

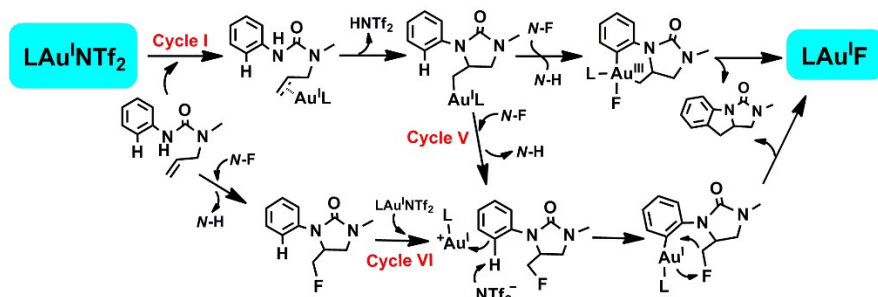
Supporting Information for

**Theoretical Investigation of Gold-Catalyzed Oxidative C_{sp3}-C_{sp2} bond Formation
via Aromatic C–H Activation**

Contents

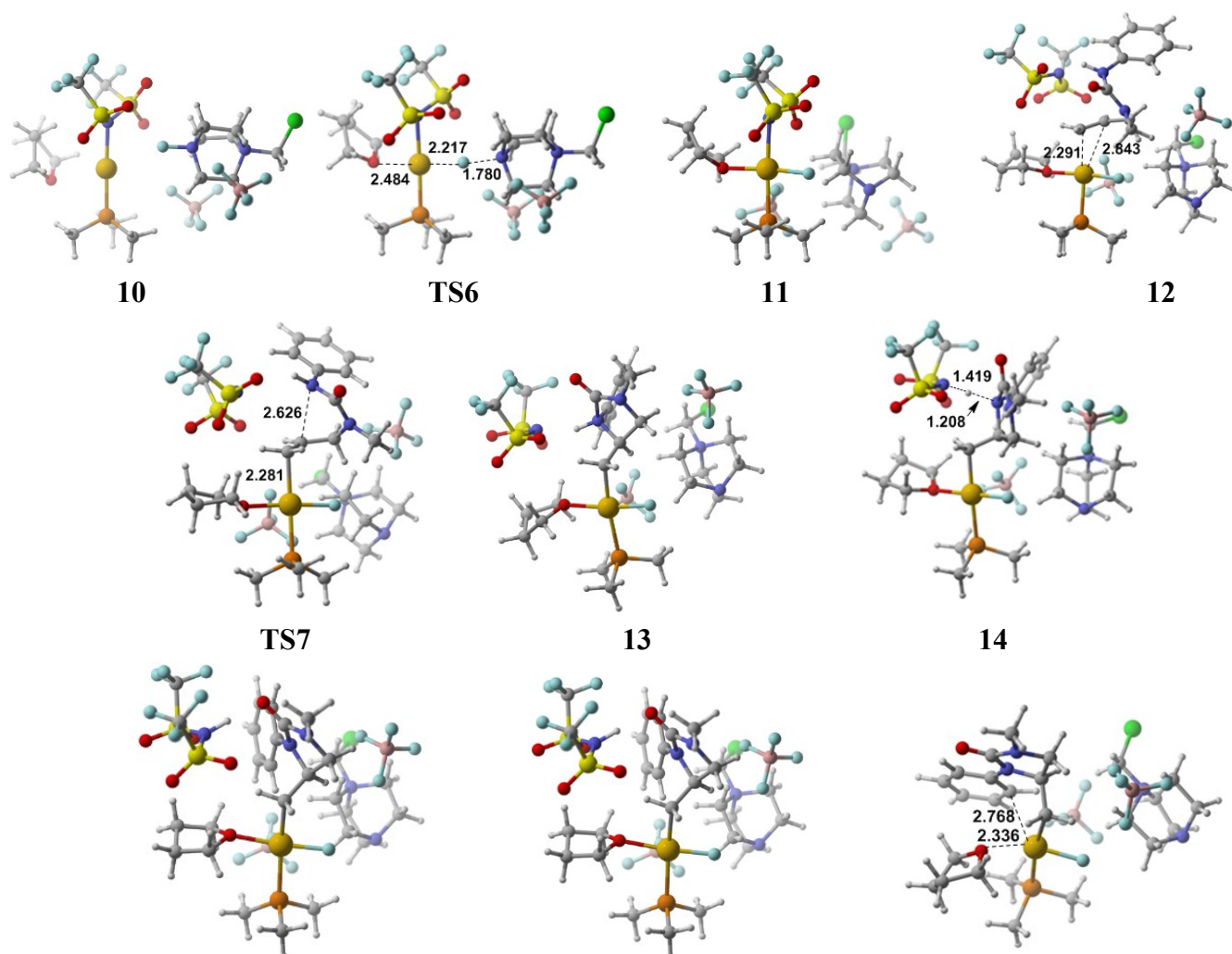
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1. Schemes



Scheme S1. Schematic diagram for Cycles V and VI.

2. Figures: Energy profiles, Structures

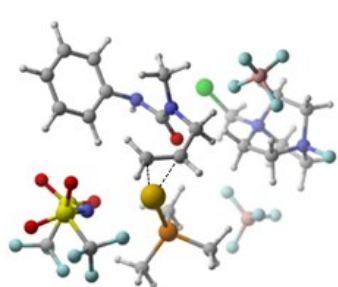


TS8

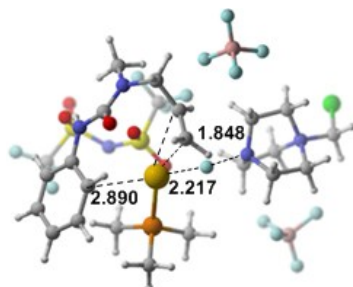
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TS9

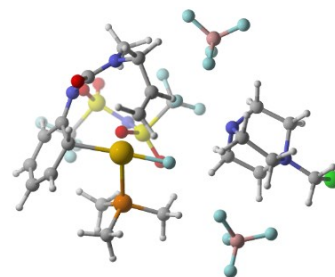
Figure S1. Structures and geometrical parameters of the stationary points along the Cycle II. Bond distances are given in Å.



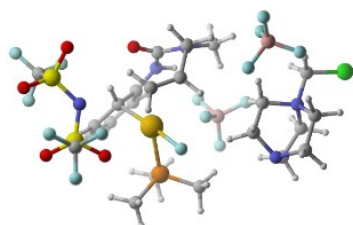
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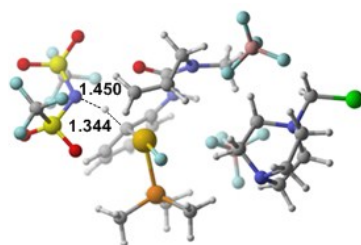
TS10



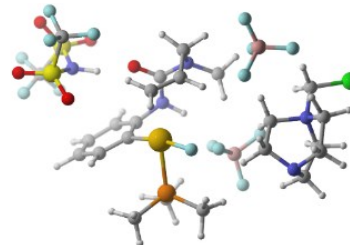
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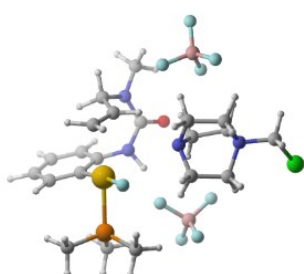
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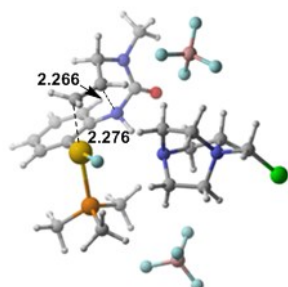
TS11



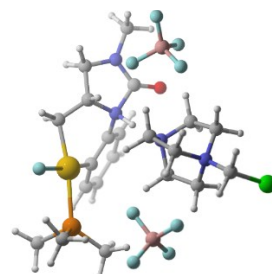
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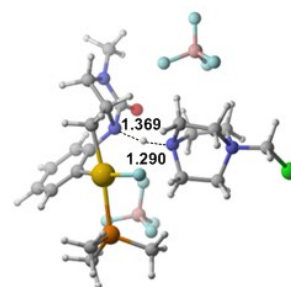
20



TS12



21



TS13

Figure S2. Structures and geometrical parameters of the stationary points along the Cycle III. Bond distances are given in Å.

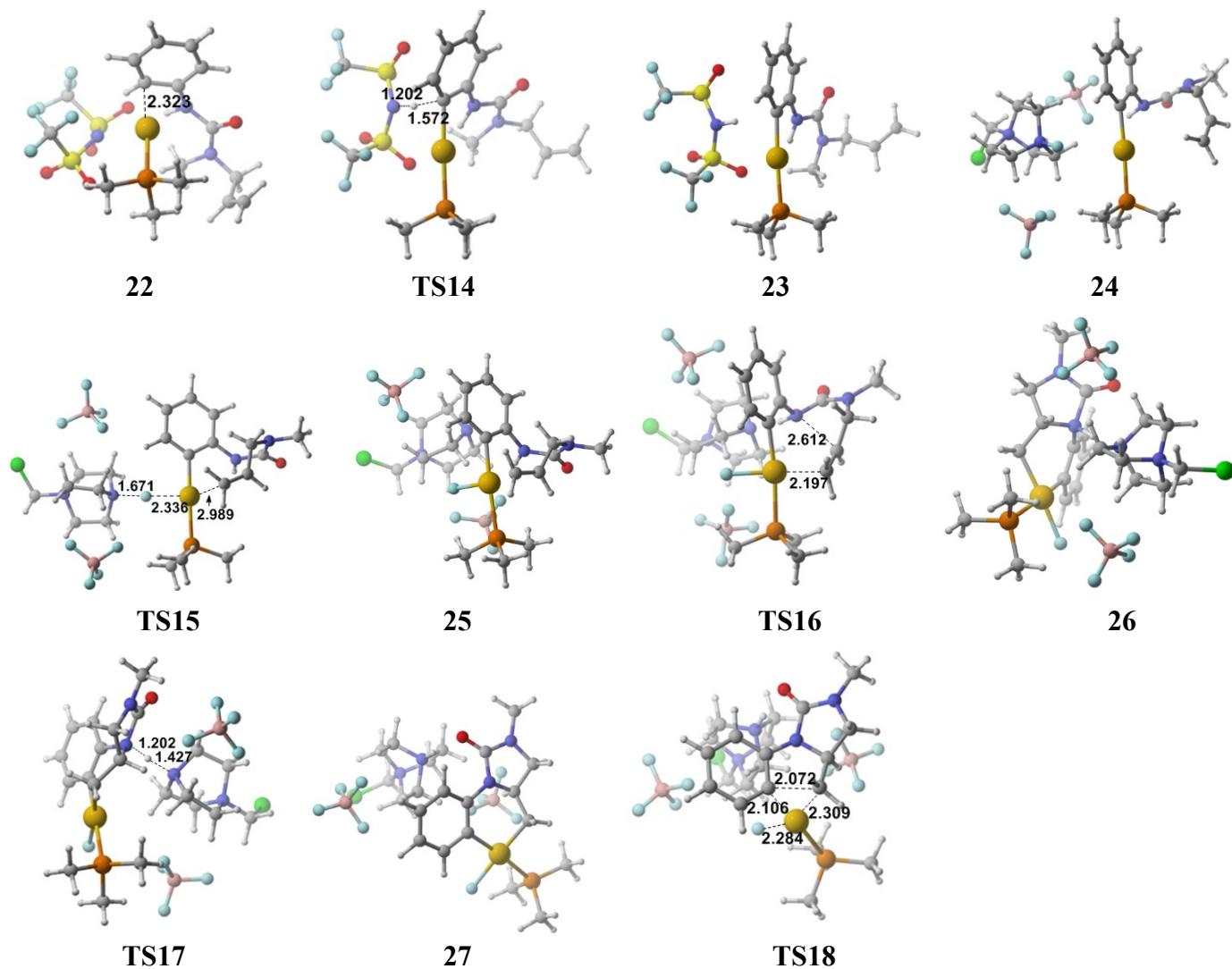


Figure S3. Structures and geometrical parameters of the stationary points along the Cycle IV. Bond distances are given in Å.

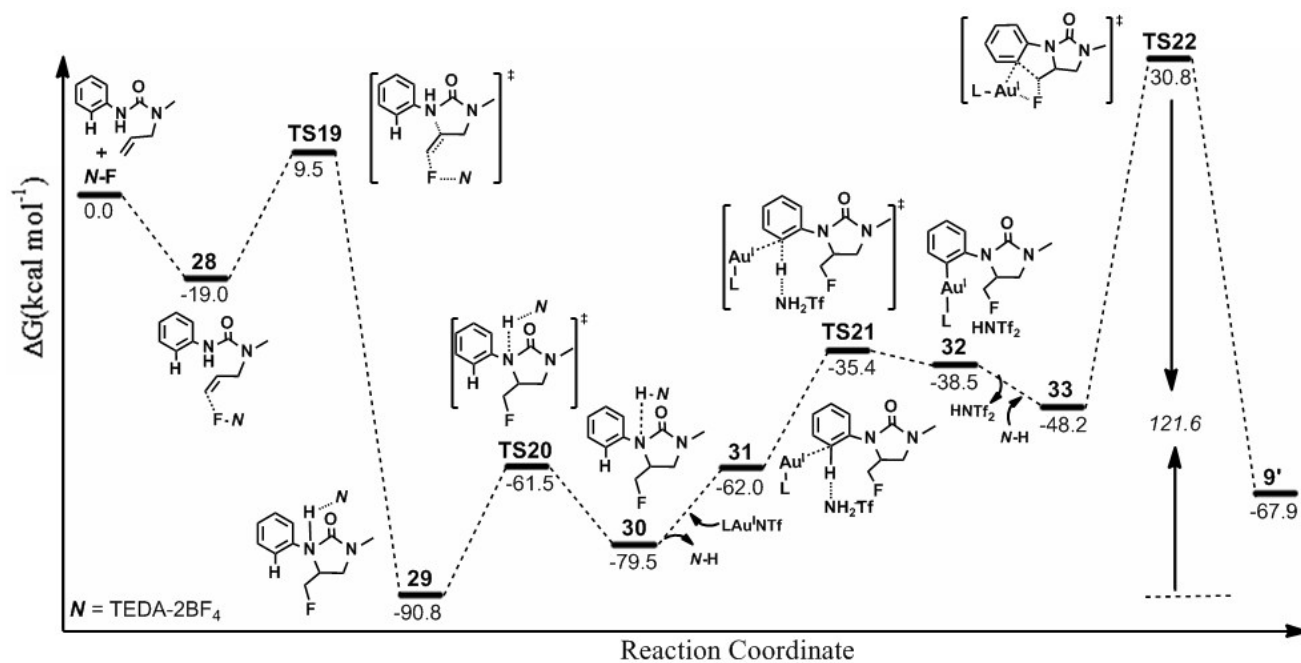


Figure S4. DFT-computed free energy profile for Cycle V. The overall free energy barrier is indicated in italics.

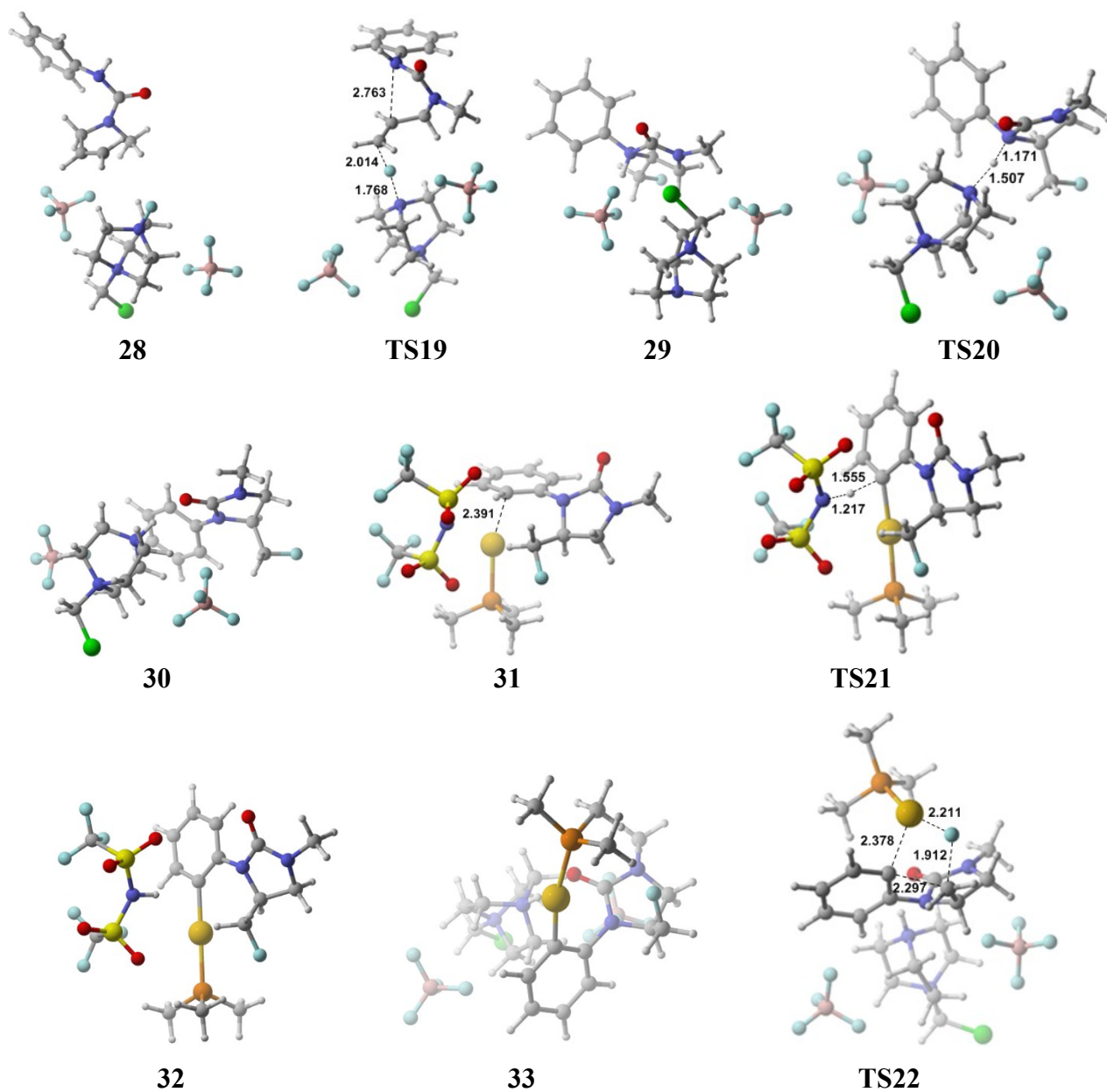


Figure S5. Structures and geometrical parameters of the stationary points along the Cycle V. Bond distances are given in Å.

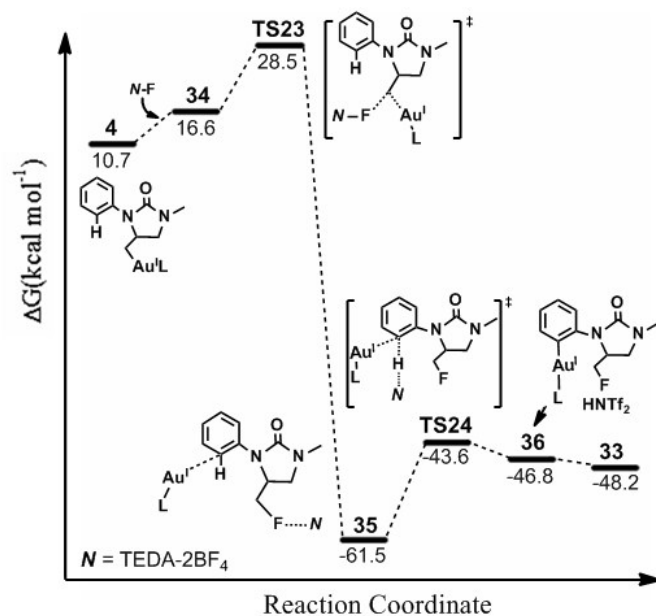


Figure S6. DFT-computed free energy profile for Cycle VI.

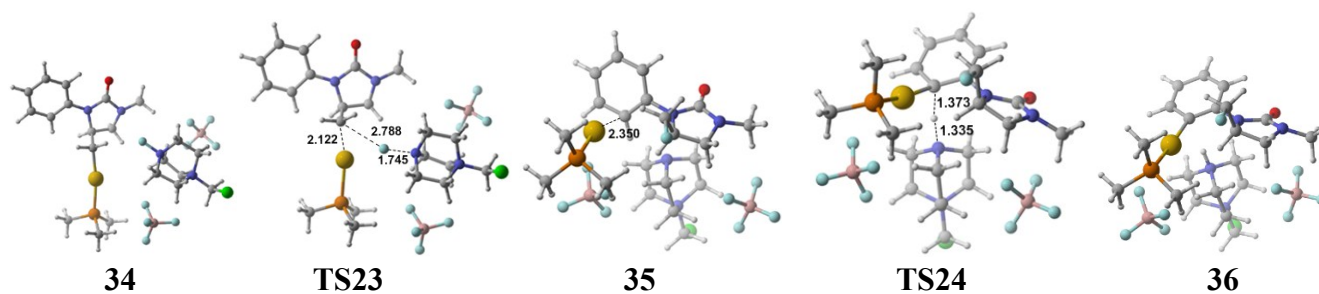


Figure S7. Structures and geometrical parameters of the stationary points along the Cycle VI. Bond distances are given in Å.

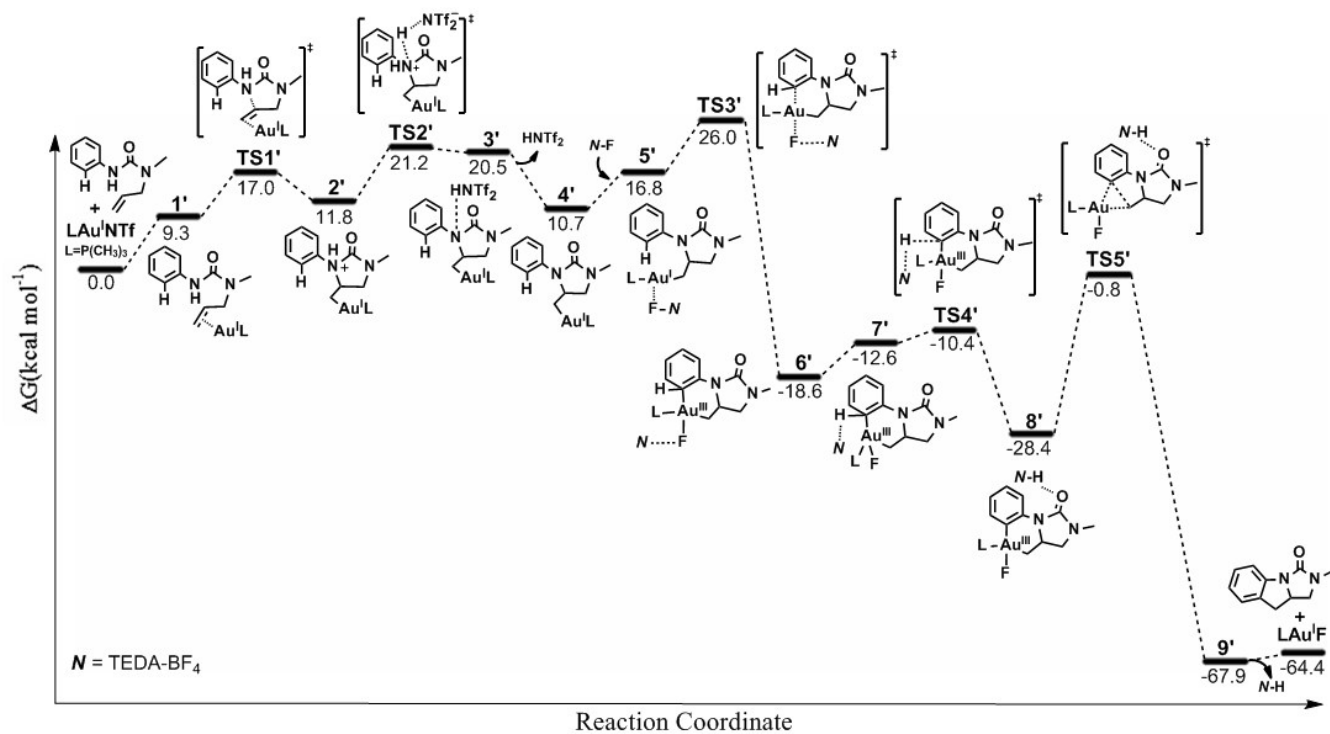


Figure S8. DFT-computed free energy profile for Cycle I'.

