

Supplementary Information

Mechanism and Origins of Regioselectivity of Selenium-Catalyzed Allylic Amination Reactions

Xiaoxiao Hu^{a,b}, Dengmengfei Xiao^{b,c}, Yu Chen^b, Yi Lu^b, Zhihan Zhang^b, and Peiyuan Yu^{*b}

^a*School of Chemistry and Chemical Engineering, Harbin Institute of Technology, Harbin 150001, China;*

^b*Department of Chemistry and Shenzhen Grubbs Institute, Southern University of Science and Technology, Shenzhen, Guangdong 518055, China;*

^c*Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, 01062 Dresden, Germany.*

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I. Free energy profiles for the direct ene reaction of intermediate **9** with the substrate **11**

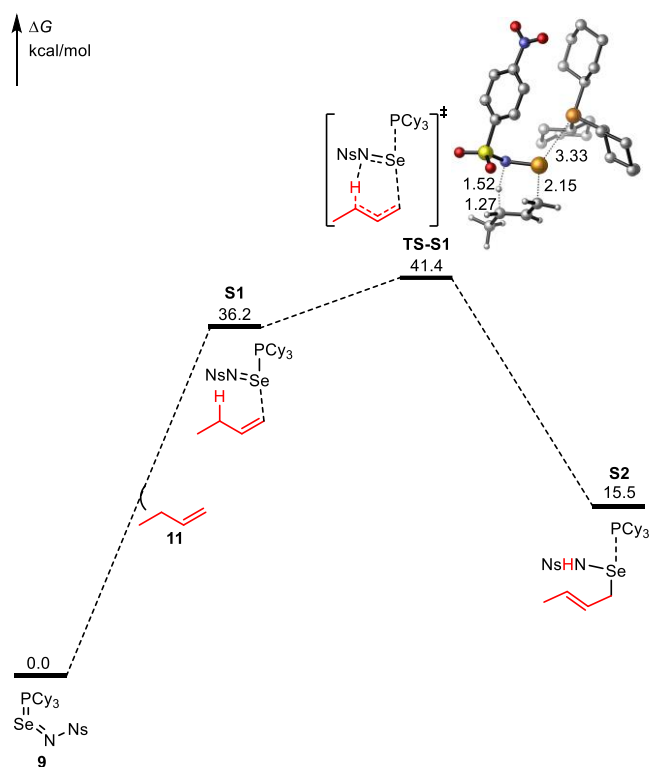


Fig. S1. Free energy profiles for the the direct ene reaction of intermediate **9** with the substrate **11**.

II. Free energy profiles for the generation of the active catalyst with the SePCy₃ ligand

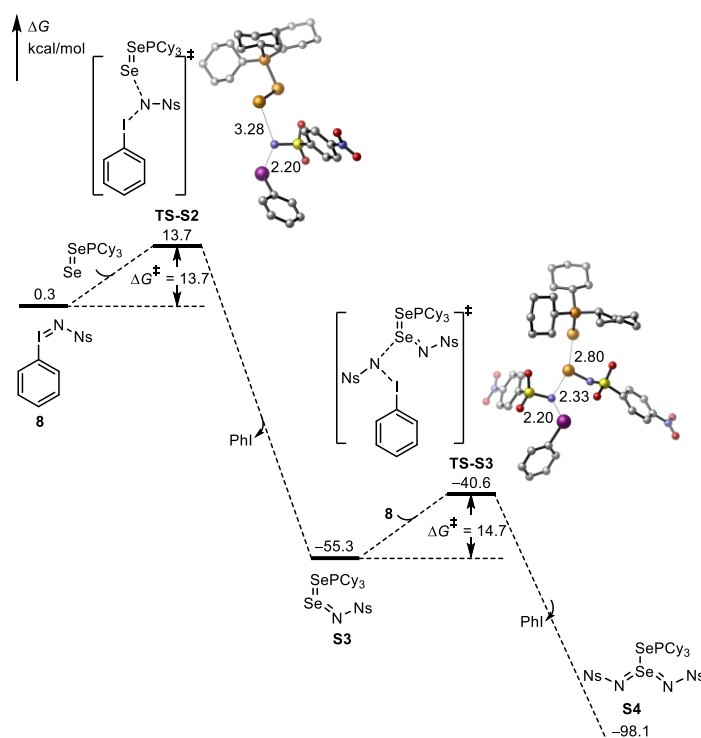


Fig. S2. Free energy profiles for the generation of the active catalyst with the SePCy₃ ligand, with selected bond lengths in Å.

III. Free energy profiles for the formation of the product with the SePCy₃ ligand

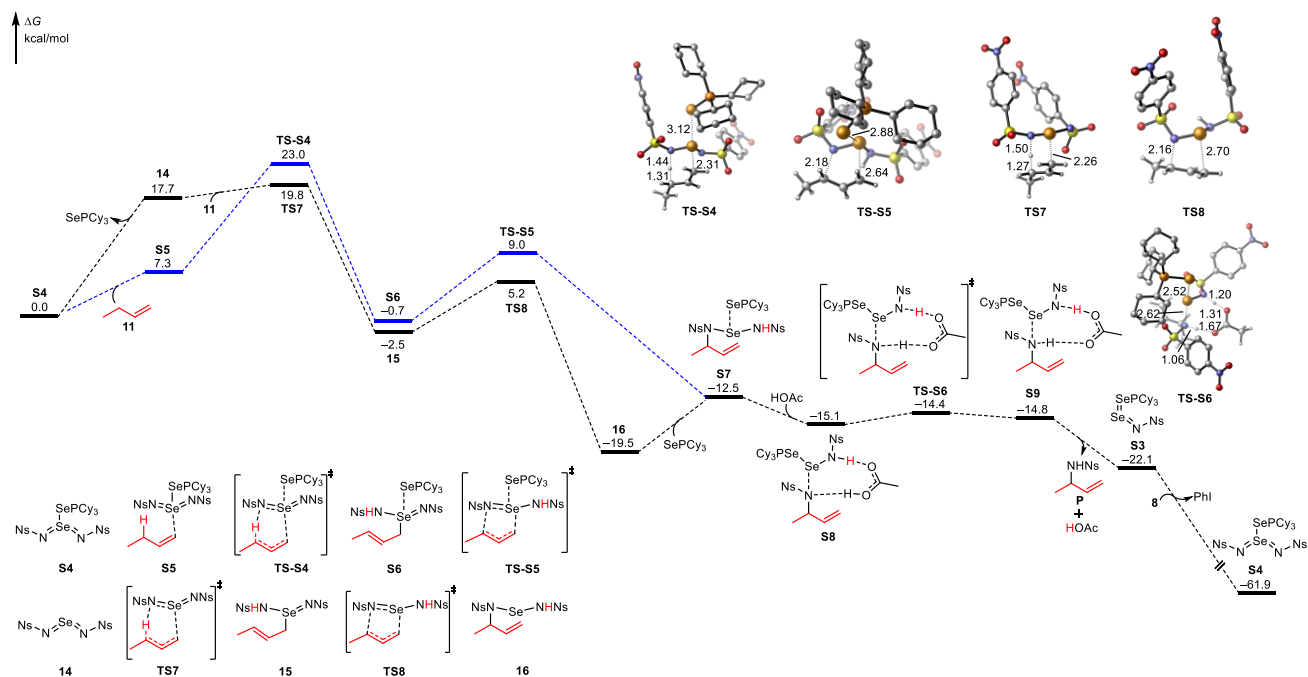


Fig. S3. Free energy profiles for ene reaction, sigmatropic shift and hydrogen transfer with the SePCy₃ ligand, leading to the formation of the final product, and selected bond lengths are given in Å.

IV. Free energy profiles for the generation of the active catalyst with the OPCy₃ ligand

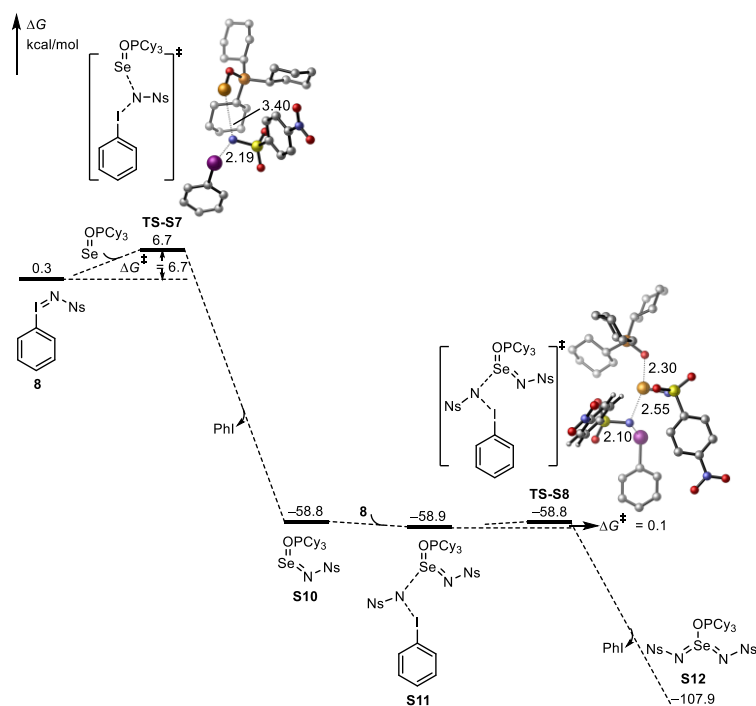


Fig. S4. Free energy profiles for the generation of the active catalyst with the OPCy₃ ligand, with selected bond lengths in Å.

V. Free energy profiles for the formation of the product with the OPCy₃ ligand

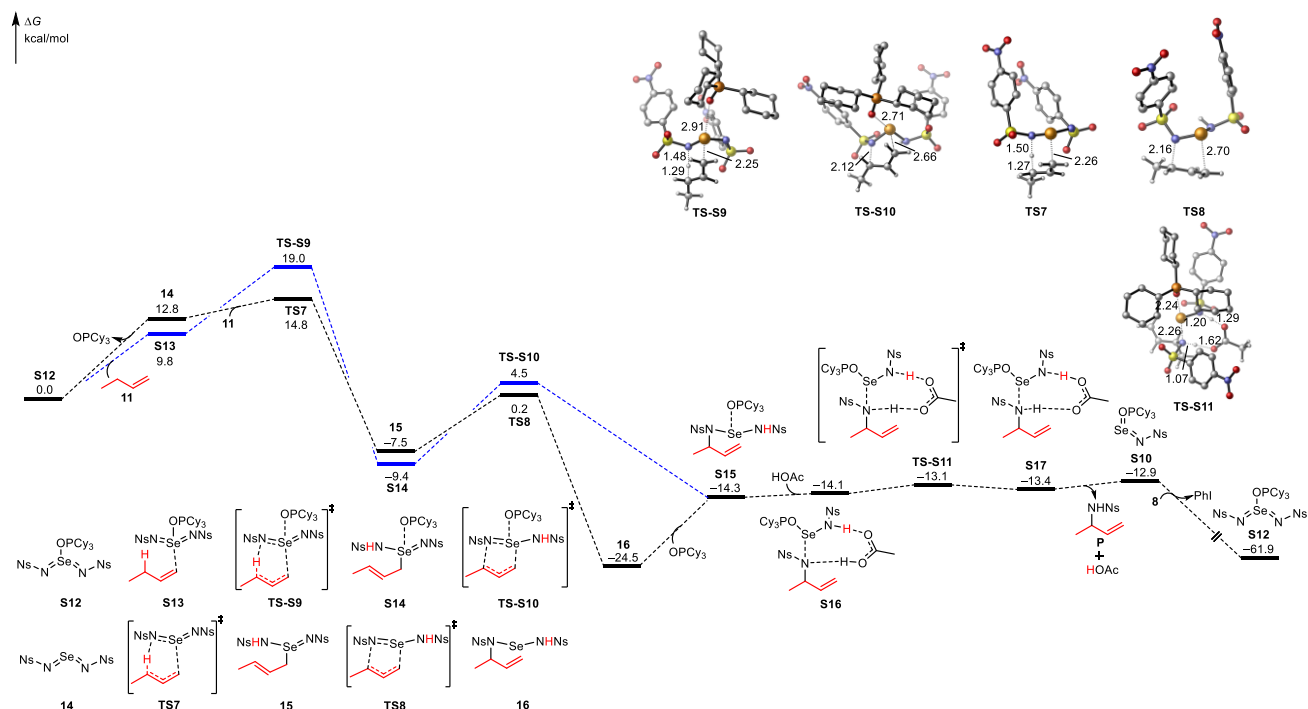


Fig. S5. Free energy profiles for ene reaction, sigmatropic shift and hydrogen transfer with the OPCy₃ ligand, leading to the formation of the final product, and selected bond lengths are given in Å.

VI. Free energy profiles for the generation of the active catalyst with the IMe ligand

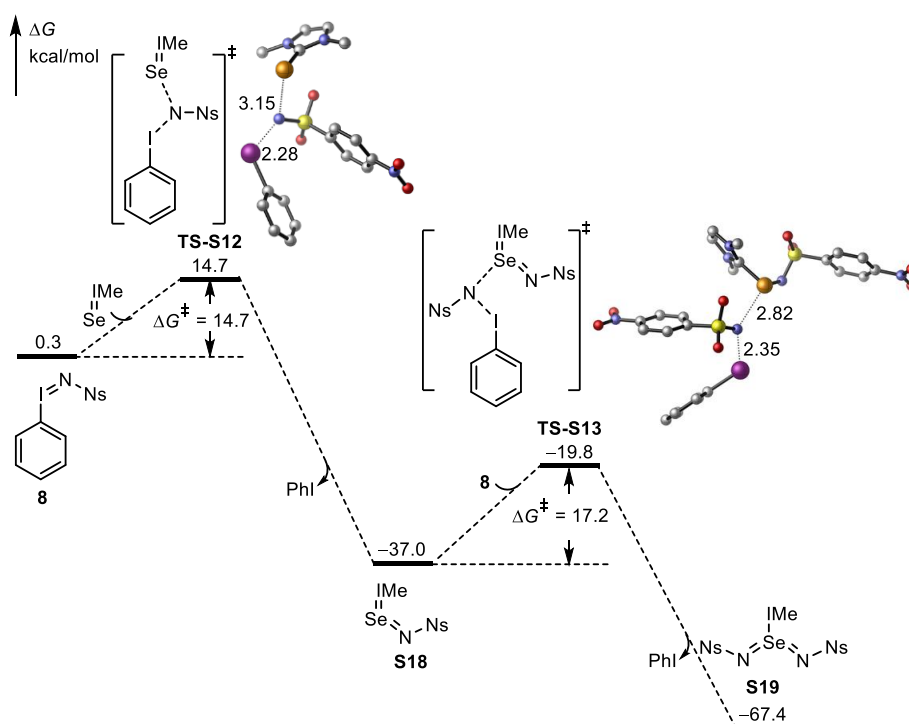


Fig. S6. Free energy profiles for the generation of the active catalyst with the IMe ligand, with selected bond lengths in Å.

VII. Free energy profiles for the formation of the product with the IMe ligand

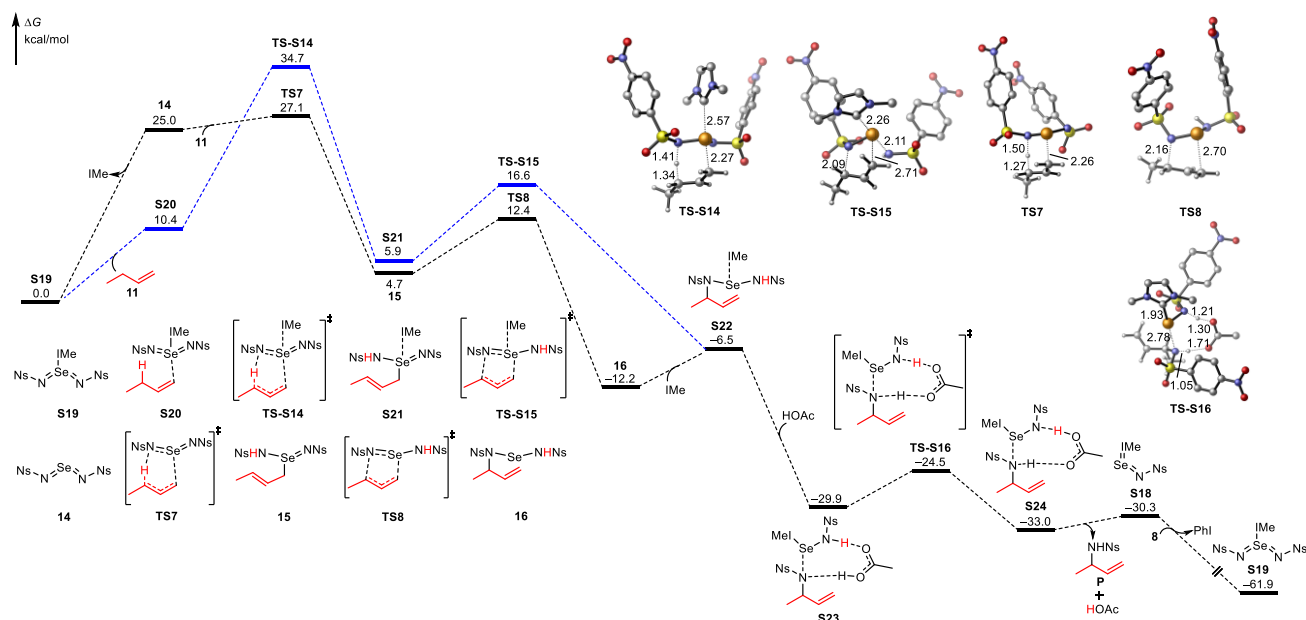


Fig. S7. Free energy profiles for ene reaction, sigmatropic shift and hydrogen transfer with the IMe ligand, leading to the formation of the final product, and selected bond lengths are given in Å.

VIII. Free energy profiles for the generation of the active catalyst with the SeIme ligand

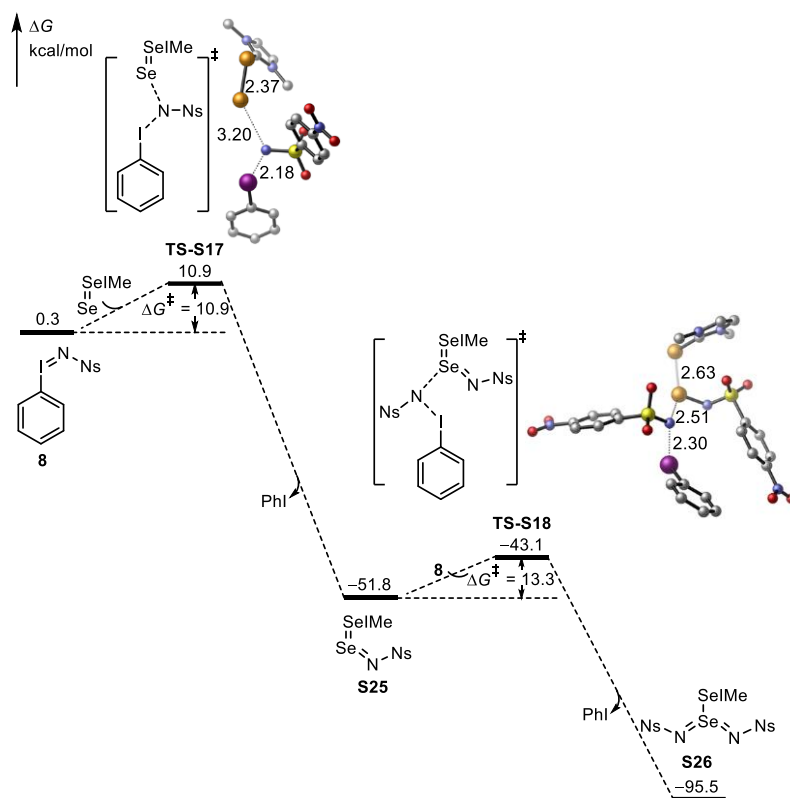


Fig. S8. Free energy profiles for the generation of the active catalyst with the SeIme ligand, with selected bond lengths in Å.

IX. Free energy profiles for the formation of the product with the SeIme ligand

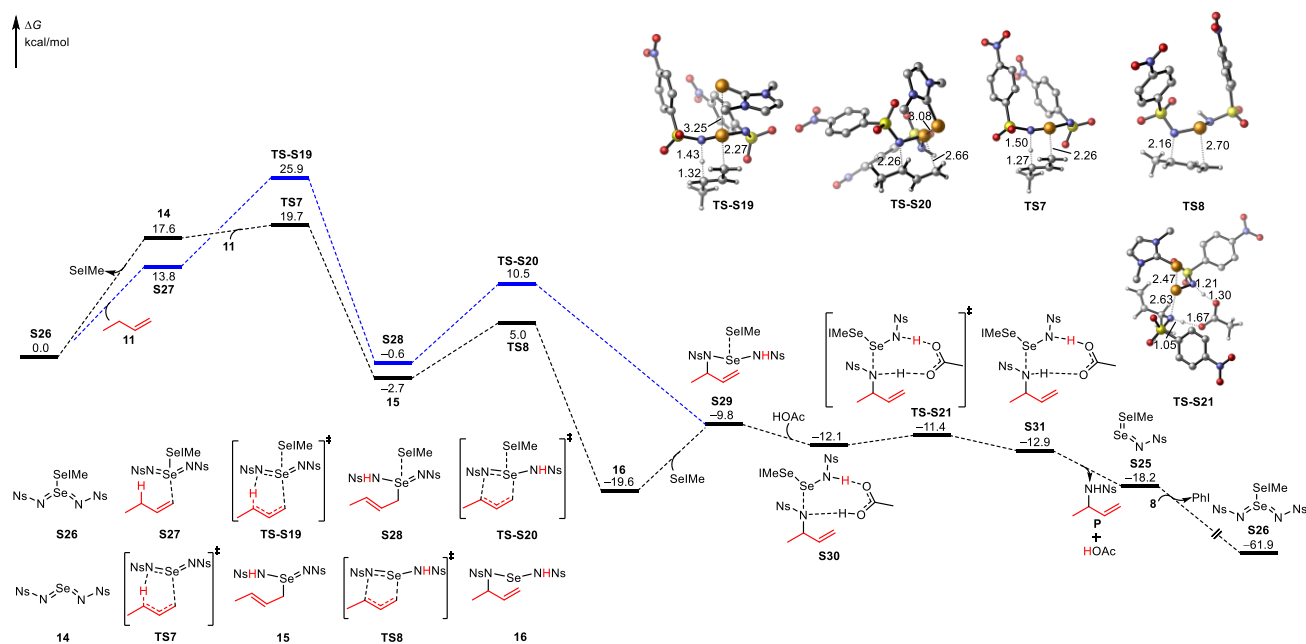


Fig. S9. Free energy profiles for ene reaction, sigmatropic shift and hydrogen transfer with the SeIme ligand, leading to the formation of the final product, and selected bond lengths are given in Å.

X. Free energy profiles for the generation of the active catalyst with the OIme ligand

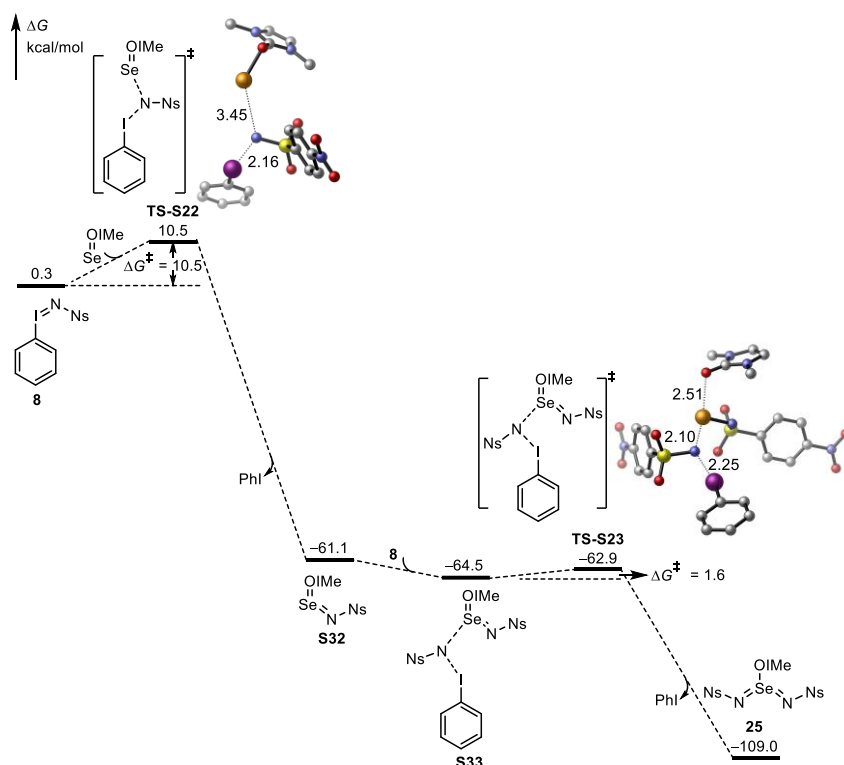


Fig. S10. Free energy profiles for the generation of the active catalyst with the OIme ligand, with selected bond lengths in Å.

XI. Free energy profiles for the formation of the product with the OIme ligand

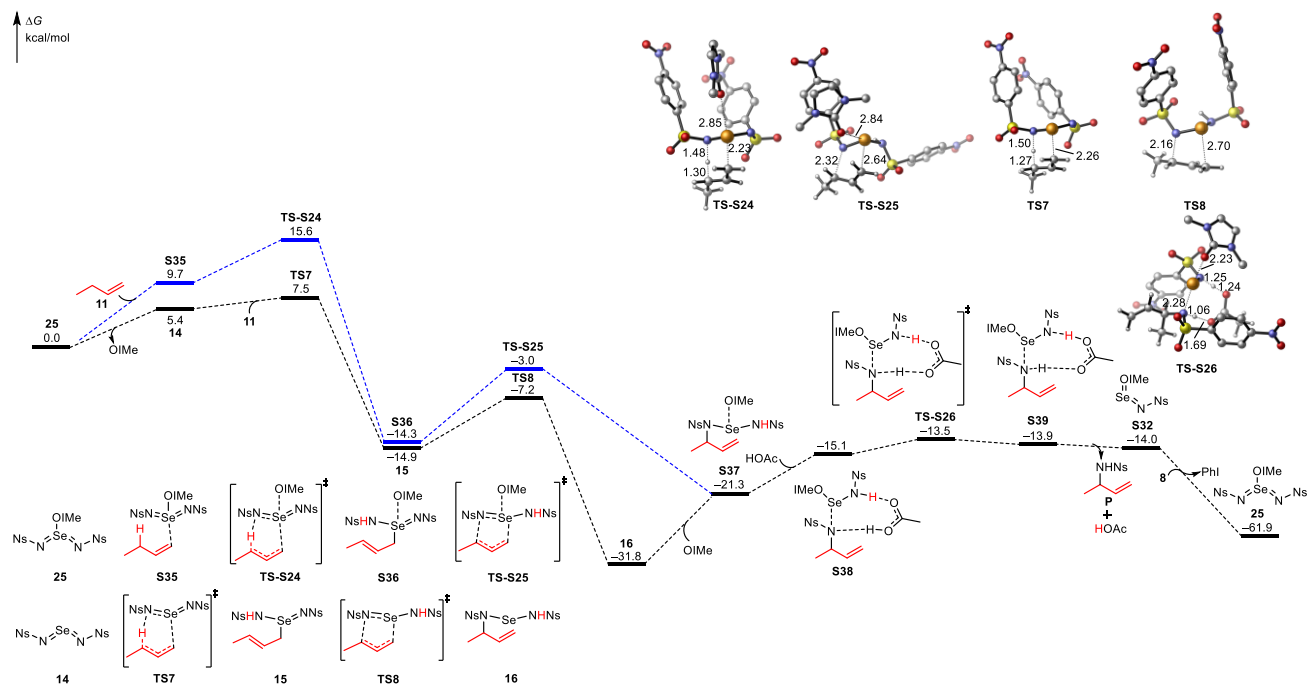


Fig. S11. Free energy profiles for ene reaction, sigmatropic shift and hydrogen transfer with the OIme ligand, leading to the formation of the final product, and selected bond lengths are given in Å.

XII. Calculated Gibbs free energy profiles of ene reaction with the substrate 42b and 44a

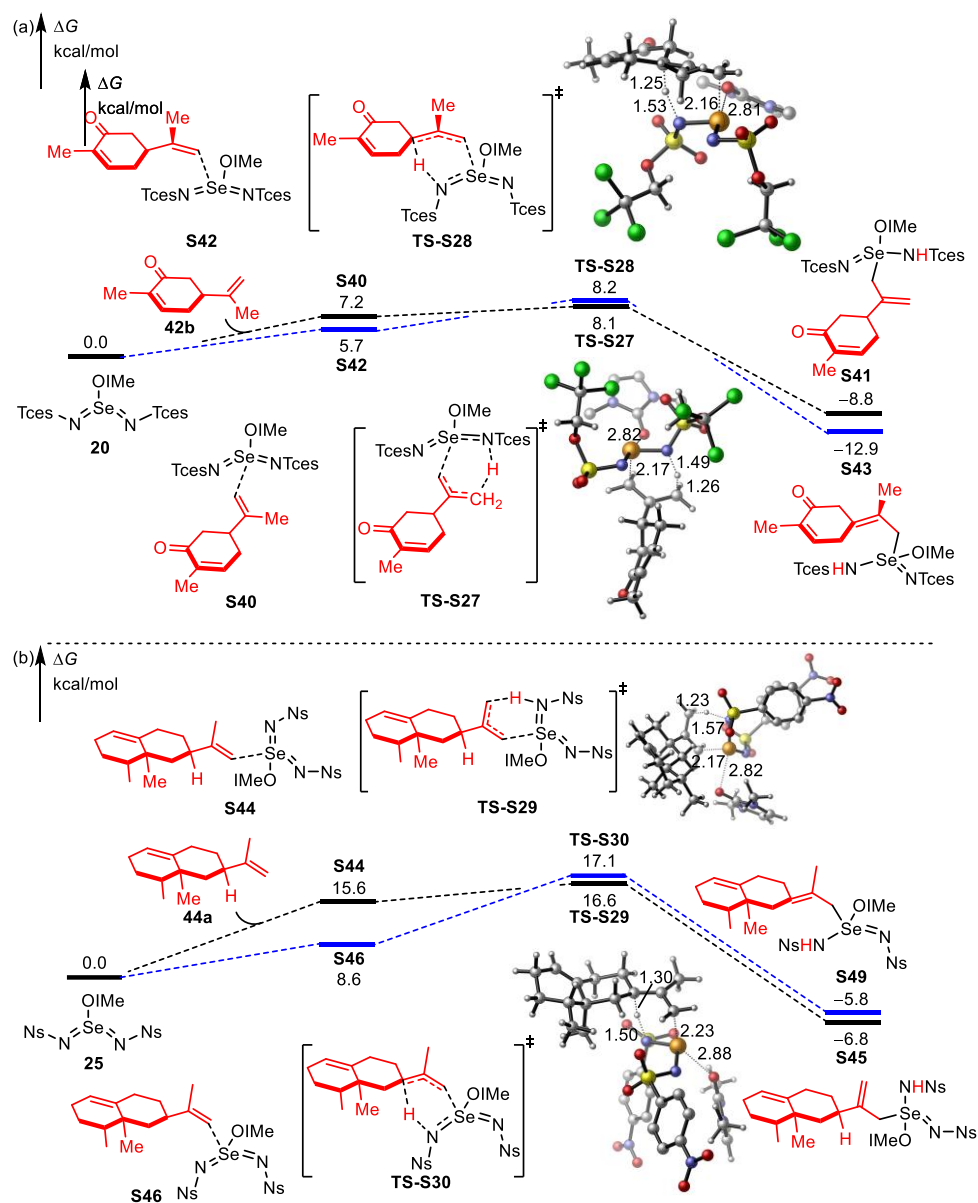


Fig. S12. Free energy profiles for ene reaction with the substrate **42b** and **44a**, with selected bond lengths in Å.

XIII. The dihedral angle of the six-membered ring in the reactant component for structures of 38, TS19 and TS20

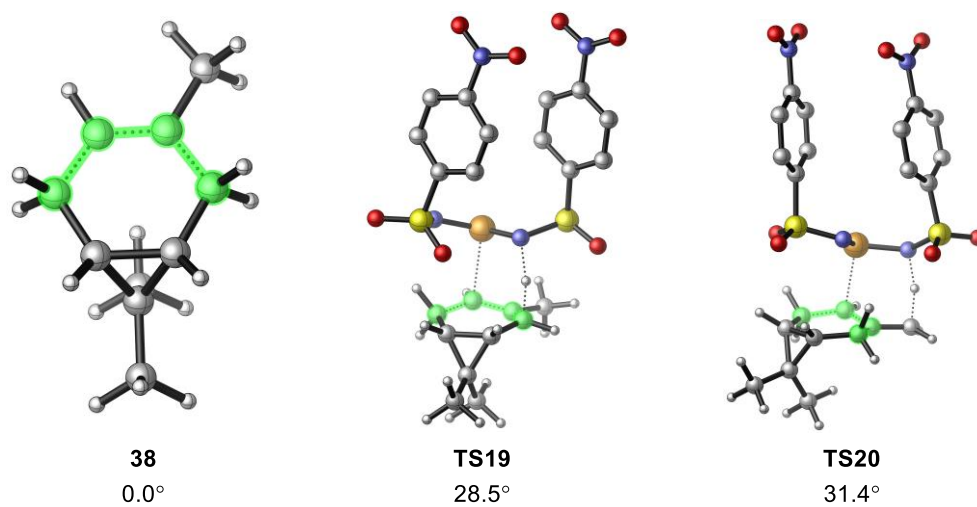


Fig. S13. The dihedral angle of the six-membered ring in the reactant component for structures of **38**, **TS19** and **TS20**.

XIV. Energies and Cartesian coordinates of all the structures

Tables S1. Energies and Cartesian coordinates of all the structures reported in the text of this manuscript.

1

0 imaginary frequency

H = -699.977998

G = -700.040213

Esol = -700.189259

C	2.46714800	-1.76700300	0.17843800
O	1.61121000	-1.48246100	-0.79441400
O	2.31340200	-1.49241900	1.36004400
C	3.69943000	-2.48371300	-0.35369500
H	4.18774200	-1.86964700	-1.11714600
H	4.39192100	-2.68194500	0.46600600
H	3.40570500	-3.42412100	-0.83099100
I	-0.35787000	-0.71832300	-0.20929200
O	-2.19937900	0.40655100	0.22274700
C	-3.20491900	-0.44620800	0.24818300
O	-3.07036500	-1.65148400	0.05706700
C	-4.54126200	0.20995300	0.54404800
H	-4.51553900	0.66634200	1.53901400
H	-4.73667400	1.00891200	-0.17799100
H	-5.33479100	-0.53748800	0.50028600
C	0.47785000	1.25861600	-0.07775900
C	-0.01101900	2.23526800	-0.94006100
C	1.46750300	1.50658400	0.86680000
C	0.52673100	3.52092400	-0.85007900
H	-0.79816400	2.01378900	-1.65108500
C	1.99487600	2.80013900	0.93417700
H	1.82755000	0.71501900	1.51409500

C	1.52809800	3.80179700	0.08206500
H	0.16031200	4.29905000	-1.51358400
H	2.77035600	3.01782100	1.66304900
H	1.94315100	4.80374900	0.14454400

10

0 imaginary frequency

H = -5527.769347

G = -5527.884893

Esol = -5528.520508

Se	-0.50278400	-0.31202800	-1.27995600
N	-1.07808200	-1.93803800	-1.67534100
S	-1.14730700	-3.13425700	-0.53323900
O	-1.86664000	-4.24668400	-1.16365900
O	-1.64927600	-2.62318800	0.76626100
C	0.54879300	-3.66469700	-0.25698600
C	0.98456900	-3.88041600	1.05021500
C	1.37442000	-3.91829800	-1.35548400
C	2.27467000	-4.35441600	1.26873400
H	0.32106300	-3.66629500	1.87968700
C	2.66537300	-4.38858200	-1.14165800
H	1.01818500	-3.73204900	-2.36254000
C	3.09077600	-4.60030900	0.16824000
H	2.65528900	-4.52863400	2.26711800
H	3.34154200	-4.58471200	-1.96389500
N	4.45771700	-5.09821900	0.39858800
O	5.15917300	-5.32043600	-0.58728700
O	4.81515000	-5.26912900	1.56390100
N	0.74094000	-0.17994300	0.04104000

S	2.24686200	-0.24517900	-0.63082800
O	3.10163700	-1.14099600	0.15604000
O	2.13665700	-0.43081700	-2.10095200
C	2.93661100	1.40867400	-0.37979200
C	3.10859700	2.25388000	-1.47798100
C	3.30930500	1.80760700	0.90830900
C	3.64295300	3.52734200	-1.28735700
H	2.84280500	1.90124500	-2.46854800
C	3.83442100	3.08045100	1.10684300
H	3.20317800	1.11937100	1.74000100
C	3.98776900	3.92180100	0.00391600
H	3.80092500	4.20805400	-2.11487200
H	4.13449100	3.42586400	2.08842900
N	4.53606000	5.27313200	0.21159900
O	4.82476000	5.60100200	1.36190700
O	4.66487100	5.99504400	-0.77652300
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C	-4.70491800	1.51387000	-1.09378600
C	-5.82255200	1.15721900	-2.09178100
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H	-3.26936900	0.14953100	-1.95009200
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H	-4.20244500	2.42655800	-1.43087300

H	-5.38199800	1.05046900	-3.09345400
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C	-0.60692000	4.54118500	0.93238300
C	-0.80877100	3.02004800	1.06063100
C	-1.81051400	2.51488300	-0.00132200
C	-1.33161700	2.90656300	-1.42151500
C	-1.14999800	4.42799200	-1.53743700
H	0.82972200	4.55450700	-0.68452500
H	-0.09350900	6.04690700	-0.54598700
H	-1.54733000	5.05128200	1.18872100
H	0.14684200	2.49775200	0.93644300
H	-2.77861600	3.00133400	0.18639400
H	-0.37374000	2.41075300	-1.61938600
H	-2.03102200	2.55155700	-2.18808600
H	-2.12682100	4.91926200	-1.41867400
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H	0.13469000	4.86723000	1.67123000
H	-1.16889300	2.79101600	2.06730000
C	-2.66270700	0.08364700	4.79344800
C	-1.59312200	-0.72737300	4.04803400
C	-1.21109500	-0.07891500	2.70675600
C	-2.48177900	0.09283000	1.84391100
C	-3.55625300	0.94245100	2.56525100
C	-3.90731100	0.30012900	3.92149000
H	-2.24584600	1.06076000	5.07951500
H	-2.94420900	-0.42006800	5.72609900
H	-1.96280300	-1.74485400	3.85979000

H	-0.74090200	0.89229900	2.89716000
H	-2.87543500	-0.91382900	1.66848100
H	-3.18114200	1.96078100	2.73313700
H	-4.46549200	1.03374400	1.95965500
H	-4.39876900	-0.66599800	3.73999000
H	-4.63853800	0.93252500	4.44016500
H	-0.69362700	-0.82997000	4.66703300
H	-0.48177100	-0.68989800	2.17372200

11

0 imaginary frequency

H = -157.172322

G = -157.206004

Esol = -157.287531

C	-1.86275900	0.01834500	-0.27808000
C	-0.72308400	-0.29748000	0.33795700
C	0.53982800	0.52037200	0.30779800
H	-0.67029300	-1.22705200	0.90880000
H	0.36612200	1.44439000	-0.25814900
H	0.79892400	0.82534400	1.33292500
H	-2.74137200	-0.61913500	-0.22334600
H	-1.96231000	0.93231000	-0.86093600
C	1.73031300	-0.24566900	-0.29394200
H	2.64114400	0.36338500	-0.27308300
H	1.93170700	-1.16723300	0.26555200
H	1.53029500	-0.52541600	-1.33416600

12

0 imaginary frequency

H = -5684.931935

G = -5685.062360

Esol = -5685.800271

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S	-1.89326700	-1.51142900	0.70819000
O	-1.46751800	-0.76560900	1.90975600
O	-1.37984300	-2.87358400	0.51126600
S	2.36356300	-1.09681900	-1.65111400
O	2.79057700	0.30592100	-1.88755600
O	2.33635100	-1.98011100	-2.82937600
C	-0.56360800	-0.89398100	-4.44294000
C	-1.38119100	-1.77774800	-3.85602300
C	-0.96019200	-3.08905200	-3.25347600
H	-2.44854900	-1.55109500	-3.80213500
H	0.12401100	-3.20445800	-3.35047300
H	-1.17338000	-3.07400200	-2.17545300
H	-0.94074700	0.03117200	-4.87372900
H	0.50533400	-1.07746700	-4.52166600
C	-1.68415300	-4.28589900	-3.89262000
H	-1.44922900	-4.36614100	-4.95998600
H	-1.38712600	-5.22248000	-3.40809100
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C	4.82657300	-1.40756700	-0.48207900
C	3.06648800	-2.85742100	0.39014700
C	5.74895600	-2.00601400	0.37228400
H	5.12700600	-0.60712500	-1.14959600

C	3.98670700	-3.45476600	1.24768700
H	2.02393500	-3.15656900	0.39742000
C	5.31116200	-3.01965400	1.22235300
H	6.78808100	-1.70200100	0.39130600
H	3.69412300	-4.24307400	1.93004200
N	6.28414400	-3.64814600	2.13452100
O	5.87720000	-4.54215500	2.87436400
O	7.44380700	-3.23799100	2.10094400
C	-3.69399700	-1.62370700	0.75643900
C	-4.39769400	-0.90264700	1.72088300
C	-4.34541000	-2.47539000	-0.13922500
C	-5.78558100	-1.01236000	1.77848900
H	-3.85773000	-0.27430700	2.41999900
C	-5.73159100	-2.58569900	-0.09010100
H	-3.77177100	-3.04637300	-0.86087300
C	-6.42707500	-1.84793100	0.86738700
H	-6.37013000	-0.47110200	2.51194800
H	-6.27582200	-3.23038800	-0.76886500
N	-7.89662900	-1.96052800	0.92128500
O	-8.44079100	-2.70842300	0.11082400
O	-8.48794400	-1.29718700	1.77198100
P	0.41536400	2.21187300	0.12944700
C	2.92778500	0.74533300	3.89107800
C	1.53832000	1.35390300	4.12284500
C	0.69711300	1.35173600	2.83511300
C	1.43331300	2.09670800	1.70128800
C	2.81819100	1.46070000	1.45166600
C	3.65595900	1.45537300	2.74197400
H	2.81862400	-0.32059800	3.64592600
H	3.52582800	0.79751600	4.80916000

H	1.64814800	2.38577000	4.48987100
H	0.49347800	0.32271500	2.52494300
H	1.58466900	3.14236300	2.01039400
H	2.68062900	0.43114600	1.10440900
H	3.36203000	1.98950700	0.66234300
H	3.87884800	2.49244400	3.03458700
H	4.62089900	0.97324600	2.54246400
H	1.00340800	0.79949500	4.90329900
H	-0.28106900	1.80352900	3.03197400
C	-3.38099800	4.56119900	1.85259800
C	-3.58335800	3.50671200	0.75632600
C	-2.38125300	2.55527300	0.64234600
C	-1.06742900	3.33949800	0.43101600
C	-0.86185500	4.38941900	1.54775600
C	-2.07330800	5.33515300	1.63816300
H	-3.35080000	4.06551700	2.83396400
H	-4.23120800	5.25371700	1.87804000
H	-3.73681100	4.01233600	-0.20871000
H	-2.29946500	1.94521100	1.55124000
H	-1.15846100	3.88196000	-0.52160800
H	-0.73811500	3.88160400	2.51209600
H	0.04963600	4.97225800	1.37743800
H	-2.14381700	5.92393200	0.71180400
H	-1.91246900	6.05285500	2.45231300
H	-4.49217700	2.92296200	0.94728500
H	-2.53352100	1.84945300	-0.17877900
C	2.27558000	5.10518900	-3.17512100
C	1.74950300	3.72224200	-3.58320200
C	0.79512700	3.14185200	-2.52651700
C	1.47968200	3.08980200	-1.14071700

C	1.97468100	4.49115900	-0.72421300
C	2.92950000	5.06657200	-1.78667400
H	1.44177300	5.82301300	-3.16246700
H	2.99203800	5.47318500	-3.91963200
H	2.59075200	3.02838800	-3.71446400
H	-0.11108300	3.76369300	-2.47912600
H	2.34348500	2.42423200	-1.24361900
H	1.11840100	5.17022400	-0.61218200
H	2.48253500	4.45513400	0.24706000
H	3.83640900	4.44681700	-1.82701900
H	3.24911100	6.07196400	-1.48506100
H	1.23419100	3.77974600	-4.54981500
H	0.47943000	2.13936400	-2.82889900

13

0 imaginary frequency

H = -5684.947857

G = -5685.074989

Esol = -5685.815847

Se	0.94481600	-1.02400900	1.13819600
N	0.26454800	0.23383300	2.20887700
N	0.65536000	-2.70057200	2.16243500
S	-1.21769100	0.01170800	2.85786400
O	-1.73737800	-1.36230000	2.60896200
S	0.74951300	-4.01959200	1.13784400
C	2.83922800	-0.83792900	1.91015300
C	2.82006000	-1.06344100	3.36648200
C	2.62969100	-0.07223300	4.25153700
H	2.89737900	-2.09227300	3.70693400

H	2.52101600	0.94606200	3.88079300
H	-0.26012300	-2.61461300	2.62757600
H	3.09237200	0.17829700	1.61315200
C	2.51522500	-0.25273900	5.73227500
H	1.51282200	0.05098100	6.06216300
H	2.67436600	-1.29391400	6.03008900
H	3.23455400	0.37896700	6.26991300
C	-2.35317700	1.11837500	1.99499100
C	-2.22743000	2.49852600	2.18594600
C	-3.36778000	0.58684200	1.19778300
C	-3.11237300	3.36203500	1.54940000
H	-1.45394800	2.88731100	2.83920300
C	-4.26603600	1.44648100	0.56680500
H	-3.45686100	-0.48821100	1.09173100
C	-4.11704200	2.81943200	0.74712800
H	-3.04783400	4.43600600	1.67226500
H	-5.07364200	1.07216300	-0.05026000
N	-5.05771000	3.73172000	0.07317000
O	-4.90000100	4.94015300	0.24350700
O	-5.93973300	3.23013900	-0.62208900
C	-0.63411700	-3.86661200	-0.01200700
C	-0.38487300	-3.40870900	-1.30750100
C	-1.92743100	-4.17287800	0.41991200
C	-1.45065500	-3.24036800	-2.18799900
H	0.63391600	-3.20936000	-1.61935500
C	-2.99636500	-4.00206300	-0.45543900
H	-2.09728900	-4.54806300	1.42350100
C	-2.73770100	-3.52861700	-1.74124700
H	-1.30058200	-2.89733000	-3.20384600
H	-4.01369800	-4.22636600	-0.15986000

N	-3.86846500	-3.32582000	-2.66748100
O	-4.99073700	-3.62988300	-2.26979000
O	-3.61627000	-2.85850000	-3.77729100
O	1.97416300	-3.78625200	0.35636000
O	0.53903000	-5.22720300	1.93175300
O	-1.17192400	0.51203600	4.23630500
H	3.39372100	-1.57594200	1.32905300
P	1.85724000	1.10282300	-1.13148700
C	5.39757400	-1.12153200	-3.47220600
C	5.71192600	-0.29557200	-2.21849500
C	4.43937000	-0.00975700	-1.40519500
C	3.35444000	0.70579600	-2.24538600
C	3.03930500	-0.14784700	-3.49219800
C	4.30726100	-0.44615000	-4.31352200
H	5.05598900	-2.12212600	-3.16931900
H	6.30408400	-1.26893600	-4.07227900
H	6.17603000	0.65713100	-2.51390100
H	4.02395800	-0.96133800	-1.04249500
H	3.76117100	1.66657600	-2.59539400
H	2.58331200	-1.09983100	-3.17974100
H	2.31148500	0.35443800	-4.13730200
H	4.69628800	0.49804600	-4.72232200
H	4.04506600	-1.07278600	-5.17547000
H	6.44398400	-0.81725400	-1.58925300
H	4.69256700	0.57560700	-0.51412900
C	2.59957600	5.14145400	1.25600900
C	1.25278600	4.95459100	0.54653800
C	1.01310800	3.48693900	0.15289100
C	2.16121800	2.92234500	-0.71228500
C	3.51314800	3.12233700	0.00833700

C	3.74626500	4.59219600	0.39822700
H	2.58008600	4.61107000	2.21950500
H	2.76814700	6.20108000	1.48500400
H	1.22917900	5.58139200	-0.35718800
H	0.91238700	2.87162700	1.05752900
H	2.19998700	3.48417400	-1.65730200
H	3.53532400	2.50392900	0.91831200
H	4.34171800	2.78343600	-0.62309600
H	3.83800400	5.19649400	-0.51628100
H	4.70238200	4.68347700	0.92908500
H	0.43120100	5.30227300	1.18587500
H	0.05943400	3.41021400	-0.37978400
C	-2.17727900	1.86541000	-3.62626700
C	-2.10176800	0.71138400	-2.61580300
C	-0.96095900	0.91941600	-1.60578400
C	0.39181500	1.11079100	-2.32739400
C	0.31467300	2.28202200	-3.32715900
C	-0.83183900	2.08044100	-4.33435900
H	-2.45956300	2.78862800	-3.09905200
H	-2.96733100	1.67335900	-4.36218300
H	-1.94964500	-0.23492300	-3.15533600
H	-1.18859600	1.79851700	-0.99008700
H	0.55299000	0.19174700	-2.90859700
H	0.14637700	3.22001800	-2.78099900
H	1.26555300	2.40100000	-3.86177900
H	-0.60906300	1.20676800	-4.96474300
H	-0.88963300	2.94415600	-5.00885900
H	-3.05554200	0.61374500	-2.08323800
H	-0.89739600	0.07284900	-0.91164100

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0 imaginary frequency

H = -4480.691187

G = -4480.768071

Esol = -4480.932677

Se	0.25879600	-1.81406300	-1.26182300
N	-0.28904900	-0.28756200	-0.63795900
N	1.36894500	-2.55602800	-0.20194800
S	-1.32060500	0.51783900	-1.73820700
O	-1.55425100	-0.35029100	-2.90482500
O	-0.78002700	1.86512200	-1.89865100
S	1.80714700	-1.99019200	1.37211300
O	2.60257300	-3.08106500	1.92297800
O	0.62825400	-1.47398900	2.06485200
C	2.91114700	-0.63210400	0.97381600
C	4.25983800	-0.91897800	0.73920000
C	2.40751300	0.67026500	0.91805100
C	5.12698200	0.12421300	0.42987600
H	4.61934500	-1.93930400	0.81316700
C	3.27646700	1.71434200	0.60769500
H	1.35894000	0.85640000	1.11482800
C	4.61626000	1.42001300	0.36753700
H	6.17964100	-0.04724200	0.24301000
H	2.93348200	2.73983300	0.55192300
N	5.53802800	2.52886200	0.03949800
O	6.71203700	2.24139700	-0.18232000
O	5.06991700	3.66427100	0.00966900
C	-2.83527000	0.61462200	-0.78293700
C	-3.88967500	-0.24482900	-1.09770100

C	-2.93015100	1.56431500	0.23819800
C	-5.07095000	-0.15944100	-0.36464200
H	-3.78863500	-0.95435000	-1.91138300
C	-4.10847100	1.64710500	0.97374100
H	-2.10135100	2.23218800	0.44455500
C	-5.15456700	0.78173800	0.65847000
H	-5.91792900	-0.80062800	-0.57436000
H	-4.22935600	2.36549100	1.77479000
N	-6.40795400	0.87097300	1.43815500
O	-6.45992500	1.71420600	2.32988300
O	-7.31388200	0.09561200	1.14227400

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0 imaginary frequency

H = -4637.918598

G = -4638.006412

Esol = -4638.278069

Se	-1.47558800	-0.76472400	-0.77010200
N	-1.19205700	-2.02300700	0.45626400
N	-2.63284300	0.41773100	0.20942200
S	-0.09135900	-1.53451300	1.59407900
O	-0.21680900	-0.06693800	1.81278300
S	-2.76340700	1.94188900	-0.51711100
C	-2.95077100	-1.77073900	-1.71987200
C	-4.04130300	-2.15144100	-0.79565100
C	-4.11995200	-3.35576000	-0.21350300
H	-4.78332900	-1.38731800	-0.57921000
H	-3.34745800	-4.09414800	-0.42821300
H	-2.25045500	0.45503700	1.16381100

H	-2.39170000	-2.61849800	-2.12270300
C	-5.19753900	-3.77930700	0.73487200
H	-4.76510800	-4.04412400	1.70867400
H	-5.93748800	-2.98826200	0.89093200
H	-5.71721900	-4.67398300	0.36736800
C	1.54355800	-1.78916000	0.87065800
C	2.12984100	-3.05402200	0.96486700
C	2.17660100	-0.74198700	0.19572900
C	3.36552400	-3.28138100	0.36590700
H	1.62673900	-3.84105600	1.51585700
C	3.41321700	-0.96410500	-0.40565800
H	1.71763200	0.24004200	0.16759100
C	3.98188500	-2.23282900	-0.31525500
H	3.85489500	-4.24591400	0.41977800
H	3.94153500	-0.17745800	-0.93011700
N	5.28756200	-2.47262400	-0.95833700
O	5.77604100	-3.59601900	-0.85175600
O	5.80326600	-1.53532600	-1.56493200
C	-1.18209300	2.76089800	-0.25534900
C	-0.17869300	2.62356700	-1.21849400
C	-0.97677400	3.47716200	0.92566000
C	1.06316600	3.21156700	-0.99019700
H	-0.37830300	2.09088500	-2.14128600
C	0.26355800	4.06681900	1.15531400
H	-1.78033600	3.58502700	1.64607300
C	1.26130800	3.91663600	0.19523400
H	1.86660500	3.14365400	-1.71328700
H	0.46539500	4.63303200	2.05590900
N	2.58026700	4.53850400	0.43645900
O	2.71622900	5.19664900	1.46434000

O	3.45457000	4.35371500	-0.40761400
O	-2.86949000	1.62399600	-1.94814600
O	-3.78399700	2.68863900	0.20928800
O	-0.21079000	-2.45948800	2.71982500
H	-3.23701500	-1.07588100	-2.51170100

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0 imaginary frequency

H = -4637.945978

G = -4638.033387

Esol = -4638.306731

Se	-0.32732300	-0.28035400	1.00664800
N	-1.22965900	-1.37001000	-0.19611800
N	1.29632100	-0.01493200	0.13650400
S	-1.89040400	-0.56303200	-1.53761700
O	-0.85005000	0.37461600	-1.97826300
S	2.47392500	-1.26084600	0.17603200
C	-4.05972700	-3.14902200	1.08140600
C	-2.85352900	-2.60014900	1.22133700
C	-1.73468300	-2.72080500	0.21535400
H	-2.60859700	-2.04340400	2.12853400
H	-2.11180100	-3.17352200	-0.70528400
H	1.12332300	0.31244800	-0.81892200
H	-4.32802300	-3.71937100	0.19423800
C	-0.56687000	-3.56009100	0.74378500
H	0.22750000	-3.62353400	-0.00507000
H	-0.14348600	-3.13004500	1.65561600
H	-0.92613800	-4.56863100	0.97128300
C	-3.26045700	0.43987800	-0.93553800

C	-4.56206600	-0.04970300	-1.06199400
C	-2.99402800	1.68127600	-0.34763300
C	-5.62499900	0.71352400	-0.58531300
H	-4.73560000	-1.00654800	-1.54020000
C	-4.05501000	2.44069600	0.13797700
H	-1.97544800	2.04111700	-0.27260700
C	-5.34999000	1.94184400	0.01110600
H	-6.65018900	0.37539900	-0.66963400
H	-3.89637300	3.40758300	0.59895300
N	-6.47489000	2.75017300	0.52312000
O	-7.60766000	2.28969100	0.39763300
O	-6.20612900	3.83041300	1.04460900
C	3.98082600	-0.28046200	0.08678000
C	4.44585900	0.35382300	1.24194300
C	4.66357100	-0.19680400	-1.12738500
C	5.61610500	1.10310900	1.17769100
H	3.90454500	0.25063400	2.17588800
C	5.83599300	0.55408600	-1.19463200
H	4.28665200	-0.72150000	-1.99831300
C	6.28666200	1.19150500	-0.04188000
H	6.01565600	1.61062300	2.04673100
H	6.39938600	0.64686500	-2.11468700
N	7.52831400	1.98904400	-0.11137600
O	8.10308300	2.05045900	-1.19592500
O	7.90569600	2.54111300	0.91999400
O	2.38136400	-1.85943100	1.50657600
O	2.40956900	-2.08056900	-1.03734800
O	-2.43765500	-1.58871200	-2.42496900
H	-4.82106600	-3.06081900	1.85143400

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0 imaginary frequency

H = -5684.989705

G = -5685.116704

Esol = -5685.859561

Se	-0.54755800	0.05221200	0.74361900
N	1.36831200	-1.10683500	1.58725700
N	0.68310000	1.08633300	-0.24441600
S	2.31922100	-1.88181600	0.55725700
O	2.31951300	-1.06733400	-0.69713400
S	1.24072600	2.51011300	0.52826700
C	0.61035800	-3.88995600	3.72235800
C	0.33200600	-2.70960300	3.16936900
C	1.31558000	-1.57405400	2.99195600
H	-0.67963200	-2.50489600	2.81190700
H	2.31318300	-1.92362400	3.28901200
H	1.45590500	0.42679800	-0.48513500
H	1.60966900	-4.12772800	4.08177000
C	0.93461400	-0.38230200	3.88355100
H	1.64954700	0.43445300	3.75569000
H	-0.05274600	0.00562000	3.61440500
H	0.91434200	-0.69028500	4.93418000
C	1.56783400	-3.44924800	0.02037500
C	2.35028400	-4.60266300	-0.03887900
C	0.22401900	-3.46832600	-0.36830500
C	1.78956500	-5.79326800	-0.49870600
H	3.38659000	-4.55755700	0.27675700
C	-0.34272500	-4.65046300	-0.82824100
H	-0.36975900	-2.56416000	-0.28343500

C	0.45220200	-5.79617000	-0.88810400
H	2.36669000	-6.70776900	-0.55856400
H	-1.37930300	-4.70517300	-1.13669900
N	-0.14751000	-7.04850900	-1.37336200
O	0.56780500	-8.04876200	-1.41675300
O	-1.33302300	-7.02314400	-1.70831900
C	2.98127400	2.50473600	0.07621700
C	3.44251800	3.46454400	-0.82573700
C	3.83139600	1.56451700	0.66452400
C	4.79602800	3.48601200	-1.15325300
H	2.74961700	4.17950300	-1.25476000
C	5.18302200	1.58095000	0.33186100
H	3.44677700	0.82651900	1.36008900
C	5.63810700	2.54288400	-0.56814900
H	5.20285900	4.21204200	-1.84577000
H	5.87395900	0.86155500	0.75270600
N	7.07344400	2.56657900	-0.91788900
O	7.80585100	1.74660000	-0.36984300
O	7.44477700	3.40829300	-1.73449200
O	0.57997800	3.63733600	-0.15323300
O	1.12066900	2.41654400	1.98838000
O	3.62866700	-2.25107800	1.13026900
H	-0.14299300	-4.66537000	3.83541100
P	-2.36053700	1.19763500	-0.31065400
C	-6.14727400	-1.61576500	0.43781900
C	-4.83648700	-1.85286300	1.20086400
C	-3.93864900	-0.60537300	1.17939700
C	-3.66631200	-0.14091600	-0.27203300
C	-4.98571300	0.11178900	-1.03275400
C	-5.87796500	-1.14301700	-0.99769700

H	-6.74238100	-0.85601900	0.96549600
H	-6.74950400	-2.53199100	0.42727000
H	-4.29517800	-2.69524600	0.74692300
H	-4.42912500	0.20234900	1.73831400
H	-3.14605300	-0.96511900	-0.78233000
H	-5.52549500	0.95193500	-0.58110500
H	-4.78257100	0.38702000	-2.07294400
H	-5.38729100	-1.94994800	-1.56097100
H	-6.82179900	-0.93187900	-1.51496000
H	-5.04241900	-2.13720200	2.23968500
H	-2.99289500	-0.81417300	1.69512500
C	-1.79623800	1.58419400	-5.01472300
C	-0.87278300	0.67252900	-4.19423300
C	-1.48976600	0.32627200	-2.83022400
C	-1.85568100	1.61093300	-2.05472200
C	-2.79544800	2.52771600	-2.86624200
C	-2.16496700	2.85366600	-4.23367900
H	-2.71482100	1.03577000	-5.27181900
H	-1.31816300	1.85289100	-5.96450800
H	0.09161000	1.17343400	-4.03254000
H	-2.39027900	-0.28463500	-2.98930200
H	-0.92257700	2.16215300	-1.87698700
H	-3.76708400	2.04222100	-3.02442800
H	-2.98661800	3.46025800	-2.32392300
H	-0.65732400	-0.25157300	-4.74377100
H	-0.79170800	-0.26710400	-2.23130400
C	-4.09784000	4.62953800	2.52968700
C	-4.44578400	4.66407400	1.03509100
C	-4.26326000	3.28297200	0.37940800
C	-2.82063800	2.77242100	0.59175300

C	-2.49105200	2.69756900	2.10268800
C	-2.68669500	4.07190300	2.76195400
H	-4.83011500	3.99857900	3.05528000
H	-4.18607900	5.63418200	2.96090800
H	-3.80014200	5.39243000	0.52387400
H	-4.96832000	2.57798500	0.83969400
H	-2.12029800	3.49311800	0.14315900
H	-3.15437400	1.96475500	2.58393900
H	-1.46756800	2.34897800	2.25611600
H	-1.94142300	4.76833400	2.35314000
H	-2.47952100	3.99072900	3.83577100
H	-5.47884800	5.00329800	0.88811700
H	-4.51712400	3.33731000	-0.68446800
H	-1.26122000	3.45843200	-4.07352800
H	-2.85859900	3.47434100	-4.81438600

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0 imaginary frequency

H = -5914.134310

G = -5914.273010

Esol = -5915.072093

Se	-0.29069500	0.83344000	-0.90837600
N	-2.39068500	-0.80626600	-2.31140800
N	0.72396100	-0.69100800	-0.59294500
S	-3.73058700	0.11077300	-1.85725800
O	-4.86228000	-0.07454700	-2.77758000
O	-3.27789400	1.49529900	-1.60776400
S	1.78204100	-1.20125900	-1.79402700
O	2.31191700	-0.01715000	-2.49312700

O	1.21493300	-2.30088800	-2.58155400
C	-2.50752600	-3.22302700	-4.89067000
C	-1.82199000	-2.41516600	-4.08252000
C	-2.22912600	-0.99205300	-3.79550100
H	-0.90054800	-2.75108300	-3.61159800
H	-3.20088100	-0.81164200	-4.26756300
H	0.11194300	-1.53461000	-0.13328100
H	-2.17051800	-4.23457600	-5.10101500
H	-3.43160800	-2.90806400	-5.37194600
C	-1.21147200	0.02274600	-4.34026700
H	-1.46055800	1.03633300	-4.00805700
H	-0.19609600	-0.21593800	-4.01049100
H	-1.22317100	0.00282500	-5.43558900
C	3.12081600	-1.90359600	-0.80467200
C	2.83498900	-2.79212500	0.23864900
C	4.43238000	-1.58909400	-1.16607600
C	3.89306600	-3.35912200	0.94466500
H	1.80532800	-3.02236600	0.50654300
C	5.49029400	-2.16238700	-0.46355600
H	4.61652800	-0.90487500	-1.98688900
C	5.20032000	-3.03430900	0.58270500
H	3.71982400	-4.04610100	1.76382100
H	6.52188400	-1.94587500	-0.71172900
C	-4.18491700	-0.60194600	-0.26515300
C	-5.46038100	-1.14713000	-0.12567500
C	-3.29038700	-0.53005700	0.80445600
C	-5.85675900	-1.63187200	1.11935400
H	-6.12493300	-1.18618300	-0.98132500
C	-3.67971100	-1.01797800	2.04586100
H	-2.30038700	-0.12056500	0.64582800

C	-4.95932900	-1.55511700	2.18158300
H	-6.83796900	-2.06226900	1.27545700
H	-3.01414400	-0.99624000	2.89924900
N	6.31779100	-3.62992200	1.33858000
N	-5.37718100	-2.05939600	3.50259000
O	6.03856200	-4.39068800	2.26355500
O	-4.57501600	-1.95886200	4.43089900
O	7.46080500	-3.32507200	1.00048600
O	-6.50234300	-2.54574400	3.59917100
O	-0.35089900	-2.62213700	0.62665800
C	-1.30720900	-3.36973100	0.18311000
O	-2.10233100	-3.08033900	-0.72957500
C	-1.43291200	-4.72515900	0.87112500
H	-2.35676700	-5.22520100	0.57441200
H	-0.58060000	-5.35555000	0.59036600
H	-1.40131200	-4.60390300	1.95883300
H	-2.31032000	-1.68468200	-1.74762000
P	0.83513300	2.22144100	0.52434500
C	1.60822500	0.34950500	4.82348200
C	2.69600500	1.22192200	4.18244300
C	2.12019900	2.10734900	3.06275300
C	1.41689500	1.23813500	1.99403600
C	0.30060800	0.37905200	2.63020300
C	0.87095500	-0.48540400	3.76848700
H	0.88866700	0.99592500	5.34732000
H	2.04984300	-0.30510900	5.58413700
H	3.48539000	0.58080200	3.76500300
H	1.39269200	2.80224000	3.50260500
H	2.15081200	0.54932200	1.55561700
H	-0.48796400	1.03331400	3.02953800

H	-0.15399800	-0.27475300	1.88302900
H	1.55640300	-1.22665000	3.33539600
H	0.05487300	-1.05382200	4.22927500
H	3.17490300	1.85848000	4.93638200
H	2.91720600	2.71671100	2.62084700
C	-2.00908400	6.01434400	1.08675200
C	-0.91475100	5.73615000	2.12649500
C	0.18022900	4.81035500	1.56617200
C	-0.43759100	3.48803000	1.05457100
C	-1.51051800	3.77629500	-0.02424600
C	-2.59747700	4.70888500	0.53576100
H	-1.58115000	6.59898800	0.25932900
H	-2.80003700	6.63201800	1.52870100
H	-1.36165500	5.26845700	3.01563700
H	0.68312700	5.32015900	0.73368400
H	-0.93891400	2.98980900	1.89715100
H	-1.03843900	4.25623200	-0.89161700
H	-1.98144400	2.85783600	-0.38406700
H	-3.14260700	4.18463100	1.33383100
H	-3.32878300	4.91530300	-0.25357200
H	-0.45591300	6.67345200	2.46406200
H	0.94036200	4.62782700	2.33337300
C	4.31916600	3.40191800	-2.43468900
C	4.70858300	2.97258600	-1.01412100
C	3.56071300	2.22062100	-0.31762600
C	2.27884000	3.08199900	-0.29211700
C	1.88465400	3.53899300	-1.71817100
C	3.04896200	4.26138600	-2.41513600
H	4.14114000	2.50776000	-3.04717600
H	5.14275700	3.95363000	-2.90385700

H	4.98101200	3.85926900	-0.42223700
H	3.36006000	1.29580200	-0.86641900
H	2.46749200	3.96954100	0.32867100
H	1.58575100	2.65725600	-2.29589400
H	1.01342200	4.20388800	-1.67838700
H	3.25522100	5.20923500	-1.89607100
H	2.74599300	4.52327400	-3.43585700
H	5.59609100	2.32841000	-1.03624900
H	3.86595200	1.94771500	0.69867900

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0 imaginary frequency

H = -5914.133665

G = -5914.272776

Esol = -5915.073906

Se	0.60769700	0.36779400	0.59018000
N	2.15406600	-3.56802500	0.77549600
N	-1.20223600	0.58472500	0.24848900
S	1.09509000	-4.69412200	0.11490800
O	0.03432700	-5.04329500	1.07294700
O	1.89707300	-5.75388600	-0.50776500
S	-1.96563800	1.42186500	1.42141100
O	-1.95238500	2.89471600	1.23426500
O	-1.61854500	0.99344300	2.81436700
C	4.95909500	-2.59508300	2.73477100
C	3.80396700	-3.22068000	2.50755900
C	3.46203900	-4.06832600	1.30228700
H	3.01006300	-3.14966100	3.25131500
H	3.33800800	-5.10192800	1.65850100

H	-1.30997200	-0.56310400	3.38040800
H	5.11901400	-2.03262000	3.65048600
H	5.79128800	-2.63042900	2.03780100
C	4.51782900	-4.06935700	0.19769500
H	4.18619100	-4.70324600	-0.62676200
H	4.68067300	-3.05478800	-0.18116000
H	5.46778300	-4.46517600	0.57317600
C	-3.65828000	0.87997100	1.10362100
C	-4.11107400	-0.32608000	1.64481600
C	-4.49337800	1.69186900	0.33484000
C	-5.41879200	-0.73487800	1.40092900
H	-3.45637100	-0.93213500	2.26122200
C	-5.80246200	1.28706900	0.08526700
H	-4.11857700	2.63371500	-0.04916100
C	-6.24051200	0.07851500	0.62170000
H	-5.80876800	-1.66129000	1.80362700
H	-6.48112400	1.88763900	-0.50736000
C	0.31040200	-3.73646700	-1.19359500
C	-0.51908000	-2.66260400	-0.86167900
C	0.52668900	-4.11691000	-2.51908700
C	-1.15009800	-1.95051800	-1.87706900
H	-0.67944800	-2.37874700	0.17174400
C	-0.09699200	-3.40418100	-3.54003300
H	1.17145000	-4.96086200	-2.73715400
C	-0.92651100	-2.33718300	-3.19798600
H	-1.78393900	-1.10439800	-1.64148500
H	0.04448700	-3.66286700	-4.58210200
N	-7.62664400	-0.35188700	0.36374800
N	-1.58383800	-1.58222200	-4.27613900
O	-8.33550900	0.38618100	-0.31914600

O	-1.20548000	-1.78335400	-5.43064100
O	-7.99076500	-1.42287200	0.84721700
O	-2.46942800	-0.78759200	-3.95944300
O	-1.35803500	-1.44913800	3.84790900
C	-0.42564600	-2.28080700	3.40748700
O	0.37654900	-1.98378400	2.52333000
C	-0.43385100	-3.61796900	4.10393600
H	0.45622900	-3.69160500	4.73989200
H	-1.32231800	-3.73796300	4.72554700
H	-0.37553800	-4.40945100	3.35183400
H	1.63068300	-2.99086900	1.44711000
P	1.54503000	2.26475100	-0.26115000
C	-0.73103000	2.21685300	-4.40519000
C	0.65328000	1.55971500	-4.31031500
C	1.07354600	1.29576300	-2.85415800
C	0.99045700	2.58783200	-2.00935600
C	-0.42573800	3.20487600	-2.08114600
C	-0.80761500	3.48466100	-3.54453600
H	-1.49553900	1.50260000	-4.07505200
H	-0.95909600	2.45448400	-5.45126800
H	1.40205400	2.21169600	-4.78486500
H	0.43194500	0.53911700	-2.38847500
H	1.70817000	3.31979400	-2.40810200
H	-1.14274400	2.51065000	-1.63018900
H	-0.47540400	4.13308100	-1.50185900
H	-0.13375200	4.25210100	-3.95547400
H	-1.81882300	3.90793600	-3.57832600
H	0.66382800	0.61587000	-4.86877900
H	2.09219600	0.88804500	-2.83416600
C	6.11302400	1.14976800	-1.08957000

