Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.
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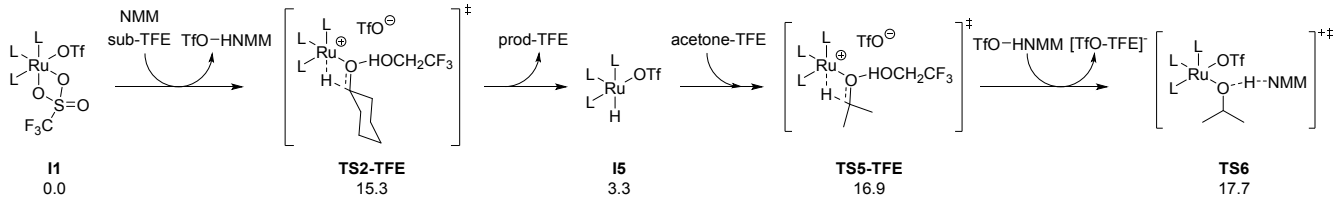
The effect of TFE using explicit solvent model



Scheme S1. The key intermediates and transition states with explicit TFE molecular. Energies are in kcal mol^{-1}.

Cartesian coordinates of optimized structures, total electronic energies and thermal corrections to Gibbs free energy

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I1, total electronic energy = -3754.5509995, thermal corrections to Gibbs free energy = 0.581916

C	3.50991500	-0.09297600	1.31191500
H	3.77842200	0.91169000	0.98173000
H	2.83318100	0.04291800	2.15733000
C	4.76861600	-0.83816100	1.77472200
H	4.54085400	-1.83778900	2.15647600
H	5.23524600	-0.27690700	2.59288100
H	5.51208900	-0.93963700	0.98067500
C	3.30258300	-0.28134500	-1.64569200
H	3.00400300	-0.99739800	-2.41726600
H	2.81432500	0.66201200	-1.89982500
C	4.82465100	-0.08591600	-1.67089100
H	5.15445200	0.65318200	-0.93616400
H	5.11995500	0.28475000	-2.65966100
H	5.37265500	-1.01292500	-1.49037000
C	2.78233000	-2.67858900	0.06732500
H	2.79734200	-2.90539300	1.13787100
H	1.88964000	-3.16174000	-0.32805200
C	4.01893300	-3.28045400	-0.61154900
H	4.02011900	-3.09948200	-1.69053400
H	4.01635200	-4.36663900	-0.46265100
H	4.95412600	-2.89445600	-0.20058300
C	0.84269700	-1.55606900	3.19769900
H	1.81880300	-1.89246700	2.83957600
H	0.95927600	-0.50360500	3.47640600
C	0.44197100	-2.39162900	4.42075700
H	-0.51823300	-2.08160100	4.84212000
H	1.19845300	-2.27480800	5.20527700
H	0.37997200	-3.45768300	4.18221100
C	-0.43831500	-3.44095000	1.37544900
H	-0.45295700	-3.55263000	0.29085200
H	0.51028100	-3.87206400	1.71279500
C	-1.61077000	-4.22551100	1.97703100
H	-1.61439900	-4.19882000	3.06998600
H	-1.53451000	-5.27593900	1.67318500
H	-2.57686500	-3.85110700	1.62542700
C	-1.94100700	-1.15568800	2.53746500
H	-2.69367700	-1.10409500	1.74908100
H	-2.21842400	-1.98377900	3.19600700
C	-1.91942300	0.15471000	3.33484600

H	-1.24504000	0.09539600	4.19446900
H	-2.92239900	0.36535500	3.72043300
H	-1.61396000	0.99802000	2.71318300
C	0.38572600	-2.79030100	-2.49894100
H	1.40296000	-2.44800000	-2.70763300
H	0.46642000	-3.54432500	-1.71016800
C	-0.21199800	-3.43895700	-3.75455500
H	-1.20493400	-3.85715300	-3.56634200
H	0.43364200	-4.26273900	-4.08005600
H	-0.29117200	-2.73530000	-4.58814900
C	-2.24270600	-2.09365500	-1.45628800
H	-2.06701200	-3.15332200	-1.23933900
H	-2.60479800	-1.63645800	-0.53586700
C	-3.31828200	-1.95245800	-2.54154900
H	-3.56379000	-0.90398300	-2.72637300
H	-4.23395400	-2.45398300	-2.20744900
H	-3.02153100	-2.40961000	-3.48939500
C	-0.79403200	-0.23309700	-3.24250800
H	-1.40621300	-0.78693100	-3.96095500
H	-1.39885500	0.60738800	-2.89327600
C	0.47944300	0.26663800	-3.93237600
H	1.07826000	0.89274500	-3.26896000
H	0.20482000	0.87437700	-4.80259600
H	1.10669000	-0.55486600	-4.29355600
C	-4.49466300	0.89854100	0.30215400
C	2.58658200	3.47251900	0.12675700
O	-1.87746000	0.78875300	0.20331900
O	-3.09957700	1.66714300	-1.80259600
O	-2.98711400	3.03287300	0.29885200
O	0.90352500	1.73668600	1.35546300
O	0.03735300	3.92741500	0.43524600
O	0.68921700	1.97578000	-1.05648100
F	-4.59397100	-0.38594100	-0.08707300
F	-4.53573400	0.92676000	1.64419100
F	-5.56733600	1.55645400	-0.16380400
F	3.44937500	2.64423100	-0.48179600
F	3.03875100	3.73582000	1.35786100
F	2.53831200	4.60826000	-0.57459400
P	2.47724300	-0.83818500	-0.06403300
P	-0.31716000	-1.60082700	1.73562200
P	-0.54940300	-1.34935200	-1.77052200
S	-2.93921600	1.70675800	-0.33439900
S	0.86188300	2.73845600	0.22976500
Ru	0.26208800	-0.10767100	0.03775600

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TS1, total electronic energy = -3430.935248, thermal corrections to Gibbs free energy = 0.886845

C	-1.57118100	2.49136200	1.87591200
H	-0.71280300	3.06699200	1.52739100
H	-2.30116700	2.52259100	1.06733900
C	-2.19035700	3.15017800	3.11548400
H	-3.08665600	2.62442800	3.45743100
H	-2.49207200	4.17198800	2.85649000
H	-1.49299300	3.21755700	3.95287900
C	0.69867600	0.82137800	2.77489300
H	0.85547700	-0.14685100	3.26088000
H	1.38006800	0.86384900	1.92299500
C	1.01795800	1.96676600	3.74400900
H	0.91616800	2.94284300	3.26112300
H	2.05809900	1.87696900	4.07840000
H	0.38581900	1.95697700	4.63430100
C	-2.10600300	-0.05394800	3.26245500
H	-3.11871000	0.29335200	3.03175100
H	-2.09407900	-1.12345000	3.06609000
C	-1.79161400	0.16289800	4.74941000
H	-0.80179400	-0.22070900	5.01367900
H	-2.52552600	-0.38668700	5.35030900
H	-1.84099600	1.21135700	5.04795400
C	-2.51040200	2.16524500	-1.78284900
H	-2.18469800	2.84272400	-0.99278700
H	-1.66349500	2.08671100	-2.47061300
C	-3.73134300	2.75231600	-2.50093200
H	-4.06599700	2.12966600	-3.33611800
H	-3.47165400	3.73535300	-2.91109600
H	-4.57825400	2.89534400	-1.82297100
C	-4.22628400	0.67701300	0.08579000
H	-4.05967700	0.06571600	0.97458200
H	-4.22610400	1.71899200	0.42405600
C	-5.59619600	0.33428700	-0.51401300
H	-5.83483100	0.94486700	-1.38876000
H	-6.37409600	0.51470900	0.23690200
H	-5.66288100	-0.71757700	-0.80802100
C	-3.30009000	-0.53267200	-2.43763100
H	-3.55878400	-1.52310600	-2.05506000
H	-4.23237500	-0.08527200	-2.79398300
C	-2.30868700	-0.64525800	-3.60047300
H	-2.11294600	0.32829400	-4.06066900
H	-2.71627100	-1.30154200	-4.37752900
H	-1.34830500	-1.06429100	-3.28537100

C	-3.25429000	-2.63555900	0.99908800
H	-3.36520100	-2.02308000	1.89520600
H	-3.88689700	-2.17632600	0.23239000
C	-3.75166500	-4.05822500	1.28634400
H	-3.78341500	-4.67403100	0.38371500
H	-4.77194200	-4.01024800	1.68399100
H	-3.13492000	-4.57253300	2.02924500
C	-1.58939300	-3.43820800	-1.22392800
H	-2.60650300	-3.29009100	-1.59926300
H	-0.92732200	-2.95319500	-1.94315900
C	-1.28311800	-4.94276700	-1.19217700
H	-0.25558600	-5.15406600	-0.88494600
H	-1.41334100	-5.35153200	-2.20094500
H	-1.95130800	-5.49452200	-0.52645100
C	-0.48022900	-3.52540700	1.48334300
H	-0.84680300	-4.54737300	1.35179000
H	0.53014500	-3.49061300	1.06979900
C	-0.44598500	-3.19360600	2.97707600
H	-0.02849900	-2.20274700	3.17223500
H	0.18115600	-3.92565100	3.49869500
H	-1.44130700	-3.23865400	3.43033100
C	0.73746400	4.37454700	-0.78090900
O	0.31596600	1.80796300	-0.43712100
O	0.92016500	2.59245100	-2.73346300
O	2.64733600	2.59617600	-0.91104100
F	0.94237300	4.55448600	0.53707200
F	-0.55406800	4.63237600	-1.04125900
F	1.48424900	5.26684000	-1.44646700
P	-0.98298200	0.71953800	1.98997900
P	-2.70006300	0.48657200	-0.99613400
P	-1.50652300	-2.43722600	0.37210100
S	1.22232200	2.64725900	-1.28907400
Ru	-0.66934200	-0.29317600	-0.08026500
O	1.50614900	-1.06989000	-0.08250600
C	1.57365100	-1.44010500	-1.45782400
C	2.56874800	-0.62584100	-2.30532400
C	1.86363800	-2.93872100	-1.66922400
H	0.57104600	-1.23462500	-1.90593600
C	2.48161500	-0.99966500	-3.79516300
H	3.58476800	-0.83531900	-1.95226400
H	2.40130400	0.44147200	-2.17102600
C	1.78970800	-3.34702700	-3.15054400
H	2.87663500	-3.14289100	-1.29808400
H	1.18222700	-3.54457800	-1.06877800

C	2.72946600	-2.49777900	-4.01800600
H	3.20262200	-0.40389800	-4.36832500
H	1.48614600	-0.73532700	-4.18075000
H	2.03043300	-4.41226000	-3.25497000
H	0.75880400	-3.22521200	-3.51227900
H	2.60488600	-2.75410700	-5.07741600
H	3.77171000	-2.73259100	-3.75819900
C	4.88493100	-1.55907900	0.44472300
C	5.35645500	-0.13921800	0.14530900
C	4.34666800	0.69529500	2.06650500
C	3.84412400	-0.68666700	2.46363600
H	6.31360800	-0.18825900	-0.38164100
H	5.65754300	-2.08774000	1.01470400
H	4.69572500	-2.11147500	-0.47788000
H	4.55148800	1.27424400	2.97122400
H	3.59760000	1.23401900	1.46874300
H	4.59282800	-1.17189000	3.10060300
H	2.90696500	-0.62714500	3.01577100
H	4.63560900	0.38830500	-0.49318400
N	3.63071900	-1.56479100	1.26765700
O	5.56994900	0.59931400	1.34358100
C	3.34220100	-2.94731700	1.73060300
H	2.43703700	-2.93599900	2.33898600
H	3.19581300	-3.59592900	0.86699600
H	4.17798100	-3.32227800	2.32907500
H	2.63262400	-1.24647300	0.60126500

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I2, total electronic energy = -3103.4761355, thermal corrections to Gibbs free energy = 0.711856

C	-0.83046400	-1.53541500	2.48077900
H	-1.71221600	-0.88798700	2.51622700
H	-0.97557600	-2.18023400	1.61275000
C	-0.74502400	-2.39942600	3.74533200
H	0.10271800	-3.09066400	3.70936100
H	-1.65517700	-3.00576800	3.82734300
H	-0.66191000	-1.80756600	4.65948000
C	0.39592100	1.10271400	3.10093100
H	1.39945000	1.51032200	3.25371700
H	-0.12036700	1.80471300	2.44178200
C	-0.33054100	0.98331800	4.44584000
H	-1.35309000	0.61207600	4.32681100
H	-0.39962400	1.97667600	4.90609500
H	0.18682000	0.33080200	5.15409200
C	2.12673200	-1.28178500	2.66923700
H	2.01840600	-2.33635100	2.39486500

H	2.95510800	-0.89318200	2.07013300
C	2.47807100	-1.15332900	4.15753200
H	2.63577700	-0.11096100	4.44991300
H	3.41157100	-1.69269700	4.35743900
H	1.70900700	-1.57438700	4.80862800
C	-0.07461000	-3.33637700	-0.97707300
H	-0.28551900	-3.48759300	0.08772100
H	-0.98487700	-2.92382700	-1.41697600
C	0.25850300	-4.68483500	-1.62675100
H	0.46960200	-4.58903000	-2.69669500
H	-0.59811800	-5.36233100	-1.52568600
H	1.11586000	-5.17385700	-1.15449600
C	2.72260700	-2.87007000	-0.36764700
H	3.30426300	-2.14006500	0.19585300
H	2.33639400	-3.58416700	0.36946400
C	3.64978700	-3.59140600	-1.35516700
H	3.13372000	-4.36137900	-1.93430100
H	4.46088500	-4.08205100	-0.80384000
H	4.11147300	-2.89504300	-2.06206400
C	1.56881100	-1.82188300	-2.86541900
H	2.48219900	-1.22357700	-2.95477000
H	1.80096800	-2.81011000	-3.27473000
C	0.43703900	-1.17299200	-3.67093400
H	-0.49190800	-1.74619400	-3.60602800
H	0.71755900	-1.10111200	-4.72837400
H	0.21867000	-0.15880700	-3.31811100
C	4.13807400	0.34820700	-0.59995300
H	4.37210300	-0.05810400	0.39008100
H	3.97766600	-0.51050500	-1.25789600
C	5.32075600	1.17268700	-1.12814500
H	5.16740700	1.47978800	-2.16704100
H	6.23392100	0.56690600	-1.09853800
H	5.50465100	2.07285100	-0.53464800
C	2.27995700	1.95483300	-2.17535100
H	2.75060300	1.24292600	-2.86369300
H	1.20635300	1.92497100	-2.38446000
C	2.79803100	3.37296000	-2.44598500
H	2.27571300	4.11697500	-1.83765600
H	2.62519400	3.62932600	-3.49783700
H	3.87004900	3.47111500	-2.25395500
C	2.85570200	2.64699500	0.68090800
H	3.33639300	3.44139800	0.10258300
H	1.86770700	3.00976700	0.97645900
C	3.72371700	2.31834300	1.90310600

H	3.35655500	1.45337600	2.46138300
H	3.73279900	3.17249100	2.58990300
H	4.76144400	2.11312900	1.62423800
C	-3.93469700	-1.85078900	0.13144700
O	-1.75009500	-0.53076400	-0.34809600
O	-2.80189200	-1.76922600	-2.25463600
O	-3.87578700	0.31034400	-1.37446400
F	-4.15153800	-1.13979500	1.25120500
F	-3.25614200	-2.96201300	0.46572400
F	-5.12399000	-2.22120800	-0.36739500
P	0.59914500	-0.41756200	2.03337500
P	1.20584000	-1.97837300	-1.03828300
P	2.49599500	1.21833600	-0.45947100
S	-2.99352900	-0.84339600	-1.11825900
Ru	0.48735600	0.12384700	-0.17613400
O	-0.17690000	2.09195500	0.21517500
C	-1.39759800	2.61684100	-0.24376900
C	-2.29287200	3.05312800	0.93668500
C	-1.15944300	3.82724100	-1.17367000
H	-1.96424600	1.87015200	-0.81937400
C	-3.60919300	3.70396700	0.47889500
H	-1.72319800	3.76680900	1.55185500
H	-2.50111100	2.18332000	1.57283400
C	-2.46942300	4.48085100	-1.64592900
H	-0.55493100	4.56789400	-0.62818200
H	-0.56212900	3.50736600	-2.03750700
C	-3.35304200	4.89253900	-0.45912200
H	-4.19802300	4.02568000	1.34807000
H	-4.21434300	2.95324600	-0.04803100
H	-2.25372900	5.35072300	-2.28020200
H	-3.02368400	3.76904000	-2.27500200
H	-4.30363000	5.30839300	-0.81758100
H	-2.85191600	5.69514600	0.10199400

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TS2, total electronic energy = -3103.4605601, thermal corrections to Gibbs free energy = 0.705292

C	1.36733100	-1.72902600	-1.44509800
H	1.30550700	-1.17756600	-2.39025500
H	1.77501300	-1.02400200	-0.71487500
C	2.33918800	-2.90864200	-1.57816500
H	2.44588100	-3.45423100	-0.63574400
H	3.32746100	-2.52167600	-1.84776300
H	2.03264200	-3.61888400	-2.34939100
C	-1.28514200	-2.56028600	-2.49509700
H	-2.18945300	-3.08749400	-2.16914300

H	-1.61957200	-1.62607200	-2.95260700
C	-0.53174600	-3.38977800	-3.54318600
H	0.33999500	-2.85298100	-3.92909300
H	-1.19530200	-3.58644100	-4.39400600
H	-0.19368400	-4.35457000	-3.15917400
C	-0.39458700	-3.52768300	0.17613300
H	0.40813900	-3.35226700	0.90229100
H	-1.33096600	-3.47964200	0.73984600
C	-0.26535000	-4.92950900	-0.43436600
H	-1.09693200	-5.15173200	-1.10965800
H	-0.28890200	-5.67679900	0.36786900
H	0.66703300	-5.06698800	-0.98569100
C	1.36424100	-0.14940000	2.07318800
H	1.54737200	-1.21633600	1.90001700
H	1.74698000	0.37122200	1.18886800
C	2.15292200	0.33144300	3.29983200
H	2.04388800	1.40849300	3.45621600
H	3.21767100	0.13336100	3.13874200
H	1.85511900	-0.17448200	4.22100400
C	-1.15348700	-1.36514400	3.08679200
H	-2.22357500	-1.15925700	3.20568300
H	-1.08137800	-2.26309000	2.46914500
C	-0.52470400	-1.64188500	4.45848200
H	0.51809000	-1.95948800	4.37026200
H	-1.07152800	-2.45372800	4.95251100
H	-0.56229600	-0.77328800	5.12234800
C	-0.83480400	1.47085200	3.20458300
H	-1.90409700	1.43616400	3.43644700
H	-0.30808200	1.25336700	4.13908200
C	-0.45353500	2.86642100	2.70963000
H	0.60738400	2.93369700	2.44753400
H	-0.64766600	3.60800700	3.49329100
H	-1.03368700	3.15185700	1.82819200
C	-3.78298900	-1.83793100	0.52710700
H	-3.55808400	-2.41733600	-0.37513600
H	-3.07976400	-2.17428500	1.29230100
C	-5.21820300	-2.12281400	0.98691200
H	-5.44507100	-1.63615800	1.93977000
H	-5.34478900	-3.20192400	1.13320800
H	-5.96475200	-1.80383300	0.25352400
C	-3.98877900	0.96257700	1.50935000
H	-3.74404000	0.42697100	2.43335600
H	-3.38063400	1.87184800	1.51068200
C	-5.47372300	1.35290700	1.50162700