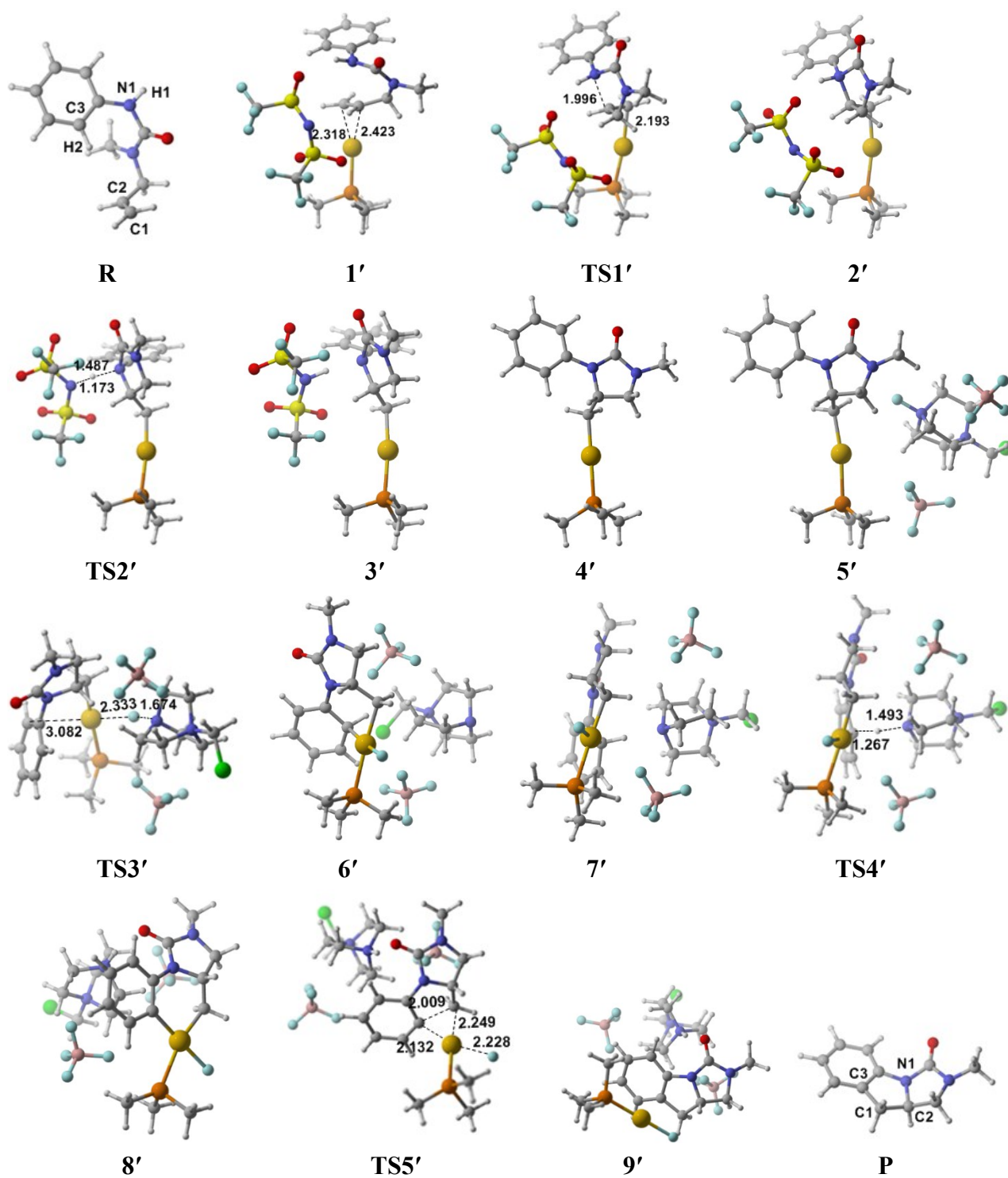


Figure S9. Structures and geometrical parameters of the stationary points along the Cycle I'. Bond distances are given in Å.

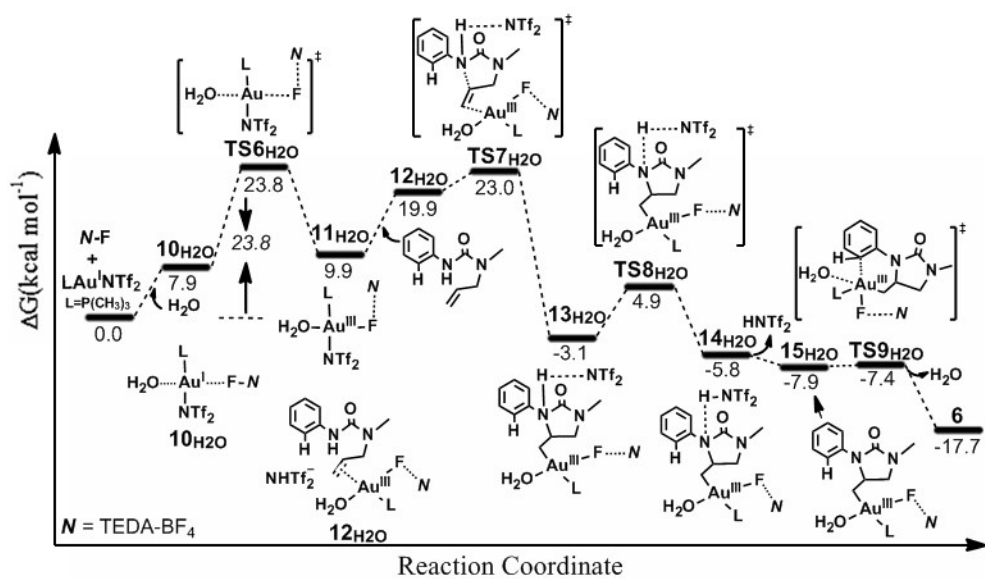
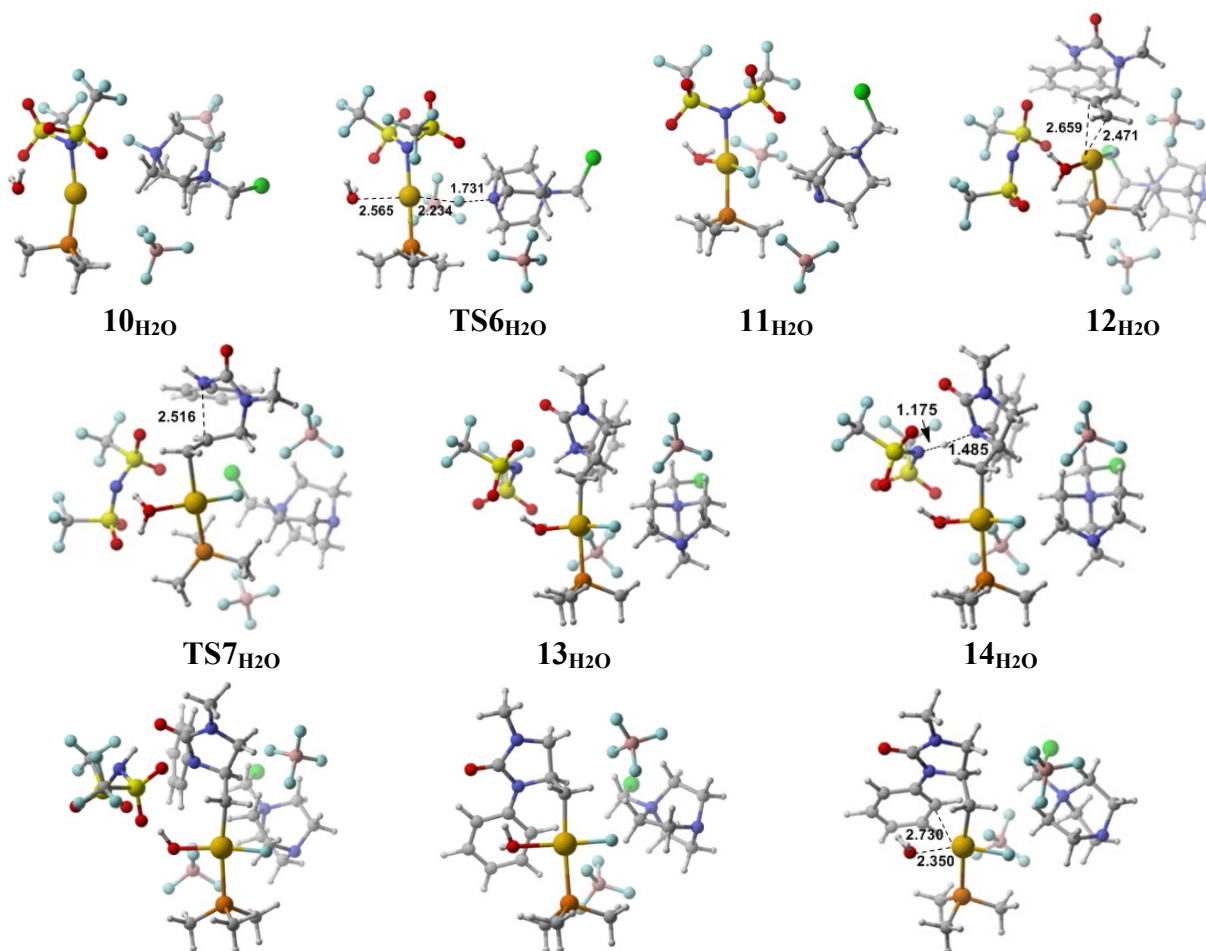


Figure S10. DFT-computed free energy profile for Cycle II_{H₂O}. The overall free energy barrier is indicated in italics.



TS8_{H₂O}

15_{H₂O}

TS9_{H₂O}

Figure S11. Structures and geometrical parameters of the stationary points along the Cycle II_{H₂O}. Bond distances are given in Å.

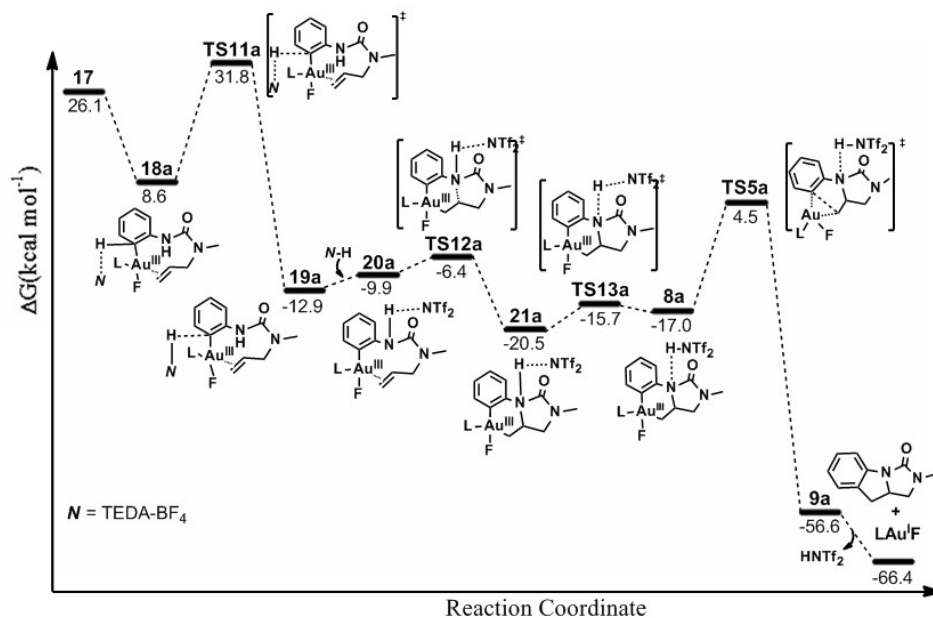


Figure S12. Alternative transition structures for the steps from intermediate **17** to final product in the Cycle III. DFT-computed free energy profile for Cycle IIIa.

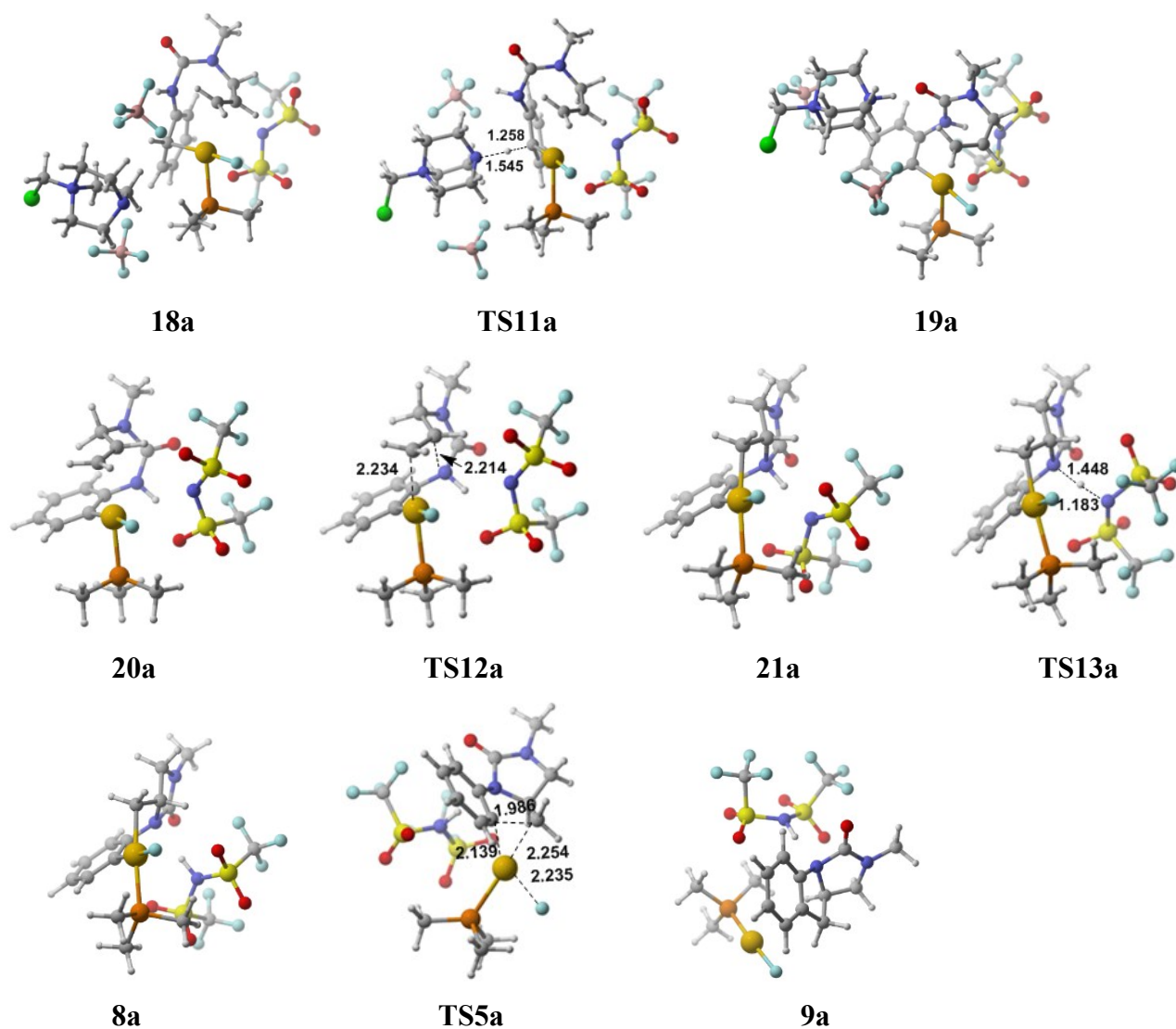


Figure S13. Structures and geometrical parameters of the stationary points in Figure S12. Bond distances are given in Å.

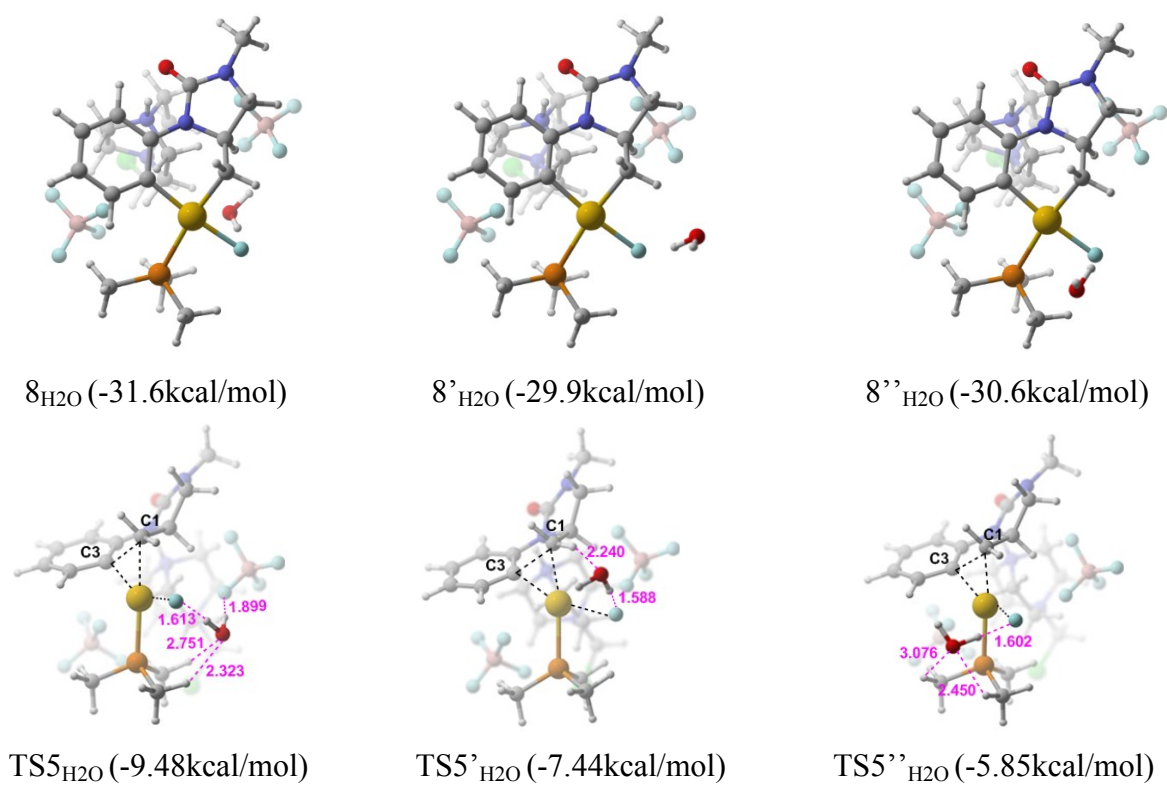


Figure S14. Optimized structures for reductive elimination mediated by one water molecule.

3. Tables: Relative Gibbs free energies calculated at M06/lanl2dz-6-31g*, M06/lanl2dz-6-311+g**

Table S1. Relative Gibbs freeenergies (ΔG , kcal mol⁻¹) for structures in Figure 1.

ΔG_{rel}	M06/lanl2dz-6-31g*	M06/lanl2dz-6-311+g**
l sol		
R1	0.0	0.0
1	5.9	5.6
TS1	19.3	21.1
2	14.5	17.8
TS2	20.6	25.1
3	16.0	20.4
4	10.7	14.7
5	16.8	25.8
TS3	23.6	27.6
6	-19.3	-15.7
7	-17.7	-13.4
TS4	-9.7	-5.3
8	-27.2	-25.2
TS5	-0.8	5.3
9	-68.9	-64.2
P	-66.4	-71.8

Table S2. Relative Gibbs freeenergies (ΔG , kcal mol⁻¹) for structures in Figure 3.

ΔG_{rel}	M06/ lanl2dz-6-31g*	M06/ lanl2dz-6-311+g**
1 sol		
10	7.4	13.0
TS6	24.8	27.0
11	7.4	11.5
12	14.8	23.8
TS7	15.3	23.8
13	-3.6	4.3
TS8	0.0	9.6
14	-4.0	4.2
15	-8.2	2.3
TS9	-4.9	5.5

Table S3. Relative Gibbs freeenergies (ΔG , kcal mol⁻¹) for structures in Figure 4.

ΔG_{rel}	M06/ lanl2dz-6-31g*	M06/ lanl2dz-6-311+g**
1 sol		
16	13.8	19.5
TS10	37.4	36.6
17	26.1	28.3
18	9.7	15.9
TS11	28.2	34.8
19	-4.1	-0.5
20	-5.0	-7.1
TS12	7.0	4.2
21	-13.1	-12.4
TS13	-6.3	-7.3

Table S4. Relative Gibbs freeenergies (ΔG , kcal mol⁻¹) for structures in Figure 5.

ΔG_{rel} l sol	M06/ lanl2dz-6-31g*	M06/ lanl2dz-6-311+g**
22	5.7	7.2
TS14	35.9	37.0
23	32.5	33.0
24	39.1	41.8
TS15	51.0	50.7
25	23.3	22.3
TS16	23.6	22.3
26	-13.1	-12.8
TS17	-12.6	-12.2
27	-23.1	-22.0
TS18	-4.7	-5.0

Table S5. Relative Gibbs free energies (kcal mol⁻¹) for several structures.

	ΔG_{rel} sol(L=PMe ₃)	ΔG_{rel} sol(L=PPh ₃)	$\Delta G_{\text{rel sol(L=PPh}_3\text{)} - \Delta G_{\text{rel sol(L=PMe}_3\text{)}}$
TS3	23.6	24.7	1.1
8	-27.2	-26.6	0.6
TS5	-0.8	1.2	0.4
TS6	24.8	25.8	1.0

4 Cartesian coordinates of the optimized structures

3.1 Cycle I and Cycle I'

R1

Num. Imaginary Frequencies: 0

C	2.70167000	-1.00666300	-0.09093300
C	1.39984800	-0.53581000	-0.27914800
C	1.17091800	0.84030600	-0.35525700
C	2.23364500	1.72787300	-0.22125900
C	3.53157100	1.25940500	-0.03734200
C	3.76042500	-0.11321500	0.01828000
H	2.87094500	-2.08120100	-0.02778200
H	0.16167200	1.21253300	-0.53061600
H	2.04323000	2.79837300	-0.27909100
H	4.35896900	1.95964800	0.05890100
H	4.77022000	-0.49518900	0.15926400
N	0.35986800	-1.48603400	-0.41808500
H	0.53515900	-2.19642100	-1.12207700
N	-1.44014600	-0.54176500	0.76457600
C	-1.01019900	-1.22366200	-0.34195400
O	-1.77505800	-1.64935500	-1.20130100
C	-2.80039500	-0.00849700	0.72986300
H	-3.17549700	0.00501600	1.76283600
H	-3.42452500	-0.69644500	0.15002800
C	-2.83542900	1.36121500	0.12222600
H	-2.32280400	2.15479100	0.67384800
C	-3.40999500	1.62430100	-1.04878600
H	-3.91423000	0.83990400	-1.61483100
H	-3.40447800	2.62060800	-1.48719500
C	-0.64481600	-0.27400400	1.94482400
H	-0.25820400	0.75647500	1.97140300
H	-1.26643200	-0.43605200	2.83457300
H	0.20492900	-0.96010200	1.99262200

LAu^INTf₂

Num. Imaginary Frequencies: 0

N	0.90106100	-0.06559600	-0.41030200
C	2.84068400	-1.61905900	0.76430100
C	1.69919200	2.26109200	0.69053200
O	2.42144100	-1.60778000	-1.85023900
O	0.63416100	-2.53168500	-0.32460000

O	0.55412000	2.10603100	-1.66497300
O	2.91284200	1.22549400	-1.41094300
S	1.63655800	-1.52344000	-0.63312800
S	1.55466900	1.36085400	-0.91812800
F	3.77166100	-0.69429400	0.63295700
F	3.39604000	-2.81821600	0.74254100
F	2.19731000	-1.44916200	1.90575700
F	2.22843700	3.44458600	0.43459600
F	2.48090600	1.59306200	1.51784300
F	0.50736400	2.42305800	1.24183300
Au	-1.25353200	-0.12511600	-0.11197700
P	-3.53050800	-0.15779500	0.20598600
C	-4.47475300	-0.31133700	-1.34155000
H	-5.55013300	-0.32384600	-1.12224600
H	-4.24594200	0.53528700	-1.99797400
H	-4.19574500	-1.23845000	-1.85385800
C	-4.17642300	1.34135300	1.00984100
H	-3.93123100	2.22048500	0.40417400
H	-5.26580700	1.26529900	1.11999200
H	-3.71761200	1.45633700	1.99796900
C	-4.09824800	-1.53562800	1.24986000
H	-3.63424800	-1.46341200	2.23955600
H	-5.19010000	-1.49764500	1.35486800
H	-3.80829100	-2.48875200	0.79452400

1

Num. Imaginary Frequencies: 0

C	3.25866200	1.23111200	3.22562700
C	3.61069700	-0.00722100	2.69716100
C	2.61681900	-0.86523200	2.22177300
C	1.27325300	-0.49432400	2.31040600
C	0.92786100	0.73170800	2.87196500
C	1.91915500	1.60317200	3.31849600
H	4.03772300	1.90043600	3.58677500
H	4.65578200	-0.31005000	2.64106500
H	0.50139800	-1.16787100	1.93462300
H	-0.12604300	1.00167800	2.93892700
H	1.64800900	2.56610400	3.74895700
C	3.98392300	-2.50954100	0.84272500
O	4.40555400	-3.65912800	0.88205200
C	3.68977300	-0.44060000	-0.52304100
H	3.51367700	0.27882900	0.28715600
H	4.28711900	0.08449100	-1.27964300

C	5.51174100	-2.03533800	-0.95973000
H	5.07744500	-2.44355600	-1.88597900
H	6.17264900	-1.20006200	-1.21685300
H	6.09273200	-2.82216300	-0.47688300
N	4.48335600	-1.56904900	-0.04146100
C	2.38377200	-0.88792100	-1.12223100
H	1.76063000	-1.54457300	-0.50836700
C	2.00598000	-0.64243700	-2.40969500
H	1.10361100	-1.09719500	-2.82112800
H	2.65665000	-0.09602500	-3.09486500
Au	0.97349600	1.04688600	-1.12811100
P	-0.08691000	3.11118900	-0.73761100
H	2.51876900	-2.93584300	2.11349300
N	2.93272900	-2.12759800	1.66069000
N	-2.24719600	-0.18387100	-0.33607600
C	-2.84664900	-2.76407400	-1.08038800
C	-4.30738500	0.07550800	1.32053700
O	-0.47538800	-2.06729800	-0.17719100
O	-1.25652700	-1.15095700	-2.38033800
O	-2.10148900	1.42129800	1.58370000
O	-2.03890800	-1.02633700	2.12983500
S	-1.53733800	-1.46419600	-0.98092800
S	-2.46631100	0.04649600	1.23958200
F	-3.20147900	-3.15946300	0.13084400
F	-2.36228400	-3.79746300	-1.75230300
F	-3.90504500	-2.28682000	-1.71400800
F	-4.66815500	0.32849700	2.56896500
F	-4.80704400	-1.09165200	0.94823900
F	-4.77414100	1.02705900	0.52790400
C	0.01633200	3.74427200	0.96342700
H	1.06904300	3.83066200	1.25545100
H	-0.46233800	4.73073700	1.01758300
H	-0.49325900	3.04760500	1.63692200
C	-1.84184100	3.16093000	-1.20843400
H	-2.41346200	2.48852000	-0.56039200
H	-2.21837600	4.18740600	-1.11006400
H	-1.94696400	2.82894800	-2.24750000
C	0.70366900	4.40408800	-1.75280100
H	0.20606000	5.36841400	-1.58657000
H	1.76148300	4.49200900	-1.48048700
H	0.63410100	4.13982400	-2.81382300