C	5.35138000	0.38352600	-0.00022400
C	3.82693000	0.50918700	-0.16066500
C	3.40320400	1.99674000	-0.19982600
C	4.16028700	2.76025500	-1.31194300
C	5.68202100	2.62174500	-1.13281200
H	5.91750600	0.68540900	-2.06708900
H	7.19403900	1.07686700	-0.91973500
H	5.64110800	0.76945900	0.98799600
H	3.50932200	0.00725200	-1.08341200
H	3.68373200	2.44338300	0.76426700
H	3.87985100	2.35347600	-2.29210300
H	3.88289500	3.82049300	-1.31634700
H	5.98383300	3.12033300	-0.20030600
H	6.19191100	3.14914800	-1.94825800
H	5.62739700	-0.67727300	-0.01121700
H	3.33270800	-0.01489200	0.66496300
C	1.50628400	5.91804200	2.75980600
C	0.92666400	4.56263500	3.19155400
C	1.44914900	3.41816200	2.30910600
C	1.13080900	3.71252400	0.82532400
C	1.75874900	5.04962500	0.37743400
C	1.24747200	6.19554300	1.27144300
H	2.59110800	5.92554700	2.94500900
H	1.08118700	6.72484000	3.36926000
H	-0.16878600	4.58281600	3.12463100
H	2.53702200	3.32438900	2.44858100
H	0.03825200	3.77979300	0.74307300
H	2.85370700	4.99367800	0.45776100
H	1.52533400	5.26666800	-0.67230400
H	0.16852000	6.32046600	1.10550700

H	1.72448200	7.13577800	0.96764900
H	1.17617100	4.35829900	4.23976700
H	1.00249900	2.46385000	2.60362400

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0 imaginary frequency

H = -699.949848

G = -700.011963

Esol = -700.160805

C	0.24764900	2.31747000	0.00557700
O	0.22998800	1.28754700	-0.86471200
O	0.20284600	2.21516800	1.21067600
C	0.33523600	3.62494400	-0.76024100
H	-0.35468000	3.62945400	-1.60771300
H	0.11467100	4.44915300	-0.08036100
H	1.35162600	3.73256600	-1.15324800
I	0.35423300	-0.59622700	0.00742000
O	2.84445700	-1.90417900	0.47370300
C	3.29341100	-0.81443000	0.09305100
O	2.53899000	0.17679900	-0.28894200
C	4.78543700	-0.52753200	0.04014700
H	5.34450700	-1.42249100	0.32091400
H	5.07202900	-0.20707900	-0.96680000
H	5.02967300	0.29078100	0.72615600
C	-1.81382900	-0.49804200	0.00505500
C	-2.53153600	-1.12649900	-1.01585300
C	-2.47843700	0.12727700	1.06421300
C	-3.92775300	-1.13515300	-0.97238600
H	-2.01303900	-1.60696700	-1.84091500

C	-3.87404200	0.11860000	1.09862400
H	-1.91368900	0.62800800	1.84456800
C	-4.59728100	-0.51283500	0.08323600
H	-4.48963900	-1.62370500	-1.76383200
H	-4.39580200	0.60443300	1.91871900
H	-5.68336200	-0.51957800	0.11493300

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0 imaginary frequency

H = -7055.022948

G = -7055.117625

Esol = -7055.306651

Se	-0.41924400	1.14661700	0.16192500
N	0.68425000	2.07865600	1.13486700
N	-0.85470700	-0.05105500	1.36191700
S	1.41821100	3.26980300	0.24488100
O	1.86999700	4.29233300	1.17205800
O	0.68152600	3.60884900	-0.97458000
S	-2.04653100	-1.05119000	0.79071100
O	-2.30946300	-0.79307000	-0.63886000
O	-3.15637200	-1.11105000	1.72592200
C	-3.17853500	2.38416300	-0.14390900
C	-5.34431000	2.00580300	-0.55978500
C	-4.73716500	2.26499500	-1.74580100
H	-6.37385000	1.78103700	-0.33074800
H	-5.13536900	2.30111500	-2.74733200
N	-4.37466100	2.07672700	0.42988000
N	-3.39717400	2.51328700	-1.48255500
C	-4.56070000	1.84560000	1.86053100

H	-3.61795900	2.07294400	2.35809400
H	-5.34791400	2.50226900	2.23996300
H	-4.80903600	0.79768000	2.03873900
C	-2.33857300	2.76243800	-2.45698100
H	-1.52992200	3.31260800	-1.97297300
H	-1.95385500	1.81619000	-2.84957100
H	-2.74394000	3.35873000	-3.27689100
O	-2.07311400	2.54702700	0.47326500
O	-1.34917700	-2.53141000	0.93877100
C	-0.24338100	-2.82091000	0.08418900
H	-0.30617800	-2.24979800	-0.84605800
H	0.69135700	-2.60409400	0.60856900
C	-0.27246500	-4.31247900	-0.27559200
Cl	1.17382400	-4.61392900	-1.31497200
Cl	-0.16989400	-5.32010200	1.20370000
Cl	-1.76347200	-4.71449300	-1.18528100
O	2.76264700	2.50585000	-0.37111600
C	3.66072000	1.92360000	0.56972500
H	3.17277200	1.72713300	1.52805800
H	4.52281700	2.57970200	0.71837400
C	4.15571200	0.58660300	0.00146700
Cl	5.00112100	0.83097900	-1.55969400
Cl	2.76616400	-0.54265500	-0.24578000
Cl	5.29098500	-0.12148900	1.20445900

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0 imaginary frequency

H = -7139.582814

G = -7139.683224

Esol = -7139.954122

Se	1.00172800	-0.07997600	-0.48363200
N	0.16438900	0.07054500	1.05412000
N	1.95025800	-1.50643600	-0.08531100
S	-0.48488000	1.56830700	1.27365300
O	0.29210900	2.62696600	0.61860200
O	-0.88597900	1.70011800	2.66366600
S	3.06468900	-1.84038800	-1.27919800
O	2.54541300	-1.54865200	-2.61568400
O	3.65740800	-3.12601500	-0.94948000
C	-2.64588100	-3.01299300	2.11577000
C	-1.54242600	-2.93092900	1.09635600
C	-1.98296400	-2.12272400	-0.14005200
C	-3.34620800	-2.66088400	-0.64659000
C	-4.40330800	-2.60487400	0.45853200
C	-3.95767600	-2.84920900	1.85321100
H	-2.33653700	-3.21848600	3.13995300
H	-0.65776800	-2.46552500	1.54343600
H	-2.14882100	-1.08866600	0.18101800
H	-3.72290300	-2.09299500	-1.50125600
H	-1.24501100	-3.95192200	0.81264300
H	-3.24284300	-3.70916200	-0.96468300
C	-5.03298000	-2.89913000	2.90509300
H	-4.60990000	-3.10011100	3.89354800
H	-5.58080100	-1.95104700	2.94437100
H	-5.77283100	-3.67329800	2.67211500
O	-5.57517400	-2.39571500	0.18098800
C	-0.98958300	-2.10468800	-1.26825600
C	-0.18793100	-3.31888400	-1.56744200
H	-1.39478300	-0.06577500	-1.80484500

H	-0.78115400	-4.23584700	-1.48759900
H	0.29838500	-3.27102100	-2.54328300
C	-0.75761000	-0.93328900	-1.96242300
H	-0.14074700	-0.94193800	-2.85763300
H	0.60917700	-3.39031900	-0.80306800
O	4.20638500	-0.65951700	-1.06872100
C	4.91044600	-0.65798500	0.17771700
H	4.35742800	-1.19360800	0.95325200
H	5.89375500	-1.11435300	0.04057800
C	5.09856000	0.79511700	0.63430900
Cl	3.50553600	1.58606300	0.91645100
Cl	6.02109400	0.73981800	2.18063400
Cl	6.02086500	1.72602100	-0.58861300
O	-1.88556700	1.39516500	0.35765200
C	-2.77365900	2.51503200	0.44929400
H	-2.23064700	3.44900200	0.27594100
H	-3.25581700	2.53522900	1.43068700
C	-3.85573200	2.38072200	-0.62666700
Cl	-4.80274800	0.87462500	-0.40253500
Cl	-3.11357500	2.38739600	-2.26997300
Cl	-4.93772700	3.80919800	-0.45619500

22

0 imaginary frequency

H = -7139.609048

G = -7139.708909

Esol = -7139.981321

Se	-0.42029900	-1.25182900	-0.76949300
N	-0.56629300	0.28313700	0.29998400

N	-0.07150800	-2.27739500	0.67760100
S	-0.65925800	1.76353900	-0.51514600
O	-1.41200900	2.64486700	0.36444900
O	-0.99487900	1.53670100	-1.90977700
S	0.41874400	-3.73473500	0.14684500
O	-0.20454700	-4.07242700	-1.14450000
O	0.40714700	-4.66093200	1.27005100
C	-6.21321600	-0.05366100	1.58785700
C	-4.78055300	-0.46282500	1.83846200
C	-3.95394000	-0.48814700	0.56910700
C	-4.19582800	0.74882500	-0.26254900
C	-5.68848500	0.93084700	-0.58495900
C	-6.65933800	0.55970800	0.47697700
H	-4.33285300	0.25562600	2.54834500
H	-6.91949800	-0.29432400	2.38182800
H	-4.76560600	-1.42394900	2.35845400
C	-8.10112800	0.91038600	0.22913800
H	-8.46474900	0.42383200	-0.68275700
H	-8.73430600	0.60530500	1.06743100
H	-8.21932900	1.98833100	0.07060500
O	-6.04176900	1.41097800	-1.64834300
C	-3.19171900	-1.55520800	0.21433000
C	-3.12663400	-2.83161900	1.03965000
C	-2.40360800	-1.57549100	-1.05452000
H	-4.11852400	-3.13403400	1.39003400
H	-2.46865500	-2.73522800	1.90893300
H	-3.65455200	0.78951100	-1.20790100
H	-3.89713900	1.64333300	0.30665800
H	-2.72957900	-3.65564000	0.44237300
O	2.02118700	-3.53798400	-0.31619100

C	2.91219600	-3.12460100	0.70977800
H	3.53475000	-3.96715300	1.02455900
H	2.37863800	-2.71948400	1.57431300
C	3.83224600	-2.02335900	0.16306600
Cl	2.86280100	-0.58302600	-0.33830200
Cl	4.77519200	-2.61470500	-1.23860200
Cl	4.95221700	-1.54807100	1.49404300
O	0.90339800	2.20520000	-0.55443700
C	1.50500600	2.73219900	0.64486800
H	0.74082600	2.99802400	1.37714300
H	2.18303900	1.97708200	1.04666800
C	2.30315400	3.99460100	0.29002700
Cl	3.06337200	4.54821700	1.83053200
Cl	1.21740200	5.26922900	-0.34566000
Cl	3.57624600	3.61810800	-0.91256000
H	-1.35444700	0.17900700	0.94931200
H	-2.37362300	-2.55935500	-1.52860200
H	-2.66145700	-0.81670000	-1.79297900

23

0 imaginary frequency

H = -7139.581148

G = -7139.682616

Esol = -7139.952529

Se	-0.34173200	-1.51671800	-1.39880200
N	-0.31123500	-0.15890500	-0.30973100
N	-0.10183100	-2.98492900	-0.52479900
S	-0.47122400	1.28889000	-1.14117000
O	-1.45793900	2.09459500	-0.43546100

O	-0.56735600	1.06123800	-2.58231100
S	0.14825200	-3.06613600	1.12205300
O	0.44382300	-4.46168800	1.40542000
O	-0.84686800	-2.32759600	1.88160000
C	-4.28398000	0.69104300	1.91210900
C	-3.62234200	-0.48340700	1.24520600
C	-3.97572200	-0.55050100	-0.25309400
C	-5.51121300	-0.44521000	-0.41981800
C	-6.08219300	0.80501700	0.25287200
C	-5.39401200	1.31178300	1.46639700
H	-2.53802500	-0.42561800	1.37737500
H	-3.81389700	1.04963600	2.82738800
H	-3.93391000	-1.40664000	1.75747900
C	-6.01493700	2.50354700	2.14412900
H	-6.04538000	3.36371000	1.46581500
H	-7.05365700	2.29627300	2.42533700
H	-5.45457900	2.78509300	3.04060400
O	-7.09713900	1.32974900	-0.18071800
C	-3.46306800	-1.77636300	-0.97644300
C	-3.58339000	-3.12098500	-0.32282900
C	-2.91959200	-1.65884000	-2.21998200
H	-3.33769700	-3.93238900	-1.01218400
H	-4.59647800	-3.28526600	0.06404300
H	-6.00037600	-1.31714700	0.04005300
H	-5.81008500	-0.42618400	-1.47194000
H	-2.90659700	-3.18513200	0.53922300
O	1.54120900	-2.19155400	1.32321900
C	2.77431400	-2.86542100	1.05354000
H	2.63060300	-3.73003700	0.40213900
H	3.22052000	-3.19258700	1.99635200

C	3.74139800	-1.88935900	0.37162300
Cl	4.04335200	-0.46169800	1.41508000
Cl	3.08533200	-1.34531400	-1.21783000
Cl	5.28259000	-2.77895200	0.10575900
O	1.01080300	1.94736600	-0.93173600
C	1.33518100	2.48292600	0.36107500
H	0.42777800	2.72536800	0.91789300
H	1.93856200	1.75245900	0.90463900
C	2.14999900	3.76936400	0.17247100
Cl	3.65628200	3.43596600	-0.74360800
Cl	2.56742700	4.34714600	1.83207900
Cl	1.18302900	5.01369000	-0.67778200
H	-3.54019300	0.33638600	-0.72981600
H	-2.67449000	-2.54079900	-2.80714200
H	-2.85535200	-0.69861200	-2.72690000

24

0 imaginary frequency

H = -7139.609078

G = -7139.707903

Esol = -7139.981392

Se	0.46700200	-0.19375200	-0.44096400
N	-0.27198700	-0.53005000	1.16265800
N	1.49149100	-1.77778900	-0.40690700
S	-0.57372800	0.85396700	1.95097200
O	0.54020300	1.81165800	2.00059600
O	-1.31771600	0.54662300	3.16116900
S	2.57253400	-1.96782300	-1.69478200
O	2.05924600	-1.34666900	-2.90521300

O	3.00974100	-3.35195400	-1.64327000
C	-4.02772300	-3.02936500	1.71433000
C	-2.76762700	-3.09990200	0.89346800
C	-2.76057800	-2.04963700	-0.22782000
C	-4.09675500	-2.10475000	-0.99829600
C	-5.30553400	-1.94662400	-0.07751700
C	-5.19020500	-2.48649600	1.30294800
H	-3.97197100	-3.45274700	2.71693100
H	-1.89666300	-2.94698200	1.54124900
H	-2.69994600	-1.07289500	0.26266500
H	-4.16495900	-1.33506900	-1.77410100
H	-2.67173800	-4.11716000	0.48138300
H	-4.18551400	-3.07706300	-1.50633200
C	-6.42190000	-2.40084800	2.16353800
H	-6.24656700	-2.83729000	3.15129500
H	-6.73323700	-1.35801700	2.29133600
H	-7.26539800	-2.91759600	1.69171000
O	-6.33899400	-1.43388600	-0.48175200
C	-1.58507800	-2.14886400	-1.19145600
C	-1.10562300	-3.30640800	-1.67991700
H	-1.70233900	-0.01829200	-1.63936400
H	-1.51121800	-4.26875000	-1.38260400
H	-0.32804500	-3.32992500	-2.43982100
C	-0.99815200	-0.85376000	-1.65996400
H	-0.49665300	-0.90825600	-2.62821900
H	0.87051500	-2.59462800	-0.33029300
O	3.74981100	-0.96313200	-1.21179200
C	4.50748400	-1.32681900	-0.03833100
H	3.95218100	-2.03017500	0.58496400
H	5.45352200	-1.76693800	-0.35839300

C	4.78429400	-0.05808900	0.77771900
Cl	3.25854800	0.67662700	1.35419500
Cl	5.78410100	-0.58294200	2.18532000
Cl	5.70526500	1.12706200	-0.20731600
O	-1.66234800	1.52739700	0.80816900
C	-1.85211600	2.93413000	0.83907900
H	-1.02520300	3.43138000	1.35374200
H	-2.80300400	3.17948700	1.32239500
C	-1.89940000	3.45845800	-0.60421700
Cl	-3.25967900	2.70077500	-1.50877400
Cl	-0.34922500	3.08821900	-1.45406400
Cl	-2.13755700	5.23605800	-0.53640400

25

0 imaginary frequency

H = -4860.817552

G = -4860.912087

Esol = -4861.203040

Se	1.67625400	0.05690000	-1.41022000
N	1.56713000	1.66846400	-1.98977000
N	0.78589900	-0.08010100	0.10036300
S	1.32322900	3.02786200	-1.03962200
O	1.31472700	4.14951500	-1.97677900
O	2.22935100	3.05156300	0.11857400
S	0.59108100	-1.66312400	0.58364100
O	0.77005500	-1.71260100	2.03892900
O	1.39400500	-2.56998900	-0.27498200
C	-1.14127200	-2.00825300	0.23044100
C	-1.45287100	-3.07951000	-0.60789300

C	-2.13759200	-1.22087100	0.81613900
C	-2.78993500	-3.37308200	-0.86806200
H	-0.65599800	-3.67172900	-1.04285700
C	-3.47463000	-1.50328700	0.54980700
H	-1.87011300	-0.39481700	1.46571800
C	-3.77426600	-2.57965500	-0.28550400
H	-3.07654100	-4.19807200	-1.50822900
H	-4.27679600	-0.90416300	0.96371600
N	-5.19032000	-2.89360000	-0.56347800
O	-6.04367800	-2.21202500	-0.00180900
O	-5.42359900	-3.81992500	-1.33880600
C	-0.34869800	2.84481900	-0.38609900
C	-0.60310900	3.29893700	0.90817400
C	-1.35952400	2.30592500	-1.18441800
C	-1.89432100	3.21025600	1.42141600
H	0.20689800	3.69935300	1.50713400
C	-2.64795400	2.19673900	-0.67126200
H	-1.13676800	1.96325000	-2.18932100
C	-2.89101900	2.64890700	0.62593700
H	-2.13403900	3.55127000	2.42100300
H	-3.45683400	1.76892400	-1.25035400
N	-4.24453300	2.50269500	1.18736500
O	-4.48210900	3.05644600	2.25867800
O	-5.05263500	1.82188200	0.55349300
C	4.00462700	-0.67292100	0.35168300
C	4.33391200	-1.52671700	2.39262300
C	4.68658800	-2.47849700	1.49014500
H	4.33657900	-1.54506100	3.47064600
H	5.05440800	-3.48205700	1.63328800
N	3.91211600	-0.41365900	1.68562800

N	4.48694100	-1.94448200	0.22880700
C	3.39907800	0.82873200	2.25968000
H	4.14612700	1.25256100	2.93645300
H	3.19101800	1.52903200	1.45084700
H	2.47402900	0.61601300	2.79984800
C	4.59392000	-2.64121400	-1.04502900
H	3.76492900	-3.34562000	-1.14964700
H	4.53952800	-1.89537900	-1.83865900
H	5.55095900	-3.16533900	-1.10246100
O	3.72923000	0.11942900	-0.60892600

26

0 imaginary frequency

H = -5066.617609

G = -5066.725718

Esol = -5067.236417

Se	0.40704600	-1.07630300	-0.20590000
N	-0.19961800	-2.48962500	-0.96826100
N	-0.72722400	-0.53447700	1.01904900
S	-1.31438200	-3.56755000	-0.27843600
O	-1.02004200	-3.73738400	1.14902300
O	-1.32479300	-4.71092800	-1.18782700
S	-0.26008000	0.94464700	1.65953700
O	1.00798100	1.38142100	1.02939900
O	-0.34813500	0.88795100	3.11940900
C	-1.56899400	2.02759800	1.06025700
C	-1.85753400	2.06476900	-0.30674800
C	-2.21603600	2.86176100	1.97126700
C	-2.80598000	2.96494400	-0.77766100

H	-1.35875800	1.38487400	-0.98899600
C	-3.16946100	3.76517500	1.50321100
H	-1.97497700	2.79857500	3.02649700
C	-3.44239600	3.80201600	0.13887000
H	-3.06083200	3.02777400	-1.82813700
H	-3.69664000	4.43258000	2.17351400
N	-4.44637100	4.76397300	-0.35992100
O	-4.66632700	4.77576900	-1.56911400
O	-4.99289400	5.49165300	0.46551600
C	-2.90841400	-2.74790700	-0.43621100
C	-3.56567300	-2.79909600	-1.66908800
C	-3.47215800	-2.11963000	0.67548500
C	-4.80993900	-2.18979300	-1.80018600
H	-3.11503300	-3.32425000	-2.50408300
C	-4.72057600	-1.51456900	0.54820400
H	-2.93658300	-2.10535500	1.61672900
C	-5.36217900	-1.55647200	-0.68756500
H	-5.35602100	-2.20511300	-2.73507400
H	-5.19875600	-1.01950600	1.38409500
N	-6.68253900	-0.90917700	-0.82353700
O	-7.14540300	-0.34894700	0.16816900
O	-7.23378700	-0.96860400	-1.92079300
C	4.17682600	-1.20538200	0.77418200
C	4.02905400	0.14027200	0.01803400
C	5.16538500	0.44129200	-1.00422500
C	6.51999800	0.23721200	-0.31011100
C	6.67946900	-1.03603800	0.49691800
C	5.53552300	-1.23933400	1.50410000
H	3.06394200	0.15401300	-0.49823500
C	5.01832300	1.93356300	-1.45914600

C	7.52377200	1.12112200	-0.39159800
H	6.70817800	-1.90891500	-0.17316300
H	5.57101300	-0.44134500	2.25689800
C	7.49223300	2.39694700	-1.18788800
C	6.29801500	2.43852500	-2.14608600
H	8.44565000	0.91257300	0.15295200
H	7.45381900	3.25621200	-0.49900300
H	6.51213300	1.82584500	-3.03199200
H	5.66107700	-2.19254000	2.03320200
H	8.43446200	2.51103800	-1.74187800
H	6.14119700	3.46145800	-2.51076000
H	4.90594300	2.52032300	-0.53448600
H	3.99477200	0.95365100	0.75269100
C	3.78224700	2.21671200	-2.32710600
H	3.69496300	3.29470000	-2.50568100
H	3.85024500	1.73016100	-3.30693800
H	2.85193800	1.89266900	-1.84867100
C	5.05377200	-0.52704300	-2.20918400
H	4.17594300	-2.01628900	0.03369900
C	3.00140700	-1.44768000	1.69824500
C	2.87393200	-0.62628000	2.94874400
H	1.89731000	-0.75108300	3.42211400
H	3.64281200	-0.93694600	3.66995700
C	2.07804800	-2.40597400	1.39742100
H	2.24551600	-3.09488800	0.57340700
H	5.76510300	-0.26125400	-2.99744000
H	5.26840600	-1.56116500	-1.92306300
H	4.04706600	-0.51114100	-2.64171300
H	7.64117600	-1.02287500	1.02239900
H	1.25452900	-2.64541000	2.06502800

H	3.02772600	0.43980600	2.75474900
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0 imaginary frequency

H = -5066.647000

G = -5066.752933

Esol = -5067.266645

Se	0.49269500	-0.64262500	0.31328000
N	-1.08910200	-1.33299900	-0.10557000
N	0.21398300	0.57567300	1.72613000
S	-1.94958800	-1.95651900	1.17074500
O	-2.12944700	-0.92210000	2.22435300
O	-1.46013700	-3.27315200	1.61552100
S	0.73034800	2.15186500	1.49973600
O	1.79810900	2.04112100	0.50030100
O	0.96316600	2.74344400	2.81375600
C	-0.65905700	3.03662900	0.75964000
C	-1.45589700	2.42376200	-0.21175400
C	-0.86816000	4.36142700	1.14918100
C	-2.47759600	3.15375900	-0.81156700
H	-1.30632500	1.38560500	-0.48765200
C	-1.88890700	5.09500200	0.54860000
H	-0.24674800	4.80362100	1.91977600
C	-2.67294900	4.47737700	-0.42209600
H	-3.11847900	2.71577100	-1.56656000
H	-2.08524100	6.12400400	0.82284900
N	-3.75864100	5.25071100	-1.05807400
O	-4.44646800	4.67484500	-1.89845300
O	-3.90380600	6.41892500	-0.70585100

C	-3.53640100	-2.19888100	0.36382100
C	-3.86200800	-3.46953600	-0.11169100
C	-4.42147400	-1.12374600	0.25798300
C	-5.09593000	-3.66833500	-0.72702900
H	-3.15995500	-4.28691600	0.00858700
C	-5.65594100	-1.31809700	-0.35446900
H	-4.14939300	-0.15476700	0.66138000
C	-5.96744200	-2.58771900	-0.83879100
H	-5.39047700	-4.63672000	-1.11164100
H	-6.37423300	-0.51434600	-0.45750600
N	-7.27640600	-2.79638400	-1.48974600
O	-8.02975100	-1.82852100	-1.57287000
O	-7.52909200	-3.92431700	-1.90830900
C	4.00890800	-1.60803900	1.04114200
C	3.83815300	-0.83788700	-0.29075700
C	5.00201900	-0.98567200	-1.31589900
C	6.33937300	-0.76570700	-0.59820500
C	6.51270100	-1.47812800	0.72693700
C	5.34274700	-1.21399900	1.68883500
H	2.92151200	-1.16613200	-0.79385300
C	4.80679100	0.10763300	-2.42063700
C	7.31395500	0.00836500	-1.09429000
H	6.59037900	-2.56465200	0.56577700
H	5.32409700	-0.14592300	1.94439000
C	7.25736000	0.73845000	-2.40881700
C	6.07726800	0.27553800	-3.27016400
H	8.22820600	0.13054000	-0.51193700
H	7.18311700	1.82145800	-2.21947300
H	6.32616700	-0.67393500	-3.76270500
H	5.49309000	-1.76940300	2.62288200

H	8.20462700	0.60266100	-2.94942200
H	5.89112800	0.99850800	-4.07439800
H	4.66351600	1.05531500	-1.87968100
H	3.70207600	0.22405500	-0.04905700
C	3.56891600	-0.09346600	-3.30924800
H	3.45501000	0.76276600	-3.98414100
H	3.65065000	-0.99045500	-3.93393900
H	2.64392700	-0.16790400	-2.72641800
C	4.97703100	-2.41371800	-1.91808700
H	4.06161100	-2.68415700	0.80660400
C	2.79807300	-1.43153500	1.95285000
C	2.84269900	-0.84548100	3.15842600
H	1.95425700	-0.75024500	3.77493100
H	3.75901500	-0.43937300	3.57162800
C	1.49070500	-1.98413000	1.47191100
H	1.59158700	-2.81998500	0.77380300
H	5.72503500	-2.52461100	-2.70932100
H	5.19622100	-3.17510300	-1.16290200
H	3.99516000	-2.65022900	-2.34385600
H	7.45642000	-1.17053300	1.19165100
H	0.79424900	-2.25397400	2.26510500
H	-0.64306400	0.39462400	2.26419100

28

0 imaginary frequency

H = -5446.733621

G = -5446.860412

Esol = -5447.496453

Se	0.05109600	0.31997000	-1.32075900
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N	0.44444400	1.79347700	-0.53876500
N	-0.46318800	-0.80097400	-0.08176500
S	0.97606300	1.88830900	1.04349200
O	1.67682700	0.66468900	1.47494700
O	-0.07235800	2.44229100	1.90562300
S	-0.82173500	-2.33012400	-0.62068200
O	-0.32671300	-2.55338800	-2.00204300
O	-2.22944800	-2.63960700	-0.34591100
C	0.18333200	-3.34169900	0.48270200
C	0.64070000	-2.84377300	1.70558000
C	0.42705500	-4.66077700	0.08724100
C	1.35823200	-3.68856200	2.55171100
H	0.46244100	-1.80861400	1.97526800
C	1.14089100	-5.50494900	0.93164900
H	0.06906500	-5.01716500	-0.87272400
C	1.59421000	-5.00205000	2.15065300
H	1.73187300	-3.34314000	3.50780300
H	1.35070400	-6.53309100	0.66429600
N	2.36408700	-5.89131800	3.04080200
O	2.56918300	-7.04196100	2.65639200
O	2.75908700	-5.42597700	4.10807600
C	2.23007500	3.16420600	0.81481400
C	2.14499300	4.32734900	1.57796300
C	3.28533400	2.93828500	-0.07409900
C	3.14130500	5.29504700	1.45462600
H	1.30701100	4.46820600	2.25145600
C	4.27913800	3.90258100	-0.20082400
H	3.31585700	2.02857700	-0.66567200
C	4.18935600	5.06368700	0.56814100
H	3.11513500	6.21391700	2.02694900

H	5.11287800	3.77500500	-0.87985500
N	5.24437700	6.08559400	0.43334500
O	5.14390200	7.10264000	1.11711100
O	6.16095500	5.85691600	-0.35487700
C	2.79021700	-1.34455000	-1.84143100
C	3.87694100	-3.28040000	-1.47314700
C	3.33487500	-3.34680500	-2.71447000
H	4.47212400	-3.99449300	-0.92622500
H	3.35702900	-4.13521800	-3.45015000
N	3.53247600	-2.04861200	-0.93062100
N	2.67644900	-2.14726500	-2.94593700
C	3.95127800	-1.52219100	0.36314300
H	3.27636800	-0.71516900	0.65143000
H	3.89599200	-2.31937600	1.10794600
H	4.97841100	-1.14564200	0.31050100
C	1.87570700	-1.80280100	-4.11029500
H	1.59628600	-0.75272500	-4.01950700
H	2.46164900	-1.94555600	-5.02237100
H	0.96944700	-2.41180100	-4.13547200
O	2.34605600	-0.17070500	-1.71070400
C	-3.78731200	0.42755700	-1.62489200
C	-3.71917400	1.29867800	-0.35623900
C	-4.73192700	0.91850000	0.77006700
C	-6.13020300	0.80038500	0.14524500
C	-6.23002700	-0.01997800	-1.12341000
C	-5.22614000	0.43985400	-2.19173500
H	-2.69507700	1.25973200	0.03285000
C	-4.72349400	2.06068400	1.84364500
C	-7.22133700	1.38596900	0.65790100
H	-6.03646700	-1.08073900	-0.90372400

H	-5.47201200	1.46067500	-2.51567500
C	-7.25321700	2.19463200	1.92559100
C	-5.97170200	2.00407700	2.74019400
H	-8.16965000	1.27028200	0.13067500
H	-7.39078200	3.26061500	1.68028900
H	-6.00748000	1.03842000	3.26248400
H	-5.30509900	-0.20599900	-3.07466000
H	-8.13465500	1.91739100	2.52136700
H	-5.89877200	2.77316700	3.51996600
H	-4.78474200	3.00560600	1.28051500
H	-3.91555200	2.34217800	-0.63802800
C	-3.45032600	2.11875200	2.70039600
H	-3.39176700	1.27019900	3.39209900
H	-2.53233600	2.12957500	2.10735700
H	-3.45539000	3.03102700	3.30936200
C	-4.33115600	-0.43841400	1.40098700
C	-2.78549900	0.81979400	-2.70141000
C	-2.51499500	-0.21462500	-3.76972200
H	-3.43622300	-0.50167700	-4.29078900
H	-1.80957000	0.15824700	-4.51978700
H	-2.10461500	-1.13602200	-3.33664300
C	-2.15059400	2.00675200	-2.73483200
H	-1.46884300	2.25487000	-3.54583700
H	-2.29312500	2.77278500	-1.98123500
H	-4.97128600	-0.67715100	2.25722900
H	-4.41365800	-1.26497400	0.69099000
H	-3.29137700	-0.41970300	1.74194600
H	-7.25102700	0.03237300	-1.52003900
H	-3.55890600	-0.61131500	-1.34632200

29

0 imaginary frequency

H = -5066.659507

G = -5066.766460

Esol = -5067.279034

Se	-0.32448000	-1.60394000	1.99392800
N	0.49399500	-0.06233300	2.30206000
N	-0.56729500	-1.51843700	0.09703800
S	-0.57600300	1.12895600	2.76782000
O	-0.20673200	1.64336300	4.08995100
O	-1.97367400	0.68940200	2.53311300
S	-1.68456900	-2.62491600	-0.55611100
O	-2.05632900	-3.55508900	0.51968400
O	-1.13146600	-3.10561000	-1.82449200
C	-3.11216400	-1.59095800	-0.89897300
C	-3.59753400	-0.73657100	0.09551800
C	-3.74025100	-1.72765800	-2.13716700
C	-4.74778900	0.00346000	-0.16202400
H	-3.07973600	-0.61774600	1.04132500
C	-4.89508100	-0.99007500	-2.39105400
H	-3.32756300	-2.39335800	-2.88694600
C	-5.37649700	-0.14098300	-1.39813700
H	-5.15294200	0.68454200	0.57582500
H	-5.41808900	-1.06158000	-3.33644500
N	-6.59934900	0.64288000	-1.66959400
O	-7.13254600	0.49867400	-2.76786600
O	-7.00392100	1.38762900	-0.78022000
C	-0.22682300	2.45231700	1.58990200
C	0.48536400	3.57053400	2.02456100

C	-0.69809100	2.35027100	0.27795300
C	0.74613800	4.60535000	1.12779100
H	0.81939000	3.62440600	3.05448100
C	-0.44066300	3.37978300	-0.62145900
H	-1.26149600	1.47782200	-0.03438900
C	0.28097000	4.48896800	-0.17967800
H	1.29465200	5.49039700	1.42520900
H	-0.78836600	3.34154900	-1.64625100
N	0.55961700	5.57900300	-1.13348200
O	0.14687000	5.44690300	-2.28476600
O	1.19016300	6.55039600	-0.72014300
C	2.88591300	-2.70787800	0.08606600
C	3.53117600	-1.37488400	0.40279400
C	3.69469800	-0.40498100	-0.81887100
C	4.35062200	-1.17836700	-1.96735200
C	3.71943400	-2.51061400	-2.30702100
C	3.55765000	-3.41771500	-1.06830600
H	2.99528600	-0.84195500	1.18973500
C	4.60360900	0.78575500	-0.36366400
C	5.42090200	-0.73285200	-2.63904200
H	2.72708400	-2.36195300	-2.75652300
H	4.56321600	-3.70884800	-0.72566500
C	6.08656000	0.59636300	-2.41033400
C	5.20693500	1.52507000	-1.56921200
H	5.84408400	-1.36324900	-3.42202300
H	7.05862200	0.44228700	-1.91462400
H	4.40102400	1.93359100	-2.19403300
H	3.04442700	-4.34093300	-1.34488200
H	6.32319300	1.06234500	-3.37674800
H	5.78966600	2.38562500	-1.21766400

H	5.44641100	0.33309800	0.18173500
H	4.54218900	-1.58537700	0.78501200
C	3.91788400	1.77826600	0.58921500
H	3.42030200	1.28829100	1.43249300
H	4.66154200	2.47014000	1.00117700
H	3.16654000	2.38240300	0.06829900
C	2.30094400	0.09752500	-1.26603100
C	1.89309200	-3.27637300	0.81858000
C	1.27821900	-4.63034900	0.50856600
H	1.22440100	-4.84076000	-0.56132100
H	1.84794300	-5.44077300	0.98447400
H	0.25533300	-4.68635800	0.89373800
C	1.41594200	-2.67976800	2.10092800
H	1.14165500	-3.44967100	2.82680300
H	2.06729900	-1.94482800	2.56793500
H	1.72045900	-0.70082800	-1.74230600
H	1.72251000	0.47647900	-0.41774200
H	2.38864100	0.89942500	-2.00626300
H	4.32206700	-3.02935100	-3.06078900
H	0.32710600	-1.59046800	-0.40005200

3

0 imaginary frequency

H = -1740.780646

G = -1740.868922

Esol = -1741.136695

C	4.00585700	1.67428800	1.17964000
O	3.70215700	1.15894500	-0.03512900
O	3.32762000	1.55010500	2.17314100

C	5.31776000	2.42678200	1.09534400
H	5.67050600	2.64245700	2.10483800
H	6.06376400	1.85154500	0.54118600
H	5.14746400	3.36402200	0.55508700
I	1.82442900	0.34956600	-0.21266400
O	-0.47000000	2.13121600	-1.06192700
C	0.41411500	3.02377100	-0.92259100
O	1.62661200	2.79057100	-0.62270000
C	0.01242600	4.48142500	-1.10781100
H	-0.44775400	4.61162400	-2.09310000
H	-0.74291200	4.74483100	-0.35901800
H	0.87159200	5.14711100	-1.00846700
C	2.71552600	-1.53346700	0.33732500
C	2.99936400	-1.78857700	1.68026300
C	2.95307500	-2.48921500	-0.65067600
C	3.54164100	-3.02577900	2.03331300
H	2.81302500	-1.03247200	2.43582400
C	3.48838800	-3.72594400	-0.28432300
H	2.71810300	-2.28388000	-1.69020600
C	3.78415900	-3.99207100	1.05406400
H	3.76932400	-3.23424800	3.07502600
H	3.67365200	-4.47804600	-1.04603200
H	4.20157400	-4.95502300	1.33496800
N	-1.13886300	-0.09837500	-2.59291300
S	-1.49438800	-1.26591600	-1.48029800
O	-1.82211300	-2.49580400	-2.19838500
O	-0.38436600	-1.24958500	-0.50200300
C	-2.97341100	-0.75948800	-0.57816100
C	-4.03120000	-1.66619500	-0.48305300
C	-3.02331100	0.50349700	0.02374600

C	-5.17132500	-1.30862100	0.23428700
H	-3.95613000	-2.63354300	-0.96670900
C	-4.16500300	0.86123300	0.73628300
H	-2.19747400	1.20371600	-0.07863200
C	-5.21568600	-0.05112600	0.83107900
H	-6.01422400	-1.98090200	0.33456000
H	-4.25164000	1.82861800	1.21511300
N	-6.42350100	0.33197000	1.58772000
O	-6.44096100	1.44826700	2.10245400
O	-7.33598800	-0.48949000	1.65486500
H	-0.88554000	0.81317900	-2.17041000
H	-1.81926000	-0.05337200	-3.34660300

30

0 imaginary frequency

H = -235.780186

G = -235.820789

Esol = -235.954941

C	-0.23589700	-0.52887800	-0.32903000
C	0.98261200	-0.04469200	-0.04278800
H	-0.33023900	-1.61348100	-0.42000200
C	2.16080000	-0.97430900	0.13322200
H	2.95909800	-0.74426200	-0.58687100
H	2.60566600	-0.86597400	1.13275200
H	1.87752900	-2.02329600	0.00054300
C	1.31507600	1.41804100	0.12750000
H	1.74732600	1.60326000	1.12088900
H	2.07491000	1.73084400	-0.60253100
H	0.45082900	2.07598100	0.01153000

C	-1.52822800	0.21710800	-0.53051500
H	-1.90937100	0.00384500	-1.54087200
H	-1.37365500	1.30049500	-0.48759100
C	-2.60498000	-0.18609700	0.49277800
H	-2.28845800	0.06105200	1.51230100
H	-3.55176600	0.32964800	0.29430500
H	-2.79817500	-1.26514900	0.45854400

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0 imaginary frequency

H = -4716.495607

G = -4716.590919

Esol = -4716.914285

Se	-1.79274900	-0.37793600	-1.00402500
N	-2.04596400	1.30193600	-1.27728400
N	-0.81603900	-0.60812400	0.43927500
S	-1.92174100	2.52298900	-0.10641000
O	-2.50293800	2.06835500	1.16214600
O	-2.42730800	3.71916100	-0.77743900
S	-0.39452500	-2.23151000	0.61303400
O	-1.07476500	-3.03274200	-0.43162000
O	-0.54191300	-2.61136400	2.01848300
C	1.36738400	-2.19876600	0.22982700
C	2.23929900	-2.88144600	1.07820500
C	1.81703700	-1.56832500	-0.93360400
C	3.59279900	-2.94584600	0.75073700
H	1.85995300	-3.34833300	1.98022900
C	3.16574400	-1.63141900	-1.26453300
H	1.12560900	-1.01700600	-1.56130200

C	4.02864000	-2.32396100	-0.41575200
H	4.30498800	-3.46505200	1.37991600
H	3.55682500	-1.15621900	-2.15540600
N	5.46121300	-2.39658100	-0.76846900
O	5.81741800	-1.83952100	-1.80455100
O	6.20198900	-3.01180300	-0.00542000
C	-0.15257200	2.75012100	0.13195300
C	0.55110100	3.52343900	-0.79603700
C	0.46941000	2.18993600	1.24894300
C	1.91555300	3.72745000	-0.61344900
H	0.03127800	3.97204300	-1.63545100
C	1.83416500	2.39771400	1.43680400
H	-0.10854400	1.60117100	1.95047600
C	2.53118800	3.15723400	0.49997300
H	2.50048800	4.32052200	-1.30525000
H	2.35802200	1.98643400	2.29055900
N	3.97893900	3.37251800	0.69692900
O	4.50147600	2.85404500	1.68159000
O	4.57027900	4.05393900	-0.13811100
C	-4.04793200	-1.48444800	0.31756500
C	-4.62058400	-0.89066300	-0.77377500
H	-3.70057900	-2.51061600	0.18478000
C	-4.71392000	-1.63986600	-2.07931500
H	-4.22332200	-2.61631200	-2.03262300
H	-5.76503500	-1.79384400	-2.35675300
H	-4.26457700	-1.06058700	-2.89794700
C	-5.20487300	0.49136900	-0.77446700
H	-6.27293500	0.44433100	-1.02634400
H	-5.09495400	1.00695500	0.17985300
H	-4.72508200	1.10857700	-1.54559000

C	-3.91069300	-0.95358600	1.71044000
H	-4.09745400	0.12128100	1.75600000
C	-4.83144900	-1.70520400	2.69323200
H	-4.63250100	-2.78273400	2.68033000
H	-4.66400400	-1.34556400	3.71360200
H	-5.88750600	-1.55201700	2.44583200
H	-2.86966000	-1.09808500	2.03169800

32

0 imaginary frequency

H = -4716.520383

G = -4716.613589

Esol = -4716.938967

Se	-1.69711700	-0.62979100	-1.19958700
N	-1.41106100	1.07584400	-1.53607600
N	-0.82654800	-0.95538300	0.46433500
S	-1.80553300	2.17961500	-0.36496400
O	-2.11110800	1.49185600	0.91931300
O	-2.77625400	3.16887100	-0.84896100
S	-0.45606700	-2.56298500	0.80581100
O	-1.14831100	-3.38734200	-0.19681100
O	-0.64225500	-2.78071900	2.23993800
C	1.29991200	-2.64609800	0.43044900
C	2.16111800	-3.20412100	1.37337900
C	1.75057900	-2.21174500	-0.82034300
C	3.51348700	-3.33576200	1.05857500
H	1.77804700	-3.52343300	2.33617800
C	3.09824200	-2.34025800	-1.13506500
H	1.06050300	-1.76512800	-1.52877000

C	3.95428900	-2.90410300	-0.18857400
H	4.22034600	-3.76240200	1.75923800
H	3.49286400	-2.01532000	-2.08962700
N	5.38615000	-3.04550300	-0.52428100
O	5.74828600	-2.65466000	-1.63168100
O	6.12020000	-3.54521800	0.32483600
C	-0.23501300	3.04378000	-0.16042100
C	0.95607800	2.31580700	-0.10926600
C	-0.25506500	4.42834200	0.01012100
C	2.15298000	2.98325100	0.12634100
H	0.93717500	1.24510500	-0.27619700
C	0.94177300	5.10213400	0.24586400
H	-1.19498000	4.96498200	-0.05412300
C	2.12293400	4.36649100	0.30273900
H	3.09932900	2.45887300	0.16986100
H	0.97219900	6.17611600	0.38084900
N	3.39134100	5.07652500	0.55195600
O	3.34188700	6.29616900	0.70057400
O	4.42025600	4.40388400	0.59723300
C	-3.84936000	-1.38107900	0.72175600
C	-3.76498500	-1.05152300	-0.72228500
H	-3.52855500	-2.38902500	0.98347400
C	-3.99088300	-2.28317900	-1.60777800
H	-3.34603100	-3.11808300	-1.32055900
H	-5.03400200	-2.60418600	-1.49480700
H	-3.82572600	-2.05781900	-2.66757600
C	-4.54781200	0.15642400	-1.21951300
H	-5.61734000	-0.07714800	-1.14388300
H	-4.35781200	1.06358000	-0.64546400
H	-4.32552200	0.37328500	-2.26885300

C	-4.31460800	-0.58319700	1.69565800
H	-4.63433300	0.42843700	1.45768400
C	-4.42238900	-0.98518600	3.13479200
H	-4.03924600	-1.99556800	3.30777100
H	-3.86175200	-0.28781500	3.77077100
H	-5.46607800	-0.94496500	3.47464300
H	-1.26995300	-0.44566800	1.23613000

33

0 imaginary frequency

H = -4716.559120

G = -4716.652219

Esol = -4716.979149

Se	1.04505800	-1.25904300	-1.61546400
N	-0.49446200	-1.29055400	-0.56769800
N	2.38285200	-1.32135200	-0.30809900
S	-1.02200600	0.09716900	0.27578300
O	-0.55354100	1.25627900	-0.47898000
O	-0.73956800	-0.05965700	1.70831000
S	3.61055900	-0.13429600	-0.51632800
O	4.01432700	-0.06134800	-1.92707100
O	4.60242400	-0.41229000	0.52810900
C	2.75340800	1.39165600	-0.12018500
C	2.41153200	1.65625200	1.20757000
C	2.49603800	2.29986800	-1.14643500
C	1.79067100	2.86125700	1.51729100
H	2.63184400	0.93547600	1.98664400
C	1.87554700	3.50753100	-0.83847600
H	2.78568800	2.06167700	-2.16301400

C	1.53299500	3.76238700	0.48611300
H	1.50271500	3.10785100	2.53116800
H	1.65353100	4.24285000	-1.60137400
N	0.86932700	5.03955500	0.81233200
O	0.65199500	5.82069600	-0.11209900
O	0.57581700	5.24414300	1.98882200
C	-2.80643000	-0.02400200	0.06704200
C	-3.59044100	-0.44143100	1.14295400
C	-3.36880800	0.32951600	-1.16278200
C	-4.97274800	-0.52373100	0.98348200
H	-3.12348300	-0.68312500	2.09112500
C	-4.74784000	0.24763000	-1.32508300
H	-2.73659300	0.67324500	-1.97406700
C	-5.52328200	-0.18194300	-0.24848100
H	-5.62054500	-0.84052000	1.79128900
H	-5.22750100	0.51213500	-2.25913300
N	-6.98765900	-0.27327100	-0.42090900
O	-7.44937300	0.03624100	-1.51697000
O	-7.64901300	-0.65536000	0.54201000
C	1.70003300	-3.51809500	0.58921400
C	1.17716400	-3.46962100	1.82747200
H	1.28745100	-4.23437000	-0.12178100
C	0.04200600	-4.38350800	2.22373200
H	-0.28579300	-5.02006900	1.39568700
H	0.34307800	-5.03518200	3.05499100
H	-0.82189100	-3.80743400	2.58322100
C	1.63559900	-2.51798800	2.90361900
H	1.76418800	-3.04560300	3.85718500
H	2.57434700	-2.01519600	2.66001600
H	0.87572900	-1.74151600	3.06262300

C	2.86699000	-2.70236400	0.07439400
H	3.58256800	-2.52078900	0.87965100
C	3.57728100	-3.41345000	-1.08164100
H	2.89016000	-3.54800000	-1.92547200
H	4.44302800	-2.84251300	-1.42794600
H	3.92146700	-4.40229300	-0.75984400
H	-0.50206200	-2.10521000	0.04832900

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0 imaginary frequency

H = -4716.497229

G = -4716.592280

Esol = -4716.915383

Se	-1.87435600	-0.35543600	-0.74652900
N	-2.16798800	1.32837200	-0.98926000
N	-0.86587200	-0.60392800	0.67513300
S	-1.90790700	2.54592800	0.16145000
O	-2.29798300	2.09295700	1.50272100
O	-2.51275400	3.73969100	-0.42731800
S	-0.46284000	-2.23077700	0.82494500
O	-1.16020500	-3.01281100	-0.22363800
O	-0.60421600	-2.63078900	2.22552600
C	1.29475700	-2.22188600	0.42458700
C	2.17495700	-2.88537100	1.27907800
C	1.73114100	-1.62473000	-0.76136800
C	3.52414500	-2.96284900	0.93611700
H	1.80465200	-3.32850600	2.19672300
C	3.07489200	-1.70174200	-1.10844700
H	1.03156400	-1.09079700	-1.39539100

C	3.94671100	-2.37405400	-0.25216100
H	4.24286600	-3.46801200	1.56929500
H	3.45575500	-1.25359500	-2.01758500
N	5.37408000	-2.46229600	-0.62182800
O	5.71751800	-1.94022900	-1.68015100
O	6.12376400	-3.05488500	0.15052300
C	-0.12355800	2.77964300	0.14578500
C	0.65609500	2.19301600	1.14431800
C	0.43630600	3.57632400	-0.85727000
C	2.03428500	2.39772900	1.13190500
H	0.18671200	1.58763800	1.90990900
C	1.81290900	3.77952600	-0.87297900
H	-0.20175000	4.04230700	-1.60008700
C	2.58605900	3.18244100	0.12189500
H	2.67844300	1.96652800	1.88796400
H	2.28985200	4.39104100	-1.62866200
N	4.04729700	3.39607200	0.10791700
O	4.50925700	4.10175500	-0.78644200
O	4.70922800	2.85218500	0.98965500
C	-4.21368200	-1.52667400	-0.19839600
C	-4.39554100	-0.61058100	0.80854200
H	-3.71483100	-2.46251100	0.05314100
C	-3.80027100	-0.82539900	2.16352100
H	-4.58611100	-0.76940500	2.92898400
H	-3.28574300	-1.78419200	2.25685300
C	-5.16912000	0.65507900	0.57498600
H	-4.68143900	1.26126100	-0.20213800
H	-6.18332500	0.43795000	0.21608600
H	-5.23175200	1.26430200	1.47837300
C	-4.83595300	-1.45128100	-1.57368300

H	-5.91250100	-1.66265300	-1.48149700
C	-4.20613400	-2.43844600	-2.56568600
H	-4.64482200	-2.32720700	-3.56197000
H	-3.12591900	-2.27700900	-2.64593700
H	-4.35695700	-3.47381900	-2.24109700
H	-4.77420800	-0.42687000	-1.96539000
H	-3.08793300	-0.01906100	2.38687600

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0 imaginary frequency

H = -4716.522413

G = -4716.615313

Esol = -4716.941567

Se	2.14916800	0.05529500	-0.93404100
N	0.65072000	-0.87877000	-0.81543900
N	2.35292600	1.07564200	0.65130500
S	0.35372700	-1.72213300	0.57657100
O	0.62838600	-0.88039300	1.77042400
O	0.91868800	-3.08448400	0.57958600
S	2.01216000	2.72750600	0.49782400
O	2.73860300	3.15615100	-0.69701300
O	2.23649000	3.30193600	1.82065300
C	0.25145100	2.83326000	0.13568900
C	-0.18014000	2.70882300	-1.18772700
C	-0.64754700	2.99349300	1.19277100
C	-1.54566000	2.72893700	-1.45925600
H	0.53992100	2.61291500	-1.99262500
C	-2.01415700	3.00790200	0.92406000
H	-0.27842800	3.11469600	2.20529000

C	-2.43577000	2.86550300	-0.39683500
H	-1.92553200	2.63896000	-2.46934000
H	-2.74697200	3.12628500	1.71281500
N	-3.88470200	2.85006900	-0.67983700
O	-4.23430300	2.91775100	-1.85470200
O	-4.64611900	2.76173300	0.28287700
C	-1.43051900	-1.89987200	0.42417700
C	-2.25706000	-0.82539600	0.75975200
C	-1.95297600	-3.12252000	0.00267200
C	-3.63780200	-0.96661200	0.65664000
H	-1.82327900	0.10458900	1.10811300
C	-3.33457900	-3.27073000	-0.10167400
H	-1.28384100	-3.94264900	-0.23113200
C	-4.14964600	-2.19008700	0.22515200
H	-4.31283900	-0.15418100	0.89852700
H	-3.78365000	-4.20169600	-0.42430400
N	-5.61384300	-2.35006900	0.11830900
O	-6.03868700	-3.43180300	-0.28402000
O	-6.31409100	-1.39277200	0.43908800
C	3.84094200	-1.12753100	-0.69616200
C	4.35282200	-1.21291400	0.71454500
H	4.50161800	-0.48365600	-1.29045300
C	3.94154900	-2.15635700	1.57329300
H	4.35370600	-2.19977700	2.57783200
H	3.17789000	-2.88650100	1.32987600
C	5.40946100	-0.19544700	1.07803800
H	5.70624500	-0.28672600	2.12655700
H	6.30691500	-0.32553700	0.45741300
H	5.04587100	0.82476700	0.91273500
C	3.54752400	-2.41769600	-1.46828900

H	2.83561000	-3.03064200	-0.90918500
C	4.82995900	-3.20864600	-1.76246800
H	4.58984600	-4.11649700	-2.32558600
H	5.53684300	-2.62081300	-2.36016500
H	5.33093700	-3.50642100	-0.83658200
H	3.05475300	-2.16611700	-2.41807500
H	1.87393500	0.60530900	1.43358300

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0 imaginary frequency

H = -4716.551845

G = -4716.644879

Esol = -4716.972727

Se	-2.00366900	0.01354700	-1.08937400
N	-0.19399200	0.52503100	-1.16947700
N	-2.02646700	-0.48180500	0.68270900
S	0.14296100	2.20133800	-1.12030600
O	-0.79345000	2.76257100	-0.14517300
O	0.25897700	2.76060500	-2.47014500
S	-2.05092000	-2.15979600	0.99428100
O	-3.04651900	-2.83186400	0.15352900
O	-2.07504200	-2.30389500	2.45255200
C	-0.42972200	-2.65776800	0.38933000
C	0.65941500	-2.60526900	1.26058500
C	-0.29766200	-3.09269400	-0.93191300
C	1.91865800	-2.97879300	0.79785400
H	0.51595600	-2.29156700	2.28880200
C	0.96204000	-3.45892700	-1.39979800
H	-1.17004100	-3.15471900	-1.57167100

C	2.04703400	-3.38865700	-0.52765700
H	2.79050000	-2.95950500	1.43989100
H	1.11309300	-3.80506000	-2.41485900
N	3.38316600	-3.77230200	-1.02599700
O	3.47206600	-4.11623300	-2.20299800
O	4.32130500	-3.71749300	-0.23387100
C	1.78990700	2.17960100	-0.39585300
C	2.85888600	2.67889900	-1.14006500
C	1.95447000	1.71057700	0.91106200
C	4.13034400	2.70402200	-0.56780100
H	2.69140400	3.04483900	-2.14685400
C	3.22142700	1.73350600	1.48350500
H	1.10388400	1.33246900	1.46740700
C	4.28602900	2.23027300	0.73127500
H	4.98908700	3.08318100	-1.10760100
H	3.39771100	1.38174100	2.49231100
N	5.63219100	2.25654200	1.34063600
O	6.55245100	2.70574300	0.66191700
O	5.74243500	1.82731000	2.48698100
C	-4.34373200	1.97474200	0.72195300
C	-4.09384200	0.80285700	1.33157100
H	-3.48980200	2.62350000	0.52157100
C	-2.65695400	0.46848100	1.66357600
H	-2.03354700	1.36451300	1.64271500
C	-5.11709600	-0.24586500	1.69172300
H	-5.07546300	-0.47598400	2.76447900
H	-6.13737800	0.06360500	1.45489700
H	-4.92553300	-1.18855300	1.16305700
C	-5.65874300	2.51438600	0.23309400
H	-6.49010300	1.85973000	0.51415100

C	-5.65828900	2.72086800	-1.29300200
H	-4.85638100	3.40250600	-1.59915100
H	-5.50220500	1.76998600	-1.81492500
H	-5.84849200	3.48289100	0.71890000
H	-2.56067400	-0.00664200	2.64382700
H	-6.60994700	3.14521400	-1.63194100
H	0.29489000	0.07496300	-1.94395700

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0 imaginary frequency

H = -4716.548944

G = -4716.642083

Esol = -4716.969668

Se	2.19688300	-0.33840000	0.86035400
N	0.47157000	0.05073200	1.39294700
N	1.93386500	-0.35782600	-1.00512000
S	0.00656500	1.60165000	1.91914400
O	1.06030600	2.52281100	1.50282000
O	-0.42953700	1.50988600	3.31455600
S	1.84582700	-1.97477900	-1.63978800
O	2.98274200	-2.77731700	-1.17348800
O	1.56526200	-1.83172900	-3.07128600
C	0.36251100	-2.59929000	-0.83213800
C	-0.87747900	-2.34752100	-1.42105500
C	0.48639000	-3.36050700	0.33309000
C	-2.03034100	-2.84476700	-0.81726100
H	-0.93330700	-1.78725500	-2.34794300
C	-0.66513200	-3.85387100	0.94257500
H	1.46813400	-3.56588500	0.74339600

C	-1.90127300	-3.58053700	0.35844800
H	-3.01308700	-2.67691800	-1.24001100
H	-0.62009200	-4.44995100	1.84571800
N	-3.12259500	-4.10336700	1.00643300
O	-2.98144200	-4.74546600	2.04468200
O	-4.19882400	-3.85812300	0.46676200
C	-1.46581700	1.89784300	0.92569900
C	-2.51444600	2.60890500	1.51319800
C	-1.51838000	1.47423300	-0.40458200
C	-3.63904000	2.91509700	0.75002200
H	-2.45360500	2.90535400	2.55444000
C	-2.64227600	1.77666900	-1.16826600
H	-0.70023000	0.89778200	-0.82239800
C	-3.68015800	2.49481300	-0.57694700
H	-4.47522300	3.46329500	1.16577800
H	-2.72740000	1.46765000	-2.20265900
N	-4.87286400	2.81386100	-1.38741400
O	-5.76889900	3.45887400	-0.84811600
O	-4.89139500	2.41352000	-2.54963900
C	3.85428900	2.47175300	-0.61109500
C	2.91771900	1.92556000	-1.40238600
H	3.77847000	3.54447100	-0.42634000
C	1.81553900	2.75830600	-2.00869800
H	1.87267600	3.79764800	-1.67353200
C	2.93381800	0.46822300	-1.79085900
H	2.62609200	0.35976000	-2.83478200
H	3.93334100	0.03381800	-1.69634100
C	4.99621100	1.80508200	0.10693500
H	4.95640500	0.71469400	-0.00118400
C	5.01366800	2.16714500	1.60201600

H	5.10163200	3.25014900	1.74475500
H	4.08530700	1.84371000	2.08252800
H	5.94665900	2.12178700	-0.34843800
H	1.86548600	2.74715000	-3.10645700
H	5.85847000	1.68996700	2.11089400
H	0.02193800	-0.68555400	1.93318500
H	0.82566400	2.37772800	-1.73275700

38

0 imaginary frequency

H = -390.578480

G = -390.624509

Esol = -390.826210

C	-0.57759200	0.54820200	-0.94968800
C	0.81248000	1.10220300	-0.66817800
C	1.80378600	0.13698600	-0.05498700
C	1.50701200	-1.14361800	0.19675500
C	0.18612000	-1.81369400	-0.07846600
C	-0.89237300	-0.90758800	-0.65625300
H	1.23962600	1.46619100	-1.61533500
H	2.27542200	-1.78296800	0.63263500
H	0.36126000	-2.64031600	-0.78375500
H	-0.17252500	-2.30070400	0.84265300
H	-1.54178900	-1.40812400	-1.37290600
C	3.16384600	0.71458100	0.24611700
H	3.83479600	-0.03237200	0.68247700
H	3.63996500	1.10790900	-0.66337900
H	3.09171500	1.55782700	0.94765300
H	0.74652800	1.99820100	-0.02919900

C	-1.56311400	0.19149700	0.14968100
H	-1.03132400	0.96106800	-1.84949700
C	-1.20775000	0.40818600	1.61149800
H	-0.15290000	0.21809900	1.82336800
H	-1.43124400	1.43993600	1.91377400
H	-1.80318600	-0.25350400	2.25443200
C	-3.03274800	0.44926800	-0.14856200
H	-3.67863900	-0.21680000	0.43905500
H	-3.31141100	1.48256600	0.09820700
H	-3.26429400	0.28684000	-1.20768400

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0 imaginary frequency

H = -4871.300251

G = -4871.399131

Esol = -4871.791412

Se	-1.22393000	-0.55338600	-0.97905100
N	-1.52213200	1.14203600	-1.02313200
N	-0.36711400	-0.97881000	0.49425900
S	-1.28560400	2.23488200	0.25265900
O	-1.76014300	1.68702400	1.52770800
O	-1.80502000	3.50226700	-0.25760400
S	0.33913800	-2.50930900	0.36444700
O	-0.14787600	-3.18429600	-0.85872900
O	0.23629600	-3.18077400	1.65994800
C	2.07180900	-2.07219800	0.11036700
C	3.02300200	-2.57567300	0.99738300
C	2.43516300	-1.28633600	-0.98684600
C	4.37099800	-2.28839400	0.78307200

H	2.70649500	-3.17893700	1.84078600
C	3.77783200	-1.00258300	-1.20706600
H	1.67886500	-0.88097100	-1.65101100
C	4.72234400	-1.50807300	-0.31389200
H	5.14278800	-2.65606900	1.44779000
H	4.10305600	-0.39890900	-2.04510600
N	6.14953000	-1.20434600	-0.54577200
O	6.96513600	-1.69261100	0.23146300
O	6.42493200	-0.49037700	-1.50712200
C	0.50747600	2.36977000	0.33569600
C	1.20382100	1.65270200	1.31038400
C	1.16187200	3.19619700	-0.58290500
C	2.59413100	1.73442800	1.34373500
H	0.66153400	1.03568700	2.01596700
C	2.55014500	3.28685300	-0.54492400
H	0.58810900	3.76576700	-1.30586600
C	3.24033900	2.53993600	0.40929200
H	3.17659600	1.18525100	2.07283600
H	3.09951600	3.91528600	-1.23493100
N	4.71512500	2.59796700	0.42446900
O	5.30545800	1.79383200	1.14525600
O	5.25817500	3.43744000	-0.28881400
C	-4.83908300	0.63267300	0.73827300
C	-4.12832900	-0.59397300	1.28446000
C	-3.73458200	-1.64610400	0.28652300
C	-3.86274900	-1.45823800	-1.05911900
C	-4.52277900	-0.27483000	-1.71195000
C	-5.02544400	0.79939500	-0.75847200
H	-3.57092800	-2.27578800	-1.71899900
H	-3.81253300	0.18533500	-2.41421000

H	-5.33746100	-0.65548500	-2.34828500
H	-4.89314200	1.80859700	-1.14094000
C	-3.18273600	-2.91933000	0.85044400
H	-2.81810600	-3.59942600	0.07641500
H	-2.36100000	-2.71759500	1.55016600
H	-3.95932900	-3.43608300	1.43096000
H	-4.71509500	-1.07697200	2.08100400
C	-6.23343900	0.59411100	0.14188200
H	-4.58894100	1.53785600	1.28527600
C	-7.02534800	-0.70260800	0.09113500
H	-6.40168300	-1.58396500	-0.08342300
H	-7.56504300	-0.86071100	1.03366300
H	-7.77545200	-0.66587900	-0.70953100
C	-7.10863100	1.81423800	0.38793400
H	-7.86030900	1.92706300	-0.40428700
H	-7.64278900	1.72937500	1.34326900
H	-6.51538000	2.73473200	0.41885800
H	-3.20110500	-0.26194400	1.77560100

4

0 imaginary frequency

H = -1740.801104

G = -1740.889311

Esol = -1741.157206

C	4.24509800	2.20409300	0.27998400
O	3.38273500	1.63164300	1.11524700
O	4.21895500	2.10544900	-0.93706400
C	5.29418100	3.00633100	1.03342000
H	5.82965400	2.35640800	1.73271900

H	5.99435800	3.44992700	0.32381800
H	4.80966200	3.79119700	1.62276200
I	1.69615600	0.60678500	0.20185100
O	-1.61952300	1.57132700	-1.64899900
C	-1.40767300	2.59598300	-0.81917000
O	-0.64184800	2.54428000	0.13319700
C	-2.22153000	3.81321600	-1.18508300
H	-2.01857100	4.10099300	-2.22175900
H	-3.28939800	3.57899600	-1.11666100
H	-1.97906600	4.63661400	-0.51279800
C	2.97663400	-1.09460700	-0.08512300
C	2.82071400	-2.20009000	0.74719400
C	3.93049200	-1.03443600	-1.09905500
C	3.66144000	-3.29727000	0.54156700
H	2.05562000	-2.22235000	1.51461900
C	4.76168800	-2.14313200	-1.28072600
H	4.04635100	-0.14165500	-1.70207200
C	4.62680400	-3.26930100	-0.46654300
H	3.55443500	-4.17253000	1.17553400
H	5.51463500	-2.11862900	-2.06329100
H	5.27565900	-4.12725500	-0.61791700
N	-0.02912000	-0.59327200	-0.76288600
S	-0.81304000	-1.77567000	0.14745400
O	-0.78401300	-3.04079600	-0.59869800
O	-0.32489300	-1.70269300	1.53196000
C	-2.52198000	-1.20303000	0.18346800
C	-3.44721400	-1.78327100	-0.68573200
C	-2.88807400	-0.20062800	1.08635800
C	-4.76955000	-1.34451000	-0.66348200
H	-3.13376300	-2.57488600	-1.35718600

C	-4.20728600	0.24310600	1.10809200
H	-2.15341100	0.22231300	1.76239400
C	-5.12302900	-0.33604200	0.23008400
H	-5.52073700	-1.76859500	-1.31797000
H	-4.53503000	1.01698700	1.79092600
N	-6.52107100	0.13529800	0.25121100
O	-6.80396600	1.03788400	1.03693100
O	-7.31361000	-0.40220400	-0.51970200
H	-1.08297500	0.78831300	-1.32963600
H	0.30129300	-1.05650600	-1.61360000

40

0 imaginary frequency

H = -4871.324707

G = -4871.422461

Esol = -4871.817037

Se	-1.48399300	0.31297900	-0.30721500
N	0.07471500	1.17293100	-0.40408700
N	-1.32893900	-0.91283800	1.13750200
S	0.61982600	1.81509500	1.02393900
O	0.68785700	0.77161800	2.08220400
O	-0.04578800	3.07611900	1.40232600
S	-1.47613000	-2.54729000	0.79482700
O	-2.33456200	-2.59586400	-0.39457100
O	-1.84331100	-3.22935800	2.03298700
C	0.16814400	-3.13686300	0.33564500
C	0.55404900	-4.39986700	0.78967100
C	0.99271400	-2.37327700	-0.49586200
C	1.78628300	-4.91816300	0.39686400

H	-0.09911600	-4.96028400	1.44896200
C	2.22441300	-2.88845700	-0.88847500
H	0.70186700	-1.38001500	-0.81924100
C	2.59719000	-4.15311100	-0.43676100
H	2.12329200	-5.89266600	0.72759800
H	2.89242100	-2.32942700	-1.53187400
N	3.90574800	-4.69713100	-0.85225500
O	4.20442700	-5.82091400	-0.45519600
O	4.61133300	-3.98937000	-1.56810000
C	2.30681600	2.21030300	0.54484300
C	3.25177400	1.18512300	0.45589500
C	2.64485100	3.54304700	0.31149100
C	4.56223800	1.49704600	0.10810500
H	2.96567100	0.16082400	0.66751700
C	3.95593600	3.86051600	-0.03803600
H	1.88988100	4.31480200	0.40968700
C	4.88808900	2.83092500	-0.13547000
H	5.32787100	0.73544700	0.02789200
H	4.26258700	4.88125000	-0.22918000
N	6.27810700	3.16497900	-0.50503500
O	7.08369000	2.23948500	-0.57970600
O	6.54129100	4.34730500	-0.71560800
C	-4.68839100	0.72306900	-1.50164500
C	-4.07221900	2.07347900	-1.51562300
C	-3.21569300	2.50384800	-0.56738500
C	-2.85568400	1.55740000	0.55631500
C	-4.02432800	0.67628400	1.00766900
C	-4.68555800	-0.02524900	-0.17858800
H	-2.34290300	2.05041200	1.38369700
H	-3.68527600	-0.05686900	1.74426600

H	-4.72664800	1.33709100	1.53032200
H	-4.49728600	-1.09461900	-0.23010200
C	-2.58814600	3.87139400	-0.57713700
H	-1.49556000	3.80414300	-0.59032100
H	-2.92014000	4.44708500	-1.44669200
H	-2.84964100	4.43341600	0.32897700
H	-4.33459800	2.74311100	-2.33449700
C	-6.00464000	0.43947500	-0.77201100
H	-4.53082400	0.13981100	-2.40894400
C	-6.79064400	1.57421300	-0.14017500
H	-6.15616500	2.40494700	0.18003000
H	-7.51644100	1.97667200	-0.85756600
H	-7.35376500	1.21821000	0.73204400
C	-6.88467300	-0.64335900	-1.37587700
H	-7.53158100	-1.09054900	-0.61044900
H	-7.53224400	-0.23207200	-2.16056600
H	-6.28823900	-1.44834800	-1.81902500
H	-0.62859300	-0.62295700	1.83423700

41

0 imaginary frequency

H = -4871.302423

G = -4871.401505

Esol = -4871.793563

Se	-1.32354800	0.70639700	1.14622000
N	-0.76191900	-0.12061800	-0.29509000
N	-0.95183100	2.38783700	1.04196200
S	-0.65771700	-1.79095300	-0.06127000
O	-1.11254200	-2.45899800	-1.28040000

O	-1.23275100	-2.16344100	1.24903900
S	-0.32312300	3.17419700	-0.32205800
O	-0.26835500	4.58237600	0.06567700
O	-1.01897600	2.75623900	-1.54510200
C	1.37088600	2.57292100	-0.41800600
C	2.32491200	3.11196900	0.45054800
C	1.70182600	1.60699400	-1.36967200
C	3.63771900	2.65491500	0.38458900
H	2.04286400	3.88721800	1.15469000
C	3.01378400	1.14268500	-1.43266400
H	0.93887700	1.22655600	-2.03746400
C	3.95304000	1.66752500	-0.54842700
H	4.41057700	3.04528300	1.03509000
H	3.31345500	0.38616700	-2.14697400
N	5.33552300	1.15318800	-0.59665800
O	6.18426900	1.74084000	0.06822700
O	5.54630800	0.16201800	-1.29567800
C	1.12790200	-2.01243300	0.06051600
C	1.82304800	-1.40154500	1.10772000
C	1.76830800	-2.83755300	-0.86303000
C	3.18805800	-1.62635700	1.24053600
H	1.30740600	-0.74464500	1.80074600
C	3.13923000	-3.06213200	-0.73540200
H	1.19750700	-3.29464800	-1.66355300
C	3.82199700	-2.45302700	0.31269100
H	3.76545800	-1.17594400	2.03821400
H	3.67845000	-3.69551000	-1.42879500
N	5.27277500	-2.69434000	0.45470000
O	5.79710400	-3.47121300	-0.33829400
O	5.85482400	-2.10831500	1.36440100

