.093004000	-0.441255000	0.864700000
6	-4.586697000	1.606237000	0.507211000
1	-5.613409000	1.480783000	0.837488000
6	-4.132714000	2.847412000	0.067225000
1	-4.802215000	3.701772000	0.043207000
6	-2.809567000	2.986328000	-0.349714000
1	-2.457335000	3.955323000	-0.694479000
6	-1.919787000	1.905955000	-0.325067000
6	-0.484461000	2.173226000	-0.721776000
1	0.210189000	2.063848000	0.115314000
1	-0.382710000	3.193515000	-1.105657000
8	0.034673000	1.271506000	-1.734700000
6	-0.585082000	1.400793000	-3.030878000
1	-0.502908000	2.440373000	-3.362585000
1	-0.029162000	0.753334000	-3.710055000
1	-1.636539000	1.100474000	-2.995416000
1	5.636308000	-1.390672000	0.113595000
6	4.700344000	-1.802046000	-0.276167000
6	3.789634000	-0.678113000	-0.792285000
1	4.228241000	-2.386140000	0.520437000
1	4.947391000	-2.495298000	-1.087539000
1	4.307729000	-0.201396000	-1.634640000
6	3.499418000	0.422737000	0.222597000
6	3.347318000	1.744832000	-0.226502000
6	3.365562000	0.175436000	1.597477000
1	3.484968000	1.968227000	-1.282959000
1	3.517408000	-0.826442000	1.987687000
6	3.056699000	2.782800000	0.660915000
6	3.069987000	1.210061000	2.488945000
1	2.969636000	3.800953000	0.290772000
1	2.985665000	0.995909000	3.550868000
6	2.910234000	2.516705000	2.024538000
1	2.699074000	3.323375000	2.720733000
6	1.508915000	-1.925398000	-0.422218000
6	2.479219000	-1.276476000	-1.373253000
1	2.690119000	-1.922004000	-2.232933000
1	1.959978000	-0.386862000	-1.900160000
1	1.178454000	-2.920384000	-0.727713000
1	1.814110000	-1.924511000	0.625449000

98
E + ZPE = -3168.567304

28	0.224491000	0.064398000	-0.693290000
15	-0.758240000	-1.442957000	0.458358000
6	0.085120000	-3.130633000	0.575207000
1	-0.722296000	-3.860704000	0.449092000
6	0.581457000	-3.208258000	2.035943000
1	0.775222000	-4.249930000	2.316517000
1	1.534571000	-2.672171000	2.134562000
6	-0.478115000	-2.559316000	2.937500000
1	-0.113318000	-2.425744000	3.962395000
1	-1.364722000	-3.204363000	3.002442000
6	-0.866538000	-1.196204000	2.323557000
1	-0.053720000	-0.487442000	2.526586000
6	-2.176155000	-0.600699000	2.844156000
1	-3.027060000	-1.262517000	2.655652000
1	-2.395324000	0.369277000	2.385537000
1	-2.106640000	-0.448450000	3.927412000
6	1.152693000	-3.431247000	-0.478817000
1	2.012165000	-2.760234000	-0.392682000
1	0.755878000	-3.352557000	-1.497154000
1	1.521551000	-4.455383000	-0.350482000
6	-2.451593000	-1.822962000	-0.182055000
6	-3.160373000	-2.925298000	0.326796000
1	-2.722840000	-3.540061000	1.106623000
6	-4.432787000	-3.256677000	-0.137063000
1	-4.955048000	-4.110741000	0.283536000
6	-5.021139000	-2.492932000	-1.142441000
1	-6.005667000	-2.746756000	-1.523358000
6	-4.331626000	-1.399913000	-1.663397000
1	-4.789780000	-0.805062000	-2.449721000
6	-3.063423000	-1.041732000	-1.189210000
6	-2.450377000	0.222111000	-1.751808000
1	-2.432409000	1.025413000	-1.012446000
1	-3.033115000	0.569281000	-2.611877000
8	-1.072191000	0.092412000	-2.182139000
6	-0.891175000	-0.782100000	-3.314119000
1	-1.544896000	-0.452889000	-4.127870000
1	0.150993000	-0.690986000	-3.621637000
1	-1.118732000	-1.818775000	-3.048411000
1	3.229921000	1.716093000	-3.241161000
6	4.066657000	1.344165000	-2.635957000
6	3.646411000	1.157028000	-1.168145000
1	4.886928000	2.063895000	-2.714818000
1	4.408974000	0.402354000	-3.079389000
1	3.292042000	2.127244000	-0.793782000
6	4.807482000	0.733368000	-0.277242000
6	5.510652000	-0.457212000	-0.514451000
6	5.201256000	1.533640000	0.802063000
1	5.236722000	-1.095528000	-1.351769000
1	4.675819000	2.466366000	0.996641000
6	6.574108000	-0.835327000	0.304797000
6	6.266480000	1.159898000	1.624082000
1	7.109196000	-1.758947000	0.101449000
1	6.558736000	1.799554000	2.452308000
6	6.955602000	-0.027509000	1.378338000
1	7.786454000	-0.319956000	2.013995000
6	1.797262000	0.053071000	0.308924000
6	2.472771000	0.150548000	-1.044199000
1	1.711050000	0.480068000	-1.819493000
1	2.796733000	-0.833733000	-1.396869000
1	2.086364000	-0.829538000	0.879092000
1	1.926296000	0.940306000	0.938342000
6	-0.418398000	2.868465000	0.280889000
6	0.148448000	2.687892000	-0.932160000
1	0.224490000	2.779679000	1.156327000

1	1.226789000	2.627907000	-1.021347000
1	-0.405048000	2.808882000	-1.858797000
6	-1.809152000	3.230139000	0.583607000
6	-2.723863000	3.645608000	-0.404365000
1	-2.406432000	3.718945000	-1.440814000
6	-2.238313000	3.214438000	1.923792000
1	-1.536124000	2.926527000	2.702784000
6	-3.540219000	3.575834000	2.266281000
6	-4.023944000	4.006578000	-0.062261000
6	-4.438547000	3.969186000	1.272978000
1	-4.712163000	4.336824000	-0.835135000
1	-3.849407000	3.561033000	3.307283000
1	-5.450734000	4.261037000	1.536974000

S22R

E + ZPE = -2859.019728

28	0.137275000	-0.699220000	0.546346000
15	-1.548856000	0.800889000	0.076358000
6	-1.903773000	1.959874000	1.518239000
1	-2.994979000	2.003263000	1.609966000
6	-1.404406000	3.335141000	1.020320000
1	-1.847553000	4.138534000	1.619506000
1	-0.316295000	3.405876000	1.152823000
6	-1.761808000	3.462692000	-0.466867000
1	-1.304723000	4.347941000	-0.923517000
1	-2.848315000	3.571833000	-0.584277000
6	-1.289176000	2.179411000	-1.186814000
1	-0.198896000	2.239010000	-1.303833000
6	-1.903544000	1.942656000	-2.568712000
1	-2.993456000	1.858879000	-2.520843000
1	-1.514730000	1.032626000	-3.039336000
1	-1.660233000	2.782493000	-3.228898000
6	-1.328851000	1.516420000	2.866919000
1	-0.238863000	1.424536000	2.832627000
1	-1.742205000	0.554067000	3.189751000
1	-1.576764000	2.252524000	3.639955000
6	-3.145200000	-0.032465000	-0.314655000
6	-4.365442000	0.657910000	-0.243207000
1	-4.382826000	1.707022000	0.034390000
6	-5.575234000	0.027713000	-0.536552000
1	-6.503116000	0.588887000	-0.480642000
6	-5.585855000	-1.317999000	-0.897363000
1	-6.522282000	-1.820470000	-1.119411000
6	-4.383281000	-2.020376000	-0.968581000
1	-4.392083000	-3.070181000	-1.250973000
6	-3.162162000	-1.395247000	-0.692805000
6	-1.896071000	-2.202520000	-0.852673000
1	-1.249538000	-1.807164000	-1.641293000
1	-2.131291000	-3.241153000	-1.106023000
8	-1.050459000	-2.226147000	0.326270000
6	-1.586433000	-2.962166000	1.446406000
1	-1.905275000	-3.950328000	1.101495000
1	-0.774359000	-3.063451000	2.166068000
1	-2.430591000	-2.429133000	1.893821000
6	2.074268000	-0.410879000	0.019677000
6	1.518058000	0.693893000	0.689936000
1	1.237062000	1.580251000	0.129712000
1	1.006115000	-1.631977000	1.215723000
1	1.958324000	-0.442577000	-1.069327000
1	1.841290000	0.891416000	1.711572000
6	3.291122000	-1.186723000	0.503371000
1	3.316768000	-1.129078000	1.598215000

6	3.284068000	-2.666387000	0.091490000
1	3.156160000	-2.788459000	-0.990126000
1	4.228376000	-3.142708000	0.370423000
1	2.468047000	-3.203432000	0.586996000
6	4.512144000	-0.428706000	-0.025715000
6	4.888360000	-0.492325000	-1.375480000
1	4.325998000	-1.109077000	-2.072186000
6	5.267373000	0.370133000	0.842895000
1	4.993875000	0.427387000	1.894269000
6	6.376805000	1.078791000	0.380775000
6	5.994568000	0.219063000	-1.841111000
6	6.742681000	1.006376000	-0.964192000
1	6.275206000	0.152936000	-2.888583000
1	6.957454000	1.682479000	1.072611000
1	7.607239000	1.555528000	-1.325677000

6	3.347311000	-1.624703000	-0.089763000
1	3.366015000	-1.882144000	-1.155760000
6	4.033257000	-2.776855000	0.683271000
1	4.028600000	-2.596030000	1.763800000
1	3.529762000	-3.730811000	0.494046000
1	5.076595000	-2.866665000	0.366065000
6	4.080587000	-0.303051000	0.090673000
6	4.207256000	0.297781000	1.351998000
1	3.789673000	-0.186299000	2.232511000
6	4.656321000	0.337360000	-1.013797000
1	4.581149000	-0.121270000	-1.997584000
6	5.339405000	1.546757000	-0.866729000
6	4.885254000	1.508054000	1.502132000
6	5.453880000	2.136952000	0.392113000
1	4.979174000	1.954360000	2.488399000
1	5.788214000	2.021421000	-1.734982000
1	5.989787000	3.074323000	0.510476000

S22S

E + ZPE = -2859.020849

28	0.467525000	-0.389379000	-0.424586000
15	-1.784787000	-0.638140000	0.021195000
6	-2.686385000	-1.676744000	-1.266620000
1	-3.612388000	-1.136552000	-1.492383000
6	-3.054447000	-2.972856000	-0.509287000
1	-3.858330000	-3.502569000	-1.032811000
1	-2.189869000	-3.650263000	-0.491654000
6	-3.453329000	-2.593664000	0.923456000
1	-3.579966000	-3.476208000	1.560772000
1	-4.416334000	-2.065649000	0.918672000
6	-2.357122000	-1.666781000	1.495654000
1	-1.487478000	-2.288780000	1.747460000
6	-2.756399000	-0.875198000	2.743005000
1	-3.607123000	-0.215337000	2.548524000
1	-1.930748000	-0.260558000	3.119320000
1	-3.042456000	-1.566225000	3.543586000
6	-1.932745000	-1.893288000	-2.582791000
1	-0.989643000	-2.427129000	-2.429887000
1	-1.711333000	-0.945757000	-3.087183000
1	-2.544322000	-2.491228000	-3.267942000
6	-2.669823000	0.978442000	0.086331000
6	-4.062107000	1.060438000	-0.073650000
1	-4.649049000	0.160997000	-0.230131000
6	-4.728257000	2.285532000	-0.022333000
1	-5.807032000	2.317790000	-0.141656000
6	-4.006122000	3.459508000	0.180804000
1	-4.513871000	4.418530000	0.214901000
6	-2.621847000	3.396769000	0.337677000
1	-2.058619000	4.312801000	0.497291000
6	-1.944141000	2.173242000	0.303423000
6	-0.453084000	2.175316000	0.541877000
1	-0.175828000	1.626332000	1.446272000
1	-0.080548000	3.198802000	0.650847000
8	0.317379000	1.545493000	-0.513280000
6	0.371157000	2.280505000	-1.754457000
1	0.637638000	3.319376000	-1.539036000
1	1.151850000	1.814018000	-2.354433000
1	-0.591356000	2.237241000	-2.272911000
6	1.892615000	-1.573641000	0.350595000
6	0.860439000	-2.315996000	-0.248858000
1	0.109168000	-2.805264000	0.363658000
1	1.715510000	-0.184540000	-1.101113000
1	1.771883000	-1.316553000	1.408648000
1	1.063290000	-2.812648000	-1.197411000

S23R

E + ZPE = -2937.571334

28	0.106183000	-1.357695000	0.360301000
15	1.037554000	0.715559000	0.220308000
6	0.259969000	1.951083000	-0.977038000
1	1.102981000	2.486685000	-1.429925000
6	-0.493177000	2.935368000	-0.057741000
1	-0.741132000	3.851605000	-0.605750000
1	-1.444924000	2.493787000	0.268013000
6	0.404083000	3.217101000	1.154681000
1	-0.119128000	3.790048000	1.928932000
1	1.270184000	3.819478000	0.849243000
6	0.879569000	1.860378000	1.719985000
1	0.034349000	1.424341000	2.269519000
6	2.079836000	1.933198000	2.666717000
1	2.966970000	2.339868000	2.172502000
1	2.345488000	0.950309000	3.071780000
1	1.843222000	2.584562000	3.515702000
6	-0.585444000	1.346448000	-2.097245000
1	-1.429446000	0.775496000	-1.700003000
1	0.005800000	0.691835000	-2.747144000
1	-0.997413000	2.144181000	-2.725941000
6	2.806544000	0.654262000	-0.314606000
6	3.501090000	1.860357000	-0.518632000
1	3.004639000	2.805854000	-0.325000000
6	4.821431000	1.883851000	-0.962602000
1	5.329714000	2.833609000	-1.099051000
6	5.475447000	0.684723000	-1.238179000
1	6.499230000	0.684815000	-1.599638000
6	4.800524000	-0.520049000	-1.057058000
1	5.310595000	-1.453921000	-1.280513000
6	3.481293000	-0.559540000	-0.584492000
6	2.904821000	-1.936842000	-0.325805000
1	2.901392000	-2.171704000	0.739290000
1	3.517045000	-2.693813000	-0.827900000
8	1.538375000	-2.144030000	-0.745220000
6	1.377990000	-2.173839000	-2.177072000
1	2.061574000	-2.918968000	-2.596556000
1	0.348402000	-2.465051000	-2.377614000
1	1.584817000	-1.190873000	-2.610794000
6	-3.083901000	-1.492139000	-0.579853000
6	0.047359000	-1.607207000	2.982982000
6	1.235850000	-2.141330000	2.663132000
1	1.346205000	-3.199110000	2.439473000

6	-1.037634000	-2.860542000	0.208225000
6	-2.006217000	-1.781372000	0.480695000
1	-2.449679000	-1.859083000	1.476885000
1	-1.400961000	-0.754583000	0.607976000
1	-0.044821000	-0.574918000	3.307066000
1	2.147937000	-1.552959000	2.720765000
1	-2.589620000	-1.512328000	-1.561183000
1	-0.919070000	-3.629031000	0.971792000
1	-1.066460000	-3.287347000	-0.796462000
1	-0.847968000	-2.217690000	3.045802000
6	-4.126502000	-2.630883000	-0.555285000
1	-4.645764000	-2.660886000	0.409582000
1	-4.880977000	-2.474144000	-1.331873000
1	-3.654474000	-3.605134000	-0.722152000
6	-3.765549000	-0.136830000	-0.431464000
6	-4.000797000	0.457751000	0.816689000
1	-3.680139000	-0.036289000	1.730489000
6	-4.231443000	0.524588000	-1.577618000
1	-4.068027000	0.075734000	-2.555455000
6	-4.905134000	1.742236000	-1.484679000
6	-4.670561000	1.680533000	0.914085000
6	-5.124240000	2.327275000	-0.235911000
1	-4.846910000	2.120416000	1.891918000
1	-5.258708000	2.233275000	-2.386997000
1	-5.649610000	3.274789000	-0.159536000

S23S

E + ZPE = -2937.570602

28	0.180649000	1.521142000	0.113648000
15	0.992695000	-0.548707000	0.674326000
6	1.636621000	-1.013630000	2.389165000
1	2.444285000	-1.733377000	2.216062000
6	0.455026000	-1.781663000	3.014035000
1	0.778240000	-2.312873000	3.916730000
1	-0.330849000	-1.077338000	3.323100000
6	-0.084318000	-2.736020000	1.941662000
1	-1.014911000	-3.223085000	2.253679000
1	0.646261000	-3.535688000	1.758860000
6	-0.312557000	-1.925293000	0.646643000
1	-1.263472000	-1.388873000	0.746317000
6	-0.377172000	-2.765725000	-0.630290000
1	0.539985000	-3.340934000	-0.788828000
1	-0.547524000	-2.146838000	-1.517523000
1	-1.213227000	-3.469712000	-0.561087000
6	2.202209000	0.116884000	3.247635000
1	1.433956000	0.843479000	3.525495000
1	3.015256000	0.647689000	2.739375000
1	2.613194000	-0.293348000	4.177059000
6	2.340804000	-1.040355000	-0.496882000
6	3.065450000	-2.224481000	-0.278829000
1	2.824650000	-2.861807000	0.565697000
6	4.091078000	-2.627573000	-1.132969000
1	4.623928000	-3.553179000	-0.936913000
6	4.426971000	-1.837222000	-2.229510000
1	5.230678000	-2.131932000	-2.897297000
6	3.723833000	-0.656895000	-2.461271000
1	3.986779000	-0.038153000	-3.315771000
6	2.677774000	-0.251584000	-1.622278000
6	1.933458000	1.004599000	-2.015725000
1	0.917571000	0.789063000	-2.357556000
1	2.458762000	1.506341000	-2.835824000
8	1.766115000	1.973117000	-0.952643000

6	3.000153000	2.560795000	-0.502234000
1	3.551317000	2.934676000	-1.371043000
1	2.734908000	3.393236000	0.146868000
1	3.611488000	1.831740000	0.039482000
6	-2.757517000	1.143105000	-1.331084000
6	-0.380948000	2.753065000	2.512117000
6	0.781798000	3.283766000	2.110799000
1	0.812381000	4.204284000	1.534090000
6	-0.890552000	2.828033000	-0.748908000
6	-1.903809000	1.870246000	-0.274179000
1	-2.526959000	2.281533000	0.524604000
1	-1.344863000	1.006524000	0.345911000
1	-0.429213000	1.882853000	3.160003000
1	1.735837000	2.869432000	2.422538000
1	-0.717821000	2.860383000	-1.826439000
1	-0.897839000	3.821785000	-0.303032000
1	-1.328712000	3.224260000	2.268133000
1	-2.083399000	0.842579000	-2.145314000
6	-3.781771000	2.140777000	-1.912950000
1	-4.372275000	1.664236000	-2.700956000
1	-4.476862000	2.480227000	-1.136444000
1	-3.282840000	3.019578000	-2.335331000
6	-3.454560000	-0.111522000	-0.821758000
6	-4.055703000	-0.170345000	0.444850000
1	-4.015667000	0.688065000	1.111275000
6	-3.563502000	-1.230390000	-1.659619000
1	-3.117989000	-1.199441000	-2.651959000
6	-4.245074000	-2.376326000	-1.247179000
6	-4.731919000	-1.318090000	0.864534000
6	-4.828357000	-2.425400000	0.020192000
1	-5.193415000	-1.341136000	1.847928000
1	-4.322281000	-3.228275000	-1.917076000
1	-5.361357000	-3.314820000	0.343511000

99RR

E + ZPE = -3168.558180

28	-0.491569000	0.260945000	0.646700000
15	1.587219000	-0.476008000	0.870176000
6	2.785857000	0.805841000	1.535286000
1	3.171300000	1.391812000	0.696990000
6	3.920136000	0.015872000	2.264612000
1	4.885216000	0.181867000	1.775554000
1	4.017818000	0.415770000	3.279611000
6	3.595645000	-1.493471000	2.323453000
1	3.971587000	-1.946486000	3.247840000
1	4.081902000	-2.022975000	1.495861000
6	2.071611000	-1.699783000	2.216686000
1	1.597362000	-1.297388000	3.121861000
6	1.681634000	-3.169970000	2.063178000
1	2.096268000	-3.602811000	1.146722000
1	0.597584000	-3.323797000	2.059885000
1	2.085064000	-3.742099000	2.906136000
6	2.071256000	1.773619000	2.496257000
1	1.616708000	1.244387000	3.341852000
1	1.298633000	2.359747000	1.992287000
1	2.803477000	2.476392000	2.909109000
6	2.322166000	-1.197367000	-0.669467000
6	3.590601000	-0.778168000	-1.101019000
1	4.130997000	-0.017290000	-0.550258000
6	4.194399000	-1.328951000	-2.233181000
1	5.177801000	-0.985088000	-2.539876000
6	3.538870000	-2.325365000	-2.950325000