H	-5.72299600	1.98459200	0.64425300
H	-5.69748400	1.92936400	2.40693600
H	-6.14119200	0.48827900	1.48971300
C	-4.46728200	0.32622900	-1.27978100
H	-5.47132100	0.09380300	-0.90923200
H	-4.43866100	1.41135500	-1.41308600
C	-4.23126200	-0.37831900	-2.61671900
H	-3.26034500	-0.10905400	-3.03765200
H	-5.00952500	-0.08314000	-3.33032400
H	-4.27704700	-1.46725200	-2.51602500
C	5.19770700	-0.47040900	0.53865700
O	3.61176500	1.48473400	-0.18645000
O	6.06091600	1.70199500	-0.64813600
O	4.67761000	0.08820600	-1.97079200
F	4.16014400	-1.32654500	0.65076100
F	5.41970700	0.05801500	1.75914700
F	6.28324700	-1.18933500	0.20170900
P	-0.40914400	-2.02673500	-0.93621800
P	-0.49967000	0.04293500	2.04774000
P	-3.30007000	-0.08386500	0.11653100
S	4.84947300	0.85576600	-0.71565800
Ru	-1.06770700	0.21160200	-0.21930000
O	-1.04989900	0.82368600	-2.29063600
C	-0.92236700	2.00688300	-1.75146200
C	0.49102500	2.58971100	-1.70364900
C	-2.01005300	3.04034400	-2.03962400
H	-1.24383800	1.88370600	-0.08143400
C	0.61758700	3.93275500	-0.97159800
H	0.76443800	2.72353900	-2.76224400
H	1.19139500	1.85044400	-1.30149400
C	-1.85625000	4.36082800	-1.27461800
H	-1.91363100	3.23925200	-3.11827100
H	-2.99536400	2.59890500	-1.89071300
C	-0.44417600	4.94093000	-1.43122300
H	1.62481300	4.33371100	-1.13314600
H	0.51508200	3.77047600	0.10767900
H	-2.60724500	5.07408700	-1.63432700
H	-2.06566900	4.19368600	-0.20934800
H	-0.35178300	5.87164200	-0.85889100
H	-0.27316100	5.19987400	-2.48579500

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I3, total electronic energy = -3103.4658872, thermal corrections to Gibbs free energy = 0.706182

C	-1.43077200	-1.58776400	1.53249200
H	-1.33685100	-1.02551100	2.46879000

H	-1.82745700	-0.88072700	0.79785100
C	-2.43705900	-2.73394700	1.69793800
H	-2.57967700	-3.28457700	0.76345100
H	-3.40740500	-2.31203100	1.98062100
H	-2.13918600	-3.44639700	2.47040700
C	1.21804100	-2.56421300	2.50648200
H	2.07059800	-3.14418500	2.13316300
H	1.63141000	-1.66640200	2.97112000
C	0.44999400	-3.36712600	3.56445400
H	-0.37116500	-2.78409000	3.99227200
H	1.12809700	-3.62502200	4.38716500
H	0.03641600	-4.29936900	3.17360600
C	0.22336200	-3.40788800	-0.16245200
H	-0.58231400	-3.18045900	-0.87096200
H	1.15185100	-3.38642600	-0.74098100
C	0.04330200	-4.81870700	0.41375300
H	0.87357200	-5.09274000	1.07149400
H	0.02462600	-5.54612700	-0.40677700
H	-0.88645000	-4.93077400	0.97507200
C	-1.36658000	0.01951700	-2.03025000
H	-1.56549500	-1.03739100	-1.81850700
H	-1.71837100	0.57322900	-1.15340400
C	-2.17097000	0.47623100	-3.25589000
H	-2.05158000	1.54655100	-3.44542600
H	-3.23449600	0.29536700	-3.07039900
H	-1.89581500	-0.05961100	-4.16684700
C	1.10526400	-1.25921400	-3.08881800
H	2.17607900	-1.07386200	-3.22959300
H	1.02905200	-2.14756500	-2.45832600
C	0.44555300	-1.53978100	-4.44487100
H	-0.59681600	-1.85034100	-4.33283300
H	0.97808700	-2.35839800	-4.94300300
H	0.47598200	-0.67567300	-5.11481200
C	0.84771200	1.59476000	-3.20825800
H	1.92364600	1.56438200	-3.40994300
H	0.34610200	1.36722500	-4.15450700
C	0.44435300	2.99185400	-2.73103900
H	-0.62064000	3.05255300	-2.48521000
H	0.64286200	3.72517500	-3.52112800
H	1.01072500	3.29273700	-1.84585500
C	3.74310200	-1.90236600	-0.58315000
H	3.44442400	-2.45824300	0.31209100
H	3.03596200	-2.18273500	-1.36731600
C	5.16341200	-2.30404100	-1.00126600

H	5.45268700	-1.84763200	-1.95220000
H	5.20939500	-3.39131800	-1.13352500
H	5.91251700	-2.03413000	-0.25094400
C	4.12231800	0.86867300	-1.60562600
H	3.81889300	0.34237200	-2.51743900
H	3.57828300	1.81694700	-1.60279300
C	5.63000400	1.15580000	-1.63717900
H	5.94001900	1.78408600	-0.79715300
H	5.87125900	1.70029700	-2.55757900
H	6.23834200	0.24848200	-1.62349200
C	4.61346700	0.22482600	1.19107100
H	5.60509300	0.02825200	0.77098300
H	4.57566300	1.29912500	1.39427200
C	4.43664500	-0.57026500	2.48707400
H	3.47674200	-0.34878900	2.95591100
H	5.23475500	-0.30530600	3.19056000
H	4.50079800	-1.64943600	2.31426600
C	-5.27009600	-0.49906400	-0.59620800
O	-3.79956000	1.53534500	0.15241900
O	-6.27283400	1.65502800	0.51052700
O	-4.87815800	0.12713800	1.91977600
F	-4.18479200	-1.29884300	-0.66602000
F	-5.48640200	-0.00342200	-1.83182400
F	-6.32414200	-1.27117800	-0.27717200
P	0.32547600	-1.93937300	0.99000500
P	0.49692800	0.17172300	-2.05823400
P	3.40029700	-0.11381400	-0.18256400
S	-5.02941700	0.86414100	0.64350400
Ru	1.19452800	0.33054400	0.20309500
O	1.36421600	0.63481500	2.36082500
C	1.12063400	1.81751900	1.89376400
C	-0.33887300	2.26617700	1.85324900
C	2.14664800	2.91840700	2.12523100
H	1.58423300	1.79369200	-0.34341100
C	-0.59065300	3.62955200	1.19097400
H	-0.67157300	2.29147500	2.90337500
H	-0.94080600	1.48059000	1.37394800
C	1.84525500	4.24746300	1.42148600
H	2.12582100	3.08859800	3.21412900
H	3.14801000	2.55474400	1.89052000
C	0.40003100	4.69724800	1.67136400
H	-1.62189600	3.94021600	1.39314200
H	-0.50174800	3.52798800	0.10307700
H	2.55184500	5.00856900	1.77331200

H	2.00952400	4.13771700	0.34132700
H	0.20375300	5.64684500	1.15948500
H	0.25505700	4.88095700	2.74565900

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TS3, total electronic energy = -3103.4636531, thermal corrections to Gibbs free energy = 0.706657

C	1.37746400	-1.31636200	-1.82941300
H	1.32789800	-0.54138000	-2.60257300
H	1.80068700	-0.82662400	-0.94732500
C	2.32669600	-2.43988600	-2.26428100
H	2.42128600	-3.21165100	-1.49427500
H	3.32362800	-2.01705400	-2.42879500
H	2.00844800	-2.92287300	-3.19114100
C	-1.30023300	-1.79997600	-3.03822100
H	-2.18259200	-2.42535500	-2.85659700
H	-1.67054500	-0.78994300	-3.22805800
C	-0.54637000	-2.29538300	-4.27959400
H	0.31051000	-1.65545800	-4.51149200
H	-1.21605200	-2.26819800	-5.14799400
H	-0.18425900	-3.32069900	-4.17529200
C	-0.43324700	-3.43267100	-0.72696400
H	0.35102000	-3.47370200	0.03860000
H	-1.38424200	-3.51602700	-0.19127700
C	-0.30784600	-4.62644400	-1.68307000
H	-1.12384400	-4.64500700	-2.41175500
H	-0.36327700	-5.55982100	-1.10971900
H	0.63646600	-4.63238100	-2.23114100
C	1.31076000	-0.83662800	2.01089800
H	1.43231800	-1.81097700	1.52312700
H	1.72319100	-0.09628700	1.31683400
C	2.12095500	-0.79147500	3.31488300
H	2.07380800	0.19237200	3.78991600
H	3.17319800	-0.99092300	3.08734600
H	1.79097600	-1.53388600	4.04488400
C	-1.28075400	-2.14845800	2.65967700
H	-2.33731600	-1.92739300	2.84699800
H	-1.25729800	-2.82548100	1.80271600
C	-0.67654400	-2.85122300	3.88217000
H	0.34479100	-3.19263800	3.69185400
H	-1.27591800	-3.73665500	4.12488800
H	-0.66399600	-2.21302500	4.77059400
C	-0.78976100	0.52747400	3.57923500
H	-1.86510100	0.52501200	3.78503200
H	-0.31170800	0.00635600	4.41536400
C	-0.27444600	1.96713500	3.50407100

H	0.79042300	2.01142000	3.25297000
H	-0.40600700	2.46094000	4.47383700
H	-0.81813200	2.54811400	2.75464900
C	-3.88398100	-1.80152900	-0.00875100
H	-3.59973600	-2.07317100	-1.03093900
H	-3.25099000	-2.39930400	0.65279400
C	-5.35913000	-2.14508000	0.23300400
H	-5.64844900	-1.98951100	1.27623400
H	-5.53122000	-3.20280500	0.00108700
H	-6.03315600	-1.55874200	-0.39892800
C	-4.02442900	0.50723000	1.85298400
H	-3.83713900	-0.32056400	2.54588800
H	-3.38532800	1.33240300	2.17763700
C	-5.49245600	0.94705700	1.94660100
H	-5.68314700	1.85125500	1.36132000
H	-5.73103700	1.17963400	2.99115600
H	-6.19165600	0.17594100	1.61487100
C	-4.41932100	0.88150800	-0.99823600
H	-5.45081600	0.67636800	-0.69393300
H	-4.25379500	1.94915300	-0.82018000
C	-4.24736800	0.54905900	-2.48269100
H	-3.23966800	0.78445400	-2.82993100
H	-4.95956800	1.13342600	-3.07720300
H	-4.44468200	-0.50859700	-2.68535600
C	5.18065500	-0.61453100	0.45892700
O	3.45037700	1.33576800	0.21853600
O	5.87958900	1.85676900	-0.07404200
O	4.65863500	0.55542200	-1.83059100
F	4.20919800	-1.53933400	0.31079000
F	5.35001200	-0.41306500	1.78117600
F	6.32072000	-1.13994900	-0.02352500
P	-0.40748700	-1.68660500	-1.39764800
P	-0.53724400	-0.54061100	2.06979700
P	-3.32166800	-0.03435900	0.20009700
S	4.74594200	0.96850700	-0.41127700
Ru	-1.08401900	0.27945600	-0.01889700
O	-0.96389500	1.30586100	-2.11138300
C	-0.73167700	2.44251500	-1.63040200
C	0.68205000	2.87443500	-1.30552000
C	-1.77540000	3.53615400	-1.69690900
H	-1.33505800	1.70775800	0.74611700
C	0.79007300	4.00548400	-0.26868100
H	1.07868200	3.23366800	-2.27025700
H	1.29122300	2.01015200	-1.02634400

C	-1.62490300	4.64434000	-0.64297900
H	-1.62126800	3.97690800	-2.69609200
H	-2.77348900	3.09658900	-1.70306000
C	-0.18091600	5.15492400	-0.56400600
H	1.82368900	4.36695200	-0.24661200
H	0.57557400	3.59946500	0.72741300
H	-2.31194400	5.46270700	-0.88594600
H	-1.92819000	4.25343000	0.33654900
H	-0.09695900	5.92411300	0.21252600
H	0.09128900	5.63353400	-1.51525100

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I4, total electronic energy = -3103.4776387, thermal corrections to Gibbs free energy = 0.708663

C	-0.49640700	-1.81981200	2.58745100
H	-1.43407500	-1.26632200	2.71507900
H	-0.64408800	-2.42937700	1.69384100
C	-0.25292500	-2.73694500	3.79208600
H	0.65310700	-3.33832200	3.66611700
H	-1.09227300	-3.43635400	3.89432200
H	-0.16608500	-2.19000300	4.73391400
C	0.46808300	0.88752800	3.27853400
H	1.40092600	1.46346800	3.31068800
H	-0.25826600	1.51303100	2.75246400
C	-0.04310200	0.62386300	4.70084500
H	-1.00439100	0.10067600	4.69199500
H	-0.20001200	1.57916900	5.21756100
H	0.65437800	0.03669700	5.30234500
C	2.41869200	-1.26069500	2.64492100
H	2.42318900	-2.29387600	2.27606700
H	3.17462100	-0.73094100	2.05958200
C	2.83735300	-1.22306200	4.12061700
H	2.90029000	-0.19617900	4.49385600
H	3.83360800	-1.66927500	4.23088500
H	2.15601500	-1.77707500	4.76963200
C	1.11821900	-3.24349700	-0.66454200
H	1.61690300	-3.41984600	0.29674400
H	0.05976600	-3.09685100	-0.44339800
C	1.27719000	-4.46798400	-1.57675300
H	0.71243000	-4.35558000	-2.50669300
H	0.88409900	-5.35525100	-1.06522500
H	2.31651800	-4.67663500	-1.84011500
C	3.58116600	-1.65466800	-0.91963900
H	4.00516200	-0.76803800	-1.40154600
H	3.70248300	-1.50586400	0.15634200
C	4.37438200	-2.89580000	-1.34903100

H	4.06538200	-3.78882700	-0.79865900
H	5.43937800	-2.73825200	-1.13944700
H	4.28219000	-3.10552700	-2.41892300
C	1.73548700	-1.70900400	-3.11094200
H	2.33814900	-0.86940300	-3.47595500
H	2.28069600	-2.62138400	-3.37432200
C	0.36851000	-1.70563400	-3.80230700
H	-0.29305400	-2.48724600	-3.41735200
H	0.49345900	-1.87295500	-4.87890600
H	-0.14236700	-0.74827400	-3.66987400
C	3.61017800	1.71631400	0.65507700
H	3.19650000	1.74265400	1.66936700
H	4.04961200	0.72237100	0.53121900
C	4.70312200	2.78176000	0.50530900
H	5.20509800	2.71568500	-0.46455300
H	5.46848800	2.64090200	1.27809800
H	4.31251500	3.79819800	0.61465600
C	2.93815400	1.86297900	-2.20131800
H	3.81442600	1.20630700	-2.15625700
H	2.22789300	1.38463300	-2.87954500
C	3.34487400	3.22206600	-2.78701500
H	2.47800900	3.86975300	-2.95031700
H	3.82221700	3.06739900	-3.76220000
H	4.05623800	3.76326600	-2.15749900
C	1.54488800	3.53358100	-0.25327000
H	2.32924000	4.19698000	-0.62866300
H	0.68302600	3.66881200	-0.91336000
C	1.19243100	3.94652300	1.17973100
H	0.40588300	3.32363400	1.60803100
H	0.84049100	4.98508300	1.19041200
H	2.06287200	3.89341200	1.84160500
C	-3.82483500	-1.67050500	0.24930500
O	-3.06114300	-0.43025600	-1.94966900
O	-1.33110100	-1.22657200	-0.29672700
O	-2.54691200	-2.87275600	-1.71820700
F	-5.03882200	-1.91496800	-0.26870200
F	-3.89830200	-0.53210500	0.96485900
F	-3.51832000	-2.67000900	1.09281500
P	0.77799200	-0.53365700	2.09708600
P	1.73896200	-1.57019700	-1.24549700
P	2.13670000	1.77381700	-0.49633800
S	-2.55579400	-1.52945100	-1.10510600
Ru	0.50122500	0.15901600	-0.31035200
O	-1.06666200	1.57361300	0.47829500

C	-1.92679200	2.36153000	0.06925600
C	-2.95027200	2.91255600	1.03786000
C	-1.99400000	2.88131700	-1.34413900
H	0.14297000	0.62378600	-1.82968700
C	-4.37455700	2.93831400	0.44551600
H	-2.63976200	3.94526100	1.25847100
H	-2.90299600	2.34618200	1.97177600
C	-3.43460700	2.93706500	-1.89728200
H	-1.59395300	3.90631100	-1.30039900
H	-1.33158200	2.28814100	-1.97681200
C	-4.39842400	3.62671900	-0.92412000
H	-5.04392100	3.44391800	1.15018100
H	-4.73601500	1.90769100	0.34432700
H	-3.42009400	3.45723700	-2.86164600
H	-3.77173400	1.91252500	-2.08539900
H	-5.41567600	3.61043900	-1.33285200
H	-4.11920400	4.68357300	-0.80872800

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I5, total electronic energy = -2793.6947998, thermal corrections to Gibbs free energy = 0.56062

C	-1.70196700	1.74549300	1.86772400
H	-2.47710500	1.83353800	1.10018500
H	-1.78224800	0.72170600	2.24220400
C	-1.97204300	2.72146600	3.01953200
H	-1.24025700	2.61088600	3.82600200
H	-2.95994000	2.51408700	3.44925600
H	-1.96660100	3.76601100	2.70002700
C	-0.26569600	3.23689100	-0.25369700
H	0.75164200	3.55510800	-0.51106600
H	-0.67429900	2.78147200	-1.16300700
C	-1.12763000	4.45222100	0.11172800
H	-2.16218800	4.16347400	0.32022200
H	-1.14990700	5.15160800	-0.73307000
H	-0.74560900	4.99523200	0.97897200
C	1.16632100	2.39169700	2.23115400
H	0.94195900	1.81613900	3.13771100
H	2.13957300	2.03705200	1.88296800
C	1.27833300	3.88439400	2.56714700
H	1.54951400	4.47516000	1.68654800
H	2.06737600	4.03378700	3.31432600
H	0.35355700	4.29505400	2.97798500
C	-0.52936600	-1.81642800	2.47174700
H	-0.42517500	-0.94367500	3.12722200
H	-1.44041200	-1.65707900	1.88912000
C	-0.67325500	-3.09230900	3.31376500

H	-0.87676400	-3.96919700	2.69292600
H	-1.52037400	-2.97778900	4.00083100
H	0.21140600	-3.30643600	3.91784700
C	2.36547100	-1.22570600	2.27150200
H	3.22117600	-1.28856600	1.59076300
H	2.24309300	-0.16620700	2.51354000
C	2.66613200	-2.01302900	3.55358000
H	1.88357600	-1.88150400	4.30617200
H	3.60347100	-1.65091800	3.99248800
H	2.78593900	-3.08474300	3.36870900
C	1.26498200	-3.45376100	0.80211300
H	2.22747400	-3.43944200	0.27983900
H	1.42934900	-3.98992100	1.74316500
C	0.22221700	-4.19039800	-0.04287600
H	-0.76432400	-4.19520900	0.43181900
H	0.52571500	-5.23381800	-0.18717300
H	0.11305000	-3.73137200	-1.02891400
C	3.50601100	1.46267300	-0.52210700
H	2.86690000	2.35301700	-0.52264100
H	3.63944400	1.18663700	0.53012800
C	4.86774000	1.79417200	-1.14374000
H	5.57394800	0.96496600	-1.04470100
H	5.30703100	2.65877000	-0.63182400
H	4.78891300	2.04938700	-2.20516900
C	3.61424700	-1.36129000	-1.37012100
H	4.16384700	-1.39348000	-0.42201900
H	2.96722100	-2.24206600	-1.38527900
C	4.59510500	-1.44641700	-2.54865100
H	4.07055800	-1.52700000	-3.50518200
H	5.21403700	-2.34501100	-2.44067600
H	5.26948300	-0.58875100	-2.60546800
C	2.26860500	0.60392700	-3.04919900
H	3.25776400	0.83736400	-3.45643100
H	1.91105600	-0.28991500	-3.57223100
C	1.30688300	1.76968700	-3.29943400
H	0.29532400	1.54005500	-2.94860400
H	1.24152700	1.98186000	-4.37288400
H	1.63841700	2.68683100	-2.80232800
C	-4.39236100	-0.20128600	-0.79657700
O	-1.90295300	-0.58797100	-0.19658100
O	-3.02580600	-2.29239500	-1.65898300
O	-2.44670100	-0.02755700	-2.58028200
F	-4.31141800	1.12019300	-0.56053900
F	-4.76261800	-0.81003300	0.33983800