C	-4.26235700	-1.24154200	-1.02484400
C	-3.97631800	0.23907600	-1.21517000
C	-4.05209300	1.10096400	0.01000100
C	-4.10563100	0.56221200	1.26501600
C	-4.29107000	-0.89538500	1.58214700
C	-4.41208500	-1.81211100	0.37408200
H	-4.14814700	1.24907800	2.11135800
H	-3.44864600	-1.24062700	2.19758100
H	-5.17311700	-0.98274000	2.23620300
H	-3.96345100	-2.78854500	0.53534800
C	-4.06487600	2.58609000	-0.20049800
H	-3.30749800	2.89102300	-0.93006300
H	-5.04110400	2.88483200	-0.60857200
H	-4.61345500	0.67607600	-1.99817900
C	-5.60425200	-1.78458800	-0.56805200
H	-3.72114500	-1.86721700	-1.72947600
C	-6.78479500	-0.86105400	-0.31300800
H	-7.49993100	-1.33212600	0.37376200
H	-6.49877500	0.10096500	0.12090600
H	-7.32116600	-0.65563100	-1.24833100
C	-6.02240000	-3.12275400	-1.16093200
H	-6.70904000	-3.65411100	-0.48900400
H	-6.53722500	-2.98445200	-2.12063800
H	-5.15785900	-3.77208300	-1.33696200
H	-2.94627500	0.34590300	-1.59999800
H	-3.90359400	3.13804300	0.72969100

42

0 imaginary frequency

H = -4871.310992

G = -4871.408394

Esol = -4871.803313

Se	0.64921200	1.06517800	-0.59673500
N	1.75148300	0.02877800	0.30838700
N	-0.86935900	0.96772300	0.56082900
S	2.62000400	-0.97657700	-0.69492300
O	4.00759600	-0.97816400	-0.21479900
O	2.33329100	-0.65437700	-2.11063000
S	-1.81020100	-0.43843200	0.34548200
O	-1.78170900	-1.21447300	1.58398800
O	-1.40576400	-0.99639900	-0.94913000
C	-3.46998200	0.22903100	0.15310200
C	-4.30063800	0.30734900	1.27232300
C	-3.89576200	0.63542800	-1.11369100
C	-5.58594800	0.82426800	1.12616100
H	-3.95037400	-0.04587100	2.23586400
C	-5.17979200	1.15210500	-1.26186700
H	-3.23838400	0.53168600	-1.96984200
C	-5.99792700	1.24152400	-0.13714100
H	-6.26594900	0.90220200	1.96525300
H	-5.55445500	1.47716900	-2.22442600
N	-7.35929100	1.79481100	-0.29284500
O	-8.06192600	1.86115600	0.71304200
O	-7.69838000	2.15551300	-1.41760900
C	1.97851400	-2.63078200	-0.37403300
C	1.00405300	-3.16682300	-1.21780100
C	2.47947600	-3.34797500	0.71571200
C	0.51028500	-4.44330600	-0.96118800
H	0.64208500	-2.59236100	-2.06161700

C	1.98620400	-4.62236200	0.97758200
H	3.25557300	-2.91524100	1.33683200
C	1.00767600	-5.14628200	0.13392700
H	-0.24505600	-4.89600700	-1.59101000
H	2.34719700	-5.21190900	1.81092800
N	0.48443100	-6.49683900	0.40772700
O	0.93626100	-7.09706600	1.38211700
O	-0.37279400	-6.94235300	-0.35397900
C	3.88973200	2.42261500	0.51663700
C	2.99292100	2.47767700	1.75241200
C	1.54749700	2.90381300	1.51745500
C	1.03828500	2.94007700	0.11066900
C	2.00662700	3.57420900	-0.89593900
C	3.39589600	2.95684000	-0.81921000
H	0.03890700	3.37941000	0.04946600
H	1.60397000	3.46883300	-1.91065300
H	2.02089400	4.65158900	-0.68827000
H	3.66518800	2.36252400	-1.68977400
C	0.73938800	3.27064200	2.52435100
H	1.09280300	3.30006600	3.55222700
H	-0.29065700	3.57570000	2.35611700
H	3.42579600	3.12050800	2.52937000
C	4.55226700	3.63671800	-0.09814800
H	4.45175300	1.49583200	0.44582300
C	4.36052700	5.00515600	0.53290100
H	4.46300000	5.80218100	-0.21511700
H	3.38700900	5.12674800	1.01843700
H	5.12603500	5.17779000	1.29993400
C	5.93552700	3.43698200	-0.69767900
H	6.13702400	4.17777600	-1.48251500

H	6.71407300	3.54308900	0.06868600
H	6.03897500	2.44097900	-1.14126900
H	2.96369200	1.46427800	2.16481700
H	-0.53154200	1.01368200	1.52888900

42b

0 imaginary frequency

H = -464.655773

G = -464.704373

Esol = -464.885289

C	-1.11034800	-1.48401600	0.35328800
C	0.38155200	-1.32071500	0.46772600
C	0.89362800	-0.05077700	-0.25173000
C	0.01711800	1.13845500	0.16476300
C	-1.46266300	0.89774700	-0.10848500
C	-1.97234000	-0.49089500	0.06328200
H	0.66690500	-1.27515900	1.53153300
H	-1.50214900	-2.48830400	0.51820700
H	0.87107000	-2.21733800	0.06844700
C	-3.45696500	-0.68745200	-0.08471200
H	-3.79151900	-0.37778400	-1.08124800
H	-3.73725300	-1.73372800	0.07112000
H	-4.00694200	-0.06376200	0.62931700
O	-2.21251300	1.81547300	-0.41102500
C	2.38927800	0.15299400	-0.05748800
C	3.28116500	-0.87257500	-0.72022000
C	2.90952300	1.16824600	0.64027100
H	2.29992700	1.92859100	1.11783800
H	3.07951600	-0.93209700	-1.79855200

H	3.11986200	-1.88033000	-0.31555300
H	0.30882000	2.06378700	-0.34033400
H	3.98502200	1.27722500	0.75509900
H	0.12032900	1.31440600	1.24692000
H	0.72802500	-0.21824600	-1.32858600
H	4.33880900	-0.62711100	-0.58617300

43

0 imaginary frequency

H = -4871.297897

G = -4871.396822

Esol = -4871.789410

Se	-1.29354300	0.53919500	-1.19105000
N	-0.85949700	2.20160900	-1.36282700
N	-0.57716800	-0.12316400	0.26993500
S	-0.41339500	3.21320000	-0.08732900
O	-1.25337400	2.94033000	1.08815200
O	-0.36469800	4.55007200	-0.67655400
S	-0.56142000	-1.80712500	0.23392200
O	-1.31277100	-2.30125100	-0.94155500
O	-0.89442400	-2.31045700	1.56729000
C	1.18888200	-2.14169100	-0.05865100
C	1.78925500	-3.16879700	0.67034000
C	1.88352800	-1.44239500	-1.04949400
C	3.11029400	-3.51636500	0.39313100
H	1.22905500	-3.68089100	1.44460600
C	3.20109800	-1.78677600	-1.32975400
H	1.40930800	-0.62269000	-1.57739600
C	3.78869800	-2.82296000	-0.60513100

H	3.61455300	-4.30754700	0.93388600
H	3.77535200	-1.27012400	-2.08852100
N	5.18524300	-3.19591400	-0.90805900
O	5.68042900	-4.11327000	-0.25779200
O	5.75891500	-2.56689500	-1.79459600
C	1.27824300	2.75435400	0.32085400
C	1.52800800	1.97042900	1.44827000
C	2.31293400	3.23511600	-0.48733100
C	2.84464400	1.64814600	1.77011500
H	0.70266400	1.61989600	2.05528200
C	3.62876700	2.91020700	-0.17143900
H	2.08871100	3.87040800	-1.33723600
C	3.86850800	2.11973900	0.95188600
H	3.08533400	1.04621800	2.63742100
H	4.46148500	3.26294100	-0.76701800
N	5.26372400	1.77525600	1.29152700
O	5.44925400	1.06381600	2.27700700
O	6.15090000	2.21922700	0.56564800
C	-4.51240700	-1.73831300	-0.02690700
C	-4.43646900	-0.85734400	-1.26479300
C	-3.68528200	1.05643600	0.18762000
C	-4.09510400	-1.19035900	1.32517600
H	-3.44529200	2.11192400	0.29549700
H	-4.07887300	0.79094600	2.24475500
H	-3.55148000	-1.88012500	1.96490000
C	-4.22676800	1.51172100	-2.21887900
H	-3.77634900	1.08192900	-3.12332300
H	-5.29295800	1.65216300	-2.44213700
H	-3.78203600	2.49414700	-2.03995700
H	-3.68852200	-1.28818200	-1.94727000

C	-5.54953100	-1.54492800	1.06571700
H	-4.22810900	-2.76809100	-0.22754400
C	-6.61645500	-0.46729900	0.95675100
H	-7.46489300	-0.82336500	0.35806300
H	-7.00558200	-0.21208700	1.95066300
H	-6.25557000	0.45869900	0.50069200
C	-6.06020100	-2.81147800	1.73800600
H	-6.41007200	-2.60219900	2.75718300
H	-6.90150800	-3.24240800	1.17959600
H	-5.27746400	-3.57505700	1.80468800
H	-5.38187300	-0.88663900	-1.82834600
H	-2.52209300	0.21787700	1.71434600
C	-3.58915200	0.23781900	1.42888900
C	-4.07253200	0.58896300	-1.03894800

44

0 imaginary frequency

H = -4871.324728

G = -4871.422088

Esol = -4871.816616

Se	-1.31675600	0.54069000	-1.11609200
N	0.25247200	1.36230500	-0.94140800
N	-1.49897600	-0.58621800	0.37014900
S	0.55911700	2.10151400	0.50704800
O	0.24635600	1.19859400	1.64635100
O	0.03268100	3.47686500	0.59460100
S	-1.67296200	-2.22921000	0.13016900
O	-2.29033600	-2.35090900	-1.19448900
O	-2.30573500	-2.78098200	1.32730500

C	-0.00776900	-2.92224500	0.04725500
C	0.21160600	-4.16416400	0.64698600
C	1.00346400	-2.25524700	-0.65051100
C	1.46663500	-4.75960800	0.54019200
H	-0.58722200	-4.64840500	1.19723400
C	2.25847100	-2.84730600	-0.75660300
H	0.83228900	-1.27815200	-1.08827500
C	2.46564100	-4.09047300	-0.16157900
H	1.67893300	-5.72088400	0.99128200
H	3.06932600	-2.36294800	-1.28628800
N	3.79830800	-4.71708500	-0.27317600
O	3.95172300	-5.81945500	0.24772400
O	4.66747000	-4.09448200	-0.87961800
C	2.35016700	2.22636100	0.38839300
C	3.13774300	1.13385700	0.75865000
C	2.91648300	3.42749700	-0.03932400
C	4.52352000	1.23762300	0.68430100
H	2.66917000	0.22233000	1.11262900
C	4.30315900	3.53545100	-0.11880200
H	2.27631300	4.26386900	-0.29606400
C	5.07985300	2.43744100	0.24270000
H	5.17285800	0.41727500	0.96377300
H	4.78492000	4.44810400	-0.44660400
N	6.54951800	2.55075500	0.16315800
O	7.21364000	1.57145600	0.49677800
O	7.01660300	3.61710600	-0.23250300
C	-4.75137500	0.01092500	-0.40823600
C	-4.13355300	1.07705600	-1.30926600
C	-3.04224200	2.08216200	0.75949200
C	-4.60035800	0.17153700	1.08851200

H	-2.43430600	2.88495000	1.16645600
H	-3.84294200	1.55960300	2.62950500
H	-4.44199200	-0.73675700	1.66792400
C	-2.57995300	3.08359800	-1.52077400
H	-2.41782800	2.84207500	-2.57857700
H	-3.42029000	3.78694400	-1.46872100
H	-1.69176700	3.58389300	-1.12859200
H	-3.84067200	0.62754500	-2.26668200
C	-5.98059100	0.29990000	0.44164300
H	-4.66536100	-1.00277300	-0.78942000
C	-6.67455500	1.64797200	0.37147700
H	-7.31688700	1.71133700	-0.51671700
H	-7.31639300	1.78886200	1.24977800
H	-5.97281400	2.48635800	0.34562200
C	-6.93326900	-0.86352800	0.66482400
H	-7.48227600	-0.74756900	1.60789300
H	-7.67176700	-0.92337900	-0.14510400
H	-6.39975800	-1.81947600	0.70208300
H	-4.87721000	1.84307600	-1.56642500
H	-1.02671000	-0.24330400	1.21543200
C	-3.81489900	1.33065800	1.56514800
C	-2.94065600	1.84441400	-0.70126500

44a

0 imaginary frequency

H = -585.906027

G = -585.962047

Esol = -586.281016

C	1.80224700	-0.09248100	0.21760800
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C	0.58318600	0.75126300	-0.19286200
C	-0.78412500	0.25978800	0.37370100
C	-0.93142100	-1.23330200	0.04529900
C	0.26449400	-2.10895900	0.36107900
C	1.57370500	-1.55535800	-0.22618200
H	0.74946300	1.79325600	0.10478600
C	-1.92612700	1.07756100	-0.32071100
C	-2.03426700	-1.76006500	-0.50440000
H	0.38748900	-2.19701900	1.45177700
H	1.53039000	-1.58609400	-1.32349400
C	-3.28885900	-0.99568300	-0.82845400
C	-3.29118900	0.38591700	-0.16891600
H	-2.04157300	-2.82593900	-0.73680500
H	-3.38565700	-0.89234000	-1.92159000
H	-3.53892000	0.28547500	0.89656000
H	2.41223700	-2.19325200	0.07827700
H	-4.16861100	-1.57397800	-0.51233000
H	-4.07533700	1.01539600	-0.60905500
H	-1.68926300	1.07327600	-1.39611400
H	0.51095600	0.74453400	-1.28909500
C	-2.01605700	2.54731900	0.12011800
H	-2.36847900	2.64053000	1.15382400
H	-1.05608900	3.06897900	0.04503300
H	-2.73020600	3.08376000	-0.51579200
C	-0.81963100	0.45651700	1.91076900
C	3.13712100	0.44514700	-0.28523200
C	4.35975200	-0.07503400	0.43668800
H	5.28168500	0.33701200	0.01504500
H	4.32641900	0.18797900	1.50322200
H	4.42847200	-1.16955500	0.38814900

C	3.25833700	1.31812100	-1.29152300
H	4.23559200	1.66230500	-1.62153000
H	2.40490600	1.72483200	-1.82443000
H	-0.11111200	-0.20145300	2.42216600
H	-0.56283600	1.48589000	2.18452600
H	-1.81255700	0.23421000	2.31569700
H	0.08478600	-3.12569300	-0.00818300
H	1.86525600	-0.09661400	1.31745500

5'

0 imaginary frequency

H = -1511.639375

G = -1511.715776

Esol = -1511.925254

C	0.84691500	1.55398900	-1.22998300
O	0.96341100	0.88779300	-0.06210000
O	1.36754700	1.22153800	-2.27136400
C	-0.03807100	2.77093800	-1.03878700
H	0.24505500	3.32204600	-0.13842500
H	0.04318000	3.40884700	-1.91992000
H	-1.07360300	2.43605500	-0.91763200
I	1.99186900	-0.91836100	-0.20985700
C	3.71258200	0.31886800	0.27172000
C	4.15287200	0.38595000	1.59540300
C	4.40162900	0.97103600	-0.75371200
C	5.31356000	1.10470300	1.89254800
H	3.60520700	-0.11364800	2.38923500
C	5.55810700	1.69011400	-0.44529300
H	4.03668900	0.92969300	-1.77530900

C	6.01347700	1.75530200	0.87428200
H	5.66505200	1.15938100	2.91915300
H	6.10215900	2.19909000	-1.23619400
H	6.91422700	2.31549300	1.10910800
N	-0.19074800	-1.42601000	-0.87227500
S	-1.23926600	-2.13057400	0.17825600
O	-1.76262800	-3.38433500	-0.38973600
O	-0.64201700	-2.10252600	1.52090100
C	-2.62982700	-0.97715700	0.23326000
C	-3.80064700	-1.27763100	-0.46447000
C	-2.50825800	0.20386500	0.97387500
C	-4.86726300	-0.38050200	-0.43566500
H	-3.87253300	-2.21206300	-1.00987800
C	-3.56793800	1.10487400	1.00451100
H	-1.59612100	0.40397900	1.52485200
C	-4.73004600	0.79805600	0.29426400
H	-5.79282400	-0.57999400	-0.96132900
H	-3.51614100	2.02710600	1.56993900
N	-5.85109200	1.75231800	0.32276600
O	-5.69851800	2.79180600	0.96403900
O	-6.87019300	1.45493200	-0.29868700
H	-0.21163700	-1.90594800	-1.77286000

5

0 imaginary frequency

H = -1511.672632

G = -1511.748897

Esol = -1511.959033

C	-4.12812300	-2.38869400	-0.19615800
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O	-3.24909500	-1.98057600	0.70814700
O	-4.11475200	-2.08437700	-1.38150700
C	-5.18782100	-3.29164000	0.41682000
H	-5.72131400	-2.75399600	1.20736300
H	-5.88950000	-3.61188100	-0.35502200
H	-4.71456900	-4.16377200	0.87896400
I	-1.51900200	-0.85986200	-0.04584700
C	-2.75911300	0.91289600	0.01092000
C	-2.46768700	1.89066400	0.95517500
C	-3.79616700	1.00839000	-0.91086700
C	-3.27135700	3.03473000	0.96497700
H	-1.63739400	1.78574400	1.64417100
C	-4.58480600	2.16235900	-0.87317200
H	-4.00192000	0.20446200	-1.60798800
C	-4.32327500	3.16986600	0.05726500
H	-3.06610100	3.81717200	1.68959200
H	-5.40299000	2.26615800	-1.58008900
H	-4.94068200	4.06338800	0.07470600
N	0.21982000	0.32280000	-0.76182500
S	1.10081200	1.33697000	0.21258000
O	1.14153400	2.68376200	-0.37237700
O	0.65154900	1.12255900	1.59696400
C	2.77664000	0.67502000	0.11326100
C	3.66696900	1.21566900	-0.81689700
C	3.15450400	-0.36340200	0.96859700
C	4.95726300	0.69825900	-0.90754900
H	3.35506700	2.04211400	-1.44586000
C	4.44269200	-0.88367200	0.88225600
H	2.45295900	-0.74246800	1.70345900
C	5.31977200	-0.34585400	-0.05901400

H	5.67916200	1.09030100	-1.61307200
H	4.77713800	-1.68572200	1.52836600
N	6.68432900	-0.89690800	-0.15369100
O	6.97987900	-1.81631900	0.60760100
O	7.43982000	-0.40367600	-0.98915100
H	0.08679900	0.74989800	-1.67847200

6

0 imaginary frequency

H = -1511.668686

G = -1511.744198

Esol = -1511.953903

C	1.15394400	-2.46894000	0.52420500
O	0.68963900	-2.03784500	-0.58236500
O	0.76197300	-2.11588100	1.67228500
C	2.29989200	-3.46811200	0.42777600
H	3.20816600	-2.94192300	0.11144100
H	2.48004400	-3.93961900	1.39581000
H	2.07994700	-4.22413300	-0.33121600
I	-1.54479300	-0.89587400	-0.67588800
C	-3.47103400	0.02886300	-0.42713800
C	-4.52604500	-0.78099400	-0.00160300
C	-3.66201700	1.37638200	-0.73476300
C	-5.80351600	-0.22795300	0.10854800
H	-4.36304000	-1.82551600	0.24515400
C	-4.94415000	1.91657500	-0.61613100
H	-2.82787200	2.00085100	-1.03104300
C	-6.01122200	1.11795900	-0.19847000
H	-6.63055600	-0.84885800	0.44079200

H	-5.10435300	2.96591800	-0.84654500
H	-7.00548000	1.54631300	-0.10888300
N	-0.87609300	-0.13137100	1.17594300
S	-0.07601300	1.37392100	1.16061300
O	-0.75770900	2.24813200	0.20171200
O	0.01425500	1.69205600	2.58493600
H	-0.21758300	-0.93840000	1.52798400
C	1.60311200	1.12793700	0.55846800
C	1.93185600	1.56041800	-0.72762000
C	2.54785700	0.53834700	1.40416900
C	3.23511100	1.39029400	-1.18937000
H	1.18077600	2.03721300	-1.34666500
C	3.84969500	0.36399500	0.94290000
H	2.26963800	0.21749200	2.40092500
C	4.16751200	0.79162900	-0.34582500
H	3.53536400	1.71313700	-2.17822900
H	4.61427900	-0.08793200	1.56220200
N	5.54884600	0.60821700	-0.83390200
O	5.80770900	1.00734200	-1.96745700
O	6.35109000	0.06716200	-0.07593800

7

0 imaginary frequency

H = -1511.670943

G = -1511.747684

Esol = -1511.957439

C	-0.37089000	3.78134000	-0.55879200
O	-1.48786600	3.42853200	-0.19783300
O	0.59070500	2.93819100	-0.92723300

C	0.06012000	5.22589600	-0.62735100
H	-0.80403800	5.87824400	-0.49766100
H	0.78609000	5.42215800	0.16985100
H	0.55564600	5.43106700	-1.58098400
I	-2.35269100	0.70133200	-0.06915100
C	-3.05637500	-1.31746600	-0.29225800
C	-3.76340100	-1.62739300	-1.45428700
C	-2.82929200	-2.25474600	0.71403700
C	-4.27632700	-2.91842900	-1.60143500
H	-3.91509700	-0.88740600	-2.23358100
C	-3.34201100	-3.54311700	0.54316800
H	-2.24480000	-1.99841700	1.59027300
C	-4.06540400	-3.87317300	-0.60514400
H	-4.83097800	-3.17464000	-2.49955900
H	-3.17150600	-4.28843900	1.31478400
H	-4.46166500	-4.87736800	-0.72586500
N	-0.27803900	0.39166900	-0.21337200
S	0.38183900	0.14354800	1.31466900
O	0.52576700	1.37814300	2.10423800
O	-0.19662400	-1.03551600	1.99297400
H	0.28044600	1.99375300	-0.75583500
C	2.00785400	-0.30865000	0.67485400
C	2.92879400	0.70068200	0.38197300
C	2.32186700	-1.66075100	0.52051000
C	4.19257900	0.34938600	-0.08611500
H	2.65690400	1.74145600	0.51747200
C	3.58625400	-2.01570300	0.05867000
H	1.58542900	-2.41539400	0.77230900
C	4.49676000	-1.00240000	-0.23886500
H	4.93732000	1.09699800	-0.32853400

H	3.87565600	-3.05086200	-0.07212200
N	5.83587700	-1.37641900	-0.73241300
O	6.08057600	-2.57490300	-0.85990800
O	6.62316300	-0.46671300	-0.98643100

8

0 imaginary frequency

H = -1282.540193

G = -1282.605165

Esol = -1282.756963

I	2.21803800	-1.29560800	-0.53091100
C	3.32957900	0.54600100	-0.21981200
C	4.32212300	0.86402900	-1.14279600
C	3.02460800	1.34023300	0.88026000
C	5.06474900	2.02927500	-0.93170000
H	4.51961700	0.23523300	-2.00498400
C	3.77361400	2.50721700	1.06105200
H	2.22194200	1.07438200	1.56155800
C	4.79000500	2.84738800	0.16572900
H	5.84758000	2.29732500	-1.63545800
H	3.55573400	3.14810000	1.91058600
H	5.36605600	3.75520000	0.31992000
N	0.20431400	-0.71921000	-0.54733800
S	-0.40381100	-0.79739000	1.01324400
O	-0.50438000	-2.16450700	1.55733600
O	0.16086000	0.23815500	1.91051800
C	-2.05024200	-0.26319900	0.50183500
C	-3.02069700	-1.23152300	0.23680900
C	-2.32909600	1.10275300	0.41449400

C	-4.30095700	-0.82646600	-0.13253900
H	-2.77124800	-2.28223400	0.33326900
C	-3.60700100	1.51262600	0.04485600
H	-1.55584600	1.82678600	0.64477000
C	-4.56810000	0.53869300	-0.22462700
H	-5.08574900	-1.54139200	-0.34562700
H	-3.86934900	2.56006100	-0.03519000
N	-5.92260100	0.97070500	-0.61813000
O	-6.13537500	2.17985500	-0.69138500
O	-6.75451300	0.09517300	-0.84966400

9

0 imaginary frequency

H = -4488.196385

G = -4488.289058

Esol = -4488.827181

Se	0.00546600	0.03401500	-1.40207000
N	0.51408500	1.79387700	-1.15277700
S	1.42024000	2.03533400	0.18513400
O	1.76138700	3.46540000	0.21117400
O	0.82792100	1.44738600	1.42210200
C	2.97686300	1.12469600	-0.04666100
C	3.59184000	0.51955700	1.05142600
C	3.56992900	1.08821300	-1.31228800
C	4.81091300	-0.13405100	0.88832300
H	3.10734700	0.55946600	2.02068800
C	4.78771500	0.43799000	-1.48568500
H	3.07136000	1.56153600	-2.15179000
C	5.38786700	-0.16490100	-0.38000100

H	5.31523600	-0.61573700	1.71691000
H	5.27429300	0.38771200	-2.45186200
N	6.67047000	-0.86313200	-0.56010000
O	7.16065800	-0.87908000	-1.68926900
O	7.17818500	-1.39325700	0.42852700
P	-1.71604900	-0.24121000	0.06295300
C	-3.76072800	-3.10219400	-3.09215900
C	-4.51341200	-1.82287500	-2.70911100
C	-3.60598200	-0.80534100	-1.99627800
C	-2.90617300	-1.42396200	-0.76537200
C	-2.16536100	-2.73060100	-1.15154900
C	-3.09705200	-3.72727700	-1.85976700
H	-2.99043100	-2.86424700	-3.83969100
H	-4.44415400	-3.81983400	-3.56180900
H	-5.35495700	-2.08124400	-2.04948900
H	-2.83900400	-0.43288900	-2.68771400
H	-3.66622200	-1.66286000	-0.00760500
H	-1.32693900	-2.48504900	-1.81838700
H	-1.73106900	-3.20221000	-0.26462200
H	-3.87296000	-4.06101000	-1.15524100
H	-2.52345700	-4.61945900	-2.13864100
H	-4.94898900	-1.35080600	-3.59801300
H	-4.20734100	0.05671900	-1.69466500
C	-4.16571900	3.82448800	0.57511500
C	-2.97331000	3.76948800	-0.39031400
C	-2.66693700	2.32712100	-0.82428000
C	-2.39388200	1.45729100	0.42436000
C	-3.59939400	1.46896600	1.38919300
C	-3.94130000	2.91681300	1.79257600
H	-5.07618600	3.50425300	0.04635200

H	-4.34386700	4.85481800	0.90660800
H	-2.08145700	4.19756500	0.08693900
H	-3.52968800	1.93617500	-1.37597800
H	-1.52782300	1.89228800	0.94297200
H	-4.47114700	1.00607100	0.90409400
H	-3.38911700	0.88896300	2.29410200
H	-3.11421200	3.31651400	2.39564600
H	-4.82800300	2.91180600	2.43898700
H	-3.17432200	4.37892300	-1.27969400
H	-1.79956400	2.30533700	-1.48691400
C	-0.41442500	-2.95892500	3.77454900
C	-1.73270100	-2.17548000	3.84736100
C	-2.24051300	-1.77861200	2.44825100
C	-1.15488100	-0.97585900	1.69589100
C	0.14545500	-1.80322600	1.57831100
C	0.64998300	-2.19238700	2.97598200
H	-0.59852700	-3.93102100	3.29335000
H	-0.05023300	-3.17622000	4.78611000
H	-1.58520000	-1.26477400	4.44502500
H	-2.48364900	-2.69058000	1.88621400
H	-0.90486500	-0.07551800	2.27083200
H	-0.04399700	-2.71637500	0.99706000
H	0.90162500	-1.23396600	1.03548500
H	0.93234800	-1.27875500	3.51771800
H	1.56116400	-2.79566400	2.88048500
H	-2.50239800	-2.76592700	4.35998800
H	-3.17239400	-1.21010100	2.54309300

HOAc

0 imaginary frequency

H = -229.113185

G = -229.145579

Esol = -229.180729

H	-1.72377500	-0.80229300	0.00003100
O	-0.77913100	-1.04652400	-0.00001100
C	-0.09225200	0.12591100	0.00002100
O	-0.64494600	1.20235700	-0.00000500
C	1.39728100	-0.11041700	0.00001100
H	1.91785300	0.84735600	0.00033300
H	1.68415500	-0.69268300	0.88183100
H	1.68421400	-0.69200300	-0.88225300

IMe

0 imaginary frequency

H = -304.787958

G = -304.826819

Esol = -304.922906

C	-0.00001100	-0.98812200	-0.00009200
C	-0.67825200	1.21832200	0.00002000
C	0.67830300	1.21831700	0.00004800
H	-1.38340500	2.03698600	0.00018400
H	1.38350400	2.03694600	-0.00029200
N	-1.06266400	-0.11928400	-0.00009600
N	1.06265200	-0.11930500	-0.00012100
C	-2.44185100	-0.57397100	0.00006500
H	-2.42331600	-1.66416000	0.00017500
H	-2.97283600	-0.21959700	0.89121800
H	-2.97301100	-0.21976200	-0.89104900

C	2.44182700	-0.57399200	0.00009100
H	2.97292800	-0.21921200	0.89101600
H	2.42326600	-1.66418200	0.00074900
H	2.97286500	-0.22023000	-0.89126700

NsNH2

0 imaginary frequency

H = -1040.806527

G = -1040.856638

Esol = -1040.949225

N	-2.95330300	-0.00041900	1.50489500
S	-2.52701600	0.00007300	-0.13377800
O	-2.94589100	-1.28594200	-0.69512100
O	-2.94580300	1.28618500	-0.69493100
H	-3.48255700	0.84131500	1.72338000
H	-3.48471000	-0.84114500	1.72205400
C	-0.72720000	0.00004900	-0.08242300
C	-0.04784300	1.21976700	-0.07160700
C	-0.04791200	-1.21971900	-0.07157500
C	1.34395100	1.22181300	-0.02931600
H	-0.60249900	2.15059600	-0.11207200
C	1.34387800	-1.22184100	-0.02929200
H	-0.60262400	-2.15051400	-0.11200800
C	2.01306800	-0.00003100	-0.00411000
H	1.91128600	2.14406100	-0.02107700
H	1.91113200	-2.14413500	-0.02103600
N	3.48872600	-0.00003400	0.04242700
O	4.05629100	-1.09039400	0.06108200
O	4.05622800	1.09035200	0.06145600

OIMe

0 imaginary frequency

H = -380.093676

G = -380.135393

Esol = -380.234814

C	0.00001100	-0.66778000	-0.00009100
C	-0.67612000	1.51429500	0.00005200
C	0.67616600	1.51428200	-0.00008900
H	-1.37585600	2.33567900	0.00031300
H	1.37595900	2.33561300	-0.00039500
N	-1.10009200	0.18577000	0.00039900
N	1.10006900	0.18569700	-0.00040300
C	-2.46250800	-0.30170200	-0.00009800
H	-3.00393800	0.03564100	0.89140300
H	-3.00242300	0.03275000	-0.89362800
H	-2.41148600	-1.39222600	0.00166400
C	2.46250700	-0.30173000	0.00018600
H	3.00328200	0.03338700	-0.89256500
H	3.00301200	0.03506500	0.89246000
H	2.41160100	-1.39226500	0.00114600
O	-0.00004000	-1.89601300	-0.00001600

OPCy3

0 imaginary frequency

H = -1122.295179

G = -1122.362019

Esol = -1122.807067

O	-0.00008600	0.12547800	2.26257000
P	0.00002800	-0.11397500	0.77127400
C	0.00026800	4.47866000	-0.27438300
C	-1.26212300	3.66939900	-0.59626100
C	-1.26579600	2.30878500	0.12017700
C	0.00006600	1.47798700	-0.19880700
C	1.26622100	2.30857800	0.11947800
C	1.26235700	3.66920300	-0.59695100
H	0.00058200	4.74093400	0.79358600
H	0.00018700	5.42475000	-0.83060400
H	-1.32189300	3.50772500	-1.68312300
H	-1.31652800	2.46242100	1.20606200
H	-0.00024700	1.22522300	-1.26987400
H	1.31759900	2.46220800	1.20533600
H	2.16987100	1.75680900	-0.16097100
H	1.32150100	3.50751200	-1.68384500
H	2.16127900	4.23324500	-0.31673600
H	-2.16080100	4.23358400	-0.31554800
H	-2.16968400	1.75713700	-0.15974300
C	-4.24276300	-1.84553800	-0.59444200
C	-3.81634900	-1.89748600	0.88031000
C	-2.68455000	-0.90159700	1.17863400
C	-1.47618700	-1.14351300	0.24607100
C	-1.90169400	-1.07355700	-1.23644200
C	-3.04481800	-2.06233900	-1.53043000
H	-4.69291400	-0.86407200	-0.80588200
H	-5.01955100	-2.59423800	-0.79565100
H	-3.47780200	-2.91545600	1.12488200
H	-3.06232400	0.12025700	1.04084700
H	-1.13335200	-2.17288600	0.43917100

H	-2.24020200	-0.05697800	-1.47811800
H	-1.05666000	-1.28672100	-1.90151600
H	-2.67012200	-3.08934200	-1.40792200
H	-3.35631400	-1.96724800	-2.57871200
H	-4.67496700	-1.69070100	1.53189500
H	-2.36126100	-0.97186400	2.22130700
C	4.24247000	-1.84594000	-0.59471500
C	3.04419800	-2.06354500	-1.53010400
C	1.90105800	-1.07472800	-1.23633700
C	1.47618400	-1.14364300	0.24642400
C	2.68487100	-0.90100500	1.17837000
C	3.81665100	-1.89698000	0.88023000
H	4.69238300	-0.86454400	-0.80698900
H	5.01930200	-2.59465000	-0.79572300
H	2.66970000	-3.09052100	-1.40676100
H	2.23928300	-0.05826700	-1.47892800
H	1.13351700	-2.17291200	0.44039100
H	3.06250700	0.12079200	1.03983400
H	2.36197300	-0.97068700	2.22120600
H	3.47828900	-2.91481900	1.12559900
H	3.35529500	-1.96912300	-2.57856500
H	1.05574200	-1.28853900	-1.90084000
H	4.67551200	-1.68969200	1.53133400

P

0 imaginary frequency

H = -1196.786917

G = -1196.846795

Esol = -1197.024617

N	-2.17154600	0.22107700	0.95640200
S	-1.39540600	1.16077600	-0.20543400
O	-1.43520100	2.55720300	0.24239400
O	-1.87870100	0.76635800	-1.53229500
C	-2.83914900	-3.07316500	0.06837000
C	-2.93956700	-1.79604700	-0.30259900
C	-3.32462700	-0.68079300	0.64219600
H	-2.78493800	-1.51117800	-1.34039700
H	-3.53980100	-1.13575300	1.61658600
H	-2.60138500	-3.85651600	-0.64649700
H	-2.99775900	-3.38922200	1.09781200
C	-4.57308700	0.07550900	0.16089600
H	-4.84842700	0.86319900	0.87188300
H	-4.39552000	0.53610000	-0.81462900
H	-5.41846300	-0.61556900	0.07237700
C	0.32309400	0.62544200	-0.07502900
C	0.64465800	-0.72872000	-0.20550600
C	1.30794200	1.59819400	0.09879500
C	1.97877600	-1.11783400	-0.15595300
H	-0.13784100	-1.47084100	-0.32598000
C	2.64675300	1.21241400	0.14659800
H	1.02334600	2.63940300	0.19947500
C	2.95680200	-0.13829700	0.01805000
H	2.27170900	-2.15625200	-0.24730200
H	3.44156800	1.93529000	0.28176600
N	4.37219700	-0.55099400	0.07262300
O	4.61947300	-1.75036300	-0.04131100
O	5.21618600	0.32941500	0.22901600
H	-2.35419200	0.81722900	1.76131800

PCy3

0 imaginary frequency

H = -1047.005011

G = -1047.070237

Esol = -1047.510891

P	0.00001600	-0.12172600	-1.02245700
C	-0.00007200	4.46262100	0.18607000
C	1.26346600	3.64153700	0.47408400
C	1.25980100	2.30563000	-0.28894900
C	-0.00001900	1.46304000	0.01533600
C	-1.25977300	2.30562900	-0.28928000
C	-1.26366400	3.64151500	0.47378300
H	0.00004700	4.76797600	-0.87080700
H	-0.00014300	5.38650600	0.77876400
H	1.32742800	3.44095100	1.55399700
H	1.30194400	2.50529900	-1.36977200
H	-0.00016100	1.21315000	1.08604300
H	-1.30160900	2.50532200	-1.37011100
H	-2.16938000	1.74733900	-0.04370300
H	-1.32787400	3.44090300	1.55367700
H	-2.16133800	4.21594300	0.21007100
H	2.16119200	4.21597800	0.21056900
H	2.16934700	1.74736800	-0.04308600
C	4.24113300	-1.79082300	0.55428300
C	3.84060400	-1.92845400	-0.92130100
C	2.69988500	-0.96615600	-1.29231900
C	1.47111400	-1.14484700	-0.36992400
C	1.88306100	-1.00872700	1.11092100
C	3.02678900	-1.97379500	1.47503600

H	4.67424900	-0.79304000	0.72068900
H	5.02442300	-2.51683100	0.80773800
H	3.51592100	-2.96244600	-1.11213500
H	3.06818200	0.06721900	-1.22465500
H	1.12088400	-2.17940500	-0.51662600
H	2.21295200	0.01928700	1.31265900
H	1.02814600	-1.19368600	1.77012100
H	2.66402100	-3.00934600	1.39317800
H	3.31688700	-1.82787800	2.52400000
H	4.70730100	-1.74974800	-1.57108200
H	2.40262000	-1.11641900	-2.33700800
C	-4.24114300	-1.79086700	0.55420100
C	-3.02689800	-1.97360400	1.47511400
C	-1.88315500	-1.00854100	1.11095200
C	-1.47102100	-1.14490400	-0.36977400
C	-2.69972200	-0.96645200	-1.29237300
C	-3.84041300	-1.92874600	-0.92131200
H	-4.67434900	-0.79308200	0.72036200
H	-5.02441400	-2.51688400	0.80768400
H	-2.66406500	-3.00915100	1.39348700
H	-2.21313300	0.01948400	1.31249000
H	-1.12068600	-2.17944800	-0.51629400
H	-3.06805400	0.06692400	-1.22493200
H	-2.40229800	-1.11689200	-2.33698700
H	-3.51563000	-2.96275100	-1.11190300
H	-4.70705000	-1.75024300	-1.57123200
H	-3.31708000	-1.82748900	2.52402600
H	-1.02834700	-1.19335900	1.77033900

PhI

0 imaginary frequency

H = -243.024351

G = -243.062953

Esol = -243.121488

I	-1.56710000	0.00000600	-0.00001600
C	0.58139700	0.00010800	0.00017100
C	1.26401000	-1.21572600	0.00007000
C	1.26396800	1.21564700	0.00005900
C	2.66140500	-1.20731500	-0.00000800
H	0.72229200	-2.15522000	0.00006700
C	2.66164500	1.20719800	0.00001600
H	0.72247900	2.15527400	-0.00019100
C	3.36184500	0.00004400	-0.00004900
H	3.19885300	-2.15181900	-0.00031900
H	3.19892500	2.15180800	-0.00010100
H	4.44812900	-0.00007500	-0.00014300

S1

0 imaginary frequency

H = -4645.333412

G = -4645.437403

Esol = -4646.080188

Se	-2.20104600	0.10147100	0.37547700
N	-2.67119500	1.19409200	-0.97216200
S	-2.59824700	2.81158800	-0.61158600
O	-3.33074700	3.15041300	0.62960600
O	-2.91921500	3.51762400	-1.85458900
C	-3.69388600	0.33919200	1.84382400

C	-4.09177600	-0.72028700	0.95360500
C	-5.11246800	-0.56703700	-0.14111900
H	-3.88532000	-1.74094500	1.27576400
H	-6.09886400	-0.76133800	0.30741400
H	-5.11896700	0.46905300	-0.49335700
H	-3.27763300	0.09647600	2.81788100
H	-4.08615100	1.34497100	1.71806000
C	-4.86073900	-1.52327400	-1.31101700
H	-4.89843100	-2.57049700	-0.98682300
H	-5.61012800	-1.38458700	-2.09549900
H	-3.87245300	-1.32986300	-1.73894000
C	-0.85217900	3.10616700	-0.25195500
C	0.02395500	3.34665000	-1.31302000
C	-0.38718600	2.97712500	1.05978200
C	1.39047800	3.42965800	-1.06828900
H	-0.37116500	3.46352700	-2.31627300
C	0.97975200	3.05278900	1.31148400
H	-1.09327800	2.83820700	1.87051400
C	1.84604600	3.25845800	0.23930000
H	2.10172900	3.60606600	-1.86546000
H	1.38125200	2.94734100	2.31152600
N	3.29350400	3.26460000	0.49053600
O	4.04278100	3.43250000	-0.47282700
O	3.67853500	3.07583600	1.64549000
P	1.04217300	-1.08303300	0.03735700
C	-0.91296800	-2.98244400	3.96988900
C	0.26351500	-2.00605600	4.09727200
C	0.50048900	-1.23627900	2.78882500
C	0.71468200	-2.17478100	1.57534600
C	-0.48309700	-3.14192400	1.46147300

C	-0.72362800	-3.91810900	2.76863000
H	-1.84601900	-2.41080000	3.84150500
H	-1.03281700	-3.56469300	4.89214500
H	1.17320400	-2.56747600	4.35606200
H	-0.36700600	-0.59295000	2.57494800
H	1.61139700	-2.78459200	1.76062600
H	-1.38998900	-2.57020900	1.21043900
H	-0.33229700	-3.85513600	0.64433900
H	0.13846600	-4.57467400	2.95595800
H	-1.59471800	-4.57674500	2.65406800
H	0.08979200	-1.30148700	4.92097600
H	1.35183300	-0.55642400	2.90467400
C	5.66068200	-0.00020500	-0.20558100
C	4.96853100	-0.50054300	-1.48002500
C	3.43626100	-0.44888900	-1.35101100
C	2.92557700	-1.23235300	-0.12122400
C	3.63806000	-0.72964100	1.15491200
C	5.17015800	-0.78114800	1.02030300
H	5.44547200	1.06877100	-0.06875500
H	6.75006600	-0.09114800	-0.30321300
H	5.28024400	-1.53638900	-1.68252700
H	3.12001300	0.60032900	-1.26558600
H	3.18209700	-2.29433700	-0.25303700
H	3.33450800	0.30624800	1.36321300
H	3.33608900	-1.32561900	2.02398100
H	5.49005700	-1.83079500	0.93607100
H	5.62989700	-0.38576100	1.93486300
H	5.28349500	0.09555300	-2.34591200
H	2.98055400	-0.83510600	-2.26979400
C	0.08891100	-3.18699800	-4.16889800

C	-0.72059000	-1.96413200	-3.71392800
C	-0.00389700	-1.18444800	-2.59869500
C	0.35225400	-2.10369100	-1.40658400
C	1.15739400	-3.33361800	-1.86636400
C	0.42854900	-4.10211900	-2.98352400
H	1.02249700	-2.84791000	-4.64223500
H	-0.46280600	-3.74681500	-4.93492000
H	-1.70230000	-2.29811600	-3.34429500
H	0.90497000	-0.72300900	-3.00790600
H	-0.61148300	-2.46352400	-1.01851100
H	2.13828900	-3.01336900	-2.24248300
H	1.35601500	-4.00419000	-1.01995100
H	-0.50093200	-4.53162900	-2.58020700
H	1.04345000	-4.94838400	-3.31684700
H	-0.92088600	-1.29915300	-4.56340700
H	-0.64109200	-0.36302000	-2.25080300

S10

0 imaginary frequency

H = -4563.435156

G = -4563.529990

Esol = -4564.070936

Se	0.15815200	-0.34349900	-2.22140700
N	1.35036000	0.31652500	-1.11398600
S	1.88752400	-0.71705400	0.11612900
O	1.39022000	-0.19232900	1.41145100
O	1.71662900	-2.15863600	-0.14785700
C	3.65358800	-0.36172500	0.05221800
C	4.12967400	0.84827300	0.56328000

C	4.51424000	-1.31178900	-0.49908600
C	5.49317500	1.12047800	0.51196000
H	3.43970300	1.55976100	1.00247500
C	5.88088400	-1.04666100	-0.54924300
H	4.11152500	-2.24709900	-0.87161800
C	6.34445100	0.16682200	-0.04555800
H	5.90426200	2.04585700	0.89553600
H	6.58369100	-1.75767400	-0.96525200
N	7.78998900	0.45139900	-0.09865100
O	8.52247900	-0.40437500	-0.59315000
O	8.17655900	1.52805000	0.35430400
O	-1.82288300	-0.01535600	-1.55283900
P	-2.30638800	0.10616900	-0.06807500
C	-6.73518400	0.58453400	-1.62911900
C	-6.06645100	1.79451100	-0.96576100
C	-4.53959800	1.63065800	-0.88000500
C	-4.14658600	0.32463200	-0.14865700
C	-4.82875400	-0.89250100	-0.81949700
C	-6.35356000	-0.71217000	-0.90507400
H	-6.41584000	0.52249800	-2.67945500
H	-7.82496300	0.70926500	-1.63871300
H	-6.47412900	1.92580400	0.04756400
H	-4.11210700	1.61220300	-1.89057600
H	-4.48473000	0.38918100	0.89662300
H	-4.41378000	-1.01658600	-1.82774400
H	-4.60370100	-1.81193400	-0.27055300
H	-6.77505100	-0.69991700	0.11100700
H	-6.79176300	-1.57991800	-1.41338900
H	-6.30049100	2.71364800	-1.51695600
H	-4.11210800	2.50011200	-0.37144600

C	-0.98998200	4.32679000	1.67669500
C	-0.29941100	3.76798400	0.42437400
C	-1.14914900	2.68647900	-0.26057600
C	-1.47962900	1.55509700	0.74435700
C	-2.20061900	2.10787300	1.99496700
C	-1.35243300	3.20627400	2.66171900
H	-1.90622200	4.85897400	1.37948700
H	-0.34686000	5.06629000	2.16992700
H	0.67135300	3.33347000	0.69996500
H	-2.07222700	3.14122000	-0.64231500
H	-0.51980300	1.13023500	1.07142800
H	-3.17635500	2.52778800	1.71375600
H	-2.39633900	1.31198400	2.72261700
H	-0.43122100	2.75295200	3.05345200
H	-1.89499700	3.61373800	3.52412600
H	-0.09118300	4.57506200	-0.28895300
H	-0.61516600	2.27459400	-1.12002900
C	-2.09278900	-4.11596400	2.10890200
C	-2.20827500	-2.84985600	2.96924000
C	-2.74600700	-1.65687400	2.15882700
C	-1.86157900	-1.40802800	0.91409700
C	-1.76654800	-2.67884300	0.03191800
C	-1.24060800	-3.86404200	0.85717100
H	-3.10034600	-4.44117800	1.80773700
H	-1.66599000	-4.93424700	2.70216900
H	-1.21914500	-2.58987300	3.37112100
H	-3.77845500	-1.87063000	1.84977500
H	-0.84627200	-1.18489900	1.27021100
H	-2.75351800	-2.92885400	-0.37880100
H	-1.10029900	-2.49150900	-0.81405300

H	-0.20155600	-3.65789700	1.14316600
H	-2.86287600	-3.02851900	3.83180900
H	-2.78570000	-0.76962300	2.80143400
H	-1.21866600	-4.76100600	0.22564600

S11

0 imaginary frequency

H = -5846.001267

G = -5846.135282

Esol = -5846.855624

Se	-0.63244300	-0.91356700	-0.19801700
N	0.14024200	-1.60678800	-1.61227700
S	0.42275600	-0.57120900	-2.91625400
O	0.19362300	0.86293600	-2.62690100
O	-0.16409700	-1.14634000	-4.13543500
C	2.21536300	-0.80342200	-3.03661400
C	3.05270700	-0.14955700	-2.12752900
C	2.72636200	-1.66777800	-4.00575300
C	4.42139300	-0.39530200	-2.16242900
H	2.63483100	0.52142300	-1.38519200
C	4.09833000	-1.91080300	-4.05376900
H	2.04665900	-2.14543300	-4.70277700
C	4.91968800	-1.28455600	-3.11719700
H	5.09980000	0.07960500	-1.46479800
H	4.53222800	-2.58223900	-4.78454000
N	6.35686300	-1.59287100	-3.11284500
O	6.80790000	-2.25327900	-4.04606500
O	7.02646600	-1.18244900	-2.16007800
I	2.19708300	-1.88647600	1.73395100

C	4.28888700	-1.52543400	2.11948300
C	4.66229900	-0.92140600	3.31793300
C	5.20123300	-1.86341800	1.12145100
C	6.02168300	-0.67286600	3.52442400
H	3.92198200	-0.62539300	4.05186700
C	6.55474400	-1.59940500	1.34664000
H	4.87881700	-2.30673300	0.18616800
C	6.96073500	-1.01080900	2.54637300
H	6.34061700	-0.20291800	4.45029300
H	7.27564400	-1.83761900	0.57061700
H	8.01352400	-0.80397500	2.71533400
N	1.58245600	-0.02260100	1.02189800
S	1.03495500	0.96772600	2.27654500
O	-0.40073100	0.76633800	2.56831000
O	1.95557900	0.97623700	3.43215500
C	1.22665700	2.52294700	1.38269500
C	0.63083200	2.70502900	0.12950800
C	1.96072900	3.53483500	2.00619000
C	0.78138500	3.93120800	-0.51459700
H	0.09050500	1.90150300	-0.35988200
C	2.09277100	4.76725300	1.37093400
H	2.41724900	3.35142200	2.97218700
C	1.50018100	4.94225200	0.12168900
H	0.35593100	4.10096900	-1.49577500
H	2.64492700	5.58258800	1.82132600
N	1.64548200	6.24651500	-0.55236700
O	2.30623800	7.11198800	0.02047500
O	1.09532500	6.38804800	-1.64232800
O	-2.81481200	-1.33148300	-0.61940500
P	-3.97181300	-0.49040400	-0.02562400

C	-7.11373300	-3.53600800	-1.77542000
C	-6.91482900	-2.19117100	-2.48573000
C	-5.61695200	-1.49967400	-2.03800200
C	-5.56753900	-1.31289500	-0.50020300
C	-5.77899900	-2.66831900	0.21319900
C	-7.07340800	-3.35769500	-0.25258500
H	-6.31795700	-4.22987000	-2.08222300
H	-8.06405400	-3.99209000	-2.07966500
H	-7.77184900	-1.53525700	-2.27114000
H	-4.75077600	-2.09828300	-2.34502200
H	-6.37414200	-0.62924300	-0.19699100
H	-4.91913600	-3.31864400	0.00662000
H	-5.82023300	-2.52711100	1.29801500
H	-7.93744000	-2.75527000	0.06551300
H	-7.16794700	-4.32785600	0.25117600
H	-6.89312400	-2.33098500	-3.57353000
H	-5.52389200	-0.53470000	-2.54732700
C	-4.50399200	3.57445700	-2.47312600
C	-3.13633600	2.87877300	-2.43099200
C	-3.25146000	1.40138100	-2.02249000
C	-3.98117900	1.26650400	-0.66475900
C	-5.37358400	1.93960200	-0.72817100
C	-5.24782000	3.41773500	-1.13908400
H	-5.11065700	3.13426000	-3.27843000
H	-4.38635100	4.63773500	-2.71654300
H	-2.48605700	3.40012500	-1.71243900
H	-3.80319500	0.85336900	-2.79733100
H	-3.38248100	1.81230800	0.08105000
H	-5.99821900	1.41964400	-1.46654800
H	-5.89857100	1.86930600	0.23155300

H	-4.70755000	3.96447100	-0.35237900
H	-6.24774500	3.86583700	-1.20054100
H	-2.63723800	2.94483400	-3.40462300
H	-2.25609300	0.95614700	-1.97347300
C	-4.11121300	-0.81597000	4.72908100
C	-4.62529800	0.46867700	4.06420300
C	-4.96799800	0.25098000	2.57873600
C	-3.76134200	-0.34054500	1.81690100
C	-3.26549200	-1.64740600	2.48170700
C	-2.91752100	-1.39990100	3.95925100
H	-4.92353400	-1.55783600	4.76254900
H	-3.83093000	-0.61262500	5.77014600
H	-3.85451200	1.24847800	4.13976700
H	-5.82657600	-0.43120000	2.50071700
H	-2.92984100	0.37808700	1.89370000
H	-4.03957100	-2.42192100	2.41984900
H	-2.39272500	-2.02857200	1.94323300
H	-2.06612500	-0.70911100	4.01385200
H	-5.51015200	0.84743100	4.59142400
H	-5.28086700	1.20463600	2.13882900
H	-2.59462400	-2.34253600	4.41987700

S12

0 imaginary frequency

H = -5603.033057

G = -5603.150422

Esol = -5603.789334

Se	0.30727200	-0.39884000	-1.51100500
N	-0.03391600	-2.07076300	-1.67391000

S	-0.58732500	-3.07951500	-0.45158700
O	-0.00333200	-2.73458500	0.85396800
O	-0.45178800	-4.43493600	-0.98405100
C	-2.35158000	-2.71517500	-0.37441300
C	-2.83758300	-1.87353700	0.62641800
C	-3.19748400	-3.28527800	-1.33009800
C	-4.19583800	-1.56844100	0.65628700
H	-2.15418800	-1.45745400	1.35575300
C	-4.55606900	-2.98428200	-1.30297900
H	-2.79349200	-3.96002700	-2.07687100
C	-5.02753900	-2.11944300	-0.31570500
H	-4.61309100	-0.91256700	1.40956100
H	-5.24646700	-3.40084600	-2.02581900
N	-6.45892500	-1.76719500	-0.30274600
O	-6.82574700	-0.90630300	0.49748700
O	-7.19669300	-2.34799900	-1.09592100
N	-0.57203700	0.24717600	-0.13513800
S	-0.76574200	1.90345300	-0.20439600
O	-0.13591700	2.52606800	0.97222000
O	-0.42045600	2.42317400	-1.54569800
C	-2.54647300	2.06362100	0.00935800
C	-3.06689500	2.19994000	1.29808800
C	-3.36983600	2.06117100	-1.11862700
C	-4.44448800	2.32468400	1.46470800
H	-2.39801800	2.22543000	2.15111500
C	-4.74711100	2.18603600	-0.95527400
H	-2.93456400	1.97914200	-2.10863900
C	-5.25917300	2.31086700	0.33454700
H	-4.89189100	2.43868100	2.44431700
H	-5.42269600	2.19447200	-1.80154200

N	-6.71889300	2.45948000	0.50860400
O	-7.14247600	2.57475400	1.65610300
O	-7.41099500	2.47048100	-0.50597000
O	2.32149200	-0.68185900	-0.80876200
P	3.35449700	0.00404900	0.14278500
C	7.77258700	-0.90850500	-1.42033800
C	6.56348100	-1.13544700	-2.33931200
C	5.34118900	-0.32727200	-1.87261100
C	4.99419300	-0.67311200	-0.40778300
C	6.19936700	-0.41118800	0.52291800
C	7.42708600	-1.20880500	0.04536500
H	8.10235200	0.13734200	-1.50784600
H	8.61729700	-1.52932400	-1.74278600
H	6.30601500	-2.20418500	-2.35242000
H	5.57367400	0.74244400	-1.95470300
H	4.78097800	-1.75227600	-0.38130700
H	6.44469700	0.65816000	0.52504300
H	5.96595000	-0.68488100	1.55788900
H	7.22156100	-2.28299600	0.15904500
H	8.28270500	-0.98435700	0.69411600
H	6.81180700	-0.86135700	-3.37193000
H	4.48137900	-0.52502600	-2.52092000
C	1.69233600	-1.98898000	4.06750900
C	1.60048800	-0.46313200	3.94363700
C	1.78590400	0.00551600	2.49053800
C	3.11859400	-0.51298000	1.90153900
C	3.22086600	-2.05324900	2.03998000
C	3.02194500	-2.49897700	3.49838600
H	0.86459900	-2.44943300	3.51255300
H	1.58739500	-2.29263600	5.11671800

H	2.36808100	0.00345800	4.57999600
H	0.95659200	-0.36656900	1.87922200
H	3.94865300	-0.05232000	2.45981300
H	2.45030300	-2.51561300	1.41325000
H	4.19385300	-2.41165900	1.68304300
H	3.85390500	-2.12395300	4.11407900
H	3.06499600	-3.59387800	3.54619800
H	0.63145500	-0.10465800	4.31234900
H	1.73866100	1.09847100	2.45305300
C	3.80135500	4.67373800	-0.60225300
C	3.94248900	4.13308500	0.82795700
C	4.26903100	2.62919400	0.83350200
C	3.19646900	1.84358100	0.04628800
C	3.07259300	2.37164600	-1.40398300
C	2.75987600	3.87711900	-1.40098900
H	4.77668500	4.61541700	-1.10889600
H	3.52682600	5.73535300	-0.57673600
H	3.00403600	4.29735300	1.37521900
H	5.25357100	2.47800500	0.37126300
H	2.22943900	2.02970800	0.53455000
H	4.00774300	2.19562700	-1.94938000
H	2.28351500	1.83270500	-1.93704200
H	1.76226300	4.03060000	-0.97268000
H	4.72541200	4.67831300	1.36974700
H	4.34264900	2.26852600	1.86691100
H	2.71471900	4.23801300	-2.43580000

S13

0 imaginary frequency

H = -5760.209673

G = -5760.340768

Esol = -5761.083006

Se	-0.70802800	-1.71456000	-0.67489900
N	-0.92626200	-2.38392200	0.89048700
N	0.99414000	-1.75780600	-1.07942300
S	0.16244700	-3.27974200	1.78944900
O	0.59786000	-4.47657200	1.05489300
O	-0.48744000	-3.43453500	3.09426100
S	1.27401600	-1.17043600	-2.63140500
O	-0.00643100	-0.74548200	-3.24593600
O	2.12437200	-2.11793100	-3.35506300
C	-1.85923700	-3.75316000	-2.35994500
C	-0.99762100	-4.62593000	-1.79932300
C	0.37269100	-4.94121100	-2.30808700
H	-1.28743700	-5.13371400	-0.87938900
H	0.56474100	-4.40943100	-3.24590000
H	1.09610400	-4.55907700	-1.57348500
H	-2.85024000	-3.58989100	-1.94231200
H	-1.62117200	-3.22651400	-3.28179300
C	0.59947600	-6.45273100	-2.48536900
H	1.62324300	-6.64612600	-2.82192600
H	0.44966000	-6.98675600	-1.54012000
H	-0.08741400	-6.87540300	-3.22729800
C	2.25391900	0.30673900	-2.31127300
C	1.77106000	1.26622400	-1.41804200
C	3.43970600	0.48647200	-3.02352700
C	2.48915600	2.44517000	-1.24858000
H	0.85653900	1.09052400	-0.85898400
C	4.16077300	1.66733200	-2.85128700

H	3.78800500	-0.28887900	-3.69660400
C	3.66770200	2.62723600	-1.97132200
H	2.15617900	3.21973000	-0.56903700
H	5.08573300	1.85095800	-3.38357900
N	4.41552500	3.88719700	-1.79814100
O	5.46500800	4.01755400	-2.42429900
O	3.93732700	4.73227700	-1.04229500
C	1.61003200	-2.23267300	2.02199400
C	2.83192600	-2.86333300	2.26365900
C	1.48493300	-0.84272900	2.03473300
C	3.95333600	-2.08931200	2.54866200
H	2.90336500	-3.94437800	2.21703100
C	2.60384300	-0.06691000	2.32192800
H	0.53691800	-0.36756900	1.80695700
C	3.81706900	-0.70295200	2.57772200
H	4.91951800	-2.53834100	2.74191700
H	2.55356100	1.01442200	2.34249300
N	4.99977600	0.12222200	2.88040600
O	4.85382200	1.34427800	2.89383400
O	6.06034800	-0.45958400	3.10190900
P	-2.25005800	1.52640100	0.46902400
C	0.04319600	5.49927100	1.75380200
C	-0.08480800	4.34098300	2.75087600
C	-0.46593000	3.02699100	2.04983100
C	-1.77434000	3.17379700	1.23286700
C	-1.62400300	4.33230600	0.21914000
C	-1.23472300	5.64659100	0.91885000
H	0.89715800	5.31405600	1.08585400
H	0.26105100	6.43537200	2.28185800
H	-0.84954100	4.58689300	3.50241900

H	0.33814500	2.72810100	1.36549600
H	-2.59102800	3.43138300	1.92427300
H	-0.84978700	4.07317200	-0.51739900
H	-2.55253100	4.48874300	-0.33980400
H	-2.06248500	5.96188300	1.57117300
H	-1.11344900	6.43549200	0.16639900
H	0.85550300	4.20169100	3.29814600
H	-0.55142500	2.22321000	2.78689000
C	-4.26305700	-1.52282500	3.45961400
C	-4.97819000	-1.26282800	2.12893200
C	-4.05724200	-0.57416300	1.10678600
C	-3.43647800	0.73005100	1.66418300
C	-2.76174000	0.47953200	3.03591700
C	-3.70851500	-0.21297000	4.03004700
H	-3.43723700	-2.23019800	3.30428000
H	-4.95227800	-1.98759200	4.17532500
H	-5.86109000	-0.63004700	2.30576200
H	-3.25344100	-1.26585000	0.83101800
H	-4.24383000	1.46628700	1.80444800
H	-1.87765400	-0.15241000	2.88819000
H	-2.41767400	1.42572100	3.46815300
H	-4.54071700	0.46428700	4.27497900
H	-3.16877300	-0.39907400	4.96635200
H	-5.34819500	-2.20211700	1.69968500
H	-4.62964800	-0.36166200	0.19791400
C	-5.12866300	1.74999500	-3.32152200
C	-3.73129300	1.13064800	-3.46956200
C	-3.15334600	0.68956100	-2.11467900
C	-3.13382800	1.88126600	-1.12804600
C	-4.54621400	2.48595900	-0.95727600

C	-5.12460600	2.91248700	-2.31804200
H	-5.83322900	0.97842300	-2.97716800
H	-5.49699700	2.09508900	-4.29536100
H	-3.05187800	1.86333900	-3.92830000
H	-3.77026000	-0.12348200	-1.71179300
H	-2.49840800	2.64873100	-1.59269400
H	-5.21306800	1.74135900	-0.50274500
H	-4.52953300	3.34607500	-0.27557600
H	-4.52249000	3.74004200	-2.72070800
H	-6.14023600	3.30366200	-2.18004700
H	-3.76333900	0.27133400	-4.15001900
H	-2.14636800	0.28892800	-2.25260100
O	-0.98540400	0.68353600	0.22080300

S14

0 imaginary frequency

H = -5760.242317

G = -5760.371460

Esol = -5761.116484

Se	-0.77851900	0.08430300	1.33951200
N	-2.59778600	0.48496100	1.88666200
N	-0.07332900	1.64271200	1.83199300
S	-3.75688300	-0.66745000	1.60257700
O	-4.65183000	-0.77666600	2.75776100
O	-3.03578500	-1.85072800	1.09915500
S	-0.32218200	2.81690900	0.70305800
O	-1.00101700	3.97819700	1.29317500
O	-0.89430900	2.24608000	-0.54986100
C	-0.17713500	-0.79891500	3.05663400

C	-0.92635700	-0.31738600	4.24470800
C	-0.54236500	0.73124300	4.98712400
H	-1.83343400	-0.86093100	4.50701100
H	0.35813900	1.27173000	4.69824000
H	-0.29332700	-1.86704500	2.86624000
H	0.87536700	-0.52188100	3.03707900
C	-1.26614500	1.23453800	6.19864900
H	-1.56088900	2.28404100	6.06737100
H	-2.16534200	0.64729200	6.41143000
H	-0.61662600	1.20266800	7.08365500
C	1.36127900	3.35165500	0.32779500
C	1.58410900	4.69607300	0.02338900
C	2.39573300	2.41365500	0.30967000
C	2.86701200	5.11469300	-0.32185000
H	0.76270500	5.40235000	0.07303800
C	3.67903200	2.82897100	-0.03299200
H	2.18775800	1.38174100	0.57476600
C	3.89224800	4.17076900	-0.34616800
H	3.08259800	6.14804900	-0.56344000
H	4.51244900	2.13862900	-0.05523500
N	5.25200000	4.60426700	-0.70947500
O	5.42338100	5.79400800	-0.97056000
O	6.13772300	3.74864500	-0.73299000
C	-4.68654900	0.01838400	0.22465700
C	-4.02301500	0.77011100	-0.74919300
C	-6.05012600	-0.26865400	0.13826700
C	-4.74545000	1.23895700	-1.84275300
H	-2.97170000	1.01685900	-0.64285600
C	-6.77208000	0.19811700	-0.95725000
H	-6.53829400	-0.83451300	0.92423400

C	-6.10417300	0.94000900	-1.92927100
H	-4.27291900	1.83461800	-2.61356500
H	-7.83164500	0.00294500	-1.06480000
N	-6.86790800	1.43311200	-3.09158700
O	-8.06851300	1.16926900	-3.13717700
O	-6.25623500	2.07353500	-3.94435600
P	1.91063200	-2.01561800	-0.41451000
C	1.32594900	-0.23219300	-4.78854500
C	0.39220600	0.20642300	-3.65161000
C	0.99091500	-0.10187100	-2.27172900
C	1.36013100	-1.59641000	-2.15009600
C	2.31143100	-2.03576000	-3.28594700
C	1.70013600	-1.71643000	-4.66210900
H	2.24282100	0.37501900	-4.76040000
H	0.85764200	-0.04410300	-5.76254200
H	-0.57142400	-0.31509000	-3.75200900
H	1.88588000	0.51637900	-2.11776700
H	0.42713000	-2.16501600	-2.27564500
H	3.26970000	-1.50817800	-3.19387400
H	2.53430700	-3.10816700	-3.22049600
H	0.80079100	-2.33271000	-4.80812300
H	2.40619000	-2.00328200	-5.45152900
H	0.17370800	1.27839300	-3.71970300
H	0.28810200	0.17567000	-1.48366300
C	-0.61098600	-6.04565600	-0.23221200
C	-1.06064000	-4.80973400	0.56144400
C	-0.42088100	-3.53362800	-0.00314300
C	1.11992600	-3.64093500	0.00348900
C	1.56897600	-4.85767700	-0.83371300
C	0.92091300	-6.14991000	-0.30086600

H	-1.01414300	-5.98211500	-1.25374300
H	-1.02889600	-6.95828500	0.21028100
H	-0.77464600	-4.92548000	1.61733200
H	-0.77575000	-3.39746200	-1.03447900
H	1.43311700	-3.80853400	1.04526700
H	1.27114700	-4.71080400	-1.88155200
H	2.66060500	-4.96429900	-0.82824500
H	1.31681100	-6.35591500	0.70439900
H	1.21747700	-6.99726500	-0.93161500
H	-2.15139500	-4.70866100	0.54242800
H	-0.75770600	-2.65311400	0.54740900
C	6.46515400	-1.76291800	0.77894400
C	6.00684500	-1.07033500	-0.51119000
C	4.47910400	-0.90289800	-0.54724600
C	3.75100400	-2.25644400	-0.37649200
C	4.21142400	-2.94067000	0.93217900
C	5.74099100	-3.10156800	0.97521300
H	6.25444500	-1.10717500	1.63623800
H	7.55090800	-1.91760600	0.76327500
H	6.32838900	-1.66331600	-1.38000100
H	4.16413800	-0.24059100	0.26879300
H	4.01193600	-2.90765200	-1.22300500
H	3.88151600	-2.33219700	1.78520400
H	3.74130500	-3.92441300	1.04404200
H	6.05062900	-3.80198400	0.18547200
H	6.03322900	-3.55898000	1.92872800
H	6.48597800	-0.08835400	-0.60989200
H	4.18021400	-0.41367700	-1.48149700
H	-2.68887500	0.99370300	2.76675700
O	1.50315300	-0.94630300	0.60675200

S15

0 imaginary frequency

H = -5760.250957

G = -5760.379243

Esol = -5761.126787

Se	0.61218800	-0.42279000	-1.12709500
N	2.28079700	-0.99731200	-2.04380600
N	0.15145700	0.89837200	-2.33252300
S	3.03601500	-2.17296100	-1.13886200
O	3.84800200	-3.04304800	-1.98771500
O	1.95490600	-2.74849500	-0.30876100
S	1.04055800	2.32942900	-2.31509900
O	1.01149000	2.92230700	-3.65549700
O	2.33074500	2.02593100	-1.67743600
C	-0.27491400	-1.10982600	-5.19481800
C	-0.13306700	0.10873100	-4.67505200
C	-0.83533200	0.56149000	-3.42137900
H	0.49744500	0.85101300	-5.16067900
H	-1.38335200	-0.28176900	-2.99592600
H	0.23205400	-1.40396900	-6.10956500
H	-0.89668200	-1.86750400	-4.72139700
C	-1.84673100	1.68884400	-3.66578300
H	-2.33006100	1.97836000	-2.72690000
H	-1.38218300	2.56711000	-4.11912200
H	-2.61597000	1.32009400	-4.35207600
C	0.14084800	3.43836700	-1.21247900
C	0.18674600	4.80730000	-1.48775200
C	-0.53246200	2.92927700	-0.09907300

C	-0.45246700	5.69504800	-0.62590200
H	0.70199800	5.16789100	-2.37119000
C	-1.17647600	3.81709600	0.75798500
H	-0.58941000	1.86181600	0.07918300
C	-1.12245200	5.18194100	0.48266100
H	-0.44459600	6.76332600	-0.80265300
H	-1.71887000	3.46621300	1.62694300
N	-1.81088100	6.11700800	1.39248900
O	-1.74552200	7.31683000	1.13243800
O	-2.40898100	5.63759800	2.35477000
C	4.18489000	-1.30455900	-0.04179700
C	3.80083200	-0.10197800	0.56083300
C	5.42712200	-1.88857200	0.21449900
C	4.67746400	0.52657200	1.43991500
H	2.84018500	0.34389600	0.32838200
C	6.30411600	-1.26434000	1.09846400
H	5.70242500	-2.81067600	-0.28510600
C	5.91084800	-0.06945800	1.69712000
H	4.42249300	1.46365900	1.91855500
H	7.27735500	-1.68225300	1.32368300
N	6.83754200	0.59340900	2.63454700
O	7.92525100	0.05595100	2.83533000
O	6.46332600	1.64094500	3.15894100
P	-2.40392300	-1.30556700	0.71493300
C	0.23102500	-2.76764800	4.39869700
C	0.89451000	-2.00938000	3.24004600
C	-0.13361500	-1.23206300	2.40400600
C	-1.24936400	-2.17294100	1.89491000
C	-1.92855800	-2.92296400	3.06201600
C	-0.88716800	-3.69178900	3.89483000

H	-0.19179500	-2.04514200	5.11282300
H	0.97934500	-3.34951600	4.95084200
H	1.41911200	-2.71742500	2.58395400
H	-0.56372800	-0.41976900	3.00530100
H	-0.74983500	-2.92249900	1.26477700
H	-2.44575400	-2.20597100	3.71367700
H	-2.69228700	-3.61807800	2.69293700
H	-0.44962300	-4.48838700	3.27607200
H	-1.38447800	-4.18716600	4.73829600
H	1.65415100	-1.31716600	3.62472200
H	0.35331900	-0.76870000	1.54341900
C	-3.39438500	-5.14832000	-1.95753300
C	-2.32750200	-4.13782000	-2.40419400
C	-1.81437100	-3.30712400	-1.21768800
C	-2.98587400	-2.57547200	-0.51802300
C	-4.02217500	-3.60880700	-0.02191700
C	-4.53824000	-4.46335100	-1.19482800
H	-2.92442400	-5.89862200	-1.30488900
H	-3.79244800	-5.69368900	-2.82223400
H	-2.75337300	-3.46549700	-3.16423100
H	-1.33232300	-3.98796400	-0.50260900
H	-3.47651900	-1.94265900	-1.27396300
H	-3.55556300	-4.26816800	0.72285500
H	-4.86903300	-3.12164100	0.47490700
H	-5.10052100	-3.81648100	-1.88429100
H	-5.24855800	-5.21143400	-0.82090000
H	-1.48703500	-4.65722500	-2.88016800
H	-1.04012700	-2.60295500	-1.53537700
C	-5.78804800	1.50784800	2.38531500
C	-4.74781800	0.96790900	3.37536900

