

- *Electronic Supplementary Information* -

**On the Mechanism of the Reaction of a Magnesium(I) Complex with CO₂. A
Concerted Type of Pathway..**

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COMPUTATIONAL DATA

Computational details

Quantum-chemical calculations: Geometry optimizations were performed with the Gaussian09 suite of programs (revision D.02)¹ using the Becke's 3-parameter hybrid functional,² combined with the non-local correlation functional provided by Perdew/Wang.³ The 6-311+G(d) all-electron basis set was used for the magnesium atom, and the 6-31G(d) for the remaining atoms.⁴ We have also considered in the present study the dispersion effects. In particular the third generation of Grimme's dispersion corrections with Becke-Johnson damping⁵ model on the B3PW91 geometries (single point calculations), with the energies denoted as ΔG^{disp} . All stationary points have been identified for minimum (Nimag=0) or transition states (Nimag=1). Intrinsic Reaction Paths (IRPs)⁶ were traced from the various transition structures to obtain the connected intermediates. Natural population analysis (NPA) was performed using Weinhold's methodology.⁷

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- (6) (a) C. Gonzalez, H. B. Schlegel, *J. Chem. Phys.* 1989, 90, 2154. (b) C. Gonzalez, H. B. Schlegel, *J. Phys. Chem.* 1990, 94, 5523.
- (7) (a) A. E. Reed, L. A. Curtiss, F. Weinhold, *Chem. Rev.* 1988, 88, 899. (b) F. Weinhold, In *The Encyclopedia of Computational Chemistry* (Eds.: Schleyer, P. v. R.), John Wiley & Sons, Chichester, pp 1792, 1998.

Table S1. Relative energies in enthalpy, Gibbs free energy, and Gibbs free including the dispersion correction, for all the pathways involved in the present study.

	ΔH (ΔH^\ddagger)	ΔG (ΔG^\ddagger)	ΔG^{disp} ($\Delta G^{\ddagger\text{disp}}$)
<i>Oxo carbonate (CO₂)</i>			
I	0.0	0.0	0.0
^{ins} TS _{I-II}	9.8 (9.8)	20.0 (20.0)	8.8 (8.8)
II	-52.9	-45.1	-47.2
^{oxo} TS _{II-III}	-25.1 (27.8)	-18.5 (26.6)	-27.2 (20.1)
III	-30.3	-35.2	-36.1
^{oxo} TS _{III-IV}	-30.2 (0.1)	-20.6 (14.6)	-32.7 (3.4)
IV	-80.8	-70.9	-76.6
<i>Concerted carbonate (CO₂)</i>			
I	0.0	0.0	0.0
^{ins} TS _{I-II}	9.8 (9.8)	20.0 (20.0)	8.8 (8.8)
II	-52.9	-45.1	-47.2
^{con} TS _{II-V}	-49.3 (2.5)	-32.3 (12.8)	-37.1 (10.2)
V	-55.1	-38.1	-39.2
^{con} TS _{V-IV}	-51.3 (3.8)	-33.9 (4.1)	-36.0 (3.2)
IV	-80.8	-70.9	-76.6
<i>Oxalate (CO₂)</i>			
I	0.0	0.0	0.0
^{ins} TS _{I-II}	9.8 (9.8)	20.0 (20.0)	8.8 (8.8)
II	-52.9	-45.1	-47.2
^{oxa} TS _{II-VI}	-42.3 (10.6)	-26.6 (18.4)	-26.7 (20.6)
VI	-119.4	-101.0	-97.6
<i>Oxo (CS₂)</i>			
I	0.0	0.0	0.0
^{ins} TS _{I-II}	9.8 (9.8)	20.0 (20.0)	8.8 (8.8)
II	-52.9	-45.1	-47.2
^{oxo} TS _{II-VII}	-16.2 (14.1)	-1.8 (28.5)	-23.8 (6.5)
VII	-70.8	-56.0	-75.6

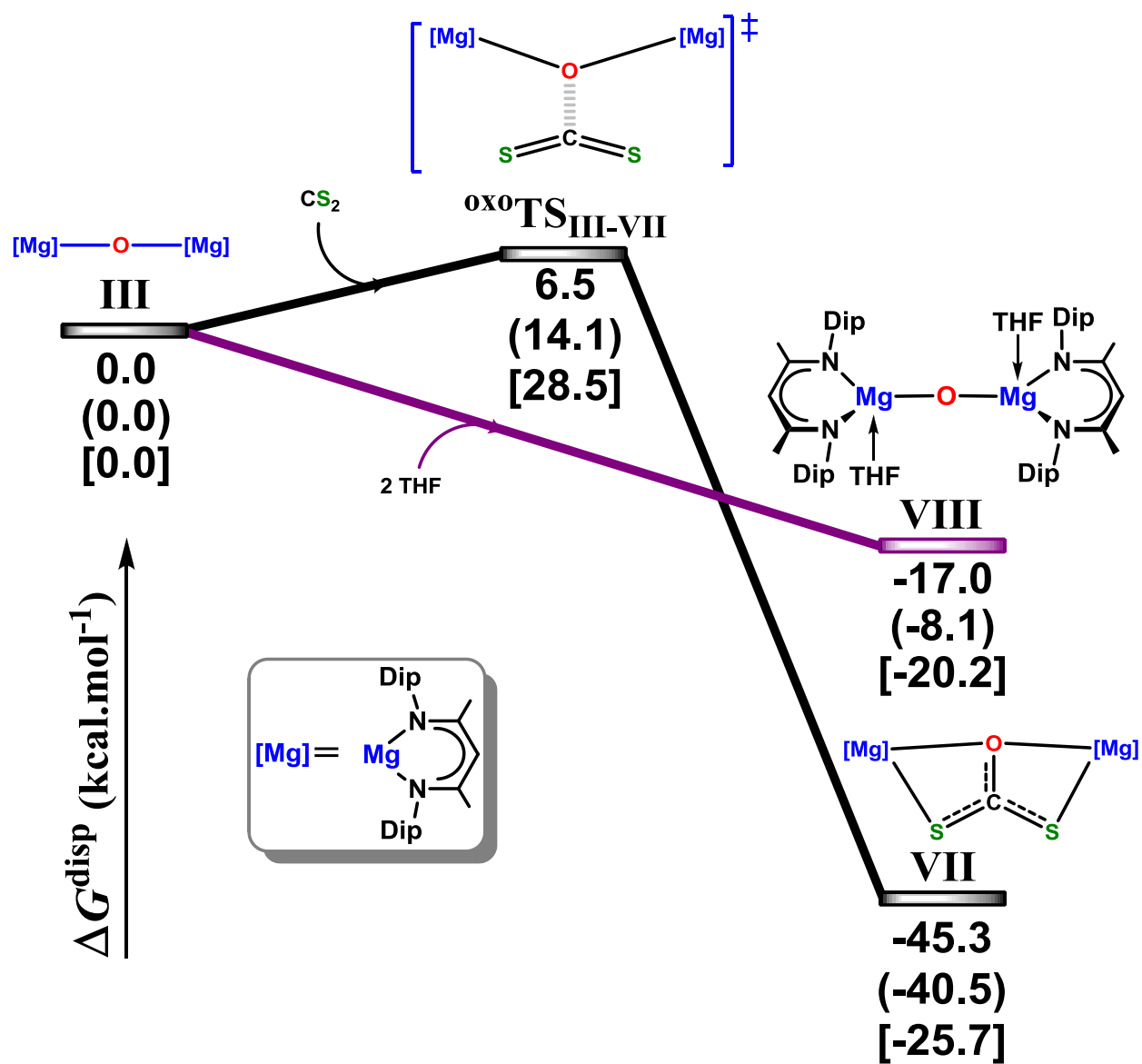


Figure S1. Energy profile for the reaction of the oxo complex **III** with CS_2 to afford complex **VII**, or the corresponding THF adduct, **VIII**. The Gibbs free energies including dispersion corrections are displayed (and given in kcal mol⁻¹) whereas the relative energies in parentheses correspond to the enthalpy without dispersion correction, while in brackets are the Gibbs free energies without dispersion correction.

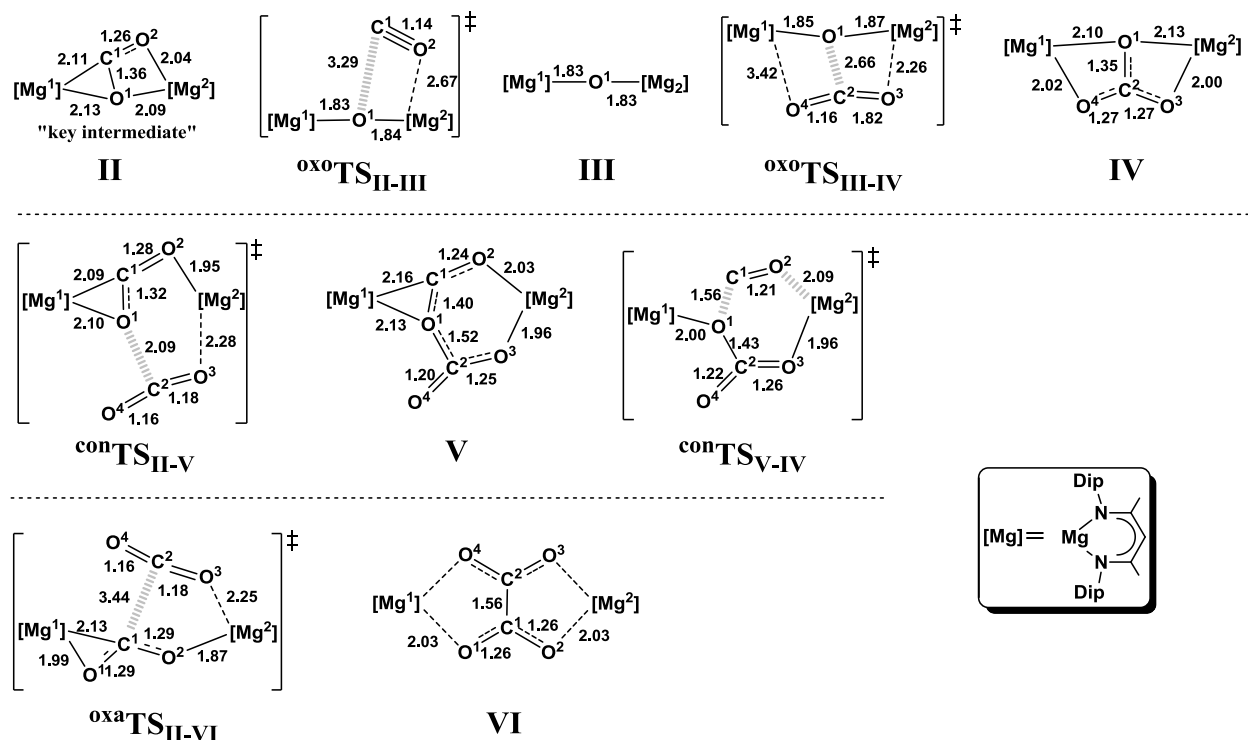


Figure S2. The most important bond distances (Å) for various model complexes, intermediates, and transition states involved in the mechanistic studies.

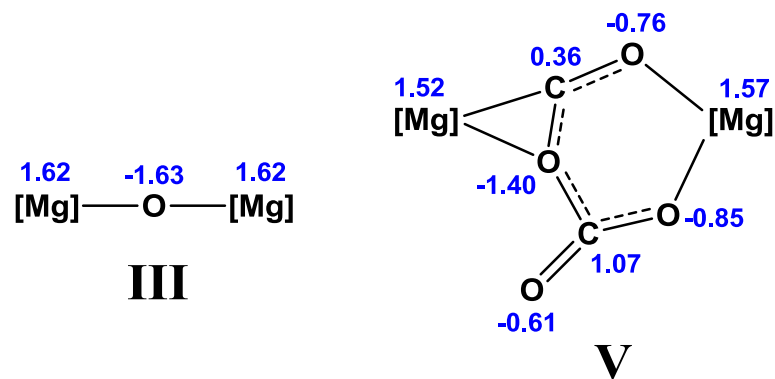


Figure S3. Natural charges of the intermediates **III** and **V** (figures in blue).

Cartesian Coordinates of Optimized Structures with their corresponding ΔH , ΔG and $\Delta G+GD3BJ$ values.

I

$H = -2876.535776$ au

$G = -2876.717951$ au

$GD3BJ = -0.4039532137$ au

Mg	1.77063400	5.75591000	10.02734300
N	1.66017300	7.87026800	10.10829500
C	0.41238600	9.98868800	10.36457500
H	1.01459000	10.25637600	11.23690900
H	-0.61967500	10.30462100	10.53543700
H	0.80901100	10.56765100	9.52336000
N	-0.13897900	5.63625000	9.13666400
C	0.48033100	8.50210400	10.07424400
C	-0.74585000	7.90755400	9.72725900
H	-1.59852400	8.57643500	9.76202800
C	-1.01860900	6.63537000	9.18591300
C	-2.41235400	6.44809600	8.62310200
H	-2.37391600	6.01758100	7.61760800
H	-2.95019900	7.39776900	8.57771100
H	-2.99480100	5.75437600	9.23815800
C	2.82994800	8.69548300	10.18846200
C	3.48128700	8.91792100	11.42384100
C	4.60080100	9.75713400	11.45576100
H	5.09371800	9.94701500	12.40661400
C	5.09516400	10.35473900	10.30408600
H	5.96468400	11.00577400	10.35187300
C	4.47158000	10.10231000	9.08799400
H	4.86782000	10.55521100	8.18191100
C	3.34262000	9.28296700	9.00377400
C	3.01379500	8.28168500	12.72377600
H	2.16712900	7.62653300	12.48747000
C	4.12240800	7.41554700	13.33878700
H	4.44579800	6.63687800	12.63902100
H	3.77107700	6.92819500	14.25535300
H	5.00247200	8.01493500	13.60126700
C	2.52661800	9.32408000	13.74139900
H	3.33338100	10.00982300	14.02686600
H	2.17103300	8.83208300	14.65516100
H	1.70278200	9.92655300	13.34437700
C	2.72385600	9.02984900	7.63513400
H	1.79487800	8.47007400	7.78283600
C	3.65489900	8.16342600	6.77385900
H	4.61098300	8.67048400	6.59477100
H	3.19834500	7.95744000	5.79805400
H	3.87500600	7.20534500	7.25682600
C	2.36915500	10.32648600	6.89250000
H	1.71149900	10.97113300	7.48578600
H	1.85411000	10.09550800	5.95218700
H	3.26398500	10.90811200	6.64101200
C	-0.50673500	4.41418400	8.48824400
C	-1.23816200	3.42114700	9.18373200
C	-1.49714100	2.20551800	8.54277600
H	-2.04969300	1.43406400	9.07405000
C	-1.06949600	1.96256900	7.24292600
H	-1.28613700	1.01162400	6.76234400
C	-0.36991200	2.95065300	6.56158600

H	-0.04825400	2.76778200	5.53897000
C	-0.07429900	4.17948800	7.16072000
C	-1.74379900	3.62295200	10.60510600
H	-1.57199900	4.66962900	10.87914100
C	-0.96577900	2.75374900	11.59937200
H	-1.09591800	1.68826200	11.37740700
H	-1.31347400	2.92548100	12.62416100
H	0.10752400	2.96958500	11.56892300
C	-3.24958000	3.34534300	10.73753000
H	-3.84226200	3.91175400	10.01050900
H	-3.59622400	3.61452900	11.74250400
H	-3.47754800	2.28323900	10.58839700
C	0.66196800	5.23553600	6.34786000
H	0.86740500	6.08243400	7.01224000
C	2.00625500	4.72431300	5.81356100
H	1.87357400	3.88003600	5.12644700
H	2.66185000	4.39147500	6.62495100
H	2.52621300	5.51698800	5.26342700
C	-0.21044300	5.75910600	5.19623600
H	-0.45131800	4.95864300	4.48601200
H	0.31327500	6.54927600	4.64412200
H	-1.15598000	6.17409900	5.56215800
Mg	3.59720000	3.68771900	11.04104100
N	5.51318700	3.07061600	10.41873900
N	3.67570200	2.40328100	12.72500300
C	7.76124400	2.10753100	10.72862700
H	7.69557800	1.47911900	9.83373700
H	8.33180900	1.56961700	11.48900500
H	8.32230000	3.00119600	10.43986100
C	6.37544700	2.45772000	11.22807300
C	6.08323300	2.07045300	12.55096800
H	6.92467300	1.66474500	13.10138800
C	4.84604600	1.97263300	13.21261600
C	4.88936400	1.26431700	14.55249600
H	4.28244900	1.78359400	15.29915900
H	5.91599000	1.18984600	14.91943800
H	4.48345200	0.24990600	14.47283500
C	5.90957700	3.36230400	9.07482900
C	5.49065700	2.50919900	8.02657900
C	5.81396900	2.84948300	6.70879300
H	5.49829500	2.19518100	5.89927500
C	6.53195300	4.00159900	6.41397200
H	6.77170800	4.25118400	5.38323600
C	6.94558300	4.82965500	7.45111900
H	7.50946900	5.73030100	7.22018500
C	6.65430700	4.53170000	8.78566700
C	4.72493000	1.21948800	8.28610400
H	4.55035000	1.14806000	9.36568800
C	5.54257500	-0.01356900	7.87122500
H	5.73489900	-0.02012000	6.79141800
H	5.00109300	-0.93496900	8.11831400
H	6.51216100	-0.04507500	8.38039000
C	3.35753400	1.21688300	7.59014400
H	2.73593400	2.05664900	7.91937800
H	2.81484300	0.29000800	7.80917100
H	3.46208600	1.28967300	6.50101200