TS1

Num. Imaginary Frequencies: 1

C	-6.02383600	0.91103800	1.73992200
C	-5.36430900	0.39532600	0.62871800
C	-4.15112700	0.95567100	0.22702000
C	-3.60312500	2.02651600	0.93543900
C	-4.27517100	2.53268100	2.04099300
C	-5.48442100	1.97747500	2.45134100
H	-6.97288900	0.47383900	2.04396500
H	-5.81013800	-0.42889400	0.07405700
H	-2.66162100	2.46450900	0.60879600
H	-3.84393900	3.37087600	2.58497200
H	-6.00591300	2.37761900	3.31826100
C	-4.14109500	-0.46710800	-1.77790900
O	-4.77818400	-0.07736100	-2.73225300
C	-3.05375500	-1.97253200	-0.24877200
H	-3.58452200	-1.96862900	0.71420500
H	-2.59963400	-2.96366300	-0.38070500
C	-4.66256600	-2.84889200	-1.97613200
H	-3.94203700	-3.54454600	-2.42512300
H	-5.26064400	-3.38891500	-1.23155900
H	-5.32124300	-2.45761700	-2.75486800
N	-3.97208200	-1.73916700	-1.35608800
C	-1.99020400	-0.90045700	-0.32026200
H	-1.76842000	-0.31583400	0.57371200
C	-0.99168700	-1.01580000	-1.31815000
H	-0.43504700	-0.10806600	-1.57184600
H	-1.25827100	-1.61551900	-2.19520600
Au	0.51501200	-2.01747500	-0.09599600
P	2.20813000	-2.88945900	1.29620300
H	-2.89866000	1.14602700	-1.38826100
N	-3.41169200	0.41851300	-0.88085400
N	1.35370500	1.68384200	-1.07040200
C	0.68052500	3.70862300	0.63466500
C	3.99220800	1.96579300	-1.02848700
O	-0.11512000	1.24566500	1.02960700
O	-0.98087500	2.47931600	-0.97220600
O	2.81901200	-0.30554300	-1.54488900
O	2.75826100	0.54796100	0.81430700
S	0.14983100	2.11254500	-0.11709200
S	2.62214600	0.80604300	-0.61857700
F	1.73390900	3.50741000	1.41071600
F	-0.31934500	4.18441900	1.36385800
F	0.98852900	4.58106600	-0.30856300

F	5.13721100	1.37289600	-0.72137000
F	3.87380500	3.07955600	-0.32459500
F	3.98081300	2.25577300	-2.31719900
C	3.91105600	-2.69146900	0.67912300
H	4.62156000	-3.12173800	1.39682500
H	4.02133000	-3.18950500	-0.29041700
H	4.11518600	-1.62343000	0.55027800
C	2.21130700	-2.05423200	2.91702600
H	1.26235400	-2.24644700	3.43047900
H	3.04207400	-2.41477000	3.53769800
H	2.31211800	-0.97587100	2.75054600
C	2.07072600	-4.66475600	1.69844000
H	2.13123000	-5.26077600	0.78104100
H	2.87787900	-4.96605000	2.37879700
H	1.10396100	-4.85751000	2.17707200

2

Num. Imaginary Frequencies: 0

C	-4.85634600	-2.61997700	2.24829700
C	-4.12859100	-2.64387600	1.06146000
C	-3.15095300	-1.67910900	0.85861400
C	-2.88431700	-0.70061000	1.81119800
C	-3.62427300	-0.68464800	2.98654800
C	-4.60934800	-1.64369800	3.20688400
H	-5.62524800	-3.37109100	2.41443300
H	-4.34476200	-3.39957600	0.30961300
H	-2.10034600	0.03798200	1.64476000
H	-3.42671800	0.08303100	3.73095200
H	-5.18678000	-1.62947300	4.12864800
C	-2.75772300	-2.70245900	-1.37724500
O	-3.69832200	-2.54244500	-2.11063000
C	-0.87590100	-3.50190800	-0.21568000
H	-1.13776900	-3.98893600	0.73495500
H	0.07969200	-3.90480400	-0.57251600
C	-2.04122900	-4.96797300	-1.94269400
H	-1.12858700	-5.15385300	-2.52101000
H	-2.20350200	-5.80230600	-1.25021800
H	-2.89350600	-4.88768800	-2.62203800
N	-1.91847500	-3.72833000	-1.20699400
C	-0.82128700	-1.97983300	-0.12656000
H	-0.61928300	-1.62107300	0.88735800
C	0.04643000	-1.34481200	-1.17355800
H	-0.24522100	-0.29545500	-1.31970100

H	-0.04468800	-1.87834300	-2.13097700
Au	2.03168600	-1.22928800	-0.45862000
P	4.17199500	-0.93483700	0.53986600
H	-2.42524700	-0.71184600	-0.79744700
N	-2.33068100	-1.65813000	-0.36973700
N	-0.75097600	1.62710900	0.04180700
C	-2.09499700	3.57244900	-1.36236600
C	1.57214200	2.90244600	0.02243800
O	-3.00771700	2.58139600	0.89793100
O	-2.84057600	1.07990400	-1.11130700
O	0.91036400	1.15900100	1.85676800
O	-0.22148400	3.40675600	1.87448200
S	-2.24366000	2.10998500	-0.24881300
S	0.25650100	2.24625900	1.13225500
F	-1.56614700	4.58418100	-0.69409300
F	-3.30078800	3.90815200	-1.78991900
F	-1.32706800	3.27755300	-2.39744000
F	2.56443200	3.35804900	0.77648900
F	1.09318300	3.89091600	-0.71351900
F	2.03761400	1.95410600	-0.77593300
C	4.56743200	0.80954300	0.90780100
H	5.50129900	0.87528300	1.48179500
H	4.67770800	1.37060300	-0.02712400
H	3.74749000	1.25421400	1.48482700
C	4.29249000	-1.73931900	2.17631000
H	4.14421700	-2.82014700	2.07308000
H	5.27398400	-1.54880100	2.62965500
H	3.50787300	-1.34050200	2.83043300
C	5.64607300	-1.53697400	-0.35558600
H	5.71197100	-1.04454400	-1.33236800
H	6.55697800	-1.32182500	0.21827400
H	5.56602000	-2.61794200	-0.51642400

TS2

Num. Imaginary Frequencies: 1

C	2.37436400	2.62698200	3.39946500
C	1.74742100	1.98160400	2.33983900
C	1.99078000	2.39315700	1.02706900
C	2.87300400	3.44795500	0.78957700
C	3.49741600	4.08397500	1.85847900
C	3.25176600	3.68116700	3.16607500
H	2.17455400	2.29428000	4.41635300
H	1.06586200	1.15697700	2.53827600

H	3.09599600	3.77295800	-0.22357100
H	4.18427300	4.90406800	1.65775000
H	3.74385900	4.18228200	3.99719300
C	1.62280900	2.28508600	-1.36170200
O	2.64679800	2.10330000	-1.98303700
C	-0.49204000	3.03620300	-0.69832400
H	-0.44389800	3.90595300	-0.02446200
H	-1.46996200	3.02571000	-1.19726900
C	0.51879400	3.86346700	-2.88719800
H	-0.35306200	3.57459300	-3.48882700
H	0.44762200	4.93343200	-2.65330900
H	1.43129200	3.68016000	-3.46089600
N	0.57939400	3.08124300	-1.67819700
C	-0.20146800	1.70853800	-0.00284800
H	-0.48539500	1.71178300	1.05363700
C	-0.79525200	0.54252500	-0.76892000
H	-0.26404500	-0.38572800	-0.53300100
H	-0.67498800	0.71005400	-1.85109700
Au	-2.81780000	0.17622000	-0.32091300
P	-5.10018000	-0.28700900	0.22542200
H	1.78514300	0.26904800	0.10290800
N	1.32606100	1.68005500	-0.05681300
N	2.18495700	-0.80313600	0.33133800
C	3.11363700	-1.59736200	-2.04386500
C	0.82649700	-3.17384900	0.72275800
O	4.20750700	-2.38776500	0.23569400
O	4.44660900	0.04691800	-0.43450800
O	0.29167600	-0.89414300	1.93326000
O	2.42259300	-2.10981900	2.55632500
S	3.67078900	-1.16884700	-0.33206100
S	1.47306800	-1.65426800	1.56467300
F	2.41831000	-2.72038500	-1.99945800
F	4.18810100	-1.76298300	-2.79099400
F	2.36462100	-0.63087500	-2.53294900
F	0.01483100	-3.77206400	1.57456700
F	1.82152100	-3.97607400	0.41030100
F	0.16182100	-2.83400400	-0.36652000
C	-6.22318000	-0.51835000	-1.19831300
H	-5.87785900	-1.36085100	-1.80827600
H	-7.24591300	-0.71800500	-0.85206500
H	-6.22195000	0.38387600	-1.82030200
C	-5.36029700	-1.79846600	1.21929300
H	-6.42693200	-1.93582600	1.44047700
H	-4.99066300	-2.67054900	0.66796200

H	-4.80256500	-1.72209900	2.15955600
C	-5.92425300	1.01615100	1.20736400
H	-6.96262600	0.73592500	1.42815000
H	-5.38291500	1.16643300	2.14832500
H	-5.91583100	1.95887200	0.64832100

3

Num. Imaginary Frequencies: 0

C	1.35576200	2.71642000	3.66007100
C	0.78704600	2.51438600	2.40644800
C	1.60278700	2.31185500	1.29135800
C	2.99421400	2.30315900	1.45272800
C	3.54997000	2.51681400	2.70814600
C	2.73660300	2.72299600	3.81918100
H	0.70475600	2.86877900	4.51934700
H	-0.29640100	2.50227200	2.31434900
H	3.63433500	2.13001200	0.59048000
H	4.63322400	2.51041000	2.81722200
H	3.17712900	2.87762800	4.80237200
C	1.47418700	2.83274900	-1.10273700
O	2.53784700	3.41482400	-1.19950600
C	-0.62924900	1.96403200	-1.64252500
H	-1.59596500	2.44564000	-1.84704500
H	-0.60928500	1.00844500	-2.19439100
C	0.66606000	3.24607300	-3.38503400
H	0.74520400	2.38562400	-4.06740100
H	-0.17379500	3.87324500	-3.70952500
H	1.59032400	3.82832400	-3.43445900
N	0.47313000	2.81163500	-2.02676900
C	-0.41047700	1.74476000	-0.14529700
H	-0.96679300	2.52213300	0.40283700
C	-0.80477100	0.35938800	0.30838700
H	-0.51163700	0.18763800	1.35422300
H	-0.26455900	-0.37748900	-0.30851500
Au	-2.86750500	-0.02023300	0.13713900
P	-5.21693400	-0.46075400	-0.01276600
H	1.90501000	0.28969300	0.08571600
N	1.04816800	2.04316300	0.00208300
N	2.48017800	-0.58549400	0.06790900
C	2.27490000	-1.08545600	-2.53743200
C	1.67894300	-3.01263000	1.02573900
O	4.36276000	-1.87850300	-1.07872900
O	4.05626500	0.60435900	-1.54614400

O	1.71106500	-0.77097300	2.44638000	H	2.52551600	4.37529800	1.25389500
O	3.92826600	-1.83029300	1.79687900	H	3.38332900	4.28569500	-0.31068100
S	3.53430100	-0.70727400	-1.23618400	N	2.22393100	2.62882600	0.11182300
S	2.56418600	-1.45939600	1.50596200	C	1.32561500	0.51912200	0.49226500
F	1.58157400	-2.14987200	-2.18838300	H	1.11553000	-0.08840400	1.38195600
F	2.90262400	-1.29767600	-3.67277900	C	0.50503700	0.06428800	-0.70578700
F	1.46993300	-0.04058700	-2.64735600	H	0.87439500	-0.90393600	-1.07366400
F	1.64048900	-3.78035400	2.09568000	H	0.65709600	0.78746500	-1.52440600
F	2.33361400	-3.61461700	0.05477600	Au	-1.55004500	-0.11357600	-0.29234700
F	0.45575500	-2.71923500	0.63397600	P	-3.89270800	-0.31724500	0.18865200
C	-6.18958600	0.81428800	-0.89004700	N	2.78650700	0.47937800	0.23520000
H	-5.83565100	0.90170200	-1.92359100	C	-4.31408100	-0.19087000	1.96340900
H	-7.25547300	0.55095000	-0.89348500	H	-3.96893500	0.77236600	2.35610000
H	-6.05809900	1.78375400	-0.39613600	H	-5.39862700	-0.27530800	2.11201600
C	-5.66860700	-2.00736300	-0.87619500	H	-3.81015100	-0.99089100	2.51781000
H	-6.75878500	-2.13602700	-0.89100000	C	-4.95760000	0.94901600	-0.58970100
H	-5.29471400	-1.97737400	-1.90592200	H	-6.00927600	0.79057600	-0.31696000
H	-5.21024200	-2.86224500	-0.36623200	H	-4.64502300	1.94620800	-0.25949500
C	-6.06531100	-0.60863500	1.59972600	H	-4.85547700	0.89732500	-1.67960300
H	-7.13491800	-0.81133600	1.45687500	C	-4.66796700	-1.89314600	-0.31857700
H	-5.61679000	-1.42434600	2.17808500	H	-5.73416500	-1.90244200	-0.05620100
H	-5.94641700	0.32258500	2.16533600	H	-4.56126900	-2.02458900	-1.40135100
				H	-4.16536700	-2.72832000	0.18241800

4

Num. Imaginary Frequencies: 0

C	5.54205100	-1.97604700	-0.23687800
C	4.86126200	-0.76513700	-0.21055600
C	3.50776200	-0.72176700	0.16301300
C	2.87395300	-1.92856900	0.50230400
C	3.57107400	-3.13069600	0.47049700
C	4.91104000	-3.16955200	0.10162800
H	6.59134500	-1.97904100	-0.53005900
H	5.36664500	0.15617700	-0.47523800
H	1.82646000	-1.94136500	0.79337400
H	3.04892300	-4.04815400	0.73908600
H	5.45354800	-4.11272300	0.07650300
C	3.26456500	1.74831300	-0.06897000
O	4.38942300	2.05788400	-0.43804000
C	1.12649900	2.00242100	0.81354900
H	1.18825000	2.21305900	1.89645500
H	0.15737900	2.36634200	0.44556200
C	2.44901300	4.04615200	0.20458100
H	1.62624900	4.59416400	-0.27141100

5

Num. Imaginary Frequencies: 0

C	4.65639600	-0.70435600	2.34830100
C	4.40886400	0.46154600	1.63224400
C	3.09407500	0.87105800	1.39079200
C	2.03652300	0.08786900	1.86423800
C	2.29150400	-1.08243100	2.57247900
C	3.60138100	-1.48220100	2.82144200
H	5.68550800	-1.00886600	2.53383300
H	5.22722500	1.07167300	1.25873400
H	1.00738800	0.39908800	1.68722300
H	1.45281100	-1.68413400	2.91833100
H	3.79949200	-2.39723600	3.37803500
N	2.84810400	2.05482700	0.66689400
C	3.39163200	3.26739400	1.07678400
O	4.30912900	3.41932800	1.87059700
C	1.83614700	3.73009200	-0.58949000
H	0.87147000	4.25045900	-0.62736800
H	2.32261800	3.83170200	-1.57851100

C	3.21483000	5.60363000	0.35393300
H	3.94626200	5.74854400	1.15431800
H	3.70802600	5.77646400	-0.61710400
H	2.40846200	6.33923100	0.46637400
N	2.69424700	4.26599300	0.44582400
C	1.68460000	2.24681800	-0.21654800
H	0.75138500	2.12611500	0.36133000
C	1.66914700	1.33225600	-1.43167200
H	2.55138000	1.57468300	-2.04787100
H	0.78882600	1.61743900	-2.03188400
Au	1.66392000	-0.75923600	-1.12578100
P	1.70820800	-3.15949600	-1.03209000
H	-3.23170900	-2.45018000	-1.15334000
C	-3.73645400	-1.48986000	-1.28698300
C	-4.38644100	-1.04324900	0.02892700
H	-4.42414500	-1.51868100	-2.13665000
N	-2.67975100	-0.48688400	-1.62625600
H	-5.47704500	-1.11596500	-0.01975000
H	-4.00542300	-1.63222100	0.87069700
N	-4.01188600	0.39859800	0.27796500
C	-1.74697000	-0.26846400	-0.48138500
C	-3.28284300	0.80328000	-2.06622500
C	-2.53573800	0.43893000	0.62210600
C	-4.82811500	1.06162800	1.35879600
C	-4.29103000	1.18982800	-0.98585600
H	-1.36544500	-1.24808400	-0.17843200
H	-0.92475900	0.35444600	-0.85326400
H	-2.47111600	1.53134100	-2.15224000
H	-3.75800100	0.62756500	-3.03443600
H	-2.26415600	1.49276500	0.71577200
H	-2.41009300	-0.09324400	1.57052300
Cl	-4.80491200	0.17554400	2.87502400
H	-5.85689300	1.12872000	0.99434400
H	-4.39216700	2.05669700	1.49373800
H	-4.20539800	2.25769300	-0.76731400
H	-5.31990600	0.95267200	-1.27469400
F	-1.94839800	-0.99444600	-2.67412400
B	-2.15901300	3.81174000	-0.61747100
F	-3.10163300	3.86549700	-1.64701300
F	-2.83711200	3.49984900	0.58526500
F	-1.46257700	4.98732900	-0.49451800
F	-1.27293400	2.73951400	-0.89555600
B	-1.68763600	-3.06648500	1.63226100
F	-0.54473100	-2.31912000	1.28765500

F	-2.33154500	-3.44887700	0.43089700
F	-1.33500600	-4.17111700	2.36429600
F	-2.56683300	-2.22992400	2.33748700
C	2.01980700	-4.04022100	0.53921400
H	2.91948400	-3.63722200	1.01901300
H	1.16500500	-3.89227500	1.20861000
H	2.15587600	-5.11253900	0.34413900
C	3.01391000	-3.81668600	-2.13660000
H	2.99409500	-4.91451300	-2.15683800
H	2.86236200	-3.43299400	-3.15258300
H	3.99584400	-3.47949700	-1.78439500
C	0.19683500	-3.96773100	-1.66727700
H	-0.02620900	-3.59008600	-2.67236800
H	0.33756700	-5.05602800	-1.71700700
H	-0.64414300	-3.74741500	-0.99886100

TS3

Num. Imaginary Frequencies: 1

C	4.06718400	1.37827300	2.91717900
C	3.33370200	2.27421800	2.14690500
C	2.12758900	1.87918800	1.56350900
C	1.67424100	0.56893500	1.75853300
C	2.41593500	-0.32842800	2.52285900
C	3.61413100	0.07380900	3.10611300
H	5.00297600	1.70233100	3.36968900
H	3.68393100	3.29221500	1.99011900
H	0.72542500	0.24098700	1.33948800
H	2.02923700	-1.33705000	2.66673900
H	4.19196700	-0.62427900	3.71015100
N	1.39340400	2.81228700	0.79444900
C	0.80431200	3.92353900	1.41160800
O	1.08671000	4.36399900	2.51466500
C	-0.08516900	3.75437200	-0.73156800
H	-1.08897400	3.57359300	-1.13779300
H	0.48693900	4.36498900	-1.45505100
C	-0.88421200	5.61417700	0.77278900
H	-0.75416000	5.91522700	1.81654200
H	-0.52934200	6.42771400	0.12069400
H	-1.94944500	5.43760600	0.57204300
N	-0.14512200	4.40159100	0.55561700
C	0.64877500	2.44589200	-0.41603000
H	-0.11285300	1.68817300	-0.17026200
C	1.51212000	1.94970000	-1.54696300

H	2.33436900	2.65614800	-1.74393000
H	0.90029400	1.84582700	-2.45548000
Au	2.41686700	0.07308700	-1.22000600
P	3.44346900	-2.10420200	-0.94144100
H	-1.02052500	-2.86104100	-0.60060300
C	-1.70899000	-2.26892300	-1.21200700
C	-3.16842900	-2.59708500	-0.83396100
H	-1.50549600	-2.43128400	-2.27472300
N	-1.51170100	-0.85245900	-0.92556400
H	-3.69496900	-3.12384000	-1.63593700
H	-3.19951900	-3.17749900	0.09163800
N	-3.89702000	-1.29575900	-0.57720500
C	-1.79449900	-0.50863900	0.46616400
C	-2.21485200	0.00539400	-1.87059200
C	-3.31284400	-0.63721800	0.65724000
C	-5.37645300	-1.48338700	-0.42174400
C	-3.70538800	-0.37208500	-1.76873800
H	-1.23268800	-1.19521900	1.10540100
H	-1.49939300	0.53113800	0.63138000
H	-2.05883700	1.05289200	-1.59695800
H	-1.81760300	-0.18299500	-2.87194600
H	-3.79845500	0.33910700	0.74601400
H	-3.54095800	-1.27817700	1.51177800
Cl	-5.78320300	-2.61841400	0.86506700
H	-5.76760100	-1.86309800	-1.36988800
H	-5.79809500	-0.50029500	-0.19099700
H	-4.31684600	0.51870500	-1.59533400
H	-4.05969200	-0.91608400	-2.64994600
F	0.14644400	-0.51831600	-1.15761600
B	-3.71006200	2.85996200	-0.40454900
F	-3.37748100	2.80870700	-1.76527600
F	-4.81692400	2.00490300	-0.18462300
F	-4.00383000	4.14622800	-0.01372800
F	-2.62053600	2.35436600	0.32970400
B	-0.80805700	-3.65088800	1.92332700
F	0.06689200	-2.53693000	1.86390900
F	-0.64925500	-4.38968000	0.74469300
F	-0.54331600	-4.41451200	3.03254300
F	-2.13137300	-3.15830400	1.96349600
C	4.71523100	-2.27250300	0.35759200
H	5.57155200	-1.63136700	0.11881700
H	4.30291100	-1.95400100	1.32229900
H	5.05168400	-3.31514600	0.42830000
C	4.25921800	-2.78904100	-2.42707700

H	4.62226800	-3.80627500	-2.23012200
H	3.54676100	-2.81595000	-3.25952600
H	5.10576300	-2.15477100	-2.71373100
C	2.17612300	-3.34596300	-0.52135300
H	1.48858700	-3.44653000	-1.37056200
H	2.63346600	-4.32245600	-0.31493400
H	1.59530400	-3.01759000	0.34967200

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Num. Imaginary Frequencies: 0

C	3.14908600	-2.55626300	2.55811400
C	3.75045900	-1.49277500	1.92675500
C	2.94339500	-0.48420800	1.35432200
C	1.49406800	-0.65640600	1.34389700
C	0.93670500	-1.76858400	2.08014100
C	1.74280900	-2.70006900	2.66179900
H	3.78844500	-3.31287400	3.01027200
H	4.82846700	-1.39354000	1.89164400
H	0.92211000	0.27315600	1.45428900
H	-0.14925000	-1.84259900	2.13155900
H	1.32180800	-3.54285000	3.20443000
N	3.43862400	0.65144000	0.81543200
C	4.81194200	0.97448600	0.60392800
O	5.76489500	0.31731300	0.97553300
C	3.51090200	2.71276100	-0.29318400
H	3.35521500	3.59155900	0.34901400
H	3.38098800	3.02977200	-1.33673200
C	6.03406500	2.83636500	-0.42530500
H	6.88572400	2.21574700	-0.13434900
H	6.07541100	3.02848600	-1.50457500
H	6.08644100	3.79566400	0.10657000
N	4.82036200	2.13652100	-0.08754800
C	2.55925800	1.56742800	0.07721900
H	1.76381700	1.94938800	0.72444200
C	2.00567100	0.85585500	-1.13749800
H	2.81549600	0.53052500	-1.80869700
H	1.29972500	1.48505700	-1.68864600
Au	1.00792200	-0.97103700	-0.76317700
P	0.11183000	-3.30975800	-0.90441800
H	-2.58075900	-1.18535200	-0.81501500
C	-2.56682900	-0.21667500	-1.31978500
C	-3.88937900	0.51658600	-1.02470400
H	-2.43782500	-0.38672300	-2.39620700

N	-1.42479500	0.55575500	-0.84317200	7			
H	-4.53433700	0.62631600	-1.90397100	Num. Imaginary Frequencies: 0			
H	-4.44192300	0.03083700	-0.21655000	C	1.97872500	-0.57334100	2.05031000
N	-3.55407400	1.91558000	-0.55235400	C	1.24031400	0.32153800	1.18855800
C	-1.61228300	0.88750300	0.56802800	C	0.80609900	1.59093400	1.76014300
C	-1.32689700	1.78144900	-1.62640000	C	1.25335000	1.96609900	3.04375900
C	-2.79873700	1.84312700	0.75892900	C	2.04574700	1.09798400	3.76100400
C	-4.76403000	2.77497300	-0.43296600	C	2.40078100	-0.18860000	3.28852000
C	-2.65275100	2.56523200	-1.58631300	H	2.14956800	-1.57852300	1.66998700
H	-1.78016000	-0.04477700	1.11804500	H	0.45151700	-0.19133000	0.60797500
H	-0.71359800	1.39179400	0.94068800	H	0.95716900	2.92508600	3.45235700
H	-0.52436600	2.40365800	-1.21643500	H	2.39471400	1.41284800	4.74348000
H	-1.07102300	1.51812600	-2.66095100	H	2.97476100	-0.86093400	3.92160400
H	-2.47163000	2.86626800	0.97935200	N	-0.02466300	2.36251400	1.02092900
H	-3.49900500	1.48026900	1.51546600	C	-0.80470300	3.46506600	1.47705400
Cl	-5.98296900	2.10728400	0.66484600	O	-0.82679800	3.89626400	2.61412100
H	-5.20700400	2.87456100	-1.42778600	C	-1.23219300	3.18997300	-0.82327500
H	-4.44419300	3.74980300	-0.05336200	H	-0.79119600	3.87937000	-1.56177700
H	-2.49331000	3.60074400	-1.26964400	H	-2.14830000	2.76287500	-1.25129000
H	-3.20396800	2.53899800	-2.53330500	C	-2.49687100	4.94209300	0.47893800
F	0.67870400	-1.11174100	-2.77833600	H	-2.57496900	5.27676700	1.51676400
B	0.19262500	4.27116900	0.59218500	H	-3.46745300	4.56110700	0.13758600
F	0.88953900	3.82833700	-0.54982900	H	-2.20050700	5.78966300	-0.15299200
F	-1.13842200	4.54248500	0.23059200	N	-1.51701100	3.88700400	0.41070800
F	0.79936700	5.39469700	1.10958500	C	-0.23298200	2.09729800	-0.40735500
F	0.19518300	3.23215400	1.54301000	H	-0.68409000	1.10529300	-0.52649800
B	-3.52382600	-2.23542500	1.43567600	C	1.08653200	2.16666200	-1.13505500
F	-2.10559700	-2.29828300	1.34384300	H	0.97612100	1.97375100	-2.20896800
F	-4.04605700	-2.59166500	0.18691500	H	1.58357700	3.13564600	-0.98068000
F	-3.96595100	-3.08776600	2.42203700	Au	2.49858300	0.72686600	-0.52936700
F	-3.88834900	-0.91143500	1.72506700	P	4.39013000	-0.89754700	-0.38113100
C	1.34949500	-4.07176200	-2.01111700	H	-2.46494800	0.44319600	1.80606600
H	1.45552200	-3.42673600	-2.89013100	C	-2.70996000	0.00699400	0.82857200
H	2.31585200	-4.13195900	-1.49494100	C	-4.01895200	-0.79149300	0.93069800
H	1.03742400	-5.07905000	-2.31595000	H	-2.83211900	0.82377600	0.10799600
C	-1.45683300	-3.47773100	-1.81677600	N	-1.61410100	-0.85732400	0.39955300
H	-1.53733700	-4.50370200	-2.20003000	H	-4.84969700	-0.28778300	0.42716500
H	-2.30460100	-3.27626100	-1.15041900	H	-4.29674700	-1.03466200	1.96095800
H	-1.46059000	-2.77706800	-2.65840300	N	-3.80775400	-2.11718800	0.22282500
C	-0.05263700	-4.51691400	0.45371100	C	-1.57753600	-2.03290400	1.26753700
H	-0.79596800	-4.15732900	1.17313200	C	-1.82508600	-1.27767500	-0.98696400
H	-0.38111100	-5.47805600	0.03592100	C	-2.79053200	-2.93785900	0.98561100
H	0.91209400	-4.65699000	0.95335700	C	-5.09676300	-2.82952200	0.01237100
				C	-3.24060200	-1.84250500	-1.16286100