C	-3.51362600	0.40230500	2.65320900
C	-3.89985800	-0.68720500	1.62523400
C	-4.94650300	-0.12954500	0.63060700
C	-6.17719300	0.43707500	1.35796600
H	-5.37137400	2.38027700	1.86151000
H	-6.67677300	1.86111200	2.92250700
H	-5.20351100	0.17533700	3.98722100
H	-2.99344800	1.21133000	2.12372700
H	-4.34010400	-1.53839400	2.16457700
H	-4.47423800	0.66219100	0.03418700
H	-5.26582500	-0.90591800	-0.07425300
H	-6.70534000	-0.38234200	1.86780600
H	-6.87893200	0.84932300	0.62208000
H	-4.43517200	1.75739900	4.06987500
H	-2.80718200	0.00575300	3.39087200
H	2.88884900	-0.19618300	-2.23259100
O	-1.72579200	-0.13255300	-0.00115800

S16

0 imaginary frequency

H = -5989.384224

G = -5989.524426

Esol = -5990.329428

Se	-0.57735000	0.14614500	-0.84332900
N	-2.36580200	0.09231900	-1.75547600
N	-0.42014400	-1.63936600	-0.46578100
S	-3.22320300	1.51522600	-1.31362300
O	-4.13810300	1.89665300	-2.39361800
O	-2.26357700	2.50818100	-0.79742200

S	0.13892100	-2.77299300	-1.58941300
O	0.58848100	-2.03863400	-2.77426200
O	-0.86149200	-3.84166000	-1.70483800
C	-0.33466400	0.95811700	-4.44704600
C	-1.59576600	0.97949900	-4.01048100
C	-2.21886300	-0.16952500	-3.25731300
H	-2.23641000	1.83849900	-4.20220000
H	-1.50998200	-0.99943600	-3.27023500
H	-1.08882100	-2.04056200	0.20971200
H	0.08095700	1.78794800	-5.01377500
H	0.31605800	0.10648100	-4.26595700
C	-3.52751400	-0.66368200	-3.88848600
H	-3.94783800	-1.49653000	-3.31708200
H	-4.27269400	0.12945600	-3.96400100
H	-3.30182400	-1.02488700	-4.89774500
C	1.58017000	-3.47083100	-0.77176500
C	2.53649400	-2.61701700	-0.21627400
C	1.72561200	-4.85924000	-0.76735800
C	3.67265600	-3.17978900	0.35902800
H	2.38893200	-1.53875500	-0.21052600
C	2.86524300	-5.41893100	-0.19417300
H	0.95312100	-5.48573900	-1.19867300
C	3.81819400	-4.56647200	0.35800200
H	4.44065700	-2.56315600	0.80885900
H	3.02048700	-6.49013000	-0.16643800
C	-4.23517500	0.96395600	0.07477200
C	-3.63805900	0.35417800	1.18090200
C	-5.60458500	1.22978600	0.03107600
C	-4.42857000	-0.00469200	2.26771200
H	-2.57619300	0.14095600	1.17219700

C	-6.39749600	0.88010000	1.12221000
H	-6.03629800	1.69850700	-0.84581500
C	-5.79420600	0.27131400	2.22007600
H	-4.00573600	-0.49542800	3.13501800
H	-7.46373000	1.06875000	1.13210300
N	5.02454100	-5.15395500	0.97113400
N	-6.63468600	-0.10259400	3.37439000
O	5.84929300	-4.38232000	1.45906300
O	-6.07832900	-0.63290800	4.33400800
O	5.13257100	-6.37891300	0.95726300
O	-7.83812000	0.13955600	3.30359800
O	-2.62447800	-2.74047100	0.95001000
C	-3.49861800	-3.05051300	0.14980900
O	-3.80060400	-2.33280100	-0.93426100
C	-4.34290200	-4.29101100	0.26879800
H	-5.38713700	-4.07753300	0.02573600
H	-3.97606400	-5.02864100	-0.45440700
H	-4.25648300	-4.70210600	1.27505300
H	-3.19920300	-1.55082900	-1.03413100
O	2.07120700	0.52170500	-0.02650100
P	2.51407900	1.84581200	0.59084500
C	2.43793300	4.18982200	-3.51774200
C	3.73804600	4.20185300	-2.70575900
C	3.75124200	3.10380500	-1.62864600
C	2.53293200	3.21096200	-0.67884600
C	1.22718900	3.19571300	-1.51416500
C	1.22095400	4.29152400	-2.59189800
H	2.37883000	3.25384000	-4.09211200
H	2.43650000	5.00899700	-4.24780300
H	3.85602500	5.18283600	-2.22157200

H	3.73464900	2.11829800	-2.11347000
H	2.59917100	4.16286800	-0.12879500
H	1.12992600	2.21381600	-1.99230100
H	0.34784400	3.32209300	-0.87991800
H	1.21233000	5.27992300	-2.10853500
H	0.29012100	4.21790000	-3.16688400
H	4.60606800	4.07354600	-3.36489400
H	4.68969100	3.16720800	-1.07022400
C	7.10802200	1.82130900	1.90648000
C	6.43634000	0.51523300	1.45613500
C	5.17315200	0.78788500	0.62253100
C	4.18610100	1.68144300	1.40388600
C	4.85402800	3.00411200	1.84198100
C	6.12550200	2.72640100	2.66446900
H	7.48547700	2.35734000	1.02300600
H	7.98059600	1.60319800	2.53444400
H	6.16691400	-0.07937200	2.34151300
H	5.46289800	1.27540900	-0.31604400
H	3.93101000	1.13154600	2.32438300
H	5.12325200	3.59896400	0.95965500
H	4.16179300	3.61823100	2.43169300
H	5.84188400	2.24321800	3.61086400
H	6.60735400	3.67556300	2.93074400
H	7.13964800	-0.09400100	0.87517600
H	4.68164800	-0.14966100	0.34374100
C	-1.01776400	2.21826200	3.73878600
C	-0.59340600	3.50058600	3.01082400
C	0.20122700	3.18838700	1.73171700
C	1.43901500	2.32235800	2.04375800
C	1.00031300	1.01955900	2.75743400

C	0.18947500	1.31636900	4.02857400
H	-1.73381900	1.67191400	3.10876000
H	-1.54291000	2.46293300	4.67050300
H	0.02416400	4.11548400	3.68279000
H	-0.44736700	2.65155500	1.03037900
H	2.08895600	2.89490400	2.72286200
H	0.40552400	0.43765300	2.04315900
H	1.86792100	0.39782800	3.01040000
H	0.84146100	1.80740900	4.76628700
H	-1.47351000	4.10296100	2.75475000
H	0.49384500	4.12691400	1.24677500
H	-0.13814600	0.37308900	4.48381600

S17

0 imaginary frequency

H = -5989.383106

G = -5989.523378

Esol = -5990.327792

Se	0.34355600	-0.50418600	1.08163100
N	2.45410000	-1.43464100	1.78309200
N	0.10981900	-1.72935800	-0.19973200
S	3.51345000	-0.12469000	2.21557500
O	4.57437100	-0.57899600	3.12032700
O	2.64974000	0.98958200	2.61965400
S	-0.68555000	-3.14907100	0.20637300
O	-0.66735600	-3.42926900	1.65694900
O	-0.20153600	-4.16341900	-0.74127900
C	0.53491800	-1.80329900	4.56126400
C	1.80486900	-1.87371700	4.16094100

C	2.21431500	-2.49577000	2.84869200
H	2.60536600	-1.48060900	4.78589200
H	1.35399300	-3.03231500	2.44257600
H	1.24899200	-1.99094500	-1.40309900
H	0.26929000	-1.36206600	5.51880200
H	-0.27401000	-2.19571500	3.95153700
C	3.39169300	-3.47094900	2.97340300
H	4.26930800	-2.99852500	3.42018300
H	3.08428300	-4.30889200	3.60829700
H	3.66521600	-3.87157900	1.99141700
C	-2.42412600	-2.85756300	-0.19169200
C	-3.23793200	-2.22011700	0.74803500
C	-2.92717400	-3.28873400	-1.42024000
C	-4.57613700	-1.99250300	0.44633100
H	-2.82143900	-1.90227700	1.69636100
C	-4.26751400	-3.06388700	-1.72877500
H	-2.27222200	-3.80515500	-2.11341300
C	-5.06594400	-2.40874400	-0.79258400
H	-5.24101000	-1.50745500	1.14971300
H	-4.69689900	-3.38397800	-2.67010600
C	4.27782000	0.27825400	0.63244300
C	3.47764600	0.60324400	-0.46493900
C	5.67061800	0.33064000	0.57692100
C	4.08831700	0.98729000	-1.65384000
H	2.39922500	0.51963900	-0.38189800
C	6.28381900	0.72431900	-0.61102900
H	6.25734000	0.06426700	1.44873400
C	5.48042000	1.04618200	-1.70197500
H	3.50850900	1.23503700	-2.53389800
H	7.36129300	0.78154000	-0.70193900

N	-6.47316400	-2.13557900	-1.12493300
N	6.12803100	1.46235300	-2.96216000
O	-6.91778300	-2.60486300	-2.17082300
O	5.39653300	1.74525600	-3.90947900
O	-7.12272000	-1.44108200	-0.33970400
O	7.35622000	1.50057500	-2.98491000
O	1.88642700	-2.18359000	-2.17591000
C	3.02850100	-2.69414200	-1.74682300
O	3.38471500	-2.72104900	-0.57024800
C	3.87448100	-3.25497900	-2.86393200
H	3.40074400	-4.16573300	-3.24700100
H	3.93046900	-2.54355600	-3.69337900
H	4.87322200	-3.49244700	-2.49603700
H	2.79001200	-1.88861100	0.90654700
O	-1.56692900	0.63516000	0.83708900
P	-1.86279900	1.95061800	0.07393000
C	0.95506000	5.60073000	1.31287900
C	1.00067000	4.30329600	2.13198900
C	0.44447700	3.10844600	1.34144000
C	-0.98498400	3.40332200	0.84103200
C	-1.03367300	4.70256700	0.00241800
C	-0.46442700	5.88834300	0.80224500
H	1.63751800	5.51372400	0.45441300
H	1.31655600	6.44456800	1.91329700
H	0.41199100	4.43282800	3.05215300
H	1.10722600	2.90124000	0.49262300
H	-1.59753800	3.58125800	1.73926000
H	-0.44577200	4.57836700	-0.91552900
H	-2.05935900	4.93253100	-0.31314500
H	-1.12467200	6.09458500	1.65726800

H	-0.47340400	6.78923700	0.17618700
H	2.02522800	4.07610100	2.44738300
H	0.45640200	2.21459800	1.96878900
C	-6.52922900	2.07986100	1.02662300
C	-6.08727900	2.41008200	-0.40483100
C	-4.67360400	1.87918400	-0.70227400
C	-3.65264000	2.42519700	0.31779400
C	-4.09163100	2.07254500	1.76008300
C	-5.50949600	2.59071300	2.05345400
H	-6.64045500	0.99109500	1.12291100
H	-7.51712700	2.51237000	1.22657200
H	-6.10269400	3.50015200	-0.55397300
H	-4.68911200	0.78345900	-0.65618100
H	-3.65089200	3.52190000	0.22081700
H	-4.05717700	0.98320600	1.87878900
H	-3.38858200	2.48172400	2.49548900
H	-5.50134300	3.69089500	2.04431300
H	-5.80310000	2.29090900	3.06712900
H	-6.79301200	1.98327300	-1.12723200
H	-4.38784200	2.15665900	-1.72329500
C	-0.23564200	0.46527100	-4.11878800
C	0.31735600	1.77560900	-3.54564200
C	0.03500700	1.90498900	-2.03931400
C	-1.47964600	1.80326600	-1.73726100
C	-2.01221600	0.45940500	-2.29876300
C	-1.73033200	0.32559200	-3.80451100
H	0.31130700	-0.38150300	-3.68230600
H	-0.06829300	0.42594900	-5.20220800
H	-0.13631800	2.62985300	-4.07011300
H	0.53559100	1.09390500	-1.49694400

H	-1.99889400	2.64119700	-2.22855600
H	-1.51469800	-0.35163400	-1.75623800
H	-3.08390900	0.34967100	-2.11747600
H	-2.29574600	1.09353000	-4.35375300
H	1.39840300	1.84632500	-3.72292500
H	0.45365300	2.84615100	-1.67125900
H	-2.10406100	-0.64503200	-4.15296500

S18

0 imaginary frequency

H = -3745.975720

G = -3746.044156

Esol = -3746.235665

Se	-1.40463600	0.55863600	1.29737100
N	-0.79987700	-1.14258500	0.86374900
S	-0.10408500	-1.18988300	-0.62522100
O	-0.02994300	-2.60902300	-1.00584900
O	-0.69355100	-0.22476700	-1.59259700
C	1.61147900	-0.63828900	-0.42182600
C	2.63552800	-1.58717500	-0.39996900
C	1.89016300	0.72347400	-0.25289800
C	3.95364800	-1.17777900	-0.21253300
H	2.38817600	-2.63345000	-0.54042800
C	3.20233800	1.14007800	-0.05850100
H	1.08211300	1.44598400	-0.26614600
C	4.21542200	0.18055300	-0.04305400
H	4.77257200	-1.88633100	-0.19710900
H	3.45536500	2.18467700	0.07398000
N	5.60460400	0.61958200	0.15481700

O	5.80956400	1.82555100	0.30088200
O	6.48341700	-0.24253300	0.16431100
C	-3.00378200	0.53494900	0.26354400
C	-4.52965600	0.91674700	-1.30967900
C	-4.91579200	-0.19005300	-0.61418000
H	-4.98859300	1.41997900	-2.14592800
H	-5.77403100	-0.83291900	-0.72985800
N	-3.34469500	1.35419000	-0.75192700
N	-3.96701800	-0.40474300	0.36492400
C	-2.46803700	2.39835500	-1.28875500
H	-2.20558000	3.10650000	-0.50152300
H	-1.57090600	1.91409000	-1.68134400
H	-3.00401000	2.92161700	-2.08168600
C	-3.92632900	-1.51129600	1.32523500
H	-3.08232300	-2.16144900	1.08135900
H	-3.77228300	-1.10298000	2.32642900
H	-4.87442700	-2.04753900	1.27594200

S19

0 imaginary frequency

H = -4785.543419

G = -4785.634778

Esol = -4785.924543

Se	1.57398100	-0.87476800	-0.82547200
N	0.56634400	-0.88936400	0.65842200
N	1.54234500	0.74611600	-1.52018700
S	0.01579100	-2.41447500	0.95266300
O	0.73771200	-3.40054400	0.10669100
S	1.95903900	2.05299900	-0.58644700

C	-1.70596200	-2.38694700	0.40261400
C	-2.07716600	-1.59042600	-0.68339100
C	-2.62848500	-3.21347800	1.04756700
C	-3.38970100	-1.62755800	-1.14358300
H	-1.34933100	-0.93290200	-1.14582600
C	-3.94371800	-3.25480000	0.59209400
H	-2.31930900	-3.80364300	1.90320400
C	-4.29934300	-2.46354700	-0.49852600
H	-3.71615900	-1.02181200	-1.97961500
H	-4.69000600	-3.88049600	1.06555600
N	-5.69069900	-2.50706100	-0.98487400
O	-6.47653900	-3.24808500	-0.39676300
O	-5.97820500	-1.80181300	-1.95061000
C	0.40732500	2.87343700	-0.16793400
C	-0.47423600	2.26827600	0.73221800
C	0.13266500	4.11425500	-0.74423900
C	-1.65615700	2.92345900	1.06443800
H	-0.23906700	1.29742000	1.15815200
C	-1.05056900	4.77199300	-0.41410700
H	0.84376300	4.55318400	-1.43463800
C	-1.92325900	4.16382600	0.48476400
H	-2.36707100	2.49287000	1.75863200
H	-1.30172800	5.73693600	-0.83640100
N	-3.17535400	4.85822100	0.83795400
O	-3.38850100	5.95126700	0.31520500
O	-3.93053800	4.30231100	1.63409500
O	2.57314600	1.63008600	0.69359600
O	2.70432500	2.97489400	-1.45237700
O	-0.00764100	-2.63780800	2.40604500
C	3.41288200	-0.96635600	-0.00431400

C	5.62507900	-1.19024900	-0.04021500
C	5.21651300	-1.19629300	1.25812000
H	6.60836800	-1.26712900	-0.47647800
H	5.77999600	-1.27281300	2.17455000
N	4.48932600	-1.05276600	-0.81215300
N	3.84140400	-1.06370000	1.26522200
C	4.45007100	-0.96703000	-2.27786600
H	3.89912500	-0.07187200	-2.57435200
H	5.47509600	-0.90924200	-2.64403400
H	3.96694000	-1.85693100	-2.69025000
C	3.04225800	-0.89255900	2.49323300
H	2.28165900	-1.66811900	2.57425600
H	3.73364100	-0.95559600	3.33449100
H	2.56862100	0.08724900	2.45639100

S2

0 imaginary frequency

H = -4645.365169

G = -4645.470359

Esol = -4646.112301

Se	-2.15964400	-0.45555100	0.32332800
N	-2.74450800	0.81240600	-0.93154200
S	-3.00223100	2.40921900	-0.39589300
O	-3.69533000	2.46459100	0.89850800
O	-3.54477000	3.11970400	-1.55772300
C	-3.88528200	-0.79226300	1.30620500
C	-4.96456700	-1.20592200	0.36992100
C	-5.98141000	-0.41242900	0.00334900
H	-4.87742800	-2.20581000	-0.05718300

H	-6.04089100	0.58863300	0.43328400
H	-3.56370900	0.50056300	-1.45940300
H	-3.59912100	-1.59037200	2.00034000
H	-4.11896700	0.11847300	1.85688600
C	-7.07995200	-0.80063200	-0.94315200
H	-8.05777400	-0.76608400	-0.44426600
H	-7.13979400	-0.10522200	-1.79083600
H	-6.93638900	-1.81171400	-1.33884200
C	-1.29442100	2.89017000	-0.11882700
C	-0.53064300	3.31069800	-1.20895200
C	-0.75475600	2.76791100	1.16152300
C	0.81832400	3.59337900	-1.02083200
H	-0.98828400	3.40730500	-2.18732700
C	0.59569400	3.04823300	1.35303700
H	-1.38208800	2.45236000	1.98611900
C	1.35806500	3.43995100	0.25556200
H	1.45284800	3.91026500	-1.83874900
H	1.06271500	2.95274200	2.32486600
N	2.80102700	3.66945800	0.44405900
O	3.46872000	3.95431600	-0.54988900
O	3.25816400	3.54224000	1.57945100
P	1.40842500	-0.95351900	0.01909100
C	-0.30083700	-3.21759300	3.87823600
C	0.66692800	-2.03880700	4.04674800
C	0.79542700	-1.22696600	2.74832100
C	1.22003600	-2.10040200	1.54193600
C	0.22862200	-3.27332300	1.38500700
C	0.10000000	-4.09160000	2.68251000
H	-1.31902100	-2.82980500	3.71887700
H	-0.33853900	-3.81944500	4.79518900

H	1.65721200	-2.42194200	4.33476400
H	-0.16956900	-0.75492500	2.50978800
H	2.20600300	-2.53737000	1.76032000
H	-0.76423400	-2.88717700	1.10666600
H	0.53859700	-3.93870000	0.57204700
H	1.06450900	-4.57531900	2.89646900
H	-0.62776500	-4.90114300	2.53882300
H	0.33637900	-1.38656700	4.86569600
H	1.50451600	-0.40328900	2.89236400
C	5.78925600	0.85958500	-0.10805400
C	5.22812300	0.25086800	-1.39966700
C	3.70624100	0.04350100	-1.31262100
C	3.29709900	-0.81468500	-0.09462100
C	3.88432700	-0.20386700	1.19803900
C	5.40617000	0.00285500	1.10553600
H	5.38795400	1.87488100	0.02071900
H	6.88029400	0.95887600	-0.17557100
H	5.71597100	-0.71731000	-1.58865200
H	3.21690500	1.02555100	-1.24131600
H	3.72569300	-1.82089400	-0.21703700
H	3.40697600	0.76702300	1.39447300
H	3.66028600	-0.84218500	2.06064600
H	5.90085200	-0.97733000	1.03038100
H	5.76935200	0.46685800	2.03142700
H	5.46309000	0.89222100	-2.25882400
H	3.34702200	-0.41238800	-2.24233900
C	0.89196000	-3.12596200	-4.22978100
C	-0.12045800	-2.06512300	-3.77447200
C	0.43372700	-1.19561000	-2.63336500
C	0.92130900	-2.05927100	-1.44692100

C	1.92778400	-3.13039900	-1.90867500
C	1.35686400	-3.99149700	-3.04978100
H	1.76449500	-2.62664400	-4.67721200
H	0.45682300	-3.75641800	-5.01594700
H	-1.03667200	-2.56679100	-3.42830600
H	1.25554600	-0.57560400	-3.01742000
H	0.02540800	-2.57828300	-1.07946400
H	2.84911900	-2.64763400	-2.26133200
H	2.21959400	-3.77200900	-1.06712600
H	0.50413300	-4.57503800	-2.67144800
H	2.10933100	-4.71879800	-3.38213200
H	-0.41429900	-1.42985900	-4.62033700
H	-0.34153800	-0.50434100	-2.28194300

S20

0 imaginary frequency

H = -4942.719190

G = -4942.824173

Esol = -4943.217482

Se	0.00872500	-1.51498100	0.64702900
N	1.32914000	-1.05396900	-0.49101700
N	-1.33486000	-1.00959100	-0.43883100
S	2.76825800	-1.45470100	0.20733700
O	3.43028900	-2.60235900	-0.42942100
O	2.62696300	-1.47060400	1.69554300
S	-2.75773200	-1.38763900	0.30183500
O	-2.58570800	-1.35579100	1.78660500
O	-3.43536900	-2.55667300	-0.27975400
C	-0.39032900	-4.47866300	-0.17728100

C	0.29066600	-4.01981800	-1.23758600
C	-0.32546400	-3.42114200	-2.46891800
H	1.37929500	-4.08465500	-1.23397200
H	-1.40567600	-3.31188700	-2.32511000
H	0.07968300	-2.41043800	-2.60442100
H	0.11930400	-4.93287500	0.66991800
H	-1.47673700	-4.43435100	-0.13406100
C	-0.03682400	-4.26202300	-3.72389200
H	1.04160000	-4.37718400	-3.88786000
H	-0.46885700	-5.26522300	-3.63514100
H	-0.46158800	-3.78802000	-4.61639900
C	-3.75585500	0.04459400	-0.15487200
C	-4.14493300	0.94761800	0.83546900
C	-4.14605000	0.21078700	-1.48776700
C	-4.92523600	2.04911300	0.48959600
H	-3.84645000	0.77328100	1.86325700
C	-4.91799300	1.31319300	-1.84006300
H	-3.85178400	-0.51725300	-2.23579600
C	-5.29169900	2.21576000	-0.84377000
H	-5.25367000	2.76985600	1.22819200
H	-5.23735000	1.48068200	-2.86118300
N	-6.10563400	3.38744300	-1.21395300
O	-6.42835400	3.50749500	-2.39449000
O	-6.40814600	4.17661400	-0.31940300
C	3.76248900	-0.00946100	-0.21859000
C	4.14810000	0.18897300	-1.54844800
C	4.14981200	0.87378000	0.79039800
C	4.91238600	1.30365400	-1.87844100
H	3.85699800	-0.52474800	-2.31142100
C	4.92231100	1.98745100	0.46693100

H	3.85738400	0.67407400	1.81529000
C	5.28343500	2.18629500	-0.86351900
H	5.22801900	1.49544600	-2.89645000
H	5.24938400	2.69314100	1.22053300
N	6.08871200	3.37115400	-1.20976100
O	6.40841000	3.51881200	-2.38795200
O	6.38726500	4.14302900	-0.29888700
C	0.05749800	0.16078600	1.77587100
C	0.09121000	2.26977800	2.45666800
C	0.09725700	1.47292400	3.56352800
H	0.10260900	3.34405600	2.35792700
H	0.11457000	1.71978500	4.61345700
N	0.06611500	1.43456000	1.35386900
N	0.07613000	0.16606500	3.11572900
C	0.04771100	1.84629600	-0.05748300
H	-0.84816700	1.44843900	-0.53420900
H	0.05788600	2.93583700	-0.09295600
H	0.91975600	1.43166700	-0.56299900
C	0.06811800	-1.05566300	3.92930200
H	0.09255300	-0.76982100	4.98110800
H	-0.84626900	-1.61433100	3.71797600
H	0.95275300	-1.64788700	3.68560500

S21

0 imaginary frequency

H = -4942.728004

G = -4942.831303

Esol = -4943.226209

Se	-0.08473000	-1.43448500	0.23388200
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N	-1.15350400	-1.28305900	-1.23625500
N	1.59979500	-1.90118300	-0.88371600
S	-0.88120700	0.06751100	-2.10999900
O	0.51040900	0.56554600	-1.94512800
S	2.96703700	-1.95997800	0.02697400
C	-1.90365100	1.40127100	-1.41836300
C	-2.75716300	2.11321300	-2.26221500
C	-1.79179300	1.73485100	-0.06443400
C	-3.50762000	3.17168700	-1.75159200
H	-2.82503800	1.83100500	-3.30692700
C	-2.53284800	2.78977200	0.45402100
H	-1.14268100	1.15763700	0.58416400
C	-3.38263500	3.49174100	-0.40182700
H	-4.17972600	3.74556600	-2.37773700
H	-2.46948900	3.07592000	1.49646100
N	-4.18120600	4.60007800	0.14741600
O	-4.06875200	4.84221300	1.34957800
O	-4.91636100	5.21276500	-0.62480500
C	3.70724600	-0.30866200	0.04601200
C	5.09688900	-0.19794000	-0.03504800
C	2.89336900	0.81723600	0.18825200
C	5.68650500	1.06190400	0.03997500
H	5.69936800	-1.08996200	-0.16435800
C	3.47563800	2.07821400	0.25832000
H	1.81713900	0.70885100	0.21043300
C	4.86434400	2.17667400	0.18931000
H	6.75999600	1.19133700	-0.01882600
H	2.87787700	2.97560800	0.35581500
N	5.48516900	3.51171400	0.27302400
O	6.71037700	3.57699500	0.18883200

O	4.73926900	4.47783400	0.42647900
O	2.47198100	-2.23167200	1.40097600
O	3.97673600	-2.84885700	-0.55417400
O	-1.40402900	-0.17020500	-3.45914300
C	-1.92756600	-1.22631300	1.65455900
C	-2.87895700	-0.77608200	3.65663000
C	-3.87811300	-0.92333300	2.74865600
H	-2.90733000	-0.55891800	4.71358900
H	-4.94986400	-0.85770300	2.85909100
N	-1.69054000	-0.96684500	2.96643300
N	-3.27459600	-1.20174200	1.53070700
C	-0.36322000	-0.92898800	3.58334900
H	-0.16689000	0.06487800	3.99566500
H	-0.30186200	-1.67148900	4.38339900
H	0.38449600	-1.15995500	2.82657400
C	-4.00439100	-1.45486700	0.28520800
H	-4.59818800	-0.57532700	0.02146900
H	-3.27289700	-1.65385000	-0.49876400
H	-4.66721600	-2.31443100	0.41911000
H	1.67671400	-1.32636400	-1.72585700
C	-0.28392400	-3.43524800	0.50503400
C	-0.71962200	-4.10235100	-0.74366300
C	-1.83480600	-4.83686900	-0.83140100
H	-0.05639000	-4.00295200	-1.59863300
H	-2.48266400	-4.92140700	0.04407300
H	-0.98478300	-3.56752700	1.32921700
C	-2.27298500	-5.58784100	-2.05308100
H	-2.35193400	-6.66437200	-1.85007500
H	-3.26663600	-5.25551300	-2.38242300
H	0.72962200	-3.69208600	0.81409200

H -1.57514400 -5.44510600 -2.88354600

S22

0 imaginary frequency

H = -4942.747518

G = -4942.851208

Esol = -4943.246570

Se	0.02183100	-1.37355500	0.36215600
N	-1.23467700	-1.49054100	-1.04044500
N	1.68178200	-1.80426400	-0.94659000
S	-1.19964200	-0.22630000	-2.17972400
O	0.15962400	0.31151900	-2.30515200
S	3.06538100	-1.96356000	-0.11982900
C	-2.18659700	1.08706700	-1.42818000
C	-3.29269300	1.55753300	-2.13807000
C	-1.79613900	1.66312200	-0.21370800
C	-4.03222000	2.62156400	-1.62358400
H	-3.56288000	1.09483000	-3.08051000
C	-2.53521100	2.72173900	0.30376300
H	-0.95495500	1.25317600	0.33114000
C	-3.64035900	3.18306000	-0.41139900
H	-4.89503800	3.01750400	-2.14474500
H	-2.26997300	3.19330300	1.24186600
N	-4.42752600	4.30198400	0.14249400
O	-4.07173800	4.76434900	1.22511100
O	-5.39234000	4.69551200	-0.50939600
C	3.83505600	-0.31922800	-0.07273600
C	5.21497700	-0.19974200	-0.24458400
C	3.03756800	0.80263700	0.17506000

C	5.81147200	1.05698200	-0.16056500
H	5.80417000	-1.08631200	-0.45132000
C	3.62399300	2.06030800	0.25895000
H	1.96550700	0.67931600	0.28308100
C	5.00526900	2.16473800	0.09295700
H	6.87847700	1.19001500	-0.28965600
H	3.03885600	2.95271700	0.44267800
N	5.63076200	3.49468800	0.18548900
O	6.84797400	3.56745500	0.02220700
O	4.89805600	4.45495900	0.42402100
O	2.66335700	-2.27031800	1.27385500
O	4.04425200	-2.83435300	-0.78260700
O	-1.93521600	-0.69596600	-3.35868400
C	-1.55873200	-1.08923400	1.93157600
C	-2.02620700	-0.96368000	4.14214900
C	-3.20530800	-0.91598500	3.47348400
H	-1.80802700	-0.93362600	5.19854000
H	-4.22100600	-0.83853800	3.82998600
N	-1.03001800	-1.07212400	3.18523300
N	-2.89800000	-0.99393000	2.12107500
C	0.40400600	-1.13805000	3.48438600
H	0.89736600	-0.20467900	3.19975300
H	0.52696000	-1.29355400	4.55724400
H	0.87410500	-1.96220900	2.94408100
C	-3.90725900	-0.98158900	1.06616100
H	-4.45475700	-0.03492700	1.08693000
H	-3.40260200	-1.09743800	0.11095300
H	-4.60224200	-1.81282400	1.20984800
H	1.78040700	-1.29259700	-1.82330700
C	-3.17378200	-4.35988000	-0.23510600

C	-2.00336400	-3.73473500	-0.36708800
C	-1.64349900	-2.86115800	-1.54259900
H	-1.20884700	-3.88430900	0.36115400
H	-2.54008500	-2.68236300	-2.14226500
H	-3.97779300	-4.23693400	-0.95853500
C	-0.57945400	-3.53943500	-2.41592700
H	-0.96884600	-4.50060600	-2.76866900
H	-0.34766500	-2.92315400	-3.28949900
H	-3.36390900	-5.04204900	0.58937900
H	0.34157100	-3.70828100	-1.85385600

S23

0 imaginary frequency

H = -5171.919168

G = -5172.033944

Esol = -5172.487460

N	2.03779300	0.81045300	0.75578300
N	-1.27766500	0.37360400	0.84512100
S	2.83128300	1.12897700	-0.65903900
O	3.12201900	2.56751800	-0.70501100
O	2.04175300	0.49829800	-1.72802200
S	-2.50923800	0.41881100	1.97286300
O	-2.92723700	1.81864400	2.14222800
O	-2.09089300	-0.39150000	3.11556000
C	4.65661200	0.82936900	3.21302900
C	3.45186000	0.47382000	2.76764600
C	2.50327700	1.39744600	2.03911600
H	3.08046800	-0.53832000	2.93164300
H	3.01715100	2.33122300	1.79084600

H	-0.86846900	-0.60424800	0.57193200
H	5.29505800	0.13458000	3.75203700
H	5.05243200	1.83151600	3.05811900
C	1.26903000	1.72815600	2.89378900
H	1.57863600	2.20644900	3.82854500
H	0.60331200	2.41192500	2.35579100
H	0.70230100	0.82464200	3.14058100
C	-3.89505500	-0.44212000	1.18914500
C	-3.70561500	-1.70733500	0.62092300
C	-5.15147200	0.16763500	1.22128800
C	-4.79880000	-2.36136200	0.05764400
H	-2.71708000	-2.16135900	0.58900300
C	-6.24615600	-0.48945500	0.66375900
H	-5.26291500	1.14237500	1.68311900
C	-6.04790700	-1.74168400	0.08706800
H	-4.69639000	-3.33784200	-0.39955600
H	-7.23725500	-0.05293200	0.67079400
C	4.42314900	0.27042700	-0.64965400
C	4.46216800	-1.10664000	-0.40452100
C	5.57955100	1.00128400	-0.92557400
C	5.68922500	-1.76223500	-0.44276400
H	3.55339600	-1.65334400	-0.16312400
C	6.80804500	0.34553600	-0.96747900
H	5.50959300	2.06867700	-1.10215800
C	6.83944000	-1.02599300	-0.72716700
H	5.76762400	-2.82569200	-0.25432800
H	7.72877900	0.87447000	-1.17966200
N	-7.19969400	-2.42921000	-0.52543300
N	8.13729100	-1.72296900	-0.77026000
O	-8.28595200	-1.85127400	-0.50311100

O	9.13887000	-1.05132400	-1.01622000
O	-7.00287000	-3.53384300	-1.02863400
O	8.14242900	-2.93500600	-0.55870800
O	-0.61249800	-2.02939900	0.12333800
C	0.52463600	-2.55504000	0.39941400
O	1.53472300	-1.93168900	0.79852400
C	0.61416800	-4.06696400	0.21562100
H	-0.11419800	-4.55999600	0.86904200
H	0.35401400	-4.33318800	-0.81497100
H	1.61611100	-4.43296100	0.44784200
H	1.72883700	-0.18731800	0.80072400
Se	-0.81409400	1.85159400	-0.11695900
C	-2.09237300	1.67219000	-1.52960500
C	-3.12418600	0.88876300	-3.33161800
C	-3.86463200	1.92980700	-2.84823200
H	-3.28767100	0.24395900	-4.18086200
H	-4.78451200	2.36635900	-3.20471600
N	-2.02791400	0.75009400	-2.51169200
N	-3.21571900	2.39980000	-1.72682400
C	-0.96510400	-0.26497400	-2.63484700
H	-1.11216200	-1.05421400	-1.89141400
H	-1.01029600	-0.67394500	-3.64487000
H	0.00529600	0.20280200	-2.45529500
C	-3.65387400	3.51316500	-0.87726300
H	-3.24316600	4.45456200	-1.25162100
H	-4.74395700	3.55514200	-0.89732400
H	-3.30579500	3.32926100	0.14059000

0 imaginary frequency

H = -5171.924002

G = -5172.038877

Esol = -5172.492862

N	0.55736400	2.46942000	0.56678000
N	0.22050800	-0.94974700	-0.93271200
S	-0.63712800	3.61084800	0.33755500
O	-0.59149100	4.08989200	-1.04837500
O	-0.64901400	4.52726300	1.48042300
S	1.10572500	-2.33889300	-0.93279800
O	1.25529800	-2.71949200	-2.34933000
O	0.58099700	-3.33741100	0.02482500
C	3.10213100	3.90732100	0.28587800
C	2.73452300	3.36133000	1.44399800
C	1.47709100	2.56284700	1.71838200
H	3.38469700	3.46180800	2.31410400
H	0.92102700	3.07794100	2.50952800
H	0.06545400	0.13226800	-2.17146200
H	4.03804800	4.45293700	0.20374900
H	2.50364800	3.83081200	-0.61699900
C	1.81673300	1.14463800	2.21017700
H	2.44229200	1.19594100	3.10816300
H	0.90614400	0.58648700	2.45044400
H	2.36928700	0.59171800	1.44526500
C	2.76181000	-1.90628300	-0.35083900
C	3.39071200	-0.75079100	-0.82730200
C	3.40698400	-2.77387200	0.53304600
C	4.68730200	-0.46104100	-0.41089400
H	2.86734900	-0.06510200	-1.48639900
C	4.70568100	-2.48983700	0.94890500

H	2.88769500	-3.65635800	0.88932100
C	5.32427800	-1.33813200	0.46735600
H	5.20172500	0.42988700	-0.74871400
H	5.23885500	-3.13830800	1.63295000
C	-2.13218000	2.60427300	0.47299500
C	-2.57703300	2.22753400	1.74336200
C	-2.76490500	2.15144100	-0.68425600
C	-3.62325800	1.31966000	1.85988800
H	-2.09625600	2.63201200	2.62752400
C	-3.83462500	1.26633800	-0.57546100
H	-2.40344800	2.46922300	-1.65523800
C	-4.21859000	0.83640100	0.69295800
H	-3.98001500	0.98423800	2.82582900
H	-4.34832500	0.88639000	-1.44986400
N	6.69451300	-1.03126700	0.91140100
N	-5.24965100	-0.20326200	0.80521400
O	7.22924200	-1.81275100	1.69831500
O	-5.44950100	-0.69489500	1.92007300
O	7.22394200	-0.01160500	0.47097400
O	-5.83503900	-0.55034400	-0.21952700
O	-0.16581700	0.78824000	-2.92475700
C	0.72198000	1.77440900	-2.95621200
O	1.63232700	1.89132600	-2.13853400
C	0.48680100	2.77298800	-4.06144700
H	-0.05730600	3.62291400	-3.63353700
H	1.44695800	3.14207000	-4.42872700
H	-0.09781700	2.34344100	-4.87734800
H	0.97641200	2.17353200	-0.32528000
Se	-0.93453900	-0.71193000	0.46478200
C	-2.22859000	-2.06592600	0.07227300

C	-3.62186300	-3.46162000	-0.96054800
C	-3.70736200	-3.70994400	0.37278000
H	-4.12506100	-3.91887000	-1.79754800
H	-4.31162900	-4.41087600	0.92609100
N	-2.71430200	-2.43209000	-1.13363000
N	-2.83092800	-2.84339600	1.00015500
C	-2.32228400	-1.86248300	-2.42739400
H	-2.25916000	-0.77801800	-2.33949600
H	-1.34633700	-2.24774500	-2.73100100
H	-3.08823400	-2.13208300	-3.15609600
C	-2.57438500	-2.77109600	2.43651900
H	-3.27893300	-2.08071000	2.90846100
H	-2.68769600	-3.76748700	2.86666300
H	-1.54838600	-2.42201900	2.57278100

S25

0 imaginary frequency

H = -6147.553838

G = -6147.626677

Esol = -6147.816959

Se	1.15763500	-1.90098400	0.19237400
N	-0.02245600	-1.01516600	-0.82352700
S	-0.44718300	0.48187700	-0.25659900
O	0.04982100	0.81118600	1.10256100
O	-0.20197600	1.49063600	-1.31499800
C	-2.24019200	0.33208200	-0.13407600
C	-2.83710200	0.27268200	1.12629800
C	-3.00450500	0.27475600	-1.30352000
C	-4.22084200	0.14968300	1.22500700

H	-2.21599700	0.33302800	2.01292000
C	-4.38641700	0.14624900	-1.21237800
H	-2.51805500	0.33778300	-2.27042800
C	-4.97174600	0.08563000	0.05279500
H	-4.72180300	0.10543600	2.18405400
H	-5.01288400	0.09730300	-2.09426500
N	-6.43427900	-0.04447000	0.15342900
O	-7.07810400	-0.09604500	-0.89446900
O	-6.92876300	-0.09415300	1.27990100
C	3.19044700	0.63649800	0.09311500
C	2.90485600	2.38148500	1.44373500
C	2.80424700	2.82693200	0.16181200
H	2.80031600	2.90265900	2.38176600
H	2.60067100	3.81034100	-0.23032400
N	3.15883600	1.02874200	1.38658400
N	2.98089000	1.73758400	-0.66479700
C	3.16323400	0.10008300	2.51485500
H	3.23756400	0.67362400	3.43914800
H	2.23311100	-0.47437100	2.48186800
H	4.01517500	-0.57578900	2.41752500
C	2.83175400	1.75881800	-2.12219800
H	1.81827000	2.08987900	-2.35397000
H	3.58661800	2.41636400	-2.56054100
H	2.96259400	0.73867200	-2.48180700
Se	3.38525300	-1.12237400	-0.53469200

S26

0 imaginary frequency

H = -7187.142757

G = -7187.238521

Esol = -7187.526226

Se	1.34239000	-0.05509800	-1.47561500
N	1.08092900	1.52720600	-2.16586000
N	0.52884400	-0.13132900	0.11460100
S	0.98823800	2.90687900	-1.24695900
O	0.91693100	4.01368800	-2.20251200
O	2.00975700	2.94417500	-0.18226000
S	0.24139800	-1.68124100	0.59855100
O	0.32849200	-1.71021900	2.06692600
O	1.05774300	-2.64780200	-0.18468400
C	-1.48063900	-2.00463200	0.17246000
C	-1.77745700	-2.98904000	-0.77110500
C	-2.48877400	-1.26132500	0.79447200
C	-3.10842400	-3.23862900	-1.10014600
H	-0.97338700	-3.55342200	-1.22933600
C	-3.81946600	-1.49877500	0.46267500
H	-2.23391900	-0.50584600	1.52924200
C	-4.10362700	-2.48839500	-0.47911800
H	-3.38274700	-3.99783400	-1.82193200
H	-4.62535100	-0.92855700	0.90927000
N	-5.51192100	-2.75464600	-0.83086800
O	-6.37590500	-2.09980800	-0.25273800
O	-5.73184300	-3.61713500	-1.68061900
C	-0.61067100	2.80797600	-0.41345100
C	-0.73630700	3.36972700	0.85762800
C	-1.69788800	2.21579300	-1.05858900
C	-1.96797000	3.32974800	1.50537600
H	0.12870800	3.81469000	1.33652200
C	-2.92915000	2.16186900	-0.41382700

H	-1.57297700	1.78660700	-2.04667700
C	-3.04028400	2.71360700	0.86259000
H	-2.10559000	3.74944400	2.49424000
H	-3.79213300	1.69765600	-0.87441800
N	-4.32783500	2.61591700	1.56825500
O	-4.45134000	3.23451600	2.62383800
O	-5.20262100	1.90878700	1.06432900
C	3.69005800	-0.83951800	0.80404300
C	3.39199900	-1.45376600	2.92232300
C	3.77864400	-2.55627800	2.22043600
H	3.12247600	-1.33900500	3.95987900
H	3.91341700	-3.57941100	2.53353100
N	3.34194500	-0.40250700	2.03840900
N	3.96047400	-2.16388200	0.91474700
C	2.90452100	0.95756800	2.37186100
H	3.52349400	1.34185200	3.18626100
H	3.00396600	1.58185900	1.48454500
H	1.85445200	0.91937700	2.66589800
C	4.24341600	-3.06053600	-0.20543100
H	3.32660100	-3.59574200	-0.46157400
H	4.56053300	-2.44944900	-1.05040500
H	5.03642400	-3.75482300	0.07926900
Se	3.80870400	0.20701300	-0.73045000

S27

0 imaginary frequency

H = -7344.313201

G = -7344.422529

Esol = -7344.814132

Se	-1.64440700	0.01723300	0.63854100
N	-2.28216800	0.67643700	-0.82611500
N	-0.19192700	0.88508100	1.12823000
S	-1.83537100	2.01810400	-1.68885900
O	-2.29941000	3.24671300	-1.02848700
O	-2.29105400	1.72813800	-3.05832400
S	0.44881800	0.20245100	2.51297400
O	-0.44671600	-0.86484800	3.02025000
O	0.86919500	1.28350200	3.40613600
C	-3.58035300	1.14607900	2.65816300
C	-3.28764200	2.33923200	2.11325800
C	-2.18068900	3.24763500	2.55495000
H	-3.88012300	2.69495400	1.26987500
H	-1.59788200	2.77836900	3.35520300
H	-1.49646400	3.39130400	1.70799600
H	-4.41671800	0.54969300	2.29966200
H	-3.01992400	0.74824500	3.50196000
C	-2.70469300	4.62196400	3.00872300
H	-1.87184300	5.27537000	3.28984600
H	-3.26400700	5.11665600	2.20609300
H	-3.36929800	4.52703100	3.87481100
C	1.93997500	-0.59794200	1.89624300
C	1.92770600	-1.97503600	1.66137200
C	3.07548500	0.17903700	1.64890000
C	3.07264400	-2.58725300	1.15550100
H	1.03469800	-2.55154100	1.87084200
C	4.22195300	-0.42955500	1.14471300
H	3.06036300	1.24284600	1.85895500
C	4.19732100	-1.80382700	0.90817500
H	3.10883500	-3.65199300	0.96164300

H	5.11962600	0.13614600	0.92866000
N	5.41315300	-2.45866500	0.38649700
O	6.42167300	-1.76893000	0.26183600
O	5.33921000	-3.65626300	0.11270000
C	-0.03395400	2.10044300	-1.72427100
C	0.56140100	3.35906900	-1.63465900
C	0.72500500	0.93972100	-1.88014900
C	1.94810200	3.46477700	-1.70608900
H	-0.05727400	4.23781700	-1.49287000
C	2.11040300	1.03940700	-1.94309800
H	0.25725200	-0.03833800	-1.91539100
C	2.69832500	2.30032000	-1.85156600
H	2.44916600	4.42223800	-1.63658700
H	2.73742900	0.16264800	-2.04543600
N	4.16721500	2.40129800	-1.87983200
O	4.66309700	3.52618500	-1.90533700
O	4.81123300	1.35122600	-1.86564100
C	-2.38240800	-2.58418100	-1.06578400
C	-4.56015300	-3.03371200	-0.80109000
C	-4.37185500	-2.61742100	-2.08245300
H	-5.45423800	-3.34199600	-0.28276100
H	-5.07292300	-2.48593100	-2.89134800
N	-3.32429000	-3.00893100	-0.18182300
N	-3.02558900	-2.34660800	-2.23402900
C	-3.03495900	-3.36651300	1.20744900
H	-3.94737100	-3.75493900	1.66147200
H	-2.24841100	-4.12309600	1.23471900
H	-2.69398700	-2.48185100	1.74863100
C	-2.40356700	-1.78096500	-3.43338900
H	-2.43052900	-0.68809000	-3.38565300

H	-1.37077500	-2.12739100	-3.47857600
H	-2.95098300	-2.13616200	-4.30846000
Se	-0.58796500	-2.34089700	-0.66277800

S28

0 imaginary frequency

H = -7344.337229

G = -7344.445421

Esol = -7344.838628

Se	0.19065700	-1.25109800	-0.03668300
N	1.51273300	0.17123300	-0.54331600
N	-1.33906900	-0.33796000	-0.07132800
S	1.91649000	1.13887400	0.75957600
O	1.66367800	0.35396000	1.97617500
O	1.34195300	2.48386300	0.60143100
S	-1.80738100	0.28074700	-1.51445000
O	-2.78823700	-0.56596400	-2.22510300
O	-0.64145600	0.73583100	-2.32203000
C	0.51487800	-2.16791900	-1.81841300
C	1.64530900	-3.11439100	-1.62914100
C	2.90485800	-2.85249900	-2.00320300
H	1.40931100	-4.05884000	-1.13912100
H	3.12018000	-1.89503500	-2.47872200
H	-0.44331200	-2.65402400	-2.00165100
H	0.70365200	-1.36921700	-2.53379100
C	4.06346100	-3.78771500	-1.83435900
H	4.85988900	-3.32263100	-1.23800900
H	3.76570500	-4.71931400	-1.34259200
H	4.50948600	-4.03969600	-2.80569100

C	-2.69440600	1.74959000	-0.95841000
C	-2.02586500	2.72289600	-0.20948900
C	-4.02543100	1.90823100	-1.34516300
C	-2.71280300	3.87190200	0.17152900
H	-0.98783000	2.59128300	0.07953800
C	-4.71574300	3.05758700	-0.96602200
H	-4.50509200	1.13580200	-1.93537900
C	-4.04621900	4.01742500	-0.21126600
H	-2.23369500	4.64801800	0.75516800
H	-5.74975000	3.21914500	-1.24404800
N	-4.77617200	5.23112500	0.19904700
O	-4.16464300	6.06906100	0.85968500
O	-5.95441400	5.33084100	-0.14208500
C	3.70241000	1.30834400	0.59283300
C	4.52758500	0.29317200	1.08385100
C	4.22598000	2.45118300	-0.01345100
C	5.90715900	0.41594000	0.95203300
H	4.09247900	-0.57008600	1.57511600
C	5.60710200	2.57764900	-0.14767500
H	3.55957900	3.23266300	-0.36126000
C	6.42117500	1.55529600	0.33381000
H	6.58426000	-0.34418400	1.32124000
H	6.05573000	3.44803300	-0.60999300
N	7.88417000	1.68503200	0.19074800
O	8.31486300	2.70194000	-0.34943500
O	8.58054000	0.76619000	0.61885900
H	1.08067700	0.73445500	-1.28901600
C	-2.74704700	-2.84832800	1.06026500
C	-4.74739600	-1.84337200	1.13560800
C	-4.05779500	-1.46814500	2.24417100

H	-5.73863800	-1.58442800	0.79905200
H	-4.33100400	-0.81718000	3.05939000
N	-3.93122800	-2.69928100	0.41577300
N	-2.83060800	-2.10402900	2.19420200
C	-4.22616800	-3.25134000	-0.90391600
H	-3.71690700	-4.21104000	-0.99815900
H	-5.30573800	-3.38992800	-0.99349700
H	-3.86373500	-2.56235200	-1.67142700
C	-1.71637400	-1.91268000	3.11624400
H	-2.08878800	-1.44233800	4.02749000
H	-1.27252700	-2.88431100	3.34102000
H	-0.96131800	-1.27607600	2.64887700
Se	-1.29575800	-3.84620200	0.51840600

S29

0 imaginary frequency

H = -7344.352474

G = -7344.460096

Esol = -7344.854849

Se	1.09909800	-1.60641500	0.28553700
N	-0.89579800	-1.86609400	0.34705000
N	1.03326000	0.08868300	1.08231400
S	-1.67825500	-2.03119800	-1.12513600
O	-1.52916200	-3.37541900	-1.70198800
O	-1.32072100	-0.85850800	-1.93344200
S	1.57239800	1.36895400	0.06414600
O	1.79627000	0.83737300	-1.28031000
O	2.64245500	2.10610500	0.75749700
C	2.05891400	-1.82433600	3.92194400

C	1.15737000	-1.10664100	3.25114900
C	1.49226000	0.17212500	2.52474800
H	0.10124000	-1.37397800	3.28283700
H	2.57867400	0.29950700	2.52307900
H	1.77288300	-2.69472600	4.50616300
H	3.11777100	-1.57873100	3.89466600
C	0.81382100	1.34695900	3.24522000
H	1.09195400	2.30930300	2.81204100
H	-0.27615400	1.24378800	3.21386200
H	1.13041200	1.34845500	4.29311000
C	0.16792900	2.49367800	-0.06669500
C	-0.94022000	2.10787900	-0.82622300
C	0.25329800	3.75476200	0.52554700
C	-2.00095100	2.99949800	-0.96681100
H	-0.97278800	1.13589300	-1.30930500
C	-0.80611000	4.64828400	0.38208200
H	1.14294500	4.03404100	1.07804500
C	-1.91741800	4.25057000	-0.35650900
H	-2.87829700	2.74250500	-1.54750600
H	-0.78049400	5.63629400	0.82440200
N	-3.04283700	5.19315500	-0.50614700
O	-4.02092100	4.81384000	-1.14738100
O	-2.93339400	6.29853900	0.02211700
C	-3.40446900	-1.86867800	-0.62037100
C	-3.82326900	-0.71668900	0.05348100
C	-4.29936800	-2.88693100	-0.95076200
C	-5.16085500	-0.58393800	0.41002700
H	-3.10766000	0.05848500	0.30509700
C	-5.64169600	-2.75795900	-0.59712100
H	-3.94019700	-3.76478500	-1.47614300

C	-6.04652900	-1.60975400	0.07778600
H	-5.52691000	0.28968500	0.93485000
H	-6.36843000	-3.52500200	-0.83408700
N	-7.46493600	-1.47377000	0.46053600
O	-8.22785800	-2.38738300	0.15141400
O	-7.79518900	-0.45598000	1.06653300
H	-1.05412900	-2.71681600	0.89178000
C	4.61005100	-0.59437600	-0.75261100
C	4.97916000	0.18352400	-2.82248700
C	5.63582500	0.99712100	-1.95559800
H	4.89642000	0.21652000	-3.89711200
H	6.23904000	1.87412600	-2.12818900
N	4.36175100	-0.80012500	-2.07177000
N	5.40681700	0.50477000	-0.68178400
C	3.48100000	-1.84897600	-2.57296600
H	3.46988600	-1.80400000	-3.66275100
H	3.85072600	-2.82188800	-2.23893200
H	2.47649300	-1.68907500	-2.17709400
C	5.84695500	1.11499700	0.56786900
H	6.68757700	1.77803500	0.35418000
H	5.02071500	1.67846400	1.00819200
H	6.15896300	0.32816200	1.25659400
Se	4.00235100	-1.61093700	0.66596100

S3

0 imaginary frequency

H = -6889.768674

G = -6889.865679

Esol = -6890.402438

Se	-1.08834300	-0.74188400	0.60233100
N	-1.58256900	0.97148800	0.83335100
S	-2.47943200	1.60569400	-0.41287600
O	-2.77799600	2.99580300	-0.03598400
O	-1.86669800	1.33048300	-1.73298200
C	-4.05551000	0.71633900	-0.41234700
C	-5.10296600	1.18932800	0.38257200
C	-4.18956800	-0.45674200	-1.16230500
C	-6.30182700	0.48460400	0.43365800
H	-4.97396500	2.11071400	0.93999100
C	-5.38482500	-1.16916400	-1.11327900
H	-3.37217000	-0.78624200	-1.79207200
C	-6.41963000	-0.68857000	-0.31194600
H	-7.13781200	0.82462700	1.03215600
H	-5.52899500	-2.07865500	-1.68314700
N	-7.68298800	-1.44042000	-0.25872200
O	-7.76472300	-2.47345100	-0.92430500
O	-8.58596100	-0.99558800	0.45043700
Se	0.61903500	-0.81389000	-1.12268000
P	2.50997200	-0.05166600	-0.19150400
C	1.69328300	-1.48960600	4.24212300
C	2.00211800	-0.00290300	4.02366900
C	1.80957900	0.41012200	2.55465500
C	2.66698200	-0.47778500	1.62082600
C	2.37074700	-1.98108400	1.84620100
C	2.55331400	-2.36665100	3.32296300
H	0.63134800	-1.67328900	4.02820600
H	1.85930300	-1.76312000	5.29117300
H	3.03800600	0.20466000	4.33267200
H	0.75695600	0.31000000	2.27930800

H	3.72702000	-0.29092800	1.84670900
H	1.34066500	-2.18456900	1.53630400
H	3.01888400	-2.60106100	1.21541900
H	3.61262400	-2.26226900	3.60167400
H	2.29935500	-3.42596500	3.45110500
H	1.35667700	0.61995400	4.65405100
H	2.07456900	1.46472900	2.43551500
C	2.46776700	4.70304500	-0.01587500
C	1.34162100	3.97441600	-0.76088900
C	1.24092000	2.49832900	-0.34843200
C	2.59796300	1.78530900	-0.52931200
C	3.75002700	2.51162400	0.20205500
C	3.81283800	3.99219500	-0.21944500
H	2.23349500	4.73804100	1.05814100
H	2.54076300	5.74404300	-0.35363100
H	1.52102800	4.03833900	-1.84437600
H	0.90423500	2.43221900	0.69185700
H	2.82804600	1.79712700	-1.60679000
H	3.59684400	2.45625200	1.28705100
H	4.71401800	2.03254500	-0.00846500
H	4.09907300	4.05076800	-1.27975500
H	4.60813600	4.49270200	0.34700600
H	0.37403000	4.45343100	-0.57576600
H	0.48175700	1.99336300	-0.95005900
C	6.12752000	-2.70929500	-1.87593600
C	6.43631400	-1.39515800	-1.14676500
C	5.25112800	-0.93538200	-0.27879600
C	3.96785200	-0.79988400	-1.13164400
C	3.64583100	-2.13208700	-1.84575900
C	4.83824500	-2.59427900	-2.70010100

H	6.01714600	-3.51653100	-1.13726200
H	6.96805300	-2.98982000	-2.52193300
H	6.67027100	-0.61231900	-1.88259600
H	5.08601900	-1.67425900	0.51603100
H	4.16104100	-0.04706100	-1.90993800
H	3.40432500	-2.90135500	-1.10068700
H	2.75580900	-2.02351900	-2.47328500
H	4.99214700	-1.87813900	-3.52047400
H	4.59527300	-3.55544300	-3.16862200
H	7.32568300	-1.50508600	-0.51431000
H	5.50173400	0.01052500	0.21415400

S30

0 imaginary frequency

H = -7573.490756

G = -7573.609446

Esol = -7574.061766

N	-2.20575800	-1.92087600	0.55663200
N	0.61371400	-0.76146800	0.09990100
S	-3.76206600	-1.62609900	-0.11476400
O	-4.81703000	-2.26900700	0.67533000
O	-3.66472500	-1.88598400	-1.55711400
S	1.74531700	-1.96857800	0.39286600
O	1.96461100	-2.70945700	-0.85395300
O	1.43518000	-2.69455300	1.63169100
C	-1.15295200	-4.79384700	-0.97696900
C	-2.11967600	-4.30327500	-0.20143800
C	-1.86824500	-3.34820600	0.93807000
H	-3.15614100	-4.59473700	-0.36855600

H	-0.79197100	-3.29110700	1.11932600
H	0.32414700	-0.15939000	0.95109700
H	-1.37582300	-5.48893700	-1.78246200
H	-0.10865700	-4.52492100	-0.83844500
C	-2.54460000	-3.77600700	2.24908700
H	-3.62309800	-3.90033600	2.12760600
H	-2.11387400	-4.73016400	2.57154700
H	-2.35943100	-3.03154600	3.03000000
C	3.22695600	-0.99268600	0.72944000
C	4.41129500	-1.37757100	0.09728600
C	3.19358800	0.05172700	1.66056000
C	5.59311400	-0.69797700	0.38695100
H	4.39845000	-2.19857600	-0.61141400
C	4.37259000	0.73681100	1.94345700
H	2.26097900	0.34653500	2.13759100
C	5.55017800	0.35208200	1.30207500
H	6.53411400	-0.96901200	-0.07598800
H	4.39213600	1.55609500	2.65154800
C	-3.91101700	0.16049000	0.09871500
C	-3.85696100	0.96108700	-1.04372900
C	-4.16122600	0.69288300	1.36464700
C	-4.03215600	2.33639800	-0.91706000
H	-3.68709800	0.50402700	-2.01181800
C	-4.33408200	2.06928600	1.49481800
H	-4.19360400	0.05287800	2.23753500
C	-4.25843200	2.86456300	0.35338200
H	-4.00285800	2.99613700	-1.77539100
H	-4.51990800	2.52701400	2.45827100
N	6.79294200	1.09091700	1.59180900
N	-4.41301400	4.32532800	0.49294200

O	7.81696700	0.73358700	1.01090100
O	-4.21399700	5.01511900	-0.50736300
O	6.72718900	2.02706400	2.38708500
O	-4.71891100	4.76436100	1.59899600
O	0.07181200	0.80458800	2.13526400
C	-0.81995200	0.44636100	2.98069900
O	-1.73982500	-0.38417800	2.77289400
C	-0.72680400	1.08340800	4.36393900
H	0.10072400	0.62071400	4.91542600
H	-0.50455500	2.15163900	4.27927500
H	-1.64867600	0.93122800	4.92914600
H	-2.02448200	-1.27558800	1.37847900
Se	-0.70425200	-0.98483200	-1.15090200
C	1.45969800	1.44735100	-2.08509300
C	3.13320500	2.67441400	-1.25016100
C	1.97095700	3.13612000	-0.71678500
H	4.15294700	2.99494600	-1.10763600
H	1.78351300	3.92398300	-0.00457200
N	2.80659200	1.62287400	-2.08580400
N	0.94531700	2.37956800	-1.24893800
C	3.75270100	0.82395200	-2.86253600
H	3.85605600	1.22791400	-3.87356900
H	4.71849700	0.83877100	-2.35599200
H	3.37238300	-0.19762200	-2.91745000
C	-0.46955000	2.51925800	-0.90293000
H	-0.68762400	3.57962200	-0.76205600
H	-1.05524800	2.12610100	-1.73259700
H	-0.67996100	1.96137000	0.01305900
Se	0.58032700	0.12516600	-3.06279800

S31

0 imaginary frequency

H = -7573.491071

G = -7573.610599

Esol = -7574.063640

N	-2.07071800	-0.67065000	1.51549000
N	0.77509400	0.52511500	0.39713200
S	-3.38568000	-1.42875300	0.76786500
O	-4.36156300	-1.94533300	1.73943900
O	-2.84700700	-2.36577000	-0.23449400
S	2.01582500	0.16998200	1.41706300
O	2.56815800	-1.19325100	1.19583600
O	1.71983100	0.55258900	2.81128000
C	-0.07405800	-3.28350900	2.52108500
C	-1.27676700	-2.72895500	2.67787400
C	-1.50245200	-1.23926400	2.78383400
H	-2.16513600	-3.35457100	2.75973300
H	-0.52951700	-0.74274800	2.85576700
H	-0.02336700	2.00078000	0.62479400
H	0.04185000	-4.36524700	2.49054100
H	0.83349300	-2.69005800	2.44473200
C	-2.33334600	-0.86103200	4.01891600
H	-2.47259500	0.22461700	4.06209900
H	-3.31539500	-1.34104300	4.00083500
H	-1.80355000	-1.17415800	4.92516800
C	3.27176200	1.32633200	0.81993600
C	3.58339300	1.34454600	-0.54357900
C	3.94242900	2.13993000	1.73182300
C	4.58840400	2.18828100	-1.00232700

H	3.03031600	0.70890700	-1.22835000
C	4.95002100	2.98998900	1.27770700
H	3.66512500	2.10728900	2.77968400
C	5.25657000	2.99640800	-0.08075300
H	4.85757300	2.23805100	-2.05008000
H	5.49291500	3.64030500	1.95232800
C	-4.14187800	-0.04066700	-0.10609400
C	-3.42998300	0.65328600	-1.08997400
C	-5.47158200	0.25856200	0.19240600
C	-4.06677900	1.67846100	-1.78286400
H	-2.39033600	0.41334200	-1.29277400
C	-6.11185200	1.27975400	-0.50632300
H	-5.98951100	-0.30420500	0.96083300
C	-5.39608000	1.97005400	-1.48076500
H	-3.55327700	2.24743600	-2.54775100
H	-7.14267700	1.54490400	-0.30768200
N	6.32411600	3.88851400	-0.56472000
N	-6.07069000	3.05408500	-2.22154100
O	6.58683800	3.86427600	-1.76714900
O	-5.41821500	3.65066100	-3.07635800
O	6.89234700	4.60146400	0.26131400
O	-7.24310300	3.29322500	-1.93826500
O	-0.31241500	2.96744400	0.75606700
C	-1.45628700	3.08773300	1.40643400
O	-2.17965600	2.15622500	1.74990800
C	-1.80325000	4.53038500	1.69473900
H	-2.78321700	4.59164500	2.16892400
H	-1.04430900	4.96492300	2.35415600
H	-1.79583800	5.11047700	0.76640400
H	-2.19069400	0.35601700	1.57934500

Se	-0.11898700	-0.86311400	-0.34562500
C	1.91494000	-3.05126100	-1.49282200
C	1.92751900	-5.08683300	-0.58532400
C	3.19522000	-4.59512000	-0.52430000
H	1.51763200	-6.02761100	-0.25381800
H	4.10127100	-5.02321800	-0.12594500
N	1.14817800	-4.12844100	-1.20128600
N	3.17325400	-3.33932800	-1.09708600
C	-0.29710900	-4.21795700	-1.42996300
H	-0.56386900	-5.26832000	-1.55699600
H	-0.84271300	-3.78311100	-0.58945600
H	-0.53088800	-3.65870000	-2.33665400
C	4.30125800	-2.40875600	-1.14848500
H	4.19629000	-1.69314800	-0.33049700
H	5.22452400	-2.98089500	-1.04576400
H	4.29756700	-1.89261400	-2.10903400
Se	1.30072500	-1.46771500	-2.29534600

S32

0 imaginary frequency

H = -3821.221973

G = -3821.293558

Esol = -3821.486964

Se	1.40733100	-1.71887200	-0.99951400
N	0.45487500	-0.26635400	-1.21810500
S	0.01605100	0.57764200	0.19240100
O	0.50648600	-0.02521000	1.45013200
O	0.30317100	2.00206000	-0.06749800
C	-1.77718000	0.39725700	0.18215600

C	-2.38164900	-0.47577500	1.08826800
C	-2.52939800	1.13216400	-0.73831300
C	-3.76645100	-0.62347000	1.07391200
H	-1.76878200	-1.01820200	1.79947400
C	-3.91290000	0.98492900	-0.76030500
H	-2.03414000	1.81614600	-1.41827100
C	-4.50660000	0.10754500	0.14671700
H	-4.27573700	-1.28563400	1.76294500
H	-4.53294500	1.53511400	-1.45698000
N	-5.97212700	-0.04817600	0.12819800
O	-6.60567500	0.60982800	-0.69596100
O	-6.47363700	-0.82738500	0.93773100
C	3.57324300	-0.02598600	-0.09182000
C	3.82873000	1.15417000	1.79088700
C	3.70416200	2.03573000	0.76643100
H	3.95707700	1.31874000	2.84872000
H	3.69989500	3.11363800	0.76180000
N	3.75736100	-0.12139900	1.25365100
N	3.54033000	1.29978300	-0.39689600
C	3.62497400	-1.37595000	1.98328400
H	4.22359600	-1.32526600	2.89512300
H	2.57207400	-1.54555200	2.22302100
H	3.99072900	-2.18469800	1.34950000
C	3.25355300	1.82283500	-1.72897300
H	2.35659600	2.44273100	-1.67824000
H	4.10652700	2.39658000	-2.10275800
H	3.06069400	0.97114500	-2.38070100
O	3.44619900	-0.99467000	-0.91690100

S33

0 imaginary frequency

H = -5103.792903

G = -5103.904215

Esol = -5104.276517

Se	-0.04643800	-0.35380800	-2.01983000
N	1.10653800	0.73736800	-1.21502100
S	1.64908600	0.23463700	0.26663300
O	2.05316600	-1.18727300	0.37816300
O	0.72192200	0.72225000	1.33181200
C	3.15944900	1.20981300	0.41179100
C	3.26695200	2.46607800	-0.19276600
C	4.19295900	0.69116000	1.19685500
C	4.42740500	3.21407800	-0.01139100
H	2.46018100	2.83296200	-0.81579400
C	5.35336600	1.43756900	1.38561300
H	4.08738700	-0.29107800	1.64418400
C	5.44944900	2.68803700	0.77774700
H	4.55273400	4.18713100	-0.46979000
H	6.17561000	1.06918900	1.98632500
N	6.67733800	3.47922100	0.97092100
O	7.56980600	2.98720400	1.66002000
O	6.73458200	4.58339100	0.43152100
I	-1.78214600	1.93408300	0.43911700
C	-3.51848800	3.00502200	-0.29880300
C	-3.95838000	4.10822200	0.42384400
C	-4.11828300	2.57931400	-1.47415300
C	-5.05637000	4.82090200	-0.06770000
H	-3.47801300	4.41643900	1.34817600
C	-5.21749200	3.30268800	-1.94567600

H	-3.74965400	1.70463700	-1.99894500
C	-5.68348300	4.41875500	-1.24803400
H	-5.41955300	5.68492200	0.48136800
H	-5.70752800	2.98549900	-2.86162100
H	-6.53844500	4.97405100	-1.62243200
N	-1.96106900	0.25720300	-0.77544300
S	-2.98964100	-0.95475500	-0.22021700
O	-4.28738800	-0.40537800	0.19325200
O	-2.90050300	-1.92005900	-1.32797700
C	-2.26986300	-1.71904600	1.24636400
C	-0.98381100	-2.26208000	1.18490800
C	-3.03446300	-1.77103100	2.41522300
C	-0.44430900	-2.85820300	2.32099000
H	-0.39509300	-2.19686800	0.27719800
C	-2.50256900	-2.38032100	3.54928100
H	-4.03011700	-1.34275000	2.42553800
C	-1.21625800	-2.91244700	3.48010800
H	0.55994800	-3.26123400	2.31573600
H	-3.06155500	-2.44634300	4.47426400
N	-0.65049200	-3.55277400	4.68248100
O	-1.33972100	-3.55953800	5.70155700
O	0.47355400	-4.04265700	4.59146300
C	1.53082600	-2.75684700	-3.06067800
C	2.44563400	-4.62423300	-2.19007600
C	1.18813000	-4.93614800	-2.58993800
H	3.20882400	-5.23363500	-1.73239600
H	0.64764700	-5.86857000	-2.54787100
N	2.65906800	-3.28340800	-2.48738600
N	0.62606000	-3.78662600	-3.13467200
C	3.82968000	-2.48670900	-2.15084300

H	4.73707200	-3.05056200	-2.38363000
H	3.79679000	-1.57806400	-2.75361100
H	3.80657800	-2.21150900	-1.09307800
C	-0.72609800	-3.63145400	-3.65546600
H	-1.43813700	-3.41292900	-2.85383100
H	-0.72252600	-2.79954300	-4.36212700
H	-1.01943600	-4.54688800	-4.17571000
O	1.36493700	-1.57112200	-3.45392800

S35

0 imaginary frequency

H = -5017.993786

G = -5018.102700

Esol = -5018.496372

Se	1.99835100	-0.83337600	0.79380200
N	2.56432300	0.52490700	1.66993800
N	1.46844000	-0.36716900	-0.80568100
S	2.88073800	2.05101500	1.03870000
O	3.71846900	1.94682900	-0.16317200
O	3.32090800	2.84350400	2.18560700
S	0.87985700	-1.69947500	-1.63720100
O	1.12944400	-2.94134900	-0.86539700
O	1.34718100	-1.61086100	-3.02128400
C	4.39254200	-2.32692400	0.20875700
C	4.85239500	-1.22379000	-0.41675600
C	4.65151500	-0.89704300	-1.86152900
H	5.39290900	-0.47728100	0.16616300
H	4.12198100	-1.71115300	-2.36796900
H	3.99886600	-0.01358200	-1.91338400

H	4.59911100	-2.50496900	1.26174600
H	3.85813600	-3.10726500	-0.32826000
C	5.97364700	-0.58213600	-2.58335400
H	6.49335700	0.25711200	-2.10716200
H	6.64720200	-1.44636000	-2.57700700
H	5.78098700	-0.30971500	-3.62609400
C	-0.90360500	-1.43725500	-1.62784300
C	-1.72812800	-2.54051900	-1.40244200
C	-1.42997000	-0.16699600	-1.87165100
C	-3.11023400	-2.36804300	-1.40264700
H	-1.28827200	-3.51368400	-1.21615100
C	-2.80892800	0.01783800	-1.84592600
H	-0.76924800	0.67344800	-2.04554900
C	-3.62338200	-1.08909400	-1.60511500
H	-3.78672200	-3.19605200	-1.23088800
H	-3.24987200	0.99599000	-1.99949700
N	-5.08174000	-0.89592600	-1.52462500
O	-5.79222100	-1.89953500	-1.52968200
O	-5.49576700	0.26011200	-1.43909600
C	1.27431100	2.69420000	0.53735800
C	0.97943500	2.81552700	-0.82058800
C	0.37508600	3.10223800	1.52522900
C	-0.26155000	3.31991200	-1.20305700
H	1.71112000	2.50678200	-1.55744400
C	-0.86433300	3.61108100	1.14853800
H	0.64778600	3.02993300	2.57231200
C	-1.16678800	3.69081600	-0.21071500
H	-0.53426700	3.42726900	-2.24595900
H	-1.59098300	3.94184200	1.88032900
N	-2.50123000	4.16992300	-0.61259700