C	7.13006500	5.48407700	9.87351500
H	6.94834000	5.00743200	10.84291300
C	6.32769100	6.78984300	9.84635900
H	6.46877700	7.32048000	8.89766400
H	6.64195900	7.46087600	10.65359800
H	5.25473500	6.60184500	9.96357600
C	8.63327600	5.78776700	9.78017600
H	8.87404300	6.36526400	8.87983700
H	9.23999500	4.87539400	9.75654400
H	8.95173100	6.38377700	10.64379800
C	2.49323600	1.94053400	13.39066800
C	1.99019000	0.65036000	13.08352500
C	0.85082600	0.19164900	13.74976400
H	0.46339400	-0.79778600	13.51769800
C	0.20611900	0.96939400	14.70434900
H	-0.67116800	0.58980600	15.22245400
C	0.68909700	2.24174000	14.97956700
H	0.18005300	2.85646300	15.71851800
C	1.81891700	2.75324000	14.33112000
C	2.63084000	-0.24358700	12.02962300
H	3.56407100	0.22933500	11.70853000
C	1.72262200	-0.36118100	10.79636000
H	0.76629300	-0.83232200	11.05518900
H	2.19890900	-0.97622400	10.02300800
H	1.50058500	0.62018500	10.36350700
C	2.98179800	-1.63973700	12.56441800
H	3.62108900	-1.58842500	13.45248300
H	3.51598300	-2.21514100	11.79866400
H	2.08453000	-2.20924900	12.83450100
C	2.27256300	4.16480600	14.66928000
H	3.13531400	4.39783700	14.03435000
C	2.72162400	4.29842400	16.13228600
H	1.89735500	4.08536500	16.82366700
H	3.06958200	5.31870000	16.33563300
H	3.54118800	3.61225600	16.37078700
C	1.16834600	5.18452400	14.35545100
H	0.87057500	5.12942500	13.30215900
H	1.51200800	6.20473500	14.56082900
H	0.27400000	5.00972300	14.96558000

^{ins}TS_{I-II}

$H = -3065.009143 \text{ au.}$

$G = -3065.199256 \text{ au}$

$GD3BJ = -0.4234198082 \text{ au}$

H	-4.32207200	1.49569300	-4.93034300
H	-4.75738600	2.94537400	-4.01992400
C	-4.61875600	1.86080300	-3.93969400
H	-5.59288500	1.42142700	-3.69740600
H	2.09328200	2.63398400	-5.46238400
H	0.94681200	3.97624600	-5.44659200
H	4.25606300	-0.48277700	-4.87333000
H	-1.89775900	1.87354200	-4.27356900
H	4.92987900	-2.03001600	-4.35749000
H	0.12656900	-5.38486600	-3.88617200
C	1.33477700	3.13973500	-4.85292200
H	3.79488100	4.22729300	-4.51741800
H	2.64424600	5.55273400	-4.26410100
C	4.24566200	-1.22419600	-4.06535900
H	0.50952000	2.44144700	-4.68531800
H	3.23879400	-1.64716500	-4.00465600
H	-2.30913600	3.26673500	-3.25587300

H	6.20618000	0.60967300	-3.73905600
C	3.05977400	4.64150900	-3.81602800
C	-2.21880700	2.17565000	-3.26864200
H	-5.74529100	-0.10690900	-2.15974000
C	-3.54408100	1.50069500	-2.90238800
H	-3.38850100	0.41759100	-2.94995000
H	1.51285000	-3.31961200	-3.42633100
H	-0.00659700	5.40102300	-4.05985400
C	0.13803700	-5.60629400	-2.81206200
H	-0.75409100	-6.19905100	-2.58250600
H	6.81382000	-0.87463400	-2.98172700
H	1.01267100	-6.23790100	-2.61662700
C	1.95168700	3.61425800	-3.53063600
H	-6.31357900	-1.74559800	-1.78071500
C	6.10638200	-0.04427700	-2.86372400
O	-0.54651200	-0.94007500	-3.59889500
H	-4.44184500	3.87712300	-1.99386200
H	3.59392900	4.92918300	-2.90531300
H	-1.43130800	1.91214000	-2.55396200
H	5.43579300	-3.14960000	-2.53758000
C	-5.72400000	-0.90373800	-1.41113700
H	-4.87691900	-3.28041000	-1.63803900
H	-0.65752800	-3.68321200	-2.30784700
C	4.66462100	-0.56575100	-2.74437900
C	-0.01762600	5.10335400	-3.01409500
C	1.47440100	-3.53357400	-2.35068000
H	2.42266300	2.74990400	-3.05202800
C	0.19471200	-4.30013400	-2.00372600
H	2.36916900	-4.10889200	-2.09109100
H	-2.35345600	-5.47554400	-1.35889300
C	-3.95781800	1.84743900	-1.47944400
H	4.01508200	0.30036700	-2.58370800
C	0.37167200	-0.33513400	-3.20196500
H	-1.67730200	6.38829800	-2.53151900
C	-4.41397600	3.13832500	-1.19675700
H	6.40694800	0.53102600	-1.98303000
H	-6.21721000	-0.50299200	-0.51926300
C	-4.04975200	-2.70513300	-1.23921100
C	0.91569100	4.16577300	-2.55943700
C	-4.30468400	-1.33085200	-1.09443200
H	-3.19628800	-5.39267800	0.17518500
H	1.53366000	-2.58830200	-1.80012600
C	4.98270100	-2.79907800	-1.61342800
C	-0.95676100	5.66500400	-2.15691400
C	-3.17132800	-4.97266000	-0.83602400
C	4.50320700	-1.48715700	-1.54116300
C	-2.96221100	-3.47261300	-0.78896500
N	-3.41357700	-0.42659200	-0.67541300
C	-3.90985900	0.89687900	-0.43207900
Mg	-1.33556800	-0.89256000	-0.47704800
H	5.26862900	-4.68181500	-0.60733000
C	-4.84500700	3.49240100	0.07646800
H	-5.20772600	4.49852000	0.27314500
C	4.89528900	-3.66345600	-0.52809600
C	0.08498300	-4.53579700	-0.50473400
N	-1.82134700	-2.97313700	-0.30325300
O	1.36961300	0.27790500	-3.03113800
H	-4.11097300	-5.22239800	-1.33385000
Mg	1.41007400	0.76907300	-0.65010800
C	0.90494800	3.80806100	-1.18885800
H	1.75538200	-5.88796600	-0.48726900
C	-0.95956500	5.30427100	-0.81463100

H	2.74207000	5.41828900	-0.85682900
N	1.86255600	2.85957000	-0.69886600
C	0.98152400	-5.41412700	0.11172600
C	3.93932500	-1.03833400	-0.32089400
C	-0.91000200	-3.91204500	0.28428600
C	-4.35471200	1.24492200	0.86581500
H	-6.47811500	-0.32606700	1.74714300
C	-4.81863400	2.54479700	1.09272900
N	3.45296100	0.30745100	-0.22612900
H	-1.68984100	5.75073800	-0.14466400
C	-0.02835400	4.39585900	-0.30251100
C	4.33853900	-3.21254100	0.66282100
C	2.98260500	3.36208000	-0.16954200
H	6.12758100	0.01316500	0.18588200
C	3.15386800	4.86206900	-0.01240000
C	4.31047300	1.22032000	0.24290100
H	-1.10203700	2.20081800	1.02635200
C	3.87359600	-1.90080500	0.79844600
H	-5.16901800	2.81744800	2.08594300
H	-6.22508700	0.92167400	2.97501600
C	4.06589600	2.60163700	0.30147400
C	-5.80105500	0.00838400	2.54047200
H	4.27882100	-3.88815200	1.51210000
H	4.20923200	5.12125400	0.10168400
C	0.89619400	-5.70344800	1.46822100
H	-4.00465200	-0.71062200	1.62912000
C	-4.37699300	0.24461400	2.01393700
H	2.62687000	5.21053700	0.88393700
C	5.66083000	0.79423200	0.78977800
C	-1.01503500	-4.21220500	1.66425800
H	-2.75501700	-3.00957800	1.90765900
H	-2.14395100	3.59002500	1.34438400
H	4.87326700	3.18517100	0.72913500
H	1.23471900	-1.64663000	1.63680200
C	-1.16830100	3.14867500	1.57356000
H	1.59681500	-6.39713800	1.92695400
C	-0.02449400	4.09220900	1.18934300
H	6.34166500	1.64642500	0.85307800
H	-5.79613100	-0.75954000	3.32369000
H	0.91346700	3.57688500	1.42203800
C	-0.10211300	-5.10779800	2.23013100
H	1.92338000	-3.06176600	2.43748300
H	5.54365000	0.38411800	1.80000200
C	-2.10542900	-3.61731400	2.54606300
C	1.93608200	-1.96698400	2.41629300
H	-0.97322000	-1.85771300	3.18276200
C	3.34503500	-1.43045200	2.14637700
H	3.27641300	-0.33756500	2.11332900
H	-3.41415200	-5.37550400	2.44802400
H	-1.13708400	2.92679400	2.64761800
H	-1.04641000	5.86835600	1.97163700
C	-3.45387000	0.67496400	3.16226700
H	-3.75863800	1.64242500	3.57903700
C	-0.07658200	5.36329500	2.05037700
H	0.69595700	6.08571000	1.76374700
H	-2.41633600	0.77066700	2.82603300
C	-1.52146300	-2.69563300	3.62552200
H	-0.17863400	-5.34575800	3.28895000
C	-2.97927900	-4.70196700	3.19437600
H	1.56458300	-1.60153800	3.38192200
H	-2.31987600	-2.28497600	4.25498700
H	-3.80372000	-4.24257200	3.75324400

H	4.30037200	-2.87995600	3.48658400
H	-3.48222600	-0.06046800	3.97492600
H	5.31243600	-1.47660400	3.12203800
C	4.28139700	-1.79847200	3.30728900
H	-0.82747300	-3.23800200	4.27879100
H	0.07051200	5.10792400	3.10669100
H	-2.40537700	-5.31549200	3.89934200
H	3.93692100	-1.32288200	4.23344900

II

$H = -3065.109046 \text{ au}$

$G = -3065.302961 \text{ au}$

$GD3BJ = -0.4090368847 \text{ au}$

H	-4.44613900	1.01239400	-5.03974600
H	-5.10971300	2.38456800	-4.13725300
C	-4.75429700	1.35104000	-4.04309800
H	-5.60353900	0.73522700	-3.72825100
H	2.31745100	2.31712800	-5.05366500
H	0.80507400	3.23810400	-5.01749600
H	4.13405900	-0.16092200	-4.45290200
H	-2.06531800	1.68186200	-4.55972400
H	4.08820000	-1.84923900	-3.91731600
H	-0.46331100	-5.22349700	-4.27302600
C	1.54612700	2.72774700	-4.39046400
H	3.72806600	4.38629200	-4.72927700
H	2.27961200	5.40194300	-4.74166200
C	3.94525900	-0.81216100	-3.59032900
H	1.04560300	1.89075600	-3.89269000
H	2.89539100	-0.69572400	-3.30100200
H	-2.64104200	3.12553900	-3.70873600
H	6.53300400	0.16016700	-3.72084800
C	2.94065200	4.81205600	-4.09552900
C	-2.38469200	2.06699700	-3.58431400
H	-6.11837800	-0.13273700	-1.73948900
C	-3.57594000	1.25499300	-3.06076100
H	-3.26560600	0.20542900	-3.02078300
H	1.18106500	-3.34800500	-3.88636400
H	0.07643700	5.28492300	-3.97596600
C	-0.43820800	-5.48453000	-3.20801900
H	-1.41927600	-5.89060100	-2.93971100
H	6.61446600	-1.54279200	-3.25199500
H	0.30116700	-6.28419000	-3.07674800
C	2.17240600	3.69403500	-3.37431100
H	-6.63996800	-1.83082000	-1.62378600
C	6.35636800	-0.53884900	-2.89446100
O	-0.44505100	-0.65657500	-2.37306400
H	-4.30320800	3.71745000	-2.24958200
H	3.41425000	5.50178500	-3.38780400
H	-1.53042200	2.00909700	-2.90511900
H	5.31641400	-3.11774200	-2.18848700
C	-6.03546600	-1.05135800	-1.15367600
H	-5.27237800	-3.46356900	-1.34162800
H	-0.84748700	-3.49466800	-2.54176200
C	4.89294000	-0.46025500	-2.43423500
C	0.10985500	5.06666400	-2.91101300
C	1.25905700	-3.66231800	-2.83920900
H	2.90113100	3.12759400	-2.78393100
C	-0.07541700	-4.25091000	-2.36588900
H	2.07155100	-4.39550600	-2.76932200
H	-4.36789200	-5.43225600	-1.32450000
C	-3.97697700	1.67871000	-1.65436200

H	4.69671600	0.57989800	-2.15155500
C	0.35396900	-0.03543100	-1.62083500
H	-1.64635100	6.23473900	-2.48017900
C	-4.33288300	3.01159700	-1.42328600
H	7.05054800	-0.28740300	-2.08463300
H	-6.46960000	-0.83784900	-0.16978100
C	-4.38769500	-2.88920000	-1.09008600
C	1.13038100	4.24978200	-2.41321600
C	-4.59663600	-1.49967400	-1.00496200
H	-2.63350100	-5.72923800	-1.05270300
H	1.54339600	-2.78850700	-2.24768200
C	4.92265000	-2.69579400	-1.26671400
C	-0.86033900	5.60301000	-2.07352300
C	-3.50276200	-5.16116000	-0.71397600
C	4.63336800	-1.32873000	-1.21043600
C	-3.25971900	-3.66705300	-0.76397500
N	-3.64010300	-0.59765700	-0.76817900
C	-4.02602800	0.76824500	-0.57231700
Mg	-1.65257000	-1.17100900	-0.81103500
H	4.94292000	-4.58562600	-0.23577700
C	-4.72545700	3.45087100	-0.16499800
H	-5.00336300	4.49049000	-0.00885300
C	4.71576600	-3.52443700	-0.17044700
C	-0.06466300	-4.57234000	-0.87758900
N	-2.05463800	-3.17558600	-0.46530100
O	0.01969900	-0.03025300	-0.30680900
H	-3.70993500	-5.47840800	0.31486500
Mg	1.82932800	1.06744800	-0.59683600
C	1.16179700	3.97829900	-1.02573800
H	1.68534400	-5.80775900	-1.04832400
C	-0.81871300	5.32835600	-0.71099200
H	3.32796900	5.56278500	-0.96990700
N	2.16404600	3.09710100	-0.50287600
C	0.93023500	-5.41539000	-0.37159600
C	4.11588300	-0.79706200	-0.00615800
C	-1.04733100	-4.07594300	0.01145600
C	-4.41982100	1.20529900	0.71543900
H	-6.65301300	0.07749900	1.93368500
C	-4.76197700	2.54916700	0.89256200
N	3.72334500	0.58027200	0.04311500
H	-1.58233100	5.74599500	-0.05997200
C	0.18440900	4.52539400	-0.16174100
C	4.22214000	-2.98667800	1.01266600
C	3.28889300	3.62590700	-0.01416700
H	6.50647200	0.51258600	0.12655100
C	3.44455100	5.13069600	0.02958900
C	4.60934800	1.49107500	0.45383000
H	-0.69767000	2.25098200	1.14348800
C	3.92202400	-1.62600600	1.12284300
H	-5.06690900	2.89467300	1.87773500
H	-6.02723400	1.25447900	3.09472800
C	4.38262000	2.87964100	0.46342700
C	-5.82822600	0.28409200	2.62452900
H	4.06318400	-3.63772600	1.86853300
H	4.42341700	5.41607400	0.42087200
C	0.97291800	-5.76315700	0.97282400
H	-4.30035900	-0.75319500	1.54714300
C	-4.46743700	0.26542900	1.91258200
H	2.67202300	5.58816100	0.65691900
C	5.97337600	1.03763700	0.92673500
C	-1.02014700	-4.43218800	1.38190400
H	-2.84170000	-3.41083100	1.81076400