H	-1.58088400	-1.68538300	2.30917600
H	-0.65269200	-2.59436000	1.10020100
H	-1.06004000	-2.01936100	-1.23102800
H	-1.71547100	-0.41578700	-1.65446800
H	-2.52489200	-3.78346000	0.33952300
H	-3.27377600	-3.31158800	1.89338000
Cl	-5.95711000	-3.17208800	1.52479700
H	-5.72133900	-2.18421000	-0.61314600
H	-4.88644000	-3.77898300	-0.48760700
H	-3.25141200	-2.79410800	-1.70611900
H	-3.92766400	-1.13148100	-1.63166300
F	3.55902400	1.22308300	-2.19119300
B	1.23867600	-3.37607300	-0.47746800
F	1.23850500	-2.00776600	-0.82613000
F	-0.02380900	-3.91316300	-0.73865900
F	2.22206100	-4.03729000	-1.19585300
F	1.50593100	-3.47859400	0.90069300
B	-4.65866200	1.53459000	-1.78679300
F	-4.48908600	2.21599200	-0.57490400
F	-3.38855100	1.14000000	-2.25037900
F	-5.28596400	2.33137700	-2.71945900
F	-5.42497400	0.36915400	-1.54986400
C	5.95345600	0.03839700	-0.28681400
H	6.80884600	-0.62210400	-0.47960900
H	5.92674700	0.83284800	-1.04031500
H	6.06291300	0.49055900	0.70558200
C	4.43299000	-1.72345000	-2.00227500
H	4.27342200	-0.95936300	-2.76988500
H	5.40201400	-2.21693900	-2.15287500
H	3.62876600	-2.46659500	-2.03981900
C	4.60045400	-2.25316300	0.82341100
H	5.50744500	-2.81750800	0.56861300
H	4.70763900	-1.85092900	1.83754000
H	3.73744600	-2.92911400	0.78886100

TS4

Num. Imaginary Frequencies: 1

C	-1.57819700	0.38026100	2.06318000
C	-0.97380200	-0.55884300	1.15873400
C	-0.17094300	-1.61289300	1.74144300
C	-0.07734900	-1.71110600	3.14571300
C	-0.70614400	-0.78589000	3.95341000
C	-1.43057900	0.29683900	3.42353100

H	-2.08940400	1.23269900	1.61677800
H	-0.08130300	0.21269500	0.58426300
H	0.50296200	-2.51469000	3.58287300
H	-0.61821800	-0.89581500	5.03313500
H	-1.87089100	1.04300000	4.08090000
N	0.55228600	-2.45775400	0.93556400
C	1.76845900	-3.10324700	1.32100800
O	2.27993800	-3.06173200	2.42511800
C	1.39227400	-3.57298200	-0.93898800
H	0.82590600	-4.49519100	-1.15179100
H	1.98906300	-3.30773500	-1.81946900
C	3.51019900	-4.40647600	0.17334800
H	3.97979400	-4.31550000	1.15648500
H	4.15622900	-3.93043300	-0.57533300
H	3.37802000	-5.46893400	-0.06960600
N	2.23653200	-3.73285800	0.22082100
C	0.47058800	-2.42127500	-0.53317600
H	0.92674100	-1.48581500	-0.89198200
C	-0.92734600	-2.54289800	-1.04202100
H	-0.96852000	-2.48191000	-2.13622000
H	-1.40561400	-3.47392300	-0.70450600
Au	-2.24395400	-1.04181600	-0.44777400
P	-4.28782100	0.36868100	-0.13505700
H	2.08197800	-0.04691400	1.76584500
C	2.25871900	0.34473900	0.75436700
C	3.44988200	1.30614300	0.75190100
H	2.45405400	-0.49490600	0.08413500
N	1.05248200	1.05574900	0.29348900
H	4.34178800	0.83578600	0.32817500
H	3.67633600	1.70990400	1.74267100
N	3.09007900	2.48507900	-0.12901500
C	0.94463100	2.31295800	1.06052800
C	1.15473700	1.34668600	-1.14817700
C	2.00414900	3.29215000	0.54931400
C	4.29066700	3.29849000	-0.47769200
C	2.53197800	1.94489000	-1.43792300
H	1.09783700	2.06620400	2.11864500
H	-0.05354800	2.74762700	0.95637400
H	0.33997500	2.02669300	-1.40621800
H	1.03230900	0.41642300	-1.71488800
H	1.59233800	3.97559500	-0.20231200
H	2.46613500	3.86901500	1.35591500
Cl	5.14045000	3.91368700	0.94726300
H	4.96480400	2.64899500	-1.04390200

H	3.96089900	4.14768900	-1.08226600
H	2.47611700	2.78229700	-2.14119400
H	3.25379600	1.20203600	-1.79386000
F	-3.47302100	-1.66487600	-1.96499300
B	-1.89766300	3.41714800	-0.54291600
F	-1.82982500	2.02098300	-0.75678700
F	-0.71997800	3.99948900	-1.02249600
F	-3.00548500	3.93566200	-1.18515100
F	-1.98946400	3.62654600	0.84414100
B	4.45692400	-1.23903400	-1.43250600
F	4.43878900	-1.52111000	-0.06213700
F	3.12333600	-1.16001800	-1.89826200
F	5.14111200	-2.21825700	-2.12031600
F	5.05230200	0.02590700	-1.62412200
C	-4.61725600	1.63641100	1.13857000
H	-4.52486100	1.19495200	2.13868100
H	-3.91472100	2.47221400	1.04658000
H	-5.64139300	2.01230700	1.01184000
C	-4.70626900	1.16847700	-1.71644200
H	-4.08176800	2.05706300	-1.85060200
H	-4.50661400	0.44106900	-2.50998600
H	-5.76651800	1.45332300	-1.72621300
C	-5.63437800	-0.84042900	0.11917300
H	-5.53163300	-1.61529300	-0.64783000
H	-5.54267200	-1.30131600	1.10984500
H	-6.61683000	-0.35789200	0.03406000

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Num. Imaginary Frequencies: 0

C	-2.45341200	0.76079200	2.19501100
C	-1.95093800	-0.32168500	1.46548800
C	-0.93391100	-1.10509700	2.04880800
C	-0.50458200	-0.80171600	3.35455000
C	-1.01778000	0.28574700	4.04599700
C	-1.99316400	1.08530900	3.46555900
H	-3.23856700	1.37267000	1.75673400
H	0.23894100	-1.43315700	3.82858200
H	-0.65528700	0.49383900	5.05130400
H	-2.40507100	1.94302800	3.99319400
N	-0.34813900	-2.19671000	1.37473500
C	0.86346200	-2.79566900	1.69244000
O	1.70319300	-2.38053900	2.50732400
C	-0.12130900	-4.08254200	0.03475300

H	-0.79370600	-4.87312300	0.40494600
H	0.22246900	-4.34240100	-0.97303200
C	2.26362800	-4.59698500	0.79000700
H	2.87683200	-4.38379000	1.67027600
H	2.80031800	-4.26239400	-0.10975900
H	2.08566100	-5.67667200	0.73254500
N	1.00867500	-3.89747200	0.92796600
C	-0.78093300	-2.70214300	0.05735300
H	-0.29317100	-2.09891700	-0.72912200
C	-2.26184200	-2.65280600	-0.11824500
H	-2.57623900	-3.07680800	-1.07918800
H	-2.80316500	-3.12273300	0.71242100
Au	-2.81256700	-0.65449400	-0.35703500
P	-3.63293000	1.58743200	-1.10467600
F	-3.68694400	-1.07877000	-2.18859500
C	-3.64297200	3.18308300	-0.21549300
H	-4.23739300	3.10599100	0.70260100
H	-2.62479500	3.50064500	0.03155800
H	-4.10590600	3.94011400	-0.86308600
C	-2.81700600	1.94335600	-2.69431600
H	-1.78106000	2.24042500	-2.50325500
H	-2.83807800	1.01863700	-3.28108800
H	-3.33942900	2.74504500	-3.23237600
C	-5.38757900	1.34288300	-1.54993400
H	-5.44545500	0.40467600	-2.11080800
H	-5.99591000	1.26074600	-0.64152300
H	-5.75617100	2.17957800	-2.15764600
H	2.05902000	-0.69693500	2.17879100
H	4.28665200	-1.07858400	1.76602200
C	3.67868100	-0.70598500	0.93692500
C	4.45380500	0.27867000	0.06014000
H	3.30266600	-1.55607600	0.36102100
N	2.49425800	-0.00394700	1.52073700
H	4.66420400	-0.15907700	-0.92133500
H	5.38198300	0.61886100	0.52792000
N	3.59148900	1.49922900	-0.16075700
C	2.91046300	1.25013900	2.20876200
C	1.50336700	0.32028400	0.44563300
C	3.41169600	2.23275600	1.14753400
C	4.13668600	2.40611300	-1.22130900
C	2.23769400	1.03807700	-0.67572800
H	3.68098900	0.98746900	2.93910100
H	2.03606700	1.65934700	2.72269800
H	0.71106900	0.92743700	0.89410800

H	1.09631300	-0.62094000	0.07135800
H	2.68786800	3.02955800	0.95662300
H	4.37896000	2.66391300	1.41885200
Cl	5.77863700	2.95976700	-0.87191200
H	4.14243400	1.84162000	-2.15818100
H	3.46330900	3.26685000	-1.27575000
H	1.68526000	1.92072900	-1.00370800
H	2.44771300	0.37105500	-1.51738200
B	0.15384600	3.58967000	0.25382100
F	-0.44763100	2.57155000	-0.50626200
F	1.34548500	3.98204600	-0.40081200
F	-0.69559000	4.66499600	0.38849800
F	0.49892500	3.06732800	1.51224600
B	3.14380800	-2.22350700	-2.20769900
F	4.13044800	-2.76214700	-1.37648100
F	1.97040600	-2.05281300	-1.43220300
F	2.89018800	-3.03546400	-3.28493400
F	3.57121100	-0.94592600	-2.63774700

TS5

Num. Imaginary Frequencies: 1

H	-1.81643200	1.69228400	1.70922400
H	-2.72203500	-0.37035200	2.56802600
C	-3.34981100	0.25656200	1.92765100
C	-4.16396200	-0.63377300	0.98634000
H	-3.97690300	0.91012500	2.54196000
N	-2.46602200	1.12450700	1.10100800
H	-5.22703700	-0.64652900	1.24762900
H	-3.76140700	-1.65214000	0.98178200
N	-4.04535500	-0.09735100	-0.42446900
C	-1.67037500	0.29608900	0.13842300
C	-3.28104800	2.12854200	0.35800600
C	-2.62223600	-0.29161900	-0.90294000
C	-5.03162300	-0.73558300	-1.35825600
C	-4.35787000	1.38517200	-0.42583300
H	-1.14774900	-0.48245100	0.70811600
H	-0.93561700	0.94862400	-0.34260900
H	-2.59730400	2.67644600	-0.29697000
H	-3.71332700	2.81669500	1.08979500
H	-2.53718300	0.22336400	-1.86473300
H	-2.46527700	-1.36669500	-1.01075000
Cl	-4.88961000	-2.48919700	-1.43320300
H	-6.03378100	-0.47494000	-1.00636600

H	-4.85249600	-0.31831700	-2.35294200
H	-4.36955400	1.71797200	-1.46806700
H	-5.35517800	1.49578000	0.01204800
B	-1.33418800	-2.94819300	1.66083500
F	-0.19595000	-2.16641400	1.41499200
F	-2.13810400	-2.93608100	0.48996700
F	-0.97534800	-4.24173100	1.97004700
F	-2.07818100	-2.36769000	2.69570900
B	-0.91821700	2.54783800	-2.40539800
F	-0.48853700	3.33265700	-3.44530300
F	-0.16213500	1.36895400	-2.30563800
F	-2.27272700	2.19960100	-2.57084800
F	-0.80484100	3.24299800	-1.17734300
C	2.77283700	-0.84951100	2.35215000
C	2.20317400	0.11198900	1.50977600
C	1.13023700	0.88118400	1.99261800
C	0.54387500	0.59217800	3.22486600
C	1.06795500	-0.43259600	4.00520200
C	2.19392800	-1.13533500	3.58360800
H	3.64861000	-1.40913800	2.02374800
H	-0.27591400	1.20487200	3.59336700
H	0.60999500	-0.65738000	4.96653400
H	2.62029600	-1.91638800	4.21026300
N	0.82420000	2.00446600	1.21180300
C	0.08269100	3.10813500	1.57365000
O	-0.97362900	3.07285300	2.22674200
C	1.90675200	3.89548000	0.35730300
H	1.91398400	4.40114000	-0.61570600
H	2.79049300	4.21988900	0.92987800
C	0.00123700	5.47309800	0.92587400
H	-0.89749400	5.46118300	1.54871800
H	0.64719200	6.29869500	1.24626200
H	-0.28696400	5.62096400	-0.12418100
N	0.67986200	4.21115400	1.07807800
C	1.83021000	2.37269300	0.20073100
H	1.41588700	2.12968300	-0.78864100
Au	2.51364000	-0.42404500	-0.53673300
C	3.06945100	1.55424500	0.45336900
H	3.76318700	1.60264900	-0.40227400
H	3.63606900	1.84397400	1.34393500
F	3.46684600	-0.05982500	-2.47846300
P	1.74576500	-2.58568200	-1.32959500
C	1.78009000	-4.04553100	-0.23303300
H	2.79962000	-4.18972800	0.14485900

H	1.10439100	-3.88101500	0.61374200
H	1.47171800	-4.94464600	-0.78340700
C	2.80011800	-3.03857000	-2.75056000
H	2.99703200	-2.11468000	-3.30573400
H	3.75909800	-3.41438200	-2.37281900
H	2.33168000	-3.80571300	-3.37985300
C	0.04546900	-2.55843200	-1.99810200
H	-0.65695500	-2.63213800	-1.15943400
H	-0.12263800	-1.61890600	-2.53937800
H	-0.12122200	-3.40686000	-2.67492500

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Num. Imaginary Frequencies: 0

H	-0.99536800	0.11628700	2.31755600
H	-3.21756100	0.81826300	2.52052800
C	-2.93906300	0.35985400	1.56819000
C	-4.01784900	-0.58559600	1.05671600
H	-2.72470100	1.14201600	0.83253400
N	-1.68793800	-0.43808600	1.76784400
H	-4.64907400	-0.09036200	0.31538300
H	-4.64423300	-0.98763600	1.85859700
N	-3.33524300	-1.76420100	0.39556300
C	-2.00399700	-1.72221900	2.46674500
C	-1.08764600	-0.74360000	0.42758000
C	-2.73950000	-2.62670600	1.47753300
C	-4.26659100	-2.50577700	-0.50908900
C	-2.19410000	-1.24935500	-0.48082100
H	-2.60781600	-1.48002000	3.34680100
H	-1.06115700	-2.17378700	2.78391200
H	-0.28443700	-1.46718100	0.59694400
H	-0.64409300	0.16591300	0.01504200
H	-2.06975800	-3.33903000	0.98265900
H	-3.54815900	-3.18002800	1.96406200
Cl	-5.70550500	-3.09649600	0.33547400
H	-4.56600100	-1.79915600	-1.28900000
H	-3.72559300	-3.36141200	-0.92165100
H	-1.84845900	-2.08229900	-1.09992600
H	-2.60860800	-0.46563200	-1.11836900
B	1.48180200	-1.25485700	2.70517000
F	1.61742900	-0.66110700	1.44375200
F	0.97381300	-2.55667000	2.51010300
F	2.69054500	-1.29306100	3.35967400
F	0.53454700	-0.50910800	3.43972200

B	-4.23388900	1.61702600	-1.59076100
F	-4.90069000	2.00333000	-0.41991400
F	-2.84609200	1.66328300	-1.34140200
F	-4.56652100	2.42491200	-2.65001800
F	-4.58099500	0.27261000	-1.86891600
C	3.96678200	3.19089300	0.01318500
C	2.61901100	2.92164000	-0.18138800
C	1.87803100	2.33368400	0.84638700
C	2.44390400	2.00355400	2.07093100
C	3.79610400	2.28803700	2.25286800
C	4.55521200	2.87298400	1.23885900
H	4.55268000	3.66062500	-0.77704900
H	1.84938800	1.52551300	2.84524900
H	4.26657600	2.03783200	3.20274500
H	5.61120600	3.08130900	1.40313600
N	0.53567000	2.17365400	0.44305100
C	-0.53947700	2.55180000	1.24844100
O	-0.73478300	2.15917700	2.39979100
C	-0.76912500	3.73059100	-0.76236200
H	-1.52420200	3.65990900	-1.55189000
H	-0.39129500	4.76756300	-0.72229200
C	-2.56227300	3.94850700	1.01774400
H	-2.67614700	3.66966100	2.07011000
H	-2.50503300	5.04337800	0.94719800
H	-3.43093400	3.59296000	0.44824300
N	-1.34727900	3.35724400	0.51809500
C	0.35094600	2.69931000	-0.93410700
H	0.00997400	1.86240500	-1.56194700
Au	1.63707000	-0.95399800	-1.63416900
C	1.73726300	3.20822900	-1.36962100
H	2.07964300	2.68458700	-2.27224900
H	1.72120800	4.28118800	-1.61523100
F	-0.21909300	-0.25665000	-2.16858700
P	3.62608800	-1.76474300	-0.85514500
C	4.51046400	-0.59992300	0.22295900
H	4.70140800	0.33928700	-0.31033000
H	3.87511000	-0.38314000	1.08911200
H	5.46161300	-1.03977500	0.55098400
C	4.83087400	-2.24225300	-2.13600800
H	4.39672500	-3.00801800	-2.78858800
H	5.08506700	-1.36694800	-2.74444900
H	5.74425700	-2.63614600	-1.67174400
C	3.39348300	-3.26335600	0.15348100
H	2.66566100	-3.05828700	0.94810900

H	3.00887200	-4.07152700	-0.47947600
H	4.34798100	-3.57505900	0.59742400

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Num. Imaginary Frequencies: 0

C	2.66773900	-0.75486100	2.22186700
C	2.02990300	0.24508900	1.48961600
C	1.06155300	1.05149900	2.11820500
C	0.73536200	0.78762100	3.46070300
C	1.36318300	-0.23339800	4.15985700
C	2.34471700	-1.00569200	3.55064100
H	3.43135700	-1.36213400	1.73906100
H	-0.01542800	1.39562400	3.95661800
H	1.08821400	-0.41084500	5.19818200
H	2.85144900	-1.79950400	4.09570900
N	0.43398300	2.11949600	1.44390800
C	-0.63510600	2.86182700	1.93098700
O	-1.54246100	2.42225800	2.65497700
C	0.57906200	4.25615300	0.53279400
H	1.40706000	4.80667600	1.00777300
H	0.26935900	4.78288200	-0.37837000
C	-1.61289100	5.08078300	1.52877000
H	-2.37149400	4.69606000	2.21580900
H	-2.06781300	5.23220500	0.54169600
H	-1.23298800	6.03593400	1.91101300
N	-0.54793900	4.11404200	1.44183000
C	0.93743600	2.79972000	0.22876500
H	0.31204400	2.48167600	-0.62103200
C	2.36543900	2.49199600	-0.07336900
H	2.67862800	2.93933800	-1.02418400
H	3.04958200	2.77365100	0.73591200
Au	2.47372200	0.44147500	-0.48468300
P	2.77676900	-1.91466800	-1.24396900
F	2.70892300	0.77818700	-2.55443500
C	3.25747000	-3.27492000	-0.12598800
H	4.21404200	-3.03848700	0.35588600
H	2.48443300	-3.43898900	0.62979200
H	3.37795200	-4.19701500	-0.71064000
C	1.39224400	-2.58664500	-2.22303000
H	0.60532700	-2.94361200	-1.55002300
H	0.98337000	-1.80367400	-2.87148400
H	1.74660700	-3.42791500	-2.83343300
C	4.15883300	-1.84795100	-2.43730900
H	3.93813200	-1.05520100	-3.15877700
H	5.08701300	-1.59439700	-1.91078100

H	4.28234200	-2.81434400	-2.94292400
H	-1.85749000	0.85471900	1.96433900
H	-4.23759900	0.66963200	1.81698000
C	-3.61368500	0.68233000	0.91805800
C	-4.18515700	-0.17826700	-0.20925600
H	-3.46451900	1.71366600	0.58495500
N	-2.27100800	0.14618800	1.30343600
H	-4.10689300	0.33113200	-1.17458600
H	-5.22248900	-0.46603800	-0.01727800
N	-3.36257100	-1.43754400	-0.31315500
C	-2.39988300	-1.18579900	1.95709700
C	-1.39726800	0.01883200	0.09239700
C	-3.25614700	-2.07402400	1.05559100
C	-3.91448300	-2.40284100	-1.31469000
C	-1.97557900	-1.05791000	-0.81475100
H	-2.86137000	-1.04958300	2.93894900
H	-1.39160200	-1.59236400	2.07930500
H	-0.39929300	-0.27512100	0.43085000
H	-1.36957700	0.99442300	-0.39370300
H	-2.80101400	-3.06135400	0.94023700
H	-4.27825300	-2.18337100	1.42870200
Cl	-5.51326800	-3.01195700	-0.86737800
H	-3.98950700	-1.88168000	-2.27251100
H	-3.21074000	-3.23892200	-1.36852100
H	-1.38476200	-1.97656900	-0.79180100
H	-2.07099000	-0.68544800	-1.83833000
B	-0.31110800	-3.86079900	0.84824800
F	0.25301700	-2.56392300	0.84626200
F	-1.12066900	-3.97470300	-0.31274800
F	0.68038600	-4.81527600	0.82388300
F	-1.12343900	-3.99688300	1.97205600
B	-2.35104100	2.91752500	-1.95017600
F	-3.16537300	3.87606100	-2.49749600
F	-2.29776300	3.05175100	-0.54474500
F	-1.04007100	3.02837100	-2.44892000
F	-2.82801800	1.62405800	-2.23993600
O	0.04904400	0.42380300	-2.52864000
H	1.00793200	0.57812000	-2.69417200
H	-0.35964600	1.30018900	-2.63444900

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Num. Imaginary Frequencies: 1