1	4.003303000	-2.772862000	-3.823879000	1	-3.850565000	3.520983000	0.384235000
6	2.278251000	-2.751564000	-2.532373000	1	-4.384455000	1.859016000	0.596587000
1	1.772294000	-3.540459000	-3.083380000	6	-2.487545000	2.034021000	-0.435470000
6	1.644979000	-2.197866000	-1.412481000	1	-1.659913000	2.753538000	-0.474549000
6	0.245270000	-2.682927000	-1.074067000	6	-3.097018000	1.888515000	-1.830707000
1	0.071115000	-2.682776000	0.002722000	1	-3.887770000	1.131208000	-1.849816000
1	0.117739000	-3.715814000	-1.429208000	1	-2.354544000	1.630101000	-2.593042000
8	-0.794082000	-1.860345000	-1.608591000	1	-3.548177000	2.840618000	-2.132423000
6	-1.018759000	-2.029727000	-3.004897000	6	-0.443308000	1.745525000	2.597082000
1	-1.234255000	-3.081155000	-3.243133000	1	0.005319000	2.484080000	1.924734000
1	-1.890563000	-1.422144000	-3.257629000	1	0.266418000	0.921086000	2.712123000
1	-0.161808000	-1.696092000	-3.603841000	1	-0.562902000	2.219446000	3.578085000
6	-3.297728000	-0.965205000	1.362508000	6	-3.077456000	-0.760343000	0.256379000
6	-0.985421000	-0.508081000	2.370183000	6	-4.022939000	-0.887642000	1.285823000
6	-2.188588000	-0.003925000	1.808990000	1	-3.967551000	-0.256196000	2.165103000
1	-2.547969000	0.936580000	2.232639000	6	-5.064685000	-1.814821000	1.210789000
1	-1.925707000	0.682569000	0.438853000	1	-5.779414000	-1.886718000	2.025178000
1	-2.809915000	-1.828421000	0.892339000	6	-5.185738000	-2.629733000	0.090045000
1	-0.524169000	0.035831000	3.192222000	1	-5.996600000	-3.347896000	0.014267000
1	-0.859758000	-1.588285000	2.420656000	6	-4.256015000	-2.511581000	-0.943261000
6	0.005267000	1.270379000	-1.047180000	1	-4.357140000	-3.138218000	-1.826036000
6	-1.405596000	1.220287000	-0.907964000	6	-3.195967000	-1.599139000	-0.882151000
1	0.437883000	0.528452000	-1.712904000	6	-2.214629000	-1.573580000	-2.041757000
1	-1.950406000	0.489666000	-1.498622000	1	-1.904902000	-0.554744000	-2.280797000
1	-1.942397000	2.153889000	-0.748671000	1	-2.694544000	-1.991000000	-2.937907000
6	0.775458000	2.531120000	-0.942142000	8	-0.994649000	-2.275143000	-1.783154000
6	0.327423000	3.645781000	-0.209092000	6	-1.121961000	-3.693374000	-1.827257000
1	-0.613594000	3.601877000	0.334256000	1	-1.514492000	-4.021170000	-2.800002000
6	1.995782000	2.638152000	-1.632384000	1	-0.118637000	-4.104641000	-1.694930000
1	2.350816000	1.793650000	-2.217742000	1	-1.776077000	-4.072592000	-1.031627000
6	2.738024000	3.818502000	-1.601140000	6	2.496316000	-1.751319000	1.566960000
6	1.070460000	4.823667000	-0.174664000	6	-0.046509000	-1.639233000	1.287003000
6	2.279572000	4.915224000	-0.869435000	6	1.225179000	-1.930629000	0.728117000
1	0.703245000	5.674204000	0.392414000	1	1.249591000	-2.781978000	0.045511000
1	3.669670000	3.884218000	-2.155998000	1	1.562122000	-0.986722000	-0.453337000
1	2.854022000	5.836442000	-0.845939000	1	2.361011000	-0.850790000	2.180295000
6	-4.048213000	-1.467696000	2.616630000	1	-0.888448000	-2.276061000	1.033065000
1	-4.830512000	-2.175394000	2.326071000	1	-0.077596000	-1.225366000	2.293027000
1	-3.365456000	-1.968985000	3.310787000	6	0.682347000	1.101518000	-1.516839000
1	-4.528211000	-0.640392000	3.150649000	6	1.580971000	0.007788000	-1.641541000
6	-4.256061000	-0.363343000	0.343130000	1	-0.134655000	1.129994000	-2.234425000
6	-4.977007000	0.808227000	0.619446000	1	2.635520000	0.184927000	-1.439279000
1	-4.862698000	1.308200000	1.579153000	1	1.386274000	-0.725872000	-2.421536000
6	-4.455522000	-0.993565000	-0.892599000	6	1.129697000	2.433547000	-1.042665000
1	-3.908758000	-1.906467000	-1.118160000	6	0.553403000	3.590344000	-1.595476000
6	-5.347163000	-0.467985000	-1.830340000	1	-0.209221000	3.491601000	-2.364465000
6	-5.864647000	1.339008000	-0.318016000	6	2.138234000	2.591615000	-0.074412000
6	-6.052498000	0.702252000	-1.546356000	1	2.614288000	1.718038000	0.363567000
1	-6.416925000	2.244882000	-0.084089000	6	2.554077000	3.861163000	0.321573000
1	-5.494771000	-0.976360000	-2.779287000	6	0.972224000	4.861268000	-1.201959000
1	-6.748390000	1.111714000	-2.272758000	6	1.971241000	5.001491000	-0.237791000

99RS

E + ZPE = -3168.559181

28	0.254283000	-0.307426000	-0.134216000	1	0.522713000	5.740437000	-1.654465000
15	-1.734860000	0.513862000	0.370933000	1	3.337420000	3.961754000	1.067486000
6	-1.817584000	1.274526000	2.092599000	1	2.299173000	5.989677000	0.070628000
1	-2.182341000	0.503881000	2.778425000	6	2.623720000	-2.956343000	2.526843000
6	-2.824520000	2.465530000	2.002902000	1	3.507674000	-2.839124000	3.160911000
1	-3.565222000	2.409105000	2.807325000	1	1.741466000	-3.042065000	3.169825000
1	-2.266482000	3.395926000	2.157953000	1	2.733526000	-3.894347000	1.971498000
6	-3.501605000	2.509291000	0.622188000	6	3.760774000	-1.564074000	0.739152000
				6	4.137236000	-2.493897000	-0.242068000
				1	3.525834000	-3.375603000	-0.421645000
				6	4.592184000	-0.458550000	0.962480000
				1	4.329688000	0.260340000	1.736421000
				6	5.761903000	-0.276506000	0.220659000

6	5.303300000	-2.313882000	-0.987462000
6	6.118376000	-1.202751000	-0.759961000
1	5.579375000	-3.046181000	-1.740982000
1	6.394578000	0.585385000	0.413073000
1	7.027626000	-1.065203000	-1.337662000

99SR

E + ZPE = -3168.558645

28	-0.459218000	-0.629945000	0.118047000
15	1.587662000	-0.323631000	0.915704000
6	1.728314000	1.152309000	2.070482000
1	1.976964000	2.033245000	1.473029000
6	2.856578000	0.809933000	3.097025000
1	3.652717000	1.560588000	3.063592000
1	2.428247000	0.858909000	4.104249000
6	3.424637000	-0.601835000	2.844837000
1	3.779635000	-1.060123000	3.775026000
1	4.286492000	-0.555940000	2.168924000
6	2.333039000	-1.479577000	2.203012000
1	1.526476000	-1.625219000	2.934323000
6	2.851962000	-2.847144000	1.757113000
1	3.631467000	-2.753887000	0.993709000
1	2.060232000	-3.494542000	1.367037000
1	3.295345000	-3.364286000	2.615443000
6	0.390523000	1.432370000	2.778348000
1	0.045040000	0.563571000	3.350832000
1	-0.393887000	1.725272000	2.075730000
1	0.524311000	2.256307000	3.488364000
6	2.926536000	-0.176395000	-0.356346000
6	3.859923000	0.869103000	-0.271358000
1	3.783744000	1.607608000	0.518426000
6	4.912795000	0.982520000	-1.181251000
1	5.619041000	1.802178000	-1.087636000
6	5.059722000	0.034857000	-2.189923000
1	5.883177000	0.102236000	-2.894499000
6	4.143139000	-1.012225000	-2.282720000
1	4.268858000	-1.763875000	-3.058003000
6	3.066802000	-1.132649000	-1.394304000
6	2.087252000	-2.272985000	-1.613657000
1	1.667218000	-2.626254000	-0.670527000
1	2.607198000	-3.121732000	-2.080593000
8	0.955136000	-1.908747000	-2.405678000
6	1.210557000	-1.852890000	-3.805810000
1	1.600575000	-2.813167000	-4.172053000
1	0.253755000	-1.649780000	-4.292029000
1	1.919095000	-1.055504000	-4.064326000
6	-3.265281000	-1.378373000	1.322545000
6	-0.793270000	-2.031038000	1.434938000
6	-1.985239000	-1.918614000	0.672167000
1	-2.148248000	-2.703835000	-0.069617000
1	-1.827832000	-0.868187000	-0.466916000
1	-2.964897000	-0.592523000	2.028068000
1	-0.807157000	-1.662502000	2.459737000
1	-0.150146000	-2.894003000	1.277439000
6	-0.210844000	0.876050000	-1.235107000
6	-1.364824000	0.116127000	-1.555533000
1	0.689991000	0.613026000	-1.781895000
1	-1.266722000	-0.632814000	-2.337786000
1	-2.337850000	0.600400000	-1.510508000
6	-0.273502000	2.284367000	-0.782854000
6	-1.415480000	2.847803000	-0.183192000
1	-2.302291000	2.241136000	-0.017919000

6	0.845461000	3.110657000	-0.989261000
1	1.729667000	2.696951000	-1.467603000
6	0.824414000	4.454646000	-0.617774000
6	-1.434505000	4.189598000	0.190767000
6	-0.315151000	4.998735000	-0.023052000
1	-2.327851000	4.608015000	0.645651000
1	1.694339000	5.078796000	-0.801692000
1	-0.335617000	6.045819000	0.264153000
6	-3.918667000	-2.517242000	2.138005000
1	-4.813201000	-2.146958000	2.647856000
1	-4.223387000	-3.344644000	1.487887000
1	-3.226580000	-2.910873000	2.889763000
6	-4.249285000	-0.765148000	0.335456000
6	-4.721352000	0.539931000	0.530368000
1	-4.385275000	1.105952000	1.397190000
6	-4.719477000	-1.486491000	-0.772331000
1	-4.390206000	-2.510010000	-0.937705000
6	-5.623554000	-0.912289000	-1.667312000
6	-5.629546000	1.116417000	-0.361316000
6	-6.079628000	0.392289000	-1.465907000
1	-5.988013000	2.127360000	-0.188757000
1	-5.978105000	-1.487583000	-2.517952000
1	-6.786539000	0.836885000	-2.160207000

99SS

E + ZPE = -3168.556558

28	0.374373000	0.108034000	0.201839000
15	-1.831307000	0.074099000	0.360103000
6	-2.413392000	0.732907000	2.028717000
1	-2.547571000	-0.123522000	2.695953000
6	-3.773962000	1.453490000	1.771985000
1	-4.529349000	1.124045000	2.492903000
1	-3.629885000	2.527016000	1.939443000
6	-4.244395000	1.229442000	0.325434000
1	-4.930456000	2.021800000	0.003926000
1	-4.790783000	0.282859000	0.232509000
6	-3.004479000	1.197047000	-0.588263000
1	-2.521226000	2.181900000	-0.558267000
6	-3.336383000	0.845872000	-2.039139000
1	-3.755265000	-0.162101000	-1.926673000
1	-2.467315000	0.917291000	-2.701070000
1	-4.087791000	1.547079000	-2.419595000
6	-1.395843000	1.685589000	2.678933000
1	-1.166117000	2.535633000	2.028384000
1	-0.453238000	1.190799000	2.932617000
1	-1.817865000	2.083995000	3.608684000
6	-2.551618000	-1.620230000	0.141832000
6	-3.467947000	-2.127380000	1.076042000
1	-3.751370000	-1.541539000	1.942751000
6	-4.051102000	-3.386196000	0.917268000
1	-4.756412000	-3.749015000	1.658998000
6	-3.735708000	-4.158761000	-0.195899000
1	-4.191679000	-5.133891000	-0.338228000
6	-2.832762000	-3.663842000	-1.136880000
1	-2.601288000	-4.257885000	-2.017581000
6	-2.221945000	-2.412787000	-0.987180000
6	-1.220561000	-1.977974000	-2.042471000
1	-1.260967000	-0.900911000	-2.208558000
1	-1.456914000	-2.467383000	-2.998103000
8	0.139522000	-2.245899000	-1.693003000
6	0.515777000	-3.610081000	-1.852707000
1	0.330999000	-3.948780000	-2.882024000

1	1.586872000	-3.669634000	-1.648109000
1	-0.019108000	-4.270422000	-1.157796000
6	2.818610000	-1.810960000	0.992762000
6	0.391326000	-1.251720000	1.631043000
6	1.735371000	-0.829262000	1.461761000
1	2.091350000	-0.095030000	2.188802000
1	1.879135000	0.107011000	0.228021000
1	2.376949000	-2.428520000	0.202448000
1	0.103202000	-2.227666000	1.246047000
1	-0.139435000	-0.944153000	2.527278000
6	0.438425000	1.526484000	-1.239717000
6	1.722073000	0.944011000	-1.064642000
1	-0.135605000	1.160232000	-2.087875000
1	2.530150000	1.581893000	-0.710474000
1	2.039926000	0.170919000	-1.760699000
6	0.173941000	2.941303000	-0.881091000
6	-0.676861000	3.708963000	-1.694765000
1	-1.139084000	3.250398000	-2.565822000
6	0.778444000	3.567386000	0.224380000
1	1.442680000	3.003132000	0.875066000
6	0.546717000	4.914054000	0.497585000
6	-0.906243000	5.057921000	-1.424200000
6	-0.297153000	5.664981000	-0.325100000
1	-1.555023000	5.634967000	-2.076786000
1	1.027485000	5.379410000	1.353272000
1	-0.473440000	6.715212000	-0.112883000
6	3.178494000	-2.739805000	2.174344000
1	3.937281000	-3.464057000	1.862734000
1	3.587261000	-2.171703000	3.017202000
1	2.297417000	-3.285986000	2.527061000
6	4.055285000	-1.127535000	0.423178000
6	4.513184000	-1.450251000	-0.861033000
1	3.974838000	-2.189067000	-1.451386000
6	4.777290000	-0.183763000	1.170197000
1	4.462563000	0.071020000	2.180009000
6	5.916448000	0.425822000	0.642811000
6	5.655487000	-0.846116000	-1.390523000
6	6.358829000	0.096717000	-0.640382000
1	5.995656000	-1.115021000	-2.386615000
1	6.463892000	1.151095000	1.238305000
1	7.248422000	0.567367000	-1.048562000

S24

E + ZPE = -3168.564612

28	-0.175259000	-0.293579000	-0.313153000
15	-0.111378000	1.635111000	0.648132000
6	-1.722822000	2.502478000	1.098149000
1	-1.634849000	3.533628000	0.738813000
6	-1.728780000	2.514713000	2.643836000
1	-2.417365000	3.281388000	3.016276000
1	-2.098133000	1.547547000	3.011397000
6	-0.292175000	2.737201000	3.131991000
1	-0.203693000	2.609099000	4.217063000
1	0.032623000	3.761959000	2.906988000
6	0.607692000	1.723877000	2.395043000
1	0.411423000	0.734802000	2.822481000
6	2.109643000	1.997613000	2.488221000
1	2.373107000	2.975180000	2.073765000
1	2.697095000	1.236887000	1.961062000
1	2.422376000	1.983597000	3.538369000
6	-2.973070000	1.880551000	0.475742000
1	-3.088529000	0.831429000	0.763891000

1	-2.947604000	1.930495000	-0.617937000
1	-3.865833000	2.421509000	0.810407000
6	0.906246000	2.835878000	-0.328186000
6	0.808191000	4.217139000	-0.095321000
1	0.097928000	4.600792000	0.629149000
6	1.620938000	5.131048000	-0.767371000
1	1.522552000	6.192545000	-0.560682000
6	2.551471000	4.676386000	-1.698327000
1	3.186668000	5.377519000	-2.230961000
6	2.653738000	3.309239000	-1.951870000
1	3.370088000	2.953779000	-2.688449000
6	1.852919000	2.381138000	-1.276750000
6	2.036202000	0.917654000	-1.611146000
1	2.434036000	0.331704000	-0.778417000
1	2.727531000	0.806315000	-2.453054000
8	0.793017000	0.257515000	-1.972681000
6	0.190537000	0.821405000	-3.156845000
1	0.941038000	0.862088000	-3.952197000
1	-0.618669000	0.158909000	-3.456856000
1	-0.196082000	1.824415000	-2.956296000
6	1.643305000	-2.371049000	1.510858000
6	-0.691081000	-1.289208000	1.177769000
6	0.360858000	-2.246812000	0.657425000
1	-0.056969000	-3.237078000	0.438475000
1	0.682668000	-1.911628000	-0.381767000
1	1.857084000	-1.373477000	1.919955000
1	-1.724860000	-1.639433000	1.108209000
1	-0.495660000	-0.930480000	2.188756000
6	-2.673952000	-1.183478000	-1.901537000
6	-1.558566000	-1.945403000	-1.904451000
1	-2.709547000	-0.324227000	-2.571944000
1	-0.766960000	-1.787777000	-2.628671000
1	-1.497433000	-2.866821000	-1.334952000
6	-3.906196000	-1.399700000	-1.135540000
6	-4.985775000	-0.519567000	-1.334478000
1	-4.879361000	0.302369000	-2.038683000
6	-4.075021000	-2.468215000	-0.233038000
1	-3.271904000	-3.182445000	-0.077041000
6	-5.275055000	-2.637665000	0.450766000
6	-6.189609000	-0.692653000	-0.654649000
6	-6.336432000	-1.750774000	0.243482000
1	-7.012670000	-0.005827000	-0.828936000
1	-5.388871000	-3.469451000	1.139885000
1	-7.273784000	-1.890530000	0.773862000
6	1.400554000	-3.321543000	2.698360000
1	2.277211000	-3.355879000	3.352343000
1	0.539444000	-2.998491000	3.294713000
1	1.206124000	-4.342287000	2.349888000
6	2.854018000	-2.784838000	0.686496000
6	4.023615000	-2.012991000	0.712040000
1	4.063370000	-1.124258000	1.340021000
6	2.839500000	-3.941073000	-0.108934000
1	1.952156000	-4.569524000	-0.139531000
6	3.957596000	-4.308735000	-0.857951000
6	5.146945000	-2.379586000	-0.033296000
6	5.115811000	-3.528818000	-0.823046000
1	6.046115000	-1.770889000	0.009843000
1	3.926699000	-5.209811000	-1.464317000
1	5.987772000	-3.819502000	-1.401801000

S25

E + ZPE = -3168.582943

28 0.663921000 0.719984000 -0.689606000
15 1.265157000 -0.952636000 0.739655000
6 2.176745000 -0.326340000 2.274026000
1 3.048280000 -0.982358000 2.387857000
6 1.194798000 -0.600091000 3.435145000
1 1.730560000 -0.600747000 4.391241000
1 0.454660000 0.209738000 3.486729000
6 0.488522000 -1.934280000 3.168196000
1 -0.340268000 -2.102394000 3.865526000
1 1.188086000 -2.768879000 3.306543000
6 -0.035804000 -1.912808000 1.714896000
1 -0.913553000 -1.259367000 1.694354000
6 -0.448328000 -3.275345000 1.151911000
1 0.383235000 -3.985687000 1.138857000
1 -0.842914000 -3.196070000 0.133289000
1 -1.242725000 -3.699663000 1.775879000
6 2.661296000 1.124111000 2.199774000
1 1.830675000 1.820581000 2.039995000
1 3.391606000 1.270955000 1.395929000
1 3.152536000 1.401301000 3.139779000
6 2.375908000 -2.211269000 -0.029561000
6 2.988104000 -3.193364000 0.766997000
1 2.837111000 -3.194005000 1.841590000
6 3.789975000 -4.188173000 0.207862000
1 4.244856000 -4.937784000 0.848353000
6 4.004087000 -4.212338000 -1.168918000
1 4.629174000 -4.979713000 -1.615150000
6 3.424670000 -3.230494000 -1.971093000
1 3.610577000 -3.234365000 -3.042237000
6 2.608863000 -2.234846000 -1.422484000
6 2.028022000 -1.193707000 -2.350013000
1 0.940496000 -1.276941000 -2.445462000
1 2.457518000 -1.295229000 -3.352896000
8 2.258121000 0.161535000 -1.894095000
6 3.654158000 0.502817000 -1.792364000
1 4.134964000 0.356809000 -2.765165000
1 3.708783000 1.555342000 -1.515138000
1 4.153491000 -0.107744000 -1.034908000
6 -3.408030000 0.198768000 0.489031000
6 -0.955486000 1.015202000 0.268326000
6 -2.070724000 0.138956000 -0.308941000
1 -2.280091000 0.421107000 -1.348976000
1 -1.759203000 -0.913109000 -0.350176000
1 -3.167053000 -0.019409000 1.539718000
1 -1.206633000 2.075560000 0.202514000
1 -0.823338000 0.807311000 1.338372000
6 0.881826000 2.701584000 -1.469734000
6 0.026033000 1.918981000 -2.223741000
1 1.941834000 2.646251000 -1.710869000
1 0.404143000 1.392978000 -3.096151000
1 -1.045214000 2.086307000 -2.203410000
6 0.540607000 3.845992000 -0.612876000
6 1.536917000 4.389105000 0.220074000
1 2.531159000 3.947628000 0.220358000
6 -0.728490000 4.455165000 -0.623875000
1 -1.500647000 4.089065000 -1.293569000
6 -0.993693000 5.554226000 0.188594000
6 1.270401000 5.485749000 1.035702000
6 0.001160000 6.068583000 1.025096000
1 2.052342000 5.891779000 1.670579000
1 -1.974118000 6.020347000 0.159587000
1 -0.207901000 6.929658000 1.652950000
6 -4.054518000 1.594819000 0.444435000
1 -4.989565000 1.603089000 1.013356000

1 -3.394766000 2.357776000 0.871772000
1 -4.292384000 1.891284000 -0.584306000
6 -4.360835000 -0.888952000 0.012415000
6 -4.713720000 -1.944732000 0.863222000
1 -4.317685000 -1.968495000 1.876809000
6 -4.898659000 -0.875835000 -1.283615000
1 -4.651489000 -0.065941000 -1.966119000
6 -5.759604000 -1.885721000 -1.713213000
6 -5.576424000 -2.957310000 0.438820000
6 -6.101667000 -2.931538000 -0.853141000
1 -5.841473000 -3.761604000 1.119890000
1 -6.168176000 -1.853565000 -2.719716000
1 -6.775663000 -3.715585000 -1.186397000

S26

E + ZPE = -3168.559566

28 -0.140121000 0.376920000 -0.166452000
15 1.452674000 -0.763945000 0.769987000
6 3.090197000 0.046965000 1.187653000
1 3.658881000 0.200120000 0.265658000
6 3.818306000 -0.936615000 2.158769000
1 4.655576000 -1.431355000 1.657464000
1 4.252592000 -0.352103000 2.976188000
6 2.830527000 -1.992410000 2.716073000
1 3.002345000 -2.176283000 3.782472000
1 2.973237000 -2.952737000 2.206800000
6 1.379015000 -1.526761000 2.489702000
1 1.183204000 -0.656998000 3.131671000
6 0.345942000 -2.603982000 2.813051000
1 0.485789000 -3.497938000 2.195852000
1 -0.682315000 -2.245840000 2.693553000
1 0.459857000 -2.913145000 3.858256000
6 2.880446000 1.420596000 1.851333000
1 2.278944000 1.344887000 2.763850000
1 2.407212000 2.139232000 1.181359000
1 3.856501000 1.826339000 2.139129000
6 1.818772000 -2.147968000 -0.404865000
6 3.122605000 -2.384869000 -0.865180000
1 3.948958000 -1.780227000 -0.509642000
6 3.394046000 -3.407480000 -1.777335000
1 4.414542000 -3.574738000 -2.108877000
6 2.359311000 -4.208407000 -2.251778000
1 2.561314000 -5.007860000 -2.958148000
6 1.054179000 -3.972778000 -1.816721000
1 0.244646000 -4.596571000 -2.187721000
6 0.763777000 -2.951609000 -0.906733000
6 -0.673938000 -2.721255000 -0.497767000
1 -0.781852000 -2.646221000 0.583525000
1 -1.302416000 -3.552025000 -0.835505000
8 -1.208618000 -1.483347000 -1.015202000
6 -1.913752000 -1.644346000 -2.254417000
1 -2.697809000 -2.400641000 -2.140243000
1 -2.385304000 -0.689380000 -2.486359000
1 -1.234208000 -1.934527000 -3.065250000
6 -3.080382000 0.677929000 1.545891000
6 -0.558741000 1.266281000 1.443777000
6 -1.909737000 1.353998000 0.795294000
1 -2.155082000 2.386374000 0.520403000
1 -1.865472000 0.852658000 -0.229541000
1 -2.715889000 -0.299068000 1.892888000
1 -0.013841000 2.206020000 1.551911000
1 -0.543292000 0.699463000 2.376080000