H	-1.86922100	3.53193900	1.45474500
H	5.20672700	3.47225700	0.84315400
H	1.28821700	-1.14413900	1.84085400
C	-0.85861700	3.18322400	1.69562500
H	1.75562500	-6.41993700	1.34480400
C	0.19196000	4.24220300	1.33378700
H	6.58199500	1.88464000	1.25071100
H	-5.85272800	-0.47388100	3.41683500
H	1.17328300	3.82865600	1.59055500
C	0.00234600	-5.26982100	1.83716300
H	1.83239500	-2.58011900	2.71151600
H	5.88751300	0.33020800	1.75810700
C	-2.06170300	-3.93248200	2.37479100
C	1.92921300	-1.48958900	2.65894300
H	-1.02439300	-2.06278100	2.83648900
C	3.39055500	-1.07589800	2.43842400
H	3.41566200	0.01767500	2.37648900
H	-3.14904400	-5.83680600	2.47210500
H	-0.82261700	2.95516800	2.76841100
H	-1.01141300	5.92335000	2.06949900
C	-3.34415400	0.58520500	2.90997900
H	-3.45182000	1.59970500	3.31236200
C	-0.00438300	5.50524300	2.18349000
H	0.71281400	6.29077900	1.91871500
H	-2.35849000	0.52066000	2.43731300
C	-1.45468700	-2.92291000	3.35913800
H	0.03412500	-5.54661900	2.88868100
C	-2.73408500	-5.07885000	3.14540900
H	1.54551100	-1.06829200	3.59684100
H	-2.21842200	-2.55296900	4.05413000
H	-3.55205300	-4.69186400	3.76519900
H	4.20794600	-2.56548200	3.82539700
H	-3.36422700	-0.11478300	3.75404400
H	5.30552200	-1.21742400	3.49868100
C	4.25234900	-1.48568100	3.64112700
H	-0.65625100	-3.38403000	3.95279100
H	0.12934300	5.26812000	3.24570800
H	-2.02858700	-5.58514000	3.81496600
H	3.89521600	-0.98516900	4.54919900

$^{oxo}TS_{II-III}$

$H = -3065.064714 \text{ au}$

$G = -3065.260645 \text{ au}$

$GD3BJ = -0.4193990456 \text{ au}$

Mg	1.29877000	5.73892500	9.85161500
N	1.40813100	7.79687800	9.49762700
C	0.55491600	9.95074000	8.64568100
H	1.05807700	10.50021700	9.44481400
H	-0.40963300	10.42206600	8.44341700
H	1.18076800	10.06058400	7.75156600
N	-0.67033200	5.56140400	9.14882000
C	0.38277700	8.48423200	8.98736300
C	-0.87643100	7.94312700	8.66872000
H	-1.58135100	8.66184100	8.26693100
C	-1.34401100	6.61581700	8.67740600
C	-2.69984100	6.41461500	8.03008400
H	-2.57762400	5.93226000	7.05242100
H	-3.20693800	7.36958800	7.87472800
H	-3.34692200	5.75985600	8.61793100
C	2.65885300	8.48688600	9.62884700
C	3.00725900	9.12266200	10.84246700

C	4.23534900	9.78918400	10.92218400	H	8.64795300	2.74255300	10.59321500
H	4.50645900	10.29360100	11.84702400	C	6.63371500	1.98385800	10.71922300
C	5.11320100	9.82194400	9.84605700	C	6.14030300	0.98982100	11.58238200
H	6.06213400	10.34673300	9.92804000	H	6.82716700	0.17460400	11.77949800
C	4.76735100	9.17950100	8.66179900	C	4.92525300	0.92274800	12.28886600
H	5.45825000	9.20103300	7.82327500	C	4.72986900	-0.32085300	13.13375100
C	3.54556000	8.51609000	8.52542800	H	4.28501100	-0.09524700	14.10589000
C	2.09011000	9.12211800	12.05718000	H	5.67659500	-0.84417700	13.28842900
H	1.21656700	8.50951700	11.81044700	H	4.04456200	-1.01053700	12.62505700
C	2.77855700	8.49816100	13.27945900	C	6.58262600	3.95599000	9.40287700
H	3.17173700	7.50166600	13.05457600	C	6.69378500	3.69815800	8.01683000
H	2.07517800	8.41361600	14.11722900	C	7.29657100	4.66359100	7.20454100
H	3.62034600	9.11263600	13.62069200	H	7.38682900	4.47944600	6.13671500
C	1.58292300	10.52985200	12.40772000	C	7.78248200	5.85435400	7.73345300
H	2.41259300	11.20017500	12.66295200	H	8.24814900	6.59163600	7.08373400
H	0.91025900	10.48855400	13.27331300	C	7.67732400	6.09199800	9.09935900
H	1.03099600	10.98470800	11.57880700	H	8.06372800	7.02073700	9.51073400
C	3.19932200	7.82571100	7.21420900	H	7.09142500	5.15427600	9.95433200
H	2.11522000	7.66920800	7.19703200	C	6.16470200	2.41389500	7.39309200
C	3.86531100	6.44420600	7.14073400	H	5.95259500	1.71091700	8.20570500
H	4.95714000	6.53580900	7.13613900	C	7.17610200	1.74118200	6.45437200
H	3.56470300	5.91989600	6.22488000	H	7.35845300	2.33968900	5.55400500
H	3.59952300	5.81694500	8.00025700	H	6.79430800	0.76757100	6.12442800
C	3.55106200	8.66184300	5.97691300	H	8.14333600	1.57681800	6.94287300
H	3.11951400	9.66826700	6.02947000	C	4.84220200	2.66805900	6.65774100
H	3.16522400	8.17435000	5.07352900	H	4.09847100	3.11734800	7.32274800
H	4.63441000	8.76868600	5.84700800	H	4.42930400	1.73087800	6.26392500
C	-1.29661500	4.27674500	9.01030500	H	4.98967700	3.35327000	5.81393000
C	-2.13063800	3.77251100	10.03624200	C	7.00319000	5.42707800	11.44842500
C	-2.73911900	2.52545800	9.85466500	H	6.82493300	4.46571800	11.94385400
H	-3.39368400	2.13753500	10.63203800	C	5.81526000	6.34635900	11.76865300
C	-2.52784900	1.77440400	8.70527500	H	5.95220400	7.33520100	11.31713400
H	-3.00999800	0.80731600	8.58471500	H	5.71089500	6.47979400	12.85287100
C	-1.69134900	2.27001500	7.71208300	H	4.86708600	5.95522100	11.37607200
H	-1.52184300	1.67977000	6.81484500	C	8.30037500	5.99972000	12.03392900
C	-1.07382000	3.51772400	7.83710700	H	8.50721500	7.01058100	11.66346400
C	-2.40099600	4.53955900	11.32334400	H	9.16459500	5.37036600	11.79234000
H	-1.78939100	5.44684000	11.30238100	H	8.22288100	6.06515100	13.12590100
C	-1.99483500	3.72241900	12.55836100	C	2.86207800	1.73074000	13.13696700
H	-2.63583500	2.84089400	12.68004100	C	1.73376500	0.96706800	12.76331400
H	-2.09610300	4.32708100	13.46814900	C	0.65767000	0.88821000	13.65286500
H	-0.96143100	3.36925000	12.49269800	H	-0.21938900	0.30694000	13.38029400
C	-3.86993500	4.97402400	11.44875500	C	0.69040500	1.53446100	14.88343900
H	-4.18211500	5.61514700	10.61810900	H	-0.15254700	1.45372500	15.56557600
H	-4.02202300	5.53625100	12.37838100	C	1.80365300	2.28990500	15.23606800
H	-4.54124500	4.10682600	11.47165300	H	1.81480300	2.79874000	16.19593000
C	-0.16518200	4.01568000	6.72327400	C	2.90059500	2.41286400	14.37751000
H	0.00946600	5.08483100	6.88751600	C	1.66495300	0.26571600	11.41477900
C	1.19701000	3.31034900	6.78791200	H	2.68833900	0.18887800	11.03057800
H	1.08203200	2.22917600	6.64019900	C	0.86221800	1.10206200	10.40835800
H	1.68333900	3.46386200	7.75856100	H	-0.18399900	1.19365100	10.72076300
H	1.86613400	3.68814600	6.00554800	H	0.87215900	0.63128300	9.41766900
C	-0.78450300	3.86773400	5.32713100	H	1.26424200	2.11772300	10.31006100
H	-0.89681900	2.81626400	5.03764900	C	1.10552900	-1.15995400	11.50305500
H	-0.14014200	4.34281200	4.57766400	H	1.64254400	-1.76407100	12.24375500
H	-1.77364800	4.33626700	5.26974100	H	1.19229100	-1.65785900	10.52986900
Mg	3.94585900	3.38211400	10.82662500	H	0.04331100	-1.16662000	11.77425200
N	5.92282200	3.02053900	10.26417300	C	4.10898400	3.24825500	14.78635900
N	3.97278600	1.85698100	12.24379300	H	4.56270300	3.62985700	13.86213700
C	8.08734000	1.84181100	10.31844100	C	5.18152000	2.40744400	15.49922000
H	8.20005400	1.72480300	9.23611700	H	4.76523400	1.92526200	16.39261800
H	8.54853600	0.98237500	10.80989700	H	6.01489400	3.04560400	15.81909300

H	5.59282300	1.62888600	14.85150300
C	3.75044100	4.45836100	15.65685100
H	2.93925100	5.04505300	15.21721700
H	4.62683300	5.10827100	15.76532400
H	3.44889100	4.15967700	16.66835300
O	2.60805200	4.52969800	10.31565200
C	1.20165800	5.43486000	13.15429500
O	0.54062900	5.98119000	12.40264100

III

$H = -2951.823096 \text{ au}$

$G = -2952.014852 \text{ au}$

$GD3BJ = -0.406264338 \text{ au}$

Mg	1.43019400	5.79081000	9.64603400
N	1.46660100	7.83550300	9.27503700
C	0.53373100	10.02140300	8.63038200
H	0.86613000	10.53281800	9.53996400
H	-0.41614200	10.45636800	8.31271500
H	1.28742800	10.23361200	7.86410300
N	-0.56140600	5.61228300	9.07295400
C	0.40373300	8.53074500	8.86222600
C	-0.86704800	7.98097100	8.61671800
H	-1.61879500	8.69515500	8.30164600
C	-1.31966800	6.65328800	8.71667900
C	-2.78342800	6.43279600	8.39720000
H	-2.90640500	5.70993500	7.58399600
H	-3.27013500	7.36713700	8.10885400
H	-3.31205100	6.01725600	9.26246800
C	2.69300300	8.54835400	9.47307300
C	2.98422400	9.10792900	10.73766000
C	4.20957300	9.75751200	10.91462300
H	4.44802500	10.19159800	11.88241300
C	5.12913700	9.85939400	9.87640800
H	6.07598800	10.37080600	10.03295800
C	4.82840300	9.30919300	8.63509200
H	5.54950500	9.39324600	7.82625300
C	3.61368100	8.65691200	8.40642400
C	2.00620400	8.99605400	11.89823900
H	1.03403600	8.70724200	11.48372500
C	2.43927700	7.88482700	12.86566200
H	2.55033100	6.92466300	12.34841700
H	1.70380100	7.75916100	13.67002900
H	3.40608400	8.12424400	13.32511500
C	1.80421300	10.32009800	12.64646800
H	2.71059000	10.63636000	13.17615700
H	1.01182300	10.21190500	13.39681600
H	1.51701300	11.12978900	11.96567700
C	3.30549800	8.06413000	7.03977600
H	2.22284600	7.90425500	6.98763100
C	3.98115400	6.69507800	6.87781000
H	5.07233500	6.79030800	6.90512400
H	3.70191200	6.23568700	5.92104400
H	3.70555000	6.00550300	7.68426500
C	3.68255100	8.99288600	5.87876000
H	3.23168400	9.98581400	5.99032700
H	3.33514300	8.56759900	4.92954900
H	4.76765400	9.12590900	5.79482800
C	-1.18854100	4.32587600	9.13494100
C	-1.76274600	3.89483600	10.35362800
C	-2.34249200	2.62480100	10.40758600
H	-2.78560300	2.27952000	11.33780000

C	-2.37029800	1.79567400	9.29040000
H	-2.83298200	0.81335700	9.34974100
C	-1.80474700	2.23138100	8.09799300
H	-1.82688300	1.57999300	7.22724600
C	-1.20856500	3.49252100	7.99458500
C	-1.73730200	4.78498600	11.58746000
H	-1.59715800	5.81669300	11.24517900
C	-0.54454300	4.43058500	12.48806000
H	-0.64591700	3.41576300	12.88784100
H	-0.48140600	5.12438600	13.33606200
H	0.40927200	4.46210300	11.94637500
C	-3.04502300	4.75159600	12.38806300
H	-3.91496100	4.96069300	11.75452300
H	-3.01605400	5.50555600	13.18368400
H	-3.20730000	3.78065500	12.87073600
C	-0.59514600	3.92648200	6.67106800
H	-0.31928900	4.98237700	6.76464900
C	0.68897300	3.13822000	6.37685900
H	0.47566800	2.06809300	6.26424500
H	1.41789500	3.24573800	7.18659200
H	1.15484800	3.48838400	5.44732600
C	-1.57648600	3.81064400	5.49606300
H	-1.84638600	2.76774200	5.29244000
H	-1.12344600	4.21535300	4.58292600
H	-2.50430900	4.36186400	5.68523600
Mg	3.92581700	3.43659100	10.93530200
N	5.93759900	3.13759100	10.50272100
N	3.87432600	1.86884800	12.30318500
C	8.13022900	2.02632400	10.65931700
H	8.23343900	1.85699600	9.58181900
H	8.60264900	1.19607800	11.18878900
H	8.68544300	2.94400700	10.88240600
C	6.67357400	2.16650300	11.04954600
C	6.19842200	1.22915000	11.98419200
H	6.93215100	0.50224500	12.31258000
C	4.92266200	1.07986500	12.55635000
C	4.76678700	-0.07790000	13.52002100
H	4.44678900	0.27079200	14.50745200
H	5.70380400	-0.62763700	13.63167500
H	3.99417400	-0.77285200	13.17257100
C	6.58175100	4.01072400	9.56771900
C	6.57072200	3.69572400	8.19063400
C	7.17472000	4.58503900	7.29670800
H	7.17396000	4.35575100	6.23397700
C	7.78036700	5.75501000	7.74118100
H	8.24940800	6.43170000	7.03085700
C	7.78784300	6.05219300	9.09976400
H	8.26337600	6.96727100	9.44224000
C	7.20057100	5.19322100	10.03274300
C	5.90387400	2.43027800	7.67243000
H	5.73900800	1.76923200	8.53016700
C	6.76913700	1.66104100	6.66561400
H	6.90096100	2.21599700	5.72930200
H	6.29258600	0.70657600	6.41202300
H	7.76558800	1.44566200	7.06826900
C	4.52827700	2.75153600	7.07042500
H	3.88506300	3.26428000	7.79479600
H	4.01999900	1.83475100	6.74670900
H	4.63087800	3.40828200	6.19802500
C	7.21115400	5.54091700	11.51394900
H	7.04081300	4.61298900	12.07125500
C	6.05625100	6.49585300	11.84774100