F	-5.34621800	-0.40424000	-1.71726900
P	-0.07007900	1.80843400	0.94796600
P	0.87595200	-1.68228500	1.24063000
P	2.45359000	0.10666700	-1.25846000
S	-2.76386900	-0.86474800	-1.40500800
Ru	0.33872700	-0.24356500	-0.42364500
H	0.38542600	-1.50838900	-1.46689500

86

I6, total electronic energy = -2986.8026414, thermal corrections to Gibbs free energy = 0.643377

C	1.54480100	-0.13316800	2.67729700
H	2.21972700	-0.90779800	2.29640300
H	1.82272300	0.77672900	2.14131600
C	1.76996000	0.07516700	4.17959500
H	1.14216400	0.87985500	4.57549000
H	2.81383600	0.36384300	4.35608300
H	1.57513500	-0.82438300	4.76814100
C	-0.27479800	-2.43574200	2.31874600
H	-1.34645200	-2.66748600	2.34669800
H	0.10842300	-2.87769700	1.39487000
C	0.44004600	-3.08341800	3.51180700
H	1.52041300	-2.91217200	3.47433100
H	0.28400100	-4.16938200	3.48832500
H	0.07473300	-2.72079200	4.47521000
C	-1.35274200	0.16545400	3.25307500
H	-1.01754100	1.19994900	3.39730500
H	-2.30420300	0.23082900	2.71912300
C	-1.60626300	-0.50371300	4.61053500
H	-2.00433900	-1.51617600	4.49090100
H	-2.35302800	0.07341700	5.17008600
H	-0.70819800	-0.56489400	5.22870500
C	0.27542600	3.12505100	0.94810600
H	-0.02424700	2.92397800	1.98440200
H	1.21773600	2.59736600	0.79016000
C	0.49764700	4.63026500	0.74387000
H	0.88801400	4.84967700	-0.25408000
H	1.23981000	4.98962100	1.46738900
H	-0.40962100	5.22189500	0.88560100
C	-2.61216400	2.63147600	0.70929500
H	-3.38721500	2.24768600	0.03842000
H	-2.65590100	2.01431300	1.61052200
C	-2.93233700	4.08573300	1.07883100
H	-2.25519500	4.47061900	1.84641600
H	-3.94946700	4.14404400	1.48499600
H	-2.88810500	4.75818800	0.21686600

C	-1.12017000	3.27646600	-1.65356200
H	-2.02469600	2.93353100	-2.16892300
H	-1.31460700	4.30564500	-1.33393500
C	0.06612700	3.25130400	-2.62233500
H	1.00295600	3.54338100	-2.13820300
H	-0.11172500	3.94816300	-3.45012400
H	0.21193800	2.25491500	-3.04847700
C	-3.73748000	-0.93260100	0.54926800
H	-3.26436400	-1.59268700	1.28491500
H	-3.78326400	0.05658600	1.01403400
C	-5.15905500	-1.42083700	0.24475600
H	-5.69860000	-0.72349000	-0.40287100
H	-5.72997300	-1.50656300	1.17726000
H	-5.16888100	-2.40432100	-0.23516700
C	-3.45174900	0.22934700	-2.13854200
H	-3.99228700	0.99944400	-1.57642700
H	-2.68234400	0.74993000	-2.71337800
C	-4.41300100	-0.46546300	-3.11283000
H	-3.88706800	-1.15762400	-3.77750100
H	-4.89360600	0.28975100	-3.74646100
H	-5.20726100	-1.02125300	-2.60776400
C	-2.58200300	-2.50202300	-1.59835500
H	-3.58715800	-2.64036700	-2.00683600
H	-1.89807100	-2.50298800	-2.45250300
C	-2.26502900	-3.66962100	-0.65804100
H	-1.26570500	-3.59305500	-0.22738500
H	-2.32001700	-4.61551300	-1.21027300
H	-2.98420000	-3.73324600	0.16491600
C	4.27652200	-0.19391800	-0.15929100
O	2.93781500	-0.08853200	-2.42573000
O	1.81900800	0.65050600	-0.29117200
O	3.58593600	2.06845200	-1.32070400
F	5.45161600	-0.25795800	-0.80606200
F	3.87519800	-1.45278000	0.09869500
F	4.47700300	0.42723600	1.01467600
P	-0.15339600	-0.58874500	2.02333300
P	-0.98064300	2.22190900	-0.11455500
P	-2.51144800	-0.78433500	-0.85618000
S	3.01820200	0.71251700	-1.18898600
Ru	-0.38849700	-0.00392400	-0.41234100
H	-0.38691900	0.29639600	-2.01352800
C	1.10459900	-2.60418700	-1.73478300
O	0.61814200	-1.98017200	-0.78566700
C	2.03645000	-3.75440400	-1.45703800

H	3.05135400	-3.46241900	-1.75258500
H	2.03256200	-4.01602400	-0.39761000
H	1.76511500	-4.62501700	-2.06352000
C	0.80777100	-2.30568200	-3.17457200
H	1.74089300	-2.26275500	-3.74356300
H	0.21902800	-3.13556600	-3.58645500
H	0.26174100	-1.36959800	-3.27810500

86

TS4, total electronic energy = -2986.784981, thermal corrections to Gibbs free energy = 0.640157

C	1.35059200	2.08626200	-0.52526800
H	1.31688400	2.63167300	0.42474900
H	1.78753000	1.11157700	-0.28832200
C	2.27109800	2.80469200	-1.51974400
H	2.34863500	2.26070200	-2.46616600
H	3.27802500	2.86359100	-1.09257700
H	1.93946400	3.82209800	-1.74014900
C	-1.33309200	3.36113200	-0.61423800
H	-2.24613600	3.33407000	-1.22118000
H	-1.65421300	3.28800600	0.42786000
C	-0.60161900	4.69470900	-0.81713000
H	0.28475000	4.76770900	-0.17969400
H	-1.26795900	5.52176100	-0.54285100
H	-0.28869900	4.85313000	-1.85152700
C	-0.50637000	1.55267000	-2.81521000
H	0.28516800	0.83602900	-3.06589800
H	-1.45295700	1.03892700	-3.01144400
C	-0.42009700	2.78262900	-3.72833500
H	-1.24319300	3.47939400	-3.54322000
H	-0.49291000	2.46489000	-4.77562800
H	0.51868200	3.32858100	-3.61429400
C	1.27082800	-1.73538300	-1.11804200
H	1.34633000	-1.00575700	-1.93265300
H	1.71411600	-1.25800000	-0.23743100
C	2.08300800	-2.99506800	-1.45461100
H	2.07538900	-3.71618500	-0.63258400
H	3.12631300	-2.71083500	-1.62570900
H	1.72450300	-3.50390000	-2.35201800
C	-1.37753600	-2.08636100	-2.43562200
H	-2.42886900	-2.30227400	-2.21596000
H	-1.35990500	-1.09360100	-2.89242700
C	-0.83516900	-3.11846000	-3.43249100
H	0.17014700	-2.86190700	-3.77759500
H	-1.48498400	-3.14661700	-4.31514600
H	-0.80649800	-4.12994400	-3.01687600

C	-0.75164600	-3.61792700	-0.07465100
H	-1.82674300	-3.82477300	-0.05019100
H	-0.31761600	-4.30672300	-0.80708800
C	-0.13633500	-3.87465900	1.30416900
H	0.93422600	-3.64559100	1.32683900
H	-0.25424800	-4.93026700	1.57462000
H	-0.62161400	-3.27297500	2.07769900
C	-3.95048600	0.43868900	-1.36755100
H	-3.66123700	1.49513100	-1.36801600
H	-3.34396000	-0.04375100	-2.13946700
C	-5.43791500	0.30406700	-1.71720700
H	-5.73476200	-0.74135300	-1.84095700
H	-5.63809700	0.81442400	-2.66674400
H	-6.08683700	0.75587200	-0.96067800
C	-4.04956100	-1.96388300	0.37830100
H	-3.88801200	-2.42395300	-0.60290200
H	-3.39664200	-2.49271800	1.07752700
C	-5.50857000	-2.15685200	0.81618800
H	-5.66972700	-1.82318500	1.84539700
H	-5.75640800	-3.22418300	0.77828200
H	-6.22093500	-1.63188000	0.17570400
C	-4.37809100	0.69137400	1.50639400
H	-5.42353100	0.47301000	1.26548000
H	-4.18136600	0.22864400	2.47907400
C	-4.17520600	2.20716300	1.58143800
H	-3.15467100	2.46257100	1.87428600
H	-4.85843200	2.63544900	2.32425500
H	-4.38983400	2.69175000	0.62349900
C	5.12843700	-0.30567300	-0.51657200
O	3.41989600	-0.58807100	1.44690400
O	5.85795100	-0.47921700	1.99641600
O	4.65213600	1.58193200	1.24357800
F	4.14757900	0.09428900	-1.35246000
F	5.28765600	-1.63368100	-0.68418200
F	6.26671800	0.29474700	-0.90689300
P	-0.44156900	1.75277800	-0.95663100
P	-0.55988200	-1.89673400	-0.76864000
P	-3.33862700	-0.23203500	0.26301300
S	4.72171000	0.10299400	1.24975500
Ru	-1.09882900	-0.10456300	0.57422400
H	-1.36443900	-1.22139100	1.74069200
C	-0.64587700	0.76434400	3.12529100
O	-0.79393700	1.57608700	2.18241800
C	0.70681900	0.17979000	3.43637000

H	0.62235800	-0.80380800	3.90551300
H	1.34990500	0.12809400	2.55572000
H	1.18674600	0.84800700	4.16676700
C	-1.72022100	0.56531500	4.16339600
H	-1.86142600	-0.49315700	4.39599200
H	-1.37177800	1.05002100	5.08594200
H	-2.66214000	1.02089200	3.86145700

86

I7, total electronic energy = -2986.7885472, thermal corrections to Gibbs free energy = 0.642959

C	-1.36519100	2.11533400	0.19973900
H	-1.28453800	2.54770200	-0.80399200
H	-1.79061500	1.11699400	0.05923500
C	-2.33106000	2.93893200	1.06117300
H	-2.45823200	2.50302700	2.05652200
H	-3.31414400	2.94515200	0.57846000
H	-2.00709500	3.97501300	1.18292600
C	1.31865700	3.41497500	0.35087600
H	2.18521900	3.43609400	1.02239400
H	1.70938000	3.25771700	-0.65690200
C	0.57895800	4.75833500	0.39750100
H	-0.25944500	4.77960000	-0.30525700
H	1.26693400	5.56172900	0.10699600
H	0.19445600	4.99731000	1.39168000
C	0.35874800	1.75284200	2.61819700
H	-0.44908500	1.05526600	2.87035600
H	1.29052700	1.25486500	2.90417700
C	0.22438300	3.04392200	3.43662800
H	1.05868000	3.72665000	3.24949900
H	0.23705100	2.80025800	4.50580600
H	-0.70489300	3.57922400	3.23151800
C	-1.30134800	-1.69168100	1.06144500
H	-1.42891600	-0.90396800	1.81318000
H	-1.69869400	-1.28400700	0.12575600
C	-2.11896200	-2.93333700	1.44587000
H	-2.05792900	-3.71335900	0.68187500
H	-3.17241100	-2.65064400	1.53755300
H	-1.80617700	-3.36864400	2.39744500
C	1.26950400	-1.89415600	2.54999500
H	2.33846500	-2.08918600	2.41093400
H	1.19148700	-0.87320200	2.93221400
C	0.69495900	-2.87105500	3.58388800
H	-0.33711100	-2.62447700	3.84694700
H	1.28855700	-2.81371100	4.50374400
H	0.72307900	-3.90960600	3.24174300

C	0.80483800	-3.61579300	0.27617200
H	1.88270100	-3.80165100	0.33278100
H	0.33517500	-4.25970000	1.02677800
C	0.28097300	-3.97710700	-1.11672200
H	-0.78794600	-3.76496100	-1.22267300
H	0.42633600	-5.04737800	-1.30213200
H	0.80969900	-3.42646900	-1.89993500
C	3.84178000	0.56237500	1.43293900
H	3.58179600	1.62200400	1.33810000
H	3.14832400	0.14110300	2.16488200
C	5.28113600	0.42046800	1.94356500
H	5.53921900	-0.62195700	2.15044800
H	5.38962800	0.97643500	2.88218000
H	6.01615300	0.82203100	1.23953700
C	4.10068100	-1.93107300	-0.17743800
H	3.83932700	-2.34581100	0.80215100
H	3.51757300	-2.49073700	-0.91372900
C	5.59551200	-2.14212200	-0.45758600
H	5.86229700	-1.84819200	-1.47674500
H	5.83079700	-3.20787000	-0.35425100
H	6.24167500	-1.59506600	0.23257300
C	4.55444000	0.67267200	-1.38037600
H	5.56195000	0.50065200	-0.98735200
H	4.50501000	0.13731600	-2.33321800
C	4.33014500	2.17192700	-1.59074000
H	3.34308500	2.36886200	-2.01346500
H	5.08726900	2.56420100	-2.27978600
H	4.42272400	2.72917400	-0.65294000
C	-5.17879900	-0.22421900	0.56105700
O	-3.60349600	-0.76868200	-1.46041500
O	-6.06803100	-0.63441800	-1.87056300
O	-4.76138300	1.45115600	-1.41304100
F	-4.13151900	0.21412200	1.29076600
F	-5.37934200	-1.51941700	0.87900300
F	-6.26533800	0.46416200	0.95379600
P	0.40060300	1.83873800	0.75224100
P	0.54607100	-1.85733500	0.83157400
P	3.39373900	-0.19611400	-0.21070500
S	-4.86991200	-0.01805500	-1.25978700
Ru	1.15881800	-0.12339200	-0.65787500
H	1.49824700	-1.42697700	-1.53847000
C	0.92039400	0.33353800	-2.84336100
O	1.10861900	1.43706100	-2.18879400
C	-0.51138400	-0.08134500	-3.14432200

H	-0.56526100	-1.09646600	-3.54614600
H	-1.15553700	-0.01055300	-2.26086300
H	-0.92161200	0.60848600	-3.89635900
C	1.94043700	-0.09688700	-3.87988700
H	1.90038100	-1.17120200	-4.07465100
H	1.69563600	0.41971200	-4.81957700
H	2.95251400	0.18797800	-3.59676000

86

TS5, total electronic energy = -2986.7832827, thermal corrections to Gibbs free energy = 0.639512

C	-1.32780600	2.13505400	0.01839700
H	-1.29456100	2.46135100	-1.02783100
H	-1.74904700	1.12611200	0.00102800
C	-2.26453100	3.04035600	0.82875900
H	-2.33852100	2.71660400	1.87136300
H	-3.26857300	2.98583500	0.39531700
H	-1.94874100	4.08607900	0.81932500
C	1.32745800	3.43471500	-0.18287200
H	2.26620500	3.53727500	0.37400800
H	1.60390200	3.13230200	-1.19640000
C	0.59406000	4.78103700	-0.24802500
H	-0.31215500	4.71556400	-0.85745800
H	1.24773700	5.52615900	-0.71747600
H	0.31436800	5.16198700	0.73647900
C	0.51284800	2.14809500	2.38229900
H	-0.28612900	1.50682000	2.77345400
H	1.45400500	1.68919400	2.69872900
C	0.42276000	3.55048000	2.99791400
H	1.25404600	4.18446000	2.67527000
H	0.47899400	3.47097200	4.09020700
H	-0.51031300	4.06162200	2.75209400
C	-1.31392200	-1.45923800	1.39200900
H	-1.42616500	-0.58849900	2.04903900
H	-1.74005100	-1.16743800	0.42613300
C	-2.11670700	-2.64781700	1.94039000
H	-2.07198000	-3.51162100	1.27105300
H	-3.16931300	-2.35828100	2.02470900
H	-1.77861500	-2.96955500	2.92787500
C	1.29851300	-1.49783800	2.82012800
H	2.35648600	-1.74538200	2.67588500
H	1.26531800	-0.43715300	3.08175300
C	0.72850600	-2.32530900	3.97912100
H	-0.28964500	-2.01931100	4.23448600
H	1.34731000	-2.17464700	4.87158600
H	0.71978500	-3.39822900	3.76610600

C	0.76786400	-3.46286600	0.79088100
H	1.84338600	-3.65507000	0.86731200
H	0.29423000	-4.00613200	1.61487200
C	0.23647800	-3.98568400	-0.54617500
H	-0.83215600	-3.78302600	-0.67279000
H	0.37640900	-5.07113600	-0.60561500
H	0.76421400	-3.53512100	-1.39184900
C	3.86215800	0.71980100	1.34022200
H	3.60258500	1.76880400	1.16052700
H	3.20027200	0.37124500	2.13637800
C	5.32125800	0.61349200	1.80097400
H	5.58332600	-0.40723000	2.09346900
H	5.47141900	1.25325400	2.67846500
H	6.02814900	0.94196500	1.03339100
C	4.02095000	-1.91876300	-0.03284800
H	3.79140100	-2.23253400	0.99147800
H	3.39913500	-2.53522000	-0.68872400
C	5.49977700	-2.18271700	-0.35030900
H	5.73027500	-1.98485500	-1.40098500
H	5.72396500	-3.23894900	-0.16069700
H	6.18017800	-1.58740600	0.26273800
C	4.45962400	0.54860700	-1.49819900
H	5.47807200	0.42964600	-1.11326700
H	4.39276800	-0.09238200	-2.38149100
C	4.21856400	2.00855800	-1.88498100
H	3.23336000	2.13627200	-2.33760700
H	4.97446700	2.32516200	-2.61327300
H	4.29685200	2.67708100	-1.02190300
C	-5.17678800	-0.14906900	0.54841900
O	-3.55073000	-0.88125400	-1.36878200
O	-6.00041300	-0.76534100	-1.86341600
O	-4.68624200	1.34267100	-1.55324600
F	-4.16064000	0.37691500	1.26424000
F	-5.36306600	-1.41315700	0.97873700
F	-6.28702500	0.55051500	0.84291800
P	0.46264400	1.94017500	0.52691600
P	0.53044500	-1.64200700	1.12433200
P	3.33593800	-0.18435700	-0.20265400
S	-4.81488100	-0.10601200	-1.27351100
Ru	1.09216900	-0.14391900	-0.59420600
H	1.30632500	-1.45585500	-1.59378700
C	0.92309300	-0.46117500	-2.86762400
O	1.09982300	0.79966400	-2.55063500
C	-0.51113000	-0.91620400	-3.11358200

H	-0.58471800	-2.00281300	-3.21041000
H	-1.19184700	-0.57942800	-2.32616800
H	-0.84974700	-0.46399600	-4.05605300
C	1.94240400	-1.10428300	-3.79962300
H	1.85815500	-2.19408900	-3.81094000
H	1.73561800	-0.73826600	-4.81413300
H	2.96131000	-0.82043000	-3.53940600

86

I8, total electronic energy = -2986.7989835, thermal corrections to Gibbs free energy = 0.649274

C	-1.35334500	0.46287400	2.65074300
H	-2.03634100	1.20668400	2.22703800
H	-1.66722800	-0.49331500	2.22840300
C	-1.48990700	0.41673400	4.17775600
H	-0.84521100	-0.34860000	4.62120600
H	-2.52385800	0.16049400	4.43851800
H	-1.25959200	1.37229300	4.65426700
C	0.50500800	2.67714700	1.94174700
H	1.57834000	2.87651900	2.01483100
H	0.20279900	2.99563100	0.94211100
C	-0.24764700	3.46929800	3.01739500
H	-1.32972400	3.31770500	2.95692900
H	-0.06284100	4.54059300	2.87114000
H	0.07256400	3.21843200	4.03207900
C	1.58176000	0.16330800	3.09135200
H	1.23604900	-0.83106700	3.39207100
H	2.49076000	0.00690700	2.50285200
C	1.92617600	1.00300000	4.32912600
H	2.31669100	1.98792900	4.05696800
H	2.70524400	0.49199900	4.90723700
H	1.06944200	1.14969300	4.99007100
C	-0.95471000	-3.05614700	1.00084300
H	-1.09576300	-2.57646600	1.97681400
H	-1.80078900	-2.74701400	0.38388400
C	-0.95461200	-4.57957800	1.17525600
H	-0.83381300	-5.10476400	0.22237100
H	-1.91189500	-4.90127800	1.60301200
H	-0.16549700	-4.92151800	1.85186900
C	1.89117700	-2.87603100	1.47254600
H	2.61053100	-2.06926800	1.61410200
H	1.37915900	-2.99716600	2.43427000
C	2.64950300	-4.16449700	1.12639100
H	1.98655900	-5.02572700	1.00938300
H	3.35605900	-4.39948600	1.93142700
H	3.22957900	-4.06096200	0.20398900