6	1.091459000	1.399287000	-1.774056000
6	-0.236723000	1.309030000	-2.114004000
1	1.748131000	0.591455000	-2.096987000
1	-0.569274000	0.503114000	-2.757331000
1	-0.881282000	2.183429000	-2.081070000
6	1.793696000	2.627341000	-1.355625000
6	3.187516000	2.693326000	-1.524619000
1	3.715113000	1.836433000	-1.937936000
6	1.130558000	3.757654000	-0.843019000
1	0.052408000	3.742095000	-0.706136000
6	1.839919000	4.908447000	-0.509901000
6	3.897632000	3.848117000	-1.198275000
6	3.226373000	4.958807000	-0.685604000
1	4.972751000	3.881506000	-1.349065000
1	1.310655000	5.771458000	-0.116253000
1	3.775957000	5.859295000	-0.428223000
6	-4.272026000	0.421770000	0.633462000
6	-4.909036000	1.470515000	-0.047531000
1	-4.560269000	2.493133000	0.078414000
6	-4.766488000	-0.877899000	0.461892000
1	-4.294755000	-1.702599000	0.992572000
6	-5.864070000	-1.127616000	-0.364816000
6	-6.002949000	1.224957000	-0.878257000
6	-6.484403000	-0.075903000	-1.039913000
1	-6.484766000	2.051671000	-1.392951000
1	-6.237973000	-2.142074000	-0.474549000
1	-7.340396000	-0.265904000	-1.680991000
6	-3.468425000	1.506569000	2.785029000
1	-4.260746000	1.005079000	3.348914000
1	-2.610053000	1.650035000	3.451062000
1	-3.841021000	2.496477000	2.498303000

S27

E + ZPE = -3168.566278

28	-0.488147000	0.255522000	0.560518000
15	1.547343000	-0.498648000	0.888640000
6	2.708510000	0.795001000	1.598479000
1	3.149653000	1.353844000	0.769403000
6	3.789298000	0.016505000	2.416905000
1	4.788050000	0.191574000	2.004418000
1	3.802177000	0.419357000	3.435399000
6	3.475415000	-1.494680000	2.457205000
1	3.802726000	-1.944090000	3.401566000
1	4.011182000	-2.020954000	1.658633000
6	1.961276000	-1.711633000	2.267196000
1	1.434962000	-1.310334000	3.143262000
6	1.591011000	-3.184992000	2.095600000
1	2.060823000	-3.616524000	1.205601000
1	0.510325000	-3.346670000	2.031205000
1	1.950324000	-3.751711000	2.961795000
6	1.949803000	1.798152000	2.485810000
1	1.430175000	1.299354000	3.311880000
1	1.222590000	2.384725000	1.918663000
1	2.666960000	2.498595000	2.928036000
6	2.366372000	-1.237634000	-0.600690000
6	3.660583000	-0.826843000	-0.959921000
1	4.170647000	-0.061449000	-0.386678000
6	4.331108000	-1.395500000	-2.044525000
1	5.332473000	-1.058141000	-2.295153000
6	3.718284000	-2.401971000	-2.785107000
1	4.234285000	-2.863400000	-3.621679000
6	2.434056000	-2.820618000	-2.438072000

1	1.961672000	-3.618114000	-3.006041000
6	1.734005000	-2.248950000	-1.367755000
6	0.313510000	-2.722909000	-1.112663000
1	0.063523000	-2.690284000	-0.051268000
1	0.206664000	-3.765387000	-1.445754000
8	-0.677390000	-1.911326000	-1.745044000
6	-0.818181000	-2.135826000	-3.144790000
1	-1.039353000	-3.192454000	-3.352284000
1	-1.659952000	-1.524414000	-3.477398000
1	0.079974000	-1.841263000	-3.702442000
6	-3.413335000	-0.962882000	1.307147000
6	-1.020477000	-0.525886000	2.190015000
6	-2.294870000	0.037524000	1.684444000
1	-2.662583000	0.861146000	2.305900000
1	-2.096686000	0.628949000	0.689390000
1	-2.924740000	-1.804702000	0.798478000
1	-0.618800000	-0.063666000	3.091924000
1	-0.973702000	-1.614636000	2.236170000
6	0.205818000	1.342184000	-1.218846000
6	-1.161689000	1.183369000	-1.178874000
1	0.774744000	0.574757000	-1.737265000
1	-1.627386000	0.337371000	-1.673908000
1	-1.810479000	2.031951000	-0.975015000
6	0.920999000	2.618120000	-1.006194000
6	0.345445000	3.721503000	-0.349517000
1	-0.659317000	3.652170000	0.059412000
6	2.220798000	2.752960000	-1.524021000
1	2.673221000	1.915305000	-2.049339000
6	2.921119000	3.952908000	-1.399567000
6	1.046386000	4.917539000	-0.220867000
6	2.337162000	5.037937000	-0.744654000
1	0.584335000	5.759926000	0.285588000
1	3.918625000	4.042075000	-1.820166000
1	2.879695000	5.973527000	-0.646777000
6	-4.081628000	-1.501791000	2.585054000
1	-4.844385000	-2.243658000	2.330604000
1	-3.347207000	-1.975636000	3.245895000
1	-4.571946000	-0.699647000	3.147822000
6	-4.414857000	-0.361811000	0.331075000
6	-5.209525000	0.739799000	0.683399000
1	-5.132081000	1.173118000	1.678237000
6	-4.556161000	-0.902671000	-0.954001000
1	-3.950397000	-1.760256000	-1.239882000
6	-5.467439000	-0.362302000	-1.864013000
6	-6.118065000	1.284279000	-0.224950000
6	-6.250343000	0.734206000	-1.501800000
1	-6.728508000	2.134122000	0.067542000
1	-5.569181000	-0.801958000	-2.852482000
1	-6.962346000	1.154685000	-2.206053000

S28

E + ZPE = -3168.568523

28	0.076633000	-0.363922000	-0.075776000
15	-1.913797000	-0.329030000	0.725075000
6	-2.148072000	-1.023574000	2.466510000
1	-3.083950000	-1.592428000	2.425009000
6	-2.387040000	0.225957000	3.340980000
1	-2.849069000	-0.058830000	4.293287000
1	-1.428644000	0.702876000	3.585105000
6	-3.268605000	1.199353000	2.545775000
1	-3.340818000	2.177002000	3.035820000
1	-4.292095000	0.805783000	2.477832000

6	-2.671421000	1.350027000	1.128684000
1	-1.796859000	2.009261000	1.189215000
6	-3.634426000	1.917419000	0.084097000
1	-4.531816000	1.300432000	-0.021381000
1	-3.163921000	1.996982000	-0.901579000
1	-3.951914000	2.923330000	0.380765000
6	-1.054056000	-1.966547000	2.971028000
1	-0.086529000	-1.463426000	3.056391000
1	-0.930228000	-2.834499000	2.313789000
1	-1.318124000	-2.344461000	3.965410000
6	-3.116087000	-1.286679000	-0.306526000
6	-4.413711000	-1.523889000	0.179133000
1	-4.712176000	-1.124896000	1.143203000
6	-5.347679000	-2.257666000	-0.550954000
1	-6.343947000	-2.415605000	-0.148957000
6	-4.992163000	-2.789338000	-1.788523000
1	-5.703924000	-3.375042000	-2.362208000
6	-3.709229000	-2.568204000	-2.285412000
1	-3.431978000	-2.983575000	-3.251135000
6	-2.770000000	-1.811759000	-1.572935000
6	-1.445556000	-1.544052000	-2.255060000
1	-1.362839000	-0.500709000	-2.569096000
1	-1.350220000	-2.170781000	-3.148222000
8	-0.275131000	-1.766974000	-1.434693000
6	-0.048845000	-3.152464000	-1.102147000
1	-0.037247000	-3.743207000	-2.023378000
1	0.927829000	-3.206593000	-0.620740000
1	-0.827546000	-3.524424000	-0.429521000
1	3.914404000	-0.101636000	3.078867000
6	3.886112000	0.704789000	2.337277000
6	3.419623000	0.185979000	0.965045000
1	4.894132000	1.124393000	2.265446000
1	3.213548000	1.484509000	2.711547000
1	3.395228000	1.042488000	0.279084000
6	4.369913000	-0.847018000	0.376930000
6	4.599802000	-2.075582000	1.015974000
6	5.037848000	-0.591783000	-0.828009000
1	4.109895000	-2.298196000	1.961437000
1	4.887600000	0.360703000	-1.332803000
6	5.468353000	-3.017873000	0.464864000
6	5.909596000	-1.531557000	-1.382439000
1	5.637965000	-3.959884000	0.979284000
1	6.422215000	-1.307994000	-2.313957000
6	6.126079000	-2.749240000	-0.737663000
1	6.806469000	-3.480899000	-1.163759000
6	0.861411000	0.632965000	1.297815000
6	1.973479000	-0.361352000	1.075250000
1	1.797115000	-0.892631000	0.076887000
1	1.941124000	-1.171948000	1.810495000
1	0.432738000	0.613161000	2.299649000
1	1.092346000	1.662693000	1.008534000
6	0.290619000	1.843128000	-2.024257000
6	1.226255000	0.867338000	-2.055526000
1	-0.650021000	1.662247000	-2.546434000
1	2.221765000	1.009760000	-1.647818000
1	1.086300000	-0.016760000	-2.667549000
6	0.390252000	3.175582000	-1.417372000
6	-0.736482000	4.017660000	-1.443841000
1	-1.652988000	3.665198000	-1.910976000
6	1.575406000	3.669042000	-0.838066000
1	2.474514000	3.060309000	-0.837970000
6	1.621141000	4.947629000	-0.290410000
6	-0.691522000	5.298292000	-0.896109000
6	0.487459000	5.766031000	-0.313750000

1	-1.571855000	5.933426000	-0.932632000
1	2.546283000	5.313502000	0.145485000
1	0.528810000	6.765731000	0.108533000

S29

E + ZPE = -3168.580912

28	-0.363600000	0.019787000	-1.005583000
15	-1.861310000	-0.632878000	0.571149000
6	-1.980122000	-2.416888000	1.197389000
1	-3.053879000	-2.609190000	1.284929000
6	-1.379263000	-2.373214000	2.620910000
1	-1.731322000	-3.231432000	3.204995000
1	-0.286207000	-2.457653000	2.562322000
6	-1.764175000	-1.038960000	3.272707000
1	-1.221712000	-0.872678000	4.210638000
1	-2.833196000	-1.031913000	3.523495000
6	-1.453716000	0.091557000	2.268048000
1	-0.366296000	0.231744000	2.234666000
6	-2.102894000	1.438639000	2.591502000
1	-3.195513000	1.376529000	2.595559000
1	-1.804312000	2.214514000	1.878087000
1	-1.782940000	1.770914000	3.585558000
6	-1.395606000	-3.508359000	0.299001000
1	-0.309235000	-3.432119000	0.220446000
1	-1.818111000	-3.480160000	-0.711572000
1	-1.627074000	-4.492625000	0.721962000
6	-3.621266000	-0.165204000	0.202918000
6	-4.660768000	-0.647206000	1.018556000
1	-4.437163000	-1.274753000	1.873772000
6	-5.996840000	-0.331695000	0.773950000
1	-6.769906000	-0.718433000	1.431088000
6	-6.329828000	0.470777000	-0.314160000
1	-7.366791000	0.712349000	-0.526377000
6	-5.315645000	0.962086000	-1.132955000
1	-5.572190000	1.593104000	-1.980250000
6	-3.968546000	0.672601000	-0.882357000
6	-2.950119000	1.359935000	-1.762041000
1	-2.428319000	2.150030000	-1.214097000
1	-3.446311000	1.824452000	-2.621367000
8	-1.896779000	0.512334000	-2.265366000
6	-2.348841000	-0.520134000	-3.161567000
1	-2.924833000	-0.067599000	-3.975134000
1	-1.456158000	-0.997559000	-3.568231000
1	-2.965056000	-1.255658000	-2.634945000
1	3.675686000	-3.569151000	-2.032416000
6	3.368387000	-3.818134000	-1.010244000
6	2.937309000	-2.563489000	-0.226783000
1	4.214318000	-4.310738000	-0.520257000
1	2.545422000	-4.539495000	-1.075760000
1	2.604317000	-2.892011000	0.767693000
6	4.095901000	-1.596420000	-0.020398000
6	4.775915000	-1.031820000	-1.112118000
6	4.520980000	-1.252352000	1.269006000
1	4.484523000	-1.293913000	-2.126867000
1	4.014768000	-1.684367000	2.129572000
6	5.843344000	-0.153500000	-0.919245000
6	5.590491000	-0.376072000	1.468944000
1	6.363223000	0.260911000	-1.779023000
1	5.907666000	-0.134667000	2.479940000
6	6.255521000	0.178079000	0.374604000
1	7.096104000	0.849806000	0.525484000
6	1.090379000	-0.777674000	-0.059603000

6	1.722033000	-1.879106000	-0.919621000
1	0.987438000	-2.660343000	-1.152543000
1	2.061110000	-1.496209000	-1.888136000
1	0.771371000	-1.223045000	0.890071000
1	1.821647000	-0.007420000	0.196764000
6	0.526541000	1.903062000	-1.478422000
6	0.935961000	0.904616000	-2.346553000
1	-0.388487000	2.432834000	-1.741174000
1	1.945941000	0.516133000	-2.297688000
1	0.430835000	0.788697000	-3.302065000
6	1.308076000	2.588123000	-0.441770000
6	0.659365000	3.554115000	0.351949000
1	-0.393492000	3.767324000	0.178049000
6	2.680947000	2.357404000	-0.228648000
1	3.221644000	1.644553000	-0.842858000
6	3.368570000	3.054590000	0.760287000
6	1.348560000	4.253645000	1.338763000
6	2.706032000	4.000243000	1.548851000
1	0.832654000	4.999472000	1.936300000
1	4.425594000	2.858577000	0.910964000
1	3.248812000	4.546190000	2.315030000

S30

E + ZPE = -3168.562717

28	-0.459481000	-0.151773000	-1.289458000
15	-1.863642000	0.720754000	0.435126000
6	-1.188838000	1.331424000	2.098187000
1	-1.627789000	0.687069000	2.864832000
6	-1.729486000	2.779532000	2.265936000
1	-1.900147000	2.999113000	3.325540000
1	-0.960179000	3.480597000	1.917211000
6	-2.994663000	2.967384000	1.425175000
1	-3.270679000	4.025196000	1.338062000
1	-3.850166000	2.450490000	1.879348000
6	-2.707267000	2.368146000	0.037267000
1	-1.909876000	2.964460000	-0.429268000
6	-3.914816000	2.338223000	-0.900588000
1	-4.703049000	1.676397000	-0.527490000
1	-3.648865000	2.023243000	-1.916148000
1	-4.340130000	3.344868000	-0.981692000
6	0.335197000	1.270584000	2.254308000
1	0.848456000	1.818972000	1.457633000
1	0.714322000	0.246182000	2.267263000
1	0.613739000	1.735921000	3.207081000
6	-3.259047000	-0.439639000	0.819325000
6	-3.822584000	-0.556489000	2.098207000
1	-3.460323000	0.052320000	2.918623000
6	-4.869635000	-1.444703000	2.356916000
1	-5.284569000	-1.507288000	3.358519000
6	-5.378342000	-2.238004000	1.333346000
1	-6.192345000	-2.930652000	1.524044000
6	-4.833945000	-2.132273000	0.052988000
1	-5.236184000	-2.742239000	-0.752275000
6	-3.785356000	-1.248473000	-0.220860000
6	-3.265245000	-1.171271000	-1.637973000
1	-3.229451000	-0.142161000	-2.004951000
1	-3.919700000	-1.730152000	-2.316137000
8	-1.916813000	-1.672253000	-1.796549000
6	-1.840853000	-3.107436000	-1.797132000
1	-2.530492000	-3.512449000	-2.546311000
1	-0.820259000	-3.370614000	-2.069417000
1	-2.085196000	-3.514100000	-0.810127000

6	0.904534000	-0.991949000	-0.248964000
6	1.700385000	-2.123427000	-0.870103000
1	1.042914000	-2.841476000	-1.373836000
1	2.397608000	-1.753795000	-1.628831000
1	0.297352000	-1.372817000	0.584215000
1	1.549638000	-0.187942000	0.108741000
6	0.506902000	1.320463000	-2.217286000
6	0.596878000	0.098301000	-2.922203000
1	1.546310000	-0.415580000	-3.013251000
1	-0.351787000	1.954732000	-2.468340000
1	-0.086696000	-0.084878000	-3.752376000
6	1.598414000	2.094166000	-1.597278000
6	1.329286000	3.406613000	-1.165805000
1	0.335959000	3.824335000	-1.317385000
6	2.899328000	1.589916000	-1.421406000
1	3.146189000	0.586837000	-1.753967000
6	3.887979000	2.367311000	-0.824183000
6	2.320798000	4.188712000	-0.577256000
6	3.604080000	3.668204000	-0.399777000
1	2.094586000	5.203815000	-0.263858000
1	4.882268000	1.953682000	-0.687387000
1	4.380050000	4.273684000	0.059143000
6	2.517545000	-2.915409000	0.200058000
1	1.812642000	-3.225688000	0.983602000
6	3.588307000	-2.058655000	0.862865000
6	3.493820000	-1.724016000	2.220021000
1	2.649390000	-2.088978000	2.801617000
6	4.700862000	-1.596241000	0.142987000
1	4.813827000	-1.855330000	-0.907347000
6	5.685486000	-0.824627000	0.761559000
6	4.475059000	-0.949463000	2.843188000
6	5.574927000	-0.496341000	2.114892000
1	4.383921000	-0.710258000	3.899245000
1	6.548016000	-0.492357000	0.189530000
1	6.345188000	0.097658000	2.598508000
6	3.103706000	-4.193951000	-0.428544000
1	2.308124000	-4.836987000	-0.822292000
1	3.785799000	-3.961952000	-1.253938000
1	3.665689000	-4.765187000	0.316988000

S31

E + ZPE = -3168.563626

28	-0.401191000	-0.151922000	-1.311070000
15	-1.921692000	0.658581000	0.386467000
6	-1.273991000	1.250559000	2.064558000
1	-1.807758000	0.669460000	2.823107000
6	-1.703019000	2.737958000	2.164074000
1	-1.808144000	3.031386000	3.214580000
1	-0.907909000	3.363289000	1.737274000
6	-2.996465000	2.949718000	1.371131000
1	-3.235224000	4.014021000	1.257069000
1	-3.848821000	2.486823000	1.885865000
6	-2.799782000	2.287756000	-0.005344000
1	-2.045694000	2.869195000	-0.553169000
6	-4.063937000	2.190254000	-0.860957000
1	-4.834498000	1.583490000	-0.375433000
1	-3.864812000	1.761485000	-1.850376000
1	-4.480004000	3.191119000	-1.022176000
6	0.229166000	1.051976000	2.284479000
1	0.820259000	1.580459000	1.529143000
1	0.516408000	-0.003399000	2.269345000
1	0.509504000	1.455624000	3.264282000

6	-3.291953000	-0.538298000	0.728065000
6	-3.996674000	-0.554396000	1.940728000
1	-3.742227000	0.141597000	2.732456000
6	-5.045343000	-1.449609000	2.163655000
1	-5.572876000	-1.433891000	3.112730000
6	-5.411232000	-2.352505000	1.169520000
1	-6.224606000	-3.052932000	1.332543000
6	-4.721496000	-2.351337000	-0.043143000
1	-5.006984000	-3.054143000	-0.822156000
6	-3.670771000	-1.459083000	-0.280929000
6	-2.982829000	-1.509783000	-1.627441000
1	-2.982946000	-0.535789000	-2.128380000
1	-3.497494000	-2.211658000	-2.293056000
8	-1.590065000	-1.895334000	-1.557276000
6	-1.401052000	-3.269792000	-1.179359000
1	-1.924136000	-3.918849000	-1.890277000
1	-0.332609000	-3.469923000	-1.226560000
1	-1.774469000	-3.451975000	-0.166644000
6	1.071353000	-1.007662000	-0.458863000
6	2.014523000	-1.940363000	-1.191428000
1	1.472493000	-2.589091000	-1.891260000
1	2.736106000	-1.377731000	-1.793522000
1	0.477498000	-1.563236000	0.282774000
1	1.609138000	-0.198157000	0.039557000
6	0.394151000	1.459579000	-2.158639000
6	0.579760000	0.291021000	-2.936734000
1	1.567942000	-0.127917000	-3.082209000
1	-0.511953000	2.036122000	-2.372689000
1	-0.108449000	0.088417000	-3.759714000
6	1.433504000	2.287775000	-1.513625000
6	1.079052000	3.566809000	-1.045562000
1	0.061215000	3.924044000	-1.187617000
6	2.766584000	1.870250000	-1.354203000
1	3.081249000	0.898989000	-1.721401000
6	3.703101000	2.696314000	-0.738024000
6	2.017256000	4.397611000	-0.436070000
6	3.333522000	3.961659000	-0.274602000
1	1.723408000	5.386295000	-0.095477000
1	4.725834000	2.350875000	-0.620889000
1	4.068201000	4.605421000	0.199811000
6	2.809301000	-2.851606000	-0.205332000
1	2.070621000	-3.403159000	0.393901000
6	3.663199000	-2.043227000	0.763872000
6	3.372211000	-2.036842000	2.134312000
1	2.536105000	-2.626638000	2.505155000
6	4.762112000	-1.293362000	0.317007000
1	5.026646000	-1.293327000	-0.738067000
6	5.541517000	-0.560073000	1.212225000
6	4.148737000	-1.303124000	3.034420000
6	5.236138000	-0.560292000	2.575192000
1	3.908699000	-1.321491000	4.094095000
1	6.396967000	0.002202000	0.846942000
1	5.847121000	0.005447000	3.272771000
6	3.635841000	-3.887127000	-0.990400000
1	2.989373000	-4.508789000	-1.620640000
1	4.373023000	-3.405259000	-1.641798000
1	4.178153000	-4.545192000	-0.304237000