H	6.17829600	7.45362700	11.33026300
H	6.01248900	6.69190300	12.92668800
H	5.08812000	6.09001400	11.53125700
C	8.54756300	6.11797100	11.99595700
H	8.74518600	7.10923700	11.57130500
H	9.38900100	5.46682300	11.73231900
H	8.53541100	6.23131600	13.08656700
C	2.64035600	1.56216500	12.96350200
C	1.71244700	0.70119200	12.33251200
C	0.49654300	0.44450800	12.97215900
H	-0.22737600	-0.21236800	12.49747400
C	0.19871600	1.00697800	14.20923500
H	-0.74974100	0.78950400	14.69477800
C	1.12210200	1.84558300	14.82269500
H	0.88548400	2.28156800	15.79040000
C	2.35091300	2.13638400	14.22147400
C	2.01958800	0.07679800	10.97927800
H	3.10704900	0.10276100	10.84604800
C	1.39649800	0.90377000	9.84488800
H	0.30277700	0.88883600	9.90454600
H	1.68815500	0.49973900	8.86710800
H	1.70067000	1.95703800	9.88719800
C	1.59025100	-1.39186300	10.87567400
H	2.00150600	-1.99406800	11.69430500
H	1.94469000	-1.81856900	9.92975800
H	0.49990800	-1.50508900	10.89085900
C	3.33364300	3.06176300	14.92432100
H	4.29177500	2.98857200	14.39811500
C	3.58276100	2.66701300	16.38669700
H	2.68625400	2.79971700	17.00350900
H	4.37104200	3.29490200	16.81898400
H	3.89592700	1.62081000	16.47750600
C	2.86856600	4.52238300	14.83450300
H	2.73026800	4.83514800	13.79403900
H	3.60132200	5.19366300	15.29945900
H	1.91002500	4.65960600	15.34989900
O	2.67823100	4.61493400	10.29025400

oxoTS_{III-IV}

H = -3140.311991 au

G = -3140.504754 au

GD3BJ = -0.4258044608 au

H	-3.17283300	2.19822000	-4.80295500
H	-3.82653400	3.50775700	-3.81534000
C	-3.71343000	2.41894900	-3.87472900
H	-4.71700600	1.98607100	-3.95686700
H	3.04490900	3.75586200	-4.08364400
H	1.80996800	5.01771300	-4.05579400
H	5.22271600	0.24985600	-3.56851400
H	-1.00232300	2.35969200	-3.49757800
H	5.75242900	-1.37083400	-3.10878700
H	1.18380600	-4.79373900	-3.66529300
C	2.16940400	4.12245500	-3.53410200
H	4.44824500	5.30545200	-2.67004200
H	3.16332600	6.49533300	-2.39065200
C	5.06799200	-0.55665400	-2.84137900
H	1.38181900	3.36513500	-3.59779500
H	4.04644500	-0.93226400	-2.95764800
H	-1.64380100	3.59562900	-2.39726100
H	7.04068400	1.13403300	-2.05903300
C	3.59011800	5.55059900	-2.03167300

C	-1.56086100	2.51702200	-2.56654300
H	-5.23145600	0.07220900	-2.73266300
C	-2.94226600	1.85996100	-2.67087600
H	-2.78693300	0.79006000	-2.84960400
H	2.02764400	-2.59025300	-2.71192300
H	0.55205200	6.16180200	-2.62881600
C	1.02119900	-5.14059000	-2.63777700
H	0.23042600	-5.89940000	-2.65767900
H	7.46775400	-0.44950400	-1.38430700
H	1.94511800	-5.63177600	-2.31136700
C	2.54657000	4.42277700	-2.07664200
H	-5.86252000	-1.58302300	-2.59725300
C	6.78646000	0.40417300	-1.28013400
O	0.40448200	-0.19213000	-3.21872000
H	-4.09459800	4.09182400	-1.67888000
H	3.96696000	5.71680700	-1.01774400
H	-0.98842600	2.09590700	-1.73230400
H	6.01743700	-2.65186600	-1.31748600
C	-5.37123000	-0.77418000	-2.05213700
H	-4.41793000	-3.12015000	-2.32187800
H	-0.21270300	-3.45950200	-2.18420100
O	2.07233900	0.96989700	-2.06653000
C	5.32165200	-0.04129500	-1.41774500
C	0.39889100	5.68094100	-1.66555200
C	1.79946600	-2.93443000	-1.69534700
H	3.01639100	3.52512800	-1.66207000
C	0.65519900	-3.95482700	-1.73482400
H	2.70920900	-3.37244700	-1.27136400
H	-3.66867200	-5.08856800	-2.01965600
C	-3.69928100	2.00344000	-1.36070600
H	4.69395600	0.84295900	-1.26672200
C	1.18189900	0.36685700	-2.55644100
H	-1.43368600	6.74407700	-1.27888200
C	-4.23078100	3.24724900	-1.00826600
H	6.98050200	0.87182000	-0.30987000
H	-6.04582100	-0.42747600	-1.26247800
C	-3.71633900	-2.57833400	-1.69854700
C	1.33165100	4.74102800	-1.21410200
C	-4.04781100	-1.22900800	-1.47347600
H	-1.91249900	-5.26018700	-1.81007900
H	1.53276200	-2.06864900	-1.07780200
C	5.40235000	-2.37595100	-0.46419400
C	-0.71900900	6.01254500	-0.90899300
C	-2.82798800	-4.86233900	-1.36022900
C	4.93936600	-1.06048900	-0.35142400
C	-2.71217600	-3.37270500	-1.11323600
N	-3.29580600	-0.36549400	-0.78337500
C	-3.86747700	0.91419600	-0.47493800
Mg	-1.31444300	-0.85224600	-0.33441900
H	5.46122700	-4.35451300	0.38396600
C	-4.93223100	3.42464100	0.17862900
H	-5.34610600	4.39790900	0.43131600
C	5.09318400	-3.33679600	0.49133500
C	0.27128600	-4.37291300	-0.32477400
N	-1.71388900	-2.90310000	-0.35831000
O	0.22344200	0.13816000	-0.08606200
H	-2.97059000	-5.40358900	-0.41912000
Mg	1.78294700	1.13939700	0.16583800
C	1.13141300	4.14296800	0.05372700
H	1.97917200	-5.65870800	-0.10674200
C	-0.91527500	5.40380200	0.32578400
H	2.86942600	5.75765500	0.93168100

N	2.07665700	3.18270800	0.53984700
C	1.08417100	-5.27087400	0.37255000
C	4.15989900	-0.71116100	0.77793800
C	-0.88253200	-3.86081800	0.31295400
C	-4.57973300	1.08379400	0.73588600
H	-6.77193600	-0.62794800	0.92540000
C	-5.10392400	2.34530600	1.03677800
N	3.67460400	0.62965100	0.91620700
H	-1.79364500	5.66028200	0.91213700
C	-0.00033200	4.47758100	0.83422700
C	4.31225300	-2.98623400	1.58733100
C	3.05374000	3.62767000	1.33452600
H	6.25335500	0.33838400	1.73950300
C	3.07511500	5.08135100	1.76510400
C	4.40007300	1.47649100	1.65198600
H	-0.93444300	1.92965400	1.42712900
C	3.84560500	-1.68003900	1.76014200
H	-5.65923600	2.48238000	1.96218100
H	-6.84768200	0.46433000	2.31461400
C	4.09383800	2.83484200	1.85255100
C	-6.30009400	-0.38204300	1.88279900
H	4.06694200	-3.74089900	2.32985500
H	4.03864500	5.34575600	2.20680100
C	0.76942500	-5.68006700	1.66336400
H	-4.31982400	-0.94960300	1.30729400
C	-4.80757400	-0.05834800	1.71594800
H	2.29665600	5.26575100	2.51535100
C	5.63928100	0.98308700	2.37313700
C	-1.21297600	-4.27185700	1.62540000
H	-2.97351400	-3.07602600	1.68197400
H	-2.23607700	3.08540900	1.76390000
H	4.78881800	3.36451200	2.49415800
H	1.10197400	-1.30684200	1.92159400
C	-1.26658000	2.71520100	2.11635300
H	1.40960500	-6.38628600	2.18662200
C	-0.23922100	3.85247900	2.20127000
H	6.24861100	1.81966200	2.72307200
H	-6.43326100	-1.24013000	2.55295200
H	0.70652900	3.41035100	2.53384600
C	-0.37365900	-5.18219100	2.27633700
H	1.48489600	-2.86101800	2.68215100
H	5.35508500	0.38388500	3.24669000
C	-2.45406300	-3.77073400	2.35065800
C	1.55443400	-1.77417400	2.80442600
H	-1.44740800	-2.14167300	3.40733000
C	3.01294100	-1.33156200	2.98543200
H	3.01020100	-0.24064900	3.08532600
H	-3.73108500	-5.45783500	1.77639900
H	-1.41429400	2.26565500	3.10691100
H	-1.66136600	5.27943700	3.07146700
C	-4.17104100	0.23683200	3.08150400
H	-4.60604100	1.13226500	3.54112800
C	-0.65874100	4.87903900	3.26279200
H	0.03442300	5.72725000	3.30923600
H	-3.09223800	0.40202500	2.99237600
C	-2.08566400	-3.00345600	3.62832600
H	-0.62358200	-5.50713500	3.28387000
C	-3.42871800	-4.91258100	2.67697400
H	0.96286400	-1.49309000	3.68537200
H	-2.98780500	-2.63937500	4.13362100
H	-4.33583000	-4.51786400	3.15067300
H	3.51579100	-2.99826800	4.32122100

H	-4.33277900	-0.60021800	3.77081600
H	4.64868600	-1.64137800	4.41479300
C	3.59235100	-1.90515700	4.28590500
H	-1.54458600	-3.64246600	4.33627900
H	-0.68391000	4.40625500	4.25196800
H	-2.98184600	-5.63683500	3.36873400
H	3.03696600	-1.51519800	5.14733600

IV

$H = -3140.392466 \text{ au}$

$G = -3140.585003 \text{ au}$

$GD3BJ = -0.4155274411 \text{ au}$

H	-3.76553700	1.32497800	-5.00989500
H	-4.60970100	2.61953000	-4.14334400
C	-4.24349800	1.58895200	-4.05880000
H	-5.11333600	0.93609800	-3.92850300
H	2.87646900	3.40424300	-4.21109700
H	1.30971100	4.22673000	-4.20347300
H	4.83366500	0.19889600	-3.72680100
H	-1.49841800	1.98776200	-4.08110000
H	4.89332600	-1.51954300	-3.30950600
H	0.23740200	-5.04008900	-3.88673200
C	1.98587100	3.60600500	-3.60303000
H	4.06585600	5.36431200	-3.20081000
H	2.56857200	6.30818300	-3.18653700
C	4.54974200	-0.53671100	-2.96391800
H	1.49100000	2.65127600	-3.40350000
H	3.45794700	-0.55414100	-2.90335700
H	-2.27587700	3.37427000	-3.29653500
H	6.96236200	0.70844800	-2.50305800
C	3.17268200	5.59824700	-2.60875300
C	-2.00566600	2.31949800	-3.16856500
H	-5.92457300	-0.10620700	-2.08936900
C	-3.23989500	1.44769200	-2.90321300
H	-2.90637300	0.40551100	-2.88592900
H	1.70943700	-3.10199600	-3.18416700
H	0.25686400	5.85987700	-2.88491300
C	0.10133000	-5.33398800	-2.83894600
H	-0.89052000	-5.78926000	-2.74528100
H	7.15516400	-0.99529000	-2.06353600
H	0.84552200	-6.10656200	-2.60909700
C	2.38559200	4.31463200	-2.30041600
H	-6.36203000	-1.82608500	-2.23081200
C	6.70577300	-0.04554500	-1.74902800
O	-0.48452400	-0.67188400	-2.28412600
H	-4.15876200	3.83123900	-2.06344900
H	3.49850300	6.10786500	-1.69513800
H	-1.28607000	2.26613700	-2.34679700
H	5.70464900	-2.80753400	-1.52620800
C	-5.90089400	-1.07489600	-1.58478300
H	-5.02856500	-3.44677300	-1.73831400
H	-0.50004600	-3.38368400	-2.20805600
O	1.39551600	0.55754500	-1.94430500
C	5.17953700	-0.16617600	-1.61335500
C	0.17058100	5.43982700	-1.88543500
C	1.63162100	-3.45782200	-2.15095300
H	3.05577400	3.64366600	-1.75188600
C	0.26386000	-4.11246500	-1.91988400
H	2.45290200	-4.16193800	-1.97384900
H	-4.12005900	-5.39500100	-1.58319900
C	-3.88206000	1.76159000	-1.55942900

H	4.79737900	0.82116900	-1.33119300
C	0.33931800	-0.03647400	-1.56146800
H	-1.71422500	6.40505200	-1.49844900
C	-4.31070100	3.06833200	-1.30403400
H	7.17870800	0.24800900	-0.80525900
H	-6.52232000	-0.98158500	-0.68647400
C	-4.21931100	-2.86151500	-1.31617200
C	1.18205100	4.59791900	-1.41077200
C	-4.49163100	-1.48308800	-1.21057300
H	-2.42619200	-5.65898900	-1.10284100
H	1.78992600	-2.60194200	-1.48868400
C	5.16311600	-2.48882300	-0.63853400
C	-0.93835400	5.75068300	-1.10848200
C	-3.34765900	-5.12543300	-0.85869200
C	4.79226100	-1.14564000	-0.51310800
C	-3.14063500	-3.62576600	-0.82846500
N	-3.62266500	-0.56398500	-0.77981600
C	-4.08941300	0.77434600	-0.56683100
Mg	-1.63776300	-1.12133700	-0.69315700
H	5.15446100	-4.45981600	0.22679200
C	-4.92843700	3.40951200	-0.10733900
H	-5.25731900	4.43084200	0.06903900
C	4.85736600	-3.42059800	0.34543600
C	0.04384400	-4.47560500	-0.45792400
N	-2.01092900	-3.11852100	-0.32660300
O	0.06893100	0.01806300	-0.23752500
H	-3.67266000	-5.48507600	0.12455200
Mg	1.86360200	1.15440200	-0.09163100
C	1.05760300	4.06466700	-0.10634600
H	1.81929100	-5.68258500	-0.38765300
C	-1.04686800	5.22373800	0.17365500
H	3.03285900	5.70670500	0.52498200
N	2.04507600	3.14708000	0.38230200
C	0.96209000	-5.32045800	0.17435000
C	4.09327600	-0.74578300	0.64989800
C	-1.07096700	-4.01336200	0.28096400
C	-4.72410600	1.10878300	0.65403300
H	-7.11314700	-0.13813600	1.32206700
C	-5.12923300	2.43121000	0.85977500
N	3.64533500	0.61030800	0.77905700
H	-1.91716100	5.46654700	0.77768300
C	-0.05908400	4.38726900	0.70041700
C	4.17334300	-3.01433100	1.48594800
C	3.06221500	3.62331600	1.10517200
H	6.34917200	0.51817100	1.31652600
C	3.11296000	5.10013700	1.43232600
C	4.41680900	1.47968400	1.43772100
H	-0.94410400	1.88003500	1.46053500
C	3.78793400	-1.68313600	1.66498500
H	-5.61659500	2.69751900	1.79501100
H	-6.76576100	0.95573100	2.66521000
C	4.12540300	2.84680000	1.60306500
C	-6.44842300	0.02664900	2.17696200
H	3.93323800	-3.74591900	2.25293700
H	4.04008100	5.35986200	1.94764500
C	0.80081200	-5.70767300	1.49887200
H	-4.70084200	-0.90240900	1.36370400
C	-4.97292500	0.08401000	1.75333900
H	2.27031600	5.38600400	2.07185400
C	5.70916900	1.00000700	2.06244200
C	-1.24643800	-4.40205900	1.63126400
H	-3.10838800	-3.37972500	1.81506300

H	-2.22526100	3.03125400	1.84698900
H	4.85961000	3.39988300	2.17716400
H	1.07229400	-1.27472300	1.97901800
C	-1.22883600	2.68650200	2.14527500
H	1.52430300	-6.36915700	1.96942400
C	-0.21162700	3.83500500	2.11051800
H	6.26085800	1.82678100	2.51491400
H	-6.60776300	-0.78952900	2.89197300
H	0.75608300	3.42116200	2.41388700
C	-0.29688900	-5.24562300	2.21587000
H	1.47316500	-2.78851200	2.79210800
H	5.51433900	0.24877700	2.83558600
C	-2.42331800	-3.92528100	2.47211100
C	1.56938800	-1.69897200	2.85842700
H	-1.46125800	-2.07673500	3.13779100
C	3.04326200	-1.27621700	2.92850000
H	3.06608600	-0.18289500	2.99160200
H	-3.52926700	-5.81617800	2.34695600
H	-1.30165700	2.26803300	3.15699500
H	-1.59562700	5.30756000	2.96534600
C	-4.08426800	0.35390100	2.97613100
H	-4.29735900	1.33816600	3.41045100
C	-0.58703100	4.91350400	3.13625200
H	0.10819700	5.76040400	3.10962800
H	-3.02225700	0.33248800	2.71111200
C	-1.96287000	-2.95066600	3.56596100
H	-0.42296800	-5.54890000	3.25279700
C	-3.20640300	-5.08845700	3.09927000
H	1.02962200	-1.36302200	3.75270500
H	-2.81791800	-2.59807300	4.15538100
H	-4.09961900	-4.71221400	3.61245200
H	3.61654800	-2.91183700	4.27324100
H	-4.25675100	-0.39988100	3.75389500
H	4.75806200	-1.56004300	4.26534200
C	3.69495000	-1.82035800	4.20724800
H	-1.25794100	-3.43341500	4.25360200
H	-0.57027300	4.49244200	4.14864300
H	-2.60550700	-5.62768200	3.84117600
H	3.19515600	-1.40507500	5.09058100