O	-2.81759600	4.04236300	-1.79616100
O	-3.22193700	4.65128100	0.25896500
C	-1.37009400	-1.28062500	2.08681900
C	-3.42227200	-1.90259500	2.83299800
C	-2.60604300	-2.97163800	2.96097400
H	-4.46793300	-1.78321200	3.07008800
H	-2.80053500	-3.96520300	3.33319900
N	-2.66827500	-0.86079400	2.29683600
N	-1.34213000	-2.59785000	2.50008800
C	-3.13564500	0.48134000	1.99525800
H	-3.53136600	0.96089200	2.89633700
H	-2.28074900	1.05022700	1.62867100
H	-3.91418600	0.46305100	1.22573200
C	-0.16512100	-3.44941700	2.49871200
H	-0.38116900	-4.39286300	1.98895800
H	0.63344500	-2.94387900	1.96045100
H	0.16586000	-3.65741300	3.52220200
O	-0.44618500	-0.58817500	1.61648000

S36

0 imaginary frequency

H = -5018.034803

G = -5018.140918

Esol = -5018.537940

Se	0.68062300	1.49886600	-0.35805900
N	2.51796600	1.89406000	0.18093100
N	-0.09490400	1.94161100	1.19410000
S	3.66542300	1.18864800	-0.82760500
O	4.98566600	1.58577800	-0.34623900

O	3.18805200	1.49327100	-2.18378500
S	0.05276100	0.72732000	2.30339400
O	-0.41603900	1.25956000	3.58355200
O	1.39804700	0.09933100	2.20450400
C	0.48941100	3.27026700	-1.28751800
C	0.73918900	4.40855800	-0.37275600
C	-0.21191800	5.27340100	-0.00087900
H	1.75763800	4.52412300	-0.01021200
H	-1.22760800	5.13142400	-0.37407500
H	1.24189600	3.15208800	-2.07200400
H	-0.51531500	3.22257000	-1.70706000
C	0.00404400	6.45302900	0.89751900
H	1.04773900	6.53127500	1.21704000
H	-0.27499500	7.38970500	0.39672300
H	-0.62299700	6.37564900	1.79567500
C	-1.11527700	-0.56008500	1.80714600
C	-0.73069500	-1.51879600	0.86514000
C	-2.41668100	-0.52234900	2.31319500
C	-1.67194700	-2.42611300	0.38871800
H	0.29574200	-1.56285000	0.52031200
C	-3.36083300	-1.43384200	1.84900000
H	-2.67404000	0.21259200	3.06819300
C	-2.97672700	-2.35373900	0.87423300
H	-1.41285800	-3.17934200	-0.34498900
H	-4.38056800	-1.43376300	2.21312700
N	-3.99012300	-3.26333200	0.32000800
O	-5.09892900	-3.28083600	0.85045400
O	-3.67384900	-3.94309600	-0.65967700
C	3.51628800	-0.59481700	-0.60586800
C	4.17942700	-1.20756500	0.45945700

C	2.70768800	-1.32236800	-1.48346700
C	4.02871000	-2.57705900	0.65915200
H	4.81629900	-0.62348200	1.11479700
C	2.55225100	-2.69242100	-1.28500200
H	2.22849200	-0.82336700	-2.31814200
C	3.21167300	-3.29227900	-0.21382700
H	4.52623500	-3.09070400	1.47214800
H	1.94483500	-3.29786800	-1.94635400
N	3.04210800	-4.74380900	-0.00259800
O	2.26824500	-5.33851100	-0.75127600
O	3.68149600	-5.26381000	0.90836800
H	2.60153700	1.56555200	1.15156600
C	-2.80823600	0.75864100	-1.51479300
C	-4.95274400	0.81822700	-0.77751400
C	-4.85575900	-0.21406200	-1.64652900
H	-5.79507100	1.18135600	-0.20980000
H	-5.59454600	-0.92772800	-1.97631600
N	-3.69648900	1.41489300	-0.68849400
N	-3.53873000	-0.25619700	-2.10130300
C	-3.33243600	2.57170900	0.11108700
H	-3.82685300	2.51758900	1.08467400
H	-2.25325100	2.55075000	0.26619900
H	-3.62339600	3.50496100	-0.38620700
C	-2.97606400	-1.21163700	-3.03913000
H	-1.92051600	-0.96439200	-3.16104300
H	-3.07550400	-2.23073900	-2.65225100
H	-3.47607800	-1.14073500	-4.01077200
O	-1.60942900	1.02926300	-1.71496700

S37

0 imaginary frequency

H = -5018.045462

G = -5018.152061

Esol = -5018.549925

Se	-0.23697500	0.17003300	0.09858600
N	-1.88018800	-0.74764300	-0.00755900
N	0.78232600	-0.58868200	-1.25352000
S	-3.02607400	-0.35378300	-1.18831700
O	-3.14990800	-1.45009300	-2.15357400
O	-2.73931200	1.01694100	-1.62016400
S	1.30889600	-2.17655700	-0.99042500
O	1.67051200	-2.74277900	-2.29233000
O	0.31809900	-2.82952800	-0.12477300
C	2.08828800	2.26346500	-2.93013800
C	1.06394000	1.53448800	-2.48845700
C	0.98824700	0.03468300	-2.61046800
H	0.17371400	2.01530300	-2.08907500
H	1.95648500	-0.34108300	-2.95377500
H	2.07448800	3.34932400	-2.89087300
H	2.97954100	1.80465300	-3.35402800
C	-0.09561400	-0.37900900	-3.61534500
H	-0.19069300	-1.46651400	-3.65818900
H	-1.06455600	0.05415200	-3.35659100
H	0.18410500	-0.01346700	-4.60981100
C	2.83358800	-2.04608400	-0.03073300
C	2.83820700	-1.37520000	1.19642700
C	3.97356100	-2.68262000	-0.52535400
C	4.01194500	-1.34332600	1.94249600
H	1.95072700	-0.86768100	1.55268200

C	5.14945500	-2.65286700	0.22179800
H	3.93302100	-3.19263600	-1.48102900
C	5.14624400	-1.98304200	1.44252900
H	4.05855100	-0.83264400	2.89605500
H	6.05474400	-3.13569000	-0.12441700
N	6.39136600	-1.94128900	2.23237700
O	7.37590100	-2.51948200	1.77533300
O	6.36962300	-1.32594800	3.29734100
C	-4.55598300	-0.31356700	-0.23617400
C	-5.40678300	-1.41906800	-0.27317200
C	-4.86653200	0.82832500	0.50677200
C	-6.59073800	-1.39067900	0.46148600
H	-5.14852500	-2.27968400	-0.88019700
C	-6.04754500	0.86103300	1.24091400
H	-4.19806400	1.68203500	0.49549000
C	-6.88638200	-0.25254000	1.20727000
H	-7.28034700	-2.22554000	0.46029700
H	-6.32944500	1.72570300	1.82855700
N	-8.13924700	-0.21948500	1.98678100
O	-8.37812500	0.79784600	2.63507500
O	-8.86433500	-1.21107900	1.94006000
H	-1.74942200	-1.75909500	0.07001800
C	2.38115500	2.85669700	0.58340600
C	3.69948900	4.66738800	0.17716100
C	2.42119800	5.10448400	0.22876500
H	4.61891800	5.20540000	0.00653400
H	2.01294400	6.09646400	0.11371700
N	3.68231100	3.29029600	0.39176900
N	1.60582900	3.99893800	0.47002000
C	4.82593900	2.40017400	0.41053600

H	5.52849700	2.68267400	1.20204100
H	4.45255400	1.39383500	0.60387100
H	5.34607700	2.41301200	-0.55343700
C	0.16516000	4.01153600	0.63880300
H	-0.20479500	2.99881800	0.47837100
H	-0.11833700	4.34460800	1.64447100
H	-0.29030300	4.67695500	-0.10034600
O	2.00558400	1.69972800	0.81520800

S38

0 imaginary frequency

H = -5247.169615

G = -5247.287794

Esol = -5247.743644

N	1.63785500	0.93296500	1.22224800
N	-0.79557900	-0.17414200	0.05270500
S	3.16599100	1.33792700	0.54076600
O	4.12966700	1.57009400	1.62169200
O	2.98463100	2.36979500	-0.49648300
S	-1.90204800	-0.14426600	1.33694400
O	-2.43320800	1.21867500	1.43873400
O	-1.33167400	-0.79643200	2.52502300
C	0.27895100	3.95928500	2.06681800
C	1.34282000	3.19416500	2.31919000
C	1.25892500	1.69778100	2.49478300
H	2.33691800	3.63390100	2.38982400
H	0.20829600	1.42320500	2.61224100
H	-0.27183500	-1.06491500	0.03889700
H	0.37072500	5.03607300	1.94640300

H	-0.72096900	3.53934200	1.99157700
C	2.00254400	1.18965700	3.73573200
H	1.92144000	0.10209200	3.81871700
H	3.05732500	1.46716600	3.72589900
H	1.53142900	1.63301400	4.62003800
C	-3.19657300	-1.22143400	0.69855700
C	-4.48547000	-0.70448000	0.56809300
C	-2.90337400	-2.55649900	0.40203100
C	-5.51064000	-1.53602900	0.12199600
H	-4.67659900	0.33276800	0.81753900
C	-3.92460900	-3.38591400	-0.05139800
H	-1.89447900	-2.94230500	0.51089400
C	-5.20973500	-2.86085000	-0.18159700
H	-6.52608800	-1.17740700	0.00887700
H	-3.74234000	-4.42368300	-0.30103000
C	3.64272200	-0.19563000	-0.29112500
C	2.96956700	-0.62734000	-1.43941200
C	4.75260500	-0.87909200	0.20967700
C	3.40843800	-1.77900300	-2.08654600
H	2.09685400	-0.09291000	-1.79556000
C	5.19628900	-2.02789700	-0.44113000
H	5.25818200	-0.50920300	1.09417900
C	4.51496600	-2.45612700	-1.57766100
H	2.91121400	-2.15200700	-2.97309500
H	6.05338100	-2.58628900	-0.08602600
N	-6.29300800	-3.74267200	-0.65786100
N	4.98178800	-3.67488000	-2.26786800
O	-7.41537400	-3.25323000	-0.77224200
O	4.37793000	-4.02110300	-3.28105700
O	-6.00538000	-4.91090600	-0.91037800

O	5.94452200	-4.26799700	-1.78446300
O	0.50184300	-2.66514800	0.48451900
C	1.21765900	-2.79776200	1.47320300
O	1.85394700	-1.79709600	2.07078000
C	1.46186400	-4.12174200	2.14944700
H	2.52552600	-4.25050200	2.36810300
H	0.92549100	-4.13609000	3.10512200
H	1.10055300	-4.93440300	1.51860000
H	1.64565100	-0.91374700	1.65512200
Se	0.28413100	1.29873400	-0.23844100
C	-1.56711900	3.21609200	-1.88224500
C	-1.40898000	5.46616700	-1.66117400
C	-2.69390200	5.12420400	-1.40787300
H	-0.92796700	6.43166300	-1.67065200
H	-3.54625800	5.73451800	-1.15356900
N	-0.71402400	4.29703000	-1.96073600
N	-2.79548600	3.74224000	-1.54773000
C	0.70542400	4.17241200	-2.25065700
H	1.00189200	4.92048300	-2.99162700
H	1.31061900	4.28941400	-1.34713600
H	0.87608000	3.17563200	-2.65900300
C	-3.96432900	2.92050900	-1.29627200
H	-3.75107300	1.92235500	-1.68113000
H	-4.16607300	2.85110500	-0.22235200
H	-4.83543800	3.33508200	-1.81260900
O	-1.28628600	2.01503500	-2.06919200

S39

0 imaginary frequency

H = -5247.167817

G = -5247.285776

Esol = -5247.741965

N	-1.23603900	0.06922600	0.73759700
N	1.99285100	-0.27055000	0.01191800
S	-2.13225000	-1.26748600	1.02448400
O	-2.19157800	-1.50781500	2.47077400
O	-1.65969400	-2.30938500	0.10042300
S	3.28889700	0.71150000	-0.43910100
O	3.60952000	0.34443400	-1.82984300
O	4.36795100	0.75232000	0.56190300
C	1.10210900	1.30759700	3.14560300
C	-0.06631100	0.71890100	2.83387900
C	-0.94773500	1.16257600	1.68648300
H	-0.46188700	-0.08550200	3.44925600
H	-0.38823300	1.88275100	1.08081700
H	1.23859200	-1.07321700	-1.28296200
H	1.67523100	1.01048000	4.01875400
H	1.50648000	2.13055900	2.56044000
C	-2.21911200	1.85430100	2.20653000
H	-2.83660700	2.19615800	1.36972600
H	-2.81137400	1.17453700	2.82664200
H	-1.94803300	2.72050400	2.81848600
C	2.55728200	2.36291100	-0.48757900
C	3.15795900	3.38220100	0.25362700
C	1.43281000	2.60407800	-1.28549900
C	2.62742400	4.67054000	0.20336200
H	4.03155700	3.15875700	0.85602500
C	0.89700700	3.88804400	-1.33351600
H	0.96834600	1.80011300	-1.84730800

C	1.50511000	4.89942800	-0.58878200
H	3.06637900	5.48879100	0.76071800
H	0.02615800	4.11581600	-1.93564500
C	-3.81660600	-0.87970300	0.49306100
C	-4.02738400	-0.36820700	-0.79252400
C	-4.87823700	-1.13896600	1.36029400
C	-5.32729800	-0.10794700	-1.21371300
H	-3.18608200	-0.16828500	-1.45050900
C	-6.18222300	-0.88070900	0.94050400
H	-4.67868300	-1.53306800	2.35047200
C	-6.38245600	-0.37037300	-0.33916900
H	-5.53577300	0.29208900	-2.19818800
H	-7.03381600	-1.06660700	1.58309600
N	0.93616200	6.25865800	-0.63837500
N	-7.76044300	-0.09519600	-0.78632300
O	1.49002100	7.13323400	0.02620800
O	-7.91180600	0.35077000	-1.92259400
O	-0.05944600	6.43440900	-1.33920100
O	-8.67339800	-0.32938700	0.00391500
O	0.84091700	-1.64829500	-2.02363800
C	-0.26808600	-1.11081900	-2.49314500
O	-0.74128600	-0.04496200	-2.09320100
C	-0.93514900	-1.95023800	-3.55417900
H	-1.57058400	-1.32305500	-4.18177600
H	-0.19666600	-2.47852800	-4.16162500
H	-1.56392200	-2.69485900	-3.05142500
H	-0.83836200	0.10866800	-0.20629600
Se	2.01658400	-0.95577800	1.63918000
C	3.25336600	-3.22800200	0.20877400
C	2.60713000	-4.46189800	-1.54293100

C	3.80783500	-3.90903800	-1.85041900
H	1.96118300	-5.10724600	-2.11623200
H	4.41158400	-3.98471900	-2.74057500
N	2.27142800	-4.04383300	-0.26509200
N	4.20027700	-3.13814600	-0.76621800
C	1.02745700	-4.30864900	0.45160100
H	0.71631000	-5.33742800	0.25585000
H	1.21699300	-4.18461700	1.51818400
H	0.24520300	-3.61158000	0.14139700
C	5.41180000	-2.32925300	-0.66500000
H	6.29580800	-2.97253500	-0.70370100
H	5.42833800	-1.59931200	-1.47671000
H	5.37915400	-1.79447200	0.28380700
O	3.29913600	-2.67203600	1.35811800

S4

0 imaginary frequency

H = -7929.356771

G = -7929.476098

Esol = -7930.111134

Se	-0.95649100	-0.58271300	1.15378700
N	-2.01996600	-1.42947900	0.06477200
S	-2.62358100	-0.65883400	-1.29316500
O	-2.57207200	-1.64436900	-2.38146700
O	-1.99865300	0.66379900	-1.49667200
C	-4.36529000	-0.38457900	-0.91100000
C	-4.71654400	0.53740400	0.07924200
C	-5.32674300	-1.09240900	-1.63348200
C	-6.06404500	0.75440300	0.35148500

H	-3.94662500	1.06866600	0.63106400
C	-6.67623800	-0.87543500	-1.36384800
H	-5.01310800	-1.79729500	-2.39495100
C	-7.01943000	0.04392600	-0.37535700
H	-6.38130600	1.45756600	1.11146700
H	-7.45547400	-1.40142800	-1.90104300
N	-8.44735600	0.27306400	-0.08694900
O	-8.72899000	1.09160100	0.78676700
O	-9.27117500	-0.36878100	-0.73789900
N	-1.75139800	0.96485000	1.52678800
S	-0.89431000	1.95848900	2.52959400
O	-1.84884000	2.86022600	3.17543500
O	0.07500700	1.20426300	3.35945100
C	0.10521900	2.89828600	1.35267200
C	-0.46402200	3.33332200	0.15179900
C	1.46640200	3.05866900	1.61489700
C	0.35269800	3.89965400	-0.82315600
H	-1.51588400	3.16519900	-0.04789400
C	2.28782900	3.62509100	0.64703400
H	1.87383100	2.70311700	2.55442300
C	1.71861100	4.00797100	-0.56671100
H	-0.04372800	4.21519600	-1.78026400
H	3.35282200	3.74531400	0.80212000
N	2.60349500	4.49460200	-1.63549300
O	3.81698500	4.31527500	-1.49512200
O	2.08672600	5.03271300	-2.61113500
Se	0.92270400	0.27208000	-0.49722400
P	2.49224700	-1.24934500	-0.18337600
C	-0.16299000	-5.09444500	-1.13032500
C	0.84797100	-5.17214700	0.02015300

C	1.29777900	-3.77758800	0.49230600
C	1.87284000	-2.95331900	-0.68288600
C	0.80819600	-2.85635800	-1.80475200
C	0.38722600	-4.25231500	-2.28779500
H	-1.09251800	-4.63512300	-0.76886900
H	-0.41778700	-6.10366800	-1.47590800
H	1.73324100	-5.74005800	-0.30315100
H	0.43635600	-3.24030600	0.91040400
H	2.76967200	-3.46365100	-1.06810300
H	-0.07201500	-2.34448700	-1.40901700
H	1.16073500	-2.25567000	-2.64594600
H	1.24346800	-4.76547800	-2.75148900
H	-0.37470500	-4.13306700	-3.06595400
H	0.42316700	-5.71621700	0.87260700
H	2.03085500	-3.89048800	1.29594900
C	4.12043200	-2.06120200	4.22760100
C	2.96497900	-1.06939100	4.03934500
C	2.23612300	-1.28337200	2.70236600
C	3.23920200	-1.20367000	1.53089600
C	4.41102300	-2.19967400	1.69962200
C	5.10924300	-1.98823500	3.05622700
H	3.71807300	-3.08230300	4.30134300
H	4.64276900	-1.86345500	5.17130500
H	3.35293700	-0.04139900	4.07731700
H	1.73929900	-2.25910600	2.71728000
H	3.65766600	-0.18848700	1.55513300
H	4.03820000	-3.23025200	1.64350700
H	5.14419200	-2.08480900	0.89226600
H	5.60119400	-1.00482500	3.05536900
H	5.90429700	-2.73481300	3.17261000

H	2.24114800	-1.15455500	4.85739500
H	1.46572900	-0.51837500	2.59315200
C	5.14015800	1.09895900	-3.33904000
C	4.54389700	-0.24575800	-3.76821800
C	3.41657100	-0.70562900	-2.82825900
C	3.88047700	-0.75475400	-1.35303900
C	4.52155800	0.58851000	-0.92704100
C	5.63572700	1.02940400	-1.89117200
H	4.38165600	1.88925800	-3.42360800
H	5.96195700	1.38078900	-4.00788900
H	5.33660300	-1.00845400	-3.78283200
H	2.56135500	-0.02240800	-2.91025400
H	4.62750600	-1.55585600	-1.24938000
H	6.47717600	0.32395100	-1.82324400
H	6.01249600	2.00617200	-1.56756800
H	4.14917400	-0.18757700	-4.78955400
H	3.06666100	-1.69188900	-3.14777900
H	3.74406900	1.36185100	-0.89513400
H	4.93766200	0.51464800	0.08366700

S40

0 imaginary frequency

H = -7519.690486

G = -7519.810528

Esol = -7520.205022

Se	-0.50865800	-0.29695600	-0.38625400
N	-1.32227500	-0.18210700	1.17714100
N	0.26315700	-1.85333300	-0.04981000
S	-2.15339800	1.21236400	1.44075000

O	-2.61093500	1.16933000	2.82287100
O	-3.07017200	1.56505600	0.35834400
S	1.36471100	-2.25485000	-1.22130100
O	1.24464100	-1.40550100	-2.41040900
O	1.39356100	-3.70651400	-1.33896200
C	-0.36132300	2.97835800	-2.30109300
C	1.21816700	4.50927500	-2.86399500
C	0.12926900	5.18997300	-2.43549500
H	2.17348000	4.86405200	-3.21808200
H	-0.04523300	6.25103500	-2.34793800
N	0.92501300	3.15029700	-2.77868900
N	-0.84316400	4.25493500	-2.08641500
C	1.79215200	2.03889600	-3.12510500
H	1.90620300	1.94578300	-4.21108300
H	2.77782000	2.17134300	-2.66914600
H	1.33957400	1.12583400	-2.73774700
C	-2.16000500	4.52456200	-1.53804200
H	-2.56935200	3.58260900	-1.17082600
H	-2.08231300	5.22748200	-0.70305300
H	-2.82701300	4.94241200	-2.30088300
O	-0.95652100	1.90600100	-2.12094600
C	-4.91405800	-2.60037400	1.74138600
C	-3.69376400	-2.65043600	0.86276900
C	-3.90026800	-1.82292200	-0.42326400
C	-5.22858900	-2.24930800	-1.09583500
C	-6.41826300	-2.13971500	-0.13828600
C	-6.16538500	-2.34592200	1.31038100
H	-4.75114700	-2.78801700	2.80217600
H	-2.82308300	-2.27494800	1.40984700
H	-4.00728800	-0.77154700	-0.13313800

H	-5.45449100	-1.64669400	-1.98029000
H	-3.47337400	-3.70042300	0.61618800
H	-5.16514200	-3.29747700	-1.42493700
C	-7.36353300	-2.27705500	2.21847200
H	-7.83920100	-1.29162500	2.15924800
H	-8.12466800	-3.00536200	1.91661300
H	-7.08268600	-2.46735400	3.25847000
O	-7.54050500	-1.93232900	-0.57402800
C	-2.76988900	-1.91909000	-1.41342200
C	-2.11832000	-3.23138700	-1.66752100
H	-2.74626000	0.19015800	-1.86212100
H	-2.81983000	-4.07017400	-1.62816400
H	-1.57612300	-3.25014200	-2.61606300
C	-2.27612000	-0.77834900	-2.00948300
H	-1.56145200	-0.84441100	-2.82616600
H	-1.37004300	-3.39696800	-0.86780200
O	2.79643600	-1.76246400	-0.54896600
C	3.36342800	-2.58935400	0.47077100
H	3.03905900	-2.23949200	1.45480700
H	3.07627200	-3.63307300	0.32424300
C	4.89240100	-2.49064000	0.39102000
Cl	5.43012900	-0.79269100	0.62839000
Cl	5.54156200	-3.51772900	1.72693200
Cl	5.48764500	-3.10007400	-1.18472700
O	-0.98598700	2.41309000	1.33034000
C	-0.13485500	2.57500900	2.46298400
H	-0.15400100	1.69937700	3.11614300
H	-0.45079500	3.45412900	3.03188800
C	1.30972600	2.80240600	1.99504600
Cl	1.41365000	4.22859800	0.91366800

Cl	1.93964300	1.35152400	1.12707900
Cl	2.30481800	3.08297800	3.47101200

S41

0 imaginary frequency

H = -7519.718688

G = -7519.836086

Esol = -7520.235016

Se	-0.34297500	-1.13704600	0.39895300
N	0.89571000	0.04868400	1.05525500
N	-0.09559400	-0.65972700	-1.38173600
S	0.85817600	-0.11131900	2.66663800
O	2.09784500	0.39636600	3.23944800
O	0.32373200	-1.44119000	3.04328200
S	-1.38612900	-0.09880900	-2.28191000
O	-2.44916200	0.22888500	-1.34438400
O	-1.58324800	-0.91495000	-3.46293600
C	-3.20258500	-3.23249800	-0.58962500
C	-5.38423200	-3.76429100	-0.90178300
C	-5.19082900	-3.62594500	0.42926300
H	-6.27521300	-4.00181900	-1.46151500
H	-5.87965000	-3.71943300	1.25407600
N	-4.16605100	-3.51867200	-1.53225100
N	-3.85150700	-3.29288800	0.62726900
C	-3.90537400	-3.55439200	-2.96114900
H	-2.93450800	-3.09213300	-3.14014000
H	-3.89616300	-4.58540100	-3.33257300
H	-4.67238700	-2.98538100	-3.49427100
C	-3.19978900	-3.07278300	1.90711200

H	-2.28060000	-2.51746000	1.73296800
H	-3.84705200	-2.47845600	2.55715800
H	-2.95832300	-4.01951200	2.40332200
O	-1.99751700	-2.99011400	-0.80047900
C	5.09000500	-0.39214000	-0.33426600
C	3.76762300	-0.88490300	-0.85708900
C	3.22729000	-2.06478700	-0.02809700
C	4.33821800	-3.11631400	0.16234100
C	5.61553300	-2.52504000	0.75621300
C	5.93801500	-1.11180400	0.42578900
H	5.36116900	0.62954500	-0.59978100
H	3.03899400	-0.06632000	-0.84203500
H	2.98351600	-1.65639500	0.95754900
H	4.02027600	-3.94270100	0.80603800
H	3.88383900	-1.17557700	-1.91364400
H	4.60041800	-3.55674600	-0.81173500
C	7.23758800	-0.57577300	0.96285000
H	7.24868000	-0.61475800	2.05790500
H	8.08226600	-1.18667400	0.62463800
H	7.39971400	0.45943800	0.64800000
O	6.36463200	-3.21063600	1.43691100
C	1.96411400	-2.69650200	-0.60458200
C	1.88761200	-3.17366700	-1.86135900
H	1.02112100	-2.96651200	1.34158200
H	2.73097800	-3.13209900	-2.54534300
H	0.98645200	-3.65675100	-2.23156100
C	0.77272100	-2.82474800	0.28857200
H	0.03871400	-3.55237000	-0.05499600
H	0.56534500	-1.25257900	-1.89626700
O	-0.75611400	1.28495700	-2.88063300

C	-0.39858100	2.29587500	-1.92450500
H	-1.28816000	2.84853900	-1.61447800
H	0.09058300	1.84300500	-1.05675400
C	0.58413900	3.25845200	-2.59822100
Cl	0.99000900	4.51597900	-1.37321600
Cl	2.08003600	2.39275700	-3.09192900
Cl	-0.16555300	4.03180300	-4.03251100
O	-0.37559400	0.86413200	3.25433900
C	-0.27361600	2.25081100	2.97615500
H	0.34966600	2.44319900	2.09724600
H	0.13212700	2.78627000	3.83967100
C	-1.68327300	2.78364200	2.68169500
Cl	-2.75494200	2.56587600	4.10567400
Cl	-2.38257000	1.92369000	1.26590700
Cl	-1.53023600	4.54343300	2.30930200

S42

0 imaginary frequency

H = -7519.693846

G = -7519.812930

Esol = -7520.209522

Se	0.32298900	-0.41042100	0.60752300
N	0.52180000	1.21794500	1.24511800
N	-1.30864500	-0.63894300	1.19489400
S	1.91792300	1.92789000	0.73385600
O	2.81386200	0.98851900	0.04984000
O	2.41533600	2.77812900	1.80936800
S	-1.82897500	-2.17761800	0.91671900
O	-2.37312000	-2.74326700	2.14801900

O	-0.86188100	-2.93795200	0.11786200
C	2.05056300	-0.87495200	3.00156500
C	3.68090900	0.10778600	4.17376700
C	2.50417100	0.38558100	4.79426300
H	4.69025400	0.39669600	4.41977500
H	2.29490900	0.96698900	5.67794800
N	3.39653000	-0.66987000	3.06403700
N	1.49807700	-0.22742600	4.06758000
C	4.35732900	-1.16649900	2.07872500
H	3.89740400	-1.95994200	1.48792600
H	4.65175300	-0.35308800	1.41125000
H	5.22982200	-1.56395100	2.60261200
C	0.06104000	-0.16030300	4.32142400
H	-0.41983100	-1.01188500	3.83917000
H	-0.11141100	-0.20210200	5.39908500
H	-0.35207100	0.75988800	3.90399900
O	1.42707800	-1.56724300	2.13133100
C	2.93462600	-4.13577400	-3.68608200
C	1.86003200	-3.10379900	-3.89999900
C	1.29609600	-2.56344100	-2.56613800
C	2.46813700	-2.18904200	-1.64790900
C	3.43914000	-3.33632100	-1.42788500
C	3.65117700	-4.28195700	-2.55409500
H	2.26830100	-2.26806200	-4.49135600
H	3.13535100	-4.80671600	-4.52198900
H	1.06163200	-3.53861900	-4.51370600
C	4.69525300	-5.34825000	-2.35846600
H	5.67264800	-4.90389600	-2.13799700
H	4.44579200	-5.98249700	-1.50024800
H	4.78785700	-5.98080600	-3.24651700

O	4.06915300	-3.44929200	-0.38099200
C	0.27110700	-1.45722100	-2.78736000
C	-1.07956500	-1.91830100	-3.27939100
C	0.52027100	-0.15575800	-2.56435400
H	1.48376900	0.21523700	-2.22812800
H	-0.99521000	-2.48411300	-4.21664900
H	-1.75322600	-1.07464300	-3.45474000
H	2.11247400	-1.85519000	-0.67429400
H	-0.23772300	0.59910400	-2.75964900
H	3.04641400	-1.35862800	-2.08065000
H	0.76195600	-3.39518500	-2.08464200
H	-1.54770200	-2.58250100	-2.54299400
O	-3.10257400	-1.91819100	-0.12220900
C	-4.43543400	-2.12318500	0.33524700
H	-4.45281900	-2.36705800	1.39943100
H	-4.87052700	-2.94537100	-0.23994400
C	-5.29234400	-0.86985100	0.09320100
Cl	-4.68997700	0.51504200	1.05205700
Cl	-6.97160900	-1.29161000	0.61507000
Cl	-5.30368400	-0.43982800	-1.65285300
O	1.41466700	2.91132100	-0.49818800
C	0.59122300	4.01702000	-0.12196100
H	-0.41134600	3.67017900	0.14627500
H	1.03949100	4.56081100	0.71365400
C	0.47977900	4.96564300	-1.31988000
Cl	-0.57560200	6.33392200	-0.79433500
Cl	-0.27640300	4.13479500	-2.72208000
Cl	2.09208100	5.59467500	-1.78740500

S43

0 imaginary frequency

H = -7519.724810

G = -7519.842627

Esol = -7520.241285

Se	-0.03990300	-1.07412200	1.03200100
N	-0.86499900	0.49878700	1.44100800
N	1.14557100	-0.25772600	-0.20918700
S	-2.11492100	0.13072000	2.40741100
O	-2.30884200	1.13432200	3.43748400
O	-2.02262100	-1.31292300	2.77452200
S	0.44253500	-0.08467900	-1.75456200
O	-0.96842100	-0.45265800	-1.66593300
O	1.33201100	-0.67220400	-2.73667100
C	1.62146000	-3.92791900	-0.65761700
C	0.76901500	-5.81072600	-1.58247000
C	1.80760600	-5.41112600	-2.35135800
H	0.10334600	-6.65389200	-1.67893400
H	2.21946700	-5.83750200	-3.25243600
N	0.64730400	-4.89450400	-0.53841900
N	2.33925400	-4.25644800	-1.78102600
C	-0.32648700	-4.92237500	0.53952000
H	-0.50808900	-3.89933500	0.87039300
H	-1.26329400	-5.34740100	0.17146800
H	0.02991500	-5.51535700	1.38942300
C	3.41358800	-3.43813700	-2.32948900
H	4.23932900	-4.08428000	-2.64053300
H	3.05536200	-2.85533200	-3.18319900
H	3.76151900	-2.74620400	-1.56172900
O	1.81003600	-2.96009100	0.11391900

C	4.78262100	2.09948100	1.48548800
C	4.04085200	1.57885800	2.69281400
C	3.27881500	0.30091600	2.40913800
C	4.08697700	-0.64954900	1.56060000
C	4.53498800	0.01256300	0.25562600
C	4.99477300	1.41854900	0.34330100
H	4.77292100	1.40967600	3.50398400
H	5.14492800	3.12450900	1.56285300
H	3.38017600	2.37087500	3.05630500
C	5.66050500	1.99898700	-0.87504800
H	5.98456200	3.02853800	-0.69692100
H	6.53038500	1.40164300	-1.17156400
H	4.97171600	1.99106300	-1.72699400
O	4.55227200	-0.61120300	-0.79846600
C	2.01855900	0.08644700	2.84941000
C	1.28064800	1.08801400	3.71975400
C	1.29288200	-1.18701100	2.55121300
H	1.90919400	-2.03759900	2.26943200
H	1.94523000	1.56294900	4.44808700
H	0.47541900	0.60675700	4.28070100
H	3.58931800	-1.58542100	1.30588000
H	0.60449000	-1.47618700	3.34958300
H	5.01240900	-0.91190500	2.10220000
H	1.92205800	-0.92350300	-0.32750600
H	0.80608700	1.87172800	3.11995900
O	0.55653400	1.51309900	-1.99374900
C	-0.33786200	2.36619200	-1.24599700
H	-0.41586800	2.03848500	-0.20415000
H	-1.32383200	2.35794100	-1.71586300
C	0.23382300	3.78471200	-1.29283100

Cl	1.84752600	3.84096300	-0.50332500
Cl	-0.92010000	4.83135500	-0.39123000
Cl	0.37485900	4.36356900	-2.98864400
O	-3.50555200	0.28214000	1.50226600
C	-3.67085500	-0.67672900	0.46443000
H	-2.77790100	-0.73387200	-0.16558400
H	-3.90004600	-1.66041100	0.88514100
C	-4.84707100	-0.24207500	-0.41493300
Cl	-4.52685500	1.35160900	-1.17724500
Cl	-6.36085300	-0.15437700	0.54510600
Cl	-5.02611600	-1.49909200	-1.70269500

S44

0 imaginary frequency

H = -5446.723959

G = -5446.849253

Esol = -5447.486668

Se	0.42899800	0.76087200	-0.31910600
N	-0.49175400	2.23165400	-0.16986900
N	-0.56626400	-0.36146100	-1.27541900
S	-1.49795600	2.85494600	-1.34048100
O	-0.95026000	2.60813100	-2.68717500
O	-1.77118200	4.22841500	-0.90254000
S	-0.23436500	-1.94184400	-0.90139900
O	0.96152000	-2.04036700	-0.02633100
O	-0.27032000	-2.75756600	-2.12110500
C	-1.66372400	-2.40288300	0.10353000
C	-2.17085100	-1.50237500	1.04436500
C	-2.18325300	-3.69117600	-0.02864000

C	-3.20649500	-1.90133900	1.88176700
H	-1.77551100	-0.49454500	1.09856400
C	-3.22176000	-4.09564700	0.80797700
H	-1.78246800	-4.36020500	-0.78203700
C	-3.70952500	-3.19524700	1.75187100
H	-3.63009000	-1.23342600	2.62122600
H	-3.65375400	-5.08626800	0.73919500
N	-4.80048000	-3.62377500	2.64806700
O	-5.20567800	-2.81073500	3.47715400
O	-5.23069800	-4.76717500	2.51362500
C	-3.06419500	1.97037100	-1.22943200
C	-3.34714100	0.94652400	-2.13475800
C	-3.98061000	2.35671800	-0.24706900
C	-4.57168800	0.28786500	-2.05278700
H	-2.61485600	0.67056700	-2.88285600
C	-5.20287300	1.69692300	-0.15800100
H	-3.74447700	3.17760700	0.42098700
C	-5.47478100	0.67276900	-1.06412700
H	-4.83335900	-0.50934100	-2.73722700
H	-5.94361100	1.96657500	0.58439600
N	-6.77203400	-0.02482700	-0.97653600
O	-7.55670100	0.34074600	-0.10292600
O	-6.98743300	-0.92954400	-1.78118900
C	1.70455700	2.91950000	2.02142200
C	0.52957700	3.20107700	3.94351100
C	0.52145800	4.38221200	3.28386600
H	0.10079900	2.92256100	4.89342500
H	0.07454800	5.32845100	3.54551700
N	1.25719000	2.29700000	3.17014800
N	1.25270900	4.21774200	2.10917800

C	1.47222000	0.88282800	3.41634900
H	1.28539800	0.33131600	2.49169400
H	2.49809800	0.68106500	3.74163500
H	0.77671800	0.54433300	4.18741200
C	1.36340800	5.17134600	1.01801800
H	0.44482100	5.18886400	0.42253700
H	1.56981600	6.16805200	1.41841700
H	2.19501400	4.85840500	0.38485200
O	2.36362700	2.39486800	1.10556800
C	3.64229600	-0.29172200	-2.15492200
C	3.91837700	-0.23169800	-0.63126000
C	5.26536500	-0.87963400	-0.18845800
C	5.36631300	-2.28362600	-0.79774800
C	5.04242900	-2.39341100	-2.27211500
C	3.68991200	-1.75655100	-2.63228200
H	3.90289400	0.80132400	-0.27862800
C	5.25860600	-0.97316800	1.37606700
C	5.70880100	-3.36977900	-0.09258900
H	5.82576600	-1.90067700	-2.86953300
H	2.87924300	-2.31774800	-2.15205300
C	6.07802500	-3.37133700	1.36508600
C	6.33014100	-1.95282600	1.88343700
H	5.72525000	-4.33541800	-0.59941200
H	5.27168200	-3.84829000	1.94530900
H	7.32469500	-1.61345800	1.56347300
H	3.53924400	-1.82769500	-3.71505700
H	6.96379700	-4.00246800	1.52376000
H	6.34290400	-1.94746900	2.98088000
H	4.28279300	-1.40652000	1.64459600
H	3.09655600	-0.75503900	-0.12949100

C	5.37348600	0.37909900	2.09866800
H	6.35820500	0.83757200	1.95001800
H	4.60995200	1.09655900	1.78131700
H	5.25334800	0.22757100	3.17896900
C	6.44773400	-0.01301000	-0.69129200
H	4.45855100	0.24973100	-2.67071900
C	2.40409600	0.47585500	-2.57472700
C	1.55467100	-0.02547200	-3.69063100
H	0.81684900	0.71531100	-4.00306400
H	2.15656200	-0.34182100	-4.55021400
C	1.99645800	1.62866500	-1.92486500
H	2.59417500	2.09325400	-1.14768000
H	6.32949700	1.03382100	-0.39063100
H	7.40101000	-0.37569900	-0.29345400
H	6.53320300	-0.03162500	-1.78258400
H	5.04530900	-3.44641800	-2.57506800
H	1.24400500	2.25070000	-2.40265500
H	1.00383500	-0.92237300	-3.35717300

S45

0 imaginary frequency

H = -5446.760841

G = -5446.885001

Esol = -5447.524695

Se	0.61358000	0.20049500	-0.56128800
N	-0.99206400	0.94080200	-0.26860000
N	0.21323900	-1.29017700	-1.69937500
S	-1.74980000	1.52515700	-1.60688200
O	-1.74344800	0.53505600	-2.71790800

O	-1.32316700	2.89389800	-1.96223100
S	0.42809300	-2.82819700	-1.10572800
O	1.40255600	-2.68387200	-0.01840700
O	0.66800100	-3.73005300	-2.23043100
C	-1.14757400	-3.32211100	-0.37343700
C	-1.91552800	-2.39648600	0.33734400
C	-1.53475300	-4.65911500	-0.49088400
C	-3.09052300	-2.81896400	0.95203900
H	-1.62159100	-1.35333600	0.38959900
C	-2.70836700	-5.08544400	0.12622800
H	-0.92815900	-5.34873400	-1.06716000
C	-3.46321000	-4.15692600	0.83926900
H	-3.71804400	-2.13234100	1.50629700
H	-3.04438000	-6.11268500	0.05927400
N	-4.70751200	-4.60420300	1.49445400
O	-5.35236100	-3.76517700	2.12105500
O	-5.01995200	-5.78700200	1.37424200
C	-3.43237600	1.62911200	-0.97656300
C	-4.45190900	1.00230200	-1.69303800
C	-3.69951100	2.38561300	0.16914800
C	-5.76980700	1.12594600	-1.25547700
H	-4.20831700	0.42619200	-2.57867400
C	-5.01209900	2.50529700	0.61278100
H	-2.89146600	2.86401500	0.71221800
C	-6.02499900	1.87475700	-0.11009200
H	-6.59052900	0.65619800	-1.78317400
H	-5.26419000	3.07612900	1.49772100
N	-7.41783800	2.00921100	0.35686600
O	-7.61422100	2.67004700	1.37575600
O	-8.29506000	1.45396300	-0.30132700

C	0.78478800	2.82745600	1.45874300
C	-0.66891900	3.27908000	3.13432100
C	-0.63048000	4.36453700	2.32396300
H	-1.22096700	3.10025000	4.04372500
H	-1.13961700	5.31295600	2.39543500
N	0.20511900	2.33291100	2.60625500
N	0.27130200	4.09174600	1.29824100
C	0.44431500	0.98320900	3.08788200
H	0.64156100	0.34354800	2.22738000
H	1.30423700	0.94220600	3.76497900
H	-0.44523200	0.62175500	3.60868400
C	0.55289900	4.91899400	0.13414500
H	-0.09834900	4.64328600	-0.70101200
H	0.40304000	5.96848600	0.39804200
H	1.59447400	4.76707500	-0.15599600
O	1.61160100	2.24949300	0.72309600
C	3.99823600	0.86759500	-1.37209500
C	4.13073000	-0.28206700	-0.34296100
C	5.23292900	-0.08863400	0.74122100
C	6.54056400	0.32261900	0.05018300
C	6.43398300	1.41776000	-0.99183000
C	5.35790900	1.11290000	-2.04682200
H	3.16734300	-0.43248600	0.15345500
C	5.42877300	-1.45577000	1.48048600
C	7.72458300	-0.24023500	0.32786000
H	6.18391800	2.37537000	-0.50946000
H	5.66169800	0.22161500	-2.61144700
C	7.95355000	-1.31106500	1.35974600
C	6.74125800	-1.47866600	2.28114500
H	8.60272000	0.09439900	-0.22647300

H	8.17696200	-2.26463700	0.85419700
H	6.73385000	-0.67736000	3.03242800
H	5.28259200	1.93780700	-2.76650400
H	8.85334200	-1.07556400	1.94574800
H	6.81718100	-2.42133600	2.83808000
H	5.53138900	-2.21352400	0.68852500
H	4.33696400	-1.20638700	-0.89872700
C	4.24072100	-1.88096300	2.35708200
H	4.10963900	-1.21271400	3.21676300
H	3.30133400	-1.91421900	1.79678200
H	4.41561700	-2.88804600	2.75380500
C	4.80548100	1.02889000	1.72614600
H	3.72518800	1.78084900	-0.82775300
C	2.87054400	0.58134800	-2.36088400
C	3.01628600	-0.17339900	-3.45961500
H	2.18211700	-0.37822200	-4.12414100
H	3.96873700	-0.61547500	-3.73466700
C	1.53161400	1.18726100	-2.07983100
H	1.56956100	2.19974700	-1.68133600
H	3.80305700	0.84423200	2.12423200
H	5.50598900	1.10539800	2.56440800
H	4.77253400	2.00781900	1.23975200
H	7.40668800	1.56346900	-1.47617800
H	0.83352600	1.11202500	-2.91282800
H	-0.54080400	-1.12777800	-2.37333500

S46

0 imaginary frequency

H = -5446.733626

G = -5446.860419

Esol = -5447.496457

Se	0.05094000	0.32018200	-1.32075800
N	0.44474000	1.79360000	-0.53885100
N	-0.46355700	-0.80063800	-0.08174000
S	0.97608000	1.88857600	1.04350700
O	1.67623200	0.66479600	1.47553400
O	-0.07232400	2.44325800	1.90520900
S	-0.82217200	-2.32976700	-0.62076600
O	-0.32701200	-2.55294700	-2.00207900
O	-2.22993200	-2.63919800	-0.34617400
C	0.18271800	-3.34143100	0.48269400
C	0.42630800	-4.66054700	0.08726900
C	0.64010200	-2.84352400	1.70557500
C	1.14002400	-5.50477800	0.93171700
H	0.06830300	-5.01691900	-0.87269700
C	1.35750400	-3.68838100	2.55175000
H	0.46194500	-1.80834000	1.97524100
C	1.59335400	-5.00190200	2.15072700
H	1.34973900	-6.53294800	0.66439200
H	1.73114100	-3.34298100	3.50785100
N	2.36310600	-5.89123200	3.04092100
O	2.75805100	-5.42593700	4.10823500
O	2.56816900	-7.04188000	2.65650200
C	2.23068500	3.16386800	0.81471600
C	2.14607100	4.32717600	1.57765900
C	3.28590400	2.93732300	-0.07409300
C	3.14283000	5.29440600	1.45423200
H	1.30810300	4.46853100	2.25106600
C	4.28014600	3.90115300	-0.20090800

H	3.31605400	2.02751400	-0.66553100
C	4.19083500	5.06243000	0.56785800
H	3.11702700	6.21338300	2.02640000
H	5.11387000	3.77309400	-0.87986900
N	5.24632000	6.08384000	0.43295600
O	6.16283700	5.85462500	-0.35518300
O	5.14626300	7.10104300	1.11655300
C	2.79000200	-1.34524200	-1.84118700
C	3.87638800	-3.28126800	-1.47273700
C	3.33440100	-3.34763300	-2.71409500
H	4.47145900	-3.99542900	-0.92577900
H	3.35642400	-4.13610200	-3.44971700
N	3.53210600	-2.04939800	-0.93029900
N	2.67617700	-2.14799100	-2.94566400
C	3.95080400	-1.52293200	0.36346800
H	3.89478300	-2.31989300	1.10844900
H	4.97816100	-1.14695900	0.31108900
H	3.27621600	-0.71548300	0.65132700
C	1.87557400	-1.80349100	-4.11010700
H	2.46170300	-1.94592000	-5.02211600
H	0.96945600	-2.41269400	-4.13557400
H	1.59586200	-0.75350900	-4.01915700
O	2.34602600	-0.17135100	-1.71046500
C	-3.78723700	0.42791500	-1.62478100
C	-3.71918300	1.29944300	-0.35640600
C	-4.73176800	0.91941300	0.77010500
C	-6.13007000	0.80082400	0.14543100
C	-6.22983200	-0.01997300	-1.12294500
C	-5.22612700	0.43969300	-2.19150600
H	-2.69504300	1.26079700	0.03261300

C	-4.72348600	2.06194000	1.84332100
C	-7.22127900	1.38636300	0.65798000
H	-6.03605900	-1.08062400	-0.90291800
H	-5.47225000	1.46034300	-2.51579900
C	-7.25323600	2.19539900	1.92542900
C	-5.97161400	2.00537200	2.73998500
H	-8.16960700	1.27033600	0.13085400
H	-7.39107500	3.26127600	1.67982400
H	-6.00715000	1.03987900	3.26259400
H	-5.30501500	-0.20650500	-3.07418200
H	-8.13456100	1.91812400	2.52135900
H	-5.89877500	2.77473300	3.51949900
H	-4.78496400	3.00667300	1.27990000
H	-3.91577900	2.34282300	-0.63849900
C	-3.45027300	2.12054500	2.69997200
H	-3.39153800	1.27227000	3.39200300
H	-2.53231900	2.13127500	2.10687600
H	-3.45544800	3.03305800	3.30858100
C	-4.33066700	-0.43721800	1.40142500
C	-2.78561800	0.82002200	-2.70151300
C	-2.51539300	-0.21446700	-3.76983400
H	-3.43662800	-0.50092500	-4.29122000
H	-1.80954200	0.15807100	-4.51966500
H	-2.10566800	-1.13613300	-3.33671700
C	-2.15056300	2.00690300	-2.73511300
H	-1.46894600	2.25488700	-3.54626900
H	-2.29285700	2.77298600	-1.98151900
H	-4.41306800	-1.26402800	0.69170600
H	-3.29086100	-0.41817600	1.74228600
H	-4.97067000	-0.67580300	2.25780400

H	-7.25087400	0.03205100	-1.51951200
H	-3.55857700	-0.61082400	-1.34591000

S49

0 imaginary frequency

H = -5446.757695

G = -5446.883412

Esol = -5447.520826

Se	0.33734400	0.42297300	-1.10653900
N	0.60139100	1.74428900	0.05678100
N	0.27197500	-1.15390500	-0.11401200
S	-0.35004900	1.81966600	1.40071000
O	0.47190700	2.36007900	2.48614000
O	-1.09571200	0.55077100	1.63072600
S	1.37819100	-2.37544400	-0.37886700
O	1.82884200	-2.18766900	-1.76089000
O	0.75993600	-3.62850700	0.05450200
C	2.75041000	-2.04924400	0.74254600
C	3.43714600	-3.14799400	1.26625900
C	3.12388600	-0.73614800	1.03593800
C	4.53682400	-2.92987900	2.09147100
H	3.10470800	-4.15525500	1.04121200
C	4.22112500	-0.51770700	1.86471200
H	2.57168300	0.10597000	0.63865300
C	4.90998400	-1.61689500	2.37198400
H	5.09706800	-3.75123200	2.52026400
H	4.53850000	0.48421400	2.12424400
N	6.07804200	-1.38311200	3.24349800
O	6.39784400	-0.21700800	3.46521900

O	6.66114800	-2.36988500	3.68934300
C	-1.61463700	3.05759200	1.03362200
C	-2.92198300	2.84021800	1.47444600
C	-1.25540700	4.24183500	0.38259900
C	-3.89185400	3.81558100	1.25145100
H	-3.17167300	1.91457400	1.98138700
C	-2.22004000	5.21811900	0.15475200
H	-0.23428000	4.38934000	0.04812300
C	-3.52327100	4.98677500	0.59420600
H	-4.91638800	3.68302100	1.57634300
H	-1.98275900	6.14576700	-0.35104000
N	-4.54877400	6.01744300	0.34924900
O	-4.19842300	7.04085500	-0.23633200
O	-5.69102700	5.78944300	0.74392300
C	4.31723500	1.31472000	-1.88140700
C	6.18197600	2.60724700	-1.71151000
C	6.54408200	1.45729000	-2.32499500
H	6.76751000	3.47265000	-1.44281100
H	7.50482400	1.13181900	-2.69249000
N	4.81770600	2.52648800	-1.43288000
N	5.40660900	0.65749300	-2.42952700
C	3.99217800	3.52589000	-0.78166800
H	4.39423700	3.77732600	0.20562600
H	3.93213300	4.43889300	-1.38544800
H	2.99269600	3.10183300	-0.66337700
C	5.30979200	-0.66662300	-3.01347700
H	6.04223700	-1.34187300	-2.55849500
H	4.30280700	-1.03981900	-2.81619700
H	5.47774100	-0.63454900	-4.09616000
O	3.15406000	0.90438500	-1.80969400

C	-2.98986300	-1.64491500	-1.99440700
C	-3.94536200	-1.42933100	-0.83689200
C	-4.09405200	-2.63018700	0.15909500
C	-4.31288200	-3.91059900	-0.65455300
C	-3.37452100	-4.12125400	-1.82182500
C	-3.34003600	-2.89799400	-2.76723800
H	-3.70296400	-0.53178900	-0.26525700
C	-5.33713500	-2.35484500	1.07071900
C	-5.27725200	-4.79996400	-0.38143300
H	-2.35181400	-4.30613400	-1.46418800
H	-4.34068000	-2.77696500	-3.20992600
C	-6.24119800	-4.70214900	0.76927800
C	-5.80659100	-3.63652500	1.77931600
H	-5.37964500	-5.67185500	-1.02882800
H	-7.24869800	-4.47171800	0.38622400
H	-4.99491200	-4.03001300	2.40558900
H	-2.64646700	-3.09652700	-3.58633200
H	-6.33393300	-5.68109200	1.26012200
H	-6.63416300	-3.39963700	2.46011700
H	-6.15131700	-2.05361600	0.39260500
H	-4.93734200	-1.25036500	-1.28137700
C	-5.14636600	-1.21888100	2.08837000
H	-4.42801100	-1.48914900	2.87012000
H	-4.79830500	-0.29005500	1.62260100
H	-6.09990900	-0.99831900	2.58236400
C	-2.79768400	-2.76412700	0.99342000
C	-1.99063100	-0.80343800	-2.35176200
C	-1.12967500	-0.96722600	-3.59158500
H	-1.56902400	-1.63531700	-4.33268500
H	-0.98060300	0.00478000	-4.08145700

H	-0.13216800	-1.35874300	-3.34930000
C	-1.64244300	0.41896900	-1.55977500
H	-1.68227200	1.33565200	-2.16096300
H	-2.17667300	0.55602000	-0.62518000
H	-1.94268800	-3.03231100	0.36738300
H	-2.55589700	-1.82257400	1.49911400
H	-2.89808200	-3.54385200	1.75554200
H	-3.67519700	-5.01108800	-2.38674900
H	-0.20801800	-1.08710400	0.78829300

S5

0 imaginary frequency

H = -8086.537555

G = -8086.670459

Esol = -8087.410087

Se	-0.29823900	1.99072700	0.34356600
N	-1.92847900	1.88988600	-0.32154800
N	0.38344400	2.81927000	-1.05839300
S	-3.00722600	1.14429700	0.66892300
O	-3.95609400	2.08160200	1.28823700
O	-2.32662800	0.18256700	1.58285500
S	1.95981000	3.26345400	-0.82693600
O	2.37942900	3.10122000	0.58798300
O	2.17093600	4.55249200	-1.48920200
C	-0.53068000	4.58631400	2.07538200
C	-1.57983600	4.75739400	1.25480500
C	-1.52315800	5.36924400	-0.11265700
H	-2.56417800	4.41988600	1.58241700
H	-0.49004500	5.62936400	-0.36808300

H	-1.84374700	4.61056300	-0.84037100
H	-0.65163000	4.15784900	3.06747300
H	0.47420900	4.89800600	1.79967300
C	-2.43133400	6.60480900	-0.23701800
H	-2.40116900	7.00256000	-1.25721800
H	-3.47394900	6.35744200	-0.00384700
H	-2.11442000	7.40032500	0.44680300
C	2.86317500	2.00786900	-1.76302600
C	4.00852900	1.44707800	-1.19731800
C	2.41448000	1.62747000	-3.03145300
C	4.70600900	0.46482100	-1.89532000
H	4.33201100	1.76879800	-0.21385000
C	3.10614700	0.64556200	-3.73369900
H	1.52165700	2.07893100	-3.45021900
C	4.23245800	0.07059000	-3.14519600
H	5.59459700	-0.00081600	-1.48749700
H	2.78412000	0.31370100	-4.71294800
N	4.93823300	-1.00355800	-3.86257900
O	5.84014300	-1.59337800	-3.26377900
O	4.58172600	-1.25597700	-5.01149600
C	-3.93019500	0.20151600	-0.56242600
C	-5.32280400	0.18982300	-0.48892800
C	-3.23914600	-0.51654000	-1.54318600
C	-6.04733000	-0.56295900	-1.41168200
H	-5.82518100	0.77729800	0.27147600
C	-3.95850600	-1.26768000	-2.46691100
H	-2.15504000	-0.47825000	-1.57722000
C	-5.35106500	-1.27908400	-2.38201100
H	-7.12949100	-0.59721500	-1.39313200
H	-3.46469800	-1.83413500	-3.24651800

N	-6.11382900	-2.07899500	-3.35836400
O	-5.47562800	-2.71153500	-4.19868800
O	-7.34040800	-2.06846800	-3.27009400
P	0.75624900	-1.64207200	1.39663600
C	4.68268600	-3.73231400	-0.22110400
C	3.38459200	-4.54557000	-0.16373800
C	2.15136600	-3.64424200	0.01184400
C	2.27312900	-2.73378500	1.26073100
C	3.58888900	-1.92629600	1.20937400
C	4.81236700	-2.83957500	1.01798600
H	4.69316400	-3.10995600	-1.12646400
H	5.54679700	-4.40304500	-0.29666700
H	3.43470300	-5.25771200	0.67324100
H	2.03235000	-3.00441300	-0.87296600
H	2.26616900	-3.35869600	2.16540300
H	3.52022500	-1.20726100	0.38316100
H	3.71844600	-1.34722800	2.12724500
H	4.93491100	-3.46991000	1.91131100
H	5.71397600	-2.21835000	0.95194100
H	3.26257500	-5.14338900	-1.07498200
H	1.25257400	-4.26597800	0.07163700
C	-2.57295900	-5.06616200	1.60112400
C	-2.80438400	-3.83611100	0.71197700
C	-1.48978500	-3.11323000	0.37912500
C	-0.75071200	-2.72397900	1.67524900
C	-0.47136800	-3.97913800	2.53564700
C	-1.79140200	-4.69827200	2.87002500
H	-2.00856300	-5.82268700	1.03619400
H	-3.53092300	-5.52782800	1.86918800
H	-3.47569300	-3.13218700	1.22346400

H	-0.85728000	-3.76787800	-0.23502700
H	-1.41773300	-2.04961800	2.22842000
H	0.17689500	-4.67002400	1.98131700
H	0.05684200	-3.72823900	3.46165200
H	-2.40674400	-4.04417000	3.50406500
H	-1.57532100	-5.59624400	3.46198500
H	-3.30574500	-4.12696500	-0.21909400
H	-1.68598200	-2.21787200	-0.21095000
C	1.42464400	1.18406800	5.21273300
C	0.38583700	0.05508000	5.27047900
C	0.65299600	-1.05216700	4.23046900
C	0.75575000	-0.43121300	2.82145000
C	1.87467900	0.62986600	2.78435100
C	1.56479400	1.74572600	3.79153200
H	2.40027600	0.79865300	5.54423100
H	1.14951600	1.97996700	5.91538900
H	-0.61394500	0.47084800	5.08277800
H	1.58685000	-1.57802700	4.47594000
H	-0.19684500	0.07801500	2.61427900
H	2.83152400	0.16938600	3.05650700
H	1.99672400	1.04551700	1.78273300
H	0.63650800	2.24539200	3.48451400
H	2.35461800	2.50373400	3.74639600
H	0.35741700	-0.39062100	6.27246100
H	-0.15724000	-1.78515500	4.28547100
Se	0.64118900	-0.46111500	-0.46312700

S6

0 imaginary frequency

H = -8086.552228

G = -8086.683159

Esol = -8087.424577

Se	-0.24978800	-0.61777800	-1.09774600
N	-1.95607300	0.28671600	-1.72105700
N	-1.06091700	-2.09521500	-0.48542100
S	-1.69133200	1.78513600	-2.38231100
O	-2.49143800	1.96128900	-3.60071000
O	-0.22874600	1.99305600	-2.42904200
S	-1.43532100	-1.94765900	1.11061500
O	-1.29546000	-0.53422900	1.56471200
O	-0.79568400	-2.99600300	1.91550300
C	0.15939500	-1.52404100	-2.87426300
C	-1.03646600	-1.68288900	-3.74011600
C	-1.81779900	-2.77330800	-3.72262600
H	-1.26403800	-0.86676700	-4.42540500
H	-1.57894500	-3.57192900	-3.02079300
H	0.94098600	-0.90432200	-3.31572900
H	0.57268700	-2.46819700	-2.52520100
C	-3.01072300	-2.98802600	-4.60387800
H	-2.87779100	-3.88157200	-5.22836800
H	-3.91465200	-3.16099000	-4.00496300
H	-3.19175100	-2.13287000	-5.26308300
C	-3.20595300	-2.32291800	1.13274600
C	-3.62958000	-3.55143600	1.64053800
C	-4.12083800	-1.37742500	0.65951400
C	-4.99057300	-3.85055800	1.66714500
H	-2.89378300	-4.25454200	2.01412500
C	-5.48060100	-1.66825100	0.68529000
H	-3.76916900	-0.42648200	0.27402400

C	-5.89205900	-2.90378800	1.18698800
H	-5.35820700	-4.79339500	2.05266500
H	-6.22103100	-0.96253300	0.32962500
N	-7.33130700	-3.21647400	1.21005900
O	-7.67179700	-4.31033700	1.65920200
O	-8.10769700	-2.36566300	0.77619200
C	-2.33106300	2.89619600	-1.11930000
C	-2.88222500	4.11274400	-1.52519100
C	-2.21343700	2.55146800	0.23087200
C	-3.31892000	5.01661300	-0.55949700
H	-2.98033600	4.33888800	-2.58145500
C	-2.65285700	3.45306500	1.19642000
H	-1.81649300	1.58460100	0.52361900
C	-3.19185100	4.67107000	0.78416700
H	-3.75548500	5.97009200	-0.82929700
H	-2.59061700	3.22143100	2.25249300
N	-3.65101600	5.62799900	1.80854600
O	-3.52055500	5.30518400	2.98798600
O	-4.13231700	6.69106500	1.41982400
P	3.53360500	-0.21258600	0.47251700
C	1.84739800	2.52787100	3.98179300
C	3.21006300	1.84417600	4.17307800
C	3.84219200	1.41989000	2.83286800
C	2.85992600	0.52757600	2.04609600
C	1.53557200	1.28241300	1.79821800
C	0.89193500	1.67166800	3.13675300
H	1.99876200	3.49695700	3.48325300
H	1.40043000	2.74827400	4.95886800
H	3.08481900	0.95061500	4.80121800
H	4.07980500	2.31634400	2.24216100

H	2.62383100	-0.36050800	2.64763100
H	1.73729700	2.20043300	1.22780100
H	0.85160500	0.67488800	1.20241000
H	0.61094000	0.75944800	3.67851800
H	-0.04011200	2.21756100	2.94860300
H	3.89912500	2.50881800	4.70901700
H	4.79087400	0.90380000	3.02229100
C	4.67425800	2.69309400	-3.13212300
C	5.23596800	3.00963300	-1.73929600
C	5.18537200	1.77842000	-0.81720600
C	3.74574500	1.22601100	-0.72684200
C	3.14942100	0.92370500	-2.11585100
C	3.24355800	2.14610000	-3.04098600
H	5.32157500	1.95061100	-3.62227600
H	4.69788800	3.59129400	-3.76118200
H	4.65382000	3.82576800	-1.28732400
H	5.85914300	1.01117800	-1.21737700
H	3.12616300	2.01465900	-0.28064800
H	3.66137600	0.06001000	-2.56099200
H	2.10221600	0.64348600	-1.98777200
H	2.56977100	2.92782500	-2.66515700
H	2.87055700	1.87695100	-4.03643600
H	6.27099000	3.36630200	-1.81180200
H	5.56223500	2.04452700	0.17809400
C	6.93938200	-3.41245300	1.13888900
C	6.39193600	-2.67065400	2.36481200
C	5.05811100	-1.96739600	2.06178000
C	5.18324700	-1.01120400	0.85128100
C	5.73265900	-1.77234100	-0.37864000
C	7.06738500	-2.46597400	-0.06156700

H	6.25933000	-4.23631100	0.87962300
H	7.91040800	-3.86650400	1.37180300
H	7.12854700	-1.92447200	2.69806600
H	4.28266700	-2.71166500	1.83867000
H	5.87307600	-0.19486200	1.10705000
H	4.98703900	-2.51553400	-0.68653100
H	5.86075800	-1.09440500	-1.23014900
H	7.83480600	-1.70679600	0.15078300
H	7.40883600	-3.01460700	-0.94807800
H	6.25081600	-3.36462100	3.20242100
H	4.72483600	-1.42394000	2.95298200
H	-2.52545800	-0.29991400	-2.33503000
Se	2.21642100	-1.80305300	-0.20721900

S7

0 imaginary frequency

H = -8086.571703

G = -8086.702064

Esol = -8087.445323

Se	0.08897000	-1.17797600	-0.89295800
N	-1.76958900	-1.10243500	-1.87425700
N	0.09236600	-3.04514000	-0.90919100
S	-1.93635600	0.39675200	-2.54324800
O	-2.09905500	0.34949900	-4.00293400
O	-0.86828300	1.24091600	-1.95449700
S	-0.03970600	-3.86088500	0.59663800
O	1.13250300	-3.62466500	1.44845500
O	-0.44100100	-5.23619400	0.27901400
C	3.25535500	-4.65994200	-1.87500800

C	2.40529600	-3.65288100	-1.67930700
C	0.91955700	-3.76497800	-1.93809000
H	2.76585700	-2.69940300	-1.29851200
H	0.61757000	-4.81372900	-1.85252200
H	4.32124400	-4.54536900	-1.69887000
H	2.92349700	-5.64011700	-2.21321400
C	0.52323900	-3.27213400	-3.33565000
H	1.09852900	-3.82207600	-4.08578100
H	-0.54169300	-3.45261100	-3.52060400
H	0.73164200	-2.20611200	-3.45953800
C	-1.42844300	-3.00740400	1.35704700
C	-2.69957800	-3.56363600	1.22977700
C	-1.19294400	-1.83971200	2.08995300
C	-3.78120300	-2.93123300	1.83980100
H	-2.83362200	-4.48271600	0.67030900
C	-2.27565600	-1.19306100	2.67756000
H	-0.18472500	-1.44733200	2.17891400
C	-3.54835600	-1.74828000	2.53541600
H	-4.78610300	-3.32936500	1.77429000
H	-2.15072200	-0.27509800	3.23843300
N	-4.69634700	-1.04737800	3.13818800
O	-5.75848500	-1.65714800	3.22287400
O	-4.51838800	0.11497900	3.50897100
C	-3.47936600	1.01167200	-1.84454800
C	-4.38534500	1.66678400	-2.67733000
C	-3.70429400	0.88486900	-0.47019500
C	-5.54146700	2.21617000	-2.12490800
H	-4.18467600	1.73817000	-3.74059400
C	-4.85361700	1.43539200	0.08808300
H	-2.99360500	0.34113300	0.14281600

C	-5.75050000	2.09571200	-0.75378600
H	-6.27299900	2.73196100	-2.73431800
H	-5.06244000	1.36130600	1.14904400
N	-6.96892400	2.68877800	-0.17023500
O	-7.12259000	2.59205000	1.04524700
O	-7.75375800	3.24621700	-0.93677900
P	2.82956100	1.21295400	0.50256200
C	-0.44796400	4.06820600	2.47626800
C	1.02681100	4.27081600	2.85485300
C	1.97912000	3.66374300	1.80682300
C	1.65296000	2.17070200	1.59402300
C	0.18625500	2.00451800	1.14461300
C	-0.76325700	2.58994500	2.20170100
H	-0.67321700	4.65532100	1.57417100
H	-1.09719700	4.45540300	3.27080500
H	1.22284600	3.79991500	3.82914900
H	1.85988900	4.20517100	0.85901300
H	1.76471600	1.65221600	2.55666700
H	0.02326800	2.52673400	0.19423700
H	-0.03579600	0.95047400	0.95153800
H	-0.66959100	2.01664400	3.13627400
H	-1.80179800	2.48076600	1.86676800
H	1.24661300	5.33886300	2.97498900
H	3.01827000	3.80499900	2.12721800
C	3.47418300	2.62262600	-4.00133300
C	3.24820700	3.68739900	-2.92007800
C	3.51930200	3.12602300	-1.51309800
C	2.64951300	1.87551600	-1.24503400
C	2.85708700	0.79537200	-2.32776700
C	2.62047700	1.37690500	-3.73132100

H	4.53855200	2.34392200	-4.01816900
H	3.24315000	3.03511400	-4.99112000
H	2.21105400	4.04769300	-2.97261500
H	4.58192800	2.86031800	-1.43984900
H	1.59344200	2.17277500	-1.29701900
H	3.86820000	0.37394500	-2.25711900
H	2.14937300	-0.01567700	-2.15284300
H	1.55656600	1.63318600	-3.82898300
H	2.82586600	0.60324300	-4.48159700
H	3.89334700	4.55803200	-3.09311200
H	3.33609300	3.90351300	-0.76276100
C	7.11361100	0.57572300	2.36914400
C	6.10260400	1.41300600	3.16240200
C	4.66831300	1.22110900	2.64183300
C	4.56544700	1.52587800	1.12857500
C	5.59765800	0.69324000	0.33244400
C	7.02426400	0.88955200	0.87049900
H	6.90680400	-0.49191600	2.52981500
H	8.13067400	0.75897500	2.73694400
H	6.37607600	2.47640500	3.09306800
H	4.34418100	0.18641400	2.81345000
H	4.76442600	2.59430400	0.96594200
H	5.31102500	-0.36393300	0.39660700
H	5.56694400	0.95957300	-0.73033800
H	7.34183300	1.92832800	0.69585400
H	7.71450000	0.25341600	0.30281600
H	6.13755400	1.15119500	4.22708100
H	3.98744400	1.86414100	3.21165400
H	-1.84756800	-1.80971300	-2.60630200
Se	2.43875500	-0.91862000	0.75827400

S8

0 imaginary frequency

H = -8315.709482

G = -8315.851729

Esol = -8316.651243

N	-2.85392200	0.53745600	1.61545100
N	0.04759800	1.55731800	0.02306600
S	-3.67485200	-0.93415100	1.44407300
O	-4.57218900	-1.18169700	2.58064400
O	-2.67888300	-1.97082300	1.10381600
S	0.90072400	2.23618600	1.29548600
O	1.79571300	1.20843000	1.86232400
O	0.02506900	2.97871400	2.21412800
C	-1.33872800	0.83575600	4.78781900
C	-2.43327200	0.51780900	4.09389900
C	-2.91342700	1.31131700	2.90391100
H	-3.06300400	-0.31272400	4.40706900
H	-2.18933600	2.10911700	2.71487200
H	-0.71908700	2.22654600	-0.43033600
H	-1.04974400	0.27685900	5.67502300
H	-0.69715400	1.66368300	4.49564500
C	-4.29285000	1.94959100	3.13979400
H	-4.23171400	2.64487200	3.98425200
H	-4.59810200	2.50795500	2.24885200
H	-5.04867000	1.19348300	3.36860100
C	1.92579600	3.45345500	0.44450200
C	3.27107300	3.53178500	0.81190900
C	1.36044600	4.33402700	-0.48391800

C	4.08201100	4.50414100	0.23171700
H	3.67131600	2.83896400	1.54345700
C	2.17490000	5.30119800	-1.06892400
H	0.31049500	4.25955100	-0.76064400
C	3.51823200	5.36962800	-0.70285500
H	5.12895400	4.60171700	0.49065000
H	1.78280800	5.99754500	-1.79977600
C	-4.67898500	-0.68565900	-0.03559500
C	-4.05763800	-0.46367500	-1.26810100
C	-6.06519800	-0.77421200	0.08747100
C	-4.84659200	-0.32370000	-2.40423200
H	-2.97784000	-0.38302700	-1.32943000
C	-6.85705300	-0.64001000	-1.05093900
H	-6.50925900	-0.94982900	1.06087800
C	-6.23162500	-0.41863000	-2.27526300
H	-4.40946700	-0.14255300	-3.37791300
H	-7.93681000	-0.70468600	-1.00346900
N	4.37743900	6.39206600	-1.32765700
N	-7.06682700	-0.28185300	-3.48305500
O	3.85887400	7.15361100	-2.14176100
O	-8.28690400	-0.35454200	-3.34427100
O	5.56307100	6.41876000	-0.99799700
O	-6.49246900	-0.10683700	-4.55671100
O	-1.54430100	3.27086300	-1.03346000
C	-2.79696900	3.33999200	-0.79017300
O	-3.48064400	2.48708800	-0.17277700
C	-3.49970400	4.59202000	-1.30681000
H	-3.16952100	5.45875800	-0.72173700
H	-3.22029300	4.77938100	-2.34846900
H	-4.58372300	4.49574300	-1.21949500