C	0.89105400	-3.24863700	-1.26864700
H	1.88573000	-2.95975200	-1.62691400
H	0.94779300	-4.31019100	-1.00958400
C	-0.14641600	-3.03755600	-2.37676700
H	-1.15085000	-3.32927400	-2.05578800
H	0.11054600	-3.64170700	-3.25485900
H	-0.19694800	-1.99261300	-2.69851200
C	3.96227700	-0.70940700	-0.33292200
H	4.11746300	-0.54812800	0.73948100
H	3.60792000	-1.73790400	-0.44578400
C	5.28651300	-0.54443400	-1.09164000
H	5.18003000	-0.80266300	-2.14941100
H	6.04262100	-1.21412200	-0.66564400
H	5.67932600	0.47467400	-1.03181900
C	2.46091900	0.07312700	-2.70754400
H	2.78718300	-0.96406800	-2.84793400
H	1.39714100	0.10215300	-2.96550800
C	3.22872900	1.00177600	-3.65643000
H	2.86925700	2.03282300	-3.59161800
H	3.08509800	0.66784700	-4.69071400
H	4.30403000	1.00483400	-3.45658400
C	3.24768100	2.10641800	-0.64550100
H	3.90426100	2.32859400	-1.49194400
H	2.37435800	2.75897000	-0.72621400
C	4.00984500	2.34589700	0.66485800
H	3.44458300	2.02466100	1.54388200
H	4.21884700	3.41546400	0.78187700
H	4.97024500	1.82219200	0.68135200
C	-4.42626000	0.46332600	-0.78927400
O	-1.95071300	-0.15836700	-0.29349800
O	-3.52304000	-2.00054200	-0.92474800
O	-2.74685400	-0.37629000	-2.66703300
F	-4.13806900	1.74994700	-1.03621000
F	-4.72036500	0.34290700	0.51600200
F	-5.51509500	0.13236200	-1.50023500
P	0.31621700	0.81850400	1.88484700
P	0.56965400	-2.25255900	0.28063900
P	2.55399100	0.39175100	-0.85685600
S	-3.00669300	-0.65329100	-1.24099700
Ru	0.34818500	0.05553100	-0.26034400
O	0.18658100	1.99952800	-1.09890900
C	-0.89712800	2.50241800	-1.83896500
C	-1.55919000	3.68821200	-1.11409100
C	-0.42104400	2.94216500	-3.23543400

H	-1.66809000	1.73632400	-1.99158200
H	-0.83259300	4.49747800	-0.96253500
H	-1.93651400	3.38550200	-0.13172600
H	0.34967400	3.71963600	-3.15193900
H	0.01148600	2.09590800	-3.78132000
H	-1.24568800	3.34595000	-3.83784800
H	-2.40200100	4.09530200	-1.68754600

105

TS6, total electronic energy = -3314.25557, thermal corrections to Gibbs free energy = 0.824398

C	-0.59715400	2.19084100	2.32986400
H	0.34121600	2.60894200	1.96344900
H	-1.37651700	2.57726900	1.67268400
C	-0.88190400	2.67981700	3.75618700
H	-1.84602100	2.32249100	4.12955600
H	-0.92249300	3.77554400	3.74952800
H	-0.10852600	2.38617000	4.46862600
C	1.20609300	-0.15440100	2.53182100
H	1.13119100	-1.21597700	2.79116600
H	1.79263500	-0.09242300	1.61312800
C	1.91942200	0.62287800	3.64560600
H	2.04638600	1.67697500	3.38258800
H	2.92093300	0.20233100	3.79393200
H	1.39627300	0.56857100	4.60253600
C	-1.67664900	-0.38779900	3.24610500
H	-2.57257600	0.24219500	3.23543000
H	-1.97442900	-1.35657700	2.85134700
C	-1.18181000	-0.59102000	4.68526300
H	-0.31762600	-1.26069600	4.72403200
H	-1.98177200	-1.05622400	5.27295200
H	-0.91071000	0.34332600	5.17936100
C	-1.87988300	2.97756100	-1.13594100
H	-1.31703700	3.34128900	-0.27563400
H	-1.14582900	2.85599000	-1.93742700
C	-2.94199400	4.00864300	-1.53586700
H	-3.49827000	3.71316900	-2.43057300
H	-2.45176100	4.96365000	-1.75893700
H	-3.66227500	4.19241300	-0.73292700
C	-3.79499900	1.57570100	0.59306200
H	-3.73645300	0.75687500	1.31262200
H	-3.48214200	2.47862400	1.12934900
C	-5.24678600	1.73397600	0.12259600
H	-5.37267300	2.56816700	-0.57244600
H	-5.88875800	1.92681900	0.98986500
H	-5.61929000	0.82848700	-0.36608800

C	-3.41958000	0.79575100	-2.22857800
H	-3.93864600	-0.14334600	-2.02305000
H	-4.19715200	1.55089900	-2.37581200
C	-2.56922900	0.68076300	-3.49863400
H	-2.12617200	1.64286700	-3.77465000
H	-3.19160300	0.35151900	-4.33818300
H	-1.75457400	-0.04164800	-3.38761200
C	-3.68552800	-2.01557100	0.68772300
H	-3.53921300	-1.61920400	1.69402800
H	-4.23481000	-1.24838700	0.13194300
C	-4.52724500	-3.29615700	0.75769500
H	-4.81447100	-3.65439800	-0.23422800
H	-5.45128400	-3.09112700	1.31048400
H	-4.00866000	-4.10765100	1.27676500
C	-2.51054100	-2.66288700	-1.87475700
H	-3.46603500	-2.16564000	-2.06666300
H	-1.79427100	-2.22223800	-2.57021500
C	-2.65582000	-4.16110600	-2.17911100
H	-1.71306100	-4.70327000	-2.06985200
H	-2.98283600	-4.28088900	-3.21862200
H	-3.39837200	-4.64948700	-1.54349500
C	-1.23015200	-3.64963800	0.56888700
H	-1.86980600	-4.49176000	0.28992400
H	-0.28658300	-3.77185600	0.03257500
C	-0.97923500	-3.68571400	2.07778900
H	-0.28740300	-2.90428300	2.40044400
H	-0.53820000	-4.65119000	2.35117600
H	-1.90540500	-3.57871100	2.65121700
C	1.94465600	3.95906400	-0.21946800
O	0.80103300	1.60469900	-0.33164200
O	1.41885400	2.70098400	-2.49198400
O	3.21472400	1.80486500	-0.98446000
F	2.30508300	3.76421600	1.06239200
F	0.77185300	4.61154300	-0.22931400
F	2.86483800	4.74237700	-0.79934500
P	-0.50229700	0.35290500	2.00027100
P	-2.46401300	1.26248200	-0.69745500
P	-2.01460900	-2.11420100	-0.14038900
S	1.84493100	2.33345300	-1.12685300
Ru	-0.66424600	-0.19218100	-0.25680700
O	1.19904100	-1.43944900	-0.76772200
C	0.99384500	-1.51345900	-2.17928400
C	2.06192700	-0.80470000	-3.02446000
C	0.84080000	-2.95609300	-2.68458300

H	0.03866700	-0.98202200	-2.41164200
H	3.00519100	-1.35847000	-3.01123900
H	2.25569600	0.20928500	-2.68251700
H	1.80744300	-3.47102300	-2.66394000
H	0.14174600	-3.53256000	-2.07991700
C	4.33969900	-2.82302400	-0.94366500
C	5.12583600	-1.51997700	-1.05180600
C	4.62753600	-0.93192700	1.14201000
C	3.83010200	-2.21171300	1.35752300
H	5.95989800	-1.66635400	-1.74407200
H	5.01076200	-3.63190100	-0.63293000
H	3.89520100	-3.09135200	-1.90419700
H	5.09202100	-0.63782900	2.08745600
H	3.98003400	-0.11268800	0.79895700
H	4.49473100	-2.98950000	1.75107700
H	3.01706800	-2.05868100	2.06665500
H	4.49261500	-0.70952300	-1.43564700
N	3.24491800	-2.72243400	0.07593000
O	5.67984500	-1.14523300	0.20544700
C	2.64914700	-4.06273500	0.31407700
H	1.85766500	-3.97128400	1.05965500
H	2.23126800	-4.44449500	-0.61738400
H	3.41514600	-4.75363300	0.67904500
H	2.30230200	-2.03342100	-0.33196700
H	0.48812800	-2.96767900	-3.72256800
H	1.72953300	-0.75710700	-4.06887600

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I9, total electronic energy = -2142.6143573, thermal corrections to Gibbs free energy = 0.697521

C	-0.90942300	2.83883100	1.43115800
H	-1.83781200	2.88004700	0.85396900
H	-1.07301600	2.06329700	2.18444000
C	-0.64410400	4.17279700	2.13944900
H	0.25232200	4.12952300	2.76647500
H	-1.48759100	4.41134300	2.79967300
H	-0.52770100	5.00734900	1.44421500
C	0.12965800	3.08662300	-1.33311000
H	1.07114500	2.98597400	-1.88690400
H	-0.61149300	2.50946400	-1.89555900
C	-0.31461600	4.55491000	-1.30199000
H	-1.28396500	4.67067000	-0.80759900
H	-0.42835400	4.92541700	-2.32846600
H	0.40302500	5.20472400	-0.79619800
C	2.00835700	2.69917900	0.95040200
H	1.94925700	2.52498800	2.03213600

H	2.74853700	1.98860900	0.57360200
C	2.51173900	4.12217500	0.67426200
H	2.63032300	4.30548000	-0.39828700
H	3.49657800	4.26069400	1.13753900
H	1.84864300	4.89110700	1.07681200
C	-0.25970400	-0.49045200	3.16611500
H	0.16836100	0.49875600	3.36777200
H	-1.26196100	-0.31105100	2.76547300
C	-0.37239800	-1.28914900	4.47292600
H	-0.87945600	-2.24659500	4.32353400
H	-0.96495100	-0.71806900	5.19816800
H	0.59769700	-1.49224400	4.93189200
C	2.51572000	-0.86241900	2.20516400
H	3.10882900	-1.38870700	1.44845100
H	2.67766600	0.20491200	2.02779200
C	3.02179500	-1.23098200	3.60583900
H	2.54301100	-0.62961900	4.38387400
H	4.10054500	-1.04266100	3.66864500
H	2.86210200	-2.28678800	3.84507700
C	0.63732000	-3.03102800	1.99316000
H	1.39083300	-3.48010200	1.33742800
H	0.96411900	-3.22605200	3.02037200
C	-0.72423900	-3.68974800	1.75034200
H	-1.51405500	-3.23886000	2.36077200
H	-0.67821000	-4.75540500	2.00422000
H	-1.02789500	-3.60532700	0.70354800
C	3.28251300	0.20958100	-1.53547400
H	2.90303400	1.21688700	-1.74295900
H	3.65249400	0.23450300	-0.50417700
C	4.44152400	-0.11261900	-2.48677700
H	4.93531000	-1.05284300	-2.22495400
H	5.19979700	0.67815100	-2.43051000
H	4.11826300	-0.17873500	-3.53050000
C	2.47325600	-2.61371000	-1.27234800
H	3.23147800	-2.53162800	-0.48409300
H	1.65506200	-3.20466200	-0.85154900
C	3.05095600	-3.36765000	-2.47902300
H	2.28426600	-3.57018600	-3.23286900
H	3.44520300	-4.33686300	-2.14980600
H	3.86787100	-2.83163900	-2.96799100
C	1.24670300	-0.93483700	-3.29296200
H	2.10475900	-1.24769300	-3.89679100
H	0.49819400	-1.73214800	-3.36980600
C	0.67174900	0.37085900	-3.84878700

H	-0.21907300	0.68614800	-3.29722200
H	0.38365100	0.24223200	-4.89894000
H	1.40029200	1.18754000	-3.80660800
P	0.36316700	2.11848900	0.25788100
P	0.73237300	-1.18153100	1.72504300
P	1.76131600	-0.88600800	-1.49177200
Ru	-0.06502400	-0.29449800	-0.19785100
H	-0.60885400	-1.78849100	-0.61915700
O	-2.02366200	0.35902000	-0.14200600
C	-3.17651100	-0.42237500	-0.33088100
C	-4.37204400	0.19539900	0.42202000
C	-3.52932600	-0.57071400	-1.82396000
H	-3.02733100	-1.44249000	0.07153300
C	-5.67586900	-0.59173500	0.20945800
H	-4.50389800	1.22810000	0.06611100
H	-4.13253700	0.25746600	1.49167400
C	-4.83010200	-1.35790200	-2.05315900
H	-3.62773000	0.43849400	-2.25202300
H	-2.69000600	-1.05581400	-2.33888400
C	-6.00636000	-0.73901900	-1.28314900
H	-6.50500100	-0.10270300	0.73689900
H	-5.57318500	-1.59226500	0.65474900
H	-5.06005500	-1.40681800	-3.12534400
H	-4.68932100	-2.39629700	-1.71895600
H	-6.91086700	-1.34638600	-1.41584600
H	-6.23039200	0.25266900	-1.70271300

86

TS7, total electronic energy = -2142.6062193, thermal corrections to Gibbs free energy = 0.698251

C	0.82667300	3.30409100	-0.05392500
H	1.89611700	3.29349600	-0.28834900
H	0.32194700	3.14167200	-1.00985700
C	0.44235100	4.67767100	0.50966800
H	-0.62732500	4.74724000	0.73130800
H	0.66861700	5.45544700	-0.23074400
H	0.99098300	4.92631000	1.42175100
C	1.95603500	1.62757900	2.11190900
H	1.61490000	1.02503300	2.96247400
H	2.68555500	1.00516400	1.58394500
C	2.65665900	2.89740800	2.61235500
H	3.04961800	3.49484400	1.78365800
H	3.50969000	2.62423000	3.24626800
H	1.99972700	3.53724300	3.20569000
C	-0.95012700	2.23342300	2.04698700
H	-1.64931800	2.76924000	1.39439400

H	-1.44617300	1.29497700	2.30172000
C	-0.71812200	3.03252300	3.33551600
H	-0.05791900	2.50018100	4.02754200
H	-1.67426900	3.18323800	3.85252400
H	-0.28725700	4.01896300	3.15034400
C	-2.31795400	1.88502300	-1.85247100
H	-1.98879900	2.61566500	-1.10506600
H	-1.54947500	1.89141300	-2.63298900
C	-3.67137300	2.31300000	-2.43118900
H	-4.04406500	1.60902200	-3.18192200
H	-3.57692000	3.29030800	-2.92052500
H	-4.43555500	2.41150300	-1.65409200
C	-3.47880700	0.29386700	0.32818000
H	-3.12280100	-0.35294300	1.13539100
H	-3.43544700	1.31588800	0.72129500
C	-4.93147000	-0.07784900	0.00097500
H	-5.35755300	0.54010800	-0.79401700
H	-5.55552000	0.05866900	0.89272000
H	-5.02506900	-1.12512000	-0.30277500
C	-2.95682200	-0.92232600	-2.27371300
H	-2.99284700	-1.91641000	-1.81441300
H	-3.99406500	-0.60749800	-2.42413400
C	-2.24824000	-1.00301200	-3.62937200
H	-2.21509400	-0.03027500	-4.13173700
H	-2.77907900	-1.69689400	-4.29194400
H	-1.22064600	-1.36255900	-3.52399900
C	-0.73494800	-1.33481500	2.90346000
H	0.03913500	-0.63045800	3.22696600
H	-1.65176900	-0.74578100	2.79228400
C	-0.94953600	-2.40348400	3.98261700
H	-1.80232900	-3.04903000	3.75327500
H	-1.15641800	-1.92332400	4.94701100
H	-0.07090000	-3.04170600	4.11920700
C	-1.61884100	-3.08841900	0.73546400
H	-2.54923800	-2.64425300	1.11082900
H	-1.68744100	-3.06615000	-0.35466600
C	-1.51360100	-4.55040100	1.19126400
H	-0.65389900	-5.05289000	0.73696000
H	-2.41116200	-5.09765000	0.87781100
H	-1.42869500	-4.65705900	2.27571800
C	1.19739600	-2.99111300	1.51231200
H	0.85342500	-3.83473300	2.11843300
H	1.50129800	-3.39974700	0.54180100
C	2.39374700	-2.32755800	2.20112000

H	2.76302400	-1.46963500	1.63226600
H	3.21887500	-3.04280000	2.30054400
H	2.13954400	-1.97929800	3.20797400
P	0.48780800	1.74058700	0.93986700
P	-2.16000000	0.21730800	-1.01783000
P	-0.25453300	-1.85987500	1.16755000
Ru	0.12740000	-0.26331000	-0.46779700
H	-0.05736000	-1.57759300	-1.43030500
O	0.93620900	0.87962700	-2.20096700
C	1.97580700	0.15353900	-1.94433200
C	2.28873800	-1.00841300	-2.89826800
C	3.25507800	0.86046700	-1.47123100
H	1.75586000	-0.67261000	-0.41755800
C	3.39797400	-1.95168900	-2.41697900
H	2.62785100	-0.51461600	-3.82353500
H	1.37057500	-1.54645500	-3.13652300
C	4.38049400	-0.08129500	-1.01866300
H	3.59774900	1.43352700	-2.34744300
H	3.01751000	1.58727400	-0.69446300
C	4.67242300	-1.17621700	-2.05424300
H	3.61234400	-2.69290300	-3.19679900
H	3.04679100	-2.51010600	-1.53918600
H	5.28585000	0.50537000	-0.81923600
H	4.09615500	-0.55165300	-0.06843200
H	5.43930800	-1.86105400	-1.67179800
H	5.08638100	-0.71650400	-2.96324300

86

I10, total electronic energy = -2142.6094641, thermal corrections to Gibbs free energy = 0.697418

C	1.23681400	3.17785700	-0.43012600
H	2.31718000	3.03053900	-0.53660800
H	0.81154900	2.89023500	-1.39505300
C	0.94704200	4.65726600	-0.14882200
H	-0.12598500	4.85744400	-0.06591600
H	1.32517300	5.26950100	-0.97738300
H	1.42681100	5.01454100	0.76601200
C	1.99199800	1.81293300	2.08119500
H	1.53366300	1.36260500	2.97023900
H	2.71018700	1.07318600	1.71289500
C	2.75008500	3.09057300	2.46357200
H	3.25746800	3.53134900	1.59970100
H	3.52306400	2.85301200	3.20525000
H	2.10253600	3.85439400	2.89923900
C	-0.82664000	2.65208800	1.61916200
H	-1.40935000	3.11531300	0.81401400