O	1.91363900	0.06634700	-3.50846400	H	3.42302800	-1.42610900	2.33598900
H	1.23047900	0.58782800	-3.06056200	H	-0.65046200	1.12730200	3.58968400
H	2.73402700	0.20317100	-2.96348400	H	0.13139900	-0.74424300	5.00841300
H	-2.12497700	1.60590600	1.76697900	H	2.21792700	-1.96893100	4.42091300
H	-3.07076500	-0.49644700	2.50723800	N	0.62799100	1.97160800	1.31962600
C	-3.65439500	0.12568100	1.82184600	C	-0.15791600	3.05590000	1.65579800
C	-4.34587700	-0.76181400	0.78155100	O	-1.24618200	2.99153600	2.24972400
H	-4.35828600	0.74866800	2.38092300	C	1.71502900	3.90301900	0.55784000
N	-2.71546900	1.03466000	1.10555500	H	1.75764900	4.41480900	-0.41130200
H	-5.42958300	-0.80734700	0.93128900	H	2.55996100	4.24829300	1.17482600
H	-3.92423300	-1.77230900	0.78780700	C	-0.22310000	5.44764300	1.10074000
N	-4.09634100	-0.19159900	-0.59894100	H	-1.16709900	5.39278700	1.64980600
C	-1.80756200	0.23426000	0.22251600	H	0.39285400	6.24811900	1.52735600
C	-3.48034700	2.03204800	0.30284200	H	-0.43008300	5.67377000	0.04552000
C	-2.62730100	-0.33494400	-0.93193500	N	0.44659800	4.17793500	1.21726500
C	-4.95162300	-0.84221400	-1.64578500	C	1.69392600	2.37778700	0.38824300
C	-4.44958200	1.28102100	-0.60598400	H	1.36545000	2.12754800	-0.63316200
H	-1.35003600	-0.54891000	0.83728200	Au	2.59612800	-0.36762500	-0.28756900
H	-1.02082100	0.89842000	-0.14740800	C	2.94749200	1.61371100	0.72255700
H	-2.75147900	2.61896800	-0.26245600	H	3.70191200	1.70519300	-0.07700600
H	-4.00661700	2.68817300	1.00182200	H	3.41546900	1.89223700	1.67079000
H	-2.46011800	0.21468000	-1.86354600	F	3.98207700	0.28395900	-1.94487200
H	-2.43056400	-1.40193100	-1.06157600	P	1.90358000	-2.46692000	-1.25801100
Cl	-4.76857400	-2.59324100	-1.69385400	C	2.03405900	-3.92820300	-0.17048400
H	-5.99304100	-0.59635000	-1.42109000	H	3.05910000	-4.02200400	0.20745200
H	-4.65475000	-0.42289400	-2.61151200	H	1.34635100	-3.80678500	0.67396000
H	-4.35757200	1.63641300	-1.63651500	H	1.77032400	-4.83944300	-0.72394200
H	-5.49050500	1.35934700	-0.27523300	C	2.85524300	-2.91564500	-2.74889700
B	-1.40389100	-2.99581500	1.66125800	H	2.71686100	-2.11341300	-3.48387600
F	-0.27090500	-2.21745300	1.37228200	H	3.91976100	-3.00061100	-2.50229700
F	-2.21615200	-3.02487800	0.50051300	H	2.49789300	-3.87121700	-3.15577000
F	-1.03055100	-4.27316200	2.01359700	C	0.16511900	-2.46811600	-1.80572200
F	-2.13560200	-2.37678600	2.68315000	H	-0.47240800	-2.46691900	-0.91315000
B	-0.99104000	2.55008600	-2.33456100	H	-0.00647800	-1.56675800	-2.40634200
F	-0.43521500	3.31266000	-3.32555100	H	-0.05326300	-3.36012400	-2.40789900
F	-0.27520800	1.33390100	-2.17532400	F-TEDA-BF₄			
F	-2.32749600	2.22648200	-2.62501300	Num. Imaginary Frequencies: 0			
F	-0.95619300	3.22355600	-1.09688600	H	1.25282300	-0.84099000	2.82613600
C	2.52010000	-0.87413900	2.59636500	C	1.27078700	-0.80348700	1.73424100
C	2.01284300	0.09269300	1.72539300	C	1.21150300	0.62505600	1.17747400
C	0.89580300	0.84712200	2.11369200	H	2.13246300	-1.34992500	1.33888500
C	0.20732300	0.53007100	3.28631400	N	0.04979400	-1.52720700	1.26015400
C	0.67234200	-0.49980200	4.09633200				
C	1.83898800	-1.18354900	3.76986100				

H	2.07624400	0.83910000	0.54595200
H	1.15437400	1.36510300	1.97948500
N	-0.03302000	0.77441000	0.34287900
C	-1.21675600	-0.89164300	1.73815600
C	0.05342700	-1.65922900	-0.22420700
C	-1.22380700	0.55819200	1.24090300
C	-0.08775300	2.11442600	-0.34210200
C	-0.02058000	-0.24270200	-0.79098800
H	-1.21502600	-0.97060100	2.82788500
H	-2.03977400	-1.46891000	1.30781700
H	-0.82756500	-2.24422700	-0.49338100
H	0.98691400	-2.15649600	-0.49381700
H	-2.13580500	0.77657900	0.68019800
H	-1.13088900	1.26537300	2.06890000
Cl	-0.12056900	3.45809100	0.79935300
H	0.81144900	2.18202600	-0.96150800
H	-1.00375400	2.11698000	-0.94100100
H	-0.94645000	-0.09000100	-1.35220600
H	0.86602200	-0.01568000	-1.39070400
F	-4.06515600	0.03625500	0.33046100
F	-2.83448700	-1.50920100	-0.79457900
F	-2.83415900	0.67298200	-1.47637200
F	-4.70532300	-0.61816000	-1.77160700
B	-3.64650000	-0.36036500	-0.94170400
F	0.09448700	-2.79415300	1.79139300
F	2.95801900	-1.48958100	-0.77674100
F	4.75135300	-0.46224700	-1.76613900
F	4.06277000	0.16227100	0.32802200
F	2.78205500	0.67830100	-1.48201700
B	3.67535700	-0.28327100	-0.93740600

H-TEDA-BF₄

Num. Imaginary Frequencies: 0

H	1.23223900	0.41843900	2.79179400
C	1.36713600	0.03854100	1.77548500
C	1.15187900	1.11447700	0.70816500
H	2.36081300	-0.40521700	1.66909200
N	0.34934100	-1.04830100	1.57042400
H	1.91273100	1.05627500	-0.07486600
H	1.14255700	2.11625300	1.14621600
N	-0.18397400	0.87942700	0.05450900
C	-1.03158700	-0.55078800	1.88431200
C	0.39867800	-1.53513800	0.15029700

C	-1.23754600	0.75989800	1.13192900
C	-0.54281800	1.95124800	-0.93247600
C	-0.09357800	-0.40734700	-0.75014900
H	-1.10846500	-0.41292200	2.96560900
H	-1.74175000	-1.31282800	1.55027500
H	-0.26207600	-2.40161800	0.07353400
H	1.43892400	-1.80636500	-0.05292500
H	-2.22277700	0.77902600	0.66004000
H	-1.12451000	1.63389000	1.77891500
Cl	-0.74724300	3.53326100	-0.17338600
H	0.26761100	2.01168600	-1.66347300
H	-1.48547200	1.64156800	-1.39427500
H	-1.09198900	-0.59687700	-1.14981800
H	0.63035300	-0.22846400	-1.54998000
F	-3.94945400	-0.54168400	0.77680600
F	-2.61737500	-2.01645300	-0.33239800
F	-3.09253600	0.01817200	-1.25915700
F	-4.72770200	-1.57970100	-1.11396700
B	-3.63074800	-1.04516800	-0.48740100
F	3.46847200	-1.73882200	0.21953100
F	5.06121800	-0.90455300	-1.20235400
F	4.06072100	0.45493400	0.34640800
F	2.86592000	-0.29504200	-1.44380200
B	3.89616200	-0.62303300	-0.53158100
H	0.57394300	-1.83215500	2.19282000

P

Num. Imaginary Frequencies: 0

C	1.51501400	0.94069300	0.05104200
C	0.94790700	-0.29341600	-0.28807300
C	1.68277800	-1.47010400	-0.28052900
C	3.03021200	-1.38693600	0.07354300
C	3.61624000	-0.16528100	0.39818100
C	2.85601700	1.00738200	0.39178800
H	1.21773200	-2.41709500	-0.54079300
H	3.63294700	-2.29368800	0.08581000
H	4.67202500	-0.12368000	0.65959400
H	3.31042300	1.96117100	0.65910100
N	-0.40339700	-0.11589200	-0.62051700
C	-0.73909500	1.31786600	-0.64093300
H	-0.83055100	1.64066200	-1.68788800
C	0.45447200	2.01494600	0.03434900
H	0.20369400	2.32817200	1.06077100

H	0.76098800	2.91660300	-0.50863900
C	-2.10718800	1.35357700	0.04863300
H	-2.82129200	2.01211500	-0.46067600
H	-2.02969200	1.68587500	1.10077100
N	-2.53532400	-0.03384600	-0.01579300
C	-1.46781500	-0.88755800	-0.17316500
O	-1.45375900	-2.09175400	0.01946300
C	-3.74439100	-0.46201400	0.63723500
H	-3.81268600	-1.55078800	0.55894400
H	-4.62103800	-0.01066100	0.15643300
H	-3.74633100	-0.18144100	1.70260700

HNTf₂

Num. Imaginary Frequencies: 0

N	-0.01098000	-0.78623900	0.71188600
C	1.91774600	0.93806400	-0.14959900
C	-2.12715900	0.78342500	0.17092700
O	1.74773200	-1.56820200	-1.02318700
O	2.33811200	-1.17378400	1.42213500
O	-2.28368800	-1.86074000	0.33414100
O	-1.01529100	-0.84525600	-1.63025800
S	1.60763900	-0.84941700	0.21792000
S	-1.40356700	-0.87090200	-0.24198200
F	1.23906000	1.27348500	-1.22498300
F	3.20970300	1.07705600	-0.35824200
F	1.53833500	1.66583900	0.87829600
F	-3.26070200	0.89925900	-0.48646000
F	-1.28543700	1.72780100	-0.19378000
F	-2.34019500	0.83964600	1.46979900
H	-0.13360500	-1.06406900	1.68950700

LAuF

Num. Imaginary Frequencies: 0

P	-1.51879900	-0.00020500	-0.00017100
Au	0.76041900	0.00005200	-0.00038900
F	2.77190300	-0.00056600	0.00148700
C	-2.25663800	1.60605600	-0.43912900
H	-3.35202600	1.53970300	-0.42296300
H	-1.92693600	2.36795200	0.27605300
H	-1.92433600	1.90055100	-1.44085900
C	-2.25819400	-1.18369900	-1.17007600
H	-3.35362300	-1.13516200	-1.12107500

H	-1.92834000	-0.94750600	-2.18791800
H	-1.92683600	-2.19830700	-0.92248000
C	-2.25608800	-0.42184700	1.61112800
H	-1.92294500	0.29872400	2.36638900
H	-3.35170200	-0.40308900	1.54726700
H	-1.92593400	-1.42188200	1.91394800

H₂O

Num. Imaginary Frequencies: 0

O	0.00000000	0.00000000	0.11945400
H	0.00000000	0.75835600	-0.47781600
H	0.00000000	-0.75835600	-0.47781600

I'

Num. Imaginary Frequencies: 0

C	5.46577200	-2.03659400	-0.88716200
C	4.81143400	-1.41830100	0.17491900
C	4.08856000	-0.24183200	-0.04513100
C	4.05869200	0.31728200	-1.32934800
C	4.72875100	-0.30146800	-2.37536300
C	5.42853300	-1.48887100	-2.16554300
H	6.02333600	-2.95360200	-0.70229100
H	4.86948100	-1.84054900	1.17690500
H	3.48786300	1.23166100	-1.49335300
H	4.69402000	0.14531300	-3.36775000
H	5.94569700	-1.97718800	-2.98912300
C	3.08587200	0.00316200	2.26537300
O	3.18323700	0.77099100	3.21170700
C	1.96062500	-2.04243600	1.35319400
H	2.65102300	-2.72445900	0.82869100
H	1.21137700	-2.67042300	1.85753800
C	2.47563200	-1.80258700	3.75326000
H	1.45107300	-1.65189000	4.12329500
H	2.70370400	-2.87501600	3.76596700
H	3.16486700	-1.28165500	4.42002800
N	2.63662000	-1.29119400	2.40302800
C	1.26527700	-1.16236800	0.35396400
H	0.79769100	-0.25937600	0.75598900
C	1.30279900	-1.37143500	-0.99521100
H	0.95142400	-0.59619800	-1.67881100
H	1.88473900	-2.19491200	-1.41345200
Au	-0.82966100	-2.08802100	-0.43577300

P	-3.12593000	-2.56912600	-0.49989300	C	3.57764400	0.28813600	2.14091700
H	3.26639300	1.42590000	0.85242600	O	4.71143300	0.38653500	2.55946300
N	3.38220200	0.42032300	0.96953200	C	1.24431200	-0.28521800	2.04312500
N	-0.19643200	2.11559200	0.69905900	H	0.65097200	0.63552000	2.14737000
C	0.03047600	4.13953900	-1.14831500	H	0.65719800	-1.11180900	2.46416300
C	-2.78402300	2.54730000	1.21871400	C	2.50266300	-0.44547300	4.21086600
O	0.75292100	1.67078700	-1.67036300	H	2.20953900	-1.48535900	4.40122100
O	2.03297500	2.97037400	0.05490500	H	1.80512300	0.22118400	4.73357600
O	-1.63167100	0.22891200	1.50733800	H	3.51410400	-0.27978100	4.58866800
O	-2.04668800	1.06000700	-0.82222800	N	2.49046400	-0.17697300	2.78972000
S	0.75081700	2.56364300	-0.51540400	C	1.59246300	-0.55935700	0.59317700
S	-1.58544100	1.32687400	0.54089900	H	1.18411800	0.11573200	-0.15746700
F	-1.12953500	3.90012100	-1.73807100	C	1.91665300	-1.86897200	0.16549500
F	0.87019600	4.65991400	-2.02894400	H	2.37498600	-1.94848800	-0.82586800
F	-0.14961500	4.99195100	-0.15489300	H	2.35851300	-2.53406400	0.91541100
F	-3.98374800	1.97976900	1.22036300	N	3.17632900	0.63945700	0.78732700
F	-2.81159300	3.62971100	0.45886900	C	4.10527800	0.55105300	-0.28172200
F	-2.45563500	2.88012700	2.45239800	C	5.04802700	-0.47536400	-0.32912100
C	-3.99264400	-2.06330700	1.01898200	C	3.97401700	1.44718300	-1.34216200
H	-5.07187100	-2.22449700	0.89870600	C	5.88321600	-0.57634300	-1.43679300
H	-3.62834900	-2.64999000	1.86945000	H	5.13774500	-1.17787800	0.49620100
H	-3.79116400	-1.00394800	1.21613500	C	4.81143200	1.33192800	-2.44440000
C	-3.92759200	-1.62175800	-1.83136900	H	3.21050000	2.22474200	-1.29704100
H	-3.53481900	-1.94371700	-2.80227100	C	5.77133700	0.32377900	-2.49285800
H	-5.01360500	-1.77877100	-1.80598000	H	6.62728600	-1.36968600	-1.47269900
H	-3.69910000	-0.55774700	-1.69240200	H	4.71182400	2.03555800	-3.26832600
C	-3.60269400	-4.30495100	-0.77146700	H	6.43008500	0.23843700	-3.35463400
H	-3.20912200	-4.92812700	0.03889500	H	2.64515800	1.52024900	0.76323100
H	-4.69630800	-4.39284500	-0.79718800	C	-3.65387600	-2.72077000	0.43228900
H	-3.18860300	-4.65988700	-1.72151900	H	-3.46300400	-3.49721100	1.18125900

TS1'

Num. Imaginary Frequencies: 1

P	-2.40391000	-2.81059800	-0.89173500	C	-3.66217000	1.66617700	0.86484300
Au	-0.16493600	-2.41876500	-0.25414800	O	0.86614900	2.53705400	0.19516200
C	-2.93763900	-1.55062900	-2.09830800	O	0.29969200	1.75751500	-2.11658100
H	-3.99928600	-1.68488000	-2.34507400	O	-1.98063900	-0.19627600	1.61341600
H	-2.77707900	-0.55045800	-1.67750300	O	-1.39836900	2.19225500	2.10993500
H	-2.33745900	-1.64157700	-3.01090400	S	-0.15381100	2.23220700	-0.81601500
C	-2.73584200	-4.40104300	-1.72311800	S	-1.90736900	1.19632000	1.17271900
H	-3.78471600	-4.44949500	-2.04354600	F	-1.44018600	4.37494100	-0.04717200
H	-2.08556000	-4.50187100	-2.59938000	F	-0.06451900	4.67458800	-1.68404000
H	-2.53000100	-5.23003000	-1.03680500	F	-1.94968300	3.67759900	-2.02603600

F	-4.29222200	1.72553900	2.02662900
F	-3.71923700	2.84699500	0.27187000
F	-4.25023700	0.75857900	0.09784300

2'

Num. Imaginary Frequencies: 0

P	-3.31378400	-2.36256900	-0.62042100
Au	-0.97617400	-2.45114300	-0.19556400
C	-3.72797000	-1.04281700	-1.81297200
H	-4.81534100	-0.96777900	-1.94562500
H	-3.33805600	-0.08880900	-1.43853300
H	-3.25781900	-1.25529400	-2.77976800
C	-4.13533900	-3.84619900	-1.30162500
H	-5.20204000	-3.65004100	-1.47249600
H	-3.66432900	-4.12856000	-2.24997700
H	-4.03099900	-4.68100600	-0.59947700
C	3.31210900	-0.71163300	2.07876400
O	4.47554500	-0.77666400	2.38046400
C	0.95428300	-0.63594800	2.06456400
H	0.56576900	0.37808100	2.23954200
H	0.20244100	-1.35850700	2.40457500
C	2.21437900	-0.95549500	4.24046800
H	1.65143600	-1.84542800	4.54392600
H	1.76032200	-0.06943500	4.70055800
H	3.25160800	-1.04669200	4.57169600
N	2.19614900	-0.82995700	2.79852500
C	1.33612700	-0.89235200	0.60497600
H	0.88618800	-0.15938300	-0.07217200
C	1.11589800	-2.29136000	0.13655800
H	1.60878800	-2.47088100	-0.82781500
H	1.48918000	-3.02621000	0.86593100
N	2.85084300	-0.42734900	0.66045400
C	3.72310700	-0.89832900	-0.40720400
C	4.36416100	-2.12743300	-0.30537200
C	3.82750300	-0.10944600	-1.54584700
C	5.14495600	-2.56194200	-1.37019900
H	4.26548100	-2.73572000	0.59020300
C	4.60911600	-0.55915000	-2.60504800
H	3.29354000	0.83889400	-1.61374700
C	5.26899500	-1.78092900	-2.51643700
H	5.65765800	-3.51874700	-1.30104100
H	4.69759000	0.05060900	-3.50118600
H	5.88222700	-2.12780200	-3.34554700

H	2.77360300	0.60835200	0.58281600
C	-4.31485000	-1.93935200	0.84681800
H	-4.20903200	-2.71919500	1.60949100
H	-5.37378700	-1.83836600	0.57444000
H	-3.94752500	-0.99161500	1.25681600
N	-0.58235600	1.95205400	-0.65637700
C	0.74933400	4.37171400	-0.70046400
C	-2.82386300	2.93379500	0.38572100
O	1.80675800	2.19869400	0.31008000
O	1.36196500	2.27337800	-2.15319900
O	-1.95654600	0.50940600	0.87893100
O	-0.72650300	2.44216900	1.90303100
S	0.89777900	2.53524900	-0.79805900
S	-1.37992100	1.84559800	0.74181300
F	0.29702600	4.73472500	0.48588300
F	1.94522900	4.90069200	-0.89892300
F	-0.08136900	4.79197200	-1.63846400
F	-3.62410200	2.91065000	1.43966200
F	-2.41744000	4.17372100	0.16667600
F	-3.48134500	2.49168100	-0.67324700

TS2'

Num. Imaginary Frequencies: 1

C	-1.98795500	4.82509900	-1.38497500
C	-1.63455500	3.85340700	-0.45673000
C	-1.99307900	2.52368500	-0.67454300
C	-2.73069500	2.17190700	-1.79913900
C	-3.08556600	3.14944000	-2.72495800
C	-2.70951000	4.47315000	-2.52370700
H	-1.70519000	5.86203100	-1.21398200
H	-1.08605600	4.12432200	0.44523600
H	-3.04892600	1.14058600	-1.94196700
H	-3.66436400	2.87186300	-3.60362700
H	-2.98731000	5.23524800	-3.24927600
C	-2.40646100	1.68999300	1.53554900
O	-3.60956100	1.83046300	1.57663200
C	-0.14313300	1.67320100	2.16352500
H	0.30152600	2.67343400	2.30772100
H	0.44269100	0.95696300	2.75670300
C	-1.94659500	1.73684600	3.94222300
H	-1.59415900	0.85439800	4.49317400
H	-1.54502400	2.63778000	4.42486300
H	-3.03901500	1.76954000	3.97316900

N	-1.53197300	1.66562200	2.56468000	C	-2.56252000	2.29464400	-1.84470100
C	-0.19170000	1.26632000	0.69303600	C	-2.83735600	3.25229800	-2.81749300
Au	2.68093000	0.83459300	0.08667800	C	-2.50894500	4.58567500	-2.59722100
P	4.61947800	-0.55466800	0.24769000	H	-1.66256600	6.00733000	-1.21310800
H	-1.96143800	0.16581600	-0.26253100	H	-1.17615900	4.29695600	0.52040000
N	-1.65725900	1.50765100	0.30110200	H	-2.84535700	1.25606600	-2.00948600
N	-2.04946500	-0.94238900	-0.63531900	H	-3.31599900	2.95212900	-3.74769200
C	-2.86104800	-2.17655900	1.59625700	H	-2.72290300	5.33379200	-3.35833500
C	0.12206700	-2.58539200	-1.05644600	C	-2.37903500	1.87246000	1.57536000
O	-3.57748300	-3.01657900	-0.81348300	O	-3.55717600	2.16645400	1.65639200
O	-4.47709900	-0.79480500	0.01944100	C	-0.13383100	1.58978600	2.18091900
O	-0.27305500	-0.23734400	-2.20979700	H	0.38836800	2.54491300	2.37529700
O	-1.74304600	-2.18711300	-2.88468100	H	0.40662900	0.79542500	2.71552600
S	-3.40788300	-1.75884500	-0.11990900	C	-1.90328500	1.74437500	3.98453200
S	-1.05269800	-1.41213900	-1.87858900	H	-1.64123300	0.81954000	4.51698500
F	-1.83879300	-3.00991200	1.54492700	H	-1.40655300	2.58824200	4.48462600
F	-3.87272100	-2.73815200	2.22405000	H	-2.98619600	1.89100500	4.02964000
F	-2.49532000	-1.07033700	2.22388700	N	-1.51423800	1.66143400	2.60317800
F	1.09661200	-2.83376100	-1.91136000	C	-0.23921400	1.28388000	0.68760200
F	-0.50714400	-3.70113500	-0.74811700	Au	2.63942200	0.79394300	0.08429500
F	0.62523700	-2.04224300	0.03931800	P	4.60315100	-0.56500400	0.25756600
C	4.27803600	-2.24147500	-0.37085500	H	-2.04214300	0.01263900	-0.38008100
H	3.90844200	-2.18559700	-1.40160300	N	-1.67190500	1.67701900	0.35389200
H	5.18339500	-2.86143400	-0.33901900	N	-2.11430700	-0.99638200	-0.69641400
H	3.49856100	-2.70491400	0.24546000	C	-2.83326000	-2.22301600	1.58250200
C	6.07563800	-0.02674500	-0.72170300	C	0.09177900	-2.61640300	-1.03851600
H	6.88422200	-0.76401300	-0.63112900	O	-3.60392800	-3.07076400	-0.82068500
H	5.79730400	0.07692900	-1.77649600	O	-4.51712000	-0.85867400	0.05871600
H	6.42976800	0.94466400	-0.35852500	O	-0.31315700	-0.28226300	-2.24651900
C	5.29905200	-0.84268000	1.91949500	O	-1.75245700	-2.26899400	-2.91246400
H	6.14283400	-1.54385400	1.87658900	S	-3.45430900	-1.82121200	-0.11384800
H	5.64098100	0.10573100	2.34904000	S	-1.07091200	-1.47039400	-1.92326300
H	4.51826200	-1.25641800	2.56772900	F	-1.77192900	-3.00051300	1.48804600
C	0.87198700	1.89167900	-0.16826500	F	-3.79451200	-2.83932600	2.23470800
H	0.97016300	2.96561000	0.04189500	F	-2.50887000	-1.09944400	2.19365600
H	0.61784600	1.77858500	-1.23006200	F	1.12776900	-2.80859000	-1.82971200
H	-0.11773200	0.17107600	0.65460200	F	-0.51900700	-3.75701300	-0.79874300
				F	0.49032100	-2.07270900	0.09636100
				C	4.35199100	-2.25917200	-0.38348000
				H	4.08595000	-2.21172100	-1.44559900
				H	5.26446300	-2.85863100	-0.26616400
				H	3.53005800	-2.74208500	0.15785700
				C	6.06349100	0.02421400	-0.66972400
				H	6.89310900	-0.68868200	-0.57498000
3'							
Num. Imaginary Frequencies: 0							
C	-1.91193300	4.96366700	-1.39618200				
C	-1.63612700	4.00824800	-0.42563200				
C	-1.95242700	2.66751400	-0.65149000				

H	5.80474000	0.13873100	-1.72848200
H	6.37913400	0.99953200	-0.28238900
C	5.24992900	-0.84414900	1.94408400
H	6.12503600	-1.50654400	1.91593900
H	5.53657300	0.11265000	2.39486500
H	4.47095100	-1.30100800	2.56500000
C	0.85004600	1.88338600	-0.16058100
H	0.97503000	2.95371800	0.05960300
H	0.59081800	1.78858900	-1.22427200
H	-0.22575100	0.19001500	0.57903100

H	-3.96893500	0.77236600	2.35610000
H	-5.39862700	-0.27530800	2.11201600
H	-3.81015100	-0.99089100	2.51781000
C	-4.95760000	0.94901600	-0.58970100
H	-6.00927600	0.79057600	-0.31696000
H	-4.64502300	1.94620800	-0.25949500
H	-4.85547700	0.89732500	-1.67960300
C	-4.66796700	-1.89314600	-0.31857700
H	-5.73416500	-1.90244200	-0.05620100
H	-4.56126900	-2.02458900	-1.40135100
H	-4.16536700	-2.72832000	0.18241800

4'

Num. Imaginary Frequencies: 0

C	5.54205100	-1.97604700	-0.23687800
C	4.86126200	-0.76513700	-0.21055600
C	3.50776200	-0.72176700	0.16301300
C	2.87395300	-1.92856900	0.50230400
C	3.57107400	-3.13069600	0.47049700
C	4.91104000	-3.16955200	0.10162800
H	6.59134500	-1.97904100	-0.53005900
H	5.36664500	0.15617700	-0.47523800
H	1.82646000	-1.94136500	0.79337400
H	3.04892300	-4.04815400	0.73908600
H	5.45354800	-4.11272300	0.07650300
C	3.26456500	1.74831300	-0.06897000
O	4.38942300	2.05788400	-0.43804000
C	1.12649900	2.00242100	0.81354900
H	1.18825000	2.21305900	1.89645500
H	0.15737900	2.36634200	0.44556200
C	2.44901300	4.04615200	0.20458100
H	1.62624900	4.59416400	-0.27141100
H	2.52551600	4.37529800	1.25389500
H	3.38332900	4.28569500	-0.31068100
N	2.22393100	2.62882600	0.11182300
C	1.32561500	0.51912200	0.49226500
H	1.11553000	-0.08840400	1.38195600
C	0.50503700	0.06428800	-0.70578700
H	0.87439500	-0.90393600	-1.07366400
H	0.65709600	0.78746500	-1.52440600
Au	-1.55004500	-0.11357600	-0.29234700
P	-3.89270800	-0.31724500	0.18865200
N	2.78650700	0.47937800	0.23520000
C	-4.31408100	-0.19087000	1.96340900