H	-3.07129800	1.20118000	0.82332600
Se	-0.58117700	-0.16677700	0.21431100
Se	0.76364000	-1.29338900	-1.46111100
P	2.28039300	-2.42633300	-0.24661000
C	5.66893600	0.19034700	-2.19703500
C	5.64087800	-1.30368300	-2.54067800
C	4.29572300	-1.95123900	-2.17003800
C	3.94937400	-1.72306300	-0.67975200
C	3.98458300	-0.21554700	-0.33549600
C	5.33229800	0.41646500	-0.71830200
H	4.93667400	0.72139800	-2.82156400
H	6.65164600	0.61486800	-2.43435200
H	6.44940200	-1.81908700	-2.00181000
H	3.49629500	-1.51612300	-2.78603700
H	4.67483000	-2.26133900	-0.05260000
H	3.17024400	0.27686600	-0.88186800
H	3.77950600	-0.04988900	0.72602300
H	6.12895600	-0.00988200	-0.09092200
H	5.29679000	1.48883600	-0.49413400
H	5.83030300	-1.45849900	-3.60973100
H	4.33278400	-3.02091100	-2.40192800
C	2.76043900	-6.86175000	-1.90066900
C	1.51954200	-6.05503100	-2.30886900
C	1.73062500	-4.54411000	-2.11589800
C	2.14452500	-4.24194500	-0.65808400
C	3.40209400	-5.03990200	-0.24200600
C	3.17953600	-6.54809600	-0.45766000
H	3.59095700	-6.62192200	-2.58078700
H	2.56755000	-7.93546800	-2.01079600
H	0.65803000	-6.37845700	-1.70725700

H	2.50622800	-4.19631300	-2.80973700
H	1.31195100	-4.56229500	-0.01735400
H	4.26247500	-4.71472100	-0.84169300
H	3.65632700	-4.84945000	0.80733400
H	2.40059300	-6.89861200	0.23429300
H	4.09659800	-7.08984200	-0.19644500
H	1.26035800	-6.25343000	-3.35558300
H	0.81421600	-3.99651200	-2.35867500
C	1.27403900	-2.53648900	4.39507800
C	0.15731100	-2.41564400	3.34782300
C	0.61669200	-2.92845200	1.97558900
C	1.88263900	-2.15346300	1.54131700
C	3.03067700	-2.38473700	2.54648200
C	2.57930300	-1.87177600	3.92908800
H	1.46407400	-3.60106000	4.60014200
H	0.95058100	-2.09043200	5.34323700
H	-0.16281800	-1.37350700	3.23182700
H	0.84362100	-4.00223700	2.03982800
H	1.63596500	-1.08425100	1.56230900
H	3.27576300	-3.45434200	2.60780200
H	3.94306600	-1.85986800	2.24143600
H	2.43464100	-0.78567200	3.86254400
H	3.37916100	-2.04649200	4.65950300
H	-0.72890500	-2.97776900	3.66352900
H	-0.19650300	-2.81178300	1.25283000

S9

0 imaginary frequency

H = -8315.708372

G = -8315.851205

Esol = -8316.651793

N	-2.45305500	0.93896400	1.75296700
N	0.27954000	1.95963100	0.15526600
S	-3.40302800	-0.45634100	1.65081000
O	-4.32779800	-0.58149300	2.78615500
O	-2.50894500	-1.59489900	1.36424900
S	1.37205400	2.48002600	1.28672200
O	2.17248200	1.38093900	1.86961900
O	0.73129200	3.43064100	2.21872500
C	-0.39648900	0.71878000	4.63433400
C	-1.60719500	0.59667000	4.08855600
C	-2.15257600	1.57582600	3.07970200
H	-2.28732600	-0.18575300	4.42254300
H	-1.35679700	2.28285600	2.82464800
H	-0.77524000	3.03992000	-0.52187100
H	-0.05843300	0.04108800	5.41446500
H	0.29539300	1.49775700	4.32377800
C	-3.35442800	2.36255000	3.62960000
H	-3.72834900	3.05993700	2.87172000
H	-4.16679100	1.69423300	3.92711300
H	-3.03882000	2.94122700	4.50408700
C	2.49307100	3.45866200	0.26294600
C	3.81599600	3.03883900	0.11951700
C	2.03190300	4.63017300	-0.34648200
C	4.69690800	3.79380700	-0.65146700
H	4.14282400	2.13256300	0.61607300
C	2.90513800	5.38468000	-1.12296500
H	1.00022500	4.94112600	-0.22647600
C	4.22466300	4.95322400	-1.26195500

H	5.73144100	3.50252400	-0.78382500
H	2.58479800	6.29407200	-1.61579000
C	-4.37347300	-0.13758800	0.15971200
C	-3.74139000	0.03141600	-1.07707700
C	-5.76300000	-0.13066000	0.28558200
C	-4.52472000	0.21853300	-2.21184500
H	-2.65714900	0.04437900	-1.14615700
C	-6.54752400	0.04916800	-0.85172000
H	-6.21508300	-0.26580500	1.26178200
C	-5.91241300	0.21942100	-2.07898400
H	-4.07940700	0.36139200	-3.18844600
H	-7.62904900	0.05962700	-0.80034700
N	5.15116000	5.75069100	-2.08258200
N	-6.74042400	0.40905600	-3.28595500
O	6.30817600	5.34563600	-2.19647200
O	-6.15715200	0.55178300	-4.35925200
O	4.71431100	6.77426800	-2.60779300
O	-7.96178000	0.41083800	-3.14394200
O	-1.25092000	3.83746900	-0.95631700
C	-2.52606100	3.93427100	-0.62332200
O	-3.13913100	3.12490900	0.06823900
C	-3.18040600	5.17232900	-1.19218600
H	-4.24820800	5.16570900	-0.97150700
H	-2.71942100	6.06425100	-0.75386000
H	-3.01751200	5.22094900	-2.27343100
H	-2.75699900	1.65744600	1.07352300
Se	-0.25689900	0.23891900	0.27252500
Se	1.45741500	-0.76131800	-1.28652500
P	1.64788600	-2.73192900	-0.30174100
C	3.33725400	-1.19477300	3.83092600

C	4.32607700	-1.59462000	2.72781800
C	3.64271500	-1.67014300	1.35255800
C	2.42244100	-2.61953200	1.39060400
C	1.42191500	-2.21056900	2.49850700
C	2.13435500	-2.14646100	3.85968500
H	2.98507700	-0.17410700	3.64228300
H	3.84186400	-1.19418300	4.80530400
H	4.77435700	-2.57112800	2.96744000
H	3.29609900	-0.67804300	1.04529700
H	2.77054300	-3.64160100	1.60094500
H	0.97919400	-1.24032800	2.25625700
H	0.59620100	-2.92894800	2.55374000
H	2.46746000	-3.15655700	4.14514900
H	1.41172500	-1.82808100	4.61956500
H	5.15291000	-0.87568400	2.67620200
H	4.36543100	-2.00934300	0.59838400
C	5.09469600	-5.14056200	-2.56922300
C	4.38111500	-3.99597400	-3.30174600
C	3.67051800	-3.04373300	-2.32560000
C	2.68809200	-3.82272700	-1.42214400
C	3.42337400	-4.95046900	-0.66163800
C	4.12863700	-5.89821600	-1.64837500
H	5.91984600	-4.72991400	-1.96940000
H	5.54704800	-5.83017500	-3.29193500
H	3.64123400	-4.41351100	-4.00013800
H	4.41609900	-2.53212800	-1.70293300
H	1.93670300	-4.28758100	-2.07607700
H	4.17446300	-4.50954600	0.00669400
H	2.73098900	-5.51999200	-0.03147700
H	3.37206400	-6.41630600	-2.25529000

H	4.66226200	-6.67381500	-1.08573200
H	5.09434000	-3.42566800	-3.90869900
H	3.13776800	-2.26488400	-2.88089400
C	-2.33247200	-5.28049500	-0.73560500
C	-2.24742400	-3.89622700	-1.39502900
C	-0.79028900	-3.43134900	-1.55245100
C	-0.06654400	-3.44877000	-0.18646900
C	-0.12252400	-4.85491200	0.44741600
C	-1.58703000	-5.30441600	0.60642600
H	-1.89666000	-6.03493400	-1.40803100
H	-3.38138000	-5.56374600	-0.58669600
H	-2.78897900	-3.16689900	-0.78055000
H	-0.27408400	-4.10183800	-2.25561600
H	-0.58963800	-2.74077500	0.47076800
H	0.40433100	-5.57094100	-0.19929800
H	0.38021300	-4.87182100	1.42130500
H	-2.08923500	-4.63339100	1.31564100
H	-1.61252800	-6.31069700	1.04251200
H	-2.73039100	-3.91189100	-2.37991500
H	-0.73793500	-2.42557200	-1.98041900

SeIMe

0 imaginary frequency

H = -2706.398413

G = -2706.442378

Esol = -2706.537723

Se	1.66749200	-0.00002300	-0.00000100
C	-0.14857800	0.00000600	-0.00000900
C	-2.30720700	-0.67810400	-0.00000200

C	-2.30718100	0.67815700	0.00000200
H	-3.12392500	-1.38270200	-0.00003000
H	-3.12387900	1.38277300	0.00000600
N	-0.98132600	-1.08865800	-0.00002400
N	-0.98128900	1.08868600	0.00001400
C	-0.49417700	-2.45722400	0.00001800
H	0.12486900	-2.63129200	-0.88463200
H	0.12498000	-2.63119000	0.88460800
H	-1.35060100	-3.13479600	0.00010000
C	-0.49409000	2.45724300	0.00000200
H	0.12481600	2.63134000	0.88474400
H	0.12521800	2.63114800	-0.88449300
H	-1.35049400	3.13484100	-0.00025700

SeOIMe

0 imaginary frequency

H = -2781.606683

G = -2781.653450

Esol = -2781.751429

Se	-1.97797600	0.00014000	-0.28352400
C	0.59836400	0.00002400	0.47644700
C	2.47599900	0.67892100	-0.52713700
C	2.47577300	-0.67965700	-0.52701000
H	3.19768900	1.38269600	-0.91038400
H	3.19708600	-1.38376700	-0.91034500
N	1.31044300	1.09388300	0.10304000
N	1.31007900	-1.09414000	0.10323700
C	0.78428400	2.44871300	0.24156200
H	1.31483300	3.10246300	-0.45280400

H	-0.28054800	2.41804000	-0.00939100
H	0.91634000	2.81243500	1.26437300
C	0.78331800	-2.44875400	0.24167200
H	1.31381300	-3.10275200	-0.45250100
H	0.91495100	-2.81245100	1.26454700
H	-0.28145400	-2.41763700	-0.00954800
O	-0.51144900	0.00031700	1.12234100

SeOPCy3

0 imaginary frequency

H = -3523.822042

G = -3523.893481

Esol = -3524.337421

Se	-0.00290800	-2.11594500	-2.20385500
O	-0.00049800	-0.17114100	-1.71518800
P	-0.00012800	0.02637200	-0.15714900
C	0.00662300	4.68375500	-0.92727000
C	1.26674000	4.04591600	-0.33085800
C	1.27402600	2.51798200	-0.50519300
C	0.00255400	1.86570300	0.09167900
C	-1.26730500	2.52194600	-0.50433900
C	-1.25512300	4.04986500	-0.33008800
H	0.00606200	4.53915200	-2.01714900
H	0.00837800	5.76691300	-0.75328900
H	1.32544100	4.28919200	0.74061500
H	1.33206900	2.26665600	-1.57158800
H	0.00316400	2.02489800	1.18069700
H	-1.32692000	2.27074700	-1.57068000
H	-2.16702200	2.11502000	-0.03307900

H	-1.31241700	4.29336600	0.74141100
H	-2.15485400	4.47271100	-0.79398300
H	2.16750700	4.46596400	-0.79528500
H	2.17280900	2.10815200	-0.03464600
C	4.26036900	-1.02859100	1.69473700
C	3.87669100	-1.56478900	0.30843700
C	2.72713000	-0.76304600	-0.32177400
C	1.50293100	-0.74863800	0.62679600
C	1.87854700	-0.18260800	2.01549600
C	3.04322700	-0.98135700	2.62873700
H	4.67560700	-0.01494700	1.59058700
H	5.05146300	-1.64508100	2.13985200
H	3.57407700	-2.61862100	0.39193000
H	3.06929600	0.26013500	-0.51992600
H	1.19155000	-1.79530200	0.74449500
H	2.17775800	0.87034500	1.92111200
H	1.02529800	-0.20585800	2.70258300
H	2.70232200	-2.00635700	2.83439500
H	3.31701100	-0.54256400	3.59665500
H	4.74465200	-1.54381300	-0.36213600
H	2.43311700	-1.20720400	-1.27748000
C	-4.26310800	-1.01876900	1.69479700
C	-3.04570300	-0.97554500	2.62864800
C	-1.87888300	-0.17946100	2.01601800
C	-1.50508000	-0.74503000	0.62669300
C	-2.72952300	-0.75534300	-0.32170400
C	-3.88101800	-1.55476100	0.30799300
H	-4.67571900	-0.00396000	1.59155300
H	-5.05573400	-1.63354800	2.13955800
H	-2.70753100	-2.00163000	2.83337000

H	-2.17500900	0.87448300	1.92292900
H	-1.19651500	-1.79267200	0.74317800
H	-3.06911400	0.26887900	-0.51883900
H	-2.43684800	-1.19944100	-1.27783100
H	-3.58096700	-2.60939800	0.39052000
H	-3.31814300	-0.53681700	3.59697400
H	-1.02559400	-0.20605900	2.70294500
H	-4.74899800	-1.53102600	-0.36245600

SePCy3

0 imaginary frequency

H = -3448.610711

G = -3448.679743

Esol = -3449.120988

P	-0.00003600	-0.11223500	0.39286100
C	0.00086300	4.37539700	-1.03695800
C	-1.25999700	3.54546300	-1.30549600
C	-1.26779700	2.24146900	-0.49097700
C	0.00021800	1.39074900	-0.73468300
C	1.26862800	2.24090400	-0.49109100
C	1.26133500	3.54490600	-1.30560400
H	0.00098100	4.70628400	0.01141800
H	0.00103300	5.28211200	-1.65516900
H	-1.31673100	3.30821900	-2.37864100
H	-1.32233400	2.46529500	0.58247200
H	0.00010100	1.02169800	-1.77046100
H	1.32335200	2.46469900	0.58235500
H	2.16888200	1.66682700	-0.73707600
H	1.31787900	3.30765000	-2.37875700

H	2.16184200	4.12524000	-1.06751700
H	-2.16022700	4.12620100	-1.06734400
H	-2.16832600	1.66779300	-0.73688400
C	-4.21573800	-2.02015500	-0.90265300
C	-3.83042400	-1.93913800	0.58151800
C	-2.72693100	-0.89835400	0.82643800
C	-1.48588400	-1.20101000	-0.03995800
C	-1.86875500	-1.25376800	-1.53553700
C	-2.98565700	-2.28584300	-1.78119800
H	-4.67953300	-1.07047100	-1.20803000
H	-4.96973600	-2.80129200	-1.06244600
H	-3.48159900	-2.92555000	0.92197200
H	-3.11270000	0.10033900	0.58211900
H	-1.12958800	-2.20167800	0.24990700
H	-2.21813500	-0.26515300	-1.86155000
H	-1.00525700	-1.50230200	-2.16140100
H	-2.59622800	-3.29200300	-1.56681000
H	-3.26346500	-2.27906400	-2.84303600
H	-4.70939900	-1.69336900	1.19060500
H	-2.43802400	-0.86467500	1.88089800
C	4.21518800	-2.02122300	-0.90254400
C	2.98495900	-2.28696000	-1.78085700
C	1.86825400	-1.25464600	-1.53537200
C	1.48553300	-1.20138900	-0.03975600
C	2.72674800	-0.89876800	0.82644300
C	3.83004500	-1.93978300	0.58164600
H	4.67907900	-1.07167700	-1.20821100
H	4.96905500	-2.80250500	-1.06223000
H	2.59539700	-3.29299900	-1.56612900
H	2.21772800	-0.26616900	-1.86169600

H	1.12907200	-2.20191500	0.25040500
H	3.11265000	0.09980800	0.58188100
H	2.43795300	-0.86482700	1.88092500
H	3.48110200	-2.92605700	0.92237500
H	4.70911700	-1.69399600	1.19058700
H	3.26263500	-2.28054700	-2.84273400
H	1.00463200	-1.50323000	-2.16104700
Se	-0.00012300	0.47981500	2.43753400

SeSeIMe

0 imaginary frequency

H = -5107.953308

G = -5108.001396

Esol = -5108.095893

Se	-2.07646800	0.26602800	-0.69314000
C	1.00462400	-0.03807500	0.25565600
C	2.55571500	1.47006300	-0.30428000
C	3.02652300	0.24521100	-0.66425100
H	2.99174900	2.45114800	-0.40844000
H	3.95325700	-0.04491000	-1.13381700
N	1.31605000	1.28043900	0.27472000
N	2.05678000	-0.67944700	-0.31739600
C	0.41521700	2.31491400	0.77875200
H	0.92074900	3.27912700	0.71048000
H	-0.50889800	2.29130500	0.18321100
H	0.16061700	2.08958400	1.81726800
C	2.10469400	-2.11470800	-0.57477600
H	2.61543400	-2.29161400	-1.52375500
H	2.63074100	-2.63722900	0.22985900

H	1.07323800	-2.47104600	-0.62631600
Se	-0.63198300	-0.79949100	0.81383500

SeSePCy3

0 imaginary frequency

H = -5850.160879

G = -5850.234808

Esol = -5850.674607

Se	-2.84754500	-0.62439500	-1.24232600
Se	-0.63000600	-0.47236400	-1.96637300
P	0.40534100	0.12305000	-0.08001500
C	-1.63117300	-3.17026300	2.70747600
C	-1.48275500	-1.75137100	3.26870100
C	-1.24694800	-0.71112000	2.15926200
C	-0.01136200	-1.08553900	1.30508900
C	-0.19850500	-2.51227700	0.72017800
C	-0.41954600	-3.53822000	1.84300300
H	-2.54017800	-3.22397100	2.09340900
H	-1.75275900	-3.89261000	3.52465100
H	-0.64099500	-1.72624800	3.97841100
H	-2.11539800	-0.65663200	1.49332400
H	0.88173800	-1.07588000	1.95015900
H	-1.06982300	-2.49451300	0.05564800
H	0.66232900	-2.80707700	0.11425500
H	0.47944900	-3.59898200	2.47599800
H	-0.55462300	-4.53110200	1.39626700
H	-2.37711300	-1.46745400	3.83737500
H	-1.12097800	0.26975100	2.62190400
C	-1.03218300	4.56767700	1.09223400

C	-1.16131800	4.05841100	-0.35037800
C	-1.14585000	2.52395800	-0.43760400
C	0.11431600	1.96137700	0.25902600
C	0.18643500	2.43815300	1.72653700
C	0.20518700	3.97650200	1.78230300
H	-1.92931300	4.28137100	1.65995700
H	-0.98782200	5.66383900	1.10799100
H	-0.33140900	4.46302100	-0.94981400
H	-2.04599700	2.09350300	0.01427500
H	0.98405800	2.39108500	-0.26419200
H	-0.69965000	2.08968300	2.26543100
H	1.05959400	2.02807300	2.24751700
H	1.11679900	4.35120400	1.29339100
H	0.25471300	4.30212100	2.82900000
H	-2.08483500	4.43505300	-0.80631800
H	-1.16033800	2.20030300	-1.48167400
C	5.10045600	-0.78674100	-0.31322400
C	4.62606400	0.54893200	0.27576200
C	3.15051300	0.49855500	0.71594300
C	2.24516400	0.03786800	-0.44723200
C	2.71665700	-1.32622500	-0.99611300
C	4.18237400	-1.25013700	-1.45311600
H	5.10730100	-1.55056900	0.47821400
H	6.13445300	-0.69561500	-0.66773100
H	4.74505100	1.34137300	-0.47733100
H	3.04767200	-0.19889300	1.55919300
H	2.34323300	0.77052700	-1.26324100
H	2.63384500	-2.08553300	-0.20780100
H	2.06643200	-1.64658900	-1.81660300
H	4.26437200	-0.55268100	-2.29938200

H	4.50066000	-2.23139900	-1.82549100
H	5.25107300	0.83535900	1.13069900
H	2.84992700	1.48629700	1.08142300

TS-S1

1 imaginary frequency

H = -4645.325767

G = -4645.429023

Esol = -4646.067463

Se	2.07900800	0.18305100	0.52587100
N	2.61685300	-0.98419300	-0.75828100
S	2.68652100	-2.60837500	-0.26228500
O	3.31278600	-2.76579500	1.06608900
O	3.22419500	-3.34746000	-1.40978500
C	3.92565400	0.34787100	1.61489900
C	4.67886500	0.77992200	0.48032300
C	5.18761200	-0.13266500	-0.47983700
H	4.64228000	1.84001600	0.22978600
H	5.54095100	-1.07672800	-0.05068700
H	4.06751700	-0.55889100	-0.88957800
H	3.67755200	1.10088300	2.36150900
H	4.11077500	-0.64685600	2.01103800
C	6.01167500	0.37334900	-1.65566500
H	7.05116400	0.56314400	-1.36291400
H	6.02410500	-0.36520100	-2.46268000
H	5.59775900	1.30377600	-2.06004500
C	0.94296300	-3.02238000	-0.07990400
C	0.21246600	-3.38330400	-1.21311800
C	0.34329200	-2.89983400	1.17471300

C	-1.15706100	-3.60199100	-1.09807100
H	0.71545000	-3.48639100	-2.16833000
C	-1.02629800	-3.11455900	1.29491700
H	0.94537700	-2.63624600	2.03618300
C	-1.75373800	-3.44518500	0.15265400
H	-1.76418600	-3.87331500	-1.95254800
H	-1.53545400	-3.01933500	2.24561800
N	-3.21238900	-3.59849900	0.26424100
O	-3.83826000	-3.88721100	-0.75586200
O	-3.72719800	-3.40352100	1.36587700
P	-1.07517900	1.13707900	0.02243800
C	0.35548400	3.10793000	4.13736200
C	-0.72826000	2.02232300	4.15221000
C	-0.78111000	1.26319100	2.81729100
C	-0.98814300	2.20643000	1.60561900
C	0.11015800	3.29218100	1.60562700
C	0.16872900	4.05224100	2.94274300
H	1.34527200	2.63008300	4.07182100
H	0.34616900	3.67489600	5.07687600
H	-1.70600900	2.48873000	4.34377600
H	0.15831500	0.70896000	2.67188000
H	-1.95523000	2.71769200	1.72541400
H	1.08808600	2.82557500	1.41146500
H	-0.05486700	4.01027000	0.79533600
H	-0.76615200	4.61705900	3.07270600
H	0.97707100	4.79459500	2.91029600
H	-0.55376900	1.31772900	4.97564500
H	-1.57063900	0.50418000	2.85227600
C	-5.53305000	-0.43224500	-0.58767600
C	-4.79619000	0.16542600	-1.79338700

C	-3.28064300	0.26370800	-1.54576400
C	-2.94952500	1.06172200	-0.26548200
C	-3.69452500	0.44673400	0.94000800
C	-5.21045600	0.35091700	0.69148100
H	-5.23656200	-1.48260800	-0.45934000
H	-6.61571100	-0.43531800	-0.76763300
H	-5.19283700	1.17071000	-2.00103600
H	-2.86242700	-0.74905000	-1.45457800
H	-3.31519200	2.09172900	-0.39336800
H	-3.30239400	-0.56031100	1.14205500
H	-3.51909300	1.03950100	1.84486300
H	-5.62639300	1.36659500	0.61114100
H	-5.69342600	-0.11802400	1.55796100
H	-4.98339700	-0.43546300	-2.69248600
H	-2.79943900	0.71815900	-2.41890100
C	-0.14275600	3.51011900	-4.04388300
C	0.78095400	2.37356600	-3.58268600
C	0.10042800	1.46562600	-2.54450700
C	-0.43169700	2.28421900	-1.34519000
C	-1.35313100	3.42788300	-1.80982300
C	-0.65882400	4.32587600	-2.84968400
H	-0.99953600	3.08362100	-4.58676700
H	0.38062200	4.16434300	-4.75301800
H	1.69040600	2.80566700	-3.13839400
H	-0.71968500	0.91836200	-3.02877200
H	0.45827800	2.73490900	-0.88522100
H	-2.26417600	3.01072300	-2.25975500
H	-1.68077400	4.03255500	-0.95395200
H	0.18679500	4.84409500	-2.37293400
H	-1.35109700	5.10713500	-3.19006100

H	1.10970000	1.77533100	-4.44215600
H	0.81121600	0.71309100	-2.18541300

TS-S10

1 imaginary frequency

H = -5760.221950

G = -5760.349277

Esol = -5761.094987

Se	-0.77800300	-0.10498100	1.46365200
N	-2.59417100	-0.05559000	2.20483400
N	-0.11157000	1.18978600	2.51746900
S	-3.64300000	-1.20915300	1.64176700
O	-4.74961100	-1.37765300	2.58357900
O	-2.79385800	-2.35717100	1.28015800
S	-0.63433400	2.72619800	2.20558900
O	-0.45099000	3.53263100	3.41886900
O	-1.97451400	2.72884300	1.57339800
C	0.03124300	-1.66925800	3.46138600
C	-0.17050900	-0.69647500	4.40486400
C	0.62258100	0.46862600	4.37149700
H	-1.08572200	-0.68833700	4.99179400
H	1.59095700	0.38383500	3.88608600
H	-0.64812100	-2.50958300	3.35386100
H	0.96459600	-1.71849800	2.90915200
C	0.50232500	1.53875700	5.41059900
H	0.90106600	2.49343100	5.06993300
H	-0.53394100	1.68840100	5.72407100
H	1.08240800	1.21488400	6.28847100
C	0.51641900	3.41247200	0.99189200

C	0.37859000	4.77081800	0.68233000
C	1.51820600	2.63043600	0.41819800
C	1.25874400	5.36127900	-0.21750800
H	-0.40320600	5.36079500	1.14885500
C	2.40984200	3.22448300	-0.47463200
H	1.61383900	1.57903700	0.66898100
C	2.26424900	4.57439500	-0.78013400
H	1.18429900	6.40870900	-0.48195200
H	3.21004600	2.65672600	-0.93230400
N	3.20616800	5.19259100	-1.72887100
O	3.06320300	6.38820700	-1.97916800
O	4.07976600	4.47456900	-2.21627300
C	-4.37141600	-0.55244800	0.12040900
C	-3.65315200	0.33239600	-0.68827600
C	-5.65260300	-0.98548200	-0.23258300
C	-4.22084700	0.78651700	-1.87568300
H	-2.67283100	0.68143700	-0.38480200
C	-6.22063600	-0.54047600	-1.42295400
H	-6.20018400	-1.64878700	0.42784200
C	-5.49151600	0.33545300	-2.22521200
H	-3.69966200	1.48056800	-2.52298100
H	-7.21064100	-0.85234600	-1.73155700
N	-6.08946200	0.80763100	-3.48818400
O	-7.21777000	0.40712500	-3.76849800
O	-5.42038200	1.56939200	-4.18447600
P	2.14658900	-1.73033500	-0.49861600
C	0.78852000	-0.04322100	-4.74486600
C	-0.03849300	0.27835700	-3.49140900
C	0.77111200	0.05646600	-2.20469800
C	1.33954000	-1.37837200	-2.14970300

C	2.18671100	-1.69372500	-3.40264400
C	1.36691000	-1.46458200	-4.68512600
H	1.61328600	0.67954800	-4.82903500
H	0.17554900	0.07701000	-5.64637800
H	-0.93321300	-0.36164800	-3.47133500
H	1.59186900	0.78464100	-2.16261600
H	0.47627300	-2.05901500	-2.16802500
H	3.07225800	-1.04543900	-3.42717600
H	2.55368500	-2.72721000	-3.37845800
H	0.54518200	-2.19475300	-4.72240100
H	1.99614200	-1.65816100	-5.56278500
H	-0.39629600	1.31492700	-3.52823800
H	0.15360200	0.23464500	-1.31922100
C	0.31027100	-6.11250600	-0.15064500
C	-0.25829700	-4.95714800	0.68699300
C	0.11975700	-3.59943600	0.07780700
C	1.65445500	-3.46307300	-0.04806000
C	2.21279700	-4.59759200	-0.93358700
C	1.82709100	-5.97301200	-0.35594000
H	-0.18672300	-6.12189000	-1.13201600
H	0.08353500	-7.07650300	0.32131200
H	0.13291700	-5.01856800	1.71328600
H	-0.33600500	-3.53549400	-0.92048800
H	2.07781000	-3.57949300	0.96142600
H	1.80206700	-4.50566700	-1.94907800
H	3.30356800	-4.53142500	-1.02755100
H	2.33847000	-6.10711100	0.60857200
H	2.19692400	-6.76682000	-1.01704000
H	-1.34899800	-5.03003500	0.76249600
H	-0.30586500	-2.77871400	0.65929500

C	6.70923000	-0.77486300	0.17336800
C	6.01527000	-0.17738400	-1.05772200
C	4.48453800	-0.24490800	-0.93098700
C	3.99367300	-1.69121000	-0.68466000
C	4.69425200	-2.28147900	0.56207000
C	6.22572200	-2.20672500	0.43888500
H	6.49103600	-0.14952000	1.05130600
H	7.79807700	-0.76003200	0.04138000
H	6.32998100	-0.72634700	-1.95743700
H	4.15808300	0.37866100	-0.08870200
H	4.25306200	-2.30633500	-1.55827600
H	4.36880000	-1.72007700	1.44830700
H	4.39385300	-3.32374400	0.71988900
H	6.55303700	-2.85969900	-0.38368900
H	6.68569000	-2.60320100	1.35272900
H	6.32465500	0.86467100	-1.20454800
H	4.02134800	0.17410000	-1.83218700
H	-2.96003100	0.90223800	2.18868600
O	1.70788700	-0.75163800	0.59285700

TS-S11

1 imaginary frequency

H = -5989.384259

G = -5989.522932

Esol = -5990.323786

Se	-0.49550700	-0.15529300	-1.21321800
N	-2.52916800	-0.84857100	-1.91787800
N	-0.16744300	-1.76922800	-0.48344500
S	-3.59483400	0.54451100	-1.90045000

O	-4.69638800	0.35930900	-2.84763300
O	-2.72322300	1.71972400	-2.01816800
S	0.65988700	-2.96503100	-1.31125600
O	0.83356400	-2.60265000	-2.72579700
O	0.05027200	-4.24330300	-0.93161300
C	-0.87437700	-0.41373600	-4.83670800
C	-2.10939000	-0.63800200	-4.38542300
C	-2.40769800	-1.58611900	-3.25012200
H	-2.96327600	-0.13080300	-4.83080000
H	-1.52405600	-2.20621800	-3.08411600
H	-0.86314900	-2.11825900	0.43296100
H	-0.69529800	0.26965300	-5.66328900
H	-0.01046300	-0.91329600	-4.40770900
C	-3.60909900	-2.50376600	-3.50316300
H	-3.79549400	-3.14029400	-2.63255200
H	-4.51384800	-1.93522900	-3.72927700
H	-3.37954000	-3.14803100	-4.35865200
C	2.30094100	-2.93970100	-0.56397500
C	3.37334500	-2.41296600	-1.28310100
C	2.46538000	-3.46152000	0.72231000
C	4.63692700	-2.38256600	-0.69733700
H	3.21140000	-2.03827100	-2.28721100
C	3.72448500	-3.43044800	1.31415600
H	1.61730300	-3.88818400	1.24756700
C	4.78674600	-2.87941300	0.59618300
H	5.49677300	-1.98572700	-1.22223300
H	3.89538600	-3.82167700	2.30940800
C	-4.27985400	0.49614800	-0.23471000
C	-3.43091300	0.44221100	0.87282100
C	-5.66476400	0.60325700	-0.10661100

C	-3.98570800	0.49829000	2.14649400
H	-2.36363900	0.31564900	0.72842600
C	-6.21985900	0.66992800	1.16973200
H	-6.29152600	0.62956400	-0.99062500
C	-5.36861400	0.62066600	2.27028400
H	-3.36832400	0.44383200	3.03393400
H	-7.28869700	0.75575700	1.31994300
N	6.11399200	-2.81435200	1.23066100
N	-5.95390600	0.69811500	3.62391000
O	7.00971700	-2.22442800	0.62369400
O	-5.17920700	0.68249900	4.57872700
O	6.24842400	-3.34248400	2.33284600
O	-7.17731700	0.77749700	3.71060300
O	-1.61687000	-2.49087300	1.41547000
C	-2.77329700	-2.90852600	1.03415000
O	-3.32901800	-2.62143700	-0.05231600
C	-3.48836100	-3.83197300	2.00468100
H	-4.54173700	-3.93579100	1.73786300
H	-3.01279700	-4.81911300	1.96780600
H	-3.38707100	-3.46007900	3.02861400
H	-2.81864400	-1.54264700	-1.15123400
O	1.50555500	0.70406800	-0.68716500
P	1.90372400	1.81854300	0.30993000
C	0.10140700	5.39251200	-2.23902200
C	1.56753800	5.48315100	-1.79903300
C	2.12826400	4.11493400	-1.37296000
C	1.27493000	3.47888000	-0.24845300
C	-0.19569400	3.37681900	-0.72398200
C	-0.75745300	4.74257600	-1.14806000
H	0.03390600	4.79147300	-3.15701400

H	-0.28317800	6.38938000	-2.48724100
H	1.65382000	6.18394300	-0.95526100
H	2.13724600	3.43869300	-2.23834100
H	1.32308500	4.13376000	0.63568300
H	-0.24274600	2.69490500	-1.58051400
H	-0.83696500	2.94567400	0.04757700
H	-0.80553400	5.40786500	-0.27290700
H	-1.78623600	4.60315100	-1.49886800
H	2.18784500	5.89128100	-2.60678200
H	3.16726700	4.23945300	-1.05595400
C	6.61796300	2.52087400	0.17461800
C	6.00124100	1.35704800	-0.61517600
C	4.49705600	1.56841200	-0.85899100
C	3.75680000	1.79834800	0.47766600
C	4.36534400	2.97905100	1.26886500
C	5.87207400	2.75809800	1.49557300
H	6.57684800	3.43663700	-0.43382200
H	7.67845800	2.32428100	0.37233900
H	6.15870400	0.41907700	-0.06406900
H	4.36003900	2.43306700	-1.51923000
H	3.91345000	0.89047900	1.08079600
H	4.22194400	3.91668800	0.71707700
H	3.86461100	3.10648200	2.23657600
H	6.01280900	1.88928300	2.15446400
H	6.29260800	3.62257100	2.02406900
H	6.51383400	1.23975700	-1.57816600
H	4.06175800	0.70670900	-1.37379100
C	-0.33910000	0.13921600	4.13192000
C	-0.42464700	1.65176700	3.88466600
C	-0.06579100	2.01495700	2.43295600

C	1.32995100	1.47754600	2.05039200
C	1.41778300	-0.04591900	2.31334300
C	1.04984600	-0.39568600	3.76295400
H	-1.08744000	-0.38590000	3.52097400
H	-0.57100300	-0.08588400	5.17984800
H	0.26245600	2.17212400	4.56829100
H	-0.81748700	1.58200700	1.76302200
H	2.06480700	1.98667900	2.69246600
H	0.73831700	-0.55365600	1.62230700
H	2.42251100	-0.42263100	2.08755200
H	1.80178800	0.02612400	4.44662700
H	-1.43025700	2.02615300	4.11458100
H	-0.11156800	3.10264000	2.30331700
H	1.08270700	-1.48419000	3.88975300

TS-S12

1 imaginary frequency

H = -3988.939853

G = -3989.024704

Esol = -3989.296924

Se	2.89724400	-0.32194900	-1.81610200
I	-1.21030600	-2.74549400	-0.22573600
C	-3.16521300	-1.85069800	-0.24251700
C	-3.68702300	-1.39293800	0.96707600
C	-3.85465200	-1.73166200	-1.44859500
C	-4.96021000	-0.81762000	0.96079700
H	-3.11025000	-1.46701300	1.88247900
C	-5.12927600	-1.16007000	-1.43033700
H	-3.41796400	-2.07505700	-2.38016800

C	-5.68046600	-0.70531600	-0.23042700
H	-5.38538200	-0.45630800	1.89290300
H	-5.68461300	-1.06579300	-2.35920200
H	-6.66973400	-0.25693500	-0.22534700
N	0.49994600	-1.24729900	0.00101600
S	0.32802200	-0.29939500	1.35462600
O	-0.55447300	-0.84884500	2.40677200
O	1.70761000	0.08987700	1.71667200
C	-0.47901200	1.23267100	0.81352900
C	-1.44414000	1.81878100	1.63562700
C	-0.09942500	1.82602700	-0.39571400
C	-2.04451700	3.01562000	1.24942500
H	-1.71779800	1.33357200	2.56580200
C	-0.69558000	3.02132200	-0.78695300
H	0.64994300	1.34662000	-1.02071100
C	-1.65960500	3.59672500	0.04284700
H	-2.79679000	3.49915100	1.86024200
H	-0.43236500	3.50791100	-1.71809800
N	-2.29533200	4.85726700	-0.37188400
O	-1.93053800	5.35947500	-1.43485600
O	-3.15497300	5.33586000	0.36841600
C	3.93915700	0.02946500	-0.34434300
C	5.13546500	1.08698100	1.24524400
C	5.08081200	-0.22799100	1.57740300
H	5.60637200	1.92133000	1.74034500
H	5.48899000	-0.75839600	2.42287000
N	4.44022600	1.23641300	0.05677900
N	4.35914700	-0.87144600	0.58948100
C	4.17854000	2.49772200	-0.61769600
H	4.21651000	2.33933900	-1.69691000

H	3.18536600	2.87312300	-0.35117600
H	4.93883200	3.22197600	-0.31675400
C	3.95991100	-2.27068600	0.59779400
H	2.87401200	-2.33321700	0.70719000
H	4.25138300	-2.74292600	-0.34345500
H	4.45754400	-2.76504600	1.43469100

TS-S13

1 imaginary frequency

H = -5028.514967

G = -5028.621825

Esol = -5028.992497

Se	1.56576400	-0.66838700	-0.51257100
N	2.64219400	-0.41822400	0.94220700
S	3.96545600	-1.38676500	1.00943600
O	3.96509500	-2.47659800	-0.00020800
O	4.16169000	-1.75193300	2.42717500
C	5.35980000	-0.31624500	0.59064000
C	5.94687100	-0.40798400	-0.67370800
C	5.81333500	0.61424000	1.53194100
C	6.99581800	0.44482800	-1.00961900
H	5.58908300	-1.15444200	-1.37382200
C	6.85872000	1.47059500	1.20327200
H	5.35576300	0.65093100	2.51437200
C	7.43185800	1.37371100	-0.06605400
H	7.47915600	0.39947900	-1.97767300
H	7.23859800	2.20152700	1.90620800
N	8.53723200	2.27735200	-0.41739900
O	8.90541600	3.08896200	0.43216300

O	9.02902900	2.17107600	-1.54126500
I	-1.70168100	2.87882200	0.23968300
C	-3.83608700	3.11400700	0.38469200
C	-4.58027900	3.10284700	-0.79468200
C	-4.42431300	3.26039100	1.64062400
C	-5.96441600	3.26992000	-0.70270700
H	-4.09831100	2.95315800	-1.75461200
C	-5.80881700	3.43476500	1.70818100
H	-3.82632400	3.24782200	2.54553700
C	-6.57613600	3.43959000	0.54124700
H	-6.56157700	3.26750800	-1.61011600
H	-6.28346700	3.56117100	2.67707200
H	-7.65252800	3.57085900	0.60249100
N	-0.85407500	0.77276100	-0.36560400
S	-1.74887300	0.12668400	-1.60450600
O	-2.31146700	1.08911000	-2.56977100
O	-0.91213300	-0.97906400	-2.13656500
C	-3.19622000	-0.68676400	-0.87013700
C	-4.32518400	-0.89219500	-1.66964600
C	-3.15822100	-1.14063700	0.45039000
C	-5.42609100	-1.56621600	-1.14770800
H	-4.33873600	-0.51519200	-2.68642800
C	-4.25596600	-1.81317700	0.98167700
H	-2.27956400	-0.94380500	1.05502000
C	-5.37115500	-2.01711600	0.17060500
H	-6.31762700	-1.74282800	-1.73669000
H	-4.26604900	-2.17341800	2.00297500
N	-6.53521500	-2.72583400	0.72991800
O	-6.45673600	-3.12065400	1.89276800
O	-7.51322400	-2.87997600	0.00028300

C	0.91377400	-2.43093100	-0.11612700
C	0.39422700	-4.58475200	-0.33585900
C	0.25989700	-4.25580200	0.97769800
H	0.23868900	-5.51969700	-0.85025800
H	-0.02641100	-4.85121800	1.83010400
N	0.80416500	-3.44541100	-0.99915200
N	0.57355900	-2.91515600	1.09957200
C	1.13667800	-3.35018400	-2.42122900
H	0.41561900	-2.70221100	-2.92213500
H	2.14454600	-2.93889500	-2.51364300
H	1.10659700	-4.35459500	-2.84583600
C	0.59165100	-2.16911100	2.36363800
H	0.22985600	-1.15645700	2.18298500
H	-0.06631300	-2.68803300	3.06378500
H	1.61195900	-2.11126600	2.74979400

TS-S14

1 imaginary frequency

H = -4942.682441

G = -4942.785458

Esol = -4943.173993

Se	-0.18284300	-1.86378200	0.71978500
N	1.11099300	-1.73495500	-0.52791400
N	-1.51707300	-1.69383400	-0.50931800
S	2.55200200	-2.01338000	0.19233900
O	3.28078200	-3.08600900	-0.50197200
O	2.37225100	-2.11579100	1.67065700
S	-3.01795100	-1.51224300	0.21659700
O	-2.91385000	-1.69020000	1.67933300

O	-3.97264700	-2.31278100	-0.55852500
C	-0.33633000	-4.12405600	0.74098500
C	-0.32212800	-4.39190500	-0.64823100
C	-1.44849800	-4.23540400	-1.47331900
H	0.65754000	-4.43747500	-1.12271900
H	-2.41789300	-4.45229900	-1.01538500
H	-1.49103200	-2.92225900	-1.19984500
H	0.55685100	-4.35998200	1.31527700
H	-1.27296300	-4.24149300	1.28597600
C	-1.37565900	-4.47883000	-2.96825300
H	-0.39544700	-4.19985500	-3.36899900
H	-1.55247400	-5.53495400	-3.20751700
H	-2.13733800	-3.89446200	-3.49478000
C	-3.43402800	0.21654600	-0.08267500
C	-3.48231600	1.10330500	0.99289900
C	-3.73899600	0.62590800	-1.38428500
C	-3.82374000	2.43518700	0.76462700
H	-3.26554200	0.74468600	1.99229500
C	-4.07804700	1.95484600	-1.61816100
H	-3.71990400	-0.08930600	-2.19931100
C	-4.10925400	2.83714500	-0.53755000
H	-3.87479400	3.15608900	1.57090400
H	-4.32287800	2.31371900	-2.61014100
N	-4.45989400	4.24893900	-0.78350900
O	-4.71003200	4.57920800	-1.94119700
O	-4.47420000	5.00831000	0.18386400
C	3.49593000	-0.50568100	-0.11691500
C	3.99029800	-0.26092500	-1.40229500
C	3.71827100	0.39316500	0.92770900
C	4.69398500	0.91255700	-1.65382400

H	3.83330600	-0.98925700	-2.19048100
C	4.42664300	1.56758700	0.68438300
H	3.34745600	0.15904100	1.91889400
C	4.89544200	1.81095300	-0.60497100
H	5.09197900	1.13822900	-2.63541600
H	4.62304000	2.28750300	1.46910400
N	5.63143300	3.05868300	-0.86871000
O	6.04144800	3.24921000	-2.01307300
O	5.78653800	3.83980300	0.07001800
C	0.02826300	0.67619900	1.03426700
C	0.35650100	2.90333200	0.76324200
C	0.32378600	2.65988600	2.09984800
H	0.49332900	3.82457600	0.21689700
H	0.42741100	3.32681200	2.94268000
N	0.17579700	1.67869600	0.13494500
N	0.12274100	1.29194100	2.24088800
C	0.15678400	1.46258400	-1.30971500
H	-0.68617200	1.99455100	-1.76061800
H	1.09144400	1.81711100	-1.75353500
H	0.05862900	0.39096200	-1.47534400
C	0.03767100	0.57965600	3.51105100
H	0.95975100	0.70828600	4.08550800
H	-0.80891700	0.94286200	4.10168600
H	-0.10133300	-0.47714100	3.28878100

TS-S15

l imaginary frequency

H = -4942.711994

G = -4942.814257

Esol = -4943.208813

Se	-0.00778000	-1.31083000	0.38305200
N	-1.25695100	-1.57849200	-0.94726200
N	1.58294200	-1.64607600	-0.95961200
S	-1.33308300	-0.37017700	-2.08493900
O	-0.01811400	0.22332000	-2.39643500
S	3.03070100	-1.76976100	-0.24144000
C	-2.30069900	0.98876700	-1.35159100
C	-3.34230600	1.51249500	-2.12172600
C	-1.97149700	1.54894200	-0.11302200
C	-4.06588700	2.60714400	-1.65215800
H	-3.57824800	1.05881800	-3.07740900
C	-2.68859400	2.64241600	0.36095100
H	-1.18202500	1.10938600	0.48330000
C	-3.72647200	3.15365600	-0.41729400
H	-4.87922400	3.03686400	-2.22381600
H	-2.46063900	3.10001700	1.31567400
N	-4.49584200	4.30284400	0.09124800
O	-4.18792700	4.74996400	1.19576100
O	-5.40171100	4.74081000	-0.61570500
C	3.72171500	-0.09465200	-0.14708900
C	5.10187700	0.08170600	-0.26627400
C	2.87082500	0.99115400	0.07764900
C	5.64321100	1.35953400	-0.14679600
H	5.73528000	-0.77587900	-0.46446700
C	3.40270100	2.27095300	0.19480900
H	1.80129800	0.82572800	0.14176900
C	4.78346300	2.43166700	0.08543000
H	6.70795800	1.53675600	-0.23450300
H	2.77438800	3.13713700	0.36063200

N	5.35166500	3.78443500	0.21536500
O	6.57048400	3.90613600	0.10057900
O	4.57282400	4.71188600	0.43524700
O	2.74572600	-2.18764000	1.15242600
O	3.99443700	-2.54801200	-1.03036700
O	-2.16121800	-0.87488300	-3.18946800
C	-1.59919300	-1.25497000	1.98694600
C	-2.09598400	-1.21969000	4.19490800
C	-3.26454100	-1.34501000	3.51595600
H	-1.89358600	-1.16531200	5.25357300
H	-4.28271500	-1.42430400	3.86512300
N	-1.08822300	-1.16988800	3.24452900
N	-2.93790800	-1.36811700	2.16620300
C	0.33759500	-1.01500900	3.55023300
H	0.65660100	0.01546100	3.36859900
H	0.49661900	-1.25564300	4.60259300
H	0.93697400	-1.68641300	2.93253000
C	-3.92024800	-1.47156000	1.08852100
H	-4.56088300	-0.58506100	1.07939800
H	-3.37776900	-1.54349800	0.14672300
H	-4.53788700	-2.36221300	1.23656100
H	1.57415400	-1.13506300	-1.84342500
C	-0.13924700	-4.01397800	0.55769900
C	-0.25611700	-4.08445900	-0.80035800
C	-1.41902600	-3.60006700	-1.44826300
H	0.63393900	-4.24683200	-1.40092200
H	-2.34019900	-3.62121900	-0.87170600
H	-1.01542800	-3.90650900	1.19097400
C	-1.58088300	-3.76153900	-2.93045200
H	-1.82242400	-4.81844200	-3.12032000

H	-2.37998800	-3.14276700	-3.33339200
H	0.80137600	-4.22356100	1.05713000
H	-0.65487800	-3.53081300	-3.46442600

TS-S16

1 imaginary frequency

H = -5171.911088

G = -5172.025482

Esol = -5172.475834

N	1.99019000	-1.17143800	-1.31954700
N	-0.94454800	-0.23187300	-0.10262900
S	3.44054300	-1.54378200	-0.53887100
O	4.48153800	-2.03546200	-1.45496500
O	3.11726900	-2.36665500	0.64052100
S	-2.14192900	-0.89759600	-1.06405100
O	-2.57219700	-2.18437100	-0.47618500
O	-1.79191000	-0.86543900	-2.49188500
C	0.37156700	-4.22082500	-1.83965700
C	1.48957100	-3.51550800	-2.01174100
C	1.50460900	-2.06428200	-2.42619500
H	2.46140600	-3.99261000	-1.88831500
H	0.47094700	-1.73422800	-2.56653900
H	-0.40466000	0.76451200	-0.52843400
H	0.40369400	-5.27661600	-1.58032900
H	-0.61220700	-3.77636000	-1.97160500
C	2.26282800	-1.84077300	-3.74434400
H	2.25576700	-0.77647300	-4.00309600
H	3.29972600	-2.17838400	-3.67268700
H	1.76531400	-2.39438500	-4.54821700

C	-3.50114100	0.26901100	-0.82205600
C	-4.76294700	-0.25831800	-0.53954800
C	-3.29680000	1.64459000	-0.97659000
C	-5.84933000	0.60282300	-0.40332600
H	-4.88390600	-1.32976500	-0.42731800
C	-4.38120700	2.50629100	-0.83304500
H	-2.30388300	2.03892400	-1.17687400
C	-5.63771500	1.97138600	-0.55051100
H	-6.84409500	0.23402800	-0.18630200
H	-4.26682900	3.57827000	-0.93620000
C	3.94105300	0.09287500	0.04077400
C	3.09949100	0.82753800	0.88046900
C	5.20529000	0.55614200	-0.32134500
C	3.53096800	2.05808900	1.36221200
H	2.11586500	0.44443100	1.12815800
C	5.64496400	1.78490400	0.16771300
H	5.82734700	-0.04137300	-0.97831700
C	4.79905800	2.51180200	1.00117400
H	2.90867700	2.66788500	2.00483800
H	6.61937200	2.18241100	-0.08716400
N	-6.78270100	2.88649900	-0.39215900
N	5.25961400	3.81209600	1.52281500
O	-7.87779000	2.38953000	-0.13114200
O	4.49903700	4.42809200	2.26899900
O	-6.57304900	4.09092600	-0.52604800
O	6.37563000	4.20053600	1.18345100
O	-0.11913000	1.97702100	-0.88828900
C	0.81137000	2.23173500	-1.75294700
O	1.68943900	1.44053300	-2.13769100
C	0.77691600	3.64403200	-2.31960600

H	1.68811200	3.85425400	-2.88232700
H	-0.08626700	3.74509600	-2.98829200
H	0.65186400	4.37458400	-1.51425900
H	1.94907500	-0.16624800	-1.61368900
Se	0.15860400	-1.46556300	0.74709200
C	-1.00835200	-1.66049200	2.27744100
C	-2.34627300	-2.57459800	3.80522600
C	-2.24086300	-1.24493700	4.08625500
H	-2.89723700	-3.35877100	4.29994400
H	-2.68575100	-0.65094700	4.86914900
N	-1.58192600	-2.81247800	2.68036500
N	-1.40269000	-0.69691700	3.13571200
C	-1.45965000	-4.08841200	1.96471200
H	-1.63889600	-3.90283300	0.90449400
H	-0.46319500	-4.51040900	2.11220100
H	-2.20990200	-4.77359000	2.36118100
C	-0.99048300	0.70503500	3.03821500
H	0.08911700	0.77960400	3.18794300
H	-1.24606800	1.09015600	2.04944800
H	-1.50758300	1.27245800	3.81251700

TS-S17

1 imaginary frequency

H = -6390.500661

G = -6390.589748

Esol = -6390.860705

Se	1.90600900	-0.39386100	-1.29300500
I	-2.76235000	-0.84499400	-1.18485100
C	-3.96687500	-2.43886500	-0.34562900

C	-4.41355900	-2.33012600	0.96759000
C	-4.24798100	-3.53701000	-1.15558900
C	-5.19751600	-3.37034300	1.47569500
H	-4.14134000	-1.47655800	1.57977400
C	-5.04402200	-4.55761200	-0.62876800
H	-3.86321700	-3.60640900	-2.16771800
C	-5.51683400	-4.47431900	0.68242200
H	-5.55661700	-3.31021600	2.49924100
H	-5.28160700	-5.42015800	-1.24509100
H	-6.12936000	-5.27452600	1.08802000
N	-0.98405200	-0.60646400	0.06179400
S	-1.29250100	0.31931300	1.41300200
O	-2.63301900	0.12142600	2.00943700
O	-0.09859200	0.08843900	2.24775000
C	-1.24143400	2.06008400	0.91842900
C	-2.24883500	2.92311000	1.35604600
C	-0.17475700	2.51621400	0.13557500
C	-2.19596000	4.27135200	1.00770200
H	-3.06071400	2.53371900	1.95987400
C	-0.12077500	3.86203200	-0.21627200
H	0.58709600	1.81893000	-0.21324400
C	-1.13057400	4.71740000	0.22779800
H	-2.95697800	4.97249800	1.32691800
H	0.68413900	4.25314500	-0.82622400
N	-1.07342700	6.14095400	-0.14387400
O	-0.12167000	6.51611600	-0.82781700
O	-1.98152400	6.87268600	0.25132000
C	4.67063500	-1.13146600	0.42039500
C	5.81083500	-2.76300100	1.45328600
C	4.71600600	-2.47350800	2.20547300

H	6.60327900	-3.47941000	1.60188000
H	4.36544700	-2.89669700	3.13351600
N	5.77106900	-1.93181100	0.34710500
N	4.02806800	-1.45905000	1.56810500
C	6.75104700	-1.92031100	-0.73315000
H	7.13562400	-2.93300400	-0.87257500
H	6.25406400	-1.57944400	-1.64389400
H	7.57865700	-1.24311600	-0.50052300
C	2.79729200	-0.83165400	2.06293600
H	1.97422300	-1.01486700	1.36946700
H	2.57700800	-1.24454100	3.04765600
H	2.94611800	0.24740200	2.13533800
Se	4.16385700	0.17040000	-0.86477100

TS-S18

1 imaginary frequency

H = -7430.106203

G = -7430.218030

Esol = -7430.586901

Se	-0.73841100	1.58510500	-0.74615800
N	0.89747800	1.83336400	-1.40713000
S	2.05138100	2.40962500	-0.36275400
O	1.63681800	2.50215000	1.05543100
O	2.66187800	3.61540100	-0.96812200
C	3.32075500	1.13106900	-0.45126000
C	3.35252000	0.13372300	0.52647200
C	4.24768000	1.15808100	-1.49705600
C	4.32211300	-0.86290100	0.45324400
H	2.62448700	0.14699600	1.33011500

C	5.21795500	0.16354100	-1.57804900
H	4.20928100	1.95919100	-2.22653200
C	5.23366300	-0.83544200	-0.60372900
H	4.38036200	-1.65111800	1.19291300
H	5.95338200	0.14882700	-2.37286700
N	6.24079000	-1.90157200	-0.70094500
O	7.09198900	-1.81141900	-1.58356900
O	6.16828800	-2.83408500	0.10451800
I	0.13817700	-2.57211800	-0.83862500
C	1.39534300	-3.85903600	0.35642800
C	2.72998900	-3.99867800	-0.01988600
C	0.84689600	-4.50771800	1.45953300
C	3.54185900	-4.85433000	0.72983300
H	3.13851500	-3.45972600	-0.86687100
C	1.67954600	-5.35364200	2.19717900
H	-0.18038800	-4.33550800	1.75642700
C	3.01632100	-5.53032000	1.83297700
H	4.58601300	-4.96403400	0.45493500
H	1.27523900	-5.86884000	3.06384800
H	3.65400800	-6.18811800	2.41641600
N	-0.54574700	-0.68956000	0.30061700
S	-1.68444300	-1.10973700	1.44903300
O	-1.31992500	-2.31243300	2.22204900
O	-1.95688800	0.14578000	2.17291500
C	-3.22793900	-1.55011300	0.60052800
C	-4.01972300	-2.56422300	1.14670900
C	-3.64012300	-0.84818500	-0.53651700
C	-5.23987200	-2.88176700	0.55436300
H	-3.67272800	-3.09940900	2.02331900
C	-4.85698800	-1.16201200	-1.13589300

H	-3.00978700	-0.07517500	-0.96395500
C	-5.63765100	-2.17335800	-0.57754900
H	-5.87847200	-3.66192300	0.94975800
H	-5.20507500	-0.64253400	-2.02002100
N	-6.92521000	-2.50945200	-1.21110700
O	-7.25123700	-1.87152200	-2.21087800
O	-7.59353100	-3.40711100	-0.70070100
C	-0.69096700	4.66700500	0.68648700
C	0.90457200	5.84280600	1.70816400
C	0.31297700	5.04573800	2.63879400
H	1.72030900	6.54269400	1.79235400
H	0.51821600	4.91494500	3.68912300
N	0.27293500	5.60448400	0.50636600
N	-0.67918000	4.33646000	1.99968500
C	0.69123600	6.17332900	-0.77829700
H	1.08469300	7.17568400	-0.59733300
H	1.45865300	5.52638100	-1.21215300
H	-0.17202900	6.22887400	-1.44063800
C	-1.48039800	3.27552300	2.61158700
H	-1.03594400	2.30169600	2.39818100
H	-1.51543200	3.45210500	3.68807400
H	-2.48866800	3.30474600	2.19707000
Se	-1.82288900	3.97911800	-0.64429500

TS-S19

1 imaginary frequency

H = -7344.297650

G = -7344.403180

Esol = -7344.793112

Se	-1.81152100	0.19046500	0.77256700
N	-2.18161000	0.82899900	-0.82272400
N	-0.33662800	1.00219200	1.47646300
S	-1.68967300	2.25100100	-1.47054500
O	-1.95735100	3.42531600	-0.61177000
O	-2.24538500	2.24582100	-2.83219500
S	0.33957500	0.05688700	2.71710300
O	-0.63361600	-0.97155100	3.13952300
O	0.87832600	1.00681800	3.69512000
C	-3.28425800	1.27840100	2.11969100
C	-2.77472800	2.59595300	2.12508500
C	-1.62327700	2.95676200	2.85402400
H	-3.09913600	3.25522100	1.32388600
H	-1.46645100	2.42840800	3.79922700
H	-0.85172100	2.16691800	2.13125700
H	-4.19404700	1.08188600	1.55750400
H	-3.13819000	0.65430500	3.00080700
C	-1.07819800	4.37128700	2.80823700
H	-0.01659400	4.38080900	3.07369100
H	-1.18948400	4.79797300	1.80700900
H	-1.60181100	5.01835500	3.52297500
C	1.73063300	-0.77723900	1.94645300
C	1.60978200	-2.12479600	1.60454600
C	2.91046200	-0.06007600	1.72785100
C	2.69646200	-2.77123300	1.01732500
H	0.68015100	-2.65119500	1.77936500
C	3.99831200	-0.70507800	1.14605100
H	2.97791100	0.98190900	2.01999200
C	3.86881200	-2.05117600	0.80466900
H	2.64729400	-3.81498700	0.73350400

H	4.92958000	-0.18894500	0.94948900
N	5.02730000	-2.74647000	0.20591500
O	6.07980800	-2.12040800	0.11577200
O	4.86327600	-3.91002300	-0.15745900
C	0.10926200	2.17046000	-1.60753500
C	0.81089100	3.37771100	-1.67400300
C	0.76471300	0.94110000	-1.67333800
C	2.19508500	3.35927900	-1.81299800
H	0.27676100	4.31824800	-1.59752100
C	2.15009700	0.91836800	-1.81051200
H	0.21858700	0.00466800	-1.61394900
C	2.84234000	2.12574000	-1.87022200
H	2.77420500	4.27297200	-1.86291900
H	2.69507200	-0.01599300	-1.85770200
N	4.31077600	2.09867500	-1.96835300
O	4.89350200	3.16941300	-2.13302300
O	4.86952200	1.00537300	-1.86809700
C	-2.49915200	-2.36359500	-1.20210000
C	-4.73446100	-2.50295000	-0.97416000
C	-4.47219000	-2.03932900	-2.22297800
H	-5.66962300	-2.71590100	-0.48087500
H	-5.13672400	-1.75382500	-3.02303700
N	-3.51180000	-2.69688100	-0.34919600
N	-3.09694100	-1.96461400	-2.35625300
C	-3.29503700	-3.20851900	0.99977700
H	-4.25758700	-3.51214100	1.41516100
H	-2.61318800	-4.06096700	0.96464500
H	-2.84665800	-2.43060300	1.62205000
C	-2.38755100	-1.41980100	-3.51043100
H	-2.35001200	-0.32861900	-3.44223800

H	-1.37609300	-1.82809900	-3.50184500
H	-2.90603600	-1.72524000	-4.42217900
Se	-0.70539000	-2.43012200	-0.79314800

TS-S2

1 imaginary frequency

H = -7132.706281

G = -7132.818730

Esol = -7133.437498

Se	-0.54481900	-0.29690600	1.39293700
I	3.61394300	-2.77173100	-0.22586000
C	5.56403800	-1.96134300	0.20021300
C	6.27331700	-1.38033900	-0.85078500
C	6.06221500	-2.00900900	1.50142100
C	7.53947300	-0.85383500	-0.58363000
H	5.84372600	-1.32817500	-1.84545400
C	7.33341600	-1.48343000	1.74587300
H	5.48136800	-2.44412100	2.30764400
C	8.06936600	-0.90854900	0.70743400
H	8.10851900	-0.39863600	-1.38933100
H	7.74095300	-1.51809900	2.75230100
H	9.05434900	-0.49626700	0.90654400
N	2.04156900	-1.23510700	-0.39025900
S	2.29842300	-0.18594300	-1.66086700
O	3.26806400	-0.64525200	-2.67907700
O	0.94318200	0.21646500	-2.08844400
C	3.03107600	1.30430500	-0.93460900
C	4.15607400	1.87310600	-1.53530400
C	2.43949000	1.87920600	0.19598400

C	4.71096700	3.03329900	-0.99866700
H	4.58213200	1.40687400	-2.41646600
C	2.99091900	3.03677700	0.73621300
H	1.56424100	1.41628500	0.64913500
C	4.11909300	3.59469500	0.13109600
H	5.58224500	3.50421900	-1.43663000
H	2.56455000	3.50932700	1.61242500
N	4.70598800	4.81485600	0.70494900
O	4.16314300	5.30090400	1.69740000
O	5.70844900	5.28054800	0.16090200
Se	-1.66812400	0.06146400	-0.65364000
P	-3.85596100	0.00980800	-0.09943300
C	-3.75579000	2.55571300	3.93074000
C	-4.50773000	1.21889500	3.92222500
C	-4.07926400	0.32876200	2.74249100
C	-4.29000200	1.06270600	1.39358900
C	-3.48725900	2.38820400	1.40819200
C	-3.91676100	3.27794300	2.58747600
H	-2.68892800	2.36851400	4.11382100
H	-4.11403100	3.18977100	4.75157300
H	-5.59090000	1.40785000	3.86377000
H	-3.01734100	0.07028400	2.83115000
H	-5.36227600	1.28909300	1.27345400
H	-2.42260400	2.14062600	1.49763900
H	-3.60964600	2.93871600	0.47309800
H	-4.96694800	3.58161400	2.45714700
H	-3.32184100	4.19951500	2.57443600
H	-4.33599800	0.67632400	4.86028500
H	-4.64215500	-0.60689000	2.77859700
C	-5.35631500	-4.38500900	1.14497800

C	-3.93879400	-4.16863200	0.59526300
C	-3.47398100	-2.71021800	0.74708700
C	-4.48436300	-1.75612300	0.06891000
C	-5.89356800	-1.94260600	0.68501800
C	-6.35530600	-3.40255800	0.51672300
H	-5.34814400	-4.24004700	2.23524300
H	-5.68144000	-5.41815800	0.96969900
H	-3.91400700	-4.44603100	-0.46910400
H	-3.38400800	-2.46002100	1.81083900
H	-4.54120900	-2.05309900	-0.99088400
H	-5.86261600	-1.70928400	1.75459600
H	-6.62940000	-1.26614300	0.24088000
H	-6.46768100	-3.62635200	-0.55450100
H	-7.34857600	-3.52413700	0.96713100
H	-3.22734900	-4.82968100	1.10487700
H	-2.47688600	-2.57912300	0.31908600
C	-6.31165500	2.30576200	-3.54272500
C	-6.65260600	0.84146800	-3.23931600
C	-6.16377300	0.39889800	-1.84601900
C	-4.65259300	0.66960300	-1.67736000
C	-4.33933400	2.15779600	-1.95440100
C	-4.81110700	2.56728500	-3.35932100
H	-6.87976100	2.96085100	-2.86576800
H	-6.62486600	2.56234100	-4.56215400
H	-6.18587400	0.19638100	-3.99776500
H	-6.72651200	0.94003900	-1.07164400
H	-4.12252000	0.07617800	-2.43904900
H	-4.86136100	2.78094100	-1.21633000
H	-3.26731200	2.34638400	-1.84279200
H	-4.24182500	2.00413000	-4.11256800

H	-4.58255700	3.62729600	-3.52356400
H	-7.73454900	0.67386600	-3.31108300
H	-6.38632200	-0.66460500	-1.72223900

TS-S20

1 imaginary frequency

H = -7344.321372

G = -7344.427848

Esol = -7344.821392

Se	1.41345600	-1.65704700	-0.07071100
N	-0.31140100	-2.61212100	-0.17020600
N	0.81257600	-0.27607500	0.89891400
S	-1.29085800	-2.40262800	-1.51316500
O	-1.49249800	-3.68677500	-2.19696600
O	-0.78931500	-1.23706800	-2.25164300
S	1.15517200	1.24425800	0.29916300
O	1.80226300	1.22613900	-1.02310300
O	1.78456600	2.03032000	1.37952600
C	1.84805000	-2.86952500	2.26139100
C	1.08123800	-1.98504300	2.99270700
C	1.41963400	-0.63085100	3.04524700
H	0.08197300	-2.28282300	3.30525400
H	2.42826900	-0.34792200	2.75202200
H	1.52120500	-3.89451600	2.10333300
H	2.90019700	-2.68487900	2.08161600
C	0.64287100	0.35517500	3.85609300
H	0.75449800	1.36414000	3.45654200
H	-0.41772300	0.09095000	3.91686200
H	1.04358800	0.36402100	4.88114800

C	-0.46914500	1.99435500	0.03451100
C	-1.13043200	1.76857400	-1.17596700
C	-1.00690800	2.83196400	1.01435100
C	-2.35924200	2.38300600	-1.40347400
H	-0.69723600	1.11297600	-1.92146000
C	-2.23535100	3.44879400	0.79030700
H	-0.45612200	3.01520000	1.92958600
C	-2.89008700	3.21220000	-0.41684300
H	-2.90317800	2.23202400	-2.32752300
H	-2.68249900	4.11023900	1.52192700
N	-4.18592900	3.87187900	-0.66175100
O	-4.75120100	3.63903700	-1.72902500
O	-4.62164700	4.61536400	0.21616900
C	-2.86406400	-1.94932700	-0.76043500
C	-2.88409700	-1.07621900	0.33074200
C	-4.03896900	-2.45754900	-1.31672700
C	-4.10833100	-0.70239900	0.87611300
H	-1.95104900	-0.71969000	0.75510800
C	-5.26653500	-2.08382100	-0.77347600
H	-3.98721100	-3.14619700	-2.15279300
C	-5.27784300	-1.21336700	0.31351600
H	-4.17163700	-0.03288700	1.72476500
H	-6.20179400	-2.45754500	-1.17115100
N	-6.57481400	-0.82837300	0.90169900
O	-7.59213000	-1.29210500	0.38991600
O	-6.55722200	-0.07000400	1.86983100
H	-0.18212600	-3.60882600	0.00380500
C	4.65967600	0.50090600	-0.53786700
C	4.87875200	1.75040500	-2.38517100
C	5.18263000	2.53529900	-1.31974200

H	4.85463900	1.97080700	-3.44043600
H	5.47972200	3.57050600	-1.26663700
N	4.57201000	0.49457500	-1.89271400
N	5.05127000	1.75228600	-0.18502300
C	4.06205500	-0.63620500	-2.65608200
H	4.13406900	-0.40222500	-3.71932200
H	4.65342200	-1.52565800	-2.42503100
H	3.02021000	-0.81355800	-2.37909500
C	5.17687500	2.20554200	1.19587700
H	5.73697200	3.14263600	1.20441000
H	4.18035200	2.35258200	1.62053400
H	5.71008800	1.44709400	1.77190800
Se	4.32152100	-0.90849500	0.59818600

TS-S21

1 imaginary frequency

H = -7573.489864

G = -7573.608309

Esol = -7574.057181

N	-1.96963200	-0.53129300	1.55539600
N	0.85755400	0.44796500	0.13898700
S	-3.34601700	-1.28358400	0.91449100
O	-4.27221300	-1.73528000	1.96296200
O	-2.88625000	-2.28008400	-0.07402600
S	2.10995900	0.12836500	1.18931400
O	2.65346100	-1.21984900	0.91588700
O	1.76391800	0.45570000	2.58282200
C	-0.03516100	-3.11431100	2.75458600
C	-1.22166200	-2.51559300	2.87052200

C	-1.40316000	-1.01626200	2.85998900
H	-2.12625300	-3.10846000	3.00210900
H	-0.41445500	-0.54783700	2.87888500
H	0.27751300	1.49560900	0.27982100
H	0.05463300	-4.19761600	2.80667700
H	0.88659100	-2.55043200	2.63634600
C	-2.20035400	-0.50784200	4.07047300
H	-2.31117300	0.57996900	4.01198600
H	-3.19301200	-0.96281000	4.11698100
H	-1.65748100	-0.75020500	4.99071300
C	3.36179100	1.31889800	0.65733600
C	4.68569800	0.87536100	0.60763400
C	3.02659400	2.64939100	0.38556500
C	5.69848700	1.76786200	0.26744600
H	4.91332000	-0.15938400	0.83647200
C	4.03828100	3.54219200	0.03964200
H	1.99365800	2.98438300	0.42650700
C	5.35487600	3.08774000	-0.01427000
H	6.73608800	1.46190800	0.21852300
H	3.81998600	4.57830000	-0.18758700
C	-4.12394300	0.07536200	0.01724500
C	-3.46149300	0.69230000	-1.04844400
C	-5.41923600	0.43496800	0.38992900
C	-4.11350900	1.69957700	-1.75242700
H	-2.44664700	0.40729400	-1.30605600
C	-6.07532600	1.43873900	-0.31910500
H	-5.89897800	-0.06759900	1.22211800
C	-5.40918700	2.05096200	-1.37726900
H	-3.63651700	2.21089700	-2.57899600
H	-7.08099000	1.74941600	-0.06533900