^{con}TS_{II-V}

$H = -3253.592209 \text{ au}$

$G = -3253.795779 \text{ au}$

$GD3BJ = -0.4148227938 \text{ au}$

Mg	1.49983200	6.05402600	9.97277300
N	1.67957900	7.67439000	8.71077900
C	0.81897000	9.47214800	7.27030600
H	1.27937600	10.26082900	7.87382500
H	-0.13327900	9.83888400	6.88089600
H	1.49268700	9.29469400	6.42481500
N	-0.44640200	5.65053400	9.42540100
C	0.63116700	8.20938100	8.08238900
C	-0.67242000	7.67689900	8.10333900
H	-1.40603100	8.25286100	7.55120300
C	-1.16911400	6.49579300	8.68736100
C	-2.62877000	6.19180800	8.42925000
H	-2.73750000	5.26354200	7.85800000
H	-3.10986100	6.99850700	7.87192600
H	-3.16981700	6.04268100	9.36917200
C	2.97088800	8.27560600	8.56209200
C	3.43330500	9.20394100	9.52425300

C	4.73604200	9.69856500	9.40353800	H	8.80894700	4.44660500	14.84783600
H	5.10326300	10.40801500	10.14127400	C	7.18275200	3.36615400	13.92893900
C	5.56892100	9.30410400	8.36359300	C	6.67831100	2.13478700	14.39702400
H	6.57810500	9.70188800	8.28915600	H	7.43117900	1.47279700	14.80929400
C	5.09888200	8.40217800	7.41581400	C	5.35308900	1.68096300	14.56438400
H	5.74925400	8.09919600	6.59830200	C	5.19079900	0.41176600	15.37349200
C	3.80586600	7.87653200	7.49092600	H	4.63322100	0.61181900	16.29507300
C	2.55819000	9.69648200	10.66922800	H	6.15941300	-0.01533200	15.64189100
H	1.57166100	9.23189900	10.55866000	H	4.61566600	-0.33788000	14.82115300
C	3.11573800	9.27928000	12.03761600	C	7.06259600	5.58954000	13.07382600
H	3.18831200	8.19122600	12.12607200	C	7.69938700	5.83433700	11.83451200
H	2.46003300	9.63929500	12.84035600	C	8.24742500	7.09812500	11.59523100
H	4.11369300	9.70139700	12.20702600	H	8.73507300	7.29320400	10.64304800
C	2.35720300	11.21930000	10.61574600	C	8.18024500	8.10869600	12.54590300
H	3.30200700	11.75405200	10.77023800	H	8.61637800	9.08375000	12.34279000
H	1.66420100	11.53885800	11.40340500	C	7.54460100	7.86213700	13.75624700
H	1.94722400	11.54512900	9.65312700	H	7.48428200	8.65460200	14.49880900
C	3.34185700	6.88666400	6.43100200	H	6.97677500	6.61693200	14.04308900
H	2.27280300	6.70635500	6.58644900	C	7.78253700	4.77912300	10.74227400
C	4.06096700	5.53858200	6.58031100	H	7.40473000	3.83991400	11.15978100
H	5.14148000	5.65056900	6.42826700	C	9.22034200	4.52592800	10.26593000
H	3.69087400	4.81673000	5.84168200	H	9.64675000	5.41021100	9.77795900
H	3.90999800	5.11165400	7.57663900	H	9.24036500	3.70752600	9.53585800
C	3.51524000	7.42921400	5.00490500	H	9.88312700	4.25415700	11.09488700
H	3.02128300	8.39863800	4.87472200	C	6.88959200	5.16479200	9.55305300
H	3.08506800	6.73016100	4.27752700	H	5.85132200	5.33098300	9.86086900
H	4.57271600	7.56051000	4.74674700	H	6.90712800	4.38478800	8.78066500
C	-1.05628600	4.45023600	9.91489200	H	7.23304700	6.09609800	9.08845400
C	-1.60178400	4.41784500	11.21996300	C	6.27761100	6.42200200	15.38050800
C	-2.10382300	3.20581400	11.70484900	H	5.93252800	5.38390200	15.42941400
H	-2.52012800	3.16899600	12.70882000	C	5.04287400	7.32850000	15.49242600
C	-2.08315300	2.05089000	10.93249500	H	5.32301800	8.38745600	15.43591600
H	-2.47951600	1.11938400	11.32935400	H	4.53714500	7.17064100	16.45261100
C	-1.55914800	2.09813000	9.64563800	H	4.32579200	7.12374700	14.69130200
H	-1.55099900	1.19528800	9.03904700	C	7.22615500	6.64862500	16.56718400
C	-1.04464100	3.28372500	9.11298500	H	7.58192200	7.68529400	16.60712300
C	-1.68146900	5.65741300	12.10063900	H	8.10675100	5.99850800	16.51425600
H	-1.28392200	6.50080000	11.52471000	H	6.71026700	6.44058600	17.51239700
C	-0.82560900	5.51809600	13.36763900	C	2.97315100	1.82194700	14.48664400
H	-1.16081900	4.67667700	13.98597800	C	2.30242800	0.84976900	13.70795500
H	-0.89657800	6.42877700	13.97546100	C	1.02465100	0.43730100	14.09777400
H	0.22880000	5.35923200	13.12282500	H	0.50257100	-0.30740900	13.50155500
C	-3.13383000	5.99751600	12.47080900	C	0.40764800	0.96080600	15.22696600
H	-3.76657900	6.11509800	11.58382100	H	-0.58513300	0.62450400	15.51591400
H	-3.17181700	6.93495000	13.03878800	C	1.07005900	1.92219600	15.97979700
H	-3.58198700	5.21484500	13.09463700	H	0.58478600	2.33788900	16.85995800
C	-0.47952600	3.28028700	7.69884400	C	2.34778400	2.37061700	15.63120600
H	-0.26724000	4.31808500	7.42051500	C	2.91131300	0.26180900	12.44421000
C	0.84511300	2.50734200	7.63378600	H	3.94403200	0.61992800	12.37679600
H	0.69852000	1.45370900	7.90141100	C	2.15549300	0.75801900	11.20218600
H	1.58683700	2.92322300	8.32251400	H	1.11407200	0.41655800	11.21059500
H	1.26560800	2.54128500	6.62102800	H	2.62008200	0.37747700	10.28303400
C	-1.47366200	2.72230700	6.66990400	H	2.12656100	1.85231300	11.15419700
H	-1.67457800	1.65711700	6.83521100	C	2.95698000	-1.27299700	12.46116400
H	-1.06786100	2.82514100	5.65620200	H	3.49085000	-1.65585300	13.33803000
H	-2.43441000	3.24819400	6.70393400	H	3.46790200	-1.64799800	11.56586700
Mg	4.49656300	3.91348700	12.83159500	H	1.95109900	-1.70878500	12.47053300
N	6.45399300	4.31770900	13.34013700	C	3.00888500	3.43933400	16.48926100
N	4.26776500	2.30090500	14.09543600	H	4.00401200	3.63228300	16.07479500
C	8.65921700	3.60264400	14.16557500	C	3.19712800	2.97831800	17.94228300
H	9.17189800	3.86369700	13.23450300	H	2.23481800	2.79415700	18.43483900
H	9.13898000	2.72126700	14.59644400	H	3.72264500	3.74741100	18.52128700

H	3.78221900	2.05362200	18.00277100
C	2.22021600	4.75609100	16.43375300
H	2.14329100	5.12917300	15.40764600
H	2.71456700	5.52389400	17.04083000
H	1.20414700	4.62729600	16.82647400
O	2.98857200	4.74170100	10.66230700
C	2.60152900	5.50747000	11.66132200
O	3.15874900	5.33621100	12.79755600
C	4.62647900	2.67360800	9.90610900
O	5.02534600	2.64781500	11.01254500
O	4.29794300	2.62136000	8.79611400

V

$H = -3253.601414 \text{ au}$

$G = -3253.804995 \text{ au}$

$GD3BJ = -0.4090577179 \text{ au}$

Mg	-1.67488200	1.14658700	-1.54498700
N	-1.62528500	2.98027300	-2.42778000
C	-2.56597700	4.85666500	-3.70521500
H	-2.30975700	5.59760000	-2.94110700
H	-3.50307800	5.15287100	-4.18126000
H	-1.76819700	4.89477700	-4.45456700
N	-3.55169500	0.66346800	-2.17691400
C	-2.66503600	3.47253000	-3.10559000
C	-3.88092300	2.79128000	-3.30731200
H	-4.61997100	3.34447900	-3.87501200
C	-4.30257900	1.51843200	-2.87778300
C	-5.71760500	1.12841000	-3.23976600
H	-5.73095800	0.21459600	-3.84167900
H	-6.21823900	1.92141700	-3.79922500
H	-6.30112100	0.91480100	-2.33747900
C	-0.45481700	3.78468800	-2.22693700
C	-0.35030300	4.57193800	-1.05487700
C	0.83972500	5.26717000	-0.82086900
H	0.93303300	5.87307300	0.07747500
C	1.90428600	5.19849100	-1.71169800
H	2.82335700	5.74300000	-1.50999300
C	1.78417500	4.43243500	-2.86491500
H	2.61720000	4.38371000	-3.56209900
C	0.61524000	3.71928200	-3.14954000
C	-1.48838000	4.68935400	-0.04945700
H	-2.34019000	4.12224500	-0.44134900
C	-1.11202100	4.08021400	1.30914700
H	-0.81764000	3.03014300	1.21312800
H	-1.96085500	4.13406900	2.00219800
H	-0.27418900	4.61939600	1.76705400
C	-1.95165300	6.14348800	0.12758600
H	-1.16311800	6.76589100	0.56700500
H	-2.81893400	6.18813800	0.79742600
H	-2.23905100	6.59915300	-0.82649100
C	0.53472500	2.91074500	-4.43746400
H	-0.47914000	2.50144900	-4.51343500
C	1.51410700	1.72773600	-4.43452400
H	2.54987900	2.07240900	-4.32883700
H	1.44199600	1.17183800	-5.37713000
H	1.31201400	1.02151300	-3.62403700
C	0.77163500	3.78807100	-5.67720100
H	0.09720800	4.65141100	-5.70648300
H	0.61295400	3.20303500	-6.59095400
H	1.79834400	4.17194800	-5.70743000
C	-4.09054500	-0.61088800	-1.79600600

C	-4.66146800	-0.76402000	-0.51044600
C	-5.07588300	-2.03745300	-0.10871000
H	-5.50653100	-2.16839800	0.88107300
C	-4.94725000	-3.13708300	-0.94813900
H	-5.27228600	-4.12021200	-0.61689100
C	-4.40612500	-2.96966500	-2.21727600
H	-4.31427200	-3.83041800	-2.87538000
C	-3.97465600	-1.71861500	-2.66942700
C	-4.84860700	0.41058300	0.44019200
H	-4.54900100	1.32165600	-0.09067200
C	-3.95733300	0.28214100	1.68375600
H	-4.19810000	-0.62113300	2.25601500
H	-4.09316500	1.14671500	2.34523100
H	-2.89659100	0.22498000	1.41750100
C	-6.31875000	0.58852200	0.84926000
H	-6.97352900	0.68859900	-0.02370200
H	-6.43600400	1.48830800	1.46527200
H	-6.67979300	-0.26312900	1.43780400
C	-3.40962600	-1.59814000	-4.07905900
H	-3.21670800	-0.53748800	-4.27554300
C	-2.07711200	-2.34658500	-4.22836800
H	-2.20094300	-3.41690300	-4.02255500
H	-1.30465800	-1.96391600	-3.55558300
H	-1.69849700	-2.24783500	-5.25317900
C	-4.40816800	-2.09059700	-5.13923000
H	-4.58440700	-3.16937400	-5.05349700
H	-4.01450400	-1.90167500	-6.14503600
H	-5.38044100	-1.59155600	-5.05771800
Mg	1.70965400	-1.33360100	1.28066600
N	3.67618500	-0.96825700	1.76874400
N	1.33387700	-2.56095900	2.88117200
C	5.72250700	-1.30970100	3.11466000
H	6.27990000	-0.89870400	2.27115400
H	6.23073600	-2.20732900	3.47831900
H	5.75349900	-0.56751600	3.92228500
C	4.28140700	-1.61715600	2.76217500
C	3.66209500	-2.58139900	3.58483400
H	4.32320500	-3.03703700	4.31446500
C	2.31952200	-2.99014700	3.67623800
C	2.00738300	-3.96094000	4.79567600
H	1.54620000	-3.43685200	5.64087500
H	2.91756600	-4.44501900	5.15777000
H	1.29805300	-4.72896500	4.47626100
C	4.39037600	0.01167000	1.00589200
C	4.99130300	-0.36052500	-0.22228400
C	5.62081500	0.63097800	-0.98158300
H	6.09342000	0.35761100	-1.92139200
C	5.65632500	1.95572500	-0.56180500
H	6.14850400	2.70993200	-1.17108800
C	5.06096100	2.30776500	0.64314800
H	5.08969000	3.34454900	0.97056300
C	4.42700000	1.35536400	1.44692200
C	5.01839800	-1.80454500	-0.70786800
H	4.27490100	-2.36326100	-0.12968800
C	6.39014700	-2.44836200	-0.44460900
H	7.18115300	-1.91741500	-0.98897600
H	6.39267400	-3.49217100	-0.78174500
H	6.65229900	-2.43872700	0.61809300
C	4.64983600	-1.95091700	-2.18975600
H	3.67840700	-1.50547700	-2.41862200
H	4.59519100	-3.01378600	-2.45319600
H	5.40206200	-1.49420500	-2.84474700

C	3.79929000	1.79724000	2.76178200
H	3.43679400	0.90201000	3.27855600
C	2.58967500	2.71295900	2.52568700
H	2.88412000	3.62976500	2.00090100
H	2.13516700	3.00351400	3.48112300
H	1.82297100	2.21648500	1.92336100
C	4.81817200	2.48150100	3.68544300
H	5.17160000	3.43004500	3.26371800
H	5.69654500	1.85005000	3.85788300
H	4.36178900	2.70449700	4.65762100
C	-0.01291500	-2.95958800	3.15989700
C	-0.60056700	-4.01417800	2.42132900
C	-1.93358100	-4.35155800	2.67821000
H	-2.38975700	-5.16697100	2.12195900
C	-2.68362500	-3.66910700	3.62798700
H	-3.71772200	-3.94887800	3.81463300
C	-2.10035400	-2.62647000	4.33908700
H	-2.69081800	-2.08991700	5.07818500
C	-0.76994100	-2.25351900	4.12733800
C	0.17562600	-4.80646800	1.37834600
H	1.15189200	-4.32570900	1.25291200
C	-0.52237400	-4.80070200	0.01169000
H	-1.47767500	-5.33840000	0.04316400
H	0.10948000	-5.28967100	-0.73893300
H	-0.72271700	-3.78152600	-0.33092400
C	0.43343600	-6.24909000	1.84094100
H	0.98790000	-6.28005700	2.78504300
H	1.01877900	-6.79293700	1.08952300
H	-0.50786300	-6.79244900	1.98965700
C	-0.19136100	-1.09200400	4.92545300
H	0.88621300	-1.05581900	4.73376100
C	-0.38608500	-1.26228200	6.43941100
H	-1.44398900	-1.20220600	6.72196100
H	0.14067100	-0.46699600	6.98049800
H	-0.00488000	-2.22529500	6.79695600
C	-0.78310100	0.24826900	4.46232800
H	-0.59981400	0.42044100	3.39757000
H	-0.33855800	1.07900600	5.02491100
H	-1.86733600	0.27523900	4.62658400
O	-0.11834800	-0.27738300	-1.22015900
C	-0.35009300	0.39232800	-0.01155200
O	0.34081300	0.13914900	0.98086200
C	0.91258400	-1.33976100	-1.57955800
O	1.44571300	-1.88560800	-0.58405400
O	1.01992300	-1.47756000	-2.76985400

^{con}TS_{v-IV}

$H = -3253.595312 \text{ au}$

$G = -3253.798443 \text{ au}$

$GD3BJ = -0.4105217254 \text{ au}$

Mg	1.37398900	5.85711200	9.89473800
N	1.52943400	7.71666700	9.06180200
C	0.70546700	9.57908200	7.65704900
H	1.43589700	10.20709600	8.17010700
H	-0.25430700	10.10202100	7.62055200
H	1.04714700	9.45075300	6.62261300
N	-0.50652700	5.46050400	9.23050700
C	0.54988400	8.22170900	8.31007400
C	-0.67114900	7.57130000	8.03704300
H	-1.34641200	8.13921300	7.40627400
C	-1.17355600	6.32909600	8.46261200