S32

E + ZPE = -3168.560073

28	-0.435702000	0.396574000	-1.095755000
15	-1.755408000	0.565424000	0.673081000

6	-1.240551000	0.630607000	2.498979000
1	-1.765513000	-0.191534000	2.991628000
6	-1.792586000	1.982351000	3.031671000
1	-2.052143000	1.889098000	4.091761000
1	-0.996139000	2.735378000	2.967364000
6	-2.980891000	2.437736000	2.181362000
1	-3.251953000	3.479756000	2.388527000
1	-3.870865000	1.829288000	2.387454000
6	-2.567079000	2.275279000	0.708505000
1	-1.737638000	2.970297000	0.516470000
6	-3.684158000	2.544405000	-0.300349000
1	-4.494609000	1.814122000	-0.212567000
1	-3.323405000	2.538752000	-1.335132000
1	-4.110771000	3.536931000	-0.117488000
6	0.252406000	0.466828000	2.808226000
1	0.873665000	1.166473000	2.239119000
1	0.611061000	-0.548489000	2.624395000
1	0.411332000	0.678627000	3.872075000
6	-3.185639000	-0.612049000	0.549071000
6	-3.860296000	-1.068322000	1.692367000
1	-3.543188000	-0.759787000	2.681084000
6	-4.965534000	-1.917113000	1.602922000
1	-5.463238000	-2.246259000	2.510130000
6	-5.423538000	-2.329610000	0.356280000
1	-6.282239000	-2.988649000	0.272554000
6	-4.765174000	-1.887829000	-0.791232000
1	-5.120717000	-2.208501000	-1.767272000
6	-3.655973000	-1.038100000	-0.720913000
6	-3.013089000	-0.616742000	-2.026827000
1	-2.931601000	0.471429000	-2.112299000
1	-3.626513000	-0.959174000	-2.869065000
8	-1.672941000	-1.104020000	-2.202903000
6	-1.600132000	-2.527545000	-2.361112000
1	-2.225761000	-2.837847000	-2.306552000
1	-0.560181000	-2.771015000	-2.575929000
1	-1.925402000	-3.047769000	-1.453873000
6	0.664501000	-0.892899000	-0.247279000
6	1.649345000	-1.245504000	-1.345746000
1	1.140927000	-1.480032000	-2.290003000
1	2.313387000	-0.397572000	-1.543825000
1	0.066488000	-1.755333000	0.069432000
1	1.173377000	-0.464577000	0.611832000
6	0.429834000	2.215680000	-1.636657000
6	0.115310000	1.465362000	-2.763807000
1	0.876066000	0.950586000	-3.343378000
1	-0.326901000	2.921639000	-1.288907000
1	-0.817632000	1.648151000	-3.294899000
6	1.784272000	2.504274000	-1.113864000
6	1.918981000	3.144697000	0.130688000
1	1.025414000	3.411411000	0.691535000
6	2.950683000	2.209086000	-1.840289000
1	2.876158000	1.765102000	-2.828577000
6	4.207850000	2.526226000	-1.327163000
6	3.174307000	3.459271000	0.646023000
6	4.325210000	3.145597000	-0.080437000
1	3.255200000	3.958869000	1.607082000
1	5.097019000	2.307267000	-1.911589000
1	5.305146000	3.399676000	0.312652000
6	2.521195000	-2.487591000	-0.971436000
1	1.832512000	-3.334460000	-0.846455000
6	3.266808000	-2.311740000	0.344728000
6	3.075395000	-3.222430000	1.391765000
1	2.384983000	-4.052849000	1.258112000
6	4.170492000	-1.256013000	0.539560000

1	4.340622000	-0.530319000	-0.252287000
6	4.860250000	-1.118450000	1.744273000
6	3.767158000	-3.090742000	2.598011000
6	4.662773000	-2.036668000	2.778133000
1	3.608655000	-3.814842000	3.392621000
1	5.556978000	-0.294607000	1.873796000
1	5.205549000	-1.932683000	3.713390000
6	3.475397000	-2.825821000	-2.131977000
1	4.187899000	-2.013145000	-2.312073000
1	4.051947000	-3.727458000	-1.901961000
1	2.921158000	-3.002580000	-3.061558000

S33

E + ZPE = -3168.571028

28	-0.070910000	-0.006840000	-0.302272000
15	-2.047874000	0.739144000	0.202585000
6	-2.139283000	1.715628000	1.804385000
1	-2.371774000	1.015799000	2.612427000
6	-3.284191000	2.765766000	1.616651000
1	-4.036129000	2.667422000	2.406255000
1	-2.851392000	3.766324000	1.726058000
6	-3.931378000	2.637916000	0.221843000
1	-4.335616000	3.598330000	-0.118092000
1	-4.770811000	1.933401000	0.245477000
6	-2.871023000	2.124589000	-0.769601000
1	-2.090007000	2.892909000	-0.861743000
6	-3.420267000	1.800987000	-2.158310000
1	-4.163256000	0.997376000	-2.118996000
1	-2.631495000	1.511872000	-2.861222000
1	-3.915181000	2.685240000	-2.574980000
6	-0.805565000	2.402952000	2.141929000
1	-0.484044000	3.081036000	1.344315000
1	0.004244000	1.690343000	2.318941000
1	-0.927874000	3.001800000	3.051467000
6	-3.336565000	-0.587769000	0.306994000
6	-4.233285000	-0.607985000	1.387369000
1	-4.172515000	0.139963000	2.169291000
6	-5.233865000	-1.576511000	1.489369000
1	-5.911385000	-1.561239000	2.337841000
6	-5.360507000	-2.546668000	0.500802000
1	-6.138618000	-3.301373000	0.563544000
6	-4.476386000	-2.540269000	-0.578159000
1	-4.578109000	-3.292854000	-1.356222000
6	-3.459648000	-1.585188000	-0.693949000
6	-2.522246000	-1.688216000	-1.883233000
1	-2.318922000	-0.707663000	-2.318173000
1	-2.988965000	-2.302239000	-2.665957000
8	-1.238310000	-2.226528000	-1.556896000
6	-1.247925000	-3.635122000	-1.341195000
1	-1.639616000	-4.161205000	-2.222763000
1	-0.211066000	-3.938889000	-1.182746000
1	-1.845929000	-3.912295000	-0.463722000
6	2.420245000	-1.446311000	1.566250000
6	-0.120878000	-1.059108000	1.280775000
6	1.162102000	-1.520432000	0.674686000
1	1.050839000	-2.505154000	0.214773000
1	1.419195000	-0.860027000	-0.244065000
1	2.423587000	-0.454375000	2.038364000
1	-0.921571000	-1.795673000	1.317835000
1	-0.019794000	-0.524265000	2.226870000
6	0.624334000	1.576083000	-1.587052000
6	0.539993000	0.369444000	-2.248996000

1	-0.226606000	2.246558000	-1.673931000
1	1.423022000	-0.226916000	-2.462593000
1	-0.322903000	0.146378000	-2.867984000
6	1.827574000	2.222412000	-1.035745000
6	1.716619000	3.548258000	-0.575361000
1	0.753679000	4.051427000	-0.627479000
6	3.089284000	1.600566000	-0.988618000
1	3.218571000	0.583363000	-1.346058000
6	4.196941000	2.286637000	-0.498203000
6	2.825449000	4.234737000	-0.087840000
6	4.070044000	3.603450000	-0.046232000
1	2.720694000	5.260986000	0.251543000
1	5.161104000	1.789195000	-0.471773000
1	4.938680000	4.135959000	0.329811000
6	2.316478000	-2.504247000	2.684748000
1	3.180313000	-2.439763000	3.352973000
1	1.408008000	-2.365772000	3.281400000
1	2.299524000	-3.515604000	2.262130000
6	3.730902000	-1.595814000	0.802990000
6	3.867372000	-2.443895000	-0.305581000
1	3.016304000	-3.012928000	-0.671418000
6	4.866696000	-0.906625000	1.252746000
1	4.783391000	-0.247529000	2.114308000
6	6.099421000	-1.056319000	0.617174000
6	5.097919000	-2.588507000	-0.951814000
6	6.218173000	-1.895810000	-0.492821000
1	5.180196000	-3.250245000	-1.809622000
1	6.967110000	-0.518201000	0.989225000
1	7.176009000	-2.012654000	-0.991325000

S34

E + ZPE = -3168.563994

28	0.254483000	0.159345000	-0.894839000
15	1.406622000	-0.385362000	0.825194000
6	1.413214000	0.741693000	2.334529000
1	2.462652000	0.887791000	2.611831000
6	0.721857000	-0.093997000	3.438148000
1	0.997450000	0.284066000	4.428966000
1	-0.367051000	0.015860000	3.346903000
6	1.110096000	-1.566586000	3.252243000
1	0.530571000	-2.227269000	3.907463000
1	2.168122000	-1.717556000	3.506438000
6	0.866595000	-1.927743000	1.772744000
1	-0.215932000	-1.986560000	1.614270000
6	1.492021000	-3.246547000	1.314705000
1	2.580191000	-3.244485000	1.427535000
1	1.259116000	-3.468393000	0.266580000
1	1.095469000	-4.071253000	1.917662000
6	0.783333000	2.115620000	2.103165000
1	-0.257785000	2.032860000	1.777846000
1	1.327202000	2.689758000	1.346605000
1	0.800469000	2.695013000	3.033467000
6	3.168344000	-0.721462000	0.365464000
6	4.198833000	-0.660965000	1.315727000
1	3.983554000	-0.375355000	2.339406000
6	5.517332000	-0.978580000	0.983780000
1	6.290907000	-0.925371000	1.743992000
6	5.832213000	-1.361498000	-0.317129000
1	6.854459000	-1.607460000	-0.587713000
6	4.821979000	-1.419168000	-1.276944000
1	5.067438000	-1.709974000	-2.295466000
6	3.495551000	-1.112995000	-0.955045000

6	2.458714000	-1.213289000	-2.050862000	6	0.616863000	-3.170779000	1.646010000
1	1.695573000	-1.968324000	-1.845085000	1	1.589143000	-3.665975000	1.573070000
1	2.936151000	-1.470795000	-3.002144000	1	0.090979000	-3.322750000	0.697055000
8	1.716320000	0.021562000	-2.250485000	1	0.041333000	-3.679932000	2.427487000
6	2.564856000	1.104259000	-2.691158000	6	2.711282000	1.900616000	1.730847000
1	3.134205000	0.775454000	-3.566082000	1	1.733237000	2.390095000	1.667084000
1	1.915537000	1.930400000	-2.970490000	1	3.249927000	2.085336000	0.794219000
1	3.248173000	1.410777000	-1.894339000	1	3.276425000	2.387769000	2.533908000
6	-2.085075000	-2.168055000	-1.365356000	6	2.867115000	-1.646807000	-0.116089000
6	-1.408275000	-0.010517000	-0.081568000	6	3.802447000	-2.373605000	0.639468000
6	-1.809140000	-0.648022000	-1.398754000	1	3.811277000	-2.289362000	1.721505000
1	-2.646333000	-0.118048000	-1.868687000	6	4.729385000	-3.219881000	0.031264000
1	-0.984338000	-0.482536000	-2.162513000	1	5.436225000	-3.773530000	0.641931000
1	-1.198796000	-2.648240000	-0.925693000	6	4.743592000	-3.347919000	-1.356345000
1	-1.870489000	0.960323000	0.120569000	1	5.462427000	-4.001201000	-1.841343000
1	-1.564773000	-0.664097000	0.776228000	6	3.838730000	-2.614876000	-2.122688000
6	-0.298113000	3.245914000	-1.598718000	1	3.864526000	-2.696088000	-3.206543000
6	-0.766278000	2.266532000	-2.400486000	6	2.897745000	-1.770961000	-1.522559000
1	0.737573000	3.562949000	-1.726743000	6	1.958717000	-0.992468000	-2.413349000
1	-0.174639000	1.877789000	-3.222755000	1	0.919361000	-1.323838000	-2.318613000
1	-1.807943000	1.964352000	-2.386080000	1	2.246578000	-1.106049000	-3.464557000
6	-1.034033000	3.997132000	-0.575808000	8	1.931505000	0.419588000	-2.097668000
6	-0.357225000	5.002730000	0.138170000	6	3.189408000	1.081992000	-2.329342000
1	0.690434000	5.197088000	-0.080437000	1	3.448852000	1.005708000	-3.390489000
6	-2.396002000	3.778029000	-0.290717000	1	3.056393000	2.130082000	-2.061958000
1	-2.95554000	3.029779000	-0.844341000	1	3.983915000	0.641749000	-1.719906000
6	-3.047554000	4.528875000	0.682913000	6	-3.388991000	0.522705000	0.743994000
6	-1.010638000	5.757989000	1.109989000	6	-1.111959000	0.686748000	0.431215000
6	-2.357564000	5.520428000	1.387810000	6	-2.002936000	-0.491521000	0.028644000
1	-0.471171000	6.533823000	1.645407000	1	-1.499412000	-1.451253000	0.208176000
1	-4.099091000	4.349099000	0.887049000	1	-2.203351000	-0.462199000	-1.049812000
1	-2.871174000	6.109043000	2.142304000	1	-3.858895000	0.454197000	0.564079000
6	-2.267145000	-2.729037000	-2.787514000	1	-1.651910000	1.631349000	0.320102000
1	-3.132049000	-2.275788000	-3.284953000	1	-0.823685000	0.630858000	1.486646000
1	-1.383131000	-2.534684000	-3.408638000	6	0.064818000	2.639400000	-1.576203000
1	-2.431674000	-3.810374000	-2.759747000	6	-0.654140000	1.631812000	-2.194587000
6	-3.269727000	-2.504857000	-0.468431000	1	1.077459000	2.816312000	-1.935797000
6	-3.115168000	-3.390971000	0.605150000	1	-0.255590000	1.151589000	-3.083822000
1	-2.140801000	-3.838486000	0.792992000	1	-1.726409000	1.545460000	-2.055039000
6	-4.541061000	-1.959963000	-0.702184000	6	-0.448502000	3.731506000	-0.736629000
1	-4.696570000	-1.277289000	-1.534599000	6	0.471797000	4.562930000	-0.070691000
6	-5.621520000	-2.288151000	0.116146000	1	1.537427000	4.375945000	-0.183021000
6	-4.194635000	-3.724405000	1.426296000	6	-1.821311000	4.015284000	-0.608234000
6	-5.451754000	-3.171378000	1.184845000	1	-2.551087000	3.422907000	-1.151611000
1	-4.052506000	-4.417990000	2.250585000	6	-2.254533000	5.078535000	0.178990000
1	-6.598727000	-1.857061000	-0.083238000	6	0.038425000	5.624732000	0.719020000
1	-6.294314000	-3.428659000	1.820201000	6	-1.328061000	5.881953000	0.849961000

S35

E + ZPE = -3168.582265

28	0.418365000	0.722901000	-0.701693000	1	0.763713000	6.256582000	1.223105000
15	1.614666000	-0.587242000	0.732052000	1	-3.316523000	5.291023000	0.258784000
6	2.574105000	0.404859000	2.023563000	1	-1.669753000	6.714300000	1.458081000
1	3.575500000	-0.041424000	2.051440000	6	-4.284662000	-1.577179000	0.108184000
6	1.854355000	0.086453000	3.352306000	6	-4.012123000	-2.947372000	0.239510000
1	2.501748000	0.332967000	4.201624000	1	-3.155410000	-3.277116000	0.823106000
1	0.958079000	0.714862000	3.443286000	6	-5.402827000	-1.195260000	-0.644446000
6	1.456394000	-1.394062000	3.340607000	1	-5.636667000	-0.138134000	-0.754016000
1	0.795854000	-1.644926000	4.178516000	6	-6.227138000	-2.147498000	-1.246867000
1	2.347720000	-2.026831000	3.443821000	6	-4.831921000	-3.902997000	-0.360872000
6	0.748069000	-1.686494000	1.998601000	6	-5.943410000	-3.506153000	-1.107326000
1	-0.259859000	-1.265261000	2.062195000	1	-4.605583000	-4.959327000	-0.242084000
				1	-7.092369000	-1.826652000	-1.820639000
				1	-6.584148000	-4.250244000	-1.571906000
				6	-3.270868000	-0.703564000	2.267275000
				1	-2.702892000	0.113130000	2.726673000
				1	-4.263149000	-0.719065000	2.729119000

1 -2.776837000 -1.648675000 2.524722000

S36

E + ZPE = -3168.560257

28 -0.259387000 -0.127032000 0.088426000
15 1.798123000 -0.301356000 0.794130000
6 2.825200000 1.237164000 1.090096000
1 3.153312000 1.634555000 0.125917000
6 4.035442000 0.785613000 1.969505000
1 4.965094000 0.807519000 1.392704000
1 4.160025000 1.511281000 2.779829000
6 3.799008000 -0.630686000 2.549881000
1 4.150833000 -0.701830000 3.585116000
1 4.361270000 -1.377258000 1.976801000
6 2.299664000 -0.979224000 2.478691000
1 1.756986000 -0.326289000 3.175984000
6 1.999032000 -2.430340000 2.847850000
1 2.510233000 -3.133055000 2.181108000
1 0.925840000 -2.649909000 2.839366000
1 2.360608000 -2.628033000 3.863224000
6 2.004994000 2.333255000 1.793284000
1 1.615139000 1.996283000 2.760281000
1 1.169810000 2.681109000 1.183343000
1 2.656053000 3.192491000 1.987643000
6 2.699456000 -1.315461000 -0.465364000
6 3.893084000 -0.858637000 -1.044087000
1 4.328104000 0.084572000 -0.734201000
6 4.559807000 -1.607975000 -2.016307000
1 5.487146000 -1.234303000 -2.440302000
6 4.037922000 -2.829860000 -2.431082000
1 4.551064000 -3.421058000 -3.183458000
6 2.844674000 -3.291036000 -1.872897000
1 2.436396000 -4.246427000 -2.193372000
6 2.161873000 -2.552308000 -0.901443000
6 0.856935000 -3.089361000 -0.356124000
1 0.818751000 -3.035981000 0.730873000
1 0.732038000 -4.140559000 -0.639739000
8 -0.290202000 -2.339410000 -0.804611000
6 -0.827311000 -2.819295000 -2.044153000
1 -1.000622000 -3.900033000 -1.983687000
1 -1.786578000 -2.323123000 -2.196160000
1 -0.156679000 -2.604113000 -2.885222000
6 -3.409348000 0.518332000 1.312735000
6 -0.864438000 0.414025000 1.788098000
6 -2.097527000 -0.305782000 1.330721000
1 -2.227940000 -1.251343000 1.866132000
1 -1.956618000 -0.640653000 0.246956000
1 -3.172287000 1.484581000 0.846039000
1 -0.940672000 1.503644000 1.852700000
1 -0.400425000 0.005023000 2.684532000
6 0.120316000 1.197323000 -1.697938000
6 -1.116664000 0.598940000 -1.742503000
1 0.946550000 0.676590000 -2.181920000
1 -1.258434000 -0.298419000 -2.331981000
1 -2.020407000 1.162144000 -1.528036000
6 0.386026000 2.619583000 -1.406279000
6 1.623469000 3.164218000 -1.790348000
1 2.359037000 2.524644000 -2.273612000
6 -0.561968000 3.473751000 -0.813066000
1 -1.532037000 3.086740000 -0.513566000
6 -0.276367000 4.820678000 -0.607400000
6 1.908848000 4.514419000 -1.588625000

6 0.960850000 5.346816000 -0.992372000
1 2.867102000 4.916948000 -1.904165000
1 -1.021911000 5.464839000 -0.150127000
1 1.178783000 6.398850000 -0.834545000
6 -4.490699000 -0.144268000 0.471281000
6 -4.952060000 -1.437602000 0.761594000
1 -4.543721000 -1.984522000 1.608494000
6 -5.057558000 0.534678000 -0.615446000
1 -4.727612000 1.545914000 -0.846727000
6 -6.054163000 -0.057207000 -1.394409000
6 -5.945543000 -2.033424000 -0.015553000
6 -6.499761000 -1.345125000 -1.097216000
1 -6.292826000 -3.033641000 0.228536000
1 -6.483990000 0.490886000 -2.228241000
1 -7.277253000 -1.807450000 -1.698506000
6 -3.876747000 0.796068000 2.753177000
1 -3.102068000 1.318107000 3.326381000
1 -4.778410000 1.415887000 2.750567000
1 -4.115755000 -0.135719000 3.278254000

S37

E + ZPE = -3168.568859

28 0.077646000 -0.062260000 0.178917000
15 2.125786000 0.437247000 0.675575000
6 2.426274000 2.279507000 0.862429000
1 2.515157000 2.741761000 -0.125761000
6 3.747311000 2.428679000 1.676985000
1 4.554588000 2.805968000 1.042163000
1 3.590293000 3.182402000 2.455765000
6 4.151965000 1.075387000 2.309311000
1 4.544149000 1.208560000 3.323535000
1 4.953442000 0.609393000 1.723874000
6 2.946228000 0.111872000 2.336762000
1 2.202345000 0.479986000 3.056235000
6 3.357858000 -1.303696000 2.741856000
1 4.063073000 -1.740315000 2.026850000
1 2.505572000 -1.980170000 2.854810000
1 3.864467000 -1.262849000 3.712762000
6 1.240454000 2.934003000 1.597763000
1 1.095403000 2.504253000 2.590730000
1 0.299585000 2.836032000 1.050259000
1 1.443299000 4.002461000 1.731472000
6 3.276184000 -0.211325000 -0.618251000
6 4.116436000 0.674520000 -1.310851000
1 4.109359000 1.733106000 -1.077339000
6 4.989374000 0.223750000 -2.303102000
1 5.630583000 0.932459000 -2.818583000
6 5.038566000 -1.131122000 -2.615597000
1 5.719665000 -1.496584000 -3.378198000
6 4.205417000 -2.021954000 -1.937371000
1 4.252462000 -3.081863000 -2.174881000
6 3.311099000 -1.591942000 -0.950126000
6 2.409703000 -2.632048000 -0.301216000
1 2.273917000 -2.433838000 0.760906000
1 2.874387000 -3.623892000 -0.394718000
8 1.084851000 -2.672237000 -0.833779000
6 0.981965000 -3.327212000 -2.093432000
1 1.358387000 -4.357877000 -2.029312000
1 -0.079153000 -3.351345000 -2.350112000
1 1.531555000 -2.795972000 -2.881875000
6 -2.867480000 -0.938326000 1.767748000
6 -0.283118000 -0.781442000 1.884238000