5'

Num. Imaginary Frequencies: 0

C	4.65639600	-0.70435600	-2.34830100
C	4.40886400	0.46154600	-1.63224400
C	3.09407500	0.87105800	-1.39079200
C	2.03652300	0.08786900	-1.86423800
C	2.29150400	-1.08243100	-2.57247900
C	3.60138100	-1.48220100	-2.82144200
H	5.68550800	-1.00886600	-2.53383300
H	5.22722500	1.07167300	-1.25873400
H	1.00738800	0.39908800	-1.68722300
H	1.45281100	-1.68413400	-2.91833100
H	3.79949200	-2.39723600	-3.37803500
N	2.84810400	2.05482700	-0.66689400
C	3.39163200	3.26739400	-1.07678400
O	4.30912900	3.41932800	-1.87059700
C	1.83614700	3.73009200	0.58949000
H	0.87147000	4.25045900	0.62736800
H	2.32261800	3.83170200	1.57851100
C	3.21483000	5.60363000	-0.35393300
H	3.94626200	5.74854400	-1.15431800
H	3.70802600	5.77646400	0.61710400
H	2.40846200	6.33923100	-0.46637400
N	2.69424700	4.26599300	-0.44582400
C	1.68460000	2.24681800	0.21654800
H	0.75138500	2.12611500	-0.36133000
C	1.66914700	1.33225600	1.43167200
H	2.55138000	1.57468300	2.04787100
H	0.78882600	1.61743900	2.03188400
Au	1.66392000	-0.75923600	1.12578100
P	1.70820800	-3.15949600	1.03209000

H	-3.23170900	-2.45018000	1.15334000
C	-3.73645400	-1.48986000	1.28698300
C	-4.38644100	-1.04324900	-0.02892700
H	-4.42414500	-1.51868100	2.13665000
N	-2.67975100	-0.48688400	1.62625600
H	-5.47704500	-1.11596500	0.01975000
H	-4.00542300	-1.63222100	-0.87069700
N	-4.01188600	0.39859800	-0.27796500
C	-1.74697000	-0.26846400	0.48138500
C	-3.28284300	0.80328000	2.06622500
C	-2.53573800	0.43893000	-0.62210600
C	-4.82811500	1.06162800	-1.35879600
C	-4.29103000	1.18982800	0.98585600
H	-1.36544500	-1.24808400	0.17843200
H	-0.92475900	0.35444600	0.85326400
H	-2.47111600	1.53134100	2.15224000
H	-3.75800100	0.62756500	3.03443600
H	-2.26415600	1.49276500	-0.71577200
H	-2.41009300	-0.09324400	-1.57052300
Cl	-4.80491200	0.17554400	-2.87502400
H	-5.85689300	1.12872000	-0.99434400
H	-4.39216700	2.05669700	-1.49373800
H	-4.20539800	2.25769300	0.76731400
H	-5.31990600	0.95267200	1.27469400
F	-1.94839800	-0.99444600	2.67412400
B	-2.15901300	3.81174000	0.61747100
F	-3.10163300	3.86549700	1.64701300
F	-2.83711200	3.49984900	-0.58526500
F	-1.46257700	4.98732900	0.49451800
F	-1.27293400	2.73951400	0.89555600
B	-1.68763600	-3.06648500	-1.63226100
F	-0.54473100	-2.31912000	-1.28765500
F	-2.33154500	-3.44887700	-0.43089700
F	-1.33500600	-4.17111700	-2.36429600
F	-2.56683300	-2.22992400	-2.33748700
C	2.01980700	-4.04022100	-0.53921400
H	2.91948400	-3.63722200	-1.01901300
H	1.16500500	-3.89227500	-1.20861000
H	2.15587600	-5.11253900	-0.34413900
C	3.01391000	-3.81668600	2.13660000
H	2.99409500	-4.91451300	2.15683800
H	2.86236200	-3.43299400	3.15258300
H	3.99584400	-3.47949700	1.78439500
C	0.19683500	-3.96773100	1.66727700

H	-0.02620900	-3.59008600	2.67236800
H	0.33756700	-5.05602800	1.71700700
H	-0.64414300	-3.74741500	0.99886100

TS3'

Num. Imaginary Frequencies: 1

C	4.61050300	1.16820600	1.40601200
C	3.74354100	2.00513700	0.70376800
C	2.44523600	2.22477800	1.17397300
C	2.01355600	1.58804000	2.33845600
C	2.88295600	0.75984000	3.04132600
C	4.18299900	0.55561000	2.58053900
H	5.62481400	1.01218800	1.04140400
H	4.06909700	2.52447600	-0.19684900
H	0.99752100	1.76070200	2.69317700
H	2.54662500	0.27483400	3.95595900
H	4.86484100	-0.07990200	3.14426300
N	1.57237700	3.06662800	0.43673200
C	0.94505400	4.14427400	1.06951500
O	1.31895900	4.68749600	2.09808800
C	-0.17732700	3.72367600	-0.92112700
H	-1.20631700	3.46890900	-1.20428400
H	0.29418700	4.29193500	-1.74522400
C	-0.91986700	5.66782600	0.51353300
H	-0.69973900	6.05986500	1.51119600
H	-0.67438700	6.43910100	-0.23363400
H	-1.98930800	5.43185300	0.44286000
N	-0.14632900	4.47265500	0.31487200
C	0.65267900	2.49151600	-0.56247500
H	-0.02246800	1.77905500	-0.04431500
C	1.34363600	1.80050100	-1.70678500
H	2.11435600	2.45015900	-2.14865000
H	0.60645200	1.53960400	-2.47929000
Au	2.24235100	-0.01451400	-1.07537500
P	3.23250000	-2.16170300	-0.51576200
H	-1.15060800	-2.94215000	-0.78507600
C	-1.89669500	-2.29979200	-1.26047600
C	-3.30987100	-2.61861700	-0.73540900
H	-1.82388800	-2.39082400	-2.34820500
N	-1.63182700	-0.90634900	-0.91204800
H	-3.92650700	-3.12004400	-1.48789000
H	-3.25662700	-3.22197000	0.17461400
N	-3.98765100	-1.31193000	-0.37580100

C	-1.78753000	-0.61022700	0.51338000
C	-2.39016700	0.01997600	-1.74429300
C	-3.28614400	-0.70845100	0.82666300
C	-5.45247200	-1.47607500	-0.10224500
C	-3.87218100	-0.35761400	-1.55544800
H	-1.19050600	-1.33293300	1.06906800
H	-1.43450800	0.41178200	0.67956800
H	-2.19576300	1.04102400	-1.40476900
H	-2.07305600	-0.09954300	-2.78444400
H	-3.74390100	0.27265300	0.98899100
H	-3.46278100	-1.37609200	1.67426400
Cl	-5.77619400	-2.65624400	1.16859900
H	-5.93179900	-1.80764700	-1.02705600
H	-5.83122400	-0.49653300	0.20399300
H	-4.47059600	0.52843500	-1.32473800
H	-4.28489600	-0.88306100	-2.42346300
F	-0.00959700	-0.61195300	-1.20178400
B	-3.74243200	2.82728300	-0.12308400
F	-3.57608700	2.81160800	-1.51348500
F	-4.81179000	1.95935600	0.20668100
F	-3.99568600	4.10115600	0.33316500
F	-2.57146800	2.31045800	0.46468900
B	-0.49261200	-3.85609300	1.42709500
F	-1.74884100	-3.38145000	1.85256600
F	0.27451000	-2.73440500	1.01885100
F	0.15308000	-4.52855700	2.43551700
F	-0.67957400	-4.66721800	0.30137800
C	3.42110000	-2.68330200	1.22256600
H	3.95643200	-3.64134800	1.26498900
H	3.98290300	-1.92432100	1.77803100
H	2.42764600	-2.79873600	1.66851500
C	4.93437700	-2.26936000	-1.17924300
H	5.36392300	-3.26391200	-1.00097900
H	4.92511900	-2.06666600	-2.25665400
H	5.56066100	-1.51310100	-0.68974000
C	2.35803500	-3.56601300	-1.29027500
H	2.20118300	-3.36725900	-2.35707400
H	2.94210900	-4.48897600	-1.17610400
H	1.38760800	-3.69246200	-0.79426700

6'

Num. Imaginary Frequencies: 0

C	0.93973700	-0.45913800	2.03292700
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C	0.07889400	-0.94721500	0.97474900
C	-0.76404600	-2.11089500	1.25612900
C	-0.70039800	-2.70178400	2.53151000
C	0.18303900	-2.21212000	3.46998200
C	1.01485400	-1.09223400	3.23754200
H	1.51318900	0.44653300	1.83227600
H	-0.53462600	-0.14487700	0.54621800
H	-1.32656400	-3.55606300	2.75649900
H	0.24278000	-2.71985300	4.43167100
H	1.67501000	-0.73045400	4.02204400
N	-1.59949100	-2.58461400	0.29656700
C	-2.80936500	-3.30011700	0.55111200
O	-3.24398800	-3.59453400	1.64538600
C	-2.72957700	-2.81599700	-1.72217000
H	-2.69959100	-3.38442000	-2.65876600
H	-3.25668200	-1.86329300	-1.88328900
C	-4.74169500	-3.97332000	-0.76488700
H	-5.01787900	-4.52522500	0.13743300
H	-5.38374300	-3.08653600	-0.85746700
H	-4.87621000	-4.61871600	-1.63978200
N	-3.35727000	-3.57670500	-0.66120200
C	-1.33154700	-2.58560400	-1.15774800
H	-0.72921600	-3.49382900	-1.34168600
C	-0.60292200	-1.39703100	-1.69059400
H	-1.16625100	-0.46669300	-1.56122400
H	-0.32441900	-1.54744200	-2.73943100
Au	1.28358900	-1.30414100	-0.76020400
P	3.65071100	-1.35007000	0.00555000
H	0.74510700	3.16531900	-1.75466300
C	-0.33001700	2.96066200	-1.78507300
C	-0.78516700	2.40417200	-0.42742900
H	-0.51933900	2.21581700	-2.56923600
N	-1.04411900	4.19655900	-2.09781000
H	-1.50263100	1.58186900	-0.51449900
H	0.06845100	2.10806900	0.18888600
N	-1.52992900	3.49991400	0.30631300
C	-0.60763300	5.23945400	-1.17272000
C	-2.47532300	3.97070400	-1.92430400
C	-0.69243200	4.75645200	0.29015300
C	-1.91136000	3.07024100	1.68280700
C	-2.82373000	3.78052600	-0.43821800
H	0.42896000	5.51351400	-1.39941800
H	-1.23512000	6.12570600	-1.32903800
H	-3.03702100	4.82122600	-2.32886200

H	-2.75709100	3.07593600	-2.49287500
H	-1.17600800	5.47665500	0.95999800
H	0.29009900	4.48416800	0.68609000
Cl	-0.50161200	2.78234200	2.72011800
H	-2.47369500	2.13553500	1.59459700
H	-2.51775500	3.86453600	2.12726400
H	-3.24302100	4.68512600	0.01840300
H	-3.50085500	2.93880400	-0.25448300
F	2.19379400	-1.76247300	-2.53032300
B	-3.74831900	0.20184400	0.05375400
F	-4.57099100	1.24648700	0.47113500
F	-3.25032100	0.49169400	-1.23237700
F	-4.42721200	-1.00431200	0.04487800
F	-2.64722300	0.12126200	0.93653800
B	2.78012600	2.49550600	0.23402700
F	2.11702800	1.49542200	-0.51802600
F	2.59213100	2.22095000	1.59491000
F	4.13250200	2.47926800	-0.06803600
F	2.21311700	3.73417300	-0.07942200
C	4.21762500	-3.08474200	-0.02943900
H	5.30130600	-3.14379800	0.13575400
H	3.70186300	-3.66622600	0.74351900
H	3.97662600	-3.50882200	-1.01140200
C	4.25679700	-0.68931400	1.59343700
H	5.34941200	-0.79143800	1.63384700
H	3.98924100	0.37130200	1.67551000
H	3.81531500	-1.24000700	2.43154200
C	4.66591500	-0.51081900	-1.24898300
H	4.55979900	0.57155900	-1.12022200
H	5.71918600	-0.79866200	-1.13745000
H	4.28779100	-0.80701500	-2.23217900

7'

Num. Imaginary Frequencies: 0

C	-1.84231300	0.52471200	2.06025100
C	-1.12248200	-0.39705200	1.21839400
C	-0.60740600	-1.61077900	1.83027100
C	-0.84684200	-1.84717400	3.19239700
C	-1.59558000	-0.94544600	3.92626900
C	-2.09274700	0.25324100	3.37714400
H	-2.12381600	1.47637700	1.61279800
H	-0.31483500	0.13584700	0.65130900
H	-0.45988300	-2.74736900	3.65528900

H	-1.80158700	-1.17541400	4.97071900
H	-2.64072800	0.95547300	4.00070000
N	0.16221800	-2.46962900	1.09109800
C	1.22586500	-3.24847200	1.62560100
O	1.59242200	-3.24281100	2.78608400
C	1.24881100	-3.49711400	-0.69428900
H	1.10922600	-4.33908700	-1.38214200
H	1.93665200	-2.77064700	-1.15897500
C	3.02757000	-4.62495200	0.69173500
H	3.26436700	-4.75594800	1.75092100
H	3.81387500	-4.03154700	0.20706900
H	2.96388400	-5.60843000	0.21122700
N	1.75833200	-3.94155300	0.58819000
C	-0.08418000	-2.84966500	-0.31440800
H	-0.87046200	-3.62404200	-0.28576100
C	-0.50611100	-1.73954000	-1.21664100
H	0.27022400	-0.97437200	-1.33607000
H	-0.82079500	-2.12153500	-2.19404300
Au	-2.24767700	-0.76065400	-0.57351400
P	-4.41571500	0.43538800	-0.30161800
H	2.18572100	-0.34298300	1.61226500
C	2.43515900	0.12418600	0.64865400
C	3.76078200	0.89284900	0.77007100
H	2.53523500	-0.66225200	-0.10574200
N	1.35570800	1.02830400	0.25803600
H	4.57253900	0.39128100	0.23394600
H	4.05711400	1.08273800	1.80631300
N	3.56827000	2.25221000	0.12381600
C	1.33906000	2.16871600	1.17345700
C	1.56093800	1.50635300	-1.10945800
C	2.57338000	3.05550800	0.93176500
C	4.86792000	2.95382600	-0.06206500
C	2.98712700	2.04891900	-1.26842900
H	1.32440100	1.78077200	2.20085600
H	0.43000500	2.75648900	1.01339200
H	0.80868400	2.27541900	-1.30719300
H	1.42584800	0.67906600	-1.81436100
H	2.32887400	3.94094800	0.33180500
H	3.06841700	3.37004400	1.85547000
Cl	5.73909900	3.21619400	1.45951200
H	5.48040100	2.32814200	-0.71805300
H	4.66912100	3.92736200	-0.51842500
H	3.01701400	3.02100700	-1.77288900
H	3.65531600	1.34354500	-1.77129300

F	-3.17698700	-1.27945600	-2.31077900	C	3.42133600	-4.50296200	0.80668600
B	-1.69264300	3.40998200	-0.39762000	H	3.76906600	-4.50753200	1.84310800
F	-1.55380100	2.04750600	-0.74285000	H	4.10378800	-3.90054000	0.19197600
F	-0.47516000	4.05364200	-0.62707700	H	3.39869200	-5.53138800	0.42871000
F	-2.70962700	3.97726000	-1.14855200	N	2.08920600	-3.94224100	0.77050300
F	-2.00906600	3.48611000	0.97014100	C	0.12019400	-3.02572900	-0.08772800
B	4.40015100	-1.34560500	-1.90187800	H	-0.67220700	-3.76936100	0.10002300
F	4.39344300	-1.95225100	-0.63777700	C	-0.32836800	-2.03170700	-1.10834200
F	3.06734700	-1.04189300	-2.25091800	H	0.48086700	-1.34459500	-1.38068100
F	4.97111000	-2.16782300	-2.84604200	H	-0.70464000	-2.53040700	-2.00947000
F	5.12354700	-0.13376300	-1.80674800	Au	-2.02008000	-0.94670100	-0.54337900
C	-5.77665800	-0.77952800	-0.29879900	P	-4.24652400	0.18533300	-0.34543100
H	-6.74655600	-0.28026700	-0.42127600	H	2.13447000	-0.23677400	1.63386600
H	-5.61289400	-1.47203700	-1.13199300	C	2.25320800	0.24144700	0.65239100
H	-5.77752000	-1.34630200	0.63911100	C	3.47134000	1.17008600	0.66356500
C	-4.65477400	1.39455400	-1.83061000	H	2.37032400	-0.53912900	-0.10519800
H	-4.39341200	0.74847200	-2.67485200	N	1.04287000	1.02147400	0.34397500
H	-5.69942500	1.72217700	-1.91181400	H	4.31026800	0.73339400	0.11451400
H	-3.99167500	2.26758700	-1.81466400	H	3.78866300	1.44980900	1.67241500
C	-4.82437400	1.61470800	1.02938600	N	3.08549300	2.45592600	-0.04150800
H	-5.83107500	2.01902200	0.85973000	C	1.00111900	2.19202200	1.23793700
H	-4.79847400	1.12013200	2.00726000	C	1.07060800	1.45940500	-1.06290500
H	-4.10099000	2.44007000	1.02159900	C	2.06977400	3.19819000	0.79909000

TS4'

Num. Imaginary Frequencies: 1

C	-1.73707600	0.42118500	2.09668700	H	1.17609600	1.83414700	2.26107500
C	-1.03823500	-0.51860800	1.27024400	H	0.01183300	2.65902500	1.20120300
C	-0.27491500	-1.55040700	1.93629900	H	0.24444200	2.15568200	-1.21131200
C	-0.23713100	-1.57020600	3.34169000	H	0.93258200	0.59210700	-1.71463500
C	-0.94066400	-0.63760100	4.08085400	H	1.64186100	3.98205700	0.16324300
C	-1.68137800	0.38315400	3.46822800	H	2.59442300	3.65385400	1.64379500
H	-2.24868500	1.24266800	1.60115300	Cl	5.23800800	3.71027900	1.05311200
H	-0.14788500	0.18935500	0.70580400	H	4.90358600	2.67542400	-1.04851500
H	0.33848700	-2.33771400	3.84475900	H	3.94548100	4.19338100	-0.86120500
H	-0.90958400	-0.70467300	5.16707500	H	2.32432200	3.02836800	-1.93626200
H	-2.19893800	1.13006700	4.06554300	H	3.11399100	1.41659100	-1.87096100
N	0.49152200	-2.44375700	1.21625800	F	-2.92300100	-1.50444400	-2.29090800
C	1.67225800	-3.05447900	1.71068800	B	-1.94438800	3.42246200	-0.30100100
O	2.21854900	-2.79812700	2.76991400	F	-1.87212500	2.06056200	-0.68084100
C	1.41887800	-3.72969000	-0.49526900	F	-0.71836000	4.02969600	-0.60267300
H	1.22697800	-4.67513500	-1.01567700	F	-2.98399100	4.03199100	-0.97541800
H	2.03530500	-3.08131000	-1.14084100	F	-2.15579700	3.46864900	1.08486700
				B	4.07400600	-1.17285400	-2.00780500
				F	4.13655900	-1.80232100	-0.75613600

F	2.71409200	-0.93894800	-2.30535100	H	-0.51899700	-2.21849200	-1.29526200
F	4.65735900	-1.94424100	-2.98432400	H	-2.07482400	-3.11240100	-1.27380500
F	4.72790800	0.07830700	-1.91320200	Au	-2.42671900	-0.72943900	-0.45611200
C	-4.79287000	1.31167200	0.98719900	P	-3.80308900	1.31450600	-0.97813900
H	-4.74876900	0.80650000	1.95958200	H	4.48513900	-0.60060400	1.54783900
H	-4.15876700	2.20625000	1.01779200	C	3.75131600	-0.35089700	0.77667500
H	-5.82978900	1.61656100	0.79221100	C	4.28737800	0.69925800	-0.19831100
C	-4.54964100	1.13140000	-1.87357200	H	3.45458600	-1.26677600	0.26076500
H	-4.01025500	2.08290300	-1.82032100	N	2.54365300	0.19429700	1.46539900
H	-4.17518100	0.53655000	-2.71313300	H	4.40698600	0.26847000	-1.19882700
H	-5.62478800	1.31766700	-1.99464500	H	5.23024100	1.14278000	0.13396700
C	-5.53314300	-1.11077100	-0.36552000	N	3.27680000	1.81495600	-0.30285000
H	-5.33236900	-1.78013700	-1.20890800	C	2.86301400	1.48907000	2.12470900
H	-5.50198000	-1.69161200	0.56354500	C	1.42185100	0.39162000	0.49338800
H	-6.52990500	-0.66503700	-0.47933100	C	3.14950800	2.51962800	1.02937700

8'

Num. Imaginary Frequencies: 0

C	-2.22353600	0.64978000	2.15269200	H	0.60916600	0.90194300	1.01971400
C	-1.72957600	-0.45555000	1.45189800	H	1.10183500	-0.59630100	0.15569400
C	-0.76509400	-1.25401600	2.09583600	H	2.33076500	3.23754900	0.92135700
C	-0.36143900	-0.94999000	3.40505600	H	4.08918100	3.04958300	1.20766800
C	-0.86178600	0.16214700	4.06636600	Cl	5.19897200	3.51922000	-1.20984200
C	-1.79753400	0.97174900	3.43651600	H	3.57055600	2.23361600	-2.34000900
H	-2.95320300	1.29720500	1.67679000	H	2.83539300	3.56611500	-1.36400900
H	2.23796200	-0.55479300	2.13405200	H	1.25502700	2.00430200	-0.94219300
H	0.36408800	-1.59371700	3.89436300	H	2.14258800	0.55986600	-1.55465700
H	-0.52747300	0.38212000	5.07877200	F	-3.14390900	-1.06010000	-2.37794600
H	-2.19710700	1.85439100	3.93195400	B	-0.32676900	3.49667600	0.55484700
N	-0.16597900	-2.35701300	1.45148500	F	-0.82185700	2.40461500	-0.18029900
C	1.09600600	-2.83900200	1.70786700	F	0.73246400	4.07101800	-0.18600000
O	1.98266900	-2.26632300	2.35946900	F	-1.32520600	4.42326600	0.77276900
C	0.13098000	-4.32732800	0.21574900	F	0.19244400	3.02920400	1.77138200
H	-0.26215900	-5.34076800	0.36085200	B	2.94667500	-2.10476800	-2.14523600
H	0.47755900	-4.23385300	-0.82643300	F	4.09966100	-2.45195300	-1.43477900
C	2.54851100	-4.58819200	0.84041400	F	1.87876200	-2.00238300	-1.21473800
H	3.20911700	-4.35496000	1.67994500	F	2.64269800	-3.04233400	-3.10149700
H	2.96815000	-4.15077900	-0.07968700	F	3.14470200	-0.83330500	-2.72341300
H	2.48214200	-5.67596100	0.73071600	C	-5.43662100	0.73932900	-1.55802800
N	1.23366900	-4.05431500	1.11945500	H	-5.25310000	-0.12431100	-2.20523800
C	-0.91286900	-3.23770800	0.54991600	H	-6.05279600	0.43180500	-0.70516600
H	-1.76607600	-3.66133800	1.10236900	H	-5.95622000	1.53127500	-2.11314200
C	-1.37646200	-2.51395800	-0.67647100	C	-3.02128500	2.02557300	-2.46490800

H	-2.07328900	2.48583000	-2.16559800	C	6.52036900	1.80868200	-1.43569500
H	-2.83125700	1.20104400	-3.15937900	H	6.64513100	0.82161900	-1.89400000
H	-3.67352800	2.77510100	-2.93156100	H	5.94528100	2.45365400	-2.10988700
C	-4.19961800	2.78567300	0.03504900	H	7.49475600	2.27114700	-1.22964500
H	-4.76810800	2.50221000	0.92879400	C	6.77310800	0.59540400	1.14657400
H	-3.28050300	3.30509900	0.33189100	H	6.35922300	0.44878100	2.15080800
H	-4.81643800	3.46795200	-0.56623000	H	6.90109800	-0.37798700	0.66069800

TS5'

Num. Imaginary Frequencies: 1

C	1.29175200	1.59463900	-0.70470500	C	-4.88440000	-1.47024900	-0.08588500
C	1.65349100	0.42385500	-0.02362900	H	-2.91623100	-2.30609500	0.36694900
C	0.92651900	0.07074800	1.12917000	N	-3.05186600	-0.35820100	1.13906700
C	0.07448200	1.00073500	1.73206000	H	-4.71596000	-1.92681400	-1.06756600
C	-0.18033200	2.21443400	1.10035800	H	-5.80829300	-1.86198500	0.34802500
C	0.37967300	2.48549400	-0.14588800	N	-5.06849400	0.00844800	-0.31285500
H	1.76793100	1.83786200	-1.65368900	C	-4.02015000	0.47296100	1.90499200
H	-0.40622500	0.75068500	2.67426100	C	-2.63275500	0.38831200	-0.09089000
H	-0.87317500	2.92287800	1.55196700	C	-5.23719700	0.72793000	1.00987700
H	0.12255000	3.40062500	-0.67457500	C	-6.21567700	0.31851500	-1.22697700
N	1.04318800	-1.26083400	1.55495100	C	-3.82856400	0.51986000	-1.02297500
C	-0.03590500	-2.00209600	2.01241000	H	-4.28045900	-0.07115400	2.81684200
O	-1.03812000	-1.54867000	2.57685900	H	-3.53268600	1.41870500	2.15733100
C	1.22817300	-3.47099300	0.73965700	H	-2.28399600	1.37381100	0.22854200
H	1.92412800	-4.27575500	1.00187100	H	-1.81595600	-0.16863200	-0.55384000
H	0.76329900	-3.70616600	-0.23176700	H	-5.33564600	1.78925500	0.76322300
C	-0.85716200	-4.29108400	1.85284400	H	-6.16351400	0.35754400	1.45691700
H	-1.56140100	-3.97095900	2.62600400	Cl	-7.76548100	-0.26500500	-0.61162900
H	-1.38116900	-4.38155700	0.88898700	H	-6.01274600	-0.16149700	-2.18791900
H	-0.43763900	-5.26400200	2.13291900	H	-6.24882600	1.40726700	-1.32820000
N	0.20013600	-3.31215500	1.75308300	H	-4.00797000	1.56449600	-1.28628900
C	1.91402300	-2.09642300	0.71517500	H	-3.70123700	-0.09403400	-1.91862700
H	2.90942100	-2.15758700	1.18053600	B	-3.72298000	3.86254400	-0.07986000
Au	3.71170400	0.01230400	-0.39581500	F	-2.72167900	3.38751400	-0.93126300
C	2.02087400	-1.44944000	-0.64870500	F	-4.96959900	3.34830700	-0.53117000
H	2.75821100	-1.97488100	-1.27983400	F	-3.76184400	5.23566600	-0.06016500
H	1.07665500	-1.43806300	-1.20083500	F	-3.48948900	3.35226000	1.21178600
F	5.51757800	-1.07332000	-1.11932100	B	-1.60646600	-2.78163100	-1.65265600
P	5.58689600	1.50637900	0.10218600	F	-0.59391000	-3.12998500	-2.51534100
C	5.44454700	3.15183900	0.89121800	F	-1.04032100	-2.08340800	-0.54063500
H	4.80729600	3.80375500	0.28264300	F	-2.53634300	-1.92613000	-2.26099300
H	4.98993600	3.05181000	1.88344500	F	-2.27676900	-3.89751400	-1.15463000
H	6.43488800	3.61512700	0.99637500				