C	-2.57447100	5.98670600	8.00796700
H	-2.56742800	5.10509500	7.35888600
H	-3.02801900	6.81533100	7.45994300
H	-3.21278300	5.73902200	8.86220400
C	2.69479300	8.49967000	9.35923600
C	2.73269200	9.23295300	10.57155200
C	3.89820100	9.93561100	10.89050900
H	3.93669500	10.50970400	11.81268600
C	5.00732300	9.91627200	10.05291000
H	5.90697400	10.46379800	10.32234500
C	4.95543700	9.19670900	8.86613900
H	5.82194400	9.18751000	8.20953900
C	3.81097600	8.48498600	8.49068300
C	1.52861200	9.32633600	11.50055600
H	0.81789100	8.54600300	11.20527300
C	1.88468700	9.08671700	12.97308300
H	2.39940600	8.13142800	13.10851000
H	0.97188800	9.07069400	13.58089000
H	2.52631900	9.88047100	13.37367400
C	0.81439800	10.67841500	11.33976400
H	1.48008900	11.50582100	11.61487100
H	-0.06894900	10.72728400	11.98858100
H	0.48493100	10.84474400	10.30907200
C	3.80916000	7.75474200	7.15430700
H	2.82909000	7.28064500	7.02971500
C	4.86936400	6.64519500	7.09984000
H	5.87862000	7.05365200	7.23222800
H	4.83973700	6.14368900	6.12453900
H	4.70229900	5.88527000	7.86747000
C	4.00898400	8.73137900	5.98359100
H	3.28223300	9.55054700	6.00180200
H	3.90682200	8.20425400	5.02732300
H	5.00987000	9.17909700	6.00701000
C	-1.13428500	4.23323100	9.62761200
C	-1.78287400	4.16403900	10.88367600
C	-2.30705100	2.93747500	11.30242900
H	-2.80515700	2.87504900	12.26729100
C	-2.20508100	1.79995600	10.51127100
H	-2.61725600	0.85418600	10.85447500
C	-1.57678900	1.88260400	9.27450500
H	-1.50225600	0.99246000	8.65419200
C	-1.03695000	3.08474700	8.80613900
C	-1.94297500	5.38052100	11.78607600
H	-1.50107600	6.24104300	11.27116800
C	-1.20067300	5.20482100	13.11895000
H	-1.59350800	4.35313600	13.68638200
H	-1.31197700	6.10207900	13.74014000
H	-0.13034600	5.03200400	12.96617100
C	-3.42184700	5.71155600	12.03902900
H	-3.97002100	5.86482100	11.10289600
H	-3.51127900	6.62699900	12.63651000
H	-3.92387900	4.90654000	12.58874500
C	-0.37390500	3.10710200	7.43457500
H	-0.09235200	4.14259800	7.21315500
C	0.90959900	2.26355900	7.40757200
H	0.69728600	1.21552500	7.65192800
H	1.65753700	2.63520600	8.11316100
H	1.35884100	2.28855600	6.40709200
C	-1.33178600	2.63832300	6.32726400
H	-1.58660700	1.57787900	6.44037300
H	-0.86190800	2.75980000	5.34399800
H	-2.27129700	3.20238500	6.32484300

Mg	4.80309900	3.76004800	12.78936000
N	6.78894000	4.04813000	13.22076400
N	4.43330400	2.48076800	14.34894600
C	8.87955100	3.53946200	14.42833200
H	9.43520800	3.81866200	13.53068100
H	9.33404300	2.64907700	14.87021800
H	8.99453500	4.36193200	15.14515900
C	7.41044200	3.31217600	14.14287600
C	6.78863800	2.32671900	14.93669900
H	7.46134300	1.79955000	15.60430100
C	5.43466500	1.96656900	15.06937400
C	5.13568200	0.94475000	16.14582000
H	4.77295500	1.44091000	17.05349000
H	6.03461300	0.38226000	16.40963000
H	4.35548500	0.24568400	15.83382700
C	7.51935000	5.04383200	12.49210200
C	8.07464400	4.72204000	11.22919700
C	8.72594300	5.73055400	10.51178300
H	9.16353400	5.49318700	9.54506000
C	8.82790400	7.02520800	11.00657500
H	9.33668400	7.79371700	10.42966900
C	8.27792600	7.32826100	12.24597800
H	8.35948700	8.34145100	12.63308600
C	7.62390200	6.35676900	13.00972800
C	8.02777100	3.31411200	10.64858700
H	7.37907500	2.70958700	11.29141100
C	9.42175400	2.66454800	10.65523500
H	10.12000000	3.22399000	10.02050100
H	9.36658300	1.63976500	10.26794700
H	9.85077500	2.61992800	11.66187500
C	7.43626100	3.27786200	9.23302200
H	6.42327400	3.68655500	9.20946500
H	7.38610100	2.24135500	8.87750600
H	8.05509900	3.83756300	8.52115000
C	7.04665400	6.74932800	14.36309300
H	6.65100200	5.84338600	14.83511600
C	5.88075800	7.73725700	14.21082200
H	6.21367100	8.67144000	13.74279600
H	5.45766700	7.98607000	15.19208400
H	5.08044500	7.32259400	13.59105300
C	8.11590700	7.33065400	15.30042000
H	8.50192900	8.28642300	14.92631600
H	8.96963400	6.65381700	15.41435000
H	7.69207200	7.51449400	16.29520300
C	3.08412400	2.11036000	14.65628800
C	2.43451700	1.12343200	13.87640100
C	1.10152500	0.81165200	14.16309700
H	0.59777700	0.04828900	13.57524400
C	0.40925300	1.45717600	15.18024800
H	-0.62677300	1.20022700	15.38719300
C	1.05237900	2.43436600	15.93070200
H	0.50712000	2.94266100	16.72266900
C	2.38671900	2.77749300	15.69319800
C	3.14618300	0.37441000	12.75791300
H	4.11729000	0.85598500	12.59877300
C	2.37569700	0.44078700	11.43261600
H	1.43104100	-0.11353300	11.48413600
H	2.97302100	0.00071100	10.62553200
H	2.14032200	1.47268600	11.15753900
C	3.42095500	-1.08790700	13.14256400
H	4.03453900	-1.16301900	14.04665600
H	3.95188200	-1.60311600	12.33272400

H	2.48525400	-1.62956900	13.32807600
C	3.03008200	3.86277600	16.54732500
H	4.09520600	3.90391700	16.29570100
C	2.91878400	3.56621700	18.05077300
H	1.87800300	3.60364300	18.39365300
H	3.47985500	4.31168000	18.62712300
H	3.31227300	2.57568400	18.30426200
C	2.43238100	5.24424900	16.23840200
H	2.55808700	5.50997000	15.18494200
H	2.92016700	6.01746600	16.84519800
H	1.35955100	5.26858800	16.46584400
O	2.40610000	4.43807500	10.85528700
C	2.54498800	5.54793100	11.93843600
O	3.45554700	5.35554100	12.71742200
C	3.54908700	3.92582200	10.16540600
O	4.42659600	3.39051700	10.89896800
O	3.51103300	4.11661000	8.95625300

${}^{\text{oxa}}\text{TS}_{\text{II-VI}}$

$H = -3253.581008 \text{ au}$

$G = -3253.786773 \text{ au}$

$GD3BJ = -0.407247554 \text{ au}$

H	-2.61150700	0.54672000	-6.03858200
H	-2.56333300	-1.20773800	-6.25911800
H	2.07536900	-5.08815100	-3.97367500
H	3.19784600	-3.04444500	-4.79173900
C	-2.93162200	-0.40856400	-5.60485700
H	-4.02635000	-0.43889900	-5.63069900
H	5.61212500	-2.05584700	-4.76888400
C	2.46758700	-4.36184000	-3.26615500
C	3.09625400	-3.20906800	-3.72158900
H	-0.42499800	-1.31362400	-4.75983700
H	-0.50979000	0.45244500	-4.62178600
H	3.37718000	-0.89346200	-5.37221500
C	5.68086700	-1.33647800	-3.94367100
H	6.16264300	-0.42866500	-4.32780900
H	-2.02660100	-3.08456600	-5.01739300
H	6.33751900	-1.76608600	-3.18059000
C	-0.85476600	-0.48954100	-4.17820300
C	-2.38924300	-0.55342400	-4.17566200
H	1.84536400	-5.47785500	-1.54563500
H	-5.42832400	-0.70284800	-3.87563000
C	2.34258100	-4.57800000	-1.89946800
H	-2.75728000	0.29901900	-3.59382800
C	3.44598900	-0.30289100	-4.45113400
C	-2.56778000	-3.06011100	-4.07412200
H	-6.80949200	0.11135400	-3.10598900
H	3.90093800	0.65941600	-4.71638000
C	3.60005600	-2.25585100	-2.83129200
C	4.28739300	-1.01300000	-3.38131500
H	-0.46218900	-0.56682400	-3.15806900
C	-2.86559700	-1.82517300	-3.48996500
C	-5.94989600	-0.53859600	-2.92805300
H	-2.70159900	-5.20546100	-3.94218300
H	2.42376800	-0.11967500	-4.10451100
C	-2.94159100	-4.25492300	-3.47193300
H	-6.31948400	-1.51839900	-2.60488900
C	2.84321800	-3.66580800	-0.96489400
H	4.42467500	-0.31625000	-2.54697400
H	-0.52230900	4.53456700	-0.77105700
C	3.47655600	-2.49315700	-1.44055900

H	-2.57659400	6.02881100	-0.79305600
H	-6.44510000	1.57498200	-1.59906400
H	0.61427100	-4.65124400	0.40836500
C	-5.02417800	0.04932400	-1.88418900
C	-3.57228500	-1.80286300	-2.26506100
H	3.94616400	4.38186000	-1.97634400
H	2.75265800	-6.15998900	0.43417800
H	7.09038400	-2.53403200	-0.14687000
C	-3.61640400	-4.22321900	-2.25767900
N	-3.86355900	-0.55599900	-1.62116700
C	-5.49480900	1.20548500	-1.23121200
O	0.27844900	2.37516700	-2.60664000
H	0.77555800	-2.93110200	0.80766600
H	-2.79832800	3.60415900	-0.47459900
C	-3.94236200	-3.01478900	-1.63470600
C	1.21694800	-3.92024700	0.96118700
H	2.46095400	4.16136900	-1.02184100
H	-3.89718900	-5.15836300	-1.77861600
H	5.91757800	-3.07924700	-1.37131000
C	-0.83384000	4.12241200	0.19669400
C	-2.85153500	5.63521600	0.19313900
C	3.51844900	4.44158100	-0.96813500
C	2.68752800	-3.97210600	0.51894000
O	2.08317200	1.28974900	-1.60417400
H	-6.66225400	-3.36551600	-1.14114300
H	-0.48119800	3.08765400	0.26902300
H	-3.93986700	5.71101000	0.29435900
C	3.30659800	-5.32977300	0.88826500
C	6.03883900	-2.76725900	-0.33159300
H	3.55760800	5.49423300	-0.66430800
H	6.21266200	4.17136500	-0.83885200
C	1.14787800	1.81568700	-2.08349100
H	4.34888400	-5.41120600	0.55939400
N	3.93252000	-1.49657900	-0.51587900
C	-2.36136400	4.18794600	0.34318500
H	-6.17338300	2.75843900	1.47967600
H	-0.33421700	4.69565800	0.98626800
H	-2.40352300	6.29442700	0.94610300
C	-4.99380900	1.89491100	-0.10901100
Mg	-2.53276500	0.20047800	-0.23739000
H	-6.79153900	3.10055900	-0.14950200
H	1.13554600	-4.16188300	2.02850400
H	5.77300400	-3.62938000	0.29221500
H	4.36470700	2.54219500	-0.45316300
C	-5.88436500	2.98522600	0.44765500
H	3.22853800	-3.20177400	1.08026900
H	3.27967200	-5.47489900	1.97485800
C	5.15232200	-1.59110600	0.01751700
H	-4.88078200	-2.01579500	-0.00459900
C	-6.00504500	-3.79304000	-0.37537600
C	-4.66362600	-3.04956600	-0.29467400
H	-5.86508300	-4.85430700	-0.61376300
C	4.30129200	3.53926300	-0.00349200
N	-3.82886600	1.63285200	0.48624500
C	5.73802600	4.06556400	0.14463600
Mg	2.60313400	-0.07335900	0.10746700
H	5.74497500	5.04954400	0.62945800
C	-0.48497100	-0.18336200	0.19068900
H	-6.52838100	-3.73845200	0.58693900
O	-1.30954200	-0.88256500	0.89524800
C	-2.79476900	3.54889500	1.65409600
H	6.35877000	3.39245400	0.74365600

H	-5.35959300	3.94543400	0.47798000
O	0.77541500	-0.34598800	0.41665700
C	5.69394600	-0.68151100	0.94721000
C	-3.49772500	2.32242300	1.69810800
C	-3.76904100	-3.65961600	0.79555300
H	-2.83321900	-3.10200100	0.90326000
H	6.69842100	-0.92297400	1.27741700
H	-3.51772100	-4.70166500	0.56143500
C	3.61110800	3.38617400	1.34563300
H	3.23734800	5.49652100	1.53283100
H	-1.91586500	5.11811600	2.83149600
N	3.92231900	0.94731800	1.29650000
C	5.14014400	0.46208000	1.55402800
C	-2.45562900	4.17430600	2.85770200
C	3.12037500	4.52110300	1.99867500
H	-4.77789900	0.06269100	2.02926600
H	-4.28614600	-3.65179100	1.76302100
C	3.46916900	2.12540600	1.97625300
C	-3.82424300	1.73283200	2.94241600
H	7.06121800	0.87517100	2.45725700
H	5.71430700	0.77478800	3.59927400
C	6.00752600	1.12594900	2.60225400
C	-4.54475900	0.39624100	3.04631300
H	-6.53996600	1.25554100	3.34710500
C	-2.78681700	3.61239900	4.08460000
C	2.48295900	4.42673500	3.23036500
H	-2.71637200	-0.80125300	3.12205800
H	0.78665600	0.08970500	2.97487700
C	2.82798400	2.01826900	3.23307700
C	-3.45959100	2.39710200	4.11741900
H	2.10202100	5.31982100	3.71962500
C	-5.87539900	0.51364100	3.80440500
H	5.89416200	2.21238000	2.60401000
H	3.22137900	-0.06999200	3.40142500
C	-3.64357100	-0.66939600	3.68872200
H	-6.39808500	-0.45062400	3.80767300
H	-2.51634500	4.11552400	5.00986100
H	-4.16242900	-1.63519300	3.72662700
C	2.33593700	3.18276100	3.83132200
C	2.65642800	0.68849500	3.95532000
C	1.18604900	0.24208600	3.98191600
H	-3.70886000	1.95011400	5.07716200
H	-5.71942700	0.80730100	4.84955000
H	-3.37827200	-0.39470500	4.71723700
H	1.08828200	-0.70485400	4.52733400
H	1.83049200	3.11120100	4.79111900
H	0.55766400	0.98564200	4.48700400
H	4.26548500	1.08241400	5.39806700
C	3.22684600	0.73300800	5.38154400
H	3.19534000	-0.26640100	5.83172800
H	2.64427400	1.39975600	6.02824400

VI

$H = -3253.703826 \text{ au}$

$G = -3253.905276 \text{ au}$

$GD3BJ = -0.4018048323 \text{ au}$

H	-3.55338100	0.53974700	-6.10869700
H	-3.20049200	-1.18534500	-6.29363300
H	1.99999500	-4.73970300	-4.19487300
H	3.05619900	-2.57413400	-4.74402800
C	-3.59483100	-0.43174900	-5.60135200