H	-1.43419600	1.81981200	1.98008700
C	-0.63357200	3.64938000	2.76855500
H	-0.09659700	3.19727900	3.60839100
H	-1.61303500	3.96968700	3.14576600
H	-0.09055100	4.54708600	2.46481300
C	-1.93186000	1.71835900	-2.32771800
H	-1.59007500	2.53452500	-1.68050400
H	-1.11063900	1.53199400	-3.02609700
C	-3.19426200	2.14860500	-3.08267400
H	-3.57321500	1.36026600	-3.74086800
H	-2.97396700	3.01914400	-3.71300400
H	-4.00237800	2.43626100	-2.40323200
C	-3.36213700	0.64107200	-0.00463600
H	-3.11996900	0.11883200	0.92493700
H	-3.23727200	1.70821800	0.21015700
C	-4.82535200	0.35127200	-0.36568000
H	-5.14417700	0.85885700	-1.27999800
H	-5.47833600	0.69627700	0.44539600
H	-5.00938600	-0.71955800	-0.49645900
C	-2.83329000	-1.05333400	-2.31388800
H	-3.02210200	-1.93226000	-1.68756400
H	-3.81221100	-0.66155300	-2.60689600
C	-2.05569100	-1.46922000	-3.56564400
H	-1.84157400	-0.61575100	-4.21781800
H	-2.64004200	-2.19026700	-4.14962100
H	-1.10439700	-1.94378900	-3.31020700
C	-1.04914400	-0.75333800	3.05647300
H	-0.22306600	-0.09569100	3.34860700
H	-1.86409600	-0.09265500	2.74238900
C	-1.50633600	-1.58276800	4.26285500
H	-2.41417300	-2.15261700	4.04531300
H	-1.73450000	-0.91828600	5.10519700
H	-0.73902800	-2.28573200	4.60158000
C	-1.93802500	-2.74764600	1.09685400
H	-2.83448400	-2.13812200	1.26290500
H	-1.87714800	-2.91873200	0.01947800
C	-2.08776900	-4.10304400	1.80189600
H	-1.26157600	-4.77804800	1.55825200
H	-3.01218400	-4.58818900	1.46556000
H	-2.14138900	-4.01747800	2.89018200
C	0.77317500	-2.83941800	2.18067600
H	0.25467800	-3.52846700	2.85381300
H	1.12055000	-3.43013000	1.32568900
C	1.96726800	-2.22133000	2.91385300

H	2.51861700	-1.52685600	2.27356700
H	2.66167600	-3.00837900	3.23060600
H	1.65583000	-1.67824300	3.81237900
P	0.64741800	1.85277000	0.76770800
P	-1.98800000	0.21169900	-1.22172200
P	-0.47780200	-1.62891600	1.50151900
Ru	0.25070800	-0.35045100	-0.31155300
H	0.07442900	-1.81820600	-1.01913400
O	0.99392000	0.56236900	-2.19529500
C	1.93688300	-0.27341000	-1.93790000
C	2.07921200	-1.51216500	-2.82818700
C	3.29688000	0.25872800	-1.46994100
H	1.65556500	-0.80492800	0.36123300
C	3.02575100	-2.58609000	-2.27547400
H	2.50428500	-1.13246200	-3.77361100
H	1.09476100	-1.91851900	-3.06182400
C	4.26706200	-0.81551200	-0.95511900
H	3.74148900	0.73042700	-2.36302000
H	3.16107100	1.05021900	-0.73233800
C	4.39935500	-1.99371900	-1.93023700
H	3.13406200	-3.39434300	-3.00948100
H	2.58130900	-3.03140300	-1.37564400
H	5.24938200	-0.36122000	-0.77387600
H	3.90727200	-1.18875900	0.01196400
H	5.05046900	-2.76556000	-1.50134000
H	4.88658500	-1.65003700	-2.85427100

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TS8, total electronic energy = -4392.4687599, thermal corrections to Gibbs free energy = 0.897913

C	3.65644000	1.62019100	0.64835800
H	3.98948700	1.11378800	-0.26329300
H	2.93371700	2.36804300	0.32266000
C	4.83067600	2.31764200	1.34659400
H	4.51150500	2.86378500	2.24009000
H	5.27046400	3.05250000	0.66087600
H	5.62524500	1.62762200	1.63875600
C	3.70508400	-1.20878600	1.53322500
H	3.45158600	-1.77598200	2.43365300
H	3.31858000	-1.77526700	0.68891700
C	5.22871300	-1.10151000	1.39795500
H	5.51246800	-0.57585300	0.48312600
H	5.65307000	-2.11145200	1.33591900
H	5.69907200	-0.60140900	2.24777500
C	2.73502500	0.90971300	3.36075300
H	2.68044300	2.00190000	3.33126800

H	1.81235100	0.57287000	3.83804900
C	3.92852200	0.48568600	4.22639600
H	4.00755000	-0.60194500	4.31445200
H	3.80150500	0.88521300	5.23991900
H	4.87831300	0.86418200	3.84161800
C	0.31043200	3.15736300	2.00007900
H	0.94240700	2.95306700	2.86863600
H	0.97956400	3.24411400	1.14378200
C	-0.41882100	4.49405300	2.21502000
H	-0.80748800	4.89840800	1.27988100
H	0.29232100	5.22911800	2.61142300
H	-1.24565200	4.42737600	2.92429600
C	-1.15261300	1.14029800	3.51755700
H	-1.97390200	0.42474200	3.42288200
H	-0.31376800	0.59493400	3.95541600
C	-1.57072200	2.25919500	4.47983100
H	-0.75198500	2.95495500	4.68392900
H	-1.86801800	1.81634500	5.43797100
H	-2.42442600	2.83535700	4.11039800
C	-2.34001200	2.06377600	1.10231300
H	-2.82753800	1.10869000	0.88203800
H	-2.89107400	2.54012600	1.92161700
C	-2.39871600	2.94554300	-0.14999900
H	-2.16394900	3.98873000	0.06940900
H	-3.41277800	2.92535200	-0.56649200
H	-1.71367200	2.60767800	-0.92778400
C	0.61428300	-2.13547500	3.44075400
H	1.67699700	-2.34607400	3.29771100
H	0.56161500	-1.16058900	3.92955600
C	-0.00441600	-3.18875100	4.36937700
H	-1.03418800	-2.93856700	4.64013400
H	0.57373500	-3.23794800	5.29993200
H	-0.00502900	-4.19070200	3.93102500
C	-1.96185800	-2.01496000	2.08800900
H	-2.09213600	-1.49928900	3.04369500
H	-2.46795400	-1.41296200	1.32815700
C	-2.64604200	-3.38774100	2.17416600
H	-2.70858900	-3.88070600	1.19968500
H	-3.67502000	-3.25099900	2.52906100
H	-2.15174300	-4.07448100	2.86558700
C	0.27972400	-3.53241700	0.87551300
H	-0.57952300	-4.19391300	1.00987200
H	0.34617100	-3.30054500	-0.18739500
C	1.54640000	-4.28232200	1.30817600

H	2.44791400	-3.67767100	1.20801600
H	1.67456400	-5.16503800	0.67109400
H	1.48632500	-4.63347600	2.34190700
C	1.29590900	4.33872900	-1.66611200
O	0.91947600	1.86734700	-0.90001300
O	-0.21260200	2.65260800	-2.99174600
O	2.26862700	2.28514700	-2.97342900
F	2.33959200	4.44781000	-0.82138400
F	0.20823400	4.82366300	-1.04189400
F	1.54308300	5.11857800	-2.73075800
P	2.65589000	0.34087500	1.57106100
P	-0.66578100	1.57277600	1.76089800
P	-0.11785600	-1.90600600	1.73302000
S	1.04090400	2.57507100	-2.21455400
Ru	0.49247500	-0.02281600	0.47990500
O	-3.33406100	-0.52018200	-0.49293000
C	-2.39005100	-0.81376100	-1.31518000
C	-2.27532200	0.04681900	-2.58023400
C	-2.18550300	-2.31728800	-1.56195500
H	-1.00936500	-0.42693100	-0.55746800
C	-1.23790700	-0.40344200	-3.61472300
H	-3.27803100	-0.02950300	-3.03194900
H	-2.12869500	1.09365000	-2.31500600
C	-1.14994600	-2.70479900	-2.62163100
H	-3.17921700	-2.64954500	-1.90203800
H	-2.00750900	-2.82932800	-0.61586800
C	-1.33915300	-1.90289800	-3.91390600
H	-1.37510800	0.18536100	-4.53013900
H	-0.22873600	-0.18672000	-3.25609400
H	-1.22561900	-3.78276900	-2.81652400
H	-0.14348200	-2.51601800	-2.24227900
H	-0.57844300	-2.19107100	-4.64839600
H	-2.31888300	-2.13458900	-4.35928300
H	-4.78445000	0.07603600	-0.82665000
C	-6.34611300	0.81964600	0.36516700
C	-6.29664600	-0.28975700	1.40978100
C	-6.45944700	-1.96052400	-0.21825300
C	-6.53288600	-0.94312900	-1.35021500
H	-6.76783900	0.06833800	2.32892500
H	-7.37464400	1.15057700	0.19763300
H	-5.73480800	1.67306000	0.66696100
H	-7.04082400	-2.84452400	-0.49200700
H	-5.41461800	-2.26059800	-0.05482400
H	-7.56965700	-0.67585100	-1.57171500

H	-6.05495600	-1.32468700	-2.25523500
H	-5.25336600	-0.55493800	1.63385500
N	-5.82079200	0.32086600	-0.95274600
O	-7.02022400	-1.43839900	0.98208700
C	-5.92225100	1.36300300	-2.01221300
H	-5.50805500	0.96214400	-2.93795300
H	-5.35299500	2.23861100	-1.69791900
H	-6.97139900	1.62822500	-2.15435000
C	3.10916900	-3.26940900	-2.09649200
O	1.66835900	-1.40228500	-0.98960700
O	3.94462400	-0.79438200	-1.86219200
O	2.06468000	-1.28402200	-3.45971000
F	2.01794700	-4.05521000	-2.13458800
F	3.80898100	-3.58328700	-0.99081500
F	3.87074400	-3.56382300	-3.16240200
S	2.65378700	-1.46033000	-2.12132100

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TS9, total electronic energy = -3296.5481995, thermal corrections to Gibbs free energy = 0.785962

C	-0.00575400	-2.48894600	-1.94202700
H	0.40077500	-1.85583900	-2.73842800
H	0.67269200	-2.37017900	-1.09112600
C	-0.00343400	-3.95825000	-2.38377600
H	-0.38393300	-4.61997200	-1.59950100
H	1.02465000	-4.26972900	-2.60292500
H	-0.59827400	-4.12394900	-3.28530000
C	-2.37659700	-1.09967100	-3.04781500
H	-3.45145400	-0.98947500	-2.86454600
H	-1.97530500	-0.09135800	-3.17502500
C	-2.13808900	-1.90816000	-4.33032500
H	-1.07286500	-1.98311800	-4.56897000
H	-2.62346900	-1.40079700	-5.17288200
H	-2.54502800	-2.92034000	-4.27870400
C	-2.73650900	-3.06647000	-0.84888700
H	-2.12278700	-3.69165900	-0.19175800
H	-3.47428900	-2.58221400	-0.20455800
C	-3.47194400	-3.94085000	-1.87290800
H	-4.13169700	-3.34715700	-2.51260400
H	-4.09973900	-4.66708600	-1.34287400
H	-2.79064500	-4.50312900	-2.51530500
C	0.16452200	-2.64793700	1.79466600
H	-0.20489800	-3.25095200	0.95928800
H	1.12130900	-2.22952400	1.46267700
C	0.37521500	-3.54942600	3.01795100
H	0.71989300	-2.99139600	3.89362000

H	1.13773300	-4.30389400	2.79074300
H	-0.53927900	-4.08266600	3.29438400
C	-2.60119200	-2.02165900	2.56088000
H	-3.42846100	-1.41552700	2.18699000
H	-2.66146800	-2.97875900	2.03251800
C	-2.80521400	-2.24360300	4.06583300
H	-2.01314800	-2.84559500	4.51805000
H	-3.75237700	-2.77238600	4.22618700
H	-2.86421800	-1.29828700	4.61372700
C	-0.37966100	-0.33965700	3.47877500
H	-0.98460700	0.56188900	3.61202300
H	-0.57977200	-0.98413300	4.33923400
C	1.10656600	0.02612000	3.44680800
H	1.74565400	-0.86163300	3.41611500
H	1.37116900	0.58908300	4.35002500
H	1.33751900	0.64724800	2.58178100
C	-4.58273400	0.09321600	-0.00409800
H	-4.55971500	-0.20666900	-1.05667400
H	-4.48036000	-0.82695600	0.57632100
C	-5.92548300	0.75976600	0.32206400
H	-6.03078400	0.95731800	1.39243200
H	-6.74491400	0.09264800	0.03028000
H	-6.06429400	1.70345200	-0.21376800
C	-3.13441700	1.73205600	2.01883700
H	-3.46468400	0.88600400	2.63203500
H	-2.09551500	1.93588700	2.28913400
C	-3.98429400	2.97391600	2.32324200
H	-3.58965500	3.86503800	1.82633700
H	-3.96182000	3.16741000	3.40229700
H	-5.03143200	2.86066400	2.03218900
C	-3.32232300	2.60165400	-0.76680400
H	-4.13962300	3.14911600	-0.28658100
H	-2.42198200	3.21389600	-0.66854900
C	-3.65662700	2.38325000	-2.24521000
H	-2.83160500	1.89689200	-2.76610900
H	-3.83742200	3.35261400	-2.72527000
H	-4.56256700	1.78305000	-2.37836000
P	-1.62354700	-1.68625300	-1.44109500
P	-1.01710600	-1.20937600	1.95112800
P	-3.02784300	1.08056900	0.26889800
Ru	-1.00809800	0.06662000	-0.04533800
O	-0.06274700	1.86687800	0.86717300
C	0.85431400	2.66859100	0.39987200
C	0.50714300	4.16521700	0.47015300

C	2.31964300	2.36031000	0.74686600
H	0.88819000	2.47567000	-0.93769700
C	1.56455500	5.10368200	-0.13131400
H	0.39028900	4.38678900	1.54176600
H	-0.47455300	4.32475700	0.01086900
C	3.33604900	3.31921800	0.11034500
H	2.38597600	2.45331400	1.84089800
H	2.54673700	1.31790500	0.50864500
C	2.97392300	4.78424600	0.38550700
H	1.29792700	6.14289900	0.09682200
H	1.55648100	5.01469800	-1.22518000
H	4.33664300	3.08657700	0.49233000
H	3.37397200	3.15633900	-0.97448600
H	3.70720500	5.45149900	-0.08373300
H	3.02019100	4.97500400	1.46738300
C	0.51027700	1.84210900	-2.05019200
O	-0.65375900	1.31376100	-1.77201600
C	0.45307400	2.98881200	-3.05806100
H	0.19460600	2.57485200	-4.04153300
H	-0.31846500	3.71232700	-2.78248700
H	1.41451000	3.50116500	-3.14977600
C	1.69427800	0.89660100	-2.24446000
H	1.53389100	0.34284800	-3.17894000
H	2.63993600	1.43658700	-2.33328000
H	1.77987100	0.17104300	-1.43130000
C	5.32492600	-0.26160100	-0.03907700
O	3.04628400	-1.54984500	0.11313700
O	4.82258800	-2.44578100	-1.40179500
O	5.08744800	-2.62009100	1.08387900
F	5.08842800	0.39192500	1.11603200
F	4.89586100	0.52402900	-1.04702500
F	6.65715700	-0.39797600	-0.16657100
S	4.47751200	-1.91524100	-0.06462500

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TS10, total electronic energy = -4082.707537, thermal corrections to Gibbs free energy = 0.74921

C	-1.91860000	0.86421600	-2.79020900
H	-1.07722800	0.39924100	-3.31474100
H	-2.42492500	0.04800100	-2.27368600
C	-2.88953800	1.52052500	-3.77916900
H	-3.75907800	1.95002700	-3.27171800
H	-3.26345900	0.75658000	-4.47168700
H	-2.42377700	2.30540700	-4.37891600
C	0.26506500	2.82339200	-2.26888500
H	0.40902200	3.73547800	-1.67929600

H	1.14489400	2.20354100	-2.11053700
C	0.16623800	3.16343500	-3.76124900
H	0.07557100	2.26046900	-4.37044300
H	1.08660700	3.67296900	-4.07186300
H	-0.67064500	3.82461500	-3.99622600
C	-2.37206200	3.23217900	-1.03500200
H	-3.34049400	2.73658700	-0.91334600
H	-2.08802300	3.59965000	-0.04742100
C	-2.51415500	4.43906300	-1.97326400
H	-1.57745600	4.99711400	-2.06055200
H	-3.26386100	5.12522000	-1.56147000
H	-2.83928300	4.16117100	-2.97746500
C	-3.80883400	-0.01908700	0.45497400
H	-4.10539500	0.90400900	-0.05446900
H	-3.41856200	-0.68125600	-0.31656000
C	-5.03813600	-0.66784200	1.10827500
H	-4.79729400	-1.61819600	1.58946100
H	-5.78343900	-0.87741800	0.33174800
H	-5.51322700	-0.02694800	1.85281500
C	-2.88132600	2.01778800	2.36825300
H	-2.13871000	2.20132900	3.14905100
H	-2.76739800	2.82025100	1.63789600
C	-4.28706000	2.10146200	2.97739600
H	-5.06647000	2.07560900	2.21137300
H	-4.38852700	3.05361800	3.51148600
H	-4.48604900	1.30237700	3.69728100
C	-2.37592900	-0.74242800	2.95255800
H	-1.60114800	-0.39080800	3.64244700
H	-3.33433500	-0.59722200	3.46306000
C	-2.17442300	-2.22862600	2.64573700
H	-2.99078500	-2.63547600	2.04649000
H	-2.14160900	-2.79669100	3.58283900
H	-1.25026700	-2.41826400	2.09817400
C	0.23426700	3.87244300	1.51968000
H	0.39390500	4.20768200	0.49016400
H	-0.84570700	3.87783300	1.68351800
C	0.89622100	4.84417000	2.50566600
H	0.64902600	4.59944100	3.54265700
H	0.53401500	5.86120500	2.31539200
H	1.98584200	4.86157000	2.41239900
C	0.64087300	1.69103100	3.42051900
H	-0.21686600	2.26366000	3.78680800
H	0.35790800	0.63981100	3.48261300
C	1.84220000	1.94666100	4.33975700

H	2.69679700	1.31199300	4.08877700
H	1.55685700	1.71460100	5.37274600
H	2.17729700	2.98691600	4.31970900
C	2.61012300	2.18211400	1.28653200
H	3.07364900	2.47650600	2.23126200
H	2.94005100	1.16469800	1.06438800
C	3.09079500	3.13313300	0.18504000
H	2.67085400	2.88688300	-0.78837400
H	4.18102700	3.06461400	0.09884700
H	2.84720100	4.17570700	0.40882000
C	-2.84559100	-3.30687000	-1.40552700
O	-1.19413400	-1.36571600	-0.83691500
O	-0.56835300	-3.68635100	-0.11347800
O	-0.51546700	-3.06340000	-2.54616600
F	-3.46473500	-2.49196100	-2.27955600
F	-3.52388600	-3.25641500	-0.24514000
F	-2.92383700	-4.56157400	-1.87431600
P	-1.13114300	1.89476800	-1.44714700
P	-2.33667700	0.44627400	1.51297700
P	0.76373800	2.08591900	1.58297200
S	-1.05734400	-2.81681700	-1.20144600
Ru	-0.32637400	0.46217000	0.28251500
H	0.42139500	-0.78072000	1.46284000
H	1.00623000	-1.28052100	1.84857300
C	3.32849600	-1.73682600	2.80631000
C	4.04817200	-1.97594600	1.48423500
C	2.66954600	-3.77903100	0.96484600
C	1.88192100	-3.62142500	2.25912700
H	5.09872200	-1.68555300	1.58403400
H	3.86584000	-2.26091600	3.61239800
H	3.31659500	-0.66846400	3.04487400
H	2.69890100	-4.83670600	0.68552500
H	2.20041800	-3.21613600	0.14998500
H	2.30048200	-4.28907500	3.02868300
H	0.83647400	-3.89249300	2.09093000
H	3.59543100	-1.37630300	0.68386800
N	1.93097500	-2.22388900	2.75386000
O	4.02384300	-3.35508700	1.13277900
C	1.30708200	-2.13228100	4.08236400
H	0.26446000	-2.45012100	4.02079100
H	1.34816200	-1.10100100	4.43972100
H	1.82808000	-2.77360500	4.80779000
C	3.82795600	0.36928000	-2.25736600
O	1.63175400	0.20533300	-0.86829800

O	1.49960300	-0.17607000	-3.34573100
O	2.57259700	-1.89758300	-1.84853100
F	4.50506800	0.38120500	-1.09546200
F	3.66833400	1.64141500	-2.66366700
F	4.57821700	-0.26432700	-3.17160000
S	2.18522800	-0.49646100	-2.08095100

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TS11, total electronic energy = -3104.642395, thermal corrections to Gibbs free energy = 0.728958