6	-1.489895000	-1.243060000	1.134571000
1	-1.394493000	-2.294250000	0.850794000
1	-1.526822000	-0.712951000	0.105230000
1	-2.870603000	0.124943000	2.042928000
1	-0.466704000	-0.024950000	2.652685000
1	0.373555000	-1.568880000	2.248986000
6	-0.193551000	1.318954000	-1.479991000
6	-0.083428000	0.011816000	-1.897940000
1	0.718480000	1.913109000	-1.484041000
1	0.871652000	-0.359797000	-2.250276000
1	-0.953121000	-0.565848000	-2.199598000
6	-1.423521000	2.118623000	-1.339147000
6	-2.716796000	1.573614000	-1.448701000
1	-2.856717000	0.509159000	-1.612185000
6	-1.297243000	3.506930000	-1.142746000
1	-0.305602000	3.948246000	-1.078822000
6	-2.420428000	4.326455000	-1.063409000
6	-3.838839000	2.392961000	-1.365872000
6	-3.695987000	3.770277000	-1.172684000
1	-4.826370000	1.951653000	-1.453918000
1	-2.300106000	5.396642000	-0.923636000
1	-4.574632000	4.405878000	-1.113910000
6	-3.031162000	-1.763760000	3.060569000
1	-3.988115000	-1.534556000	3.538858000
1	-3.018298000	-2.837840000	2.842274000
1	-2.228974000	-1.549557000	3.775428000
6	-4.038742000	-1.176741000	0.823436000
6	-5.110338000	-0.273041000	0.804038000
1	-5.074098000	0.610945000	1.437043000
6	-4.115866000	-2.314100000	0.005515000
1	-3.314840000	-3.049447000	0.012614000
6	-5.224864000	-2.534605000	-0.814054000
6	-6.224800000	-0.494648000	-0.006668000
6	-6.283512000	-1.625501000	-0.823300000
1	-7.048334000	0.214402000	0.003049000
1	-5.264518000	-3.422966000	-1.438414000
1	-7.149153000	-1.800101000	-1.455657000

S38

E + ZPE = -3168.567103

28	-0.325408000	-0.470207000	-0.806161000
15	-1.689827000	-0.410704000	0.838425000
6	-1.532711000	-1.770723000	2.140377000
1	-2.563140000	-2.054279000	2.383530000
6	-0.934305000	-1.048932000	3.367414000
1	-1.099800000	-1.641339000	4.274648000
1	0.152511000	-0.947787000	3.249940000
6	-1.581510000	0.339790000	3.464950000
1	-1.085061000	0.968996000	4.212427000
1	-2.629367000	0.243683000	3.780346000
6	-1.515109000	1.004322000	2.071749000
1	-0.489469000	1.354704000	1.903080000
6	-2.469163000	2.182892000	1.871879000
1	-3.513809000	1.893042000	2.020233000
1	-2.377067000	2.611823000	0.868618000
1	-2.235084000	2.975186000	2.591676000
6	-0.790552000	-3.038342000	1.711536000
1	0.259975000	-2.841256000	1.477763000
1	-1.255280000	-3.504379000	0.835320000
1	-0.814054000	-3.773791000	2.523869000
6	-3.457335000	-0.501471000	0.293401000
6	-4.472656000	-0.675155000	1.249491000

1	-4.219395000	-0.734811000	2.302917000
6	-5.815920000	-0.764823000	0.886584000
1	-6.574957000	-0.891021000	1.652745000
6	-6.172580000	-0.698620000	-0.458275000
1	-7.212889000	-0.780536000	-0.757937000
6	-5.180006000	-0.531609000	-1.421954000
1	-5.458988000	-0.481237000	-2.471611000
6	-3.829706000	-0.415689000	-1.068316000
6	-2.850369000	-0.132272000	-2.186634000
1	-2.466392000	0.888831000	-2.131817000
1	-3.343199000	-0.254965000	-3.157031000
8	-1.663097000	-0.960179000	-2.189151000
6	-1.923150000	-2.353674000	-2.454257000
1	-2.486616000	-2.441245000	-3.388451000
1	-0.953638000	-2.840353000	-2.563098000
1	-2.485757000	-2.808018000	-1.633411000
1	2.668027000	-1.721396000	-3.431779000
6	3.394156000	-1.963136000	-2.644960000
6	3.144664000	-1.118661000	-1.383595000
1	4.396684000	-1.778070000	-3.042159000
1	3.315272000	-3.035622000	-2.434082000
1	3.204266000	-0.060656000	-1.669317000
6	4.195601000	-1.355076000	-0.306294000
6	4.412703000	-2.632851000	0.230598000
6	4.975735000	-0.294246000	0.169251000
1	3.830624000	-3.480007000	-0.125443000
1	4.828245000	0.703462000	-0.238891000
6	5.379526000	-2.841132000	1.213925000
6	5.946442000	-0.498101000	1.152018000
1	5.535435000	-3.839510000	1.613395000
1	6.544459000	0.338943000	1.501749000
6	6.150517000	-1.773337000	1.678539000
1	6.906656000	-1.936369000	2.441113000
6	1.220930000	-0.392768000	0.231179000
6	1.724446000	-1.363599000	-0.810628000
1	1.032341000	-1.318745000	-1.718884000
1	1.642228000	-2.399436000	-0.465805000
1	1.225452000	-0.788597000	1.246215000
1	1.702637000	0.589994000	0.216911000
6	0.021594000	2.341421000	-1.857964000
6	0.464360000	1.298967000	-2.595676000
1	-1.033004000	2.608987000	-1.938543000
1	1.516665000	1.037561000	-2.646602000
1	-0.184950000	0.817185000	-3.318708000
6	0.793731000	3.223521000	-0.975890000
6	0.110669000	4.210769000	-0.242299000
1	-0.968195000	4.299650000	-0.346742000
6	2.194881000	3.152554000	-0.851884000
1	2.755978000	2.429588000	-1.436358000
6	2.879049000	4.024147000	-0.009938000
6	0.795085000	5.083641000	0.601213000
6	2.182161000	4.989744000	0.723336000
1	0.248150000	5.841593000	1.154402000
1	3.960645000	3.960546000	0.067079000
1	2.720381000	5.671914000	1.374791000

S39

E + ZPE = -3168.578939

28	-0.331731000	0.399347000	-0.838097000
15	-1.481117000	-0.921716000	0.620025000
6	-0.694728000	-2.465518000	1.381980000
1	-1.489018000	-3.218618000	1.363545000

6	-0.429301000	-2.081409000	2.855829000
1	-0.331892000	-2.985085000	3.468553000
1	0.524851000	-1.544268000	2.932330000
6	-1.574625000	-1.182838000	3.340972000
1	-1.351715000	-0.730616000	4.314298000
1	-2.491460000	-1.772292000	3.472691000
6	-1.806725000	-0.082777000	2.281167000
1	-0.993460000	0.648473000	2.364263000
6	-3.136578000	0.664167000	2.401557000
1	-3.994823000	-0.005135000	2.288131000
1	-3.223000000	1.460858000	1.654308000
1	-3.206204000	1.134128000	3.389020000
6	0.512257000	-3.054441000	0.649727000
1	1.368966000	-2.377745000	0.660938000
1	0.280783000	-3.299075000	-0.393040000
1	0.820177000	-3.984707000	1.140681000
6	-3.123157000	-1.518556000	-0.008754000
6	-3.855591000	-2.457503000	0.739902000
1	-3.469613000	-2.821025000	1.685802000
6	-5.090586000	-2.940717000	0.309206000
1	-5.629384000	-3.659938000	0.918651000
6	-5.620053000	-2.502549000	-0.902050000
1	-6.573562000	-2.880931000	-1.257488000
6	-4.910486000	-1.573427000	-1.659493000
1	-5.321975000	-1.229416000	-2.605212000
6	-3.681221000	-1.062610000	-1.224681000
6	-3.051146000	-0.019514000	-2.069297000
1	-3.133308000	0.996310000	-1.583521000
1	-3.558637000	0.087119000	-3.038009000
8	-1.639949000	-0.144959000	-2.318698000
6	-1.313051000	-1.302333000	-3.111706000
1	-1.863490000	-1.260627000	-4.057124000
1	-0.241319000	-1.256670000	-3.310038000
1	-1.559476000	-2.226018000	-2.579034000
6	1.107850000	0.629807000	0.399555000
6	2.386629000	0.032194000	-0.202429000
1	2.183534000	-0.938347000	-0.675698000
1	2.782410000	0.668733000	-1.000591000
1	0.902451000	0.127124000	1.351447000
1	1.220469000	1.692210000	0.628852000
6	-0.488657000	2.400949000	-1.534082000
6	0.504174000	1.699659000	-2.198845000
1	1.549336000	1.914603000	-2.013877000
1	-1.496547000	2.332418000	-1.942381000
1	0.282016000	1.237003000	-3.156533000
6	-0.331633000	3.498390000	-0.569824000
6	-1.478006000	3.991255000	0.081601000
1	-2.447215000	3.546452000	-0.135305000
6	0.906481000	4.112268000	-0.302431000
1	1.800347000	3.780734000	-0.821599000
6	0.992271000	5.169628000	0.598764000
6	-1.392025000	5.046408000	0.986000000
6	-0.153941000	5.636697000	1.249175000
1	-2.288246000	5.415608000	1.475704000
1	1.952756000	5.640691000	0.785499000
1	-0.083380000	6.466432000	1.946241000
6	3.524326000	-0.190733000	0.839685000
1	3.112668000	-0.821298000	1.641095000
6	4.680032000	-0.958877000	0.213278000
6	5.456545000	-0.403683000	-0.815195000
1	5.246949000	0.602389000	-1.171216000
6	4.990117000	-2.253279000	0.650308000
1	4.406668000	-2.699751000	1.453292000
6	6.042390000	-2.974229000	0.082461000

6	6.507735000	-1.120182000	-1.387133000
6	6.804670000	-2.409522000	-0.940140000
1	7.098878000	-0.669545000	-2.179863000
1	6.268187000	-3.974176000	0.443071000
1	7.625886000	-2.966205000	-1.382583000
6	3.985914000	1.129831000	1.481730000
1	4.369402000	1.827333000	0.727444000
1	3.165758000	1.626446000	2.011684000
1	4.790760000	0.946593000	2.200478000

S40

E + ZPE = -3168.562369

28	-0.399580000	0.187623000	-1.038784000
15	-2.393221000	0.123501000	0.280353000
6	-2.548156000	1.012296000	1.944185000
1	-3.086626000	0.332983000	2.611231000
6	-3.478816000	2.210049000	1.655352000
1	-3.902673000	2.589525000	2.591963000
1	-2.897762000	3.030332000	1.212805000
6	-4.557060000	1.746076000	0.676922000
1	-5.181558000	2.575108000	0.323821000
1	-5.226416000	1.025698000	1.166409000
6	-3.851261000	1.065495000	-0.512988000
1	-3.369543000	1.850138000	-1.113375000
6	-4.807353000	0.276702000	-1.411401000
1	-5.218118000	-0.598102000	-0.898016000
1	-4.337148000	-0.058454000	-2.341367000
1	-5.647177000	0.920652000	-1.696531000
6	-1.239981000	1.411580000	2.630909000
1	-0.670405000	2.126832000	2.029202000
1	-0.602659000	0.548017000	2.842246000
1	-1.468312000	1.894502000	3.588038000
6	-2.959762000	-1.626446000	0.513827000
6	-3.555294000	-2.087279000	1.695961000
1	-3.727418000	-1.414932000	2.528241000
6	-3.953675000	-3.418394000	1.843132000
1	-4.415230000	-3.739883000	2.772032000
6	-3.763203000	-4.321226000	0.802061000
1	-4.071627000	-5.357021000	0.905551000
6	-3.170216000	-3.881512000	-0.381995000
1	-3.024911000	-4.581949000	-1.200852000
6	-2.763174000	-2.553547000	-0.542756000
6	-2.133283000	-2.153165000	-1.856942000
1	-2.599122000	-1.261350000	-2.283280000
1	-2.242365000	-2.956732000	-2.593760000
8	-0.729004000	-1.822146000	-1.751799000
6	0.122333000	-2.975758000	-1.639845000
1	-0.077172000	-3.661454000	-2.470934000
1	1.149434000	-2.620434000	-1.704928000
1	-0.038126000	-3.491591000	-0.687211000
6	0.918748000	0.041872000	0.336619000
6	2.333320000	-0.347281000	-0.037802000
1	2.345902000	-1.185900000	-0.742344000
1	2.851126000	0.484597000	-0.525170000
1	0.455288000	-0.739241000	0.957067000
1	0.885124000	0.997772000	0.859986000
6	0.013856000	1.977766000	-1.807151000
6	0.698245000	0.938980000	-2.475540000
1	1.775249000	0.843163000	-2.403428000
1	-0.979841000	2.234665000	-2.192775000
1	0.277866000	0.529852000	-3.395620000
6	0.616397000	3.082324000	-1.032821000

6	-0.230027000	4.002078000	-0.387110000
1	-1.308058000	3.887647000	-0.480292000
6	2.004842000	3.279176000	-0.938212000
1	2.683712000	2.622498000	-1.472860000
6	2.525015000	4.341529000	-0.201008000
6	0.287983000	5.065177000	0.348791000
6	1.670757000	5.234129000	0.450407000
1	-0.384516000	5.767526000	0.832837000
1	3.600653000	4.483698000	-0.149781000
1	2.079099000	6.065564000	1.017135000
6	3.176467000	-0.778456000	1.208985000
1	2.632775000	-1.598815000	1.698016000
6	4.519172000	-1.334520000	0.757048000
6	5.491761000	-0.511958000	0.168631000
1	5.298499000	0.550379000	0.038490000
6	4.809713000	-2.695717000	0.916089000
1	4.072107000	-3.349481000	1.377450000
6	6.035199000	-3.223409000	0.505361000
6	6.716743000	-1.034918000	-0.245070000
6	6.992875000	-2.393713000	-0.078243000
1	7.458540000	-0.380093000	-0.694187000
1	6.242038000	-4.280805000	0.646237000
1	7.948397000	-2.800301000	-0.396960000
6	3.330841000	0.358867000	2.234380000
1	3.791353000	1.246682000	1.785939000
1	2.363238000	0.661014000	2.650298000
1	3.966948000	0.038109000	3.065079000

S41

E + ZPE = -3168.562736

28	-0.318833000	0.090833000	-0.951203000
15	-2.392123000	0.134293000	0.277219000
6	-2.566250000	0.911183000	1.995204000
1	-2.980953000	0.134681000	2.644981000
6	-3.606849000	2.049216000	1.828439000
1	-4.127514000	2.227312000	2.775906000
1	-3.078359000	2.978997000	1.579113000
6	-4.574305000	1.696130000	0.694274000
1	-5.201878000	2.550287000	0.412850000
1	-5.253982000	0.889957000	0.999734000
6	-3.725327000	1.229637000	-0.502964000
1	-3.171592000	2.099192000	-0.884811000
6	-4.522697000	0.614041000	-1.654340000
1	-5.063885000	-0.282619000	-1.336996000
1	-3.886087000	0.345356000	-2.505651000
1	-5.260562000	1.336459000	-2.020979000
6	-1.254048000	1.396486000	2.620060000
1	-0.761664000	2.146557000	1.991818000
1	-0.552394000	0.575174000	2.793362000
1	-1.462523000	1.862313000	3.590173000
6	-3.174122000	-1.543715000	0.369052000
6	-4.110134000	-1.879638000	1.359017000
1	-4.392452000	-1.156466000	2.115987000
6	-4.714989000	-3.137856000	1.397550000
1	-5.437615000	-3.363109000	2.176200000
6	-4.392604000	-4.092437000	0.437593000
1	-4.855728000	-5.074195000	0.457596000
6	-3.465117000	-3.776540000	-0.555248000
1	-3.214100000	-4.519383000	-1.308565000
6	-2.852727000	-2.519668000	-0.607613000
6	-1.874709000	-2.256727000	-1.731887000
1	-2.151032000	-1.375215000	-2.321992000

1	-1.854423000	-3.107041000	-2.422847000
8	-0.523931000	-2.001340000	-1.289360000
6	0.119929000	-3.150355000	-0.713164000
1	0.112374000	-3.973770000	-1.435903000
1	1.148968000	-2.864899000	-0.502037000
1	-0.382945000	-3.461389000	-0.208205000
6	1.061466000	0.018799000	0.360077000
6	2.473432000	-0.359773000	-0.030228000
1	2.480692000	-1.195640000	-0.739633000
1	2.974449000	0.476605000	-0.527729000
1	0.613021000	-0.746026000	1.011574000
1	1.014353000	0.995346000	0.845905000
6	0.011536000	1.857169000	-1.208602000
6	0.727362000	0.810784000	-2.431867000
1	1.807675000	0.753251000	-2.372913000
1	-0.986522000	2.071046000	-2.202991000
1	0.311570000	0.344865000	-3.327765000
6	0.586124000	3.007300000	-1.074292000
6	-0.281803000	3.929409000	-0.461224000
1	-1.357193000	3.788252000	-0.548272000
6	1.969280000	3.239789000	-0.985355000
1	2.664446000	2.578613000	-1.492705000
6	2.464007000	4.340561000	-0.287913000
6	0.210819000	5.030267000	0.235883000
6	1.588935000	5.236010000	0.330876000
1	-0.478593000	5.733027000	0.694973000
1	3.536098000	4.508809000	-0.241333000
1	1.977189000	6.096437000	0.867635000
6	3.339809000	-0.779714000	1.203254000
1	2.816226000	-1.609554000	1.699027000
6	4.685405000	-1.312859000	0.732978000
6	5.637025000	-0.472796000	0.135218000
1	5.425543000	0.586847000	0.011726000
6	4.999358000	-2.669822000	0.882699000
1	4.278959000	-3.337850000	1.352094000
6	6.227143000	-3.176823000	0.453199000
6	6.864332000	-0.974928000	-0.296882000
6	7.163757000	-2.329928000	-0.139682000
1	7.589615000	-0.306778000	-0.753242000
1	6.452170000	-4.231447000	0.586575000
1	8.120955000	-2.720285000	-0.473252000
6	3.486806000	0.358723000	2.228602000
1	3.927057000	1.254490000	1.775629000
1	2.518664000	0.644154000	2.655388000
1	4.137525000	0.048325000	3.051803000

S42

E + ZPE = -3168.558847

28	-0.316342000	0.167973000	-0.726077000
15	-2.279660000	0.340004000	0.287086000
6	-2.665067000	1.235682000	1.914954000
1	-3.122910000	0.492370000	2.572317000
6	-3.721257000	2.315183000	1.549229000
1	-4.388674000	2.490648000	2.399869000
1	-3.201880000	3.262856000	1.354684000
6	-4.483572000	1.895137000	0.290406000
1	-5.080940000	2.719486000	-0.116566000
1	-5.177538000	1.072479000	0.506119000
6	-3.434902000	1.434949000	-0.737076000
1	-2.817905000	2.306257000	-0.998369000
6	-4.020179000	0.841645000	-2.019291000
1	-4.564406000	-0.088154000	-1.825988000

1	-3.252938000	0.644066000	-2.776225000
1	-4.726418000	1.553515000	-2.460771000
6	-1.471488000	1.834265000	2.666696000
1	-0.877718000	2.500904000	2.032562000
1	-0.813497000	1.064699000	3.076890000
1	-1.848113000	2.4271133000	3.508243000
6	-3.143199000	-1.301642000	0.347541000
6	-4.105586000	-1.588232000	1.328558000
1	-4.350602000	-0.860314000	2.092459000
6	-4.792435000	-2.803832000	1.350239000
1	-5.532211000	-2.987577000	2.123573000
6	-4.530253000	-3.765513000	0.380453000
1	-5.058180000	-4.714182000	0.384942000
6	-3.577229000	-3.498854000	-0.602384000
1	-3.369926000	-4.247794000	-1.362686000
6	-2.878188000	-2.287445000	-0.638686000
6	-1.863218000	-2.098348000	-1.747511000
1	-2.039352000	-1.178555000	-2.314593000
1	-1.933322000	-2.929919000	-2.459202000
8	-0.506148000	-1.997811000	-1.286735000
6	-0.003112000	-3.222521000	-0.732370000
1	-0.117247000	-4.031894000	-1.463269000
1	1.056513000	-3.071320000	-0.529650000
1	-0.527213000	-3.486519000	0.192401000
6	0.628937000	-0.065694000	0.904697000
6	2.003030000	-0.435331000	0.380824000
1	1.934250000	-1.183080000	-0.417842000
1	2.491862000	0.444030000	-0.049953000
1	0.186606000	-0.862236000	1.514402000
1	0.631944000	0.869430000	1.461371000
6	0.202895000	1.888364000	-1.790668000
6	0.604573000	0.747281000	-2.474851000
1	1.642416000	0.430833000	-2.514577000
1	-0.780296000	2.292182000	-2.039950000
1	-0.027138000	0.338574000	-3.262466000
6	1.079938000	2.861044000	-1.101236000
6	0.500256000	3.881085000	-0.325864000
1	-0.583603000	3.939979000	-0.246863000
6	2.479689000	2.835150000	-1.226822000
1	2.953123000	2.095366000	-1.865415000
6	3.270209000	3.781555000	-0.576743000
6	1.289325000	4.826986000	0.325066000
6	2.680061000	4.775780000	0.207093000
1	0.820505000	5.609738000	0.914459000
1	4.349389000	3.754172000	-0.697853000
1	3.298102000	5.515726000	0.706824000
6	2.945227000	-1.030973000	1.482325000
1	2.414826000	-1.879322000	1.936373000
6	4.207343000	-1.578309000	0.833322000
6	5.149299000	-0.728753000	0.233245000
1	4.995285000	0.347777000	0.246905000
6	4.445141000	-2.958822000	0.804511000
1	3.732989000	-3.634096000	1.275223000
6	5.589486000	-3.480119000	0.197714000
6	6.292925000	-1.245282000	-0.375428000
6	6.516736000	-2.623798000	-0.396278000
1	7.013377000	-0.570805000	-0.830274000
1	5.757650000	-4.553602000	0.194461000
1	7.409158000	-3.025372000	-0.867645000
6	3.244042000	-0.012005000	2.594789000
1	3.716191000	0.892748000	2.195222000
1	2.328481000	0.291193000	3.114691000
1	3.924449000	-0.443998000	3.335178000