9'

Num. Imaginary Frequencies: 0

C	1.08213500	0.51305700	-1.67552500
C	1.14216000	-0.63785400	-0.90300900
C	0.89805700	-0.54861400	0.47326200
C	0.62421200	0.65643400	1.10533500
C	0.56579300	1.80639700	0.31220300
C	0.78279600	1.73539200	-1.06304500
H	1.24578800	0.46276000	-2.75156100
H	0.45724800	0.69635500	2.18059900
H	0.31700500	2.76261100	0.77091100
H	0.69100600	2.63663400	-1.66676900
N	0.97194800	-1.82703700	1.05933400
C	-0.11451200	-2.38423000	1.70542800
O	-0.93475000	-1.75400500	2.38782300
C	0.71837700	-4.06214500	0.32794600
H	1.35689000	-4.92307800	0.56061100
H	0.07330700	-4.32229700	-0.52726900
C	-1.25200600	-4.53630500	1.82016000
H	-1.74338200	-4.10360700	2.69663900
H	-1.96905000	-4.57630600	0.98592300
H	-0.91991500	-5.55212600	2.06418600
N	-0.11473300	-3.71758900	1.47525600
C	1.52685200	-2.78188100	0.06725700
H	2.59906400	-2.90655600	0.25888900
Au	4.45424800	-0.13518600	-0.20626600
C	1.37013300	-2.07524200	-1.29331300
H	2.28343200	-2.20357300	-1.88347900
H	0.50980000	-2.46401200	-1.85832800
F	4.33894200	-2.10541300	-0.70517700
P	4.68325400	2.06257600	0.38219600
C	4.09782100	3.25686300	-0.86145800
H	4.62493600	3.09395600	-1.80813200
H	3.02341700	3.11082700	-1.02648500
H	4.27959600	4.28197900	-0.51340100
C	6.41847600	2.53283700	0.68173900
H	6.83246300	1.91637800	1.48748900
H	7.00721800	2.36188300	-0.22648000
H	6.48322700	3.59187000	0.96315500
C	3.81381700	2.53090500	1.91335500
H	2.73582700	2.37488300	1.78173500
H	4.16213000	1.90381500	2.74180200

H	4.00536200	3.58634700	2.14739100
H	-1.91980800	-0.57039300	1.61636600
H	-3.96851900	-1.56411200	2.19961100
C	-3.76347400	-1.31981900	1.15281400
C	-5.02498600	-0.89718800	0.39809400
H	-3.27819900	-2.17421100	0.67853400
N	-2.78930700	-0.18549600	1.16291400
H	-5.11982300	-1.44605400	-0.54538700
H	-5.93061400	-1.03049200	0.99585700
N	-4.91130500	0.56455700	0.04652100
C	-3.35106600	0.94073400	1.95718000
C	-2.46088300	0.30585300	-0.21337100
C	-4.65939100	1.38502100	1.29570700
C	-6.11194400	1.08016300	-0.68950400
C	-3.74873200	0.71053900	-0.91705500
H	-3.50610500	0.58787900	2.98026200
H	-2.62590900	1.75979000	1.94677900
H	-1.79432100	1.16603900	-0.10341700
H	-1.95509000	-0.50699300	-0.73737000
H	-4.60492700	2.42886000	0.97267700
H	-5.52202900	1.23693600	1.95038600
Cl	-7.60293200	0.95849600	0.25183600
H	-6.21954200	0.48715500	-1.60151400
H	-5.90882500	2.13059400	-0.91970100
H	-3.71660100	1.75200100	-1.24193300
H	-3.95846600	0.04352400	-1.75747800
B	-2.83521000	4.00659600	-0.44891800
F	-2.12758600	3.26282700	-1.39631900
F	-4.22292600	3.73346500	-0.61709000
F	-2.60396400	5.35397000	-0.59028100
F	-2.46720000	3.56900800	0.83636200
B	-2.51366000	-3.09610100	-1.51120900
F	-1.80481000	-3.75707000	-2.48844500
F	-1.59701300	-2.48663900	-0.61023700
F	-3.31537400	-2.07552900	-2.05163600
F	-3.32305300	-3.96235500	-0.77779400

3.2 Cycle II and Cycle II_{H2O}

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Num. Imaginary Frequencies: 0

N	1.86062500	-1.19027200	0.10674300
C	2.93694500	-3.40703500	1.41892200
C	2.91341200	-2.10107500	-2.23027200
O	0.38647300	-2.75989900	1.58833500
O	2.11171900	-1.20099500	2.57225600
O	0.82814200	-0.54252300	-2.09948600
O	0.54262500	-2.91980800	-1.32883900
S	1.66149000	-2.06942600	1.49604100
S	1.33007800	-1.69549400	-1.36593800
F	2.58456300	-4.32089300	0.53453200
F	2.99990000	-3.95271000	2.61956400
F	4.11260800	-2.89763500	1.10088600
F	2.61113300	-2.54158200	-3.43695600
F	3.58739300	-3.02531300	-1.57224600
F	3.64325800	-1.00315800	-2.32843800
Au	1.68103300	0.99947100	0.44923300
P	1.40012800	3.25792300	0.82905800
H	-2.36079200	-2.71654500	-0.19476200
C	-2.93879200	-1.92470200	0.29170500
C	-4.40681200	-1.85178900	-0.14153600
H	-2.85441900	-1.99679800	1.37903400
N	-2.31281000	-0.63605000	-0.11488700
H	-5.06995500	-1.72740900	0.71862000
H	-4.69367500	-2.73363800	-0.72023200
N	-4.61576700	-0.64249500	-1.02984100
C	-2.21437600	-0.53786600	-1.60606600
C	-3.03446900	0.52740000	0.48014400
C	-3.63104800	-0.69011200	-2.16989200
C	-6.04615300	-0.57037500	-1.49094700
C	-4.36269000	0.64488800	-0.26016500
H	-1.54645200	-1.34222600	-1.92608800
H	-1.76755500	0.43772400	-1.81938900
H	-2.40723700	1.40691100	0.31285900
H	-3.16498100	0.31308800	1.54414800
H	-3.85556800	0.14232200	-2.84352900
H	-3.77106700	-1.64267400	-2.68700000
Cl	-6.48539800	-1.91325100	-2.54592400
H	-6.66045900	-0.58745100	-0.58519000
H	-6.16483300	0.36998600	-2.03626800
H	-4.32877100	1.44952800	-1.00100000
H	-5.17679400	0.79729800	0.45193600
F	-1.03405600	-0.61782100	0.39222500
B	-5.63202600	-0.20671000	2.78550000
F	-4.49542900	-1.04532500	2.73841100

F	-5.21045800	1.11011600	2.59004300
F	-6.46806200	-0.56574800	1.69302200
F	-6.30282000	-0.35915200	3.97014800
C	5.08545800	1.34968000	1.06768500
C	4.93556200	1.86679800	-1.20497200
C	5.93852000	0.73649800	-1.03286600
C	5.46091000	0.11274000	0.27321800
H	5.96448300	1.78203500	1.57465600
H	4.30800600	1.16618100	1.82524300
H	4.02684600	1.51557900	-1.72488400
H	5.33347500	2.72955100	-1.75515800
H	5.94338700	0.04202300	-1.87981100
H	6.95407100	1.13963800	-0.91338800
H	4.57042100	-0.50822800	0.09235900
H	6.21406700	-0.50481400	0.77510000
O	4.58217200	2.28501400	0.11387700
C	2.60981700	3.94839700	2.00053600
H	2.41242700	5.01813600	2.14851700
H	2.53245700	3.42877200	2.96244600
H	3.61476100	3.80527700	1.58948800
C	-0.21853500	3.71055700	1.53012700
H	-0.21681300	4.77835700	1.78693500
H	-1.01296600	3.52053600	0.79978600
H	-0.40874300	3.12402100	2.43618200
C	1.55825000	4.25852200	-0.68021600
H	0.76122800	3.97492800	-1.37647800
H	1.46621900	5.32378500	-0.43150700
H	2.53481700	4.07441200	-1.14168800
B	-2.15483500	3.06292600	-1.71458900
F	-1.72539600	4.17913100	-2.38777400
F	-1.04340600	2.27347000	-1.31728800
F	-2.86910700	3.39657200	-0.55710400
F	-2.97984100	2.26202500	-2.52984100

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Num. Imaginary Frequencies: 1

N	2.07531300	-1.08070800	0.03812000
C	2.88130400	-3.31456700	1.51166000
C	3.11216500	-2.20690000	-2.21777500
O	0.38528300	-2.46206400	1.49183400
O	2.16703100	-0.98893600	2.50744600
O	1.21610900	-0.41752200	-2.22594600
O	0.64350600	-2.73209600	-1.39135800

S	1.71436300	-1.87911200	1.44739500	H	5.34892200	1.92929100	1.70890900
S	1.55192100	-1.59509900	-1.43619600	H	4.03350300	0.73539600	1.93423200
F	2.48178900	-4.25187100	0.67499300	H	3.79477200	1.19049300	-1.71225800
F	2.85856500	-3.77937700	2.74645700	H	4.58733100	2.77535700	-1.50750500
F	4.10426600	-2.92254300	1.20604200	H	6.08983700	0.44705500	-1.73969800
F	2.80922300	-2.64895800	-3.42313900	H	6.60837900	1.76394000	-0.66784100
F	3.64264300	-3.18016800	-1.50235400	H	4.89228000	-0.65560400	0.12225600
F	3.97502000	-1.20951400	-2.31552800	H	6.41222100	-0.13001400	0.89492900
Au	1.54415000	1.10284400	0.37485800	O	3.89168800	1.90059300	0.23431000
P	0.95966000	3.28228400	0.97313300	C	2.14251600	3.79464100	2.25552000
H	-1.59922900	-2.30226300	-0.10961200	H	1.93934300	4.82946500	2.56009300
C	-2.36603500	-1.63780800	0.30059400	H	2.05390800	3.13391500	3.12549200
C	-3.79588000	-2.00495100	-0.15998400	H	3.15774200	3.71842800	1.84990300
H	-2.31221900	-1.63325100	1.39208500	C	-0.69547500	3.49019300	1.67682100
N	-2.12557000	-0.29205300	-0.19850900	H	-0.74682100	4.46615800	2.17726800
H	-4.48696700	-2.07430800	0.68373800	H	-1.44329600	3.46215600	0.87625900
H	-3.80887900	-2.92924200	-0.74368500	H	-0.89565100	2.69852900	2.40746700
N	-4.33566200	-0.90861100	-1.06187500	C	1.12632300	4.47675600	-0.38186600
C	-2.02905800	-0.25971000	-1.65656400	H	0.36007800	4.26998100	-1.13702800
C	-3.06112900	0.67679500	0.35796000	H	0.99183200	5.49051000	0.01789800
C	-3.39213500	-0.70768100	-2.22227600	H	2.12335300	4.39121800	-0.82885000
C	-5.73687700	-1.22238400	-1.49001000	B	-2.42423800	3.32562200	-1.79146000
C	-4.41792700	0.41379000	-0.31223900	F	-2.17690400	4.44317200	-2.55215200
H	-1.22536700	-0.93816900	-1.95698600	F	-1.20097400	2.68337000	-1.47087700
H	-1.78376900	0.76118800	-1.95387800	F	-3.05870300	3.65676300	-0.58581200
H	-2.71856700	1.68764100	0.12341500	F	-3.23405800	2.40599800	-2.48240900
H	-3.11897600	0.51791700	1.43901300				
H	-3.81951200	0.06874800	-2.86528300				
H	-3.32783300	-1.65374400	-2.76627800	11			
Cl	-5.83800900	-2.66982200	-2.50114500	Num. Imaginary Frequencies: 0			
H	-6.31561200	-1.37282300	-0.57381000	N	-2.66788400	-0.81477800	-0.42556500
H	-6.10730400	-0.36709600	-2.06120600	C	-5.18493700	-1.77031400	-1.12914300
H	-4.63652200	1.18061900	-1.06310800	C	-2.32200300	-2.86513000	1.34380600
H	-5.22035500	0.34910100	0.42663900	O	-3.28190200	-1.33653600	-2.92520300
F	-0.52677500	0.31407600	0.29569200	O	-4.24032400	0.63121500	-1.66110100
B	-5.48497300	-0.68399000	2.75099600	O	-0.36436400	-1.52241200	0.22611900
F	-4.13238600	-1.08066800	2.72269400	O	-1.72614800	-3.11565200	-1.21547000
F	-5.54967600	0.68824200	2.50262500	S	-3.74920900	-0.74273600	-1.69052300
F	-6.15422400	-1.35389900	1.69221800	S	-1.63839800	-2.09096800	-0.19421600
F	-6.06184000	-1.00943100	3.95471500	F	-4.87220000	-3.04809000	-1.19301200
C	4.70476300	1.19655400	1.19889700	F	-6.19058600	-1.51046000	-1.94052800
C	4.48254400	1.77132000	-1.08004600	F	-5.51040200	-1.44207300	0.10739400
C	5.80192300	1.04591400	-0.86901800	F	-1.63282700	-3.96331600	1.57424800
C	5.51149600	0.21632300	0.37771700	F	-3.59923700	-3.15398900	1.18395000

Num. Imaginary Frequencies: 0

N	-2.66788400	-0.81477800	-0.42556500
C	-5.18493700	-1.77031400	-1.12914300
C	-2.32200300	-2.86513000	1.34380600
O	-3.28190200	-1.33653600	-2.92520300
O	-4.24032400	0.63121500	-1.66110100
O	-0.36436400	-1.52241200	0.22611900
O	-1.72614800	-3.11565200	-1.21547000
S	-3.74920900	-0.74273600	-1.69052300
S	-1.63839800	-2.09096800	-0.19421600
F	-4.87220000	-3.04809000	-1.19301200
F	-6.19058600	-1.51046000	-1.94052800
F	-5.51040200	-1.44207300	0.10739400
F	-1.63282700	-3.96331600	1.57424800
F	-3.59923700	-3.15398900	1.18395000

F	-2.18789000	-2.03350900	2.36484800
Au	-1.62009200	1.17871500	-0.37912000
P	-0.68417900	3.30884300	-0.67203900
H	3.46003800	-2.02561200	-2.78887600
C	4.09539800	-1.31787200	-2.24270600
C	4.66220800	-1.96582100	-0.96417400
H	4.93106200	-1.02705000	-2.88834100
N	3.29994900	-0.13423500	-1.92911500
H	5.74488500	-1.84334600	-0.87529200
H	4.39600000	-3.02270300	-0.86593600
N	4.06203000	-1.25467700	0.22753100
C	2.14105900	-0.53167600	-1.13614900
C	4.12264800	0.79404700	-1.16082500
C	2.55565000	-1.30875500	0.13103400
C	4.57657700	-1.79888000	1.51277500
C	4.48395100	0.20649900	0.21123700
H	1.47566400	-1.14687300	-1.75268900
H	1.58487400	0.36510100	-0.84103800
H	3.57716800	1.73522000	-1.01646600
H	5.04108600	1.00361100	-1.72050100
H	2.16421700	-0.86308000	1.05180800
H	2.27680700	-2.36605600	0.09234700
Cl	4.12077700	-3.49537000	1.78681900
H	5.66742600	-1.72523400	1.47848600
H	4.15294300	-1.19307100	2.31903600
H	3.93750200	0.68085200	1.03030100
H	5.55861900	0.24339300	0.40569800
F	-0.89776400	0.88444100	-2.17678400
B	7.79164900	-0.07270600	-0.79696100
F	7.11971200	-0.37451100	-1.99129000
F	7.36700900	1.17813700	-0.34123900
F	7.43186300	-1.04451000	0.17222900
F	9.15847700	-0.09304500	-0.98800600
C	-3.86832100	1.62603600	1.62038200
C	-1.75748700	1.09058100	2.68281100
C	-2.90926800	0.87074900	3.63802500
C	-4.09220300	0.60817600	2.70994700
H	-4.18225900	2.63684900	1.90919800
H	-4.28562900	1.37487200	0.64040300
H	-1.27480300	0.16089400	2.36524600
H	-0.99134000	1.79656500	3.01021600
H	-2.70386600	0.03974800	4.32033900
H	-3.08863100	1.77080300	4.23974300
H	-4.04862300	-0.41009400	2.30045000

H	-5.06161500	0.74459100	3.19912400
O	-2.40032000	1.68901300	1.48948500
C	-1.78517000	4.03199700	-1.90239900
H	-1.43197300	5.04146300	-2.14977500
H	-1.77135100	3.40277300	-2.79927200
H	-2.80592900	4.08734900	-1.50778700
C	0.97918900	3.17122700	-1.33351900
H	1.23559800	4.13448900	-1.79450900
H	1.67160000	2.94450900	-0.51525900
H	0.99462300	2.38480200	-2.09707200
C	-0.73538400	4.25123800	0.85635900
H	-0.11818600	3.76539900	1.62163700
H	-0.33687500	5.25176900	0.63995500
H	-1.76975800	4.33703500	1.20476500
B	1.70713900	1.84689000	2.04986000
F	1.05682000	2.63391500	2.99859100
F	0.73050400	1.37212900	1.12583700
F	2.62809800	2.61095000	1.33555700
F	2.32949400	0.75812100	2.64433800

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Num. Imaginary Frequencies: 0

C	0.11887000	5.45017100	-0.83348700
C	0.34181100	4.30966600	-1.59755300
C	1.47905700	3.52951100	-1.36462100
C	2.39604000	3.91946300	-0.37834000
C	2.16750600	5.06907900	0.36273900
C	1.02573500	5.84163400	0.14502500
H	-0.78575600	6.02467000	-1.02196100
H	-0.37792100	4.03878000	-2.36604000
H	3.27250100	3.29928100	-0.19509000
H	2.88698200	5.35900100	1.12726500
H	0.84570100	6.73650600	0.73763800
C	1.01636800	1.82546400	-3.15711900
O	1.54566200	1.54410600	-4.22074700
C	-0.69312500	1.36136200	-1.49838100
H	-0.85005100	2.30951400	-0.95910900
H	-1.67334000	0.85973700	-1.50129800
C	-1.16047400	1.08050200	-3.94100300
H	-1.09081500	-0.01245800	-4.05414200
H	-2.19203600	1.36163000	-3.70934900
H	-0.85804100	1.54507700	-4.88237600
N	-0.30063600	1.56841400	-2.87637800

C	0.25549100	0.49898500	-0.75751200	H	-2.74523400	0.01313500	0.79889800
H	0.38526000	0.68212100	0.31493200	H	-3.12399400	1.50843900	-0.12200900
C	0.93435200	-0.56994600	-1.31034500	B	-3.32744000	3.74781700	-1.55115700
H	1.77593800	-0.98260100	-0.75177400	F	-3.43550200	2.46455000	-2.13210300
H	0.98733300	-0.68269100	-2.39837900	F	-4.60354900	4.24450000	-1.30717500
H	2.73179400	2.07149700	-2.12506600	F	-2.61319900	4.58765900	-2.38787700
N	1.74985300	2.35094800	-2.07939900	F	-2.64814900	3.60971000	-0.31447200
N	3.64584400	0.92419400	0.29657600	B	-1.79153900	-1.87478900	2.36563100
C	4.22394900	1.77563400	2.72797200	F	-0.84703400	-1.10567900	1.65049400
C	6.18659600	0.16278000	-0.39453100	F	-2.37224700	-1.08997700	3.35076600
O	3.82422900	-0.78154100	2.26218700	F	-2.78004500	-2.27881900	1.43884000
O	1.87180600	0.77895100	2.06406300	F	-1.18863400	-3.00042200	2.90591500
O	4.23076800	0.63856400	-2.07865300	Au	-0.59875600	-2.21046100	-0.85528700
O	4.11293400	-1.43001100	-0.65655200	P	-1.99333000	-4.18311000	-0.77795700
S	3.28066000	0.49279300	1.80206900	F	-2.12137400	-1.25646600	-1.66856100
S	4.38814700	0.00410500	-0.77013400	C	-1.56807100	-5.22603500	0.63237600
F	5.51251800	1.66700100	2.44308000	H	-0.53884000	-5.58401100	0.51159900
F	4.04070000	1.58034200	4.02361700	H	-1.65245500	-4.65456400	1.56347000
F	3.80231200	2.98583500	2.40275500	H	-2.25200400	-6.08513200	0.65011500
F	6.87673200	-0.48690800	-1.31779400	C	-1.59588000	-5.08997300	-2.29617400
F	6.44215300	-0.35661800	0.79474400	H	-1.83328700	-4.47168500	-3.16913900
F	6.53044800	1.43925100	-0.40127700	H	-0.53473900	-5.36067300	-2.32071200
H	-7.11642900	1.90852400	-0.03325800	H	-2.19594000	-6.00905300	-2.33253700
C	-6.05509100	1.64736700	-0.12146500	C	-3.76653500	-3.85394900	-0.83609200
C	-5.26573100	2.27440000	1.04150600	H	-4.09693100	-3.43143200	0.11518900
H	-5.68127100	2.04219300	-1.07308300	H	-3.97755600	-3.15815000	-1.65435200
N	-5.90933400	0.19339400	-0.12777700	H	-4.27722100	-4.80744600	-1.02535800
H	-4.66577000	3.13234200	0.72236900	C	2.01592600	-3.85594300	-0.92445400
H	-5.90234300	2.56313700	1.88380200	O	0.95637300	-3.35210300	-0.05140000
N	-4.31273500	1.22333300	1.57032900	C	1.51150400	-3.04716800	1.28754300
C	-6.18996600	-0.32532400	1.20704600	C	2.86968000	-3.73255400	1.28875700
C	-4.53404700	-0.13787900	-0.48221300	C	2.86618700	-4.63156700	0.04870600
C	-5.10936000	0.11355100	2.21521700	H	1.52569900	-4.45061700	-1.70178100
C	-3.28478700	1.80342200	2.48047500	H	2.55381200	-3.00943500	-1.36974000
C	-3.54493600	0.64269900	0.39337400	H	1.56944700	-1.95857500	1.40453800
H	-7.17882500	0.03528800	1.51629400	H	0.77287600	-3.43722900	1.99195600
H	-6.23168900	-1.42152100	1.17082200	H	3.65863300	-2.97782000	1.20893000
H	-4.38542400	-1.21394900	-0.34903000	H	3.02337000	-4.30201800	2.21045900
H	-4.35002300	0.10621100	-1.53505500	H	3.87339500	-4.79847600	-0.34662500
H	-4.38936700	-0.67513400	2.45387200	H	2.40552300	-5.60588300	0.25773900
H	-5.52824900	0.50915300	3.14592500				
Cl	-3.99759300	2.61573800	3.89090000				
H	-2.72098500	2.53945700	1.89910600				
H	-2.65466900	0.98143900	2.83289800				

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Num. Imaginary Frequencies: 1