C	-0.68079300	-0.48280900	2.94669000
H	-1.44687200	0.29250200	2.83466800
H	-1.03470400	-1.32547000	2.35047800
C	-0.56294300	-0.91012700	4.41472100
H	0.16066700	-1.72092400	4.54451400
H	-1.53433000	-1.28501000	4.75960500
H	-0.27499200	-0.08965200	5.07582800
C	0.96784700	1.95580100	2.57833600
H	2.02311900	2.22555700	2.45784100
H	0.42398700	2.50035400	1.80217200
C	0.46277900	2.39010300	3.95958500
H	-0.60153300	2.17147400	4.08882800
H	0.58663100	3.47467100	4.06684900
H	1.00834300	1.91483400	4.77822200
C	2.27587100	-0.70022900	2.83951800
H	1.99503200	-1.75848600	2.89897600
H	3.08551900	-0.64065600	2.10972600
C	2.80581500	-0.21032600	4.19370900
H	3.14482100	0.82876700	4.14024900
H	3.66953400	-0.81909300	4.48718400
H	2.06468400	-0.28411000	4.99187100
C	0.26071700	-3.32887100	0.48172100
H	0.81537700	-3.35817600	1.42789200
H	-0.69112000	-2.84598700	0.69897100
C	0.00333700	-4.75419100	-0.02566100
H	-0.60003400	-4.75769900	-0.93691700
H	-0.55389300	-5.31382700	0.73527700
H	0.92365400	-5.30603000	-0.22969800
C	2.99145700	-2.57697600	-0.24614600
H	3.59307600	-2.00646000	-0.95982300
H	3.21440100	-2.16955000	0.74268200
C	3.41569900	-4.05121100	-0.28738100
H	2.92129800	-4.64088600	0.48943400
H	4.49555800	-4.12182700	-0.11020700
H	3.21386800	-4.52124100	-1.25431300
C	1.05976900	-2.82005800	-2.33875700

H	1.87567100	-2.36061600	-2.90750500
H	1.28441900	-3.88984500	-2.28363200
C	-0.26613400	-2.60637800	-3.07176200
H	-1.11167300	-3.03886900	-2.53156100
H	-0.22344400	-3.07948300	-4.05993900
H	-0.47755700	-1.54399500	-3.21994600
C	3.99387400	0.97268100	0.07040000
H	3.71474400	1.45860000	1.01152400
H	4.13365100	-0.08666700	0.30044800
C	5.30959800	1.56157300	-0.45397900
H	5.67021700	1.02724700	-1.33764700
H	6.08342000	1.47555000	0.31787300
H	5.21935500	2.62114400	-0.71089500
C	3.05355700	0.35249200	-2.66531700
H	3.68573600	-0.50579500	-2.41329900
H	2.15078100	-0.05489000	-3.12756000
C	3.77389900	1.24222500	-3.68789200
H	3.12642800	2.04297700	-4.05697900
H	4.06217300	0.63243200	-4.55238000
H	4.68398700	1.69883000	-3.29056300
C	2.40558600	2.90194700	-1.42155600
H	3.29077200	3.13094100	-2.02157000
H	1.52864300	3.03292700	-2.06074400
C	2.32852400	3.86879000	-0.23839100
H	1.40768700	3.72085500	0.32483800
H	2.33612100	4.90098900	-0.60936000
H	3.18159900	3.76291900	0.44014600
C	-3.53415100	-2.55363800	-0.01839900
O	-1.62609200	-0.77564000	0.07911300
O	-3.25567600	-0.65379000	-1.83312600
O	-3.96785200	-0.02065000	0.49150800
F	-3.26433800	-2.87068000	1.26040700
F	-2.87051700	-3.41602100	-0.80869300
F	-4.84758600	-2.72603900	-0.22671600
P	0.82362100	0.17308600	2.04957700
P	1.20947800	-2.13276500	-0.60597300
P	2.48930300	1.08162500	-1.02423400
S	-3.05587100	-0.78903400	-0.37806200
Ru	0.48507500	0.10001100	-0.32983600
H	-0.01683400	0.25645900	-2.03417300
O	-0.40172700	2.15439700	-0.67698400
C	-1.73286400	2.59278100	-0.46580500
C	-1.72907600	3.90625200	0.34108000
C	-2.45902100	2.81574400	-1.80733200

H	-2.30794900	1.85438500	0.11095200
C	-3.14394000	4.47663400	0.53854700
H	-1.10867200	4.63884100	-0.19537800
H	-1.25331900	3.73934300	1.31476200
C	-3.87622900	3.38504300	-1.62464500
H	-1.85570300	3.51365800	-2.40734300
H	-2.50437900	1.86823400	-2.35614000
C	-3.86232400	4.68179100	-0.80267000
H	-3.09380200	5.42221100	1.09369700
H	-3.73129800	3.78376600	1.15843300
H	-4.34257600	3.55831100	-2.60309100
H	-4.49901400	2.63956000	-1.11091500
H	-4.88647900	5.03951400	-0.63580200
H	-3.34465000	5.46702800	-1.37296500
H	-0.27790700	1.05109000	-1.65309400

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TS2-a, total electronic energy = -3065.364798, thermal corrections to Gibbs free energy = 0.697597

C	2.36186600	-2.28844800	-0.78848800
H	2.60001000	-1.77861600	-1.72738700
H	2.68966100	-1.60493400	-0.00452900
C	3.14455000	-3.60252800	-0.66938000
H	2.97496200	-4.09347100	0.29415900
H	4.21840500	-3.38768900	-0.73602100
H	2.90474600	-4.31789200	-1.45901500
C	-0.07189500	-2.89208300	-2.35593100
H	-1.08901300	-3.27441800	-2.21832900
H	-0.17297000	-1.96687200	-2.93202800
C	0.76748600	-3.89136900	-3.16167300
H	1.76945000	-3.50287700	-3.36661500
H	0.28528200	-4.07035100	-4.13069200
H	0.87263100	-4.85800600	-2.66385100
C	0.14681100	-3.69459800	0.53494600
H	0.91218900	-3.59978300	1.31467100
H	-0.80074000	-3.45263500	1.01734500
C	0.08831700	-5.14104900	0.02771400
H	-0.68677700	-5.27043600	-0.73429300
H	-0.15812900	-5.81189300	0.85977000
H	1.03722900	-5.47721300	-0.39590100
C	1.71979700	-0.53571500	2.58514900
H	1.88819100	-1.53298800	2.16463800
H	2.34737400	0.14478000	2.00714400
C	2.13651100	-0.51900100	4.06046000
H	1.95611500	0.45138000	4.53354400
H	3.21095200	-0.72425200	4.13927300

H	1.61695700	-1.28357800	4.64499500
C	-1.03212700	-1.26953000	3.22934100
H	-1.98316600	-1.44189200	2.72526900
H	-0.49399200	-2.22403900	3.19629900
C	-1.32781900	-0.87676200	4.68398900
H	-0.42550500	-0.67546600	5.26581800
H	-1.86183600	-1.69735000	5.17774300
H	-1.96868000	0.00830800	4.74089400
C	-0.28921000	1.54780300	2.98438100
H	-1.34042700	1.81760300	2.83189800
H	-0.15085300	1.40867000	4.06068000
C	0.62026500	2.67937800	2.49576100
H	1.67702200	2.46001200	2.67712300
H	0.37929000	3.60628700	3.02920000
H	0.49730400	2.86700800	1.42622500
C	-3.13823000	-2.31912700	0.31601900
H	-2.66761800	-2.96157400	-0.43574600
H	-2.63701300	-2.54066500	1.26012300
C	-4.62533800	-2.67240900	0.44552300
H	-5.10360300	-2.12680600	1.26385100
H	-4.72623400	-3.74195900	0.66475400
H	-5.18818200	-2.47399700	-0.47110300
C	-3.62681900	0.52321600	1.02082300
H	-3.51706500	0.06704700	2.01166400
H	-3.06621400	1.46158600	1.05578400
C	-5.10474400	0.83464100	0.74706800
H	-5.23684300	1.38852200	-0.18706400
H	-5.49662600	1.46289200	1.55578300
H	-5.72782800	-0.06147800	0.69721400
C	-3.62584200	-0.39834600	-1.75548200
H	-4.67849800	-0.52944500	-1.48716400
H	-3.52022300	0.63084900	-2.09893200
C	-3.26745700	-1.34997000	-2.89881200
H	-2.24754400	-1.18001200	-3.24543800
H	-3.94575900	-1.17514800	-3.74272800
H	-3.37008500	-2.40172700	-2.61370400
C	4.33784200	1.29380400	-0.03979300
O	3.26117200	0.62814400	-2.35837500
O	1.83071500	0.69540100	-0.29294700
O	2.63250000	2.82812000	-1.33498700
F	5.38512800	1.90295800	-0.61574500
F	4.68175800	0.01997000	0.21658800
F	4.09158600	1.90191000	1.13474600
P	0.49616800	-2.30519300	-0.67525700

P	-0.04115800	-0.09998800	2.14297900
P	-2.66227800	-0.57580000	-0.16073700
S	2.84966700	1.37788900	-1.15515400
Ru	-0.39692900	-0.03293900	-0.20032500
O	-0.61482700	0.61076400	-2.28921700
C	-0.63201200	1.73507500	-1.63426100
C	-1.78206500	2.72606000	-1.78375300
H	-0.86607000	1.51398200	0.10174300
H	-1.80992600	2.97232200	-2.85670700
H	-2.74474200	2.26978500	-1.54540700
C	-1.59509500	4.01519200	-0.97687400
H	-1.58285800	3.77665400	0.09572900
H	-0.61319800	4.45121700	-1.20775800
C	-2.68618800	5.05901400	-1.24863500
H	-3.66921500	4.62379400	-1.02100000
H	-2.69836600	5.29819500	-2.32086200
C	-2.50029100	6.34671400	-0.44143400
H	-3.29347800	7.07153800	-0.65673800
H	-2.51774800	6.14625200	0.63676000
H	-1.54120900	6.82538700	-0.67309400
H	0.32704200	2.25044700	-1.50203000

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TS2-b1, total electronic energy = -3142.751496, thermal corrections to Gibbs free energy = 0.733348

C	1.51567000	-1.36768200	-1.54210600
H	1.40337100	-0.76998800	-2.45385800
H	1.85354800	-0.67305700	-0.76845700
C	2.59918900	-2.43688500	-1.73805000
H	2.75117900	-3.02975100	-0.83109200
H	3.54829000	-1.93977200	-1.96567900
H	2.36915100	-3.12214800	-2.55696600
C	-1.03026600	-2.40185300	-2.65521000
H	-1.87751600	-3.03643300	-2.37032800
H	-1.45878900	-1.48102400	-3.05940600
C	-0.19436100	-3.08435800	-3.74598300
H	0.62081300	-2.44073300	-4.08978200
H	-0.83279700	-3.29078700	-4.61362800
H	0.23646400	-4.03373600	-3.42123100
C	-0.01618400	-3.42695200	-0.04079800
H	0.79701700	-3.21400500	0.66346600
H	-0.92428800	-3.51183100	0.56034300
C	0.22601600	-4.76903000	-0.74410700
H	-0.60517900	-5.03116500	-1.40561600
H	0.30546700	-5.56236600	0.00886500
H	1.14554800	-4.77976900	-1.33251300

C	1.33313000	0.06790200	2.03533600
H	1.65652500	-0.96028600	1.83712100
H	1.62025700	0.64981100	1.15524000
C	2.07058400	0.63210200	3.25775300
H	1.83494800	1.68762600	3.42165700
H	3.14988500	0.56098900	3.08578100
H	1.84384700	0.08962800	4.17821900
C	-0.93746900	-1.53902700	3.02201500
H	-2.02514500	-1.53009200	3.15309800
H	-0.71294500	-2.38351300	2.36646800
C	-0.25748800	-1.75945700	4.37951300
H	0.82371800	-1.88700900	4.27735700
H	-0.65091500	-2.67480700	4.83727500
H	-0.44075000	-0.94046300	5.08100900
C	-1.05124700	1.30436500	3.27860600
H	-2.09351900	1.09093800	3.53746100
H	-0.46403900	1.12698100	4.18503100
C	-0.91035400	2.76497100	2.84888300
H	0.11258800	3.00713000	2.54260300
H	-1.17128700	3.42714900	3.68266400
H	-1.57470000	3.00175300	2.01407800
C	-3.49384100	-2.36462200	0.55629400
H	-3.21911000	-2.86216400	-0.38074900
H	-2.70531600	-2.59933100	1.27274900
C	-4.82674500	-2.92121400	1.07246100
H	-5.08498100	-2.51460600	2.05443300
H	-4.74552800	-4.00913600	1.18100800
H	-5.65934400	-2.72429500	0.39085600
C	-4.16541700	0.31740500	1.65638700
H	-3.79271600	-0.19316500	2.55107400
H	-3.73330300	1.32221000	1.67410700
C	-5.69591400	0.42860300	1.71249800
H	-6.09050800	1.02645300	0.88607500
H	-5.98430900	0.93000100	2.64383000
H	-6.19454100	-0.54306100	1.69460700
C	-4.65020800	-0.33363300	-1.12878500
H	-5.54822700	-0.82729300	-0.74239100
H	-4.89889500	0.72901300	-1.18489300
C	-4.31646100	-0.87775000	-2.51840200
H	-3.44221800	-0.37727100	-2.94006200
H	-5.16590000	-0.71458500	-3.19204200
H	-4.11969800	-1.95407500	-2.49557600
C	5.39583700	-0.29794800	0.72450600
O	4.54306700	1.83119400	-0.53913700

O	7.00035900	1.35975100	-0.51474300
O	5.46926200	-0.06674600	-1.88574400
F	4.17648100	-0.87885900	0.70217800
F	5.50285700	0.36925500	1.89190200
F	6.31275900	-1.28212300	0.73155900
P	-0.22231100	-1.87018000	-1.05771400
P	-0.54142200	0.00160100	2.04043200
P	-3.35319000	-0.53816600	0.20002700
S	5.63020000	0.84084200	-0.72455400
Ru	-1.22519800	0.19741800	-0.20570600
O	-1.38517800	0.91889500	-2.23969100
C	-1.55946900	2.08579800	-1.69578100
C	-0.36917600	3.06133800	-1.69404700
C	-2.90876700	2.77585500	-1.87535800
H	-1.71634200	1.79769000	0.02814000
C	-0.61068000	4.30793800	-0.82334900
H	-0.34248600	3.39893600	-2.74394800
C	-3.11843200	4.01008900	-0.99133600
H	-2.91509500	3.08616400	-2.93181900
H	-3.71393700	2.05378900	-1.75989800
C	-1.94961900	4.99388200	-1.12167800
H	0.21706700	5.00912300	-0.98412900
H	-0.57315000	4.01880500	0.23397100
H	-4.06260500	4.49542200	-1.26527500
H	-3.21743200	3.69433400	0.05579500
H	-2.09315700	5.84570900	-0.44623600
H	-1.93154100	5.40091800	-2.14246100
C	0.95863600	2.37788700	-1.37987400
H	0.90332600	1.85935600	-0.41215500
H	1.23083700	1.64522800	-2.14202600
H	1.76700500	3.11231100	-1.31194600

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TS2-b2, total electronic energy = -3440.493164, thermal corrections to Gibbs free energy = 0.706781

C	1.19769500	-1.73819100	-1.50891400
H	1.22431700	-1.06381200	-2.37012000
H	1.59289100	-1.16622800	-0.66715400
C	2.11812500	-2.94251400	-1.74716100
H	2.13576400	-3.61766300	-0.88622200
H	3.14223400	-2.58306900	-1.89877700
H	1.83429700	-3.52169900	-2.62874200
C	-1.42207800	-2.25312900	-2.80533100
H	-2.36240700	-2.78341400	-2.61485500
H	-1.69628600	-1.24562000	-3.12815000
C	-0.63667100	-2.94198100	-3.92902900

H	0.28028000	-2.39627900	-4.17078500
H	-1.25052200	-2.96415400	-4.83764000
H	-0.36567800	-3.97224600	-3.68918100
C	-0.70792400	-3.65471000	-0.26786600
H	0.09631300	-3.63877400	0.47726800
H	-1.64440800	-3.65004700	0.29410500
C	-0.64291300	-4.94616800	-1.09389700
H	-1.47096800	-5.00957000	-1.80628200
H	-0.72392000	-5.80909400	-0.42217500
H	0.29177400	-5.04698800	-1.64897300
C	1.09767600	-0.68607800	2.17180300
H	1.21720600	-1.75359600	1.95205600
H	1.53257100	-0.15222000	1.32691800
C	1.87777900	-0.31610600	3.44072000
H	1.83777500	0.75800100	3.64338300
H	2.93122900	-0.58230700	3.30095500
H	1.51758200	-0.84060500	4.32877100
C	-1.47491200	-1.88784100	2.93461300
H	-2.54923900	-1.69329300	3.02317200
H	-1.36468800	-2.70526700	2.21801400
C	-0.91606000	-2.32780300	4.29387800
H	0.13614100	-2.61812500	4.22785400
H	-1.47333800	-3.20298600	4.64813000
H	-1.00972300	-1.55127500	5.05842000
C	-1.07240600	0.89565100	3.43617000
H	-2.14671600	0.85356000	3.64468000
H	-0.56692400	0.54239100	4.34023100
C	-0.65599400	2.33674400	3.14100100
H	0.40551100	2.41526200	2.88488200
H	-0.83093400	2.96329500	4.02334900
H	-1.23332400	2.75684800	2.31398400
C	-3.96195000	-2.07580500	0.32161100
H	-3.72294400	-2.52276100	-0.65004800
H	-3.25391100	-2.49454800	1.03764400
C	-5.38685100	-2.46245100	0.73772800
H	-5.62495100	-2.11600500	1.74739900
H	-5.47717500	-3.55499900	0.73784800
H	-6.14720800	-2.07395000	0.05397400
C	-4.25656500	0.58200400	1.64069300
H	-3.98898700	-0.04427400	2.49862100
H	-3.68466400	1.50870100	1.74714100
C	-5.75624300	0.91012200	1.67287900
H	-6.03363200	1.62142300	0.88986400
H	-6.00010000	1.37407400	2.63572500

H	-6.38798700	0.02572000	1.56514800
C	-4.73229500	0.23297200	-1.20210300
H	-5.69960200	-0.17404500	-0.88903400
H	-4.84547500	1.31887900	-1.16177000
C	-4.41569700	-0.22039500	-2.62778300
H	-3.46877300	0.19764100	-2.97607700
H	-5.21056400	0.11307200	-3.30511200
H	-4.35840600	-1.31053400	-2.70192200
C	4.52740100	-0.06303300	0.19071300
O	6.83189200	1.11822500	-0.20773300
O	6.67418000	-0.62742000	1.57840300
O	6.59698600	-1.29395800	-0.83251200
F	4.05804700	0.27571400	-1.02692200
F	4.12415000	0.88130900	1.06348800
F	3.93318100	-1.22320200	0.54613700
P	-0.61868000	-2.00298300	-1.13929100
P	-0.75091200	-0.37702000	2.10858200
P	-3.53133400	-0.26948800	0.13871400
S	6.37871000	-0.23660700	0.18099300
Ru	-1.29064400	0.13633600	-0.12998700
O	-1.26699000	1.05536700	-2.10428800
C	-1.27924700	2.15011900	-1.40744100
C	0.00135700	3.03497400	-1.36090000
C	-2.52043700	3.04022200	-1.48908800
H	-1.48301500	1.73876400	0.32221500
C	-0.06495600	4.16396000	-0.30995200
H	0.00821100	3.50094300	-2.35754900
C	-2.59170300	4.16393400	-0.45150400
H	-2.47319000	3.48271700	-2.49622900
H	-3.40889300	2.41619500	-1.46669500
C	-1.32344900	5.02232100	-0.47679000
H	0.82894200	4.78633700	-0.40631000
H	-0.04531300	3.72437400	0.69187100
H	-3.47579600	4.78103500	-0.64873500
H	-2.72351400	3.72914100	0.54775400
H	-1.35561900	5.77750200	0.31659200
H	-1.26917200	5.56532600	-1.43006600
C	1.33010400	2.30791700	-1.28715100
F	1.51531200	1.42429500	-2.28982100
F	1.49127500	1.62435300	-0.11778800
F	2.36453800	3.18101700	-1.35378700