S43

E + ZPE = -3168.572953

28	-0.002881000	0.273134000	-0.076857000
15	-2.104333000	0.805004000	0.082816000
6	-2.463898000	1.972665000	1.508792000
1	-2.717400000	1.367774000	2.383943000
6	-3.672624000	2.858920000	1.062694000
1	-4.502740000	2.769325000	1.770587000
1	-3.357187000	3.907777000	1.089143000
6	-4.129499000	2.494920000	-0.365233000
1	-4.563322000	3.361884000	-0.876621000
1	-4.908715000	1.724122000	-0.338774000
6	-2.923738000	1.956715000	-1.159855000
1	-2.199827000	2.774413000	-1.290265000
6	-3.301682000	1.404275000	-2.534335000
1	-3.975629000	0.545295000	-2.449900000
1	-2.428042000	1.105676000	-3.122675000
1	-3.825629000	2.177063000	-3.107805000
6	-1.245970000	2.837196000	1.875086000
1	-0.913848000	3.446278000	1.027320000
1	-0.393804000	2.244245000	2.218585000
1	-1.520315000	3.525800000	2.682084000
6	-3.264832000	-0.625249000	0.258383000
6	-4.245091000	-0.617255000	1.263973000
1	-4.326071000	0.216410000	1.951488000
6	-5.152154000	-1.668785000	1.407155000
1	-5.897819000	-1.630755000	2.195645000
6	-5.103008000	-2.749450000	0.532491000
1	-5.809678000	-3.568494000	0.626331000
6	-4.139210000	-2.767808000	-0.475470000
1	-4.108605000	-3.603069000	-1.170719000
6	-3.209669000	-1.731914000	-0.626411000
6	-2.172114000	-1.862806000	-1.726509000
1	-1.954012000	-0.896615000	-2.182746000
1	-2.558623000	-2.519785000	-2.518702000
8	-0.910277000	-2.353662000	-1.272357000
6	-0.896754000	-3.756985000	-1.029105000
1	-1.208901000	-4.311653000	-1.925465000
1	0.132987000	-4.027405000	-0.787409000
1	-1.547914000	-4.036308000	-0.190828000
6	2.006513000	-2.098986000	1.249788000
6	-0.110554000	-0.627180000	1.595940000
6	1.353399000	-0.695692000	1.321028000
1	1.930571000	-0.021182000	1.962553000
1	1.573856000	-0.244156000	0.274515000
1	1.353396000	-2.715538000	0.620793000
1	-0.649455000	-1.573334000	1.526342000
1	-0.405251000	-0.056638000	2.476145000
6	0.825617000	1.760298000	-1.388790000
6	0.675579000	0.542879000	-2.019600000
1	0.020681000	2.484419000	-1.500956000
1	1.514805000	-0.131436000	-2.169525000
1	-0.172858000	0.375505000	-2.674829000
6	2.054638000	2.328045000	-0.807384000
6	1.992525000	3.610571000	-0.231402000
1	1.047372000	4.148171000	-0.227870000
6	3.295252000	1.661398000	-0.829935000
1	3.386185000	0.678628000	-1.283091000
6	4.427468000	2.260141000	-0.286842000
6	3.127412000	4.209845000	0.310160000
6	4.348251000	3.533743000	0.286371000
1	3.060577000	5.203674000	0.742717000

1	5.375027000	1.731246000	-0.315626000
1	5.236489000	3.998622000	0.704035000
6	2.045349000	-2.730103000	2.651306000
1	2.496932000	-3.725976000	2.611284000
1	2.630104000	-2.125822000	3.353501000
1	1.034452000	-2.826637000	3.061423000
6	3.368200000	-2.035412000	0.570048000
6	3.501410000	-2.440687000	-0.766054000
1	2.636981000	-2.844085000	-1.290506000
6	4.501603000	-1.539564000	1.230273000
1	4.433589000	-1.224069000	2.268064000
6	5.730399000	-1.451936000	0.573914000
6	4.728175000	-2.351215000	-1.428043000
6	5.847778000	-1.854807000	-0.758322000
1	4.811296000	-2.681129000	-2.459961000
1	6.599440000	-1.076784000	1.107625000
1	6.806157000	-1.793638000	-1.265909000

S44

E + ZPE = -3168.566645

28	-0.476360000	0.453128000	0.537096000
15	1.532055000	-0.428499000	0.860276000
6	2.893063000	0.768530000	1.352778000
1	3.314401000	1.207299000	0.445568000
6	3.952614000	-0.067317000	2.140815000
1	4.903295000	-0.100188000	1.599581000
1	4.156390000	0.444242000	3.087502000
6	3.438502000	-1.499397000	2.414540000
1	3.779129000	-1.865907000	3.389620000
1	3.828482000	-2.197079000	1.664761000
6	1.898700000	-1.515077000	2.356947000
1	1.512962000	-0.932259000	3.203967000
6	1.313030000	-2.925213000	2.417395000
1	1.644453000	-3.534947000	1.570375000
1	0.217773000	-2.929183000	2.440019000
1	1.655989000	-3.422698000	3.331528000
6	2.342224000	1.921828000	2.210609000
1	1.886558000	1.558218000	3.138541000
1	1.610382000	2.526708000	1.669683000
1	3.170035000	2.580489000	2.495838000
6	2.175738000	-1.416067000	-0.571482000
6	3.469724000	-1.171407000	-1.059745000
1	4.085928000	-0.398848000	-0.615556000
6	4.007188000	-1.914302000	-2.112582000
1	5.012212000	-1.699861000	-2.463795000
6	3.258077000	-2.933177000	-2.692792000
1	3.668822000	-3.528582000	-3.502602000
6	1.971341000	-3.187472000	-2.219060000
1	1.389002000	-3.991227000	-2.662781000
6	1.404499000	-2.440023000	-1.178708000
6	-0.030548000	-2.747220000	-0.789729000
1	-0.201445000	-2.599099000	0.277700000
1	-0.255084000	-3.799787000	-1.015349000
8	-0.988138000	-1.904226000	-1.431700000
6	-1.237966000	-2.228152000	-2.795277000
1	-1.527675000	-3.283446000	-2.901933000
1	-2.070956000	-1.599348000	-3.117721000
1	-0.366553000	-2.032092000	-3.433224000
6	-3.208400000	-0.567789000	1.627867000
6	-0.931794000	0.171563000	2.520755000
6	-2.115548000	0.464138000	1.876028000
1	-2.441920000	1.505790000	1.868406000

1	-1.888310000	0.792537000	-0.295305000
1	-2.724990000	-1.527482000	1.403895000
1	-0.385747000	0.945533000	3.055322000
1	-0.741788000	-0.847276000	2.848544000
6	0.133742000	1.185518000	-1.147544000
6	-1.351474000	1.252015000	-1.215072000
1	0.557087000	0.421620000	-1.796002000
1	-1.769435000	0.621140000	-1.998892000
1	-1.765874000	2.259974000	-1.252577000
6	0.919027000	2.441076000	-1.144985000
6	0.462772000	3.625163000	-0.533046000
1	-0.506102000	3.647290000	-0.039170000
6	2.173256000	2.468133000	-1.783369000
1	2.534192000	1.569934000	-2.278726000
6	2.939298000	3.631937000	-1.815766000
6	1.230125000	4.787931000	-0.561329000
6	2.472001000	4.796159000	-1.201438000
1	0.855685000	5.691357000	-0.088650000
1	3.896185000	3.634281000	-2.330070000
1	3.064880000	5.705473000	-1.230319000
6	-4.020689000	-0.752223000	2.935080000
1	-4.805353000	-1.500245000	2.785224000
1	-3.372828000	-1.082304000	3.753756000
1	-4.502624000	0.182965000	3.239249000
6	-4.124231000	-0.219918000	0.459891000
6	-4.839136000	0.987326000	0.428384000
1	-4.743220000	1.701041000	1.243963000
6	-4.300256000	-1.126300000	-0.593853000
1	-3.752294000	-2.064814000	-0.585512000
6	-5.163558000	-0.835867000	-1.652692000
6	-5.697795000	1.283233000	-0.631449000
6	-5.863433000	0.371236000	-1.675867000
1	-6.245936000	2.221236000	-0.634865000
1	-5.295624000	-1.557232000	-2.454703000
1	-6.538280000	0.597298000	-2.496346000

S45

E + ZPE = -3168.559876

28	-0.350821000	0.744316000	0.198744000
15	1.801220000	0.399065000	0.522813000
6	2.821979000	1.975524000	0.390191000
1	2.974730000	2.223731000	-0.664561000
6	4.171669000	1.672991000	1.105761000
1	4.963958000	1.485606000	0.375857000
1	4.474665000	2.562075000	1.668669000
6	4.021954000	0.451780000	2.049749000
1	4.481982000	0.640754000	3.026086000
1	4.534775000	-0.418717000	1.625730000
6	2.531977000	0.099633000	2.240914000
1	2.060656000	0.888749000	2.840477000
6	2.332319000	-1.231326000	2.963529000
1	2.794086000	-2.061343000	2.419751000
1	1.277004000	-1.469801000	3.133557000
1	2.814999000	-1.180420000	3.946244000
6	2.098864000	3.166021000	1.047882000
1	1.907191000	2.995466000	2.112488000
1	1.149326000	3.399034000	0.560505000
1	2.737613000	4.053645000	0.975324000
6	2.645070000	-0.834357000	-0.585099000
6	3.639760000	-0.387863000	-1.473207000
1	3.878559000	0.666174000	-1.543914000
6	4.360656000	-1.272925000	-2.274552000

1	5.121174000	-0.890655000	-2.948915000	1	2.146138000	1.891378000	2.664534000
6	4.119583000	-2.640484000	-2.181026000	6	2.191080000	-0.151734000	3.454985000
1	4.696449000	-3.345340000	-2.772197000	1	1.557643000	0.162258000	4.291309000
6	3.128646000	-3.098701000	-1.315324000	1	2.979179000	-0.783276000	3.880777000
1	2.949323000	-4.167105000	-1.231822000	6	1.374276000	-1.008418000	2.435555000
6	2.356002000	-2.222418000	-0.539501000	1	0.306178000	-0.876185000	-2.622532000
6	1.213373000	-2.821688000	0.263355000	6	1.708647000	-2.500994000	2.574251000
1	0.892686000	-2.149777000	1.059228000	1	2.762382000	-2.699619000	2.352035000
1	1.536562000	-3.764621000	0.730095000	1	1.106654000	-3.139186000	1.922150000
8	0.033522000	-3.045366000	-0.505011000	1	1.521979000	-2.813870000	3.608310000
6	0.047041000	-4.196585000	-1.339688000	6	3.947608000	1.704844000	0.541571000
1	0.325329000	-5.096000000	-0.771047000	1	3.274638000	2.558764000	0.415418000
1	-0.970882000	-4.313542000	-1.718189000	1	4.273046000	1.369122000	-0.448077000
1	0.730392000	-4.084570000	-2.190843000	1	4.836707000	2.064308000	1.072219000
6	-2.430128000	-0.798382000	1.874445000	6	2.221242000	-1.614980000	-0.394371000
1	-1.589485000	-1.504942000	1.878065000	6	3.550780000	-1.773251000	-0.806766000
6	-0.750632000	1.119376000	2.189694000	1	4.323416000	-1.102943000	-0.445633000
6	-1.892271000	0.601701000	1.617008000	6	3.913729000	-2.794952000	-1.688540000
1	-2.624712000	1.318090000	1.249442000	1	4.951040000	-2.900326000	-1.992174000
1	-1.479848000	-0.517005000	-0.996546000	6	2.947248000	-3.675444000	-2.166198000
1	-0.623773000	2.193224000	2.307633000	1	3.221710000	-4.476728000	-2.845670000
1	-0.144137000	0.502712000	2.847483000	6	1.617764000	-3.522731000	-1.765901000
6	-0.024073000	0.989470000	-1.660891000	1	0.863564000	-4.214202000	-2.133618000
6	-0.827445000	-0.272172000	-1.868423000	6	1.234951000	-2.498638000	-0.895394000
1	0.959657000	1.000443000	-2.123288000	6	-0.223026000	-2.343557000	-0.518050000
1	-0.186446000	-1.137517000	-2.020515000	1	-0.341589000	-2.185206000	0.557238000
1	-1.536070000	-0.176642000	-2.701307000	1	-0.780681000	-3.253174000	-0.768433000
6	-0.720813000	2.270928000	-1.600829000	8	-0.837183000	-1.211486000	-1.148955000
6	-2.095087000	2.325982000	-1.264958000	6	-1.537713000	-1.546442000	-2.346095000
1	-2.690387000	1.419563000	-1.232045000	1	-2.336116000	-2.267182000	-2.133214000
6	-0.029567000	3.494595000	-1.790903000	1	-1.992513000	-0.627650000	-2.721618000
1	1.016658000	3.468119000	-2.084860000	1	-0.861465000	-1.952122000	-3.109517000
6	-0.675511000	4.708693000	-1.630720000	6	-0.638326000	1.849819000	1.602080000
6	-2.734444000	3.558070000	-1.082647000	6	-1.730225000	1.175947000	1.118880000
6	-2.030746000	4.744874000	-1.259656000	1	-2.367831000	1.709930000	0.424064000
1	-3.792027000	3.582736000	-0.836783000	1	0.174205000	0.414948000	-3.272641000
1	-0.136017000	5.636103000	-1.799082000	1	-0.491059000	2.903560000	1.373502000
1	-2.532756000	5.700053000	-1.137756000	1	-0.117516000	1.484939000	2.483129000
6	-3.427491000	-1.254473000	0.814599000	6	1.321452000	1.444950000	-1.710198000
6	-3.246789000	-2.472820000	0.147596000	6	1.203503000	0.562456000	-2.941290000
1	-2.361835000	-3.067078000	0.357267000	1	2.362681000	1.654906000	-1.477852000
6	-4.571418000	-0.495396000	0.519480000	1	1.651822000	-0.420102000	-2.781174000
1	-4.756608000	0.440065000	1.043582000	1	1.746071000	1.041527000	-3.767993000
6	-5.501135000	-0.937456000	-0.422760000	6	0.461870000	2.603632000	-1.553617000
6	-4.179294000	-2.919901000	-0.791898000	6	-0.939137000	2.395791000	-1.655525000
6	-5.308024000	-2.153492000	-1.082014000	1	-1.323173000	1.506078000	-2.146563000
1	-4.025201000	-3.871766000	-1.293238000	6	0.922762000	3.877695000	-1.103862000
1	-6.383085000	-0.338344000	-0.632098000	1	1.992308000	4.048461000	-1.020146000
1	-6.035318000	-2.501793000	-1.809664000	6	0.031580000	4.893038000	-0.829950000
6	-3.072163000	-0.839921000	3.285649000	6	-1.835871000	3.456468000	-1.389590000
1	-3.904888000	-0.132967000	3.362625000	6	-1.361373000	4.683827000	-0.969370000
1	-3.461784000	-1.841883000	3.491069000	1	-2.901689000	3.306304000	-1.537446000
1	-2.337165000	-0.584071000	4.056007000	1	0.399136000	5.867979000	-0.522765000
				1	-2.050388000	5.499533000	-0.771772000
				6	-2.380187000	-0.026518000	1.776850000
				1	-1.604895000	-0.710351000	2.139652000
				6	-3.328809000	-0.821621000	0.885724000
				6	-4.249687000	-0.199328000	0.031231000
				1	-4.279857000	0.884714000	-0.048521000
				6	-3.368261000	-2.218301000	0.991881000
				1	-2.684477000	-2.721935000	1.672544000
				6	-4.280724000	-2.975033000	0.254291000
				6	-5.162311000	-0.950860000	-0.711816000
				6	-5.179855000	-2.342608000	-0.606242000

S46

E + ZPE = -3168.572440

28	0.154673000	1.060004000	-0.158111000
15	1.730175000	-0.242786000	0.727272000
6	3.291183000	0.592413000	1.357038000
1	4.015729000	-0.222646000	1.492970000
6	2.844705000	1.049720000	2.757337000
1	3.704679000	1.420077000	3.326590000

1	-5.868839000	-0.445935000	-1.364946000
1	-4.295428000	-4.056431000	0.360452000
1	-5.895535000	-2.926475000	-1.177726000
6	-3.154145000	0.482304000	3.026805000
1	-2.479065000	0.976945000	3.732813000
1	-3.932095000	1.196980000	2.738157000
1	-3.641071000	-0.357366000	3.532552000

S47

E + ZPE = -3168.564699

28	0.613591000	1.065437000	-0.291957000
15	1.592130000	-0.477033000	0.913573000
6	2.754341000	-0.089112000	2.323448000
1	3.262646000	-1.034781000	2.559174000
6	1.739524000	0.200469000	3.446114000
1	2.251521000	0.286879000	4.410922000
1	1.265392000	1.173031000	3.257657000
6	0.693108000	-0.930702000	3.467434000
1	-0.247149000	-0.589151000	3.912754000
1	1.058141000	-1.744819000	4.103299000
6	0.455257000	-1.502549000	2.030457000
1	-0.572781000	-1.310686000	1.710876000
6	0.711198000	-3.017174000	1.986326000
1	1.740518000	-3.260585000	2.271292000
1	0.530437000	-3.452787000	1.000281000
1	0.045139000	-3.516832000	2.699875000
6	3.802817000	1.011418000	2.155945000
1	3.334175000	1.995136000	2.052664000
1	4.453249000	0.849119000	1.290663000
1	4.440216000	1.046124000	3.046664000
6	2.408763000	-1.620188000	-0.261479000
6	3.776437000	-1.907487000	-0.157431000
1	4.355718000	-1.511184000	0.669829000
6	4.421433000	-2.705132000	-1.105390000
1	5.480851000	-2.919061000	-0.999997000
6	3.701160000	-3.218346000	-2.179830000
1	4.191167000	-3.835182000	-2.926965000
6	2.339556000	-2.933520000	-2.296198000
1	1.781132000	-3.340561000	-3.135188000
6	1.674304000	-2.140892000	-1.354403000
6	0.180403000	-1.963360000	-1.521608000
1	-0.379499000	-2.424010000	-0.696039000
1	-0.126347000	-2.473729000	-2.441140000
8	-0.234378000	-0.580457000	-1.620262000
6	-1.510238000	-0.495001000	-2.279831000
1	-2.258236000	-1.102847000	-1.763297000
1	-1.816982000	0.549812000	-2.257142000
1	-1.413570000	-0.828465000	-3.320610000
6	-1.304617000	1.670101000	1.371977000
6	-2.484563000	1.224005000	0.905181000
1	-2.928195000	1.733243000	0.049293000
1	2.304691000	1.173422000	-2.825121000
1	-0.883571000	2.603770000	1.014220000
1	-0.875114000	1.256219000	2.280646000
6	2.219537000	2.004456000	-0.793629000
6	2.962265000	1.441409000	-1.993469000
1	2.899637000	2.277324000	0.010583000
1	3.537062000	0.549774000	-1.728784000
1	3.671625000	2.194712000	-2.363594000
6	1.134823000	2.955730000	-0.961027000
6	0.063906000	2.555420000	-1.809929000
1	0.236352000	1.825052000	-2.595295000

6	0.975764000	4.131658000	-0.169449000
1	1.791623000	4.441241000	0.478282000
6	-0.175019000	4.885600000	-0.256493000
6	-1.109298000	3.348667000	-1.879116000
6	-1.233812000	4.487706000	-1.108782000
1	-1.898559000	3.076639000	-2.574821000
1	-0.269145000	5.798622000	0.324457000
1	-2.127414000	5.100950000	-1.177196000
6	-3.325793000	0.141669000	1.542026000
1	-2.692782000	-0.409236000	2.249171000
6	-3.882042000	-0.855478000	0.530749000
6	-4.754930000	-0.450009000	-0.490238000
1	-5.049714000	0.593624000	-0.572160000
6	-3.545517000	-2.212781000	0.616542000
1	-2.891006000	-2.552192000	1.416958000
6	-4.057853000	-3.141334000	-0.293806000
6	-5.266829000	-1.372943000	-1.403051000
6	-4.917955000	-2.722784000	-1.309763000
1	-5.946520000	-1.039430000	-2.182417000
1	-3.793511000	-4.191262000	-0.200706000
1	-5.323288000	-3.442169000	-2.015427000
6	-4.460966000	0.806105000	2.363889000
1	-4.045570000	1.459285000	3.137872000
1	-5.115335000	1.410166000	1.726671000
1	-5.075475000	0.038047000	2.844119000

S48

E + ZPE = -3168.566579

28	-0.492234000	-0.622556000	0.101945000
15	1.544689000	-0.285041000	0.913416000
6	1.683747000	1.224588000	2.022304000
1	1.871505000	2.100601000	1.396784000
6	2.863733000	0.951426000	3.008598000
1	3.653465000	1.699759000	2.887921000
1	2.488296000	1.062497000	4.031671000
6	3.427479000	-0.471018000	2.811749000
1	3.803259000	-0.885154000	3.754418000
1	4.274644000	-0.455866000	2.116518000
6	2.328904000	-1.385567000	2.235860000
1	1.543291000	-1.507702000	2.993187000
6	2.863782000	-2.763909000	1.844832000
1	3.615179000	-2.693490000	1.051598000
1	2.078493000	-3.453007000	1.518857000
1	3.348924000	-3.221782000	2.714256000
6	0.365817000	1.464217000	2.781674000
1	0.088381000	0.600044000	3.396813000
1	-0.462384000	1.696707000	2.107715000
1	0.490930000	2.316475000	3.458954000
6	2.872106000	-0.177132000	-0.373514000
6	3.782516000	0.891285000	-0.354008000
1	3.700036000	1.667687000	0.398088000
6	4.819090000	0.982704000	-1.285245000
1	5.508811000	1.820476000	-1.242257000
6	4.970064000	-0.007763000	-2.251065000
1	5.780101000	0.043740000	-2.972327000
6	4.074182000	-1.076582000	-2.279984000
1	4.202437000	-1.859953000	-3.022889000
6	3.015895000	-1.178157000	-1.368083000
6	2.059700000	-2.350194000	-1.513730000
1	1.689887000	-2.687444000	-0.544402000
1	2.584682000	-3.197766000	-1.977073000
8	0.885077000	-2.044149000	-2.267416000

6	1.085851000	-2.022452000	-3.677243000
1	1.495164000	-2.979781000	-4.029748000
1	0.105205000	-1.868744000	-4.133376000
1	1.756375000	-1.210108000	-3.986099000
6	-3.203486000	-1.392617000	1.384825000
6	-0.761476000	-2.086996000	1.518209000
6	-1.936846000	-2.005561000	0.802033000
1	-2.079995000	-2.709030000	-0.019260000
1	-1.813558000	-0.669181000	-0.899475000
1	-2.902429000	-0.607158000	2.090692000
1	-0.714533000	-1.664513000	2.519527000
1	-0.046701000	-2.877709000	1.310204000
6	-0.178324000	0.818499000	-1.169137000
6	-1.397700000	0.121372000	-1.649684000
1	0.703639000	0.595635000	-1.764280000
1	-1.229768000	-0.480817000	-2.541724000
1	-2.277127000	0.758583000	-1.748147000
6	-0.263837000	2.245145000	-0.776693000
6	-1.406067000	2.798359000	-0.166283000
1	-2.273513000	2.173184000	0.031936000
6	0.826708000	3.096387000	-1.034371000
1	1.708503000	2.693680000	-1.526178000
6	0.779466000	4.448456000	-0.697476000
6	-1.452130000	4.148880000	0.172907000
6	-0.359186000	4.979530000	-0.088193000
1	-2.345577000	4.556997000	0.637003000
1	1.626937000	5.090276000	-0.921424000
1	-0.400044000	6.033419000	0.170612000
6	-3.940280000	-2.487609000	2.198425000
1	-4.842108000	-2.069184000	2.655942000
1	-4.245864000	-3.319605000	1.554932000
1	-3.297475000	-2.885445000	2.990391000
6	-4.133448000	-0.765108000	0.354643000
6	-4.591500000	0.547609000	0.528640000
1	-4.278001000	1.111104000	1.405464000
6	-4.578803000	-1.483693000	-0.765075000
1	-4.264893000	-2.514541000	-0.913725000
6	-5.440551000	-0.897886000	-1.693830000
6	-5.457743000	1.135979000	-0.396589000
6	-5.880351000	0.415603000	-1.514459000
1	-5.805647000	2.153151000	-0.239547000
1	-5.776087000	-1.471571000	-2.553272000
1	-6.554713000	0.869138000	-2.234872000