H	-4.64788900	-0.67032500	-5.41657300	C	6.17271400	-2.67415800	-0.57760500
H	5.01844700	-1.38285500	-5.05994700	H	2.53157000	4.76012600	0.31796900
C	2.42042900	-4.12269200	-3.40461500	H	5.66344700	4.48093700	0.12195000
C	3.01450100	-2.90371200	-3.70839200	C	0.18773800	0.51579600	-0.54890700
H	-0.83279600	-0.74751200	-5.23322400	H	4.68081900	-5.50096300	0.20270100
H	-1.28775200	0.95931000	-5.12330900	N	3.94468400	-1.66685500	-0.31285700
H	2.74096200	-0.19232100	-4.62010200	C	-2.84636400	4.37863600	-1.00405500
C	5.37622500	-0.99297300	-4.09945500	H	-7.10693900	2.82759800	-0.06978100
H	5.88934600	-0.04466700	-4.29994200	H	-0.83476400	5.22747700	-1.11898900
H	-1.89164600	-2.80717700	-5.09085100	H	-3.06873200	6.55424800	-0.89242300
H	6.11561700	-1.70304200	-3.71273600	C	-5.16702500	1.88342500	-0.23907800
C	-1.32400200	-0.00207300	-4.59628000	Mg	-2.57958300	0.42236000	-0.47376300
C	-2.77961900	-0.38930200	-4.29900000	H	-5.74190400	3.95989200	-0.11255900
H	1.91633400	-5.50708100	-1.84653000	H	1.39607800	-4.89086400	1.89075300
H	-5.71538300	-1.37869800	-3.47615200	H	7.11503900	-2.74156900	-0.02943600
C	2.37356900	-4.54894000	-2.08292700	H	4.44144400	2.36378300	0.41657100
H	-3.21000100	0.39739800	-3.66955000	C	-6.07692800	2.98499400	0.25732700
C	3.20002800	0.21339500	-3.71032300	H	3.31370300	-3.56735800	1.03480300
C	-2.36872000	-2.86735500	-4.11544100	H	3.64095700	-5.94927600	1.56633600
H	-7.07125900	-0.44374300	-2.80114200	C	5.21536300	-1.71331700	0.09160500
H	3.69727900	1.15350900	-3.98042000	H	-4.70749100	-2.23053200	0.02732400
C	3.56143600	-2.08888800	-2.71225300	C	-5.44899800	-4.20937300	-0.30518200
C	4.21584800	-0.77346700	-3.11548400	C	-4.28852600	-3.20328800	-0.25317400
H	-0.73885800	0.09816100	-3.67784400	H	-5.08990600	-5.22665600	-0.50166000
C	-2.88088100	-1.70303700	-3.53427600	C	4.02571000	3.26502400	0.88063700
C	-6.17823000	-1.02194500	-2.55242300	N	-3.88972300	1.86706100	0.14876900
H	-2.05202400	-4.99010600	-3.94299800	C	5.18449600	4.25464300	1.08232600
H	2.40136900	0.44600700	-3.00033600	Mg	2.58311300	-0.38127300	0.51429900
C	-2.45927400	-4.09723200	-3.47508700	H	4.83183900	5.20193400	1.50773900
H	-6.49703400	-1.91053800	-1.99462300	C	-0.18392600	-0.47461800	0.59128700
C	2.90208700	-3.77263500	-1.04688700	H	-5.97847200	-4.22806600	0.65500400
H	4.63114600	-0.31453100	-2.21131600	O	-1.41192000	-0.64676500	0.80289600
H	-1.47162300	4.65043800	-2.66660800	C	-2.83440300	4.07046800	0.48801300
C	3.49323300	-2.52613500	-1.36726900	H	5.95142000	3.85584600	1.75545500
H	-3.66818500	5.83689100	-2.39354000	H	-6.06032100	3.04505600	1.34999500
H	-6.80409000	1.10890000	-1.31205100	O	0.77655500	-1.01431500	1.19833300
H	0.86905400	-5.23679700	0.23625300	C	5.76277000	-0.90412500	1.10674700
C	-5.21173400	-0.20349900	-1.72436200	C	-3.39471400	2.88659100	1.02672400
C	-3.50160100	-1.79595600	-2.26476300	C	-3.28786400	-3.60837600	0.84045800
H	3.46974000	4.11956100	-1.03993900	H	-2.49063700	-2.86818000	0.95409300
H	3.19702500	-6.42027400	-0.08101200	H	6.81350300	-1.08016900	1.30672200
H	6.39413600	-2.34163000	-1.59815400	H	-2.82397700	-4.57571400	0.61160400
C	-3.07892400	-4.17748100	-2.23382500	C	3.39859800	2.85881200	2.20858900
N	-3.94367900	-0.60169200	-1.60670200	H	2.80294000	4.87430900	2.65906400
C	-5.75453300	0.93776000	-1.10128600	H	-1.82253500	5.90690700	0.96139300
O	-0.77247300	1.02533000	-1.18151000	N	3.89784800	0.47920100	1.82409400
H	0.83790500	-3.57299000	0.84855300	C	5.17581400	0.10130100	1.89978500
H	-3.38066000	3.56644000	-1.50941400	C	-2.25998000	4.99642200	1.36447100
C	-3.61166400	-3.04592700	-1.60861400	C	2.81374100	3.84468600	3.00932600
C	1.40130400	-4.51023500	0.86185800	H	-4.45286400	0.82360800	2.25153000
H	2.19236000	3.13610600	-0.30812800	H	-3.79955400	-3.70611400	1.80630200
H	-3.15315100	-5.14183100	-1.73647200	C	3.40388400	1.52149300	2.67489400
H	5.73885300	-3.67449400	-0.66207700	C	-3.39129800	2.66291800	2.42510100
C	-1.42792400	4.43503200	-1.59155700	H	6.01386500	1.85646300	2.84908100
C	-3.59364000	5.68664600	-1.30977200	H	7.12763600	0.47353700	2.75684000
C	2.99042800	3.85150600	-0.09021000	C	6.08637200	0.76659000	2.90785700
C	2.84488600	-4.30874700	0.37815800	C	-4.01895000	1.42685700	3.05662200
O	1.41529300	0.71711000	-0.73587000	H	-5.92334000	2.41135200	3.53496200
H	-6.17379100	-3.96021400	-1.08807900	C	-2.23578300	4.77952100	2.73681200
H	-0.89838000	3.48749400	-1.45924900	C	2.24841900	3.53745600	4.24098400
H	-4.60873700	5.68779900	-0.89754000	H	-2.19632100	0.21385800	3.09416700
C	3.63901100	-5.61715200	0.52099200	H	0.91339200	-0.82270900	3.69282500

C	2.84591600	1.19928900	3.93573600
C	-2.80366900	3.62237300	3.25546700
H	1.79566200	4.31861200	4.84660500
C	-5.15724700	1.79701200	4.02083600
H	5.79627400	0.48876300	3.92734600
H	3.39511700	-0.85480200	3.79030100
C	-2.97733400	0.55857000	3.77783800
H	-5.64353700	0.89072000	4.40155200
H	-1.78126400	5.51180800	3.39949000
H	-3.45617100	-0.32700500	4.21386200
C	2.27237700	2.22425500	4.69474500
C	2.85699700	-0.21593400	4.49949900
C	1.43786800	-0.78383500	4.65169400
H	-2.79311100	3.45795300	4.33052000
H	-4.78250500	2.35874600	4.88482600
H	-2.49533300	1.11103900	4.59352000
H	1.47808800	-1.80288200	5.05659200
H	1.83618600	1.98586200	5.66219100
H	0.84133000	-0.17550700	5.34239700
H	4.61283500	0.12326000	5.77702700
C	3.59908900	-0.28690500	5.84388400
H	3.67608000	-1.32754100	6.18145100
H	3.06930700	0.27362100	6.62344400

oxoTS_{III-VII}

H = -3786.153442 au

G = -3786.349244 au

GD3BJ = -0.4464758279 au

H	-1.73155200	-1.72358800	-6.80929000
H	-0.37188500	0.21400100	-6.10377200
C	-1.94767900	-1.21794700	-5.87129600
H	0.10061400	2.37056800	-5.87050300
H	-3.57046200	-2.52202600	-5.37310700
C	-1.18816400	-0.12719600	-5.47170200
C	-2.98418900	-1.66328100	-5.05859300
H	-1.42557000	3.10629400	-5.36384500
C	-0.44624100	2.76703900	-5.00676800
H	0.10866100	3.64080900	-4.64541900
H	1.30495500	0.67443900	-4.24802400
C	-1.45054300	0.54679300	-4.27358800
H	-6.01229900	-1.03293700	-4.37937200
H	3.88319400	4.70174100	-3.67741100
H	-4.31802700	1.65584800	-4.24065100
H	-5.00058000	-3.39822400	-4.02459200
C	-3.27890400	-1.03638300	-3.84462700
C	-0.57108700	1.72492600	-3.88593300
H	-3.24400700	3.00285000	-3.89479800
H	5.35801000	0.36773100	-3.77190900
H	5.18478800	2.60518000	-3.51921500
C	0.81628200	1.23923000	-3.44424900
C	-2.50674400	0.08824000	-3.45581000
C	-4.06384500	2.40181700	-3.48327000
H	1.46034400	2.08665100	-3.18548900
C	-5.75718800	-0.87567200	-3.32392600
C	3.73806900	4.03083700	-2.83426800
H	-4.92247900	3.06004900	-3.33171800
C	-4.59400100	-3.07978300	-3.05711600
H	-1.03296300	2.22115300	-3.02481300
C	-4.42174300	-1.55725200	-2.98214500
H	-3.64767100	-3.60872000	-2.90209800
C	4.46622300	2.85169700	-2.74108900

H	0.73467100	0.59060300	-2.56557500
H	-5.72693900	0.20125200	-3.13753400
H	3.90769100	-0.36841100	-3.07789300
C	4.96239700	-0.14406100	-2.88636200
H	5.50248400	-1.09355700	-2.78919000
H	-6.56810100	-1.29506300	-2.71534000
H	2.24058600	5.25885400	-1.91504800
H	-5.30221000	-3.41335500	-2.28998200
H	7.03873700	1.61262900	-2.19062200
C	2.81840900	4.34086000	-1.83932000
N	-2.79140200	0.71813500	-2.19905200
H	-4.18309800	-1.29874700	-1.94291500
C	-3.62846600	1.75861400	-2.18153100
C	4.29923200	1.97354500	-1.66525200
C	5.13431000	0.70300700	-1.61749200
C	6.62037900	1.00973200	-1.37522000
S	-1.19233800	-2.81670200	-1.31866600
H	7.20050600	0.08081400	-1.31469200
H	-0.01097400	4.26448100	-1.15175300
S	1.84704500	-2.19609100	-1.59756200
C	2.62016400	3.50077600	-0.73913700
H	-4.80565300	3.19253800	-1.18513500
C	-4.15929800	2.33982400	-1.01110000
H	4.78006300	0.10932800	-0.76815800
C	0.29178900	-2.30847900	-1.34258900
H	6.77216100	1.56119700	-0.44116100
C	3.37365400	2.30600900	-0.64665600
H	1.49722700	6.05897500	0.00933200
H	4.22033300	-4.00737100	-1.17846500
Mg	-1.76857800	0.25924000	-0.44241700
H	5.83432400	-3.26702300	-1.18163700
H	0.02927500	2.60128100	-0.52394600
C	0.16368400	3.65527500	-0.25639200
H	-5.18138600	-3.27111100	0.27403500
H	-7.15802400	-1.71089900	0.59293400
H	5.55360600	-4.75695700	-0.28598700
C	5.10107000	-3.79698700	-0.56240300
O	0.00092400	-0.12659100	-0.07936100
C	1.57660800	3.88633600	0.29835300
H	-4.87637900	-0.81354100	0.31573000
C	1.72616700	5.33097000	0.79636800
H	-0.59561800	3.92576100	0.48740700
H	-6.98497500	-0.20448700	1.50980400
H	2.74091900	5.54017600	1.15336800
C	-4.11125400	1.90280600	0.32737800
N	3.19065100	1.40722800	0.45570300
C	-6.64210200	-1.24264100	1.43994200
Mg	1.77397400	-0.13107900	0.46118700
C	-4.67261000	-2.78786100	1.11671100
H	5.41165000	2.98877800	0.86566400
C	-5.12000100	-1.32495600	1.25274600
N	-3.31408400	0.93110900	0.78319700
H	1.70112700	3.22243700	1.16008100
H	1.03101200	5.51882100	1.62341100
H	-3.59217300	-2.86186100	0.95222600
H	-5.63747100	3.37225200	0.76905500
H	-4.90734700	-3.36375400	2.02001800
H	4.07738500	3.79782500	1.66618700
H	-6.96400700	-1.76097600	2.35119500
C	4.75009300	-2.95329200	0.67001400
H	4.47018000	-1.95129600	0.32277400
C	4.70834800	2.90353300	1.70019300

C -5.06575500 2.59350100 1.27837900
 C 3.87535200 1.64345400 1.57954100
 H 4.11190700 -5.55143700 1.11415400
 H 6.84391000 -2.42485400 0.96146400
 H -0.67765400 -1.93756100 1.69560900
 H -5.76905900 1.87368900 1.71082800
 C 3.56475100 -3.49973500 1.45546900
 C 3.39829000 -4.88137400 1.58562300
 H 6.28763200 -3.75564400 1.99451800
 C 5.99764300 -2.79312300 1.55482900
 C -3.50665200 0.47659300 2.13001100
 C -4.36669100 -0.62138000 2.37183900
 H -4.52922000 3.04517800 2.11884900
 H -1.98246600 2.60138500 1.96691200
 H 5.27344100 2.91513000 2.63464600
 N 2.78269700 -1.22244800 1.92724600
 H -0.17215000 1.00923100 2.43954800
 C 2.62903000 -2.63909500 2.08503300
 H 2.21947700 -6.49677200 2.38555900
 C 2.33380600 -5.41881100 2.30063500
 C -0.81959700 -2.33299000 2.70713900
 C 3.90423200 0.78921800 2.70011200
 H -1.20036000 -3.35925000 2.63125600
 H -1.58010700 -1.72471400 3.20887000
 H 0.28185700 2.62845300 3.01800600
 C 1.54508300 -3.17611100 2.81430700
 C 1.41708300 -4.56691200 2.90115400
 H 5.83200500 -2.08376900 2.37041700
 C -0.41140700 1.79213100 3.16775600
 C 3.47854300 -0.54740000 2.84461200
 C -1.86570100 2.25463600 2.99929000
 H 0.86637100 -1.26565300 3.46569100
 C -2.82166700 1.09011100 3.20526100
 H 0.58114200 -4.98783100 3.45461100
 C 0.50161900 -2.29867100 3.48737500
 H 4.44685000 1.18276000 3.55213700
 C -4.52817000 -1.07815300 3.68372200
 H -5.19057400 -1.91955500 3.87458700
 H -0.23999600 1.39118200 4.17424400
 H -1.51719600 4.29192000 3.66801400
 C -2.16289200 3.44343400 3.92446400
 H -3.20422000 3.77562700 3.84459600
 C 3.85642100 -1.21641800 4.15128800
 H 4.23016900 -2.23168700 3.99550800
 C -3.01372400 0.59291500 4.49837900
 H 2.97193000 -1.30140100 4.79423400
 C -3.86188700 -0.48005400 4.74593400
 C 0.26920200 -2.67460200 4.95788900
 H -1.97443300 3.19854300 4.97637500
 H -0.19724500 -3.66203900 5.05581000
 H 4.61188000 -0.63898600 4.68929900
 H -0.40649800 -1.94968800 5.42661700
 H -2.48906500 1.05960200 5.32867100
 H 1.20418200 -2.69298300 5.52995500
 H -4.00130600 -0.84773300 5.75954100