N	6.42287600	4.03348000	-0.38472000
N	-6.10237000	3.11368700	-2.13142900
O	7.57379900	3.60033100	-0.43980800
O	-5.49780700	3.63431000	-3.06720700
O	6.09984300	5.19672100	-0.61801700
O	-7.24227600	3.41112500	-1.77884800
O	-0.13965300	2.71812300	0.41564600
C	-1.15610900	3.00311300	1.15745000
O	-1.97568300	2.18957100	1.62823300
C	-1.32838900	4.48562100	1.45419100
H	-2.27320100	4.66880100	1.96878300
H	-0.50032100	4.82854200	2.08529400
H	-1.28736900	5.06239300	0.52465200
H	-2.03054400	0.52125300	1.53634600
Se	-0.21742700	-0.95147100	-0.36118800
C	1.69845700	-3.22968100	-1.51098400
C	1.86129300	-5.16298400	-0.41567400
C	3.11519500	-4.64930800	-0.54107000
H	1.51263700	-6.06851700	0.05505800
H	4.06919700	-5.02383000	-0.20528300
N	0.99550200	-4.28178000	-1.03169600
N	2.99906100	-3.45357400	-1.22116800
C	-0.46519100	-4.40553400	-1.07306700
H	-0.72389300	-5.46548800	-1.08088500
H	-0.91212500	-3.90755200	-0.20982800
H	-0.81949300	-3.92418800	-1.98519300
C	4.10300800	-2.55138400	-1.54077000
H	3.67820500	-1.58065000	-1.79189300
H	4.74039000	-2.45106800	-0.66202300
H	4.67539200	-2.94387200	-2.38599700

Se	0.96766100	-1.73192900	-2.37797000
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TS-S22

l imaginary frequency

H = -4064.155412

G = -4064.242466

Esol = -4064.517954

Se	2.34714300	-0.97050300	-1.52829900
I	-2.53295700	-0.24362700	-1.12909600
C	-3.99749900	-1.54696100	-0.20521800
C	-4.27575800	-1.39710500	1.14921000
C	-4.60888900	-2.50613900	-1.00879700
C	-5.23175200	-2.24848500	1.71169800
H	-3.75396100	-0.65794500	1.74871700
C	-5.57002800	-3.33601900	-0.42516000
H	-4.35138300	-2.61519700	-2.05716100
C	-5.87936900	-3.20763900	0.93031000
H	-5.46602000	-2.15470200	2.76829000
H	-6.06426500	-4.08843000	-1.03321600
H	-6.62227900	-3.86074400	1.37913600
N	-0.71415800	-0.51181400	0.00152100
S	-0.66855100	0.46772100	1.34984200
O	-1.96647700	0.64031900	2.04054700
O	0.47337600	-0.08299500	2.10194300
C	-0.18818100	2.12842300	0.81353500
C	-0.90086100	3.23045700	1.29221400
C	0.90694300	2.27975300	-0.04494900
C	-0.51731600	4.51395000	0.90797000
H	-1.74463400	3.07468800	1.95488800

C	1.29056300	3.56108500	-0.43211800
H	1.44027200	1.40585400	-0.42152100
C	0.57344200	4.65612600	0.05237800
H	-1.04338000	5.39395700	1.25654500
H	2.12823700	3.71937100	-1.10022500
N	0.97867800	6.01187200	-0.35729400
O	1.94884700	6.11648400	-1.10649300
O	0.32222900	6.95969500	0.07456400
C	4.22527100	-2.01490300	0.13098500
C	4.36436500	-3.95248500	1.23600200
C	4.18361000	-2.96449300	2.15089600
H	4.48011400	-5.01726000	1.36132100
H	4.10431100	-3.00521200	3.22551000
N	4.39586500	-3.35444000	-0.01590600
N	4.10970800	-1.76429400	1.45887400
C	4.48297400	-3.99940000	-1.32180600
H	4.27400400	-5.06351100	-1.19860300
H	3.73423600	-3.54349300	-1.97665200
H	5.48006700	-3.86771700	-1.75157500
C	3.79233000	-0.44789400	2.01054500
H	2.71192800	-0.34848800	2.14554900
H	4.31738100	-0.32606800	2.96115000
H	4.13714300	0.30386500	1.30006800
O	4.23317100	-1.14376200	-0.81705500

TS-S23

l imaginary frequency

H = -5103.791198

G = -5103.901527

Esol = -5104.273507

N	-1.12087700	-0.31116200	0.76107200
S	-1.24585400	-0.90995500	-0.77917700
O	-0.19989300	-0.34115600	-1.68237700
O	-1.45622000	-2.36799600	-0.87473200
C	-2.80702600	-0.12900400	-1.24414800
C	-2.84077100	0.71179800	-2.35714600
C	-3.96985300	-0.42934800	-0.52686600
C	-4.04968100	1.28164900	-2.75426300
H	-1.92556100	0.90514400	-2.90502400
C	-5.17845600	0.13977700	-0.91392500
H	-3.92834300	-1.10106000	0.32376700
C	-5.19697900	0.98949500	-2.02105300
H	-4.11555800	1.93862500	-3.61266200
H	-6.09960700	-0.06235900	-0.38169200
N	-6.47538000	1.59656600	-2.42905400
O	-7.47547000	1.31749400	-1.76863200
O	-6.46531600	2.34773000	-3.40334200
C	-1.84883800	-3.03321500	2.53738100
C	-3.85482100	-3.83933900	1.87618700
C	-4.09285700	-2.76902900	2.67593900
H	-4.53943100	-4.50571700	1.37509900
H	-5.02205100	-2.33562100	3.01186600
N	-2.47919600	-4.00891600	1.79777300
N	-2.85950400	-2.27881100	3.09386400
C	-1.75992300	-4.96178600	0.96671300
H	-2.22514700	-5.94822100	1.04891400
H	-1.74944800	-4.62347300	-0.07215100
H	-0.73393100	-5.00952500	1.33395000
C	-2.61100100	-1.09199400	3.89408800

H	-1.60349900	-1.17008200	4.30509600
H	-2.66971600	-0.18992100	3.27703300
H	-3.33709300	-1.03825200	4.71022000
O	-0.61961700	-2.87612600	2.68608500
I	0.95529400	2.11057900	-0.53727900
C	1.29849400	3.98539300	0.42519900
C	2.59737300	4.46822800	0.58217800
C	0.17970100	4.69516300	0.86651400
C	2.77019400	5.71110600	1.19495300
H	3.45182800	3.88129000	0.26955200
C	0.37440700	5.93887700	1.46954600
H	-0.82062300	4.29211200	0.74981000
C	1.66565600	6.44524000	1.63258500
H	3.77496900	6.09985200	1.33211200
H	-0.48512700	6.50437400	1.81744100
H	1.81159300	7.41162900	2.10646600
N	1.57096000	0.84086400	1.21181100
S	3.25269300	0.46213600	1.22521700
O	4.01786900	1.66792000	0.88179300
O	3.40285700	-0.20227300	2.52534700
C	3.61864000	-0.75600700	-0.05213700
C	4.06037300	-0.31518300	-1.30288400
C	3.45675400	-2.11571400	0.23005200
C	4.33166000	-1.24892000	-2.29916500
H	4.21304500	0.74253000	-1.48325600
C	3.72742200	-3.05203000	-0.76504900
H	3.14322600	-2.43615700	1.21580700
C	4.15426700	-2.60066000	-2.01162700
H	4.67972900	-0.95038600	-3.27990100
H	3.61482300	-4.11419200	-0.58858400

N	4.44450100	-3.59273100	-3.06540600
O	4.29416800	-4.77973200	-2.78468600
O	4.82039200	-3.16776100	-4.15623600
Se	0.39893600	-0.87172400	1.56443200

TS-S24

l imaginary frequency

H = -5017.988394

G = -5018.093217

Esol = -5018.485762

Se	2.15773700	-1.01841300	0.86441100
N	2.47105600	0.44509300	1.76957500
N	1.75103200	-0.65414100	-0.87265800
S	2.88378100	1.88898900	1.09656000
O	3.71904900	1.73427400	-0.11429200
O	3.36223600	2.72385900	2.20068400
S	0.98841500	-1.98155900	-1.59758500
O	1.19291600	-3.19707000	-0.77760900
O	1.42066600	-1.98268500	-2.99976000
C	4.17895100	-1.86301600	0.44434000
C	4.70806500	-0.96807700	-0.52007900
C	4.28247300	-0.97518300	-1.86322000
H	5.22240400	-0.08482700	-0.15080200
H	4.01930300	-1.95425400	-2.27433200
H	3.07633100	-0.63034300	-1.53105900
H	4.59927500	-1.83232700	1.44715000
H	3.85009200	-2.84821600	0.11468400
C	4.83680200	0.01516100	-2.86984500
H	4.98931900	0.99492000	-2.40876400

H	5.79336900	-0.33476600	-3.27679600
H	4.14507200	0.12987600	-3.70989300
C	-0.76821600	-1.59884100	-1.56629000
C	-1.65693800	-2.65590100	-1.36613700
C	-1.21206600	-0.29847000	-1.80737900
C	-3.02606600	-2.40394500	-1.39409500
H	-1.27909100	-3.65449100	-1.17803200
C	-2.57849500	-0.03677100	-1.81414900
H	-0.49936800	0.50444000	-1.94891000
C	-3.45988200	-1.09666300	-1.60143700
H	-3.75247100	-3.19239000	-1.24143300
H	-2.96008500	0.96551500	-1.97040000
N	-4.90678700	-0.82214300	-1.56095500
O	-5.67186800	-1.78385000	-1.59586300
O	-5.25868000	0.35498800	-1.48042500
C	1.33120500	2.61846800	0.53975600
C	1.06604900	2.72347500	-0.82578600
C	0.43073700	3.09492900	1.49583900
C	-0.14106000	3.27661300	-1.24776200
H	1.79914300	2.36912800	-1.54034300
C	-0.77173300	3.65873000	1.08175900
H	0.67588300	3.02962200	2.55013000
C	-1.04545000	3.72008800	-0.28503200
H	-0.38749300	3.37071100	-2.29849300
H	-1.49445900	4.04345900	1.79070400
N	-2.34254800	4.25844200	-0.72629700
O	-2.63745600	4.12893600	-1.91557300
O	-3.05925700	4.79035400	0.11952200
C	-1.54347100	-1.12647300	2.01760500
C	-3.58796400	-1.50218600	2.94767400

C	-2.85081200	-2.61902700	3.13604600
H	-4.60225700	-1.27340500	3.23558000
H	-3.09812700	-3.55023400	3.62138500
N	-2.79340400	-0.58226300	2.26651300
N	-1.59462400	-2.39786500	2.56967600
C	-3.17484000	0.75690000	1.85792500
H	-3.54246300	1.32868100	2.71626900
H	-2.28289600	1.24003600	1.45782500
H	-3.94989900	0.73333700	1.08409200
C	-0.49276300	-3.34065900	2.55628800
H	-0.74391000	-4.23214200	1.97139700
H	0.36648000	-2.85586900	2.09624500
H	-0.23221900	-3.64156700	3.57685400
O	-0.60140000	-0.58412000	1.42284700

TS-S25

1 imaginary frequency

H = -5018.016706

G = -5018.122839

Esol = -5018.518383

Se	0.03502100	0.48039400	-0.68551700
N	1.84353300	0.06528400	-0.09808500
N	-0.56895300	1.52834800	0.63038700
S	3.07319700	1.15093600	-0.49408900
O	3.21117500	2.24680700	0.47456300
O	2.91598500	1.45613500	-1.92108900
S	-0.73398500	0.82035300	2.10246900
O	-1.18071800	1.86534400	3.03292600
O	0.44270000	-0.00864200	2.45906200

C	0.03221500	2.75399300	-2.03144100
C	0.35785500	3.57381100	-0.96554300
C	-0.55148300	3.77653800	0.06800800
H	1.39873600	3.84247700	-0.80586600
H	-1.59855200	3.56651800	-0.12762100
H	0.77580800	2.50488600	-2.78044500
H	-1.00203100	2.50656300	-2.25265200
C	-0.23168300	4.53994600	1.30842900
H	-0.69477200	4.07212100	2.18110300
H	0.84755700	4.60990200	1.46989900
H	-0.63850500	5.55920800	1.22085000
C	-2.11074100	-0.33598200	1.90875800
C	-1.88378500	-1.59809000	1.35156300
C	-3.39799900	0.08799100	2.24348800
C	-2.96586100	-2.43049400	1.08353600
H	-0.87262700	-1.92303000	1.13647800
C	-4.48432000	-0.74359300	1.98447200
H	-3.53515500	1.06051500	2.70325700
C	-4.25084300	-1.97968500	1.38417200
H	-2.83295800	-3.41194400	0.64571100
H	-5.49804200	-0.44862400	2.22575400
N	-5.39969000	-2.82747100	1.03397100
O	-6.52477400	-2.41108800	1.30940700
O	-5.17139200	-3.89632200	0.46666800
C	4.51680600	0.08973400	-0.29886900
C	5.31293500	0.22882900	0.83858600
C	4.82004500	-0.83542000	-1.30144500
C	6.43408200	-0.58601400	0.98663200
H	5.05916500	0.97072000	1.58761200
C	5.93890800	-1.64903800	-1.15832300

H	4.19218300	-0.90586000	-2.18271800
C	6.72369400	-1.51051000	-0.01349200
H	7.07965000	-0.51243400	1.85285500
H	6.21336000	-2.37801200	-1.91045000
N	7.91048100	-2.37440700	0.14029200
O	8.14400000	-3.18391800	-0.75561500
O	8.59071300	-2.23160700	1.15435600
H	1.77457300	-0.04576900	0.92548700
C	-3.54481800	0.17641600	-1.85060900
C	-5.67965000	-0.60595900	-1.76140000
C	-4.90679200	-1.60121400	-2.25153900
H	-6.73631200	-0.58151800	-1.54593600
H	-5.16194700	-2.60832000	-2.54158100
N	-4.85031000	0.48834600	-1.51530900
N	-3.59496300	-1.12941800	-2.30499600
C	-5.24634200	1.77798500	-0.98639000
H	-5.68858200	1.67163700	0.00972700
H	-4.34650400	2.39066800	-0.91612200
H	-5.96724300	2.26772100	-1.64983600
C	-2.44149900	-1.84174200	-2.82018100
H	-1.54302600	-1.36650400	-2.42555500
H	-2.47151200	-2.88361800	-2.48914400
H	-2.40891200	-1.81397700	-3.91563600
O	-2.55112600	0.91365200	-1.76477700

TS-S26

l imaginary frequency

H = -5247.168868

G = -5247.285202

Esol = -5247.737832

N	0.04769900	-1.41757400	1.21723900
N	-0.40639100	1.10499700	-0.24469300
S	1.37224000	-2.19413100	2.07035600
O	1.11526400	-3.62906000	2.19261900
O	1.63417700	-1.36033600	3.24497700
S	-1.85864800	1.94398100	-0.20748300
O	-1.82469500	2.87884900	-1.33924700
O	-2.13027300	2.43303200	1.15292600
C	-2.14678400	-2.15633200	4.03032000
C	-1.54705900	-1.39492100	3.11645800
C	-1.35572200	-1.75419000	1.66428100
H	-1.17772600	-0.40519400	3.37888800
H	-1.93522600	-1.03567400	1.07168800
H	-0.01924500	0.60091500	-1.31698600
H	-2.27590400	-1.80472100	5.04976000
H	-2.52621200	-3.14983200	3.80965900
C	-1.79590700	-3.15818400	1.23992500
H	-1.30283800	-3.93646100	1.82446900
H	-2.87946700	-3.24740900	1.37054900
H	-1.56718700	-3.31528600	0.18152000
C	-3.13584100	0.73157600	-0.60484200
C	-4.11983600	0.44588200	0.34376300
C	-3.13916300	0.13250300	-1.86905300
C	-5.12689100	-0.46497500	0.02881900
H	-4.09229700	0.93839600	1.30944600
C	-4.13987900	-0.78103000	-2.18433000
H	-2.36715900	0.37566600	-2.59147700
C	-5.11640700	-1.06334300	-1.22892200
H	-5.91118500	-0.71160600	0.73367600

H	-4.17861600	-1.27059400	-3.14939700
C	2.72281600	-1.96073700	0.90024900
C	3.62499800	-0.91769800	1.11974400
C	2.87079800	-2.86273100	-0.15422600
C	4.69643700	-0.75853800	0.24548600
H	3.48827100	-0.24732000	1.95969400
C	3.94294500	-2.70462700	-1.02978500
H	2.15888300	-3.66687700	-0.29475900
C	4.83051200	-1.65301000	-0.81506800
H	5.42311900	0.03343200	0.37586800
H	4.09735700	-3.37747900	-1.86378200
N	-6.17883700	-2.02998200	-1.56367700
N	5.96206500	-1.47835300	-1.74909500
O	-6.15475600	-2.53711900	-2.68379600
O	6.72301400	-0.53384100	-1.54793300
O	-7.02227800	-2.27023200	-0.70120700
O	6.06796900	-2.28500400	-2.67027100
O	0.31840000	0.10928900	-2.40888900
C	0.41169200	-1.17821200	-2.44062900
O	0.24569300	-1.94582100	-1.46855000
C	0.77841100	-1.76127900	-3.79455100
H	0.27258200	-1.21984300	-4.59836300
H	1.85795800	-1.64647100	-3.95214400
H	0.53117100	-2.82389500	-3.83366800
H	0.14135500	-1.59763400	0.17986600
Se	0.53435800	0.80737600	1.25792600
C	1.14799100	3.70036000	0.49496700
C	0.35127100	5.50895300	-0.57294100
C	1.11906500	4.82077700	-1.45208800
H	-0.21430200	6.41882600	-0.69503500

H	1.34689000	5.01328000	-2.48828000
N	0.36952300	4.81424300	0.62908800
N	1.61415200	3.70527200	-0.78930000
C	-0.37607100	5.13375700	1.83861200
H	-1.44733400	5.01767000	1.65959000
H	-0.07015200	4.42515900	2.60805200
H	-0.14801000	6.15399700	2.16016700
C	2.43672700	2.64653100	-1.35895100
H	1.91184300	2.16647300	-2.18863100
H	3.39576400	3.05115000	-1.69625300
H	2.60418700	1.90370300	-0.57922100
O	1.40695200	2.85472600	1.40428300

TS-S27

1 imaginary frequency

H = -7519.692759

G = -7519.809143

Esol = -7520.203663

Se	0.05051200	-0.93105600	-0.06409600
N	0.99716400	0.02333000	1.15172700
N	0.28511200	0.21478000	-1.42248200
S	1.10727300	-0.76560600	2.56895900
O	1.81991700	0.08333200	3.51460300
O	1.45923500	-2.18357900	2.41211200
S	-1.05558400	0.63945000	-2.30842900
O	-2.29450500	0.29471100	-1.61072600
O	-0.86065500	0.32306000	-3.71331000
C	-2.34149800	-3.01208000	-1.97976600
C	-4.43507700	-3.57761300	-2.63638700

C	-4.31247800	-3.93416900	-1.33768600
H	-5.27132200	-3.66333900	-3.31231400
H	-5.01952000	-4.39079500	-0.66309900
N	-3.22707900	-3.00861600	-3.03415700
N	-3.02742000	-3.58349900	-0.92682600
C	-2.91566700	-2.46193500	-4.34391100
H	-1.99756900	-1.88031900	-4.26035700
H	-2.78075100	-3.26232000	-5.08031400
H	-3.72242900	-1.80045600	-4.67203400
C	-2.45153900	-3.79021500	0.38979700
H	-1.62718900	-3.08977500	0.51327000
H	-3.19952300	-3.58440400	1.15945300
H	-2.07615500	-4.81292100	0.51073700
O	-1.16337700	-2.60478900	-1.98184500
C	5.30070800	0.59117900	0.20597800
C	4.04009900	0.27892700	-0.55358000
C	3.69602300	-1.22075000	-0.46373300
C	4.93935900	-2.06272200	-0.84340100
C	6.16249600	-1.69410200	0.00212600
C	6.27207500	-0.29759800	0.49337800
H	5.41540500	1.62211500	0.53888800
H	3.20644100	0.86554800	-0.15402100
H	3.45599900	-1.44113200	0.58187200
H	4.76632300	-3.13674400	-0.72734000
H	4.16764200	0.59169200	-1.60111800
H	5.19770100	-1.88829000	-1.89849600
C	7.50891600	0.04277900	1.28025200
H	7.57518900	-0.57315400	2.18411400
H	8.41256900	-0.16681200	0.69692800
H	7.51255700	1.09629700	1.57451200

O	7.03224000	-2.52473500	0.21381800
C	2.52937100	-1.65820000	-1.30803800
C	2.28401400	-1.14409000	-2.60430100
H	1.70784300	-2.88587800	0.27068100
H	3.08336400	-0.61169600	-3.11624300
H	1.64845200	-1.74252400	-3.25925500
C	1.48952300	-2.43376200	-0.69523700
H	0.82654900	-2.99865800	-1.34696700
H	1.43121600	-0.30008500	-2.22518600
O	-0.89259100	2.27725400	-2.27013900
C	-0.98418300	2.88116000	-0.97662000
H	-2.02906700	2.94878600	-0.66246800
H	-0.40373400	2.30583500	-0.24879000
C	-0.39975600	4.29422200	-1.06191900
Cl	-0.55853000	5.01692800	0.58438300
Cl	1.33291500	4.24144800	-1.52946800
Cl	-1.31339600	5.28904200	-2.24412700
O	-0.48173700	-0.90705500	3.12074600
C	-1.07315500	0.28770600	3.61297500
H	-0.61803700	1.17921500	3.17153500
H	-0.97913400	0.33454000	4.70187700
C	-2.56432100	0.28869100	3.25124200
Cl	-3.38931600	-1.14717400	3.95289900
Cl	-2.77722000	0.28666500	1.46472800
Cl	-3.28500400	1.79000700	3.94146700

TS-S28

1 imaginary frequency

H = -7519.692158

G = -7519.808993

Esol = -7520.202399

Se	0.02556600	-0.97578200	0.84020500
N	-1.20131200	0.00100000	1.74277600
N	1.02025800	0.40969400	0.29280300
S	-2.25268000	-0.99422800	2.50284100
O	-2.60054800	-0.49444900	3.82077000
O	-1.83216600	-2.40846300	2.33526700
S	1.26039000	0.51996500	-1.34003000
O	0.33509900	-0.36151500	-2.05692500
O	2.67734000	0.55777600	-1.66224300
C	2.03657200	-3.30757200	-1.26555900
C	1.38993100	-4.88396500	-2.76080400
C	2.54398500	-4.34006200	-3.21071000
H	0.76504800	-5.65759600	-3.17838600
H	3.11736200	-4.54658100	-4.10067200
N	1.07218500	-4.24824700	-1.56146200
N	2.94981400	-3.37783400	-2.28929500
C	-0.07650100	-4.50490900	-0.71318500
H	-0.24487600	-3.62235200	-0.09729100
H	-0.96085100	-4.68240400	-1.33110400
H	0.08680100	-5.36980700	-0.05996100
C	4.09458600	-2.48345900	-2.41650800
H	4.84862300	-2.97101000	-3.03890000
H	3.79780600	-1.53210400	-2.86623600
H	4.51814700	-2.27690500	-1.43291400
O	2.07155500	-2.56127200	-0.26423700
C	4.45862100	2.22793300	1.78078500
C	3.49298400	1.59031300	2.74376200
C	2.94985600	0.25442000	2.23197100

C	4.02491000	-0.62672800	1.57583000
C	4.97771900	0.12247500	0.64815400
C	5.11350700	1.59226800	0.79198100
H	3.98485700	1.45322200	3.72214200
H	4.61823700	3.29720400	1.91440900
H	2.67060400	2.29246000	2.92129700
C	6.03135000	2.28163700	-0.17916300
H	6.11790500	3.34884700	0.04506400
H	7.02870900	1.82933400	-0.16292600
H	5.65106000	2.16760800	-1.20057700
O	5.65866900	-0.50584100	-0.15050400
C	1.87474000	-0.37271400	2.94564000
C	1.05379900	0.37149400	3.94350300
C	1.31940200	-1.60584200	2.45265100
H	1.95505700	-2.28893600	1.89764400
H	1.62046300	1.11329400	4.50811400
H	0.55401900	-0.31244600	4.63485800
H	3.59472700	-1.43503300	0.98204600
H	0.58481400	-2.09835000	3.08652900
H	4.64342500	-1.08597000	2.36245800
H	2.18869300	0.52180200	1.28045100
H	0.23557700	0.88025000	3.39672800
O	0.78964100	2.07696300	-1.60324400
C	-0.57943600	2.38353200	-1.33020900
H	-0.90513200	1.90019100	-0.40362000
H	-1.21221600	2.07035100	-2.16513400
C	-0.70029000	3.90199300	-1.16057400
Cl	0.28069700	4.46696200	0.23528900
Cl	-2.44044400	4.26320100	-0.85499900
Cl	-0.16743500	4.75030500	-2.65126600

O	-3.67075800	-0.82193800	1.65019700
C	-3.65634600	-1.35349100	0.33257000
H	-2.71058300	-1.12259800	-0.17075400
H	-3.81193900	-2.43589500	0.35216200
C	-4.78561900	-0.70730000	-0.47775300
Cl	-4.53128100	1.06067600	-0.61834300
Cl	-6.37715800	-1.03915800	0.27709900
Cl	-4.73078100	-1.45811900	-2.12354800

TS-S29

1 imaginary frequency

H = -5446.725711

G = -5446.847609

Esol = -5447.484423

Se	0.55022200	0.76244700	-0.23944100
N	-0.68512600	2.03056700	-0.19330300
N	-0.14928200	-0.65450300	-1.17290800
S	-1.55987600	2.49430000	-1.50867200
O	-0.91483800	2.10576900	-2.78436500
O	-1.91009700	3.90498900	-1.28811500
S	0.05988800	-2.11208100	-0.38906800
O	1.08791200	-2.00816200	0.67121900
O	0.19597600	-3.15524800	-1.41201000
C	-1.51837700	-2.36279700	0.45187900
C	-2.13167600	-1.29573100	1.11370700
C	-2.05111100	-3.65185400	0.48978900
C	-3.29275000	-1.52517800	1.84354200
H	-1.72123300	-0.29506100	1.04041900
C	-3.21473200	-3.88593100	1.22003500

H	-1.56183100	-4.45447300	-0.05087700
C	-3.81004500	-2.81924900	1.88874700
H	-3.80083900	-0.72546200	2.36752300
H	-3.66133500	-4.87077600	1.27721600
N	-5.03355800	-3.06595900	2.67530700
O	-5.53828000	-2.10598100	3.25533300
O	-5.46741900	-4.21556200	2.70673900
C	-3.11995200	1.58811900	-1.44589100
C	-3.25223100	0.38815600	-2.14756700
C	-4.17837700	2.12173000	-0.70554500
C	-4.46311900	-0.29799200	-2.10227900
H	-2.41590100	0.00068000	-2.71612400
C	-5.39045800	1.43871200	-0.65560500
H	-4.05381600	3.07019900	-0.19519500
C	-5.51013500	0.23904800	-1.35572400
H	-4.60794300	-1.22961900	-2.63488700
H	-6.23710100	1.82062900	-0.09879600
N	-6.79517800	-0.48286900	-1.31300000
O	-7.71488300	0.02797800	-0.67613300
O	-6.86805800	-1.55231000	-1.91692100
C	1.45582200	3.23435200	1.84123700
C	0.15977000	3.64487200	3.65701900
C	0.09722000	4.73399400	2.85738000
H	-0.29956700	3.44573500	4.61251400
H	-0.43609000	5.66373800	2.97817800
N	0.99650600	2.71847300	3.03572200
N	0.90335200	4.49147600	1.74724900
C	1.29052200	1.36240700	3.46378600
H	1.23715900	0.70063700	2.59699600
H	2.28967400	1.28411300	3.90496200

H	0.54683600	1.05183800	4.20096200
C	0.98759200	5.30676000	0.54686100
H	0.10799900	5.15392800	-0.08721500
H	1.07182700	6.36151000	0.82355700
H	1.88341000	5.00642700	0.00095400
O	2.20572900	2.66519300	1.02442300
C	3.74777800	-0.16896800	-2.08158000
C	3.84855100	-0.41256600	-0.54634400
C	5.28627900	-0.78037000	-0.06836100
C	5.77838000	-1.96330200	-0.91203700
C	5.63413100	-1.81483000	-2.41322200
C	4.20727300	-1.42349900	-2.83676300
H	3.50534900	0.46584200	0.00783400
C	5.18681900	-1.18286100	1.44324200
C	6.29108300	-3.08206900	-0.38322600
H	6.32760200	-1.04558500	-2.78640300
H	3.52236300	-2.25204200	-2.61286700
C	6.50631100	-3.31853400	1.08604700
C	6.40166000	-2.01645500	1.88387800
H	6.58162000	-3.89042600	-1.05533000
H	5.76627400	-4.04799400	1.45212900
H	7.32067900	-1.42899000	1.75118400
H	4.17702900	-1.25831200	-3.92117500
H	7.48589400	-3.79009900	1.24630300
H	6.32702300	-2.23355300	2.95698100
H	4.30470200	-1.83464200	1.52778000
H	3.17688300	-1.23929200	-0.29075800
C	4.97689100	0.00440500	2.39841500
H	5.88661200	0.60813200	2.49744100
H	4.16859200	0.67185000	2.08151800

H	4.72696000	-0.36901700	3.39884900
C	6.23647300	0.42834900	-0.25691700
H	4.43813900	0.65783700	-2.32466600
C	2.39695500	0.36630600	-2.48056100
C	1.49522100	-0.31500800	-3.34015300
H	0.76546900	0.31633500	-3.85297400
H	1.86377100	-1.15302000	-3.92566300
C	1.87205700	1.50915300	-1.78376700
H	2.54546100	2.08861200	-1.15766300
H	5.82171300	1.33469200	0.19729300
H	7.21132800	0.23351400	0.20193300
H	6.42436900	0.64685900	-1.31281500
H	5.92164800	-2.74919800	-2.90774700
H	1.13962800	2.09494300	-2.33659800
H	0.73362500	-0.73783900	-2.46491600

TS-S3

1 imaginary frequency

H = -8172.312382

G = -8172.447371

Esol = -8173.163999

Se	0.01295400	-0.13317100	-0.11797900
N	0.53914900	1.47816700	-0.71694500
S	0.33469300	2.65902100	0.41392600
O	1.18650500	2.46918200	1.62323200
O	-1.07884000	3.01022900	0.69096300
C	1.04424300	4.04395900	-0.50033100
C	0.71378600	4.24507100	-1.84443600
C	1.86479400	4.94103600	0.18615200

C	1.21780600	5.35610500	-2.51366800
H	0.08827400	3.52473000	-2.35884600
C	2.36856100	6.05834700	-0.47647100
H	2.10653800	4.75314400	1.22636300
C	2.03622300	6.24584000	-1.81657000
H	0.99201800	5.54221400	-3.55625900
H	3.00877400	6.77576600	0.02165600
N	2.57220500	7.42115700	-2.52281900
O	3.30067800	8.18517200	-1.88979000
O	2.26052700	7.56931900	-3.70399000
I	3.44154200	0.47090300	1.55519300
C	5.40140900	-0.34155000	1.27331400
C	5.87230700	-1.32684700	2.14224100
C	6.17605500	0.15500100	0.22319500
C	7.16785100	-1.81353500	1.95424400
H	5.23943400	-1.72159000	2.92743000
C	7.46938700	-0.34316000	0.05253700
H	5.78603000	0.91167100	-0.44919700
C	7.96373600	-1.32313500	0.91602500
H	7.55084500	-2.57985400	2.62208800
H	8.08516500	0.03482200	-0.75843100
H	8.97016200	-1.70775400	0.77774800
N	2.15877200	-0.89185600	0.40101200
S	1.99365100	-2.43113800	1.12307200
O	3.08742400	-2.70003000	2.07444700
O	0.60359600	-2.67115500	1.54653600
C	2.26838200	-3.46462200	-0.33285300
C	3.52183300	-4.05282800	-0.51298800
C	1.22359600	-3.66890700	-1.23791300
C	3.73940400	-4.86401300	-1.62380600

H	4.30659100	-3.88430300	0.21570000
C	1.43876000	-4.47608200	-2.35135100
H	0.25886100	-3.20098200	-1.07583600
C	2.69366200	-5.05898700	-2.52433900
H	4.69367500	-5.34458900	-1.79953900
H	0.65767400	-4.65942100	-3.07843500
N	2.92252300	-5.91681700	-3.70099800
O	1.98217100	-6.08348700	-4.47576900
O	4.04025600	-6.41307200	-3.83483100
Se	-2.51263700	-0.48408000	-1.27478300
P	-4.16431700	-0.38662400	0.17936700
C	-4.21427800	4.21910300	1.48856000
C	-4.49570700	3.14831600	2.55034200
C	-3.97835900	1.76216300	2.12140200
C	-4.59855500	1.34938000	0.76717500
C	-4.25804600	2.41686900	-0.30120300
C	-4.78209500	3.79892600	0.12626400
H	-3.13023000	4.35508700	1.39677400
H	-4.64143500	5.18118700	1.79950800
H	-5.57912800	3.08773200	2.73800600
H	-2.88774400	1.79955200	2.02267300
H	-5.69319300	1.30254100	0.89004800
H	-3.17026500	2.45744400	-0.41223600
H	-4.66748200	2.14847900	-1.27913000
H	-5.88241600	3.78049400	0.17110800
H	-4.51330800	4.53500800	-0.64155600
H	-4.02798800	3.42329700	3.50387300
H	-4.22116900	1.03591000	2.90275000
C	-3.59317900	-2.72014800	4.32318600
C	-2.39659200	-2.56562800	3.37490800

C	-2.59828700	-1.40267300	2.38951000
C	-3.90685000	-1.59538000	1.59294700
C	-5.12549200	-1.73803000	2.53554900
C	-4.90237000	-2.88620000	3.53894200
H	-3.66639700	-1.83070100	4.96654900
H	-3.44579100	-3.57758600	4.99168900
H	-2.24858300	-3.49653500	2.80944200
H	-2.62741500	-0.46007600	2.94632300
H	-3.79707600	-2.53962400	1.04140600
H	-5.28311100	-0.80293600	3.08806200
H	-6.04501800	-1.92948500	1.97026300
H	-4.87843200	-3.83905900	2.99009900
H	-5.75942000	-2.94082500	4.22214000
H	-1.47091500	-2.40072600	3.93725000
H	-1.74274200	-1.34436700	1.71418600
C	-7.26006400	-2.10510200	-3.00649200
C	-7.42730600	-0.65316800	-2.54324800
C	-6.15583300	-0.11596800	-1.86273300
C	-5.71448300	-1.01711900	-0.68807700
C	-5.56362600	-2.48430500	-1.14981000
C	-6.84094800	-3.00075700	-1.83456600
H	-6.49319000	-2.15132400	-3.79301000
H	-8.19216500	-2.47269300	-3.45313800
H	-8.26994900	-0.59134800	-1.83849300
H	-5.34016800	-0.05800900	-2.59511200
H	-6.49515600	-0.96992200	0.08603900
H	-7.65774700	-3.04340300	-1.09870600
H	-6.67502800	-4.03009800	-2.17569800
H	-7.68213300	-0.00459100	-3.39047000
H	-6.34367700	0.90347800	-1.51207600

H	-4.71828800	-2.54886200	-1.84659500
H	-5.32396700	-3.13563700	-0.30217900

TS-S30

1 imaginary frequency

H = -5446.722102

G = -5446.846872

Esol = -5447.479214

Se	-0.09779700	-0.14361200	-1.78646600
N	0.88060100	1.09777400	-1.00260000
N	-1.22261400	-0.87656800	-0.56917600
S	0.31971600	2.00846800	0.24951900
O	0.27873000	1.29132600	1.53303800
O	-0.88757200	2.78158800	-0.13292700
S	-1.22752000	-2.54807100	-0.55658800
O	-0.72698300	-3.09561000	-1.83429700
O	-2.55372600	-2.96984000	-0.08524000
C	-0.04104300	-2.96135200	0.73708900
C	-0.29346300	-4.09451800	1.51349700
C	1.10939200	-2.19031000	0.91049700
C	0.63681800	-4.47832900	2.47588200
H	-1.21123500	-4.65498300	1.37427700
C	2.04055900	-2.57236600	1.87074300
H	1.26845000	-1.29955800	0.31875400
C	1.78993800	-3.71166800	2.63287600
H	0.48081000	-5.34821000	3.10152700
H	2.94489500	-2.00166300	2.03800000
N	2.78025900	-4.11906000	3.64640000
O	3.78936600	-3.42616600	3.76800800

O	2.53946700	-5.12982600	4.30473500
C	1.68501400	3.18545300	0.34125200
C	1.83749000	4.14723500	-0.66075500
C	2.53836100	3.13703800	1.44319900
C	2.87551900	5.06841400	-0.56982200
H	1.14771800	4.17560800	-1.49685900
C	3.58019500	4.05806300	1.54098500
H	2.37650100	2.38913400	2.21141700
C	3.73134300	5.00383000	0.53008400
H	3.03068500	5.82924400	-1.32450100
H	4.26523300	4.05562000	2.37969700
N	4.83625000	5.97607000	0.62633500
O	5.58199700	5.89668400	1.60108800
O	4.94585700	6.80472500	-0.27616400
C	3.38941900	-2.04443200	-1.84499000
C	5.47024400	-2.23399300	-0.94426800
C	4.99863700	-3.48737900	-1.13727300
H	6.41011700	-1.89361900	-0.53837000
H	5.45018800	-4.44498300	-0.92969900
N	4.48496900	-1.34253400	-1.36816700
N	3.72045100	-3.37933800	-1.68295600
C	4.55287500	0.10653000	-1.37429400
H	4.86402600	0.47774200	-0.39245400
H	5.25793000	0.46754000	-2.13231600
H	3.55302200	0.48270400	-1.59879200
C	2.82843800	-4.46130900	-2.05656600
H	2.72926100	-5.17334500	-1.23101800
H	1.85157300	-4.02611400	-2.27578000
H	3.19726700	-4.99002000	-2.94313200
O	2.34187400	-1.58235500	-2.31186600

C	-3.63724400	0.09678700	-1.53377800
C	-3.93151300	1.33120500	-0.65480600
C	-4.57385300	1.05726400	0.74042000
C	-5.74767300	0.09134300	0.55023700
C	-5.43607500	-1.16827000	-0.22528700
C	-4.80600800	-0.88926900	-1.60084500
H	-3.02987700	1.92630900	-0.51055400
C	-5.08187900	2.43370800	1.29477100
C	-6.97884600	0.31694700	1.02831200
H	-4.74282800	-1.80354600	0.33865300
H	-5.57170200	-0.45645800	-2.26359600
C	-7.37029200	1.50433500	1.86486800
C	-6.13713500	2.23918100	2.39607000
H	-7.76106700	-0.41440400	0.81982000
H	-7.99342500	2.19113700	1.26880600
H	-5.70024700	1.66981000	3.22753500
H	-4.49268300	-1.83807900	-2.04602300
H	-8.01085900	1.17711700	2.69590000
H	-6.42297900	3.21607100	2.80655500
H	-5.59467300	2.93265400	0.45668700
H	-4.63836000	1.94431700	-1.23345900
C	-3.96715100	3.37495900	1.77980200
H	-3.51767800	3.01475600	2.71197600
H	-3.15801100	3.49517700	1.05336100
H	-4.38590400	4.36817200	1.98238800
C	-3.52728600	0.42668800	1.69310800
C	-2.82948600	0.24942000	-2.70119200
C	-2.88803700	-0.76604500	-3.80922000
H	-3.91325500	-0.93422900	-4.15164000
H	-2.27375500	-0.46258300	-4.66079700

H	-2.50552700	-1.73605300	-3.45391800
C	-1.69418900	1.11593800	-2.70032600
H	-1.21273300	1.27793600	-3.66215300
H	-1.66584800	1.97354100	-2.03406300
H	-3.26082500	-0.58914600	1.39159800
H	-2.60054600	1.00675600	1.71266400
H	-3.92195300	0.36780200	2.71327100
H	-6.35046800	-1.75571600	-0.36713800
H	-2.61119800	-0.46918300	-0.96516800

TS-S4

1 imaginary frequency

H = -8086.515932

G = -8086.645462

Esol = -8087.382728

Se	-0.20809600	2.20027900	0.70974300
N	-1.78486700	2.06437300	-0.12032400
N	0.50882900	3.15982200	-0.65339600
S	-2.91467100	1.42480800	0.86601400
O	-3.80597800	2.43923700	1.46737100
O	-2.31114500	0.45608400	1.82806800
S	2.17126900	3.36630700	-0.50464900
O	2.61734100	3.09416700	0.87885700
O	2.47720300	4.66062300	-1.12211100
C	-0.62965300	4.06328700	2.00980800
C	-1.26612500	4.86547000	1.04177700
C	-0.55855900	5.55828000	0.03632100
H	-2.33492800	4.70371900	0.90565700
H	0.42559900	5.94144200	0.32394400

H	-0.11055700	4.44733000	-0.50111500
H	-1.24776800	3.61429000	2.78397100
H	0.39596200	4.28825800	2.29831000
C	-1.28135900	6.38631800	-1.00936300
H	-0.67117000	6.48379900	-1.91260900
H	-2.23524200	5.92759500	-1.28925300
H	-1.48433700	7.39878500	-0.63887900
C	2.83481000	2.05876100	-1.54763800
C	3.95458900	1.36016800	-1.09830700
C	2.24592300	1.79144500	-2.78604200
C	4.49234600	0.35469800	-1.89661500
H	4.38295400	1.59140400	-0.12976100
C	2.77399300	0.78019000	-3.58195300
H	1.37007400	2.34475200	-3.10567300
C	3.88270900	0.07477200	-3.11704900
H	5.35772300	-0.21659600	-1.58524700
H	2.33877100	0.52582200	-4.54017000
N	4.42373600	-1.01886500	-3.94302400
O	5.34216400	-1.69039100	-3.47024600
O	3.92578800	-1.19754100	-5.05207800
C	-3.89588300	0.52735700	-0.35160100
C	-5.28681400	0.56566400	-0.24842700
C	-3.25042200	-0.20229700	-1.35396200
C	-6.05747100	-0.14685600	-1.16477800
H	-5.75104500	1.16145200	0.52961700
C	-4.01758900	-0.91065100	-2.27428000
H	-2.16559400	-0.20582900	-1.40099500
C	-5.40742500	-0.87212700	-2.16096700
H	-7.13950600	-0.14294000	-1.12356600
H	-3.56052900	-1.48467600	-3.07065300

N	-6.21953300	-1.62638300	-3.13318600
O	-5.62425200	-2.26751700	-3.99833500
O	-7.44330000	-1.57213000	-3.01907700
P	0.71526100	-1.83665900	1.15624200
C	4.50556800	-4.08583500	-0.54882600
C	3.16378300	-4.82634900	-0.53566100
C	1.98460100	-3.86811200	-0.30241000
C	2.15142800	-3.03531900	0.99318900
C	3.51774200	-2.31596400	0.99525000
C	4.68589200	-3.28526700	0.74549700
H	4.54432300	-3.40553300	-1.41088400
H	5.33165100	-4.79643400	-0.67449900
H	3.17564700	-5.58981600	0.25662300
H	1.89447800	-3.17156100	-1.14624400
H	2.09149400	-3.70228600	1.86533400
H	3.49503400	-1.54211800	0.21711900
H	3.67875800	-1.80564300	1.94880100
H	4.76726000	-3.97972500	1.59511700
H	5.62447200	-2.71716600	0.71988700
H	3.00915900	-5.36073300	-1.48107700
H	1.05371000	-4.44303500	-0.27245100
C	-2.84240900	-5.05370600	1.16073400
C	-2.96385800	-3.77486500	0.31983100
C	-1.59117900	-3.14110500	0.04577700
C	-0.85831100	-2.84697500	1.37079800
C	-0.68590300	-4.15795900	2.17420300
C	-2.05844100	-4.79795400	2.45566400
H	-2.32478200	-5.82608700	0.57284800
H	-3.83679100	-5.45378700	1.39411900
H	-3.59571700	-3.04633100	0.84752900

H	-0.99215900	-3.82535500	-0.56919400
H	-1.49577500	-2.15847000	1.94430900
H	-0.07863000	-4.86526600	1.59442300
H	-0.15626000	-3.99423600	3.11800700
H	-2.63808400	-4.13079500	3.10978200
H	-1.91733400	-5.73476700	3.00939100
H	-3.46447000	-3.99161800	-0.63194100
H	-1.69688800	-2.22059300	-0.52914900
C	1.58039400	0.62568700	5.19466300
C	0.48589900	-0.45096700	5.18697200
C	0.67351800	-1.48383800	4.05685900
C	0.78580700	-0.76712700	2.69598000
C	1.95280900	0.24158800	2.72284900
C	1.71821700	1.29069400	3.81840600
H	2.54245400	0.16706700	5.46730000
H	1.36327300	1.37537000	5.96566800
H	-0.49375100	0.02972900	5.05556100
H	1.57877600	-2.07991700	4.24295900
H	-0.14033000	-0.19333100	2.54499100
H	2.89222200	-0.27962100	2.94175500
H	2.07505400	0.71491700	1.74662800
H	0.80232300	1.85108200	3.58258700
H	2.53966800	2.01640400	3.81430800
H	0.45325800	-0.97057700	6.15279800
H	-0.17614200	-2.17207000	4.07383000
Se	0.65920600	-0.51627300	-0.56755300

TS-S5

1 imaginary frequency

H = -8086.538042

G = -8086.667723

Esol = -8087.409133

Se	0.03278500	-0.32187300	-1.04693200
N	-1.97593500	0.08012500	-1.34589700
N	-0.14151500	-1.99997100	-1.67010400
S	-2.21537300	1.71715600	-1.42779400
O	-2.22465600	2.23470700	-2.80819600
O	-1.26732700	2.29065500	-0.45222300
S	-0.10904300	-3.21735800	-0.54088300
O	0.88688300	-3.03547300	0.52606000
O	-0.11396200	-4.47411700	-1.30508400
C	0.66062700	0.23333700	-3.55003500
C	0.06555400	-0.88886800	-4.08779700
C	0.51332300	-2.17051300	-3.74177600
H	-0.90988100	-0.79705200	-4.56371900
H	1.53251400	-2.26501200	-3.37617600
H	0.21679500	1.21489500	-3.69380000
H	1.68243500	0.21016100	-3.18303100
C	-0.11133400	-3.41555300	-4.28569100
H	0.42272200	-3.70539300	-5.20299800
H	-0.03325800	-4.23889300	-3.57391400
H	-1.16339600	-3.25819700	-4.54400200
C	-1.72645300	-3.06433700	0.25354200
C	-2.83372900	-3.69759700	-0.31267100
C	-1.85141900	-2.25560500	1.38477400
C	-4.09359300	-3.51095200	0.25072200
H	-2.70165100	-4.33639400	-1.17920400
C	-3.10708900	-2.05688900	1.94843400
H	-0.96724800	-1.81438700	1.82843000

C	-4.21012400	-2.67662700	1.36129200
H	-4.97697600	-3.98614200	-0.15778300
H	-3.24527100	-1.43819000	2.82680900
N	-5.54377200	-2.43237400	1.93142900
O	-6.48187700	-3.10226400	1.50599600
O	-5.64136100	-1.55979400	2.79811300
C	-3.88701100	1.93692700	-0.78754000
C	-4.73242500	2.83828800	-1.43680500
C	-4.29203900	1.25165900	0.36128400
C	-6.00836900	3.06425600	-0.92516200
H	-4.39194600	3.34475900	-2.33287700
C	-5.56894800	1.46677800	0.87269400
H	-3.62361400	0.54067500	0.83256100
C	-6.40125500	2.37644700	0.22036800
H	-6.69587900	3.75480400	-1.39735200
H	-5.92353900	0.93704000	1.74897900
N	-7.75340200	2.61885400	0.76044400
O	-8.06896700	2.02794700	1.79044600
O	-8.47876400	3.40099900	0.14685600
P	3.54927800	0.50837300	0.63746900
C	1.90379700	-0.48180200	5.01749400
C	3.41821000	-0.53191500	4.76599500
C	3.82670100	0.28403500	3.52439400
C	3.03607200	-0.20289500	2.29135100
C	1.52052200	-0.04489800	2.54794800
C	1.10525000	-0.88340100	3.76762100
H	1.62125200	0.54016900	5.31038800
H	1.64221900	-1.13109800	5.86191600
H	3.73027700	-1.57594800	4.62039500
H	3.61466600	1.34720100	3.70381200

H	3.23172800	-1.27335700	2.14252300
H	1.29323200	1.01019800	2.75592300
H	0.94327700	-0.32502000	1.66178300
H	1.26317100	-1.94646100	3.54075700
H	0.03125800	-0.75593800	3.95556200
H	3.96234600	-0.16216100	5.64402800
H	4.90802400	0.19785600	3.37049100
C	2.70115000	5.09860300	-0.28241300
C	3.09202000	4.70149300	1.14739900
C	3.76340800	3.31720500	1.18263600
C	2.85261500	2.24952500	0.53525800
C	2.42075800	2.63843600	-0.89430800
C	1.79145200	4.04041300	-0.92051400
H	3.61330700	5.21558200	-0.88683700
H	2.20200100	6.07530800	-0.27871600
H	2.19318900	4.68472300	1.78031900
H	4.71560100	3.37403200	0.63988200
H	1.93299900	2.18822200	1.13184200
H	3.27943500	2.59261500	-1.57645700
H	1.69144900	1.90588000	-1.24475100
H	0.82973900	4.00541900	-0.39253200
H	1.56034700	4.31083000	-1.95810200
H	3.77034700	5.44496400	1.58460100
H	4.00611300	3.04759700	2.21772000
C	8.00825400	-0.34261000	-0.63382700
C	7.53147500	-0.87661000	0.72278600
C	5.99774900	-0.86587600	0.83099600
C	5.41825000	0.54483600	0.56766700
C	5.90941700	1.08395600	-0.79645000
C	7.44328100	1.05852200	-0.89871500

H	7.67527000	-1.02467300	-1.42912800
H	9.10441100	-0.32468000	-0.67228400
H	7.95941500	-0.26121900	1.52817600
H	5.56629400	-1.56054800	0.09905900
H	5.74820100	1.22553200	1.36514900
H	5.46504100	0.46808500	-1.58867900
H	5.54904000	2.10605600	-0.95929200
H	7.86945100	1.76672400	-0.17262800
H	7.74472300	1.41279200	-1.89228300
H	7.89707700	-1.89823700	0.88357100
H	5.69825700	-1.23047200	1.82016200
H	-2.26150700	-0.37011700	-2.21880300
Se	2.87204000	-0.80457400	-0.94704500

TS-S6

1 imaginary frequency

H = -8315.709033

G = -8315.850551

Esol = -8316.647819

N	-2.37137300	0.94190700	1.73346200
N	0.29990900	1.89594600	0.16554500
S	-3.37920800	-0.41886500	1.61719900
O	-4.29418200	-0.53135200	2.76059200
O	-2.52178900	-1.58239400	1.30724800
S	1.40565400	2.47541400	1.27620900
O	2.19681200	1.35979000	1.82584600
O	0.76275400	3.40745900	2.21719100
C	-0.34954900	0.65894200	4.64232600
C	-1.55220500	0.55348400	4.07525000

C	-2.07868400	1.55277500	3.07686100
H	-2.24018500	-0.23202900	4.38483600
H	-1.27612200	2.25775700	2.84000400
H	-0.46905400	2.68306600	-0.30609600
H	-0.02629400	-0.03400800	5.41529100
H	0.34933300	1.44259700	4.36020700
C	-3.27531600	2.35050800	3.62319100
H	-3.63486900	3.05010500	2.86136100
H	-4.09554000	1.69185000	3.91935200
H	-2.95373800	2.92453800	4.49861700
C	2.49767000	3.45424400	0.22653300
C	3.86959000	3.20823700	0.29611900
C	1.97106900	4.46570900	-0.58424000
C	4.74266900	3.98569000	-0.46113700
H	4.23941400	2.41356600	0.93373500
C	2.84219300	5.23895100	-1.34615200
H	0.89866800	4.62798900	-0.64372100
C	4.21203500	4.98789000	-1.26933600
H	5.81365200	3.82821900	-0.43521200
H	2.47753000	6.02619600	-1.99409000
C	-4.35307600	-0.05416500	0.14106200
C	-3.72580900	0.12090300	-1.09679000
C	-5.74064200	-0.01604900	0.27868000
C	-4.51218300	0.34102300	-2.22289700
H	-2.64286400	0.11297000	-1.17197800
C	-6.52863100	0.19820500	-0.85017500
H	-6.18917200	-0.15313500	1.25613600
C	-5.89844000	0.37020600	-2.07958200
H	-4.07020500	0.49095600	-3.19982100
H	-7.60914400	0.23376300	-0.79049000

N	5.13280000	5.80759100	-2.07708700
N	-6.73082400	0.59117500	-3.27820900
O	6.33566700	5.55778100	-2.00105300
O	-6.15297000	0.72283300	-4.35573300
O	4.64432800	6.69107200	-2.77973800
O	-7.95050100	0.62579600	-3.12581900
O	-1.14129700	3.67379500	-0.82893000
C	-2.36688000	3.85859100	-0.48398200
O	-3.06590400	3.07740700	0.19723100
C	-2.97976700	5.16342000	-0.97140000
H	-4.05391900	5.18198700	-0.77875900
H	-2.50542300	6.00274200	-0.44957800
H	-2.78502600	5.29508700	-2.04038800
H	-2.66401000	1.70421400	1.06408200
Se	-0.29851700	0.18423500	0.32866700
Se	1.40057200	-0.77742600	-1.26122800
P	1.60304300	-2.76744200	-0.31505100
C	3.35649400	-1.27576500	3.80557000
C	4.32933700	-1.66871100	2.68604100
C	3.62703000	-1.73191700	1.31981100
C	2.40417700	-2.67788800	1.36629200
C	1.42151300	-2.27840800	2.49348800
C	2.15367600	-2.22713800	3.84467100
H	3.00207900	-0.25321000	3.62979000
H	3.87430900	-1.28135300	4.77282400
H	4.77862300	-2.64772500	2.91247700
H	3.28131400	-0.73613300	1.02371700
H	2.75137500	-3.70348200	1.55984500
H	0.97749100	-1.30429900	2.27004400
H	0.59517700	-2.99570100	2.55378600

H	2.49057900	-3.23958300	4.11621600
H	1.44257600	-1.91501900	4.61783600
H	5.15696000	-0.95125300	2.62825800
H	4.33842600	-2.06752300	0.55359400
C	5.02243500	-5.12147500	-2.67592700
C	4.29468800	-3.96698000	-3.37827700
C	3.59602900	-3.03352300	-2.37560100
C	2.62929400	-3.83170500	-1.47166800
C	3.37820200	-4.97080300	-0.74162200
C	4.07211400	-5.89862300	-1.75499600
H	5.85473700	-4.71841800	-2.08088900
H	5.46658700	-5.79670900	-3.41696200
H	3.54576400	-4.37469600	-4.07273300
H	4.34941600	-2.53041900	-1.75552900
H	1.86941800	-4.28687500	-2.12241600
H	4.13735300	-4.53983900	-0.07590500
H	2.69596200	-5.55356900	-0.11245600
H	3.30859100	-6.40861500	-2.35998300
H	4.61607500	-6.68199200	-1.21353000
H	4.99704500	-3.38391400	-3.98565800
H	3.05310500	-2.24732500	-2.91041500
C	-2.37764900	-5.31553900	-0.73728800
C	-2.30275300	-3.92238400	-1.37897500
C	-0.84825300	-3.45253600	-1.54627500
C	-0.10899700	-3.48774000	-0.18871300
C	-0.15493500	-4.90247300	0.42671300
C	-1.61694200	-5.35655800	0.59571800
H	-1.94844400	-6.06035500	-1.42448300
H	-3.42422900	-5.60251700	-0.58002900
H	-2.83879000	-3.20153200	-0.75006000

H	-0.33848800	-4.11224700	-2.26407700
H	-0.62676200	-2.79049500	0.48394300
H	0.36583900	-5.60854000	-0.23558100
H	0.35883000	-4.93157900	1.39463300
H	-2.11225400	-4.69641900	1.31995900
H	-1.63566700	-6.36859800	1.01846000
H	-2.79553500	-3.92633500	-2.35897900
H	-0.80307800	-2.44099900	-1.96126900

TS-S7

1 imaginary frequency

H = -4806.378658

G = -4806.488508

Esol = -4807.112077

Se	1.05058500	0.31388300	-2.23464600
I	-3.61806600	-1.02217400	-1.18051700
C	-4.29126800	-2.78681000	-0.12520100
C	-4.49766100	-3.94879700	-0.86595900
C	-4.48886000	-2.71799800	1.25069700
C	-4.95508000	-5.08523200	-0.19372100
H	-4.31068400	-3.97923700	-1.93417200
C	-4.93488300	-3.87203400	1.90169400
H	-4.27984900	-1.80593400	1.79954400
C	-5.17280800	-5.04668900	1.18500300
H	-5.12911700	-6.00051000	-0.75235100
H	-5.09450500	-3.84472900	2.97587700
H	-5.52228100	-5.93574400	1.70203600
N	-1.66977800	-0.46695400	-0.34228800
S	-1.82680800	0.41545700	1.06226900

O	-2.95919600	0.02562400	1.93142900
O	-0.45798600	0.38216500	1.62315300
C	-2.13953200	2.13743100	0.60147700
C	-3.19785500	2.82453800	1.19919600
C	-1.30043000	2.75453000	-0.33399700
C	-3.42914400	4.15657800	0.85905500
H	-3.82618700	2.31498400	1.92093300
C	-1.52937200	4.08424400	-0.67642700
H	-0.48882800	2.19499900	-0.79852600
C	-2.58960300	4.76287900	-0.07278500
H	-4.23876400	4.72457700	1.30019500
H	-0.90590700	4.59601500	-1.39916900
N	-2.83335500	6.16994900	-0.43520300
O	-2.07580200	6.68774600	-1.25449400
O	-3.78034600	6.74262300	0.10362700
O	2.89838000	-0.12667200	-1.66742500
P	3.13177100	-0.38196300	-0.12743100
C	7.58512000	-1.52094900	-1.20617600
C	6.68796900	-2.61076600	-0.60697200
C	5.19797800	-2.23610400	-0.68368400
C	4.91740100	-0.87001100	-0.01321700
C	5.83425800	0.22546000	-0.61245800
C	7.31846700	-0.16911900	-0.53285400
H	7.38531300	-1.43634400	-2.28410400
H	8.64179700	-1.79732700	-1.10232100
H	6.96650000	-2.77276900	0.44509200
H	4.88160900	-2.18936500	-1.73347000
H	5.12998100	-0.95895200	1.06295200
H	5.54929600	0.38854100	-1.65905800
H	5.68525200	1.17739200	-0.09348300

H	7.62525000	-0.22124900	0.52251800
H	7.92665400	0.61790700	-0.99585800
H	6.84680600	-3.56645800	-1.12192300
H	4.60588100	-3.02313700	-0.20756400
C	0.95424700	-4.32948100	1.39082900
C	0.59815000	-3.74070700	0.01791800
C	1.70927600	-2.82101200	-0.51530000
C	1.99564200	-1.69891600	0.51157800
C	2.39339000	-2.28507500	1.88619300
C	1.28588200	-3.22269300	2.40174100
H	1.82236900	-4.99845300	1.28682000
H	0.12875500	-4.94662400	1.76847100
H	-0.33136000	-3.16045400	0.09183900
H	2.61184100	-3.41676200	-0.70021700
H	1.05860500	-1.14244000	0.64357000
H	3.33678200	-2.84432600	1.80312900
H	2.55543700	-1.49188500	2.62357600
H	0.38717800	-2.62232400	2.59708500
H	1.59356700	-3.65811600	3.36134300
H	0.41505400	-4.54628200	-0.70509700
H	1.40165000	-2.37553200	-1.46546000
C	3.31002600	3.76251500	2.21215800
C	3.15095500	2.46348500	3.01466900
C	3.59960000	1.23442200	2.20354700
C	2.81834300	1.15729500	0.86948600
C	3.02144400	2.45309400	0.04576800
C	2.57851600	3.67730900	0.86475900
H	4.37981400	3.94903500	2.03358500
H	2.93810200	4.61413900	2.79565100
H	2.09748900	2.33427700	3.29932000

H	4.67718300	1.31217200	2.00225900
H	1.74870700	1.08128600	1.10653100
H	4.07868400	2.56761400	-0.22608500
H	2.45326800	2.39110900	-0.88691000
H	1.49512600	3.61835100	1.04037900
H	3.72688900	2.51590100	3.94753300
H	3.45541600	0.33162600	2.80670800
H	2.75171500	4.58919100	0.27936600

TS-S8

1 imaginary frequency

H = -5846.002595

G = -5846.135111

Esol = -5846.855843

Se	-0.63089600	0.95064100	0.11014400
N	0.13045600	1.70440500	1.50200800
S	0.42868600	0.72223300	2.83859100
O	0.21433000	-0.72511100	2.60676600
O	-0.16293200	1.33891200	4.03479400
C	2.21922200	0.96871700	2.96050000
C	3.07400000	0.21010400	2.15550600
C	2.71312900	1.94380900	3.82904900
C	4.44291100	0.45612300	2.19061300
H	2.66758600	-0.54960400	1.49753500
C	4.08388000	2.19079100	3.87623800
H	2.02149100	2.49897700	4.45305000
C	4.92361600	1.45415400	3.04122500
H	5.13528200	-0.10235800	1.57324100
H	4.50435600	2.94442500	4.53071800

N	6.36202400	1.75517500	3.03567300
O	6.79290900	2.52934800	3.88727700
O	7.05440900	1.22293500	2.16233000
I	2.25921900	1.83315600	-1.86959100
C	4.34458400	1.36054000	-2.14416900
C	4.73215000	0.66563100	-3.28791800
C	5.23531600	1.72706400	-1.13668300
C	6.08653000	0.35312700	-3.42943200
H	4.00479200	0.35258900	-4.02757800
C	6.58392300	1.39847600	-1.29688700
H	4.89926800	2.24237800	-0.24423800
C	7.00522100	0.71827600	-2.44179300
H	6.41714900	-0.18703500	-4.31185900
H	7.28752800	1.65886300	-0.51228700
H	8.05395400	0.46152500	-2.55961800
N	1.46864700	0.07803500	-1.03494500
S	0.98168400	-1.02184600	-2.23503600
O	-0.45403800	-0.88797200	-2.55353000
O	1.92852600	-1.05126800	-3.36819400
C	1.21260300	-2.52958100	-1.27092400
C	0.63127000	-2.66771900	-0.00584000
C	1.96096100	-3.55378900	-1.85651500
C	0.81119000	-3.86158600	0.68966400
H	0.08243600	-1.85325900	0.45522200
C	2.12313600	-4.75409700	-1.16886000
H	2.40564900	-3.40553500	-2.83391900
C	1.54459500	-4.88563100	0.09211700
H	0.39705500	-3.99560400	1.68114900
H	2.68764800	-5.57741000	-1.58837300
N	1.72251200	-6.15551700	0.82171100

O	2.39508100	-7.03234500	0.28070000
O	1.18603000	-6.25904900	1.92260500
O	-2.85383700	1.33036900	0.57716600
P	-4.00848100	0.46642300	0.02474400
C	-7.17169200	3.51122500	1.73508500
C	-6.95230700	2.18471200	2.47335000
C	-5.65138500	1.49650500	2.02935300
C	-5.61235300	1.27590500	0.49596600
C	-5.84443700	2.61334900	-0.24459100
C	-7.14223500	3.29948100	0.21627000
H	-6.38069700	4.22000900	2.01936900
H	-8.12419800	3.96407600	2.03750900
H	-7.80435900	1.51547800	2.28108400
H	-4.78859200	2.11024400	2.31555500
H	-6.41356200	0.57669400	0.21446300
H	-4.98980100	3.27673100	-0.05869000
H	-5.89192500	2.44870200	-1.32590400
H	-8.00248900	2.68111100	-0.08088500
H	-7.25143400	4.25727600	-0.30791600
H	-6.92280600	2.34920800	3.55756400
H	-5.54434000	0.54406400	2.55917700
C	-4.44780800	-3.54425600	2.57924900
C	-3.09345700	-2.82525400	2.50523200
C	-3.23998900	-1.36113800	2.06048200
C	-3.98492500	-1.27435200	0.70719400
C	-5.36343000	-1.97119200	0.80131200
C	-5.20738000	-3.43560300	1.24932800
H	-5.05440700	-3.09409600	3.37908900
H	-4.30843400	-4.59856500	2.84902900
H	-2.44131100	-3.35334400	1.79319800

H	-3.79493400	-0.80442600	2.82682800
H	-3.38260100	-1.82808800	-0.02996300
H	-5.99143300	-1.44330600	1.53123600
H	-5.89801200	-1.93584300	-0.15503900
H	-4.66491500	-3.99312900	0.47170200
H	-6.19831800	-3.89995300	1.33275000
H	-2.58391100	-2.85802800	3.47526700
H	-2.25455600	-0.89649800	1.99070500
C	-4.21611200	0.67196800	-4.73671100
C	-4.72623900	-0.59357500	-4.03294400
C	-5.04845000	-0.33747900	-2.54893300
C	-3.82992500	0.26811200	-1.81786600
C	-3.34128600	1.55713400	-2.52138900
C	-3.01194200	1.27221600	-3.99633400
H	-5.02650400	1.41543700	-4.77915000
H	-3.94925700	0.44132400	-5.77568200
H	-3.95944300	-1.37825500	-4.09911200
H	-5.90349900	0.34967400	-2.47707100
H	-3.00191400	-0.45487500	-1.89039000
H	-4.11427700	2.33369100	-2.46929000
H	-2.46219300	1.95158300	-2.00331600
H	-2.16268900	0.57787100	-4.04414500
H	-5.61914200	-0.98180900	-4.53939100
H	-5.35943700	-1.27850700	-2.08138300
H	-2.69223800	2.20178400	-4.48497700

TS-S9

1 imaginary frequency

H = -5760.199046

G = -5760.326222

Esol = -5761.067230

Se	0.15549900	-2.02791000	-0.77619200
N	0.18795000	-2.47065300	0.91881700
N	1.83987400	-1.60083000	-1.34032100
S	1.52875800	-2.83998800	1.78948600
O	2.49673100	-3.67982500	1.05113400
O	1.03642200	-3.32320000	3.08525400
S	1.77384900	-0.80582700	-2.84546500
O	0.42868800	-0.99377900	-3.43461900
O	2.95636500	-1.22730700	-3.60285000
C	0.07582900	-4.02828400	-1.79285200
C	1.36038900	-4.55328000	-1.51561900
C	2.51705000	-4.10441000	-2.18811600
H	1.49232800	-5.08699100	-0.57776800
H	2.37419700	-3.81361800	-3.23296800
H	2.42243500	-2.91854100	-1.68172500
H	-0.77422800	-4.45686300	-1.26691500
H	-0.13657000	-3.66350900	-2.79700200
C	3.88622700	-4.67142100	-1.86212000
H	4.66920100	-3.97554200	-2.17765500
H	3.98866200	-4.84352900	-0.78761300
H	4.05184600	-5.61795800	-2.39121000
C	1.96945900	0.93943700	-2.45350700
C	1.05763000	1.55791900	-1.59576200
C	2.98889700	1.64650500	-3.09268000
C	1.15989000	2.93066800	-1.39393100
H	0.27703500	0.99935300	-1.08621900
C	3.09388900	3.02048600	-2.88221600
H	3.68176700	1.12603500	-3.74388400

C	2.17097500	3.63775900	-2.04206600
H	0.47099100	3.45609700	-0.74483100
H	3.86717900	3.61036400	-3.35822900
N	2.25858100	5.09663000	-1.83576700
O	3.17588200	5.69581300	-2.39234600
O	1.40279300	5.62247300	-1.12532800
C	2.36336500	-1.26672500	2.08373500
C	3.65393200	-1.30990100	2.62044000
C	1.71929300	-0.05601300	1.82626200
C	4.30920600	-0.12164700	2.92462400
H	4.14161700	-2.26395700	2.78949800
C	2.37047700	1.13601300	2.13791000
H	0.71945000	-0.03707700	1.40482800
C	3.65180700	1.08391800	2.68039900
H	5.30881600	-0.11330400	3.34080700
H	1.90425300	2.09697200	1.96042500
N	4.33912700	2.34611100	3.00211800
O	3.74100300	3.39703700	2.77228500
O	5.47015600	2.27496300	3.48130000
P	-2.75445000	0.54178300	0.44596900
C	-2.49911300	5.22881100	1.22472100
C	-2.07576300	4.25521300	2.33152500
C	-1.84061800	2.83904500	1.78245500
C	-3.08645400	2.29228000	1.04101300
C	-3.49796700	3.27931600	-0.07654300
C	-3.72579300	4.69859700	0.47247600
H	-1.66597000	5.36328900	0.51946800
H	-2.71147100	6.21867000	1.64680400
H	-2.85577400	4.21994300	3.10664200
H	-0.99878100	2.85188900	1.07895800

H	-3.91891100	2.22363200	1.75790500
H	-2.70748000	3.31303900	-0.84035700
H	-4.41002200	2.94237100	-0.58079400
H	-4.59143700	4.68404700	1.15133400
H	-3.98989800	5.36984500	-0.35428200
H	-1.16260100	4.61050700	2.82458000
H	-1.54266300	2.16979600	2.59459900
C	-2.96817300	-2.78445900	3.77444800
C	-3.77384600	-3.02175700	2.49228700
C	-3.34698300	-2.07194400	1.35993100
C	-3.40767300	-0.58355600	1.78108500
C	-2.64706900	-0.35445100	3.11061400
C	-3.09648800	-1.32278300	4.21702300
H	-1.91097100	-3.02307900	3.59639000
H	-3.31743500	-3.45422000	4.57026600
H	-4.84481400	-2.87819500	2.70228200
H	-2.32209700	-2.31164100	1.05538700
H	-4.46219700	-0.30152400	1.92889200
H	-1.57345800	-0.48915600	2.93065800
H	-2.79180800	0.67533400	3.45594200
H	-4.14259100	-1.11033700	4.48551700
H	-2.49826300	-1.13929600	5.11798200
H	-3.65896600	-4.05866000	2.15204700
H	-3.99485300	-2.24240400	0.49322000
C	-5.51334100	-0.96856900	-3.14075700
C	-3.99075200	-0.89448200	-3.33003700
C	-3.24978700	-0.88103000	-1.98296100
C	-3.75677000	0.28668800	-1.10359600
C	-5.28365000	0.19395000	-0.88864500
C	-6.02438300	0.16359900	-2.23736900

H	-5.77524100	-1.93674100	-2.68847300
H	-6.01997300	-0.93230200	-4.11311100
H	-3.73524800	0.01612300	-3.89090400
H	-3.42243000	-1.83733900	-1.47323700
H	-3.55803100	1.20389600	-1.67633900
H	-5.52203400	-0.71970100	-0.32771600
H	-5.64919100	1.03378300	-0.28387400
H	-5.88199600	1.12803800	-2.74652200
H	-7.10283900	0.05794400	-2.06520400
H	-3.64049500	-1.73905800	-3.93636400
H	-2.17157400	-0.79817600	-2.14289800
O	-1.26807700	0.33073100	0.16409100

TS1

1 imaginary frequency

H = -1740.781874

G = -1740.868435

Esol = -1741.135578

C	4.77388000	1.45538700	-0.28760600
O	3.83361500	1.26762900	0.66518400
O	4.67474800	1.09211300	-1.43893600
C	5.96350700	2.18640600	0.30171900
H	6.29592200	1.69882000	1.22224100
H	6.76969000	2.20600200	-0.43282300
H	5.66621500	3.20892900	0.55611300
I	2.01600800	0.50238700	0.01371300
O	-0.94809700	2.37647000	-0.23318400
C	-0.02930300	3.23248000	0.00355700
O	1.20817700	3.00687400	0.04301900