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TS2-b3, total electronic energy = -3178.689429, thermal corrections to Gibbs free energy = 0.71286

C	-1.06125000	2.65408100	0.50010400

H	-1.79743700	2.32118600	-0.23745700
H	-1.18851700	1.99762300	1.36593600
C	-1.36583500	4.09603100	0.92797100
H	-0.69292900	4.44084000	1.71918400
H	-2.38644000	4.14274900	1.32598700
H	-1.30519300	4.80383300	0.09837400
C	0.53789200	2.78024900	-1.99560900
H	1.57598900	2.93666900	-2.30974300
H	0.18897500	1.89040500	-2.52764300
C	-0.32853900	3.98034300	-2.39770400
H	-1.37974400	3.82300100	-2.13825200
H	-0.28003500	4.11251400	-3.48564300
H	-0.00125700	4.91566800	-1.93823600
C	1.77595400	3.42960500	0.65028800
H	1.43136900	3.47765000	1.68972400
H	2.75506500	2.94983200	0.67711600
C	1.93748600	4.84776400	0.08753500
H	2.30726600	4.83435200	-0.94238800
H	2.67178000	5.39607800	0.68997200
H	1.00583400	5.41719300	0.10578400
C	-0.27548600	-0.05594800	3.07952900
H	-0.29493600	1.03515700	3.18781200
H	-1.09027300	-0.31181700	2.39718800
C	-0.52044200	-0.72320900	4.43964300
H	-0.59742200	-1.81071800	4.35084000
H	-1.47020600	-0.36300600	4.85293700
H	0.26068500	-0.50017200	5.17012600
C	2.59076800	0.66627900	2.93265200
H	3.54906500	0.32184600	2.52690400
H	2.43055800	1.66887400	2.53092900
C	2.67579600	0.74198500	4.46245100
H	1.77109100	1.17505600	4.89877300
H	3.51562500	1.38598500	4.74951300
H	2.84313500	-0.23554700	4.92391400
C	1.86430600	-2.07915700	2.82383800
H	2.91568500	-2.18138100	2.53700300
H	1.84954000	-1.98976700	3.91468500
C	1.08943400	-3.32670100	2.40007900
H	0.03208400	-3.26815600	2.67716500
H	1.51035200	-4.21246000	2.89041600
H	1.14381700	-3.48594000	1.31988900
C	4.26997500	1.07626800	-0.44520800
H	3.84818700	1.93191200	-0.98323100
H	4.15187400	1.29356900	0.61992600

C	5.76080900	0.93770800	-0.77798200
H	6.24230600	0.16092200	-0.17720900
H	6.27299300	1.88233200	-0.56027100
H	5.93430500	0.70856000	-1.83371300
C	4.01248300	-1.83717800	-0.06347000
H	4.39778000	-1.49193800	0.90326800
H	3.22352100	-2.55992100	0.16094800
C	5.12377700	-2.54582700	-0.85048200
H	4.74112300	-3.00195900	-1.76838300
H	5.54208600	-3.35206400	-0.23629800
H	5.94658200	-1.88069100	-1.12291800
C	3.42104100	-0.60705100	-2.64310000
H	4.48100600	-0.84916300	-2.76678500
H	2.86034300	-1.49926900	-2.93290900
C	3.05084500	0.56043400	-3.56091500
H	1.98307700	0.77648600	-3.51234400
H	3.29836200	0.30492000	-4.59823400
H	3.60527900	1.47103400	-3.31099900
C	-5.20964100	-0.73733100	0.15806700
O	-3.43971200	0.80207500	-1.01765000
O	-5.85053400	1.23588100	-1.46705300
O	-4.87414400	1.79447300	0.77735900
F	-4.37421200	-1.09552800	1.15198400
F	-5.08653400	-1.64157000	-0.83039100
F	-6.46511300	-0.80178500	0.62894500
P	0.61745400	2.23254800	-0.21021200
P	1.30218100	-0.43176800	2.13954300
P	3.13532400	-0.35668300	-0.81573500
S	-4.81654100	0.97437100	-0.44880200
Ru	0.90908900	-0.21172300	-0.17237600
O	0.19293600	-0.48331900	-2.21668300
C	-0.09795200	-1.63390600	-1.68306300
C	-1.44591800	-1.68625800	-0.94420900
C	0.31138500	-2.90699300	-2.41587700
H	0.86954200	-1.88574400	-0.30952200
C	-1.75873700	-3.01431200	-0.25857000
H	-2.22615500	-1.45807800	-1.68061200
C	-0.04008500	-4.20675800	-1.68127200
H	-0.24756300	-2.86777400	-3.36327300
H	1.37059700	-2.86414800	-2.68011000
C	-1.49607300	-4.20204700	-1.19564000
H	-2.80050600	-2.99980300	0.07654600
H	-1.13177800	-3.10559600	0.63372000
H	0.13831400	-5.05633500	-2.35049600

H	0.62917100	-4.33673700	-0.82084000
H	-1.72588500	-5.13838900	-0.67457400
H	-2.17096400	-4.15018700	-2.06154400
O	-1.37969100	-0.61269000	0.02171900
H	-2.05683600	0.05510100	-0.24026200

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TS2-c1, total electronic energy = -3327.878668, thermal corrections to Gibbs free energy = 0.696357

C	-0.97288800	2.39371900	-0.71315200
H	-1.37067700	1.85926900	-1.58271600
H	-1.33769600	1.84533100	0.15714600
C	-1.52764700	3.82271500	-0.66256100
H	-1.17938400	4.36270800	0.22353700
H	-2.62128800	3.77484400	-0.60652400
H	-1.26657800	4.41223800	-1.54423900
C	1.36999200	2.37710900	-2.53258200
H	2.44323300	2.60018300	-2.51846000
H	1.26706800	1.38984100	-2.99135900
C	0.62133700	3.40699100	-3.38857800
H	-0.44441000	3.17036200	-3.46174000
H	1.02672300	3.39313300	-4.40775300
H	0.71744900	4.42710700	-3.01047000
C	1.61526000	3.52520700	0.20967000
H	1.00376500	3.62237200	1.11475900
H	2.59770000	3.18099600	0.54151100
C	1.77990400	4.89176600	-0.46854500
H	2.43667200	4.83065500	-1.34156100
H	2.24035000	5.59403400	0.23680400
H	0.82912600	5.32260700	-0.78890400
C	-0.54257000	0.63204400	2.69140400
H	-0.48512000	1.72435700	2.60889700
H	-1.25430000	0.31198800	1.92778200
C	-1.08732600	0.23032500	4.06859800
H	-1.24171500	-0.85016600	4.14239600
H	-2.06045700	0.71006800	4.22691600
H	-0.43342800	0.53406600	4.88921500
C	2.33328800	1.19670800	2.96618300
H	3.33003700	0.78135600	2.78182600
H	2.27664400	2.12314700	2.39050800
C	2.17591100	1.51395900	4.45866200
H	1.23413100	2.02867200	4.66913600
H	2.98750900	2.17911100	4.77692300
H	2.22387400	0.61909700	5.08606800
C	1.43695400	-1.50156100	3.21839700
H	2.51760100	-1.67622800	3.20342300

H	1.18169000	-1.22550500	4.24602200
C	0.69824300	-2.78095800	2.82584100
H	-0.38724000	-2.64050200	2.81284100
H	0.92038500	-3.57944100	3.54335100
H	1.00526500	-3.12863900	1.83502200
C	4.50321600	1.22034800	-0.09554500
H	4.14411400	1.90130200	-0.87492800
H	4.17548900	1.64509000	0.85732900
C	6.03469200	1.14721700	-0.12906100
H	6.43260100	0.56887500	0.70953600
H	6.45153900	2.15853300	-0.05502700
H	6.41137900	0.70524600	-1.05637200
C	4.24822200	-1.55258700	0.92416700
H	4.36845800	-0.98384300	1.85288700
H	3.45361100	-2.28033500	1.11063500
C	5.54571600	-2.30604600	0.59898200
H	5.41897000	-2.98392400	-0.25017400
H	5.83209200	-2.91730200	1.46300200
H	6.38277600	-1.63976400	0.37697800
C	4.19285500	-1.01635600	-1.93325500
H	5.25329900	-1.22896800	-1.76719800
H	3.70150600	-1.97974400	-2.10000800
C	4.04063700	-0.12440800	-3.16771700
H	2.98997700	0.03820600	-3.40924600
H	4.51671500	-0.60697100	-4.02973200
H	4.52503900	0.84825000	-3.03247200
C	-4.94496700	1.27209400	0.31663200
O	-5.46788500	-1.28568400	0.50314100
O	-7.03484300	0.13822700	-0.81633600
O	-4.75011800	-0.38505500	-1.71604700
F	-3.68933700	1.03632000	0.75176400
F	-5.69056900	1.60892300	1.38022700
F	-4.90203700	2.32781100	-0.51515200
P	0.87427300	2.10182600	-0.75255800
P	1.14380300	0.00604700	2.15276500
P	3.52658800	-0.35042000	-0.32314000
S	-5.63262300	-0.22506200	-0.54243700
Ru	1.22246300	-0.22821400	-0.18458300
C	0.18370700	-4.38677400	-1.90735900
C	1.01778600	-3.33718700	-2.04000900
C	0.58346100	-1.98105800	-1.63336500
C	-0.89384200	-1.94427900	-1.23019600
C	-1.28792300	-3.21241400	-0.47233300
H	0.40623300	-5.36825100	-2.31681300

H	1.96100400	-3.46263000	-2.55867200
O	-1.02515300	-4.37084500	-1.29389800
H	-0.67558200	-3.29969500	0.43156600
H	-1.49188700	-1.86914100	-2.14979300
O	1.02308100	-0.92078800	-2.25118400
O	-1.05606800	-0.76270000	-0.43963600
H	-1.77834200	-0.95854400	0.20485700
C	-2.75942700	-3.23380100	-0.07882700
H	-3.38948700	-3.11606300	-0.96898800
H	-3.00169200	-4.19600900	0.39256400
O	-2.94710700	-2.14925200	0.83372200
H	-3.88191200	-1.83409000	0.75180200
H	1.21549400	-1.94201700	-0.15978600

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TS2-c2, total electronic energy = -3327.869526, thermal corrections to Gibbs free energy = 0.696913

C	1.88665500	-2.05143300	0.37811900
H	2.50805200	-1.26595600	-0.05672000
H	1.64826100	-1.71909600	1.39219800
C	2.69176000	-3.35466800	0.46863900
H	2.13231900	-4.14668900	0.97580100
H	3.60077700	-3.17172100	1.05394700
H	3.00173900	-3.73081800	-0.50833800
C	0.75632600	-1.93236500	-2.36178400
H	-0.09431600	-2.33737200	-2.91992000
H	0.78490000	-0.86078000	-2.58245500
C	2.06105900	-2.57822600	-2.84478400
H	2.93458600	-2.14343300	-2.35172700
H	2.17355900	-2.39660400	-3.92082200
H	2.08332100	-3.65941000	-2.69051700
C	-0.44021200	-3.71924800	-0.27278200
H	-0.22241700	-3.95433400	0.77584700
H	-1.52453600	-3.62699800	-0.34267500
C	0.01621700	-4.87225100	-1.17626100
H	-0.21216600	-4.67519700	-2.22829900
H	-0.51577900	-5.78855300	-0.89338900
H	1.08632100	-5.07388700	-1.09406500
C	-0.13971500	-0.72561900	3.34486400
H	0.25181900	-1.73594200	3.17581300
H	0.61101200	-0.03353600	2.95670500
C	-0.32724300	-0.47819200	4.84806700
H	-0.62776800	0.55270300	5.05547000
H	0.62633900	-0.64803600	5.36227000
H	-1.06691000	-1.14191300	5.30095300
C	-2.53129200	-2.18197700	2.39453600

H	-3.50564600	-2.01664700	1.92145700
H	-2.00684900	-2.91287700	1.77460500
C	-2.73746700	-2.76192200	3.79963300
H	-1.78902100	-3.03420600	4.27134200
H	-3.34053900	-3.67508100	3.73078000
H	-3.26522600	-2.07268200	4.46535000
C	-2.78527800	0.56407100	3.11492600
H	-3.75886500	0.45474100	2.62612600
H	-2.89678500	0.15068500	4.12246400
C	-2.41020100	2.04432000	3.19965300
H	-1.42351100	2.19586200	3.64807300
H	-3.14112500	2.57832800	3.81836000
H	-2.40142500	2.51281100	2.21263500
C	-3.52496600	-2.09902500	-1.14738100
H	-2.77876100	-2.60722300	-1.76614100
H	-3.43999600	-2.52970100	-0.14740000
C	-4.92779100	-2.37074800	-1.70519900
H	-5.71040100	-1.96361300	-1.05861400
H	-5.09035900	-3.45300300	-1.77149900
H	-5.06627400	-1.95809900	-2.70891800
C	-4.38756400	0.54432100	-0.18434000
H	-4.74178100	-0.14788200	0.58870500
H	-3.94969100	1.39467600	0.34464100
C	-5.57172900	1.03528000	-1.02823800
H	-5.26823700	1.80323500	-1.74594300
H	-6.32326700	1.48460200	-0.36822800
H	-6.06109500	0.23147400	-1.58346400
C	-3.08877300	0.22534700	-2.79532800
H	-4.14662200	0.14274100	-3.06344400
H	-2.82496300	1.28173400	-2.83829400
C	-2.24230900	-0.53025700	-3.82269300
H	-1.17710900	-0.37834400	-3.64515000
H	-2.46940800	-0.15255200	-4.82694700
H	-2.44525800	-1.60613800	-3.82912500
C	5.68161100	-0.29451200	-0.36336900
O	3.68029900	0.68021200	1.01595000
O	5.68625200	2.12626500	0.66890100
O	4.13265100	1.64664600	-1.24419100
F	4.90769600	-1.22990900	-0.94809200
F	6.22120800	-0.83751300	0.73951600
F	6.67575100	0.00864300	-1.21313800
P	0.27025400	-2.00865800	-0.55828900
P	-1.61368600	-0.56577200	2.19855200
P	-2.94855000	-0.32925300	-1.01934600

S	4.69483400	1.22272600	0.05624400
Ru	-0.91071900	0.08529500	0.04311000
C	-0.27334400	4.20309800	1.22368100
C	0.78750900	3.39185400	1.21513000
C	0.92388400	2.28195100	0.21931500
C	-0.29859000	2.14158500	-0.71420500
C	-0.97943600	3.50423900	-0.93840500
H	-0.43955800	4.97514000	1.96942300
H	1.56185000	3.51370900	1.96590100
O	-1.27676700	4.17508300	0.30074200
H	-0.20349400	4.10101800	-1.45180900
H	-1.50081500	1.59712200	0.43244200
O	1.01425000	1.00187000	0.88489100
H	1.95749500	0.70786400	0.84852200
O	-0.17422900	1.28137100	-1.67344300
C	-2.27127400	3.59459000	-1.74982100
H	-2.99100700	2.85371600	-1.39674600
H	-2.69526100	4.58944900	-1.55226400
O	-2.09615700	3.37721100	-3.13872300
H	-1.50611000	4.06680500	-3.47787500
H	1.81468800	2.40701900	-0.40897300

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TS2-c3, total electronic energy = -3327.86389, thermal corrections to Gibbs free energy = 0.693172

C	-0.04007400	-2.59336000	-2.04326100
H	0.42757900	-1.94919300	-2.79728900
H	0.60172700	-2.53282300	-1.15883300
C	-0.07652600	-4.04630600	-2.53310600
H	-0.52362800	-4.71367900	-1.78993000
H	0.94760300	-4.39416500	-2.71195300
H	-0.63239700	-4.15602600	-3.46732700
C	-2.25619300	-1.01489200	-3.19094600
H	-3.31064900	-0.76139200	-3.03148700
H	-1.72207800	-0.06561600	-3.28851400
C	-2.08314700	-1.81722300	-4.48767700
H	-1.02942100	-2.02908700	-4.69185200
H	-2.46433000	-1.22716800	-5.32961300
H	-2.62520300	-2.76486800	-4.47700200
C	-2.86081800	-3.04325600	-1.07899800
H	-2.32917400	-3.68052100	-0.36303000
H	-3.62403000	-2.51058200	-0.50337300
C	-3.55588500	-3.89988800	-2.14475400
H	-4.16043700	-3.28816200	-2.82059300
H	-4.23338100	-4.60734600	-1.65210100
H	-2.85280200	-4.48027600	-2.74579500

C	0.14593700	-2.91868400	1.71261000
H	-0.44334300	-3.60461200	1.09241400
H	0.98657600	-2.59402500	1.09332900
C	0.69603300	-3.64882900	2.94628600
H	1.35017000	-3.00609700	3.54166400
H	1.29403300	-4.50686600	2.61776000
H	-0.09141500	-4.02702900	3.60086200
C	-2.60218000	-2.05511900	2.48612200
H	-3.16063200	-1.16597600	2.80019000
H	-3.09329400	-2.42408000	1.58296100
C	-2.68499300	-3.12613000	3.58124200
H	-2.25787700	-4.07735000	3.25248200
H	-3.73779000	-3.30894700	3.82628000
H	-2.18255600	-2.82541800	4.50501500
C	-0.32944700	-0.64496600	3.54013000
H	-1.05983600	0.12895800	3.80012100
H	-0.40056400	-1.41536900	4.31504100
C	1.08183300	-0.05106900	3.52641600
H	1.83785800	-0.78896900	3.24108200
H	1.33820600	0.31329700	4.52782500
H	1.16195500	0.79410600	2.83702300
C	-4.24989500	0.27560100	0.18124200
H	-4.27395900	-0.05287300	-0.86322100
H	-4.16777200	-0.62951800	0.78643600
C	-5.54606100	1.01860800	0.52963700
H	-5.59939900	1.26635400	1.59352100
H	-6.40433900	0.37701500	0.29916700
H	-5.66503300	1.94317100	-0.04300800
C	-2.67284100	1.93426800	2.08753900
H	-3.07324000	1.15218500	2.74218000
H	-1.62324500	2.06077900	2.36774000
C	-3.41998700	3.25524700	2.31827000
H	-2.96469700	4.07991200	1.76229000
H	-3.37163000	3.51267000	3.38259800
H	-4.47512200	3.20138000	2.04006300
C	-2.87806300	2.66200000	-0.74401500
H	-3.71546800	3.22473600	-0.31959700
H	-1.99502100	3.29864500	-0.65632500
C	-3.14990500	2.37702800	-2.22273800
H	-2.29749400	1.88804700	-2.69598800
H	-3.32877000	3.32289400	-2.74691300
H	-4.03472900	1.75021300	-2.37008900
C	3.54768800	-1.48459400	-0.36622600
O	5.59779700	0.11572800	-0.08842400

O	5.62989200	-2.08899200	1.09628700
O	5.90084900	-2.00048400	-1.39023200
F	3.11987000	-0.85533200	-1.48085200
F	2.89515600	-0.92703000	0.68098200
F	3.14810700	-2.76920600	-0.44784100
P	-1.63749300	-1.73056900	-1.58486100
P	-0.93397600	-1.40968700	1.95248200
P	-2.63942400	1.18732300	0.37250500
S	5.39370700	-1.34812400	-0.16289900
Ru	-0.77456500	-0.07730300	0.00367000
C	2.31154900	4.09806500	1.49975400
C	2.23932100	5.22142600	0.77983800
C	1.46783400	5.29245000	-0.50667600
C	1.24492800	3.87648500	-1.04201200
C	0.77096200	2.94602000	0.09108600
H	2.87816900	4.00944800	2.42151300
H	2.75764500	6.10960300	1.12570300
O	1.69825100	2.91518900	1.18930300
H	-0.19299600	3.31125800	0.46052000
H	2.20932500	3.50859000	-1.42797100
O	2.19746700	6.08974700	-1.43901000
H	1.67116800	6.10412700	-2.25300400
O	0.26886600	3.94451900	-2.07028000
H	0.01257600	3.02236900	-2.26582200
C	0.68149900	1.50769700	-0.42593500
H	1.65985000	1.01038300	-0.34831900
H	0.06458500	0.92311300	1.00885500
O	-0.01410500	1.27924400	-1.52985100
H	0.47392000	5.74110800	-0.33857600