VII

$H = -3786.240379 \text{ au}$

$G = -3786.435512 \text{ au}$

$GD3BJ = -0.4426799191 \text{ au}$

H -2.44004400 -1.13754200 -7.20125300

H -0.69879300 0.40301700 -6.36342300
 C -2.51497000 -0.72163600 -6.19954900
 H 0.01198600 2.52778500 -5.90836400
 H -4.33886100 -1.75056500 -5.74293800
 C -1.54177700 0.14744000 -5.72568200
 C -3.58086800 -1.06271100 -5.37587800
 H -1.24292500 3.41094500 -5.03240800
 C -0.31742900 2.83706200 -4.90922100
 H 0.44992100 3.50692600 -4.50396800
 H 1.16043100 0.49043300 -4.80970500
 C -1.61925200 0.70338400 -4.44440700
 H -6.41633000 -0.69321300 -4.75805800
 H 3.68331100 4.34612600 -3.95108500
 H -4.42426200 2.21554500 -4.09308400
 H -5.24998700 -2.94761500 -4.10191800
 C -3.69816700 -0.54551700 -4.08280800
 C -0.50694100 1.62823000 -3.98105400
 H -3.08010200 3.29606900 -3.77237000
 H 5.23854500 0.05880800 -3.76121100
 H 5.05686200 2.31254300 -3.65596500
 C 0.81503200 0.86093700 -3.83663600
 C -2.71437700 0.36297400 -3.62044400
 C -3.96329700 2.83329000 -3.31743000
 H 1.59700700 1.51020000 -3.42816800
 C -6.20069700 -0.36409200 -3.73414000
 C 3.56369900 3.73064500 -3.06300900
 H -4.66004900 3.62602600 -3.03643300
 C -5.00602000 -2.49907700 -3.13162700
 H -0.78292000 2.01099200 -2.99257500
 C -4.88332600 -0.97157500 -3.22670700
 H -4.07593900 -2.95575000 -2.77883300
 C 4.33316600 2.58724600 -2.89242300
 H 0.70651400 -0.00816300 -3.18021200
 H -6.17031100 0.73044700 -3.73482700
 H 3.86413700 -0.70381100 -2.94366800
 C 4.91035300 -0.40411000 -2.82302900
 H 5.50759100 -1.31140700 -2.67696600
 H -7.03887300 -0.67559400 -3.09853200
 H 2.02562700 4.96683800 -2.22536900
 H -5.80938800 -2.77188400 -2.43658600
 H 6.94185800 1.47089200 -2.32922200
 C 2.63484900 4.07687600 -2.08827500
 N -2.83706600 0.89492800 -2.29026100
 H -4.71443700 -0.58944000 -2.21384500
 C -3.55428400 2.00590300 -2.11677500
 C 4.20161700 1.78020500 -1.75706700
 C 5.08561800 0.54778200 -1.63128300
 C 6.56299100 0.93066300 -1.45308700
 S -1.39445600 -2.36169800 -1.34074800
 H 7.17919600 0.03283500 -1.32277500
 H -0.20663500 3.95239400 -1.35643100
 S 1.63240300 -2.29423100 -1.16060400
 C 2.46965300 3.30941200 -0.93134700
 H -4.57256900 3.40180100 -0.91761100
 C -3.99868100 2.48384800 -0.86588600
 H 4.78091500 0.00783500 -0.72752300
 C 0.08096200 -1.63209600 -0.87032600
 H 6.71180700 1.57116100 -0.57668900
 C 3.26872600 2.15230500 -0.75944900
 H 1.23587800 5.86707500 -0.37519000
 H 4.44074800 -3.15156600 -0.66450500
 Mg -2.03275500 -0.09567800 -0.66065400

H	6.19309900	-2.86709800	-0.58060900
H	-0.08642500	2.33467900	-0.65212500
C	0.00989600	3.40312700	-0.43263600
H	-5.24278900	-3.42672000	0.11441600
H	-7.06534700	-1.68694100	0.36630600
H	5.51389800	-4.41541900	-0.05488500
C	5.34128200	-3.33267100	-0.06955700
O	0.01751700	-0.46591700	-0.23482100
C	1.41708700	3.73031900	0.08464600
H	-4.68550600	-1.03470500	0.16743700
C	1.50232100	5.21559300	0.46528500
H	-0.75421900	3.67485900	0.30469900
H	-6.75797200	-0.16895800	1.22784300
H	2.50724300	5.50055400	0.79585400
C	-3.96556500	1.89225400	0.41096300
N	3.12505400	1.33248700	0.41035800
C	-6.53271600	-1.24099300	1.21495400
Mg	2.05243600	-0.43489000	0.38287400
C	-4.73866200	-3.00697100	0.99255400
H	5.26506300	3.03723100	0.72579300
C	-5.02286400	-1.50205300	1.09951500
N	-3.25050900	0.80822700	0.74101000
H	1.57552500	3.14292900	0.99469700
H	0.80310900	5.43661200	1.28049500
H	-3.66648500	-3.20571500	0.89338900
H	-5.44135200	3.35361900	1.01220700
H	-5.10345800	-3.55139000	1.87167400
H	3.87154900	3.88087900	1.37503500
H	-6.94122700	-1.67918500	2.13376100
C	5.19631100	-2.77390400	1.35398300
H	5.04900300	-1.69179900	1.27181700
C	4.52873600	3.02122100	1.53637600
C	-4.84596400	2.55125600	1.45256800
C	3.75733100	1.71749900	1.52772600
H	4.81452600	-5.34300000	2.01761900
H	7.33584200	-2.50716800	1.64983100
H	-0.61602200	-2.91630100	1.64626000
H	-5.52527100	1.81987700	1.90267300
C	3.97813700	-3.36405100	2.05247300
C	3.95864900	-4.73806200	2.30805000
H	6.73570900	-4.07308300	2.21204400
C	6.49333100	-3.00582800	2.14439200
C	-3.41405400	0.26534400	2.05981400
C	-4.25737500	-0.85666200	2.24548400
H	-4.25439300	2.97060300	2.27193200
H	-1.90534200	2.42055100	2.01383700
H	5.05289400	3.16049300	2.48402900
N	2.85423700	-1.17538400	2.14535700
H	-0.09155200	0.76738000	2.34015100
C	2.85766900	-2.58461800	2.43161800
H	2.87543100	-6.41821000	3.10965100
C	2.87040100	-5.34782700	2.91935200
C	-0.74793000	-2.92289300	2.73283000
C	3.79983900	0.98622500	2.72891400
H	-0.98804500	-3.95233100	3.02598000
H	-1.61249000	-2.29773300	2.98131400
H	0.38916600	2.35724600	2.96967500
C	1.74153100	-3.19738800	3.04398800
C	1.77392900	-4.57591400	3.27861700
H	6.42630200	-2.61817600	3.16660800
C	-0.30635400	1.52092300	3.10490400
C	3.47235200	-0.35965100	2.99932100

C	-1.76265900	1.99647600	3.01296800
H	0.65960000	-1.37078400	3.17451500
C	-2.72040400	0.82270600	3.16204700
H	0.91844700	-5.05181600	3.75209200
C	0.50555500	-2.41688700	3.45988800
H	4.29659700	1.49650500	3.54644300
C	-4.41293800	-1.37761900	3.53458500
H	-5.07065800	-2.23008900	3.68557900
H	-0.10059000	1.06967600	4.08256900
H	-1.37946000	3.98108900	3.80775900
C	-2.01134100	3.11449200	4.03607900
H	-3.05472200	3.44854900	4.03944600
C	3.93986400	-0.88197200	4.34122900
H	4.86101700	-1.46411700	4.22724800
C	-2.90377800	0.25812500	4.42801800
H	3.20108800	-1.54933800	4.79142000
C	-3.74899500	-0.82815800	4.62362100
C	0.28419700	-2.45008900	4.97982800
H	-1.76539200	2.79478600	5.05537400
H	0.11525400	-3.47399400	5.33469300
H	4.14585700	-0.05811900	5.02906200
H	-0.59834700	-1.85663300	5.24566200
H	-2.37677500	0.68169100	5.27953300
H	1.14272100	-2.04755600	5.52911100
H	-3.88546200	-1.24545200	5.61813600

VIII

$H = -3416.314657 \text{ au}$

$G = -3416.529837 \text{ au}$

$GD3BJ = -0.4977539652 \text{ au}$

Mg	1.54834000	4.38866500	4.01495600
O	1.55093100	4.10310700	5.84972700
N	0.30529100	3.52348400	2.49510300
C	0.05274600	2.96189000	0.10350500
H	0.31858200	1.91179600	0.26552800
H	0.44995500	3.28112100	-0.86310600
H	-1.04031400	2.99782600	0.05297800
O	3.44800900	3.53572400	3.38714600
N	1.68187600	6.21136600	2.87524300
C	0.57651400	3.83666300	1.22720000
C	1.31735700	4.96356500	0.81728600
H	1.48594900	5.02863700	-0.25201400
C	1.72560200	6.10043300	1.54615500
C	2.25142300	7.24860900	0.70239100
H	1.74683100	8.18948400	0.93993600
H	2.12646300	7.04512100	-0.36376900
H	3.31680600	7.41312300	0.89913600
C	-0.67194800	2.50077300	2.71600400
C	-0.27664400	1.16071100	2.93389800
C	-1.25722100	0.18915000	3.15666800
H	-0.95273500	-0.84057200	3.32826700
C	-2.60873400	0.51040700	3.16140200
H	-3.35774400	-0.26008900	3.32855500
C	-2.99134000	1.82951200	2.95104100
H	-4.04901400	2.08460300	2.95505500
C	-2.04852400	2.83697400	2.72539700
C	1.18483500	0.74789000	2.94568800
H	1.76845400	1.60327600	2.59102100
C	1.64080200	0.43708300	4.37679400
H	1.52687100	1.31127000	5.02765200
H	2.69404800	0.12950900	4.38785900

H	1.05668100	-0.38031700	4.81316500	O	-0.34611800	4.67025100	8.31236400
C	1.47615600	-0.43437100	2.01051800	N	1.42009300	1.99477000	8.82424900
H	0.98499400	-1.35359800	2.35069100	C	2.52558500	4.36949000	10.47217300
H	2.55413500	-0.63720900	1.97895800	C	1.78473200	3.24261400	10.88215600
H	1.13843600	-0.23829800	0.98616000	H	1.61618000	3.17758500	11.95146500
C	-2.54323100	4.25865600	2.49828800	C	1.37641600	2.10574600	10.15334000
H	-1.67223600	4.88677600	2.28724300	C	0.85059300	0.95760000	10.99714100
C	-3.21967300	4.81357000	3.75918400	H	1.35522800	0.01672900	10.75967000
H	-4.09156300	4.21118200	4.04271600	H	0.97548900	1.16114800	12.06329700
H	-3.56538900	5.84092100	3.59248200	H	-0.21477500	0.79304200	10.80034300
H	-2.52596800	4.81807400	4.60562700	C	3.77396800	5.70535500	8.98330200
C	-3.49656300	4.36273700	1.29816200	C	3.37861800	7.04542400	8.76555200
H	-3.03466500	3.99152200	0.37706300	C	4.35916000	8.01702100	8.54277900
H	-3.78512500	5.40755600	1.12982800	H	4.05464500	9.04674600	8.37125700
H	-4.41654800	3.78846300	1.46163600	C	5.71067900	7.69579100	8.53792400
C	1.91906700	7.51489700	3.41888400	H	6.45966000	8.46631300	8.37075800
C	3.22744400	7.94959900	3.73313800	C	6.09333300	6.37668300	8.74817700
C	3.41208000	9.25110900	4.21145000	H	7.15101400	6.12162300	8.74407900
H	4.41712000	9.58914800	4.45279300	C	5.15055400	5.36918400	8.97380900
C	2.34297300	10.12258800	4.37495900	C	1.91712800	7.45821200	8.75394000
H	2.50897000	11.13708500	4.72972200	H	1.33353800	6.60269400	9.10834500
C	1.05599300	9.67806100	4.09457900	C	1.46109100	7.76950400	7.32296500
H	0.21791600	10.35559800	4.23760200	H	1.57507000	6.89556800	6.67177900
C	0.81681100	8.37989900	3.63369700	H	0.40782200	8.07700600	7.31206500
C	4.43911900	7.04211400	3.58991800	H	2.04512700	8.58711000	6.88686900
H	4.11589600	6.14375900	3.05426100	C	1.62581100	8.64013500	9.68954300
C	4.94246600	6.60263600	4.97155000	H	2.11698100	9.55948300	9.34971200
H	5.23327000	7.46617400	5.57922100	H	0.54783300	8.84296600	9.72117900
H	5.82368100	5.95517000	4.87534500	H	1.96352900	8.44368000	10.71382900
H	4.16998100	6.05821800	5.52478000	C	5.64529900	3.94748600	9.20073300
C	5.58025900	7.68529600	2.78811000	H	4.77434700	3.31935900	9.41195400
H	5.24523200	8.04790500	1.80968100	C	6.32141900	3.39265800	7.93963200
H	6.38457800	6.95763500	2.62269700	H	7.19309500	3.99521400	7.65580000
H	6.02049900	8.53634900	3.32105300	H	6.66738400	2.36537600	8.10624500
C	-0.61300800	7.93768000	3.35371700	H	5.62742800	3.38799700	7.09342400
H	-0.60874400	6.84247400	3.31792300	C	6.59892200	3.84331000	10.40062000
C	-1.58471200	8.36565900	4.46120200	H	6.13727900	4.21454300	11.32183900
H	-1.22662200	8.05496400	5.44801300	H	6.88743300	2.79846200	10.56885500
H	-2.56934500	7.91383300	4.29573800	H	7.51892200	4.41749900	10.23694500
H	-1.73019300	9.45225700	4.48476900	H	1.18285200	0.69121000	8.28069100
C	-1.11592500	8.44224400	1.99210800	C	-0.12553100	0.25654400	7.96641600
H	-1.08297500	9.53810900	1.94428500	C	-0.31022400	-1.04501000	7.48824500
H	-2.15436300	8.12983300	1.82479700	H	-1.31527900	-1.38301700	7.24691500
H	-0.51472400	8.04878000	1.16704000	C	0.75883300	-1.91658300	7.32490900
C	4.04111500	3.37335100	2.07985700	H	0.59278900	-2.93111800	6.97027700
H	4.08246400	4.34990200	1.59129300	C	2.04582000	-1.47211100	7.60534200
H	3.38508900	2.72451100	1.49007000	H	2.88386100	-2.14973700	7.46251100
C	5.41274100	2.74401400	2.31666400	C	2.28506000	-0.17391100	8.06608000
H	6.18010400	3.51960000	2.42587900	C	-1.33718500	1.16407000	8.10955800
H	5.71137600	2.08791400	1.49324000	H	-1.01391800	2.06251400	8.64503600
C	5.21260800	2.00674100	3.64324200	C	-1.84064200	1.60330000	6.72788800
H	4.69763700	1.05317300	3.47973900	H	-2.13138600	0.73964300	6.12035700
H	6.14922900	1.80552100	4.17180500	H	-2.72191700	2.25069100	6.82403700
C	4.31855000	2.97656600	4.39795700	H	-1.06824600	2.14772100	6.17454000
H	3.67718100	2.54413700	5.16585500	C	-2.47827000	0.52102800	8.91156000
H	4.90225800	3.78940100	4.84307400	H	-2.14317900	0.15859300	9.89002900
Mg	1.55358800	3.81740600	7.68447300	H	-3.28258200	1.24871700	9.07689600
N	2.79676200	4.68262800	9.20425600	H	-2.91854000	-0.33011900	8.37879300
C	3.04939200	5.24430800	11.59581500	C	3.71490100	0.26814500	8.34621000
H	2.78352300	6.29439000	11.43376500	H	3.71074600	1.36334000	8.38224800
H	2.65224000	4.92510400	12.56245700	C	4.68656800	-0.15968500	7.23863300
H	4.14245600	5.20840500	11.64628900	H	4.32863000	0.15151100	6.25192300

H	5.67132500	0.29178100	7.40433500
H	4.83170900	-1.24631800	7.21463700
C	4.21771100	-0.23679200	9.70771700
H	4.18477500	-1.33267100	9.75524500
H	5.25612700	0.07559000	9.87521500
H	3.61641400	0.15643000	10.53283600
C	-0.93914200	4.83267800	9.61968400
H	-0.98048000	3.85614300	10.10828100
H	-0.28306800	5.48152700	10.20940100
C	-2.31078300	5.46200800	9.38293600
H	-3.07815500	4.68641400	9.27383000
H	-2.60935900	6.11816200	10.20633800
C	-2.11075300	6.19919400	8.05629100
H	-1.59579400	7.15278100	8.21969900
H	-3.04741400	6.40035600	7.52778100
C	-1.21673900	5.22933100	7.30158100
H	-0.57543400	5.66168400	6.53358400
H	-1.80047900	4.41645100	6.85657800

H	11.98365400	0.79994200	0.16957400
H	10.84679300	1.85708500	-0.69519600

CO₂

H= -188.488908 au

G= -188.513197 au

GD3BJ= -0.0016110417 au

C	-0.15896000	-0.02890200	0.00000000
O	1.00890400	-0.02890200	0.00000000
O	-1.32682300	-0.02890200	0.00000000

CS₂

H= -834.352773 au

G= -834.379731 au

GD3BJ= -0.0051880734 au

C	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	1.55943200
S	0.00000000	0.00000000	-1.55943200

CO

H= -113.249934 au

G= -113.272375 au

GD3BJ= -0.0007103159 au

C	-0.09826800	-0.02890200	0.00000000
O	1.03874900	-0.02890200	0.00000000

THF

H= -232.239314 au

G= -232.273611 au

GD3BJ= -0.0155303282 au

C	10.91831400	0.97423900	-0.04808000
O	10.39020200	-0.15147700	-0.74395100
C	9.48851600	-0.86251700	0.09721000
C	9.72683000	-0.34719300	1.51578800
C	10.10844300	1.10945200	1.24243600
H	8.45171800	-0.66859100	-0.22197300
H	9.68049400	-1.93639600	-0.01307800
H	8.85126100	-0.45786100	2.16335100
H	10.56541100	-0.87986000	1.98093300
H	10.67665500	1.57452100	2.05422600
H	9.20788600	1.71159600	1.06992100