S49

E + ZPE = -3168.560794

28	-0.432671000	-1.060384000	-0.237742000
15	-0.995165000	0.716618000	0.901581000
6	-2.513536000	0.399838000	1.960758000
1	-3.414491000	0.498165000	1.348996000
6	-2.475112000	1.460338000	3.099008000
1	-3.189278000	2.264825000	2.901230000
1	-2.797940000	0.984113000	4.030715000
6	-1.048552000	2.047937000	3.246906000
1	-0.737003000	2.089244000	4.296470000
1	-1.029254000	3.078851000	2.876041000
6	-0.017766000	1.226978000	2.438061000
1	0.164305000	0.270450000	2.948146000
6	1.311531000	1.974908000	2.312691000
1	1.187348000	2.922673000	1.779264000
1	2.096902000	1.396356000	1.817632000
1	1.677163000	2.214140000	3.317867000

6	-2.489694000	-1.030432000	2.534220000
1	-1.601904000	-1.209405000	3.151331000
1	-2.532815000	-1.795476000	1.755754000
1	-3.362673000	-1.168265000	3.181887000
6	-1.304840000	2.280530000	-0.039957000
6	-2.577219000	2.874810000	0.009841000
1	-3.375430000	2.413549000	0.579164000
6	-2.851704000	4.071454000	-0.652600000
1	-3.846089000	4.503898000	-0.593491000
6	-1.842073000	4.713660000	-1.363462000
1	-2.033184000	5.659788000	-1.860845000
6	-0.576008000	4.133710000	-1.425610000
1	0.216985000	4.646432000	-1.963394000
6	-0.289190000	2.910764000	-0.803505000
6	1.096760000	2.321655000	-1.006959000
1	1.343332000	1.607779000	-0.222245000
1	1.849199000	3.123628000	-0.973405000
8	1.245013000	1.581512000	-2.218903000
6	1.424423000	2.364967000	-3.393798000
1	2.250728000	3.079723000	-3.269187000
1	1.675115000	1.668217000	-4.196894000
1	0.514577000	2.912894000	-3.669423000
6	2.592902000	-1.432821000	-0.631255000
1	2.341511000	-0.654754000	-1.365009000
6	0.692928000	-2.437265000	0.833384000
6	1.532206000	-1.409628000	0.469157000
1	1.682256000	-0.609984000	1.189193000
1	0.225815000	-1.662468000	-2.149518000
1	0.699452000	-3.383610000	0.298923000
1	0.235275000	-2.461092000	1.819501000
6	-1.679471000	-0.742215000	-1.635447000
6	-0.581766000	-1.058929000	-2.622907000
1	-2.174307000	0.214339000	-1.783005000
1	-0.112847000	-0.152709000	-3.000903000
1	-0.936411000	-1.689454000	-3.448152000
6	-2.548098000	-1.842492000	-1.196098000
6	-2.078738000	-3.177767000	-1.179880000
1	-1.134301000	-3.435995000	-1.648639000
6	-3.856028000	-1.592950000	-0.715033000
1	-4.249020000	-0.580436000	-0.762711000
6	-4.645882000	-2.622355000	-0.227447000
6	-2.871995000	-4.208022000	-0.662883000
6	-4.149423000	-3.935131000	-0.182841000
1	-2.497435000	-5.227435000	-0.667383000
1	-5.656374000	-2.414504000	0.112590000
1	-4.772103000	-4.738346000	0.199417000
6	3.931444000	-1.022707000	-0.016400000
6	4.615713000	0.097841000	-0.503512000
1	4.183090000	0.675266000	-1.317899000
6	4.502408000	-1.758647000	1.031979000
1	3.984648000	-2.630027000	1.426397000
6	5.733252000	-1.387256000	1.572614000
6	5.848697000	0.470891000	0.035859000
6	6.410592000	-0.271549000	1.074900000
1	6.370599000	1.338331000	-0.358760000
1	6.165105000	-1.970184000	2.381344000
1	7.370710000	0.015194000	1.494087000
6	2.711321000	-2.777353000	-1.371546000
1	1.780476000	-3.067962000	-1.874044000
1	3.487614000	-2.707641000	-2.138606000
1	2.990326000	-3.585280000	-0.687621000

S50

E + ZPE = -3168.576547

28	-0.075375000	1.080736000	-0.121692000
15	1.840012000	0.203895000	0.647658000
6	3.234571000	1.447691000	0.919869000
1	4.155391000	0.850507000	0.922376000
6	3.002303000	1.897378000	2.373278000
1	3.854146000	2.492055000	2.722287000
1	2.120717000	2.549763000	2.435838000
6	2.822592000	0.628989000	3.207071000
1	2.457827000	0.843876000	4.217281000
1	3.798555000	0.140345000	3.319818000
6	1.856442000	-0.348716000	2.483921000
1	0.844028000	-0.175046000	2.861157000
6	2.234943000	-1.808279000	2.767102000
1	3.217157000	-2.055944000	2.352689000
1	1.512180000	-2.527918000	2.375262000
1	2.284650000	-1.955081000	3.852575000
6	3.407509000	2.611637000	-0.054743000
1	2.509358000	3.235938000	-0.099643000
1	3.653545000	2.280650000	-1.068503000
1	4.232538000	3.247146000	0.287253000
6	2.515463000	-1.190728000	-0.349883000
6	3.802105000	-1.112319000	-0.903632000
1	4.411385000	-0.226380000	-0.763736000
6	4.336132000	-2.166328000	-1.648083000
1	5.335510000	-2.078571000	-2.063748000
6	3.590685000	-3.325705000	-1.839883000
1	4.002212000	-4.158517000	-2.402172000
6	2.304349000	-3.409866000	-1.304763000
1	1.721532000	-4.315889000	-1.451557000
6	1.741223000	-2.354767000	-0.578956000
6	0.300886000	-2.476156000	-0.118545000
1	0.143037000	-1.992188000	0.847719000
1	0.031486000	-3.534779000	0.001512000
8	-0.616036000	-1.838932000	-1.004002000
6	-0.979721000	-2.632237000	-2.127774000
1	-1.399532000	-3.593085000	-1.801970000
1	-1.752401000	-2.080485000	-2.666282000
1	-0.129063000	-2.812032000	-2.798295000
6	-0.877505000	1.910853000	1.586603000
6	-1.449337000	0.662612000	1.568613000
1	-0.934937000	-0.153109000	2.071860000
1	-0.320770000	-0.079462000	-3.077964000
1	-1.464305000	2.785106000	1.310705000
1	0.012802000	2.110926000	2.177437000
6	0.742342000	1.420803000	-1.888274000
6	0.679006000	0.337533000	-2.949592000
1	1.722641000	1.890480000	-1.857215000
1	1.361944000	-0.485387000	-2.729748000
1	0.982740000	0.773504000	-3.911473000
6	-0.348009000	2.366371000	-1.739961000
6	-1.656015000	1.836045000	-1.567395000
1	-1.865140000	0.800417000	-1.825999000
6	-0.157836000	3.768457000	-1.548732000
1	0.840911000	4.180877000	-1.660179000
6	-1.230318000	4.596882000	-1.293893000
6	-2.744577000	2.708260000	-1.338165000
6	-2.537718000	4.067112000	-1.195495000
1	-3.753321000	2.308400000	-1.301054000
1	-1.075510000	5.667275000	-1.192841000
1	-3.378166000	4.734878000	-1.031253000
6	-2.933478000	0.421909000	1.350858000
1	-3.305391000	1.166411000	0.642603000

6	-3.297902000	-0.962294000	0.830823000
6	-2.937406000	-2.123525000	1.529490000
1	-2.358134000	-2.049710000	2.447563000
6	-4.082016000	-1.099136000	-0.320936000
1	-4.398559000	-0.210522000	-0.863613000
6	-4.490143000	-2.356893000	-0.770863000
6	-3.337811000	-3.382947000	1.082739000
6	-4.116052000	-3.504476000	-0.071060000
1	-3.058519000	-4.269175000	1.646420000
1	-5.109373000	-2.437395000	-1.660193000
1	-4.441457000	-4.483627000	-0.410916000
6	-3.649285000	0.693722000	2.703250000
1	-3.295532000	0.015789000	3.487234000
1	-3.473190000	1.721737000	3.035783000
1	-4.726923000	0.539377000	2.589570000

S51

E + ZPE = -3168.563098

28	0.441837000	0.868932000	-0.356181000
15	2.015215000	-0.085573000	0.841804000
6	3.230512000	0.878885000	1.882660000
1	4.010805000	0.160014000	2.170214000
6	2.367016000	1.167767000	3.126055000
1	2.983967000	1.583225000	3.930484000
1	1.626366000	1.939264000	2.875881000
6	1.680876000	-0.140280000	3.566927000
1	0.760933000	0.065838000	4.123223000
1	2.343959000	-0.679529000	4.252131000
6	1.393248000	-1.067063000	2.338500000
1	0.314580000	-1.202000000	2.211280000
6	2.041528000	-2.448373000	2.522227000
1	3.129720000	-2.373020000	2.622595000
1	1.833526000	-3.132247000	1.695395000
1	1.655887000	-2.907725000	3.439877000
6	3.892425000	2.128920000	1.301116000
1	3.159888000	2.924886000	1.134551000
1	4.408046000	1.935728000	0.355058000
1	4.634923000	2.512691000	2.009853000
6	2.926044000	-1.231764000	-0.258439000
6	4.317063000	-1.136511000	-0.401069000
1	4.879807000	-0.429788000	0.199401000
6	5.007390000	-1.941905000	-1.309563000
1	6.086123000	-1.853981000	-1.397809000
6	4.306243000	-2.850226000	-2.096936000
1	4.829248000	-3.478609000	-2.811357000
6	2.919945000	-2.949482000	-1.966781000
1	2.378008000	-3.663496000	-2.581528000
6	2.211265000	-2.154977000	-1.059191000
6	0.723379000	-2.396265000	-0.931544000
1	0.461077000	-2.780526000	0.064682000
1	0.433674000	-3.163766000	-1.657823000
8	-0.078315000	-1.220782000	-1.180485000
6	-1.421107000	-1.603453000	-1.522544000
1	-1.879115000	-2.195501000	-0.722772000
1	-1.997131000	-0.690895000	-1.658682000
1	-1.418519000	-2.183060000	-2.453952000
6	-1.265061000	1.315547000	1.521885000
6	-2.209929000	0.363894000	1.638485000
1	-1.965479000	-0.554143000	2.175245000
1	1.592325000	0.810597000	-3.185812000
1	-1.499134000	2.286434000	1.093348000
1	-0.341562000	1.236380000	2.084975000

6	1.615743000	2.023533000	-1.354257000
6	2.275724000	1.409278000	-2.577087000
1	2.317509000	2.622095000	-0.776734000
1	3.116828000	0.767823000	-2.299862000
1	2.668706000	2.212688000	-3.215634000
6	0.295588000	2.625044000	-1.436318000
6	-0.743781000	1.805700000	-1.959293000
1	-0.503039000	0.976189000	-2.618209000
6	-0.051925000	3.874656000	-0.842986000
1	0.738958000	4.500595000	-0.438424000
6	-1.361593000	4.304314000	-0.830929000
6	-2.082420000	2.269186000	-1.930254000
6	-2.389336000	3.494803000	-1.372818000
1	-2.864057000	1.670246000	-2.388860000
1	-1.608167000	5.277558000	-0.416027000
1	-3.413137000	3.857428000	-1.375001000
6	-3.649970000	0.508419000	1.205369000
1	-3.706045000	1.349975000	0.505030000
6	-4.208688000	-0.729288000	0.511260000
6	-4.166832000	-1.994137000	1.117307000
1	-3.726700000	-2.111530000	2.104976000
6	-4.817845000	-0.615695000	-0.744948000
1	-4.883692000	0.360900000	-1.220242000
6	-5.357443000	-1.732044000	-1.388397000
6	-4.703030000	-3.112945000	0.477585000
6	-5.296619000	-2.986551000	-0.780578000
1	-4.666274000	-4.082479000	0.966920000
1	-5.831141000	-1.618758000	-2.359716000
1	-5.718765000	-3.856198000	-1.275796000
6	-4.504205000	0.875895000	2.448366000
1	-4.461058000	0.087166000	3.207187000
1	-4.148587000	1.806674000	2.901803000
1	-5.551633000	1.003332000	2.157148000

S52

E + ZPE = -3168.568578

28	0.272148000	-0.396901000	-0.208040000
15	-1.620102000	0.531094000	0.439515000
6	-1.580188000	1.126440000	2.228997000
1	-1.994704000	0.330559000	2.854854000
6	-2.477153000	2.402166000	2.293974000
1	-3.168557000	2.346870000	3.141314000
1	-1.829059000	3.267248000	2.475577000
6	-3.227179000	2.607321000	0.968777000
1	-3.522241000	3.654965000	0.837676000
1	-4.150007000	2.014799000	0.943683000
6	-2.302888000	2.168204000	-0.182513000
1	-1.431428000	2.834346000	-0.203908000
6	-2.993813000	2.201409000	-1.546229000
1	-3.827985000	1.493737000	-1.595135000
1	-2.309492000	1.988384000	-2.373484000
1	-3.403763000	3.202869000	-1.719833000
6	-0.154809000	1.426462000	2.721276000
1	0.342918000	2.168667000	2.088578000
1	0.476986000	0.533709000	2.753190000
1	-0.201714000	1.833308000	3.737977000
6	-3.057249000	-0.631999000	0.266827000
6	-3.957280000	-0.809947000	1.328548000
1	-3.819477000	-0.277011000	2.262421000
6	-5.058349000	-1.662470000	1.218524000
1	-5.736285000	-1.775283000	2.059324000
6	-5.282792000	-2.352451000	0.031974000

1	-6.138133000	-3.013554000	-0.069425000
6	-4.398165000	-2.183129000	-1.033763000
1	-4.579037000	-2.711942000	-1.966435000
6	-3.283622000	-1.341327000	-0.941460000
6	-2.364266000	-1.241490000	-2.146478000
1	-2.054171000	-0.211154000	-2.325829000
1	-2.896520000	-1.585652000	-3.043854000
8	-1.142868000	-1.974930000	-2.006009000
6	-1.294033000	-3.382363000	-2.172306000
1	-1.718261000	-3.616048000	-3.158435000
1	-0.294527000	-3.817880000	-2.105845000
1	-1.933234000	-3.821853000	-1.395623000
6	2.307510000	-1.989964000	-1.551982000
6	-0.209011000	-1.892834000	1.176755000
6	1.055282000	-2.160822000	0.702967000
1	1.141775000	-2.860104000	-0.129326000
1	1.676837000	-0.893835000	-0.962339000
1	2.132992000	-1.160418000	2.249314000
1	-1.072833000	-2.398448000	0.759590000
1	-0.332077000	-1.501042000	2.183549000
6	0.640246000	0.999360000	-1.487673000
6	1.616592000	-0.084112000	-1.794964000
1	-0.148770000	1.084404000	-2.233759000
1	2.657538000	0.243190000	-1.795074000
1	1.368542000	-0.661889000	-2.685686000
6	1.164483000	2.321665000	-1.057984000
6	0.630170000	3.500862000	-1.607070000
1	-0.158299000	3.431889000	-2.352751000
6	2.209506000	2.443289000	-0.122317000
1	2.662711000	1.551726000	0.304104000
6	2.695045000	3.695403000	0.249667000
6	1.118661000	4.754381000	-1.238879000
6	2.149811000	4.856871000	-0.304054000
1	0.699161000	5.649444000	-1.689247000
1	3.505491000	3.765675000	0.969783000
1	2.533250000	5.831426000	-0.016871000
6	2.495676000	-3.274184000	2.399996000
1	3.377614000	-3.173176000	3.039987000
1	1.620964000	-3.456087000	3.032753000
1	2.643924000	-4.151653000	1.761395000
6	3.567959000	-1.674804000	0.757233000
6	3.989094000	-2.490243000	-0.304233000
1	3.414884000	-3.373069000	-0.577572000
6	4.357795000	-0.569960000	1.101000000
1	4.061664000	0.058341000	1.938884000
6	5.527554000	-0.274471000	0.396354000
6	5.155017000	-2.196379000	-1.012992000
6	5.926695000	-1.084723000	-0.666979000
1	5.465689000	-2.841687000	-1.829940000
1	6.127830000	0.584538000	0.682773000
1	6.836342000	-0.859028000	-1.215634000

S53

E + ZPE = -3168.559669

28	-0.084919000	0.179709000	0.757024000
15	1.641824000	0.512314000	-0.555779000
6	1.210541000	0.983073000	-2.326116000
1	1.013531000	0.070975000	-2.897068000
6	2.444614000	1.752187000	-2.897979000
1	2.895070000	1.200878000	-3.729230000
1	2.093346000	2.702799000	-3.313365000
6	3.491548000	2.012362000	-1.793055000

1	3.998373000	2.972677000	-1.941697000	6	-5.385398000	-3.333307000	-0.145280000
1	4.269630000	1.240699000	-1.816615000	6	-6.498688000	-2.493463000	-0.219699000
6	2.812357000	1.979875000	-0.410032000	1	-5.511940000	-4.385361000	0.094479000
1	2.132650000	2.838620000	-0.323003000	1	-7.187254000	-0.484280000	-0.591735000
6	3.825321000	2.024255000	0.734923000	1	-7.493698000	-2.889289000	-0.038210000
1	4.496559000	1.159471000	0.709168000			
1	3.356236000	2.068398000	1.722842000	S54			
1	4.446789000	2.921283000	0.633443000	E + ZPE = -3168.571392			
6	-0.056262000	1.855246000	-2.372040000	28	0.008157000	-0.799548000	0.369104000
1	0.055073000	2.767425000	-1.777839000	15	-1.947439000	-0.435093000	-0.603970000
1	-0.941840000	1.328558000	-2.007694000	6	-1.737446000	-0.678751000	-2.459236000
1	-0.249730000	2.155394000	-3.408078000	1	-1.266972000	0.212855000	-2.886198000
6	2.754035000	-0.971701000	-0.649655000	6	-3.158640000	-0.918264000	-3.050630000
6	3.079711000	-1.512576000	-1.905077000	1	-3.474643000	-0.068499000	-3.663290000
1	2.670048000	-1.083381000	-2.811534000	1	-3.113176000	-1.780132000	-3.724787000
6	3.944500000	-2.600370000	-2.032223000	6	-4.181361000	-1.172346000	-1.919842000
1	4.173692000	-2.992371000	-3.018677000	1	-4.894500000	-1.957632000	-2.194321000
6	4.521672000	-3.159984000	-0.896558000	1	-4.771747000	-0.267510000	-1.735862000
1	5.212578000	-3.993354000	-0.981349000	6	-3.466852000	-1.560670000	-0.605884000
6	4.212136000	-2.631633000	0.355823000	1	-3.055471000	-2.573909000	-0.703835000
1	4.681678000	-3.052545000	1.241121000	6	-4.442672000	-1.527524000	0.572376000
6	3.321667000	-1.560740000	0.509988000	1	-4.828464000	-0.517092000	0.743093000
6	3.005549000	-1.109039000	1.925989000	1	-4.008817000	-1.896335000	1.503881000
1	2.714468000	-0.058750000	1.949851000	1	-5.301284000	-2.168946000	0.343125000
1	3.900278000	-1.219778000	2.555962000	6	-0.823405000	-1.887761000	-2.738817000
8	1.911296000	-1.804006000	2.527857000	1	-1.240257000	-2.810568000	-2.319298000
6	2.227895000	-3.097951000	3.030733000	1	0.184368000	-1.761469000	-2.333430000
1	3.077846000	-3.052269000	3.726672000	1	-0.734432000	-2.032852000	-3.821199000
1	1.344946000	-3.447427000	3.570438000	6	-2.663829000	1.253779000	-0.340276000
1	2.460541000	-3.808021000	2.226737000	6	-2.939052000	2.079999000	-1.440861000
6	0.181200000	1.665268000	1.908307000	1	-2.726878000	1.741209000	-2.448459000
6	-0.252473000	0.663627000	2.943827000	6	-3.497412000	3.349282000	-1.277773000
1	-1.075359000	1.013158000	3.575049000	1	-3.700408000	3.963700000	-2.149911000
1	-0.668554000	-0.270192000	2.462382000	6	-3.802638000	3.811775000	-0.001217000
1	1.164520000	2.098673000	2.066864000	1	-4.251084000	4.790808000	0.138289000
6	-0.386494000	-1.834265000	0.154997000	6	-3.531244000	3.002495000	1.101937000
6	-1.619610000	-1.238620000	0.206654000	1	-3.781627000	3.356816000	2.098794000
1	0.079782000	-2.074690000	-0.795312000	6	-2.950761000	1.735629000	0.962429000
1	0.063115000	-2.305150000	1.024426000	6	-2.628585000	0.951260000	2.222496000
1	-2.146095000	-1.248105000	1.162696000	1	-2.723542000	-0.120898000	2.053820000
1	0.575360000	0.304332000	3.554333000	1	-3.333471000	1.224645000	3.020455000
6	-0.819549000	2.604286000	1.366987000	8	-1.287109000	1.130606000	2.687042000
6	-2.194844000	2.281965000	1.337608000	6	-1.077744000	2.325287000	3.434364000
1	-2.556940000	1.371423000	1.806856000	1	-1.757931000	2.372726000	4.296550000
6	-0.420331000	3.844765000	0.824262000	1	-0.047257000	2.293060000	3.794582000
1	0.626330000	4.134245000	0.878640000	1	-1.214667000	3.224978000	2.820225000
6	-1.347711000	4.714558000	0.262898000	6	-0.611995000	-2.470643000	1.105490000
6	-3.121816000	3.151452000	0.761315000	6	-1.242255000	-2.397477000	2.490963000
6	-2.703022000	4.365805000	0.217614000	1	-0.954197000	-3.279453000	3.077691000
1	-4.175461000	2.887427000	0.759437000	1	-0.948343000	-1.508859000	3.057658000
1	-1.020454000	5.672937000	-0.129918000	1	-1.151608000	-3.141821000	0.436767000
1	-3.427036000	5.048448000	-0.216949000	6	0.441001000	1.207875000	-0.107416000
6	-2.528222000	-0.913443000	-0.975559000	6	1.670073000	0.626208000	0.062299000
1	-2.638003000	0.177901000	-1.037570000	1	0.100271000	1.494485000	-1.097845000
6	-1.992908000	-1.419646000	-2.326300000	1	-0.064801000	1.684825000	0.725449000
1	-1.909933000	-2.511279000	-2.331780000	1	2.091327000	0.633773000	1.063053000
1	-2.678859000	-1.132974000	-3.128417000	1	-2.331562000	-2.396896000	2.425566000
1	-1.008553000	-1.001501000	-2.561078000	6	0.830340000	-2.624168000	0.998469000
6	-3.923004000	-1.470798000	-0.692240000	6	1.657443000	-1.824996000	1.828227000
6	-4.107652000	-2.825426000	-0.379414000	1	1.223543000	-1.269653000	2.654709000
1	-3.248371000	-3.489824000	-0.320242000	6	1.455871000	-3.449577000	0.015278000
6	-5.046017000	-0.637607000	-0.761156000	1	0.829656000	-4.052204000	-0.636901000
1	-4.919410000	0.414760000	-1.007614000				
6	-6.326232000	-1.143897000	-0.529420000				