10

acetone, total electronic energy = -193.0890976, thermal corrections to Gibbs free energy = 0.055311

C	0.00000000	0.18315700	-0.00000200
O	-0.00001800	1.40456700	0.00000000
C	-1.28679300	-0.61458200	-0.00000800
H	-1.32614600	-1.26725300	0.88024900
H	-2.14962400	0.05451600	-0.00020000
H	-1.32598600	-1.26762800	-0.87998200
C	1.28680300	-0.61455500	0.00000400
H	1.32605300	-1.26751400	0.88004500
H	1.32615000	-1.26730900	-0.88018900
H	2.14964300	0.05453200	0.00011600

12

iPrOH, total electronic energy = -194.2883561, thermal corrections to Gibbs free energy = 0.080559

H	-0.00000300	0.07190800	-1.46987700

C	0.00002100	0.03912000	-0.37300300
O	-0.00017500	1.41764400	0.02297400
C	1.27091200	-0.66689000	0.09940500
H	1.31735000	-1.69465700	-0.27776800
H	2.16038200	-0.13173100	-0.24873200
H	1.30422000	-0.70998400	1.19588500
C	-1.27076500	-0.66717700	0.09939800
H	-1.31709900	-1.69489300	-0.27790800
H	-1.30393700	-0.71038700	1.19587200
H	-2.16026000	-0.13199200	-0.24861400
H	-0.00026000	1.43026700	0.99254800

18

NMM, total electronic energy = -326.9765668, thermal corrections to Gibbs free energy = 0.132577

C	0.10497100	0.32295200	1.19939600
C	0.10497100	-1.20226200	1.17187000
C	0.10497100	-1.20226200	-1.17187000
C	0.10497100	0.32295200	-1.19939600
H	0.65682100	-1.60169300	2.02832200
H	1.14979400	0.68313400	1.27782200
H	-0.43359400	0.67277400	2.08819500
H	0.65682100	-1.60169300	-2.02832200
H	-0.93262000	-1.57154400	-1.22116800
H	1.14979400	0.68313400	-1.27782200
H	-0.43359400	0.67277400	-2.08819500
H	-0.93262000	-1.57154400	1.22116800
N	-0.55500800	0.84494200	0.00000000
O	0.74578700	-1.70143200	0.00000000
C	-0.60142300	2.30080700	0.00000000
H	-1.13734000	2.65523300	-0.88731000
H	-1.13734000	2.65523300	0.88731000
H	0.40188300	2.76794100	0.00000000

8

TfO, total electronic energy = -961.5586032, thermal corrections to Gibbs free energy = -0.005115

C	-0.94383000	-0.00012200	0.00018400
O	1.24065400	-1.27997800	-0.66999200
O	1.23987900	1.22029700	-0.77361300
O	1.24118500	0.06003400	1.44319900
F	-1.43389000	-1.05828200	0.67549800
F	-1.43389100	-0.05580000	-1.25390500
F	-1.43375500	1.11390800	0.57881000
S	0.91269100	-0.00003300	-0.00009300

27

TfO-HNMM, total electronic energy = -1289.013626, thermal corrections to Gibbs free energy = 0.160943

C	-2.25721800	-0.77861100	-0.18300600

O	-0.97164600	0.75940300	1.52703300
O	-0.50997200	1.03855700	-0.90431200
O	-2.69716400	1.80900500	0.03023500
F	-3.20086200	-1.09283000	0.71790900
F	-1.29974200	-1.72521900	-0.12965700
F	-2.81090500	-0.81690600	-1.40458000
S	-1.54715200	0.89968700	0.17125200
C	2.41887700	0.36730900	1.19470900
C	2.03088700	-1.10000900	1.34022600
C	2.33710500	-1.51465800	-0.93883300
C	2.76990800	-0.08016200	-1.21592100
H	2.33692500	-1.44865400	2.32998900
H	3.48722800	0.51142300	1.37485400
H	1.83971000	0.99384900	1.87523400
H	2.84989000	-2.18271400	-1.63548200
H	1.25231700	-1.61984200	-1.09005800
H	3.85347800	0.02831000	-1.12463400
H	2.45147900	0.24678900	-2.20825400
H	0.94158400	-1.21351000	1.25288000
N	2.14479000	0.84587900	-0.20733500
O	2.69625300	-1.91356800	0.37891100
C	2.57701400	2.25967800	-0.40460600
H	2.31928700	2.56389600	-1.41977200
H	2.05208800	2.88610000	0.31769800
H	3.65488100	2.32817500	-0.25129300
H	1.10641500	0.83616100	-0.37324200

19

sub, total electronic energy = -310.9662831, thermal corrections to Gibbs free energy = 0.143995

O	-2.39282200	-0.09978100	-0.12869500
C	-1.03641200	-0.01811000	0.31988300
C	-0.31522000	-1.27187000	-0.17493500
C	-0.34348800	1.25316400	-0.18605200
H	-1.00902100	-0.01351200	1.42386300
C	1.17078400	-1.25628300	0.21602300
H	-0.41313700	-1.31398300	-1.26874200
H	-0.81432700	-2.16225700	0.22604800
C	1.14211900	1.28165200	0.20753100
H	-0.44189300	1.28364400	-1.28010600
H	-0.86206700	2.13782600	0.20823600
C	1.87181400	0.01923600	-0.27668700
H	1.67072000	-2.14588400	-0.18564000
H	1.25858600	-1.31660900	1.31015300
H	1.62073300	2.18077100	-0.19889300
H	1.22648100	1.35071800	1.30148300

H	2.91542800	0.03188600	0.06124700
H	1.89667000	0.01597800	-1.37579300
H	-2.84317600	0.70292600	0.17313000

17

prod, total electronic energy = -309.7640792, thermal corrections to Gibbs free energy = 0.120448

O	2.31222600	0.00000100	-0.33650800
C	1.15737800	0.00000100	0.06313300
C	0.39321800	-1.28434300	0.33777800
C	0.39321600	1.28434400	0.33777300
C	-1.02007100	-1.26528000	-0.28197400
H	0.30126500	-1.37478100	1.43042100
H	0.98678900	-2.13151900	-0.01805000
C	-1.02007700	1.26527900	-0.28196800
H	0.30127200	1.37479000	1.43041700
H	0.98678400	2.13151900	-0.01806400
C	-1.79286700	-0.00000300	0.11344700
H	-1.56433700	-2.16473000	0.02718400
H	-0.93236600	-1.30915600	-1.37580600
H	-1.56434400	2.16472400	0.02719900
H	-0.93238000	1.30916400	-1.37580100
H	-2.78011700	-0.00000400	-0.36354700
H	-1.96515600	-0.00000600	1.19898000

18

sub-a, total electronic energy = -272.8656185, thermal corrections to Gibbs free energy = 0.133123

O	-3.15940700	-0.17923700	-0.07811000
C	-1.92147900	0.52581200	0.01217300
C	-0.70311300	-0.39543500	-0.03300500
H	-1.90745400	1.21076300	-0.84396300
H	-0.75455800	-1.09347500	0.81587300
H	-0.75800200	-1.00425100	-0.94521800
C	0.62654700	0.36757400	0.01125600
H	0.67298300	1.06578000	-0.83684400
H	0.66195800	0.98710000	0.91896500
C	1.85755000	-0.54734900	-0.02200200
H	1.82253700	-1.16766000	-0.92815400
H	1.81330000	-1.24378700	0.82667700
C	3.18116100	0.22152100	0.01824100
H	4.04011900	-0.45860600	-0.00629700
H	3.27207400	0.90157100	-0.83739900
H	3.26247000	0.82566700	0.92999300
H	-1.88829800	1.14677600	0.92235500
H	-3.20587100	-0.76872500	0.68891000

16

prod-a, total electronic energy = -271.658422, thermal corrections to Gibbs free energy = 0.109078

O	3.04498100	-0.17045000	-0.41379800
C	2.06766900	-0.22787000	0.30843200
C	0.81374600	0.58601100	0.13519800
H	0.73136200	1.24048600	1.01643600
H	0.91992200	1.21946000	-0.75167900
C	-0.44292200	-0.30149900	0.05268500
H	-0.36824000	-0.95232800	-0.82863200
H	-0.47565500	-0.96513100	0.92749400
C	-1.74143700	0.51138900	-0.01938500
H	-1.70056700	1.18244600	-0.88780400
H	-1.80995900	1.15805800	0.86592000
C	-2.99089100	-0.36855200	-0.11099300
H	-3.90194200	0.23832800	-0.15873400
H	-2.96658300	-1.00189400	-1.00585800
H	-3.07694300	-1.02920200	0.76004200
H	2.05176400	-0.92349400	1.17758200

22

sub-b1, total electronic energy = -350.2594154, thermal corrections to Gibbs free energy = 0.170137

O	1.65689800	-1.62040000	-0.06128600
C	0.55465800	-0.77644600	0.29348300
C	0.69887500	0.64417600	-0.28897800
C	-0.78056400	-1.41999400	-0.10294100
H	0.60404700	-0.70608500	1.38956200
C	-0.51586500	1.50819500	0.10516300
H	0.69513100	0.53846400	-1.38688700
C	-1.98231900	-0.54841800	0.28956400
H	-0.78048500	-1.57316500	-1.19314200
H	-0.84968200	-2.41282400	0.35731200
C	-1.85244400	0.86629700	-0.29172600
H	-0.41961700	2.50151800	-0.35133600
H	-0.49860800	1.66545000	1.19402500
H	-2.91422500	-1.01921900	-0.04625800
H	-2.04113400	-0.48550900	1.38549100
H	-2.68696400	1.49404400	0.04452400
H	-1.92009100	0.81533900	-1.38782000
H	1.64054800	-1.71166500	-1.02658700
C	2.01889100	1.30071300	0.12796200
H	2.87316700	0.67628700	-0.14897000
H	2.14071600	2.28000000	-0.34911800
H	2.05462500	1.45342900	1.21432500

20

prod-b1, total electronic energy = -349.0575549, thermal corrections to Gibbs free energy = 0.146724

O	1.24072700	1.75460000	-0.37063500
C	0.44703300	0.94119200	0.07921100

C	0.83653300	-0.50290500	0.38851100
C	-1.00077900	1.30331400	0.36745900
C	-0.17460400	-1.47051600	-0.27771200
H	0.71131000	-0.61098600	1.47786900
C	-1.97904200	0.30506600	-0.28620000
H	-1.13734100	1.27463100	1.45814800
H	-1.17934500	2.32939100	0.03298500
C	-1.62830600	-1.14109800	0.08420600
H	0.07223300	-2.49718600	0.01742300
H	-0.04740000	-1.41719100	-1.36825500
H	-3.00430800	0.54699200	0.01587100
H	-1.93417900	0.42247900	-1.37718100
H	-2.30630400	-1.83457600	-0.42752000
H	-1.77912200	-1.28959900	1.16259400
C	2.28469600	-0.81396300	0.01469500
H	2.98086700	-0.13672300	0.51790700
H	2.54063900	-1.84036300	0.29827500
H	2.44395700	-0.71020800	-1.06406100

22

sub-b2, total electronic energy = -648.0064941, thermal corrections to Gibbs free energy = 0.143755

O	-0.01891200	2.27646100	-0.07279700
C	0.60942200	1.04128800	0.26154000
C	-0.10169600	-0.18468700	-0.35877600
C	2.09548900	1.04602800	-0.11709400
H	0.51968100	0.96880400	1.35209200
C	0.60177800	-1.49355800	0.06289400
H	-0.06008500	-0.09477800	-1.45283100
C	2.80335600	-0.25483000	0.28535200
H	2.17615300	1.19009400	-1.20481400
H	2.56846000	1.91312900	0.35732500
C	2.08999100	-1.47592600	-0.30801000
H	0.10239000	-2.34417000	-0.40984900
H	0.49267900	-1.62096500	1.14792200
H	3.85010700	-0.22747200	-0.03893000
H	2.81495300	-0.33732500	1.38098600
H	2.56321200	-2.40190700	0.03863600
H	2.18913800	-1.46065000	-1.40225700
H	0.01901100	2.37155600	-1.03702000
C	-1.57887800	-0.22746800	-0.00840500
F	-2.29138400	0.76363800	-0.59027400
F	-1.79549700	-0.13687100	1.32894200
F	-2.15769400	-1.39044500	-0.41132200

20

prod-b2, total electronic energy = -646.8013638, thermal corrections to Gibbs free energy = 0.120483

O	0.06363700	2.07295000	0.38506500
C	0.62190200	1.09946100	-0.08969300
C	-0.11286500	-0.20957000	-0.40675000
C	2.10306900	1.06864600	-0.40600900
C	0.60031800	-1.40699300	0.27137900
H	-0.06138800	-0.34966100	-1.49467900
C	2.79799400	-0.14582700	0.24620700
H	2.20583900	0.99698100	-1.49822400
H	2.54529700	2.01517800	-0.08389100
C	2.08435000	-1.45509100	-0.10963000
H	0.09496800	-2.33237200	-0.01974200
H	0.49791900	-1.30775900	1.35887400
H	3.84528800	-0.17682200	-0.07278300
H	2.79978800	-0.01428900	1.33592000
H	2.56302700	-2.29596600	0.40451400
H	2.17789200	-1.64539100	-1.18730900
C	-1.58655500	-0.15691400	-0.05561500
F	-2.24158300	0.82407500	-0.71321900
F	-1.80258100	0.02708100	1.26643400
F	-2.20328200	-1.32179800	-0.38905300

20

sub-b3, total electronic energy = -386.1824933, thermal corrections to Gibbs free energy = 0.146477

O	-1.81874700	-1.45897300	0.06685200
C	-0.65298200	-0.71942900	-0.29637500
C	-0.65998600	0.70229400	0.27805400
C	0.62802100	-1.46563300	0.10585400
H	-0.70078400	-0.63657700	-1.39023000
C	0.61388300	1.46456600	-0.11665200
H	-0.69666800	0.61653100	1.38012500
C	1.90204600	-0.70252400	-0.28389800
H	0.61209400	-1.61645400	1.19590300
H	0.61017400	-2.46156200	-0.35120000
C	1.89078900	0.71915300	0.29472300
H	0.58707900	2.46490500	0.33570500
H	0.59949600	1.60747900	-1.20580600
H	2.78722000	-1.25057800	0.06019300
H	1.97254800	-0.64771200	-1.37922700
H	2.77379400	1.27720100	-0.03836600
H	1.94767400	0.66651200	1.39100700
H	-1.82498100	-1.52113200	1.03439900
O	-1.83092600	1.36394600	-0.19952200
H	-1.80088600	2.27103700	0.13861700

18

prod-b3, total electronic energy = -384.9774032, thermal corrections to Gibbs free energy = 0.123269

O	1.32457900	1.70170400	-0.39691000
C	0.50943800	0.92821800	0.07410500
C	0.83888500	-0.53017900	0.38589900
C	-0.92221400	1.32623300	0.39101200
C	-0.18533200	-1.45613500	-0.30511900
H	0.71624400	-0.64208100	1.47848300
C	-1.93601800	0.37018600	-0.27388600
H	-1.05053200	1.28101400	1.48176900
H	-1.07156000	2.36302700	0.07672800
C	-1.62879500	-1.09338800	0.06732000
H	0.03797700	-2.49420400	-0.02857600
H	-0.04201600	-1.37141700	-1.39033400
H	-2.95025500	0.63758900	0.04265300
H	-1.89588100	0.50716800	-1.36244800
H	-2.32445000	-1.75769400	-0.45790100
H	-1.78311800	-1.25999000	1.14221800
O	2.17132600	-0.80193700	-0.00642300
H	2.34056900	-1.73116000	0.20808900

20

sub-c, total electronic energy = -535.3724801, thermal corrections to Gibbs free energy = 0.129834

C	-1.18942400	1.89071000	-0.03540600
C	-2.02216400	0.86015100	0.14208000
C	-1.51313900	-0.54156000	0.31363100
C	-0.08003700	-0.62860300	-0.21433900
C	0.75658100	0.55111000	0.30539400
H	-1.52502100	2.91320300	-0.18304800
H	-3.09295500	1.03510300	0.15746000
O	0.17373600	1.81861600	-0.05827900
H	0.81240300	0.49136600	1.40184000
H	-0.12612400	-0.56116900	-1.31439200
O	-2.37545000	-1.43924000	-0.38794300
H	-1.99346800	-2.32231100	-0.26943100
O	0.45309900	-1.87777100	0.20087400
H	1.41943000	-1.81658800	0.09091200
C	2.16601100	0.59333800	-0.28151800
H	2.09601200	0.65659700	-1.37567800
H	2.68352000	1.49089100	0.08217400
O	2.85420800	-0.59537100	0.12668600
H	3.66277600	-0.66928400	-0.40090300
H	-1.48828100	-0.81855000	1.38130900

18

prod-c1, total electronic energy = -534.1736564, thermal corrections to Gibbs free energy = 0.107292

C	1.34181300	1.78907500	-0.00576800
C	2.13076600	0.69295600	-0.05859100

C	1.56386500	-0.64741100	0.03515100
C	0.06457800	-0.67332300	0.36867800
C	-0.64572100	0.52388700	-0.28742100
H	1.73617000	2.80169600	0.01803200
H	3.20694100	0.80901700	-0.12182300
O	-0.00046600	1.78242700	0.02393700
H	-0.60844300	0.39131200	-1.37791500
H	-0.00574600	-0.55522300	1.46721900
O	2.22143500	-1.67647300	-0.06795500
O	-0.49805200	-1.89182800	-0.06307600
H	-1.46345400	-1.75866300	-0.03941500
C	-2.09060200	0.70527300	0.17175900
H	-2.10650500	0.84913700	1.26009600
H	-2.51060200	1.60248000	-0.30155700
O	-2.82034100	-0.46572100	-0.20866800
H	-3.65717300	-0.46974700	0.27860300

18

prod-c2, total electronic energy = -534.1575395, thermal corrections to Gibbs free energy = 0.104781

C	-1.03961900	1.86911500	-0.18094400
C	-1.92476700	0.95667700	0.23186300
C	-1.53363900	-0.47535400	0.52372800
C	-0.12587400	-0.69016100	-0.00863000
C	0.83953200	0.46028800	0.25797400
H	-1.31011800	2.88913200	-0.43844200
H	-2.96694500	1.23549600	0.34650600
O	0.30237000	1.66475700	-0.33771500
H	0.89298700	0.61446700	1.34684700
O	-2.43341800	-1.39575500	-0.06284000
H	-1.87083800	-2.04586700	-0.52139000
O	0.15131900	-1.68649700	-0.65255500
C	2.24183900	0.25534700	-0.31058800
H	2.17345800	-0.10596000	-1.34015300
H	2.75027300	1.22871600	-0.32248700
O	2.96400700	-0.72043900	0.42284300
H	3.20527700	-0.32672100	1.27462900
H	-1.49316400	-0.64127100	1.61620800

18

prod-c3, total electronic energy = -534.1584644, thermal corrections to Gibbs free energy = 0.105788

C	-1.02278400	1.92518800	-0.08047100
C	-1.90120100	0.93153100	0.08240100
C	-1.46922600	-0.49187100	0.29626600
C	-0.01972800	-0.65622800	-0.16299100
C	0.83231400	0.51428600	0.36594000
H	-1.30761900	2.95739400	-0.25973500

H	-2.96321300	1.15126900	0.05210800
O	0.33924200	1.79558900	-0.04863300
H	0.84459100	0.46852800	1.46777200
H	-0.00910900	-0.62988400	-1.26332700
O	-2.34008900	-1.35270900	-0.43607300
H	-2.03259800	-2.25649500	-0.26682100
O	0.45954900	-1.89426700	0.33217100
H	1.39611100	-1.94922000	0.07674400
C	2.26877400	0.44470400	-0.11293800
H	2.73827000	1.42168400	-0.33823600
O	2.88038400	-0.60073500	-0.24310900
H	-1.50801000	-0.75195000	1.36740000