C	-0.50212800	4.66023100	0.26030900
H	-1.13286400	4.99619700	-0.56947900
H	-1.11985900	4.68118500	1.16546000
H	0.34499300	5.33740800	0.38295700
C	2.73599800	-1.52631100	0.02561300
C	2.32849500	-2.37191300	1.05851100
C	3.57474900	-1.96347400	-1.00183100
C	2.77615200	-3.69481200	1.05654700
H	1.65846100	-2.01949800	1.83562900
C	4.02108900	-3.28590100	-0.98218700
H	3.89031600	-1.28282500	-1.78466800
C	3.62159500	-4.14815000	0.04227000
H	2.46055800	-4.36728100	1.84882100
H	4.67927100	-3.64063200	-1.77031300
H	3.96872500	-5.17759300	0.04796000
N	-0.41412400	-0.12611700	-0.72029000
S	-1.26850100	-1.21302200	0.27029600
O	-1.08569300	-2.55138200	-0.29486000
O	-0.85395000	-0.90380700	1.63950500
C	-3.00507800	-0.76739500	0.08155200
C	-3.90014700	-1.78723600	-0.25118400
C	-3.42759800	0.54545200	0.31919500
C	-5.25874100	-1.49353900	-0.34534800
H	-3.53217900	-2.79077100	-0.43215500
C	-4.78563800	0.83785300	0.21571500
H	-2.71456300	1.33623400	0.53636400
C	-5.67495500	-0.18570500	-0.10841600
H	-5.98847600	-2.25253100	-0.59794900
H	-5.15911700	1.84078800	0.38028000
N	-7.11402900	0.12877200	-0.21235500

O	-7.45846200	1.28855400	0.00339200
O	-7.87529600	-0.79027900	-0.50818700
H	-0.67031500	0.93846400	-0.54888400
H	-0.50372200	-0.39926900	-1.70054100

TS10

1 imaginary frequency

H = -7139.583524

G = -7139.681706

Esol = -7139.949654

Se	-0.47221300	-1.11953500	-0.76816700
N	-0.79103700	0.37876200	0.20207200
N	-0.23380300	-2.14771400	0.68107100
S	-0.59834200	1.78750800	-0.69180300
O	-1.34570200	2.81301000	0.02518400
O	-0.78529100	1.54869500	-2.11937800
S	0.13972300	-3.67535400	0.23362100
O	-0.54105100	-4.07738700	-1.00464100
O	0.09740400	-4.50774100	1.42811200
C	-5.57207700	0.23000900	1.82391100
C	-4.06649200	0.11560400	1.85950900
C	-3.47964000	-0.05282000	0.45984300
C	-4.04565500	1.02838200	-0.47069100
C	-5.57729400	0.94567200	-0.51990000
C	-6.28640400	0.58130700	0.73815100
H	-3.64919400	1.03208500	2.30536700
H	-6.09351800	0.01663400	2.75653600
H	-3.76703100	-0.69551600	2.52911400
C	-7.78861100	0.65721700	0.70922100

H	-8.19485800	-0.01205900	-0.05734100
H	-8.21888300	0.38584100	1.67757700
H	-8.12247200	1.66666000	0.44399100
O	-6.18009100	1.22048700	-1.54330700
C	-3.22201200	-1.36480900	-0.04092800
C	-3.31479200	-2.57604300	0.83492300
C	-2.54609400	-1.51046100	-1.30230700
H	-4.28025900	-2.61471300	1.34951000
H	-2.51764600	-2.55414500	1.59320900
H	-3.67452300	0.98747500	-1.49573100
H	-3.77495700	2.01695600	-0.07892700
H	-3.17512900	-3.49328800	0.25972600
O	1.73411400	-3.59722500	-0.27237300
C	2.68921200	-3.26474000	0.73000200
H	3.26177000	-4.15689200	0.99853500
H	2.21521700	-2.85279100	1.62471600
C	3.66507700	-2.21488900	0.17865400
Cl	2.79706400	-0.68556200	-0.22846500
Cl	4.50008700	-2.82766300	-1.28261000
Cl	4.87308700	-1.88079100	1.47510000
O	1.00889300	2.09375800	-0.54686000
C	1.48354300	2.70115500	0.66423900
H	0.65158800	3.06906400	1.26722400
H	2.06378800	1.96057600	1.21877200
C	2.39451000	3.88783900	0.31511800
Cl	2.98754200	4.54326900	1.89082700
Cl	1.48131000	5.15293900	-0.56304800
Cl	3.78849100	3.34444500	-0.67294800
H	-2.20303800	0.22969500	0.50666400
H	-2.45583200	-2.51615300	-1.70614000

H	-2.67269900	-0.73914700	-2.05908800
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TS11

l imaginary frequency

H = -7139.583811

G = -7139.681453

Esol = -7139.950578

Se	-0.87354000	-0.06665400	0.55992500
N	-0.17664500	-0.18067700	-1.08433700
N	-1.91820500	-1.53432800	0.36695300
S	0.45237300	1.23700000	-1.56055200
O	-0.37378800	2.40901500	-1.24122600
O	1.01624500	1.08160500	-2.89266500
S	-3.04386700	-1.65722100	1.60743600
O	-2.50451600	-1.16572700	2.87361100
O	-3.62863800	-2.98315900	1.48728200
C	3.16530300	-3.09079600	-2.05599800
C	1.91494300	-3.08423900	-1.21716900
C	2.07865300	-2.18402300	0.01520900
C	3.39426700	-2.55114500	0.75388000
C	4.59926500	-2.42939400	-0.18310800
C	4.39827100	-2.77614800	-1.61240600
H	3.03796100	-3.37112300	-3.10082800
H	1.06822300	-2.73302200	-1.81740800
H	2.18756600	-1.15340100	-0.33903400
H	3.58112000	-1.91204200	1.62101400
H	1.68460900	-4.12103100	-0.92579200
H	3.34180200	-3.58954500	1.11331100
C	5.62130300	-2.75356000	-2.48904900

H	5.37692800	-3.03939900	-3.51613900
H	6.07017000	-1.75414400	-2.50060600
H	6.39057200	-3.43310200	-2.10515400
O	5.68782200	-2.08968400	0.25509400
C	0.95467100	-2.20363800	1.01243900
C	0.01938700	-3.25420400	1.12924500
H	1.44033100	-0.21363400	1.73275000
H	0.20110000	-4.18314200	0.59462100
H	-0.45049900	-3.39090500	2.10581200
C	0.67614100	-0.98896800	1.74023000
H	0.14526100	-1.08494800	2.68740800
H	-0.95917800	-2.63615300	0.56828600
O	-4.15436900	-0.52291300	1.19731400
C	-4.87315900	-0.72100700	-0.03116900
H	-4.34468700	-1.40923000	-0.69434200
H	-5.86824900	-1.10821600	0.19777700
C	-5.01084800	0.63195000	-0.74149300
Cl	-3.40086200	1.29718700	-1.16309100
Cl	-5.95569900	0.32248000	-2.24659000
Cl	-5.89761100	1.79610800	0.29769500
O	1.75447500	1.32374400	-0.46217200
C	2.53409100	2.51249300	-0.55832800
H	1.89120500	3.39783100	-0.53440100
H	3.13093500	2.50737300	-1.47607300
C	3.48830800	2.57353800	0.63867500
Cl	4.58786000	1.15373400	0.65608800
Cl	2.55344200	2.62389900	2.18287500
Cl	4.45179000	4.08391100	0.47768600

TS12

1 imaginary frequency

H = -5066.620240

G = -5066.724149

Esol = -5067.234696

Se	0.57744500	-1.21810300	-1.14426100
N	-0.74249200	-2.25397300	-1.67936000
N	0.14000100	-0.42137900	0.41929000
S	-1.57982600	-3.24471300	-0.64616800
O	-0.79084600	-3.55239800	0.56994100
O	-2.10107300	-4.34180300	-1.46388600
S	0.41673900	1.23745400	0.43564900
O	1.24528200	1.64137000	-0.71708600
O	0.84774800	1.59137200	1.79224600
C	-1.22597600	1.92863100	0.16761000
C	-2.04576700	1.40089600	-0.83316400
C	-1.60101500	3.04668900	0.91311400
C	-3.26241900	2.01598000	-1.10723400
H	-1.74956100	0.50986800	-1.37518100
C	-2.82020500	3.66476900	0.64111100
H	-0.94841400	3.42072200	1.69411100
C	-3.62415200	3.14154400	-0.36794600
H	-3.92845700	1.63964800	-1.87334900
H	-3.15131100	4.53573600	1.19280700
N	-4.90941700	3.80364900	-0.66807100
O	-5.60650500	3.31132600	-1.55276100
O	-5.19614900	4.80641300	-0.01820800
C	-3.02139800	-2.31565500	-0.08665400
C	-4.15328500	-2.28124800	-0.90642300
C	-3.00114900	-1.68383300	1.15773500

C	-5.28459700	-1.59170800	-0.47905500
H	-4.15035300	-2.80795100	-1.85433400
C	-4.13131500	-0.99453200	1.59064800
H	-2.11321700	-1.73714100	1.77532400
C	-5.25179400	-0.95992400	0.76355000
H	-6.18463900	-1.54647800	-1.07962200
H	-4.15914200	-0.49499100	2.55098500
N	-6.45244500	-0.23756700	1.22543600
O	-6.38133200	0.35231800	2.30279800
O	-7.44796600	-0.26975400	0.50528600
C	3.98823800	-1.55831500	0.70477900
C	3.93324900	-0.18915200	-0.03670000
C	5.33614000	0.40444300	-0.36837900
C	6.18205600	0.39723800	0.91393000
C	6.18718700	-0.88981200	1.71561900
C	4.76659000	-1.39620300	2.01755000
H	3.35154100	-0.27994400	-0.96021300
C	5.12261800	1.87603600	-0.86700000
C	6.88219000	1.45951500	1.33373700
H	6.72614700	-1.67903500	1.16892700
H	4.25873100	-0.66991900	2.66463600
C	6.97500700	2.77476700	0.61171000
C	6.43664200	2.67411500	-0.81806200
H	7.43541900	1.37948800	2.27036800
H	6.41444400	3.53822100	1.17448900
H	7.18720800	2.19796300	-1.46340700
H	4.80836800	-2.34782800	2.56214400
H	8.01746500	3.12237800	0.60833300
H	6.26950600	3.67683100	-1.23026900
H	4.43814800	2.34501800	-0.14509600

H	3.39556200	0.51733400	0.60470200
C	4.46544300	1.99331300	-2.25081800
H	4.26802800	3.04816600	-2.47245800
H	5.11353100	1.60969100	-3.04738000
H	3.50365600	1.47493800	-2.30267400
C	6.02739800	-0.46099600	-1.45108600
H	4.53766000	-2.26078900	0.06090300
C	2.60282100	-2.13207100	0.84094600
C	1.77686500	-1.93328800	1.97408400
H	0.98368400	-2.67033100	2.11984900
H	2.22731700	-1.55455400	2.88781300
C	1.97170800	-2.69100500	-0.32419100
H	2.60681700	-2.88111000	-1.18833700
H	6.95253700	0.00998700	-1.79719300
H	6.29993700	-1.45218500	-1.07467500
H	5.37651000	-0.60617900	-2.32048200
H	6.73473500	-0.73976900	2.65247000
H	1.22604900	-3.46016300	-0.12792300
H	1.03907700	-1.05300900	1.47373300

TS13

1 imaginary frequency

H = -5066.617721

G = -5066.723203

Esol = -5067.232005

Se	0.19196600	-1.38074700	2.01250800
N	0.47465400	0.33803800	2.41331300
N	0.30622100	-1.32167800	0.20288500
S	-0.94202500	1.03967100	2.88836800

O	-0.75998900	1.77105500	4.14509700
O	-2.04017800	0.03357400	2.80695600
S	-0.31938800	-2.71627300	-0.52974500
O	-0.33542900	-3.82941000	0.44600200
O	0.39986500	-2.89171500	-1.79806700
C	-2.02607900	-2.27967200	-0.91297000
C	-2.85071000	-1.72279700	0.06840700
C	-2.49827200	-2.58503800	-2.19083900
C	-4.18614200	-1.47589000	-0.23570500
H	-2.47271200	-1.45797400	1.04933400
C	-3.83519200	-2.33798100	-2.49476200
H	-1.82608100	-3.00302300	-2.93152400
C	-4.65399300	-1.79135300	-1.50999200
H	-4.85557800	-1.03981000	0.49507600
H	-4.24508700	-2.55899100	-3.47232000
N	-6.07171600	-1.53023400	-1.83192600
O	-6.45768400	-1.81504900	-2.96392700
O	-6.77415400	-1.04682400	-0.94728000
C	-1.27526500	2.28275700	1.62115800
C	-1.71010200	3.54694000	2.02132400
C	-1.15468400	1.94310800	0.27138200
C	-2.03677100	4.49411800	1.05263300
H	-1.77993900	3.78074000	3.07765000
C	-1.48092600	2.88476300	-0.69935500
H	-0.78877200	0.96245400	-0.01338800
C	-1.91754500	4.14473200	-0.29036700
H	-2.37545500	5.48719000	1.32048500
H	-1.39739400	2.66432000	-1.75623400
N	-2.25645200	5.14576300	-1.31837600
O	-2.13641900	4.81448300	-2.49726300

O	-2.63714100	6.25065600	-0.93524200
C	3.08953100	-1.66475000	0.18998000
C	3.50711100	-0.18205000	0.37170600
C	3.63103700	0.68523200	-0.92083300
C	4.32780700	-0.12538100	-2.01762000
C	3.76891400	-1.50755700	-2.26288700
C	3.76052800	-2.36948700	-0.99186400
H	2.80980300	0.31420700	1.04944800
C	4.48885100	1.94429000	-0.54846200
C	5.35710500	0.34065200	-2.73764000
H	2.73954400	-1.44843700	-2.64062100
H	4.79847100	-2.59960700	-0.70745300
C	5.94563500	1.71905200	-2.60777000
C	5.02925000	2.64659800	-1.80463800
H	5.80201800	-0.31102500	-3.49067300
H	6.93545200	1.65471400	-2.12746000
H	4.19213900	2.97535600	-2.43464300
H	3.26177200	-3.31943300	-1.20445100
H	6.13375300	2.13566900	-3.60684900
H	5.57023800	3.55520500	-1.51215300
H	5.36730500	1.56370200	-0.00357600
H	4.48909400	-0.20074400	0.86421300
C	3.77718300	2.94823800	0.37279800
H	3.32901300	2.47541600	1.25327300
H	4.49407500	3.69604200	0.73079700
H	2.98222800	3.48719000	-0.15444500
C	2.22240700	1.09747900	-1.41505500
C	2.85716400	-2.44363000	1.36983600
C	2.92900400	-3.94035400	1.33168300
H	2.11091800	-4.34181000	0.71572900

H	3.86920800	-4.27929400	0.88528700
H	2.82934600	-4.37082700	2.33077100
C	2.26274100	-1.83615000	2.52491500
H	2.13834100	-2.47765000	3.39511300
H	2.52765200	-0.81303000	2.77623200
H	1.62747100	0.23145700	-1.71630000
H	1.66379600	1.61151400	-0.62780000
H	2.29566800	1.76440500	-2.28018400
H	4.35316400	-2.01741900	-3.03676600
H	1.86492100	-1.56209200	-0.03165200

TS14

1 imaginary frequency

H = -4716.491952

G = -4716.584205

Esol = -4716.904424

Se	-1.94802500	-0.37554200	-1.08771200
N	-1.97747800	1.30346300	-1.59909800
N	-1.23379100	-0.48249000	0.57700500
S	-1.73297600	2.56371600	-0.54262000
O	-2.49742100	2.40175600	0.70948500
O	-1.89791300	3.78287600	-1.33560200
S	-0.58930200	-2.04598900	0.83488600
O	-1.27353300	-3.00763700	-0.05411200
O	-0.57735000	-2.25394000	2.28362400
C	1.11225600	-1.88233800	0.27097500
C	2.13124700	-1.81283400	1.22126200
C	1.37840600	-1.86526200	-1.10080600
C	3.45411300	-1.71883100	0.79009900

H	1.88790400	-1.84067100	2.27740500
C	2.69721300	-1.76755000	-1.53233100
H	0.56999900	-1.92783000	-1.82140500
C	3.71047000	-1.69433400	-0.57752300
H	4.27858900	-1.66424000	1.49024900
H	2.95216600	-1.75196400	-2.58466000
N	5.11146900	-1.59758700	-1.03862100
O	5.29826300	-1.47708000	-2.24782800
O	5.99209100	-1.65317800	-0.18658200
C	0.00978200	2.41711800	-0.09372300
C	0.94527600	2.08031800	-1.07448500
C	0.39066100	2.66423500	1.22506000
C	2.28667900	1.96177900	-0.72586100
H	0.62310400	1.90128100	-2.09476500
C	1.73370000	2.56008300	1.57811400
H	-0.36283900	2.90845600	1.96506400
C	2.65516200	2.19536000	0.59875100
H	3.04173300	1.68799500	-1.45212100
H	2.07032700	2.73598000	2.59232100
N	4.06584800	2.02018900	0.98244400
O	4.39708900	2.36295800	2.11566900
O	4.82567800	1.52590100	0.14834200
C	-4.09430400	-1.25693000	0.75615900
C	-4.38513800	-0.77159900	-0.53373600
H	-3.99471300	-2.34121900	0.83808800
C	-4.72141100	-1.78929400	-1.60742200
H	-4.17408900	-2.72626700	-1.46744500
H	-5.79646700	-2.01416100	-1.58536000
H	-4.50035400	-1.40124300	-2.60736800
C	-4.91101300	0.62273400	-0.76897000

H	-6.00909900	0.58141300	-0.75001700
H	-4.57750600	1.34243700	-0.02109700
H	-4.61480700	1.00250100	-1.75143400
C	-3.62318000	-0.51818200	1.86722300
H	-3.80174500	0.55936400	1.85087300
C	-3.59387600	-1.14672100	3.25005600
H	-3.32689400	-2.20676300	3.20672500
H	-2.86323900	-0.64417300	3.88958100
H	-4.57683400	-1.05574500	3.72908700
H	-2.38976300	-0.48511600	1.42912200

TS15

1 imaginary frequency

H = -4716.496995

G = -4716.588575

Esol = -4716.909762

Se	-1.95534600	-0.50719200	-0.74458000
N	-2.15571000	1.13429700	-1.35089700
N	-1.16655900	-0.48517300	0.90109200
S	-1.81291900	2.45405000	-0.40865300
O	-2.37580400	2.34704900	0.95090700
O	-2.13660500	3.62220100	-1.23062600
S	-0.48101000	-2.01076100	1.23366500
O	-1.17359700	-3.03955100	0.42891400
O	-0.42428100	-2.12133200	2.69124000
C	1.19810400	-1.87032500	0.60233800
C	2.24505800	-1.67837600	1.50386100
C	1.41937400	-1.98741900	-0.77265400
C	3.55030500	-1.60006300	1.01911200

H	2.03750100	-1.60441100	2.56549300
C	2.72066000	-1.90745600	-1.25789200
H	0.58938900	-2.14646600	-1.45281000
C	3.76230600	-1.71388900	-0.35184100
H	4.39534100	-1.45715400	1.68129800
H	2.94170600	-1.99879200	-2.31401900
N	5.14618400	-1.64708000	-0.86789400
O	5.29508400	-1.69658200	-2.08680300
O	6.05193300	-1.55924400	-0.04506800
C	-0.01878300	2.38256600	-0.20346600
C	0.53213900	2.79766400	1.00945900
C	0.78458100	1.93172500	-1.25307400
C	1.91271700	2.75263700	1.18418000
H	-0.11970400	3.12334900	1.81201600
C	2.16410200	1.87343000	-1.08148000
H	0.33085000	1.62116100	-2.18813500
C	2.70288300	2.27758100	0.13946600
H	2.37856200	3.05777600	2.11303000
H	2.82131200	1.51821000	-1.86538400
N	4.15742300	2.17116900	0.34156800
O	4.81221600	1.59504600	-0.52832000
O	4.62840500	2.65115000	1.37064000
C	-4.00065400	-1.15435600	-0.05630300
C	-4.19721500	-0.28492400	1.07173400
H	-3.67653200	-2.16591700	0.19741100
C	-3.47514500	-0.55311600	2.25329800
H	-3.62702900	0.10869500	3.10349800
H	-3.30257000	-1.59714600	2.52022500
C	-5.01793200	0.95830000	0.91885800
H	-4.79879300	1.48481500	-0.01347500

H	-6.07933800	0.66849300	0.88743100
H	-4.86599000	1.64705800	1.74976500
C	-4.86735200	-1.05939300	-1.30258900
H	-5.91934000	-1.14558500	-0.99621800
C	-4.54719000	-2.14594700	-2.33595900
H	-5.16469800	-2.02354400	-3.23057400
H	-3.49671800	-2.10606700	-2.64610000
H	-4.73265800	-3.14651000	-1.92950500
H	-4.76248500	-0.06467300	-1.75306700
H	-2.26007100	-0.33558700	1.77818700

TS16

1 imaginary frequency

H = -4716.511222

G = -4716.604277

Esol = -4716.928633

Se	-2.03729300	-0.48369500	-0.70654700
N	-1.12211200	0.86374500	-1.62665100
N	-1.13911000	-0.56816200	0.85159400
S	-1.00595100	2.49601000	-1.22707200
O	-2.03574100	2.73528600	-0.21339200
O	-0.98102600	3.24736500	-2.48074800
S	-0.84441800	-2.13553700	1.31212200
O	-1.87218400	-3.04518400	0.75844800
O	-0.57825600	-2.11696200	2.75444100
C	0.70871500	-2.56002400	0.49059700
C	1.89968300	-2.51673800	1.21693000
C	0.69328800	-2.90950800	-0.86404600
C	3.10203000	-2.81697800	0.57903700

H	1.87455900	-2.26464000	2.27133700
C	1.89083500	-3.20735000	-1.50603100
H	-0.24722700	-2.96349100	-1.40140300
C	3.07616300	-3.15200300	-0.77264200
H	4.04658400	-2.79879100	1.10862500
H	1.92248000	-3.48933300	-2.55120500
N	4.34592500	-3.46542000	-1.45338600
O	4.29553600	-3.74215300	-2.65119100
O	5.37597600	-3.42737200	-0.78324000
C	0.61370500	2.70377200	-0.46203700
C	1.44605400	3.70777000	-0.96264300
C	0.98040800	1.91041600	0.62801700
C	2.67913700	3.93120800	-0.35364500
H	1.12937700	4.29954300	-1.81379700
C	2.21339900	2.13406300	1.23494200
H	0.32332600	1.12047700	0.98528900
C	3.03830600	3.13988800	0.73415000
H	3.35625000	4.69868100	-0.70719100
H	2.54127000	1.54372800	2.08147700
N	4.34639800	3.37363700	1.38014400
O	5.05110300	4.27192100	0.92515200
O	4.64534100	2.65458800	2.33106900
C	-4.14059800	0.53971400	0.39167600
C	-3.97038200	-0.16966500	1.60632500
H	-3.71835100	1.53878700	0.33970900
C	-2.93688100	0.23844700	2.41265300
H	-2.42987600	1.17973300	2.23506900
C	-4.71330000	-1.46025200	1.86357200
H	-4.49522500	-1.84281400	2.86383400
H	-5.79777300	-1.32745500	1.77628100

H	-4.40718800	-2.23250900	1.14686100
C	-5.20849500	0.21966400	-0.61626300
H	-5.29641300	-0.86522200	-0.75412300
C	-5.03449200	0.92628200	-1.96460600
H	-4.99046800	2.01340300	-1.83951400
H	-4.10625300	0.61567400	-2.45717500
H	-6.16590000	0.53322400	-0.16580200
H	-2.65784100	-0.30683000	3.30846700
H	-5.86681400	0.69307700	-2.63568900
H	-0.38981100	0.53408000	-2.25139400

TS17

1 imaginary frequency

H = -4716.504083

G = -4716.597767

Esol = -4716.921516

Se	-0.44342900	-1.83139200	0.60349400
N	0.32479200	-0.55640100	1.73557700
N	-0.44987100	-0.97945000	-0.97684800
S	1.92383300	-0.39605000	2.18960000
O	2.57564600	-1.66728400	1.86655500
O	1.93333700	0.13659500	3.55110000
S	-1.94231300	-1.04459800	-1.70949700
O	-2.62120600	-2.32007800	-1.38482100
O	-1.73882100	-0.66027500	-3.10911100
C	-2.90658700	0.26388700	-0.92202900
C	-3.00648000	1.50533900	-1.55160500
C	-3.51784000	0.01858000	0.31215600
C	-3.72240200	2.52899000	-0.93402700

H	-2.53787300	1.65534300	-2.51791600
C	-4.23001700	1.03927000	0.93460800
H	-3.44701600	-0.96260700	0.76869600
C	-4.31663200	2.27868700	0.30070900
H	-3.82725300	3.50520700	-1.39101600
H	-4.72442400	0.89029000	1.88659200
N	-5.07088400	3.36096600	0.96015900
O	-5.57791500	3.11577500	2.05373300
O	-5.14284900	4.44128100	0.37754300
C	2.59817900	0.88856100	1.12081200
C	3.62332100	1.68240800	1.64408200
C	2.13376100	1.04993800	-0.18643600
C	4.21276100	2.65038800	0.83592200
H	3.94376000	1.55142100	2.67173700
C	2.72104400	2.02250400	-0.99350300
H	1.31117000	0.45065100	-0.56870500
C	3.75119800	2.80019900	-0.47014600
H	5.00878400	3.28713900	1.20113400
H	2.38762500	2.18640600	-2.01077900
N	4.37227600	3.82886600	-1.32861600
O	5.27652700	4.50399900	-0.84122100
O	3.94635500	3.94277000	-2.47601500
C	1.16477300	-3.64789300	-0.24248600
C	1.65683900	-2.96775000	-1.38612000
H	1.83840600	-3.71531600	0.60970500
C	3.05512100	-2.38635500	-1.35961100
H	3.32402400	-2.03018200	-0.36220900
C	0.80472800	-2.70793800	-2.42693200
H	1.11277700	-2.09513000	-3.26777700
H	-0.16409000	-3.18194600	-2.52265200

C	0.03343200	-4.65287000	-0.26432200
H	-0.87713800	-4.21431300	-0.69620100
C	-0.27547400	-5.25132600	1.11212300
H	0.60040300	-5.75955300	1.53037800
H	-0.58036600	-4.47526200	1.82342800
H	0.32566600	-5.45521300	-0.95812000
H	3.78963300	-3.15130300	-1.64320300
H	-1.08954800	-5.97902000	1.04283400
H	-0.29811000	0.16122500	2.09804500
H	3.15471000	-1.55799500	-2.06761300

TS18

1 imaginary frequency

H = -4716.517158

G = -4716.610484

Esol = -4716.934168

Se	1.11268100	-1.37416300	-0.83232100
N	-0.50947200	-0.93442500	0.11552000
N	2.24937100	-1.19360900	0.55055300
S	-1.17616800	0.60260200	-0.24841900
O	-0.91603400	0.82842900	-1.67053800
O	-0.80653000	1.58963000	0.77130400
S	3.53137600	-0.15541500	0.23463100
O	4.14565400	-0.46445900	-1.06919800
O	4.35232700	-0.15748700	1.45403700
C	2.79917800	1.48799700	0.10050300
C	2.67057400	2.25977900	1.25694500
C	2.36744900	1.95381800	-1.14340300
C	2.09090600	3.52187800	1.17283700

H	3.03524800	1.87645500	2.20321700
C	1.77957100	3.21237500	-1.23024100
H	2.49497000	1.34275400	-2.02895900
C	1.65016300	3.97178900	-0.06969600
H	1.97355100	4.15355400	2.04421500
H	1.42298400	3.60722200	-2.17291900
N	1.02646600	5.30391500	-0.15968400
O	0.65299000	5.68645100	-1.26755200
O	0.91816300	5.95488900	0.87896400
C	-2.93346600	0.25998900	-0.04682000
C	-3.57681900	0.67521200	1.11976300
C	-3.61931900	-0.39316000	-1.07438000
C	-4.93741900	0.41495500	1.27386000
H	-3.02137700	1.20630300	1.88476500
C	-4.97736100	-0.65432400	-0.92386700
H	-3.09803800	-0.67758100	-1.98176400
C	-5.60943600	-0.24956200	0.25148000
H	-5.47758500	0.72037600	2.16128600
H	-5.54973500	-1.15552900	-1.69438900
N	-7.04962900	-0.53288100	0.41540900
O	-7.61943200	-1.12166400	-0.50105800
O	-7.58506800	-0.16547100	1.45888200
C	2.46314000	-3.99162100	0.08601400
C	1.10792300	-4.15527100	-0.14591400
H	3.14158900	-4.24068000	-0.72927600
C	0.63690900	-4.78998500	-1.42687600
H	1.42303100	-4.81697900	-2.18617500
H	0.31012200	-5.82259900	-1.23590200
H	-0.22819700	-4.25595000	-1.83416900
C	0.05467400	-4.00735900	0.91772100

H	-0.23703500	-5.00772000	1.26982900
H	0.38982200	-3.43818100	1.78660700
H	-0.84679100	-3.53232800	0.51971500
C	3.01444600	-3.31400600	1.17649600
H	2.40227600	-3.11605100	2.04796700
C	4.49196600	-3.24814300	1.38882100
H	5.04182100	-3.28212000	0.44386400
H	4.78250600	-2.34917300	1.93331700
H	4.78892500	-4.12259600	1.98933000
H	-0.25474800	-0.95234800	1.10818800

TS19

1 imaginary frequency

H = -4871.293841

G = -4871.391755

Esol = -4871.779306

Se	-1.39008600	-0.21324200	-1.51478800
N	-1.22392300	1.53200500	-1.56616100
N	-1.03842700	-0.87116200	0.14548700
S	-0.87325000	2.53165200	-0.28177700
O	-1.50948400	2.09901700	0.97082300
O	-1.09815500	3.88636500	-0.79176900
S	-0.33832100	-2.42387600	0.05825600
O	-0.61353300	-3.03691000	-1.25550500
O	-0.72822600	-3.11844500	1.28790700
C	1.43285400	-2.10442500	0.12305200
C	2.17182700	-2.67592600	1.15851900
C	2.04277300	-1.38727700	-0.90962500
C	3.55943800	-2.53432500	1.15897800

H	1.66513800	-3.22773400	1.94219900
C	3.42584100	-1.24926400	-0.91374400
H	1.44779100	-0.93158300	-1.69382400
C	4.15965400	-1.82743300	0.12175200
H	4.17423700	-2.96462100	1.93975900
H	3.94021800	-0.70617200	-1.69647100
N	5.63099200	-1.69059200	0.10914400
O	6.26090300	-2.27923500	0.98294900
O	6.12472600	-1.00485600	-0.78295500
C	0.90420200	2.36159400	-0.02982200
C	1.36798900	1.66593200	1.08775700
C	1.78326700	2.97291500	-0.92910900
C	2.74028100	1.56127700	1.30325300
H	0.65616500	1.22355900	1.77458800
C	3.15483000	2.87429000	-0.71593300
H	1.39357400	3.53417400	-1.77153400
C	3.60816600	2.16170400	0.39445800
H	3.14213100	1.02863500	2.15606100
H	3.87058600	3.33887300	-1.38293300
N	5.06076200	2.03768500	0.61518900
O	5.43526300	1.26523800	1.49808900
O	5.80444600	2.70849100	-0.09554500
C	-4.02276800	0.03552700	1.51201400
C	-3.62904300	-1.26700500	0.88963900
C	-3.86745700	-1.48973600	-0.49261800
C	-3.89676800	-0.37883800	-1.35920000
C	-4.30708200	0.99604900	-0.90856400
C	-4.39846800	1.18622000	0.60280900
H	-4.02156400	-0.58747900	-2.42124700
H	-3.60077600	1.73102800	-1.32170500

H	-5.26828900	1.22409600	-1.39541200
H	-4.04902400	2.15941300	0.93058100
C	-3.82231900	-2.87831300	-1.06676700
H	-3.25195800	-2.90830400	-2.00055600
H	-3.37740900	-3.59322100	-0.37033200
H	-4.84473500	-3.21339200	-1.28891300
H	-3.67983700	-2.14857700	1.53315200
C	-5.46926800	0.55185400	1.46701600
H	-3.45967400	0.28719300	2.40661000
C	-6.59404600	-0.26806300	0.86264600
H	-6.28049300	-0.87942700	0.01208500
H	-7.02942700	-0.94023500	1.61257500
H	-7.39658000	0.39273800	0.51051800
C	-5.90834900	1.35121300	2.68537200
H	-6.71270300	2.05042600	2.42272600
H	-6.28652800	0.68964800	3.47515000
H	-5.08183500	1.93588000	3.10278100
H	-2.32759800	-1.12979400	0.71440000

TS2

1 imaginary frequency

H = -1511.666421

G = -1511.741358

Esol = -1511.948730

C	0.56860300	3.50430900	0.55962400
O	1.68066300	3.15136000	0.08325200
O	-0.32512600	2.70513600	1.00738300
C	0.23952700	4.98706800	0.58732600
H	1.15136200	5.58661300	0.55551800

H	-0.36525500	5.22675300	-0.29547400
H	-0.35098600	5.22844600	1.47501300
I	2.44540700	0.69907200	0.07274600
C	2.89960900	-1.38733400	0.31597100
C	3.31139800	-1.82019300	1.57791500
C	2.83707700	-2.25789400	-0.77253400
C	3.67794100	-3.15689300	1.74904400
H	3.34757400	-1.13440000	2.41857900
C	3.20423200	-3.59206700	-0.58539800
H	2.48366200	-1.91484500	-1.73760800
C	3.62478900	-4.03993000	0.66909900
H	3.99885000	-3.50450900	2.72685300
H	3.15647600	-4.28091800	-1.42393800
H	3.90932100	-5.07942100	0.80556300
N	0.36214600	0.39671300	0.21501400
S	-0.37463400	0.18933800	-1.32151000
O	-0.45671600	1.43922600	-2.08231700
O	0.19261500	-1.00372200	-1.96527000
H	0.01266700	1.43197500	0.64745800
C	-2.00786500	-0.20575500	-0.67645500
C	-2.78304400	0.81226700	-0.11114700
C	-2.47380500	-1.51579600	-0.80115500
C	-4.06181700	0.50374300	0.34545500
H	-2.38394100	1.81592800	-0.00560800
C	-3.75683500	-1.82082200	-0.35330400
H	-1.84037900	-2.27299200	-1.24908300
C	-4.52479300	-0.80467800	0.21214600
H	-4.69796800	1.25449200	0.79709500
H	-4.16568800	-2.82014400	-0.43421300
N	-5.88323800	-1.12894100	0.69168800

O	-6.26579100	-2.29099800	0.56903100
O	-6.54446900	-0.21696800	1.18317700

TS20

l imaginary frequency

H = -4871.289063

G = -4871.385552

Esol = -4871.774786

Se	1.30521900	0.57405500	-1.08948500
N	0.92055700	-0.27581500	0.43570500
N	1.30424700	2.33815400	-0.70510300
S	0.62909000	-1.87872000	0.11494500
O	1.09178900	-2.67424100	1.25454800
O	1.09502900	-2.20971800	-1.25803000
S	0.50521000	3.02688200	0.65253300
O	0.58420500	4.46354600	0.38595200
O	1.01737600	2.48024500	1.91154600
C	-1.20379700	2.50983500	0.46778600
C	-2.00671900	3.15165400	-0.47924500
C	-1.70742200	1.53550700	1.33005400
C	-3.34828200	2.79575300	-0.57998300
H	-1.59045600	3.92929400	-1.11030200
C	-3.05032900	1.17831100	1.22989500
H	-1.05315900	1.07319300	2.05889200
C	-3.84175100	1.81042200	0.27462300
H	-4.01115500	3.26777700	-1.29440600
H	-3.48514000	0.42486900	1.87429300
N	-5.26289800	1.42267000	0.16360900
O	-5.96718300	2.06564000	-0.61043400

O	-5.64741400	0.47853300	0.85158300
C	-1.16910300	-2.03722800	0.04861800
C	-1.86059000	-1.45533100	-1.01823100
C	-1.82816900	-2.78851700	1.02078500
C	-3.23370900	-1.64134800	-1.12565100
H	-1.32927900	-0.86678900	-1.75932400
C	-3.20818700	-2.96961500	0.92338200
H	-1.26002900	-3.23426100	1.82965600
C	-3.88452700	-2.39687400	-0.14975700
H	-3.80467500	-1.22056200	-1.94399100
H	-3.75833200	-3.55010400	1.65361900
N	-5.34085700	-2.60599100	-0.26960400
O	-5.88770700	-3.29112400	0.59129500
O	-5.90920100	-2.08857200	-1.22837600
C	4.26879900	-1.09008300	0.99534200
C	4.04816000	0.41057700	1.09870000
C	3.99812400	1.17023400	-0.19788700
C	3.65748300	0.48423500	-1.39526100
C	3.99965500	-0.97185900	-1.62343200
C	4.23329700	-1.78093200	-0.35550500
H	3.63687200	1.09718700	-2.29826600
H	3.20863100	-1.45039600	-2.20893900
H	4.89268300	-0.97960900	-2.26797300
H	3.73955700	-2.74789500	-0.36950300
C	3.92313600	2.57814100	-0.19874600
H	4.15482000	3.11216500	0.72119500
H	4.19094700	3.10793700	-1.11440300
H	4.78151700	0.88391000	1.76387100
C	5.53193200	-1.71155100	0.43414500
H	3.79126300	-1.63728300	1.80397400

C	6.67897800	-0.83703200	-0.04545000
H	7.28578100	-1.36738600	-0.79071000
H	6.35058400	0.10316200	-0.50003600
H	7.34197900	-0.58008600	0.79039400
C	6.00090900	-3.00553800	1.08253200
H	6.59226800	-3.60677100	0.37977200
H	6.63085600	-2.80137900	1.95807500
H	5.15470700	-3.61632600	1.41499000
H	3.06553200	0.57035400	1.57465500
H	2.59815600	2.62040500	-0.37987800

TS21

1 imaginary frequency

H = -4871.292077

G = -4871.388875

Esol = -4871.778497

Se	-1.42312700	0.50410700	-1.27846600
N	-0.66506300	2.08236700	-1.39921600
N	-0.99290100	-0.29737000	0.28771700
S	-0.25622100	3.03084700	-0.09810300
O	-1.08944900	2.73837900	1.08538000
O	-0.17592800	4.39975300	-0.61256100
S	-0.79166100	-1.97090100	0.10585100
O	-1.46525600	-2.44531600	-1.11864600
O	-1.11367500	-2.58204300	1.39811400
C	0.98850900	-2.14231500	-0.14931100
C	1.62418900	-3.21168200	0.48435200
C	1.67706500	-1.29062100	-1.01712600
C	2.97454000	-3.44626400	0.23323300

H	1.06834100	-3.84412800	1.16732400
C	3.02534500	-1.52182000	-1.26884500
H	1.18046400	-0.44241800	-1.47322800
C	3.64800700	-2.60041600	-0.64341300
H	3.50511800	-4.26537700	0.70242800
H	3.59507400	-0.88374000	-1.93261000
N	5.07620100	-2.85371300	-0.92135100
O	5.59826100	-3.81877900	-0.36845400
O	5.64701700	-2.08537300	-1.69225500
C	1.42549200	2.54870600	0.33582400
C	1.63923000	1.67897100	1.40683300
C	2.48881400	3.08201500	-0.39861200
C	2.94311600	1.32421500	1.74550000
H	0.79377100	1.29414500	1.96412900
C	3.79299300	2.72906500	-0.06458300
H	2.29248900	3.77865700	-1.20620600
C	3.99560000	1.85362900	1.00196600
H	3.15375900	0.65647200	2.57154900
H	4.64564900	3.12379400	-0.60300400
N	5.37689900	1.48184000	1.36317500
O	5.52717200	0.67432900	2.27903400
O	6.29094500	2.00080000	0.72573200
C	-4.52282400	-1.49226600	-0.05634400
C	-4.37917900	-0.49833500	-1.20763900
C	-3.53755900	1.19762100	0.48637900
C	-4.01866000	-1.12492300	1.32515300
H	-3.24360900	2.21773800	0.71354000
H	-3.25651800	0.59200000	2.50635500
H	-3.54299200	-1.91827700	1.89400200
C	-4.03521800	1.96708300	-1.86666200

H	-3.88461700	1.61374200	-2.89267300
H	-5.07840000	2.30061500	-1.78946500
H	-3.38708700	2.83161900	-1.69865300
H	-3.78365400	-0.96698800	-2.00105800
C	-5.51814900	-1.29843800	1.07403500
H	-4.35038000	-2.52059500	-0.36250100
C	-6.47637000	-0.12101300	1.08616700
H	-7.33107000	-0.31499300	0.42544200
H	-6.87364800	0.03696600	2.09625200
H	-6.01814000	0.81881000	0.76545200
C	-6.13026200	-2.56546700	1.65434800
H	-6.43264300	-2.41288600	2.69798500
H	-7.02291000	-2.86179100	1.08863900
H	-5.42472200	-3.40277300	1.62853400
H	-5.36165300	-0.30602200	-1.66633400
H	-2.12983800	-0.03367600	1.14275800
C	-3.36425400	0.21349900	1.48785100
C	-3.78692600	0.86283600	-0.86207600

TS3

1 imaginary frequency

H = -4731.155909

G = -4731.263889

Esol = -4731.884115

Se	1.40343400	-0.28199300	-1.58346800
I	-2.65659100	-2.77784300	-0.46785200
C	-4.65727600	-1.99942100	-0.60031500
C	-5.28822700	-1.60683600	0.57974800
C	-5.26813500	-1.88891000	-1.84882800

C	-6.59096700	-1.10873000	0.49719000
H	-4.77206700	-1.67121500	1.53135000
C	-6.57390600	-1.39560200	-1.90720400
H	-4.74800600	-2.18000800	-2.75505800
C	-7.23317500	-1.00744500	-0.73885100
H	-7.10075500	-0.79904100	1.40512700
H	-7.06889000	-1.30963500	-2.87037400
H	-8.24622500	-0.61944800	-0.79301500
N	-1.04277600	-1.20685700	-0.07538100
S	-1.36570300	-0.32800900	1.30495600
O	-2.31623800	-0.95983000	2.24494300
O	-0.04769700	0.09919000	1.82461400
C	-2.18419500	1.19469400	0.75558500
C	-3.21996700	1.72408100	1.52891000
C	-1.74926700	1.83427400	-0.41004400
C	-3.83528400	2.91100300	1.13628500
H	-3.53776500	1.20246100	2.42475000
C	-2.36006800	3.02008000	-0.80777500
H	-0.94715300	1.39564500	-0.99695600
C	-3.39431600	3.53879400	-0.02709000
H	-4.64206200	3.35138500	1.70896100
H	-2.05425500	3.54203300	-1.70605700
N	-4.04706500	4.78838900	-0.44950300
O	-3.63839000	5.32810200	-1.47733000
O	-4.96403700	5.21977100	0.24974400
P	2.96092700	0.05300000	-0.11780000
C	6.50265900	-0.23734700	-3.26426600
C	6.26934000	-1.41269700	-2.30645200
C	4.87944300	-1.34112200	-1.65244900
C	4.66035700	0.00170700	-0.91807200

C	4.90311700	1.18365300	-1.88136400
C	6.28911100	1.10061900	-2.54518700
H	5.80124500	-0.31271300	-4.10769700
H	7.51327000	-0.28442000	-3.68938000
H	7.04431400	-1.40560400	-1.52523400
H	4.10110300	-1.44687800	-2.41861000
H	5.37782000	0.07390200	-0.08773200
H	4.11979500	1.17877300	-2.65070500
H	4.81843100	2.13601500	-1.34853900
H	7.06690200	1.22712500	-1.77710800
H	6.40587800	1.93660400	-3.24648700
H	6.37180400	-2.36713900	-2.83829500
H	4.75262800	-2.18412600	-0.96474800
C	3.47816100	-3.72421000	2.81314600
C	2.14165200	-3.48192000	2.09748900
C	2.29973200	-2.56923600	0.86960100
C	2.95189400	-1.23020400	1.27402300
C	4.32196600	-1.48700100	1.94400900
C	4.15914900	-2.39757600	3.17574600
H	4.14385500	-4.30258100	2.15486600
H	3.32699600	-4.33058000	3.71541100
H	1.43029700	-3.01765800	2.79532100
H	2.91932200	-3.07442000	0.11546600
H	2.28214100	-0.76414700	2.00849800
H	4.99780300	-1.97696800	1.23063400
H	4.80999000	-0.55451000	2.24581400
H	3.55822800	-1.87299400	3.93251600
H	5.14277200	-2.58094800	3.62748500
H	1.69798300	-4.43734300	1.78870500
H	1.32705900	-2.38068800	0.40989400

C	3.01796400	4.53936600	1.59374500
C	3.52235900	3.39458300	2.48226400
C	3.89632300	2.14488900	1.66153900
C	2.71304800	1.69260700	0.77743200
C	2.24323000	2.84597300	-0.13477900
C	1.85613000	4.07520600	0.70400300
H	3.84182900	4.89622100	0.95748400
H	2.71070600	5.39109200	2.21370200
H	2.73815700	3.12274300	3.20318400
H	4.76838400	2.37392200	1.03254000
H	1.86644300	1.44108300	1.43093700
H	3.04007200	3.12968900	-0.83387400
H	1.39816300	2.51219600	-0.74290800
H	0.98991500	3.82458500	1.33291300
H	1.53667700	4.88769900	0.03902600
H	4.39080900	3.71804600	3.07055600
H	4.20095800	1.35018400	2.34959800

TS4

1 imaginary frequency

H = -5770.742226

G = -5770.873088

Esol = -5771.590943

Se	-1.22198800	-0.28370600	-0.68808600
N	-1.28729100	-1.94501400	0.07012900
S	-1.46976700	-3.20621800	-0.96636800
O	-1.68301500	-2.83456900	-2.38475600
O	-2.39773900	-4.17823000	-0.35249200
C	0.15472200	-4.00600900	-0.90359600

C	1.09105100	-3.73991500	-1.90639400
C	0.46067900	-4.85826100	0.16229800
C	2.36137200	-4.30419900	-1.83035300
H	0.81241300	-3.10588600	-2.74110000
C	1.72397500	-5.43640400	0.24097700
H	-0.29543000	-5.07079000	0.90990000
C	2.66055300	-5.13745300	-0.75104900
H	3.11130400	-4.11945000	-2.58958400
H	1.99481800	-6.10559300	1.04850800
N	4.00513200	-5.71732000	-0.65373900
O	4.19996000	-6.58409300	0.19586700
O	4.87078900	-5.29262600	-1.42682800
I	2.45049300	0.19542300	2.47282000
C	4.04551600	-0.30140000	1.12914100
C	4.07434500	-1.57397400	0.56002100
C	5.01551700	0.66211400	0.85249900
C	5.12669200	-1.89400300	-0.30248500
H	3.30183700	-2.30275500	0.77849200
C	6.05771400	0.32425700	-0.01405500
H	4.96753300	1.65029900	1.29634600
C	6.11408000	-0.94802500	-0.58695700
H	5.17015400	-2.88387400	-0.74817700
H	6.82374000	1.06115400	-0.23813600
H	6.92879100	-1.20394900	-1.25792200
N	0.67825400	0.79440300	1.04428200
S	0.58083100	2.46132800	1.03599000
O	-0.65981800	2.75926900	0.27516900
O	0.74811800	3.10196700	2.35433900
C	1.93321100	3.09324600	0.00840000
C	2.17461300	2.51077100	-1.24008300

C	2.69801200	4.16831100	0.46586000
C	3.19273500	3.00992600	-2.04593800
H	1.57911000	1.66426100	-1.56599900
C	3.72184100	4.67300400	-0.33507100
H	2.48587600	4.59601000	1.43949700
C	3.95035000	4.08438200	-1.57725300
H	3.41171200	2.58406700	-3.01717400
H	4.33634600	5.50595600	-0.01630400
N	5.03716600	4.60885900	-2.42260500
O	5.70076000	5.54615200	-1.98131500
O	5.21638700	4.07487100	-3.51629100
P	-3.27262700	0.58376800	-0.04618900
C	-5.96682400	-3.10375900	-1.30473600
C	-5.86465500	-1.90453900	-2.25634800
C	-4.65500000	-1.01684900	-1.91591900
C	-4.69798300	-0.56221600	-0.43623500
C	-4.83287700	-1.76096500	0.53270400
C	-6.04405100	-2.63120800	0.15248500
H	-5.08402200	-3.74440200	-1.42693600
H	-6.84618800	-3.71082400	-1.55411500
H	-6.78910100	-1.30926800	-2.19882500
H	-3.73263200	-1.57505000	-2.10783600
H	-5.57956600	0.08301600	-0.29803400
H	-3.92669800	-2.37252000	0.50706500
H	-4.95571600	-1.40057800	1.55951800
H	-6.97252600	-2.05914000	0.30571600
H	-6.08726800	-3.49052700	0.83230600
H	-5.77267900	-2.24365600	-3.29522600
H	-4.63985600	-0.14583500	-2.58218400
C	-4.32339700	4.11904600	-3.09582000

C	-2.85718100	3.71581200	-2.89052400
C	-2.72248400	2.30988600	-2.28090000
C	-3.51542500	2.21367300	-0.95678600
C	-5.00000500	2.58560700	-1.18446000
C	-5.11655400	3.99727600	-1.78787700
H	-4.77837300	3.46837100	-3.85705100
H	-4.38607800	5.14377600	-3.48216400
H	-2.36638200	4.43791900	-2.22288500
H	-3.08726900	1.55898700	-2.99361300
H	-3.07092900	2.93900200	-0.26436800
H	-5.46032600	1.86664200	-1.87408200
H	-5.57137400	2.53859400	-0.25084000
H	-4.74198700	4.73251300	-1.06131100
H	-6.17503000	4.23236500	-1.95554400
H	-2.31398300	3.75015000	-3.84290200
H	-1.66573200	2.09875500	-2.09939300
C	-3.56777600	1.04218100	4.69890800
C	-4.21943200	2.09950900	3.79706300
C	-4.46733600	1.57069700	2.37085400
C	-3.15276900	1.02779900	1.76449300
C	-2.53174000	-0.06979100	2.65859100
C	-2.28025100	0.49281400	4.06809500
H	-4.27520900	0.21506400	4.85936700
H	-3.35847300	1.47108700	5.68678000
H	-3.56535400	2.98093000	3.73912600
H	-5.22198700	0.77309200	2.40384700
H	-2.42836400	1.85221000	1.71439500
H	-3.20447400	-0.93205200	2.72708300
H	-1.59731600	-0.43016500	2.22262000
H	-1.52777700	1.29220400	4.00709800

H	-1.85395100	-0.29583400	4.70070700
H	-5.16997200	2.44041900	4.22656400
H	-4.88154000	2.37909000	1.75785100

TS5

1 imaginary frequency

H = -5684.905309

G = -5685.031982

Esol = -5685.767228

Se	-0.17750700	-1.03006000	-1.74240900
N	-1.69665600	-0.79056300	-0.88733800
N	0.59452700	-2.54912700	-1.13013000
S	-2.17376500	-1.86827800	0.26091900
O	-1.32257400	-1.84232300	1.46757700
O	-2.48565800	-3.19242200	-0.32056600
S	2.26350200	-2.57464600	-1.35683600
O	2.67152800	-1.45461300	-2.22965800
O	2.63808400	-3.93966500	-1.73819300
C	-0.95927700	-2.03005700	-3.67369600
C	-1.38311100	-3.28048900	-3.18729500
C	-0.47950900	-4.31828800	-2.86106300
H	-2.39111300	-3.34716400	-2.78340900
H	0.43097700	-4.36315000	-3.46659300
H	0.01698100	-3.63980900	-1.87170300
H	-1.70969500	-1.28920100	-3.93692000
H	-0.02676800	-1.96696100	-4.23310000
C	-0.97391900	-5.65321900	-2.33675100
H	-1.29890700	-6.30214900	-3.15973400
H	-0.17213200	-6.17243000	-1.80351000

H	-1.81032600	-5.51283400	-1.64637800
C	2.88196100	-2.27972600	0.30852400
C	4.21465500	-2.61656600	0.56537900
C	2.05785200	-1.71987500	1.28619800
C	4.74251300	-2.37637200	1.83004800
H	4.82425800	-3.07508900	-0.20596800
C	2.58501600	-1.48781700	2.55562900
H	1.01753500	-1.50199000	1.07588600
C	3.91629800	-1.81279400	2.80206900
H	5.76811900	-2.62317600	2.07412600
H	1.97563600	-1.06907000	3.34650300
N	4.47393400	-1.55818400	4.14427300
O	3.73213400	-1.04686600	4.98093900
O	5.64745600	-1.86929500	4.34098400
C	-3.74060200	-1.09510900	0.70642500
C	-4.02563700	-0.92015200	2.06092300
C	-4.67528500	-0.77365600	-0.28173400
C	-5.26249400	-0.40013200	2.43918000
H	-3.27965800	-1.18325700	2.80234700
C	-5.90896000	-0.24927100	0.08863800
H	-4.43217400	-0.91771900	-1.32817200
C	-6.18079200	-0.07272300	1.44532400
H	-5.52028700	-0.24673200	3.47966600
H	-6.65706900	0.02060300	-0.64619700
N	-7.48846700	0.48301900	1.83989800
O	-8.28046100	0.76684900	0.94232800
O	-7.70640700	0.62932900	3.04123900
P	0.96137600	1.91652600	-0.44997600
C	-2.06966900	2.61376000	3.13128500
C	-2.34621200	3.33280200	1.80418400

C	-1.53953800	2.72308500	0.64426100
C	-0.02432400	2.71550200	0.94676000
C	0.23514900	1.96905300	2.27553700
C	-0.56676600	2.57923600	3.43783400
H	-2.44886200	1.58363900	3.06824700
H	-2.61539500	3.10013800	3.94984800
H	-2.08513200	4.39674900	1.90683400
H	-1.87522600	1.69433500	0.45926000
H	0.30631700	3.75732100	1.06631400
H	-0.05174400	0.91443500	2.15293100
H	1.30240700	1.98158100	2.52666600
H	-0.20954700	3.60271700	3.62535700
H	-0.37640000	2.01014500	4.35671900
H	-3.41739800	3.29729400	1.56725200
H	-1.74786200	3.28625600	-0.27234500
C	-0.55822700	4.83882900	-3.96247100
C	-0.40857700	3.33111600	-4.21041600
C	-0.36496300	2.54434600	-2.89034100
C	0.75677500	3.05669400	-1.95440200
C	0.58667300	4.57061800	-1.70408300
C	0.54127600	5.35881200	-3.02607900
H	-1.54160500	5.03478500	-3.50983800
H	-0.53843700	5.38495300	-4.91401900
H	0.51965500	3.14571400	-4.77098200
H	-1.33685000	2.63256200	-2.38551000
H	1.70368100	2.91724800	-2.49722700
H	-0.34504800	4.75202100	-1.15207700
H	1.39724400	4.95367000	-1.07623500
H	1.51591600	5.27541300	-3.52942700
H	0.38971600	6.42552200	-2.81629800

H	-1.23129400	2.96453100	-4.83824200
H	-0.22647000	1.47543200	-3.09565200
C	5.62845800	2.97349500	0.12216600
C	5.18700100	1.63098500	-0.47794600
C	3.74320500	1.68862800	-1.00712600
C	2.76185700	2.14808700	0.09407800
C	3.20020700	3.51747500	0.65339000
C	4.64118700	3.45835700	1.19345200
H	5.68728500	3.72484100	-0.67959500
H	6.63767200	2.89004900	0.54511800
H	5.25651400	0.84688300	0.29048200
H	3.70855100	2.39776700	-1.84716300
H	2.84863500	1.41806700	0.91373700
H	3.15386300	4.27159100	-0.14356600
H	2.52465000	3.85575300	1.44751800
H	4.67433600	2.77608300	2.05570300
H	4.93859000	4.44652600	1.56770000
H	5.86588500	1.33336500	-1.28732700
H	3.45027900	0.71189500	-1.40621300

TS6

1 imaginary frequency

H = -5684.933818

G = -5685.059823

Esol = -5685.800297

Se	0.18499200	-1.59502100	0.76449800
N	-0.04116600	-1.17785800	2.50331300
N	-0.94123600	-3.21968300	0.68131200
S	-1.56218800	-0.69250500	2.96773700

O	-2.61294900	-1.52459300	2.33783800
S	-1.35954200	-3.58364800	-0.89655700
C	2.17631500	-3.15550900	1.78113600
C	1.44961100	-3.40267600	2.91252300
C	1.19336300	-2.36080000	3.82721800
H	0.86892200	-4.31878100	2.99142600
H	1.87349100	-1.51394700	3.81262500
H	-1.76844500	-3.05428300	1.27129400
H	2.81260600	-2.27964100	1.70778300
C	0.49028100	-2.61681800	5.12319400
H	0.07818600	-1.70846600	5.55874300
H	-0.31337300	-3.35081400	5.01448600
H	1.23275600	-3.03360700	5.82150600
C	-1.78460500	0.98141300	2.32975600
C	-1.05978900	2.02149400	2.91854300
C	-2.71662200	1.22325300	1.32096500
C	-1.26572400	3.32635900	2.48538300
H	-0.35994500	1.81217500	3.72000700
C	-2.92131500	2.52816400	0.87327500
H	-3.28455000	0.39786900	0.90921100
C	-2.18849000	3.55493800	1.46435300
H	-0.73262500	4.16184700	2.92158900
H	-3.63221800	2.75062600	0.08591900
N	-2.39196200	4.93796100	0.99648600
O	-1.83533700	5.83889100	1.62192400
O	-3.10130200	5.10541700	0.00506500
C	-2.60934700	-2.36950000	-1.36715400
C	-2.20160500	-1.11331500	-1.82561600
C	-3.95909200	-2.67960400	-1.18644700
C	-3.16154300	-0.13815700	-2.08113800

H	-1.15095800	-0.90673800	-1.98954800
C	-4.92411600	-1.71152700	-1.45411900
H	-4.24557300	-3.66943400	-0.84821900
C	-4.50457000	-0.45253400	-1.87944700
H	-2.88739000	0.85027200	-2.42909200
H	-5.98094800	-1.91228700	-1.32920000
N	-5.51842300	0.59221800	-2.11481700
O	-6.69831600	0.25127600	-2.11670900
O	-5.11635000	1.74389400	-2.28510300
O	-0.14854000	-3.29174700	-1.68080100
O	-2.00010900	-4.89697200	-0.91820700
O	-1.53933200	-0.56223100	4.42855000
H	2.27983100	-3.89510400	0.99372600
P	2.48041500	0.51739000	-0.74147400
C	3.40844400	-3.23644700	-3.54556600
C	4.18148900	-3.07004100	-2.23189800
C	3.50184300	-2.04174800	-1.31454100
C	3.31968600	-0.66217600	-1.99167000
C	2.55090000	-0.84940400	-3.31818300
C	3.22891100	-1.88046500	-4.23871600
H	2.42093900	-3.66768400	-3.32979100
H	3.92617400	-3.93931600	-4.21049500
H	5.20979000	-2.74318100	-2.44843700
H	2.50922600	-2.41036800	-1.02552700
H	4.31176400	-0.25133500	-2.23417300
H	1.52809800	-1.19282400	-3.10334600
H	2.46542000	0.10087700	-3.85576300
H	4.21197000	-1.49495700	-4.54833900
H	2.63596600	-1.99396300	-5.15529000
H	4.26385200	-4.03288400	-1.71087900

H	4.07760100	-1.93849800	-0.38715600
C	5.70092900	2.43494900	2.17948500
C	4.67563200	3.36450600	1.51834100
C	3.49701700	2.57705400	0.92094500
C	3.96162400	1.49358700	-0.07693700
C	4.99819500	0.56923100	0.59770400
C	6.17614500	1.35882600	1.19483700
H	5.24104400	1.95002300	3.05357500
H	6.55478400	3.01221600	2.55586300
H	5.16851700	3.93853900	0.71992100
H	2.93268700	2.09467200	1.73285400
H	4.45729300	1.98895900	-0.92462700
H	4.50586800	-0.00291600	1.39924100
H	5.38432100	-0.16313500	-0.11954500
H	6.73851600	1.83676000	0.37926200
H	6.87116900	0.66696500	1.68781700
H	4.30023700	4.09900100	2.24236700
H	2.80533200	3.27459500	0.43655100
C	0.40844700	4.28976600	-2.88523100
C	-0.44424300	3.27704000	-2.10690000
C	0.40765500	2.45568800	-1.12265900
C	1.57005600	1.75095500	-1.85607000
C	2.43072700	2.76772200	-2.63235800
C	1.57648400	3.60081400	-3.60492400
H	0.80479900	5.04008000	-2.18515100
H	-0.21404000	4.83532600	-3.60498300
H	-0.92594600	2.59195600	-2.82252400
H	0.79676900	3.12330500	-0.34216200
H	1.09357800	1.09494200	-2.59769700
H	2.92569600	3.44789500	-1.92588700

H	3.23064700	2.25631200	-3.18288600
H	1.17974700	2.94192500	-4.39163100
H	2.20618100	4.34431400	-4.11044600
H	-1.25491000	3.79174100	-1.57791900
H	-0.20989900	1.70907900	-0.60774400

TS7

1 imaginary frequency

H = -4637.884798

G = -4637.970799

Esol = -4638.238405

Se	-2.10791500	-0.81061500	-1.25005900
N	-2.29683200	0.80698600	-1.89048200
N	-1.39506500	-0.75837500	0.41154300
S	-2.30007000	2.15303900	-0.92327500
O	-3.12869800	1.96812200	0.28726400
O	-2.57234700	3.28437400	-1.80945400
S	-0.63912100	-2.23775600	0.78849800
O	-1.17295900	-3.29740500	-0.09127500
O	-0.71022200	-2.37499000	2.24379400
C	-4.17752300	-1.47139200	-0.61449600
C	-4.39076500	-0.67784600	0.53447800
C	-3.75871400	-0.95880100	1.76898300
H	-4.81347100	0.31316200	0.38892600
H	-3.59844700	-2.02075300	1.98204900
H	-2.59822400	-0.70325200	1.30955900
H	-4.72597700	-1.22581800	-1.52092600
H	-3.93298500	-2.52568400	-0.49016000
C	-4.00829900	-0.09078300	2.98923600

H	-4.07529000	0.96390400	2.70831100
H	-4.93945900	-0.38196000	3.48988900
H	-3.19456800	-0.20691800	3.71099200
C	1.07372600	-1.93934800	0.32611300
C	2.00916900	-1.67904300	1.32756500
C	1.42660000	-1.97107500	-1.02556200
C	3.33550800	-1.44030900	0.96944200
H	1.70018100	-1.67116400	2.36679300
C	2.74879300	-1.73013500	-1.38491900
H	0.68340700	-2.18978600	-1.78531500
C	3.67765100	-1.46540700	-0.37930700
H	4.09742900	-1.23357400	1.71074300
H	3.07021100	-1.74632300	-2.41893100
N	5.08170500	-1.20922500	-0.76280800
O	5.90466300	-1.10414800	0.14077000
O	5.33013300	-1.12613500	-1.96419400
C	-0.59400900	2.27753500	-0.34643800
C	-0.34829900	2.75481000	0.94121900
C	0.44779200	1.90087300	-1.19677400
C	0.96460900	2.84462600	1.39686800
H	-1.17824400	3.02471100	1.58434100
C	1.76066700	1.97823200	-0.74425600
H	0.22910700	1.53919700	-2.19555400
C	1.99450400	2.43872700	0.55074600
H	1.19763200	3.20005400	2.39298800
H	2.59536700	1.68239000	-1.36723400
N	3.37865500	2.46720300	1.05262700
O	4.24689000	1.93663000	0.35843300
O	3.58151500	3.00456200	2.13946500

TS8

1 imaginary frequency

H = -4637.907863

G = -4637.994147

Esol = -4638.266052

Se	-1.70519400	-0.14985700	-1.03589200
N	-2.04952800	-1.56278800	0.00488700
N	-2.33006600	1.25176600	0.14164200
S	-1.06059100	-1.72368300	1.33853100
O	-0.93275200	-0.43530000	2.05755300
S	-1.91367300	2.79571700	-0.37550000
C	-4.25106500	-0.57716200	-1.83989600
C	-4.62000300	-0.93468100	-0.57019800
C	-4.13290600	-2.12896700	0.00026100
H	-5.06004700	-0.18911000	0.08762500
H	-3.83422200	-2.92074300	-0.68076500
H	-1.98020500	1.03614900	1.08624000
H	-3.86231600	-1.31644600	-2.53424800
C	-4.52378800	-2.55806800	1.37892800
H	-3.79311000	-3.23657700	1.81860700
H	-4.66214700	-1.70217500	2.04619600
H	-5.48622700	-3.08739500	1.30650300
C	0.57762800	-2.10730700	0.68285400
C	0.88660000	-3.43798400	0.39416900
C	1.49968700	-1.08037100	0.46948600
C	2.13812400	-3.74832600	-0.13118300
H	0.16051300	-4.21814900	0.59399100
C	2.75440900	-1.38450100	-0.05326800
H	1.24458500	-0.06196000	0.73650000

C	3.04569800	-2.71440300	-0.35258500
H	2.41937400	-4.76707800	-0.36694200
H	3.50001700	-0.61694100	-0.22560200
N	4.36903700	-3.04308800	-0.91802100
O	4.60819100	-4.22666100	-1.15198800
O	5.14532900	-2.11293900	-1.12351000
C	-0.13121100	2.91593100	-0.12432600
C	0.72897300	2.50354000	-1.14603700
C	0.35319100	3.34152600	1.11514200
C	2.10171400	2.48441500	-0.91219000
H	0.32897800	2.21902200	-2.11264900
C	1.72643100	3.33784400	1.34794400
H	-0.33665800	3.67927600	1.88105700
C	2.57265500	2.89068300	0.33498500
H	2.80341300	2.16616900	-1.67339600
H	2.14404300	3.66220500	2.29306800
N	4.02471800	2.83660300	0.59397200
O	4.43982300	3.37446600	1.61684100
O	4.72296100	2.24596700	-0.22954800
O	-2.15786900	2.78041300	-1.82207100
O	-2.55268100	3.74968300	0.52641100
O	-1.52193300	-2.91224800	2.06224200
H	-4.48566400	0.39882000	-2.25368500

TS9

1 imaginary frequency

H = -5914.134507

G = -5914.272416

Esol = -5915.069847

Se	0.24874300	0.76576200	0.93666400
N	2.23078400	-0.85035300	2.31729900
N	-0.79923500	-0.74286600	0.72336400
S	3.62738000	0.00411900	1.94163100
O	4.70602800	-0.19035000	2.92352000
O	3.24905400	1.39345200	1.61337100
S	-1.82683800	-1.17440100	1.97320400
O	-2.21999200	0.01709500	2.74510300
O	-1.29437800	-2.34567900	2.68185100
C	0.63156900	1.06700500	4.63484600
C	1.75637000	0.38614300	4.41349200
C	1.79907000	-0.97035100	3.74863300
H	2.71765200	0.80386600	4.71212400
H	0.77632000	-1.34870600	3.65868300
H	-0.23484400	-1.66729500	0.21102300
H	0.65030300	2.03988600	5.12081600
H	-0.34489500	0.67747600	4.35747200
C	2.62168500	-1.99782600	4.53999700
H	2.62301500	-2.96041500	4.01721700
H	3.65524600	-1.66777100	4.67114500
H	2.16970300	-2.14512100	5.52734300
C	-3.28497000	-1.74323600	1.07238100
C	-4.52806300	-1.20983000	1.41570600
C	-3.15497400	-2.73898700	0.09706100
C	-5.67206300	-1.67080800	0.76652700
H	-4.59047000	-0.44755900	2.18429400
C	-4.29596100	-3.19543000	-0.55663700
H	-2.17515300	-3.13159600	-0.16182800
C	-5.53433700	-2.65299200	-0.21085700
H	-6.65577000	-1.28548700	1.00442800

H	-4.24182800	-3.96041900	-1.32131400
C	4.11964800	-0.78613700	0.39712800
C	3.24750300	-0.75958100	-0.69328300
C	5.39567600	-1.33963500	0.31017100
C	3.66169500	-1.30431800	-1.90265200
H	2.25658800	-0.33823200	-0.57030300
C	5.81714500	-1.88081800	-0.90340400
H	6.04098400	-1.34252200	1.18162600
C	4.94228200	-1.85044100	-1.98656600
H	3.01520600	-1.31977500	-2.77085300
H	6.79987000	-2.32046300	-1.01933400
N	-6.74091300	-3.13185600	-0.90949900
N	5.38511100	-2.41666700	-3.27406900
O	-7.82012400	-2.63505600	-0.58952100
O	4.60126400	-2.35904600	-4.22144900
O	-6.59458000	-3.99513600	-1.77339400
O	6.51084200	-2.90830900	-3.32524400
O	0.11351900	-2.71033200	-0.49536500
C	1.04623500	-3.48842000	-0.03505400
O	1.85394900	-3.20524700	0.86404400
C	1.10380400	-4.86122600	-0.69083500
H	2.01926900	-5.38392300	-0.40799200
H	0.24077500	-5.45421000	-0.36528100
H	1.04166500	-4.76753400	-1.77962600
H	2.14696000	-1.74721700	1.78877700
P	-0.58059400	2.13927000	-0.70691600
C	-1.50089700	-1.17771300	-3.95987400
C	-0.22211800	-0.34233500	-4.09956200
C	0.14097100	0.34282200	-2.77073400
C	-1.02727400	1.22381400	-2.26955600

C	-2.32282100	0.38863600	-2.13351800
C	-2.66519100	-0.31220500	-3.45965100
H	-1.31710200	-1.99241300	-3.24592100
H	-1.75849300	-1.64208100	-4.91923300
H	-0.35711700	0.41853900	-4.88254600
H	0.35192900	-0.43087900	-2.02332900
H	-1.20218700	2.02507900	-3.00408500
H	-2.17819800	-0.36069800	-1.35057900
H	-3.16240700	1.01954700	-1.82284000
H	-2.91661700	0.44188400	-4.22052300
H	-3.56433500	-0.92339200	-3.31625500
H	0.61594800	-0.97377700	-4.41828100
H	1.05226500	0.93906300	-2.89819000
C	2.73050800	5.52617700	-1.16422300
C	2.19859000	4.84277200	-2.43227000
C	0.84343600	4.15507700	-2.18355700
C	0.95851400	3.15179000	-1.01680400
C	1.45596300	3.85407300	0.27114500
C	2.80460500	4.54670500	0.01527300
H	2.06787200	6.36421700	-0.90148100
H	3.71844200	5.96036900	-1.35907300
H	2.92321300	4.09073800	-2.77548100
H	0.09377300	4.91984600	-1.93975000
H	1.70873200	2.39568000	-1.28345000
H	0.71881700	4.60389100	0.59097000
H	1.57273900	3.13594200	1.08816600
H	3.56345200	3.77676300	-0.17537700
H	3.11767900	5.06781400	0.92727000
H	2.09277000	5.56989700	-3.24660300
H	0.50697800	3.65703900	-3.10108600

C	-4.68027100	4.34383000	0.30256500
C	-3.76023300	4.96068900	-0.76052900
C	-2.75852100	3.93146900	-1.31762700
C	-1.94790500	3.29640200	-0.16444300
C	-2.86901700	2.65910100	0.89692600
C	-3.86971200	3.69387100	1.43311400
H	-5.31991000	3.58400300	-0.16983800
H	-5.35274600	5.11001500	0.70672400
H	-3.20512200	5.80209000	-0.32101600
H	-3.31170400	3.15217400	-1.85572000
H	-1.38725000	4.10124600	0.33310000
H	-3.41946200	1.82020500	0.44996400
H	-2.26988400	2.23460300	1.70605900
H	-3.32373300	4.47259400	1.98568600
H	-4.53695600	3.21106500	2.15671900
H	-4.35027800	5.37413800	-1.58759400
H	-2.09925800	4.41390000	-2.04799200