6	2.830369000	-3.529616000	-0.062639000
6	3.059834000	-1.917365000	1.735878000
6	3.639870000	-2.764366000	0.807326000
1	3.682659000	-1.335786000	2.408737000
1	3.295176000	-4.195596000	-0.783815000
1	4.720809000	-2.854007000	0.753712000
6	2.691003000	0.346177000	-1.030676000
1	2.963329000	-0.716279000	-0.985592000
6	2.198787000	0.653216000	-2.456154000
1	1.979037000	1.718934000	-2.579997000
1	2.977855000	0.393493000	-3.178605000
1	1.300132000	0.083226000	-2.714431000
6	3.967126000	1.134773000	-0.723729000
6	3.920345000	2.511624000	-0.463286000
1	2.962782000	3.027109000	-0.449572000
6	5.213702000	0.497494000	-0.736248000
1	5.268322000	-0.569409000	-0.941370000
6	6.387061000	1.215680000	-0.499717000
6	5.090748000	3.231786000	-0.223055000
6	6.328325000	2.585628000	-0.240494000
1	5.036146000	4.298431000	-0.023576000
1	7.345841000	0.704871000	-0.518585000
1	7.239908000	3.146099000	-0.054462000

S55

E + ZPE = -3168.567221

28	-0.807349000	1.257633000	-0.309957000
15	-1.980901000	-0.249684000	0.763319000
6	-1.291395000	-0.777186000	2.440873000
1	-0.799645000	-1.743380000	2.294679000
6	-2.517290000	-0.926848000	3.391120000
1	-2.401108000	-1.803775000	4.036897000
1	-2.547202000	-0.052608000	4.053199000
6	-3.819147000	-0.984392000	2.582311000
1	-4.691253000	-0.769263000	3.210966000
1	-3.974896000	-1.984672000	2.158633000
6	-3.714790000	0.043387000	1.439441000
1	-3.669659000	1.048492000	1.881481000
6	-4.884417000	-0.022436000	0.455830000
1	-4.923915000	-0.988511000	-0.058019000
1	-4.845322000	0.769375000	-0.298635000
1	-5.826801000	0.099147000	1.001556000
6	-0.250711000	0.196926000	3.011596000
1	-0.675741000	1.196511000	3.155469000
1	0.626479000	0.289562000	2.367118000
1	0.080991000	-0.160063000	3.993721000
6	-2.157977000	-1.783814000	-0.264500000
6	-2.027624000	-3.066349000	0.288084000
1	-1.819318000	-3.191928000	1.344634000
6	-2.173398000	-4.215359000	-0.493635000
1	-2.070919000	-5.194017000	-0.034258000
6	-2.454085000	-4.099499000	-1.851367000
1	-2.571381000	-4.985434000	-2.468019000
6	-2.587105000	-2.830439000	-2.416742000
1	-2.816638000	-2.737968000	-3.475509000
6	-2.442161000	-1.669740000	-1.649889000
6	-2.606706000	-0.327477000	-2.333984000
1	-3.283743000	0.328364000	-1.784057000
1	-3.024449000	-0.466585000	-3.338326000
8	-1.376262000	0.415418000	-2.438041000
6	-0.549253000	-0.011852000	-3.527276000
1	-1.094309000	0.083829000	-4.474136000

1	0.320333000	0.647438000	-3.546715000
1	-0.218835000	-1.048921000	-3.397151000
6	-1.630586000	2.781611000	0.507897000
6	-2.868798000	3.335891000	-0.177279000
1	-3.058190000	4.357995000	0.178423000
1	-2.777723000	3.382995000	-1.266464000
1	-1.754917000	2.735805000	1.592347000
6	1.106589000	-0.359130000	-0.556891000
6	2.235493000	-0.113297000	0.125255000
1	0.645872000	-1.340070000	-0.594752000
1	0.739019000	0.379895000	-1.271962000
1	2.666540000	0.885026000	0.068713000
1	-3.757711000	2.743785000	0.058522000
6	-0.298985000	3.204843000	0.102131000
6	0.026870000	3.025497000	-1.274941000
1	-0.757468000	2.998094000	-2.026667000
6	0.747140000	3.539242000	1.012053000
1	0.505516000	3.666785000	2.063596000
6	2.031062000	3.749846000	0.557080000
6	1.357897000	3.240851000	-1.713422000
6	2.345481000	3.591391000	-0.814053000
1	1.589693000	3.164766000	-2.772134000
1	2.809230000	4.048521000	1.253774000
1	3.359272000	3.773843000	-1.157928000
6	3.020040000	-1.086689000	0.974361000
1	3.016994000	-0.675275000	1.995875000
6	2.424611000	-2.502641000	1.034924000
1	3.026572000	-3.132928000	1.695673000
1	1.397790000	-2.491669000	1.419233000
1	2.414474000	-2.973498000	0.046133000
6	4.481132000	-1.106891000	0.520219000
6	5.512942000	-0.840895000	1.427793000
1	5.271666000	-0.601826000	2.461465000
6	4.813945000	-1.413310000	-0.806649000
1	4.024855000	-1.617714000	-1.526795000
6	6.147305000	-1.459044000	-1.213600000
6	6.848509000	-0.886328000	1.023618000
6	7.169036000	-1.195655000	-0.298683000
1	7.636807000	-0.680809000	1.742479000
1	6.389031000	-1.700497000	-2.245096000
1	8.207650000	-1.231916000	-0.614693000

S56

E + ZPE = -3168.566496

28	0.325212000	-0.131027000	0.007052000
15	-1.771471000	0.472298000	0.329017000
6	-2.061194000	1.292552000	2.007940000
1	-2.454901000	0.534371000	2.690915000
6	-3.119141000	2.414291000	1.776877000
1	-3.875241000	2.399144000	2.568799000
1	-2.611910000	3.383883000	1.845245000
6	-3.753178000	2.279053000	0.385687000
1	-4.205575000	3.223494000	0.061151000
1	-4.554325000	1.529440000	0.388326000
6	-2.647850000	1.852213000	-0.598034000
1	-1.902539000	2.656129000	-0.643524000
6	-3.173896000	1.571128000	-2.006140000
1	-3.873643000	0.728835000	-2.016321000
1	-2.374287000	1.364282000	-2.724689000
1	-3.715089000	2.450645000	-2.373217000
6	-0.772702000	1.859299000	2.626524000
1	-0.272525000	2.559914000	1.950254000

1	-0.054884000	1.079080000	2.898905000	28	-0.054842000	0.750479000	-0.752187000
1	-1.022716000	2.403761000	3.544431000	15	-1.384282000	0.237791000	0.902443000
6	-2.932306000	-0.970738000	0.192587000	6	-0.441866000	-0.283786000	2.451074000
6	-3.909060000	-1.189649000	1.176102000	1	-0.211969000	-1.350176000	2.374459000
1	-3.986459000	-0.529465000	2.032063000	6	-1.393345000	0.000881000	3.658912000
6	-4.817439000	-2.246507000	1.083493000	1	-1.640623000	-0.926737000	4.184488000
1	-5.560904000	-2.385413000	1.862744000	1	-0.854524000	0.628018000	4.377201000
6	-4.770018000	-3.104835000	-0.009756000	6	-2.678978000	0.720756000	3.197781000
1	-5.475178000	-3.925677000	-0.099037000	1	-3.041838000	1.416417000	3.962988000
6	-3.809353000	-2.895703000	-0.999549000	1	-3.483904000	-0.003028000	3.025473000
1	-3.781849000	-3.555039000	-1.863670000	6	-2.405794000	1.474699000	1.882384000
6	-2.881776000	-1.850206000	-0.920470000	1	-1.693192000	2.288679000	2.078609000
6	-1.860548000	-1.724357000	-2.037827000	6	-3.673165000	2.062160000	1.261295000
1	-1.686426000	-0.680794000	-2.302343000	1	-4.395555000	1.279280000	1.007590000
1	-2.237663000	-2.232818000	-2.936215000	1	-3.471913000	2.653254000	0.362100000
8	-0.568612000	-2.241229000	-1.705377000	1	-4.155632000	2.728716000	1.985005000
6	-0.497132000	-3.663611000	-1.718155000	6	0.891088000	0.466359000	2.606676000
1	-0.788249000	-4.061437000	-2.700407000	1	0.751181000	1.551198000	2.618949000
1	0.544292000	-3.928970000	-1.523609000	1	1.604687000	0.229967000	1.813379000
1	-1.135620000	-4.114894000	-0.947500000	1	1.351300000	0.180407000	3.559175000
6	2.367392000	-2.295939000	1.093126000	6	-2.546238000	-1.160610000	0.520001000
6	-0.008219000	-1.509396000	1.568846000	6	-2.550552000	-2.304581000	1.336967000
6	1.341282000	-1.246420000	1.505776000	1	-1.862073000	-2.391429000	2.168366000
1	1.731722000	-0.441799000	2.132462000	6	-3.444083000	-3.354951000	1.123264000
1	1.808000000	-0.539203000	-0.643955000	1	-3.418454000	-4.222453000	1.775931000
1	1.900681000	-2.950374000	0.345807000	6	-4.371249000	-3.274327000	0.089130000
1	-0.408158000	-2.428426000	1.148469000	1	-5.084971000	-4.075583000	-0.077157000
1	-0.632237000	-1.028532000	2.314005000	6	-4.378871000	-2.147575000	-0.731817000
6	0.614852000	1.172954000	-1.389295000	1	-5.112289000	-2.075778000	-1.530875000
6	1.710838000	0.178988000	-1.549957000	6	-3.472566000	-1.094478000	-0.553486000
1	-0.114908000	1.148588000	-2.196418000	6	-3.509513000	0.040330000	-1.560974000
1	2.714659000	0.607711000	-1.542852000	1	-3.190865000	0.982448000	-1.112439000
1	1.564691000	-0.499927000	-2.389645000	1	-4.538267000	0.178486000	-1.925095000
6	0.956052000	2.549012000	-0.952292000	8	-2.628663000	-0.156957000	-2.665351000
6	0.300498000	3.655977000	-1.522169000	6	-3.103568000	-1.061669000	-3.655556000
1	-0.436627000	3.493210000	-2.304894000	1	-4.094032000	-0.757810000	-4.024107000
6	1.945390000	2.796698000	0.020432000	1	-2.389721000	-1.022440000	-4.481204000
1	2.498202000	1.968421000	0.458308000	1	-3.162249000	-2.092430000	-3.282241000
6	2.252108000	4.097230000	0.415452000	6	-0.481385000	2.592718000	-0.845520000
6	0.610042000	4.957787000	-1.130393000	6	-0.746958000	2.418326000	-2.328286000
6	1.582061000	5.183315000	-0.154063000	1	-0.331773000	3.244025000	-2.919753000
1	0.099931000	5.796202000	-1.595943000	1	-0.257308000	1.505973000	-2.737623000
1	3.021199000	4.264895000	1.164081000	1	-1.297260000	3.046032000	-0.288943000
1	1.826213000	6.196514000	0.150926000	6	0.337351000	-1.038598000	-1.726930000
6	2.680341000	-3.167302000	2.337155000	6	1.276157000	-0.956716000	-0.729424000
1	3.401878000	-3.947113000	2.074422000	1	-0.592920000	-1.579822000	-1.588002000
1	3.116770000	-2.565984000	3.142081000	1	0.599864000	-0.822598000	-2.760351000
1	1.771367000	-3.642816000	2.719503000	1	1.035335000	-1.422954000	0.224169000
6	3.649626000	-1.731189000	0.495416000	1	-1.807941000	2.308597000	-2.547864000
6	4.137018000	-2.225786000	-0.721325000	6	0.859915000	3.042973000	-0.438995000
1	3.586321000	-3.007658000	-1.240519000	6	1.981971000	2.869340000	-1.279475000
6	4.390094000	-0.738094000	1.155427000	1	1.853852000	2.508615000	-2.294962000
1	4.056099000	-0.355159000	2.117359000	6	1.069449000	3.635549000	0.829049000
6	5.572371000	-0.242297000	0.603944000	1	0.211973000	3.822781000	1.471129000
6	5.322081000	-1.735207000	-1.274525000	6	2.337970000	4.011012000	1.244054000
6	6.040945000	-0.737670000	-0.615315000	6	3.261906000	3.233146000	-0.851008000
1	5.683104000	-2.135379000	-2.217806000	6	3.445212000	3.797270000	0.409301000
1	6.133427000	0.523889000	1.131749000	1	4.109201000	3.098877000	-1.517118000
1	6.963295000	-0.354961000	-1.042261000	1	2.473159000	4.482487000	2.213229000
				1	4.437023000	4.096160000	0.735111000
				6	2.764079000	-0.658521000	-0.903836000
				1	3.004635000	0.257009000	-0.347631000
				6	3.192025000	-0.447359000	-2.366905000
				1	3.026083000	-1.350567000	-2.962904000

S57

E + ZPE = -3168.561786

1	2.652184000	0.378816000	-2.843481000
1	4.259916000	-0.214786000	-2.408924000
6	3.566575000	-1.786399000	-0.254582000
6	4.527632000	-1.497618000	0.721706000
1	4.693217000	-0.465442000	1.023675000
6	3.372312000	-3.122713000	-0.633076000
1	2.630387000	-3.368796000	-1.389488000
6	4.124692000	-4.143149000	-0.051614000
6	5.283609000	-2.516894000	1.303911000
6	5.083009000	-3.842868000	0.919041000
1	6.028898000	-2.273706000	2.056115000
1	3.964329000	-5.173094000	-0.358130000
1	5.670230000	-4.637480000	1.370200000

S58

E + ZPE = -3168.575695

28	-0.133605000	0.984398000	-0.254117000
15	1.205247000	-0.682011000	-0.824991000
6	0.202295000	-2.246981000	-1.102408000
1	-0.096684000	-2.668152000	-0.138619000
6	1.105558000	-3.231069000	-1.900242000
1	1.404479000	-4.079011000	-1.276206000
1	0.518155000	-3.647983000	-2.725042000
6	2.355104000	-2.502245000	-2.440281000
1	2.608656000	-2.835026000	-3.452971000
1	3.223587000	-2.731386000	-1.811851000
6	2.154736000	-0.968821000	-2.437085000
1	1.437598000	-0.689145000	-3.220286000
6	3.488843000	-0.266099000	-2.702137000
1	4.215501000	-0.478691000	-1.910963000
1	3.402439000	0.816629000	-2.813266000
1	3.908068000	-0.651820000	-3.638508000
6	-1.084737000	-1.919235000	-1.883730000
1	-0.864179000	-1.483381000	-2.865036000
1	-1.741709000	-1.236765000	-1.339249000
1	-1.645701000	-2.844345000	-2.053022000
6	2.444408000	-1.017438000	0.508038000
6	2.447744000	-2.252540000	1.175281000
1	1.732109000	-3.021920000	0.906808000
6	3.371789000	-2.531124000	2.184143000
1	3.352334000	-3.496638000	2.680914000
6	4.321787000	-1.576172000	2.534369000
1	5.055829000	-1.786778000	3.306324000
6	4.330312000	-0.344568000	1.878671000
1	5.084958000	0.393163000	2.139674000
6	3.398117000	-0.033380000	0.880931000
6	3.446452000	1.355135000	0.259286000
1	3.093775000	1.337113000	-0.770423000
1	4.485345000	1.715758000	0.248142000
8	2.612537000	2.320171000	0.903456000
6	3.146305000	2.854733000	2.109317000
1	4.140893000	3.291263000	1.939463000
1	2.463039000	3.643066000	2.432762000
1	3.219159000	2.097747000	2.901513000
6	-0.167377000	1.741723000	-2.047260000
6	1.017774000	2.598381000	-2.476052000
1	0.682089000	3.365090000	-3.186911000
1	1.508803000	3.112241000	-1.644124000
1	-0.496284000	1.067123000	-2.840766000
6	-0.059557000	0.974360000	1.858966000
6	-0.910328000	-0.050200000	1.549415000
1	0.995911000	0.793914000	2.023949000

1	-0.443564000	1.923059000	2.220326000
1	-0.477688000	-1.044008000	1.454943000
1	1.770630000	1.996134000	-2.987947000
6	-1.275409000	2.374706000	-1.347218000
6	-0.966803000	3.113911000	-0.174142000
1	0.057016000	3.423271000	0.024587000
6	-2.646157000	2.152219000	-1.665067000
1	-2.891079000	1.566989000	-2.547097000
6	-3.644825000	2.729104000	-0.906203000
6	-2.002650000	3.680571000	0.599138000
6	-3.325172000	3.496738000	0.235752000
1	-1.754835000	4.289601000	1.463757000
1	-4.684650000	2.602953000	-1.194470000
1	-4.120393000	3.954952000	0.816328000
6	-2.417923000	-0.015518000	1.753748000
1	-2.810891000	0.922482000	1.345620000
6	-2.712075000	-0.002751000	3.278911000
1	-2.312513000	-0.896744000	3.768900000
1	-2.264501000	0.875498000	3.754912000
1	-3.793123000	0.019265000	3.448391000
6	-3.144190000	-1.175804000	1.084011000
6	-4.213228000	-0.939943000	0.211179000
1	-4.504173000	0.083650000	-0.009386000
6	-2.802036000	-2.506643000	1.370409000
1	-2.000045000	-2.723215000	2.073324000
6	-3.496272000	-3.567348000	0.787391000
6	-4.913414000	-1.998510000	-0.372596000
6	-4.554580000	-3.316332000	-0.089378000
1	-5.742399000	-1.791784000	-1.043905000
1	-3.220472000	-4.590352000	1.028741000
1	-5.100512000	-4.141333000	-0.537782000

S59

E + ZPE = -3168.567103

28	-1.098874000	1.051511000	-0.343130000
15	-1.880244000	-0.871684000	0.339747000
6	-2.211446000	-1.061423000	2.181976000
1	-1.280554000	-1.392088000	2.653137000
6	-3.333325000	-2.140663000	2.329165000
1	-3.004822000	-2.957085000	2.980700000
1	-4.191024000	-1.676205000	2.828004000
6	-3.767548000	-2.680238000	0.952212000
1	-4.815734000	-3.000607000	0.963929000
1	-3.175804000	-3.562607000	0.679966000
6	-3.555943000	-1.592624000	-0.119415000
1	-4.262464000	-0.769851000	0.059235000
6	-3.748216000	-2.124693000	-1.540997000
1	-3.019502000	-2.907551000	-1.776861000
1	-3.673810000	-1.341015000	-2.300637000
1	-4.745751000	-2.568902000	-1.632290000
6	-2.637692000	0.262424000	2.840028000
1	-3.572149000	0.638833000	2.409150000
1	-1.883218000	1.047494000	2.746278000
1	-2.818908000	0.093927000	3.907595000
6	-0.679216000	-2.200212000	-0.128505000
6	-0.322311000	-3.224982000	0.759766000
1	-0.750657000	-3.262312000	1.755457000
6	0.578469000	-4.226986000	0.389817000
1	0.831379000	-5.010692000	1.097718000
6	1.139874000	-4.219910000	-0.884019000
1	1.836444000	-4.997227000	-1.183335000
6	0.796358000	-3.205063000	-1.779397000

1	1.226938000	-3.202937000	-2.777832000
6	-0.101008000	-2.192770000	-1.422988000
6	-0.430383000	-1.119071000	-2.438230000
1	-1.508051000	-0.985615000	-2.550164000
1	-0.029128000	-1.392008000	-3.420364000
8	0.075725000	0.182828000	-2.070113000
6	1.389612000	0.449714000	-2.581122000
1	1.398150000	0.331397000	-3.671109000
1	1.623892000	1.485020000	-2.331888000
1	2.139750000	-0.210159000	-2.132349000
6	-2.813521000	1.903233000	-0.494866000
6	-3.541410000	1.745736000	-1.821510000
1	-4.321773000	2.515134000	-1.900537000
1	-2.888173000	1.856798000	-2.692331000
1	-3.494206000	1.784432000	0.351086000
6	0.689519000	1.303242000	1.519493000
6	1.722457000	0.887106000	0.764613000
1	0.319167000	2.319802000	1.447439000
1	0.339991000	0.722718000	2.367228000
1	-4.038062000	0.774682000	-1.897875000
6	-1.862823000	2.988489000	-0.306407000
6	-0.775141000	3.046315000	-1.224329000
1	-0.865676000	2.600592000	-2.210868000
6	-1.832360000	3.834142000	0.840040000
1	-2.659085000	3.792596000	1.543869000
6	-0.793351000	4.721077000	1.030685000
6	0.283193000	3.960685000	-1.001304000
6	0.281400000	4.779236000	0.111744000
1	1.081955000	4.043458000	-1.733241000
1	-0.801845000	5.387861000	1.888229000
1	1.087133000	5.489643000	0.270657000
1	2.089850000	1.560690000	-0.007848000
6	2.497860000	-0.409232000	0.910657000
1	2.094478000	-1.119127000	0.174183000
6	2.349903000	-1.058410000	2.301100000
1	2.719338000	-0.390936000	3.086535000
1	1.306835000	-1.308000000	2.523590000
1	2.929816000	-1.984742000	2.344093000
6	3.968244000	-0.196881000	0.561320000
6	4.623739000	-1.076464000	-0.309614000
1	4.071598000	-1.906594000	-0.746639000
6	4.700647000	0.856217000	1.127396000
1	4.211344000	1.546736000	1.811061000
6	6.052480000	1.026295000	0.827253000
6	5.976861000	-0.910180000	-0.611049000
6	6.694475000	0.143575000	-0.043930000
1	6.469445000	-1.603596000	-1.287218000
1	6.605614000	1.846954000	1.275692000
1	7.747228000	0.275310000	-0.276645000

.....