C	0.11994400	5.46481500	-0.79363400	C	-6.05169500	1.64991200	-0.11726500
C	0.31402300	4.29968500	-1.52736100	C	-5.25994500	2.27579300	1.04459700
C	1.46376600	3.53093500	-1.31746300	H	-5.67750800	2.04295000	-1.06956400
C	2.41804800	3.95282700	-0.38037200	N	-5.90958600	0.19543000	-0.12262700
C	2.21505400	5.12423000	0.33297000	H	-4.66204400	3.13496400	0.72516500
C	1.06372000	5.88825000	0.13529100	H	-5.89455600	2.56226600	1.88917200
H	-0.79267400	6.03162900	-0.96684700	N	-4.30451200	1.22445200	1.56829800
H	-0.44065600	4.00523100	-2.25257100	C	-6.18575900	-0.32098600	1.21415300
H	3.30702200	3.34493400	-0.21694300	C	-4.53618100	-0.13880900	-0.48182500
H	2.96391400	5.44415900	1.05581800	C	-5.09886100	0.11517700	2.21665100
H	0.90667600	6.80261500	0.70414400	C	-3.27131200	1.80324300	2.47337100
C	0.99550100	1.85406800	-3.12695700	C	-3.54331000	0.64459000	0.38670000
O	1.54422800	1.63552000	-4.19379200	H	-7.17186600	0.04355800	1.52768900
C	-0.71167900	1.34486400	-1.49342600	H	-6.23141700	-1.41709500	1.17948500
H	-0.89569400	2.28265500	-0.94704800	H	-4.38741600	-1.21459800	-0.34605000
H	-1.67141100	0.80690900	-1.50692300	H	-4.35586200	0.10155400	-1.53622500
C	-1.17198200	1.11082600	-3.94651400	H	-4.37873700	-0.67469700	2.45056700
H	-1.11693700	0.01747500	-4.06243100	H	-5.51182500	0.51048900	3.15013000
H	-2.20202400	1.40551000	-3.72582600	Cl	-3.97616800	2.61732100	3.88673800
H	-0.84868100	1.57635500	-4.88037600	H	-2.70889000	2.53809600	1.88911400
N	-0.31775100	1.57637900	-2.86816900	H	-2.64089400	0.98034700	2.82326800
C	0.27395200	0.50608800	-0.77074800	H	-2.73898800	0.01736300	0.78696300
H	0.44075500	0.70452600	0.29430400	H	-3.12938800	1.51111600	-0.13295000
C	0.91890000	-0.58627500	-1.32730300	B	-3.33450200	3.76478800	-1.54782900
H	1.77912200	-0.99036000	-0.79043100	F	-3.43622000	2.48528800	-2.13699300
H	0.94532800	-0.70480400	-2.41609000	F	-4.61192000	4.25269600	-1.29549100
H	2.69063200	2.04626200	-2.05149400	F	-2.62727700	4.61612300	-2.37978200
N	1.70922800	2.32771100	-2.00259800	F	-2.64829300	3.62129500	-0.31569400
N	3.64625800	0.91909900	0.28587000	B	-1.78465100	-1.87085500	2.36186800
C	4.23045600	1.76570900	2.71750500	F	-0.84576600	-1.09903400	1.64243900
C	6.18655100	0.15366500	-0.40509100	F	-2.36165600	-1.08768100	3.35101800
O	3.81605800	-0.78922800	2.24954700	F	-2.77752500	-2.27667000	1.44089600
O	1.87249600	0.78299100	2.05230800	F	-1.17651000	-2.99518500	2.89892300
O	4.23074000	0.63891700	-2.08764000	Au	-0.60033800	-2.22130000	-0.85687800
O	4.11091700	-1.43461400	-0.67113400	P	-2.00195500	-4.19241400	-0.76800600
S	3.27988700	0.48868800	1.79097200	F	-2.12390100	-1.27106500	-1.67726700
S	4.38804100	-0.00068800	-0.78153000	C	-1.57222500	-5.24056100	0.63801900
F	5.51929700	1.64341000	2.43926200	H	-0.54164700	-5.59394000	0.51415600
F	4.03909800	1.57635600	4.01287300	H	-1.65533100	-4.67152200	1.57060000
F	3.82251500	2.97847400	2.38567200	H	-2.25240300	-6.10252000	0.65602600
F	6.87568200	-0.49259600	-1.33146400	C	-1.61453200	-5.10103900	-2.28877000
F	6.44084700	-0.37211000	0.78157900	H	-1.85287800	-4.48054500	-3.16001200
F	6.53234200	1.42965300	-0.40551400	H	-0.55399700	-5.37404700	-2.31755200
H	-7.11219400	1.91429900	-0.02858600	H	-2.21715000	-6.01833800	-2.32498300

C	-3.77662400	-3.86563700	-0.81819700
H	-4.10366600	-3.44494800	0.13506600
H	-3.99002100	-3.16668400	-1.63328300
H	-4.28898200	-4.81789900	-1.00868600
C	2.00996900	-3.87038500	-0.92866700
O	0.95589400	-3.36041000	-0.05358400
C	1.51610500	-3.05347700	1.28207700
C	2.87270500	-3.74217300	1.27981300
C	2.85982300	-4.64703300	0.04413400
H	1.51417300	-4.46483500	-1.70285700
H	2.54986600	-3.02713800	-1.37821200
H	1.57710500	-1.96478500	1.39648000
H	0.77878000	-3.44029700	1.98964900
H	3.66299200	-2.98970900	1.19146700
H	3.03026500	-4.30724300	2.20358500
H	3.86446900	-4.82247900	-0.35393800
H	2.39344600	-5.61730600	0.25940600

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Num. Imaginary Frequencies: 0

C	0.02826100	-4.44213200	0.65611700
C	-0.36278500	-3.62741100	-0.40183700
C	-0.67998400	-2.30153000	-0.13532600
C	-0.58459900	-1.76383100	1.14004000
C	-0.20055600	-2.59178800	2.18866000
C	0.09763700	-3.93057100	1.94901400
H	0.27497500	-5.48321000	0.46185900
H	-0.42940500	-4.04210300	-1.40561600
H	-0.80570500	-0.71268600	1.31866900
H	-0.12470800	-2.17366100	3.18943700
H	0.39749600	-4.57596200	2.77269900
C	-1.53916500	-2.16857100	-2.47048400
O	-2.58093300	-2.76033800	-2.52215800
C	0.63117000	-1.33914900	-2.74936100
H	1.32648000	-2.06189500	-2.30731000
H	1.16051400	-0.75778600	-3.51211900
C	-0.38183800	-2.85508000	-4.51180600
H	-0.34155000	-2.21490800	-5.39975800
H	0.54463800	-3.43878900	-4.44213300
H	-1.24586300	-3.52105800	-4.58046500
N	-0.51129200	-2.04491100	-3.31379700
C	-0.03154300	-0.45144200	-1.70404300
H	0.63197500	-0.26070900	-0.85059100
C	-0.63068800	0.81354700	-2.28337200

H	-1.72470300	0.84715700	-2.27204400
H	-0.23960000	1.03727400	-3.28083900
H	-1.98910800	-0.89997600	-0.86771500
N	-1.12530200	-1.38717700	-1.21407900
N	-3.73361800	-0.65775700	-0.13589800
C	-4.40096500	-2.72594400	1.43278600
C	-5.93063200	-1.05502700	-1.81018700
O	-5.59544400	-0.38206700	1.65716300
O	-3.17199500	-0.58286700	2.31438600
O	-3.73429800	0.22727000	-2.42860300
O	-5.31408200	1.29540800	-0.79244400
S	-4.25642200	-0.88604100	1.38789000
S	-4.60397300	0.11038200	-1.25943500
F	-5.39051600	-3.12153200	0.65080600
F	-4.65594100	-3.08663700	2.68007200
F	-3.27433400	-3.28622000	1.03073600
F	-6.55661400	-0.49351100	-2.83334500
F	-6.79363900	-1.26626400	-0.83261900
F	-5.39774100	-2.19902200	-2.19164500
H	6.83127100	-0.63310200	-0.61575200
C	5.73903200	-0.71706400	-0.66341200
C	5.27862000	-1.96968800	0.10702000
H	5.44039300	-0.80677000	-1.71394300
N	5.13749400	0.49323000	-0.10775000
H	4.94774700	-2.77833100	-0.55416400
H	6.04428500	-2.35646400	0.78776100
N	4.10633300	-1.56877900	0.97446500
C	5.35593400	0.52246300	1.33518800
C	3.70069800	0.47709400	-0.36684800
C	4.58547400	-0.61263900	2.04048200
C	3.38825800	-2.74543700	1.53731300
C	3.08164100	-0.84258600	0.11641000
H	6.43343000	0.43711200	1.52333300
H	5.01388900	1.48513100	1.73317700
H	3.23543600	1.31576300	0.16264500
H	3.50874900	0.60662300	-1.43836900
H	3.68521600	-0.25919700	2.55361300
H	5.20558900	-1.18496200	2.73758600
Cl	4.42850900	-3.79268600	2.52435400
H	3.00474400	-3.32319500	0.68983300
H	2.57715400	-2.36816900	2.16752200
H	2.20618500	-0.68147900	0.75403200
H	2.85201400	-1.53339300	-0.69759900
B	3.49414500	-3.26095500	-2.68659500

F	3.68617800	-1.87014800	-2.77800200	C	-0.34846200	-1.73318600	1.23887100
F	4.71798200	-3.89168100	-2.53742000	C	0.00444800	-2.39971500	2.40896300
F	2.80537500	-3.71596600	-3.80093600	C	0.11945400	-3.78632300	2.41820500
F	2.70678900	-3.51306100	-1.52870000	H	0.00207100	-5.57857300	1.22661600
B	1.23898800	1.18744200	2.36994800	H	-0.63718900	-4.40661000	-0.83869000
F	0.73099300	1.04928000	1.04292600	H	-0.41783700	-0.64786500	1.25721800
F	1.47432400	-0.09210900	2.87503600	H	0.20887500	-1.80989300	3.30061300
F	2.43990100	1.89744300	2.29975100	H	0.39301600	-4.31087200	3.33220200
F	0.31373700	1.86840400	3.13847300	C	-1.17673400	-2.45546600	-2.36317900
Au	-0.00348900	2.47628600	-1.16267200	O	-1.87451900	-3.44387100	-2.45329200
P	1.00050500	4.44617900	0.03263000	C	0.30846500	-0.70376000	-2.83577300
F	1.73465100	2.19687800	-2.05449200	H	1.37492000	-0.96757300	-2.82788900
C	0.55197200	4.84563500	1.75410100	H	0.17249000	0.17567200	-3.47694900
H	-0.50619500	5.12599000	1.81848300	C	-0.40187100	-2.28883600	-4.67061300
H	0.73176500	3.97938100	2.40155400	H	-0.59772800	-1.46847600	-5.37185100
H	1.16148400	5.69241700	2.09679400	H	0.59827300	-2.70202900	-4.85062100
C	0.70592600	5.99493000	-0.88823700	H	-1.15273200	-3.07145600	-4.80929100
H	1.00699800	5.86739600	-1.93443200	N	-0.49394100	-1.80686800	-3.31358900
H	-0.35835000	6.25684100	-0.85509200	C	-0.24695400	-0.45155600	-1.42985100
H	1.28559700	6.81513700	-0.44521600	H	0.56307800	-0.38557100	-0.69651700
C	2.80851900	4.23753300	0.05581000	C	-1.13384700	0.77082400	-1.34746300
H	3.06033500	3.53448100	0.85780900	H	-1.81061400	0.74397000	-0.48289500
H	3.13609000	3.81962300	-0.90186800	H	-1.69861900	0.95579100	-2.27068700
H	3.30064600	5.20033000	0.24174400	H	-2.39118300	-1.42189900	-0.81859400
C	-2.87373800	3.59597600	-0.81447300	N	-1.03040400	-1.70410200	-1.10749300
O	-1.93089300	2.57287800	-0.34294900	N	-3.56487200	-1.20439100	-0.63160200
C	-2.09154000	2.33291100	1.09615100	C	-4.34440700	-2.78948700	1.38328700
C	-3.40391300	3.00576400	1.42143200	C	-5.72123600	-1.74745800	-2.26090000
C	-3.42635300	4.19211300	0.45877200	O	-5.41534800	-0.39848000	0.97701500
H	-2.32420200	4.29348700	-1.45500200	O	-3.00882900	-0.51415300	1.74067400
H	-3.63401000	3.06634900	-1.40133100	O	-3.41615700	-0.72640400	-3.05900200
H	-2.08208100	1.24690700	1.23771300	O	-4.93925900	0.73002000	-1.66383000
H	-1.23385900	2.76824800	1.62098300	S	-4.10463700	-1.01338900	0.92988800
H	-4.24626900	2.33464500	1.21090700	S	-4.33834400	-0.55816500	-1.95078700
H	-3.44796800	3.30584400	2.47307800	F	-5.25680400	-3.31491000	0.58838800
H	-4.42972400	4.60359500	0.30985200	F	-4.75525700	-2.83406700	2.63555500
H	-2.77246300	5.00013000	0.81744500	F	-3.20460100	-3.43491200	1.25506600
				F	-6.32157000	-1.36639500	-3.37277100
				F	-6.57373400	-1.72135100	-1.25671700
				F	-5.22556100	-2.95710200	-2.40434900
				H	6.67518400	-0.39486300	-0.58254500
				C	5.58811400	-0.52011800	-0.65626700
				C	5.16976500	-1.86385700	-0.03357700
				H	5.30736900	-0.50634600	-1.71549000
TS8							
Num. Imaginary Frequencies: 1							
C	-0.10247400	-4.49535800	1.24076900				
C	-0.46165100	-3.83901500	0.06802700				
C	-0.59157300	-2.45146200	0.06887500				

N	4.92652300	0.59748700	0.00969700	H	3.74207700	4.99991600	-0.03486100
H	4.83224500	-2.59640300	-0.77411400	C	-2.70411900	3.82796500	-0.51278900
H	5.95814500	-2.30964500	0.58152700	O	-1.56723600	3.25544200	0.20015500
N	4.00869700	-1.60471500	0.90264200	C	-2.00467300	2.63664500	1.46502700
C	5.14935800	0.50918500	1.45051800	C	-3.50739700	2.81570000	1.44994300
C	3.49665300	0.52181000	-0.26837200	C	-3.70718600	4.06057000	0.58986900
C	4.48288200	-0.75005800	2.05169900	H	-2.33357200	4.72464200	-1.02147500
C	3.36223600	-2.87344700	1.33750600	H	-3.06473800	3.09666500	-1.25123900
C	2.91908900	-0.82751500	0.18329500	H	-1.66575900	1.59738100	1.48455700
H	6.23108400	0.49508400	1.63209800	H	-1.49053800	3.18550600	2.26091300
H	4.72651500	1.39741800	1.93200700	H	-3.99529100	1.95388500	0.97238000
H	2.98000600	1.32815600	0.26232000	H	-3.91219500	2.91597600	2.46170400
H	3.32349000	0.65969000	-1.34133200	H	-4.72557800	4.15468900	0.20065800
H	3.59282000	-0.51087200	2.64623400	H	-3.45670500	4.97204000	1.14875500
H	5.17025200	-1.35600200	2.65012700				
Cl	4.45928200	-3.94993400	2.22714100				
H	3.01288500	-3.38786000	0.43500800	14			
H	2.52106400	-2.61762200	1.99024000	Num. Imaginary Frequencies: 0			
H	2.10766600	-0.70682500	0.91212900	C	-0.83397400	-3.77665900	1.56980900
H	2.58970000	-1.46126300	-0.64426100	C	-0.97742200	-3.46209000	0.22557200
B	2.88691100	-3.16123500	-2.57722900	C	-0.65310400	-2.17720500	-0.22971300
F	3.44223700	-1.87062500	-2.68647300	C	-0.17893800	-1.23214400	0.67897100
F	3.85074800	-4.02427900	-2.05422100	C	-0.03710400	-1.55716800	2.02493100
F	2.44013600	-3.59052800	-3.81302600	C	-0.36239800	-2.83104500	2.47805900
F	1.80913300	-3.09435100	-1.66513200	H	-1.08538400	-4.78141100	1.90606200
B	1.35406200	1.50894900	2.59205300	H	-1.32836700	-4.21013100	-0.47982300
F	0.76423400	1.30699200	1.30997000	H	0.10623800	-0.23731800	0.33799300
F	1.55414300	0.25611000	3.16792100	H	0.35180700	-0.80443400	2.70916400
F	2.57891000	2.15926900	2.40704300	H	-0.24927200	-3.08564900	3.53029600
F	0.50790900	2.29735700	3.35163300	C	-1.66628700	-2.39549300	-2.47354700
Au	0.00669400	2.50246100	-0.96657600	O	-2.67536700	-3.04359600	-2.15323000
P	1.39588800	4.46011400	-0.31128400	C	-0.02725000	-1.34495600	-3.71721400
F	1.43818700	1.79677300	-2.12196200	H	0.80468500	-2.03974500	-3.90000500
C	0.89417300	5.04788800	1.33767000	H	-0.01135700	-0.54873800	-4.47063900
H	-0.12008000	5.46298400	1.27918900	C	-2.04612900	-2.40037500	-4.90404100
H	0.88947800	4.20121500	2.03752600	H	-2.17309100	-1.52336900	-5.55089000
H	1.58222000	5.82218100	1.69995500	H	-1.53686200	-3.18941500	-5.47392100
C	1.27780000	5.90365300	-1.41750700	H	-3.03096800	-2.76136500	-4.59183500
H	1.63360600	5.63032100	-2.41711600	N	-1.30744500	-2.03959700	-3.72380800
H	0.23510800	6.23280400	-1.49252900	C	0.01137100	-0.80139800	-2.28162200
H	1.88865200	6.73016600	-1.03194800	H	1.05046600	-0.75346300	-1.92855200
C	3.17107000	4.07721500	-0.19936400	C	-0.74081700	0.51968400	-2.16927100
H	3.33223000	3.39372200	0.64275200	H	-1.70876400	0.40479800	-1.66948400
H	3.50643700	3.59656400	-1.12564400	H	-0.87493000	1.02259900	-3.13682700

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C	-0.83397400	-3.77665900	1.56980900
C	-0.97742200	-3.46209000	0.22557200
C	-0.65310400	-2.17720500	-0.22971300
C	-0.17893800	-1.23214400	0.67897100
C	-0.03710400	-1.55716800	2.02493100
C	-0.36239800	-2.83104500	2.47805900
H	-1.08538400	-4.78141100	1.90606200
H	-1.32836700	-4.21013100	-0.47982300
H	0.10623800	-0.23731800	0.33799300
H	0.35180700	-0.80443400	2.70916400
H	-0.24927200	-3.08564900	3.53029600
C	-1.66628700	-2.39549300	-2.47354700
O	-2.67536700	-3.04359600	-2.15323000
C	-0.02725000	-1.34495600	-3.71721400
H	0.80468500	-2.03974500	-3.90000500
H	-0.01135700	-0.54873800	-4.47063900
C	-2.04612900	-2.40037500	-4.90404100
H	-2.17309100	-1.52336900	-5.55089000
H	-1.53686200	-3.18941500	-5.47392100
H	-3.03096800	-2.76136500	-4.59183500
N	-1.30744500	-2.03959700	-3.72380800
C	0.01137100	-0.80139800	-2.28162200
H	1.05046600	-0.75346300	-1.92855200
C	-0.74081700	0.51968400	-2.16927100
H	-1.70876400	0.40479800	-1.66948400
H	-0.87493000	1.02259900	-3.13682700

H	-3.52336900	-2.07638200	-1.08934300	F	2.53627900	-3.35560600	-3.69597400
N	-0.74183600	-1.86022100	-1.59427600	F	2.53853200	-3.16054900	-1.41407000
N	-4.17696000	-1.36086600	-0.65179400	B	1.79407600	1.70942900	2.89115400
C	-5.15731200	-3.31621700	0.92517800	F	1.19276800	1.54690500	1.61683700
C	-6.25276900	-1.17502600	-2.41376900	F	1.97378900	0.44420700	3.46289400
O	-5.74133400	-0.72623300	1.26852000	F	3.04225200	2.31633700	2.72131800
O	-3.39074700	-1.52885300	1.76616600	F	0.96284600	2.49396400	3.67362600
O	-3.84905000	-0.15618700	-2.81925900	Au	0.13989100	2.09145500	-1.07394200
O	-5.28880300	0.91554800	-1.03520300	P	1.15697500	4.18726200	-0.13635100
S	-4.59451400	-1.55272500	0.96789800	F	1.75458400	1.88197600	-2.18610300
S	-4.80210600	-0.25289400	-1.73357400	C	0.56564800	4.89125800	1.43667500
F	-6.19762700	-3.42669700	0.12586100	H	-0.49699300	5.15234500	1.35864700
F	-5.48552800	-3.65492100	2.15329700	H	0.69896800	4.15702800	2.24131700
F	-4.16731300	-4.06824800	0.48884400	H	1.13368700	5.80069700	1.67410500
F	-6.78983400	-0.44976300	-3.37171800	C	0.89721300	5.50577600	-1.37479400
F	-7.12651500	-1.38323600	-1.45112800	H	1.31842300	5.18231400	-2.33456800
F	-5.81946700	-2.32293900	-2.89482700	H	-0.17373900	5.69857400	-1.51077700
H	6.75198900	-0.68037700	-0.65145100	H	1.39027700	6.43553100	-1.06271400
C	5.65740800	-0.69729500	-0.58527800	C	2.96605500	4.09829800	0.03353500
C	5.20010900	-1.93571400	0.20626700	H	3.20962600	3.55273400	0.95217100
H	5.24788200	-0.75014900	-1.60049700	H	3.38638700	3.57297900	-0.83202700
N	5.18535600	0.53497500	0.04052400	H	3.38232700	5.11230100	0.09179700
H	4.76273000	-2.70043100	-0.44181500	C	-2.72399800	3.06945700	-0.51917100
H	6.00062100	-2.37971700	0.80685700	O	-1.68353400	2.16935300	-0.02512100
N	4.13610700	-1.48953000	1.18113500	C	-1.83649200	1.90321400	1.40378200
C	5.52369400	0.52761300	1.46074600	C	-3.30480100	2.17857600	1.62188200
C	3.73279600	0.59869000	-0.09202600	C	-3.58765000	3.35791400	0.69433500
C	4.76503500	-0.58653700	2.21445600	H	-2.23928200	3.95803300	-0.94213900
C	3.40423000	-2.63568600	1.78425300	H	-3.25188800	2.52484800	-1.31290500
C	3.08301900	-0.68547000	0.43314000	H	-1.54547000	0.85971500	1.56175900
H	6.60832800	0.39555000	1.55979800	H	-1.16266800	2.56382300	1.96643300
H	5.24741100	1.49469600	1.89714800	H	-3.90090600	1.30880600	1.31677100
H	3.36377700	1.44828700	0.48997000	H	-3.52672500	2.39699000	2.67106900
H	3.44836100	0.74875700	-1.13990200	H	-4.64506200	3.42827800	0.41979100
H	3.94002900	-0.19899100	2.82286100	H	-3.28597700	4.30199200	1.16554400
H	5.41818000	-1.20671600	2.83668900				
Cl	4.47379700	-3.76647400	2.64136700				
H	2.90146600	-3.16745900	0.96863700	15			
H	2.67889400	-2.23271700	2.49829700	Num. Imaginary Frequencies: 0			
H	2.28839100	-0.47687300	1.15516300	H	-6.38905500	0.38423200	0.13679100
H	2.71854700	-1.34638000	-0.35944200	C	-5.40059700	0.56819300	-0.30294700
B	3.16958500	-2.76232600	-2.61282600	C	-4.44172800	1.18323700	0.73314000
F	3.08144700	-1.36121500	-2.71290100	H	-5.52331000	1.27403800	-1.13418100
F	4.51201700	-3.13437100	-2.56310300	N	-4.87917700	-0.69448600	-0.81514200

Num. Imaginary Frequencies: 0

H	-3.88724000	2.03756000	0.33470100	H	0.47746600	3.90448900	-1.01281800
H	-4.94561700	1.47756200	1.65934500	C	2.93694000	5.23848100	-0.54690200
N	-3.41892600	0.13602000	1.09813500	H	2.57166900	5.60629400	-1.51321400
C	-4.85042200	-1.68048400	0.26176700	H	2.58396400	5.91955500	0.24262300
C	-3.51746300	-0.47750500	-1.29552100	H	4.03035400	5.23666000	-0.55146700
C	-4.13745400	-1.12613000	1.51145600	N	2.47950600	3.89229000	-0.32010300
C	-2.47004800	0.63036900	2.13296300	C	1.12235200	2.05365500	-0.00107900
C	-2.56586400	-0.17917000	-0.12879000	H	0.32643100	1.71411100	0.66938900
H	-5.87668100	-1.97095300	0.51748600	C	0.96991200	1.45904500	-1.38593300
H	-4.32376400	-2.57184500	-0.09977300	H	1.69447600	1.88756800	-2.09190300
H	-3.16664600	-1.36815000	-1.82936900	H	-0.05427400	1.58210400	-1.75491000
H	-3.51735000	0.36611500	-1.99565100	Au	1.24246000	-0.62661200	-1.62427000
H	-3.38355700	-1.80823300	1.91475400	P	1.23371100	-3.12243700	-2.04343800
H	-4.83582100	-0.84200900	2.30509400	N	2.44239300	1.87136500	0.60969700
Cl	-3.25456200	0.94494900	3.69941200	F	-0.67999400	-0.66914800	-2.07719100
H	-2.04659800	1.56638500	1.75669000	C	1.90452200	-4.29274400	-0.81317600
H	-1.71592200	-0.14841200	2.28286500	H	2.97933400	-4.14323200	-0.66437500
H	-1.93851100	-1.03203800	0.14466900	H	1.38167400	-4.15009400	0.13896700
H	-1.94288200	0.69819900	-0.32319900	H	1.73835000	-5.31870500	-1.16825000
B	-2.24223100	3.26927800	-1.33572300	C	2.05605300	-3.58303200	-3.61261600
F	-2.02303700	2.23879300	-2.25693300	H	1.59442000	-3.02808600	-4.43799300
F	-3.61006100	3.47578500	-1.18260200	H	3.12327400	-3.33192000	-3.58221200
F	-1.60300800	4.42807900	-1.74587700	H	1.95069800	-4.65916300	-3.80352500
F	-1.70046000	2.86250200	-0.08153000	C	-0.48981300	-3.66506900	-2.27586300
B	-0.86530500	-3.00684300	1.43725400	H	-1.03307300	-3.53453600	-1.33276300
F	-0.07227700	-4.05127200	1.88571700	H	-0.96549600	-3.05019100	-3.04659100
F	-0.13698500	-2.24175100	0.49445500	H	-0.50959800	-4.72056800	-2.57643400
F	-2.01978200	-3.47610000	0.81296600	C	4.11830500	0.32110900	-2.33728500
F	-1.20953800	-2.16675100	2.50597600	O	3.32457300	-0.32388200	-1.30750500
C	2.21563700	-1.41384700	2.31255100	C	4.14969300	-1.40852800	-0.79790100
C	1.87806000	-0.28774700	1.56491200	C	5.56815500	-0.84679000	-0.81823800
C	2.79934000	0.75475400	1.37949800	C	5.46419800	0.43982800	-1.65863600
C	4.05802500	0.65102200	1.99610500	H	4.12928700	-0.32689300	-3.22825200
C	4.37232600	-0.46946200	2.75475200	H	3.63882900	1.27374700	-2.57715300
C	3.46399400	-1.51432400	2.91564000	H	3.75721900	-1.66448400	0.19074200
H	1.48845800	-2.21832000	2.40530700	H	4.03990400	-2.26382500	-1.48086200
H	0.88413800	-0.25498200	1.12435300	H	5.91306700	-0.62433100	0.19677800
H	4.78189400	1.44778000	1.86578600	H	6.25733000	-1.57316600	-1.26184000
H	5.35427400	-0.52440800	3.22363900	H	5.45457200	1.32084800	-1.00601100
H	3.72661200	-2.39154400	3.50355100	H	6.27690600	0.54676800	-2.38358700
C	3.26838500	2.95040200	0.28348000				
O	4.47385500	3.04453000	0.47130400				
C	1.07628900	3.58221900	-0.15400300				
H	0.66216600	4.05916800	0.75052400				

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Num. Imaginary Frequencies: 1

H	-6.41772500	0.33727100	-0.25245500	H	4.04796900	-2.63600200	2.88351200
C	-5.41616200	0.53829300	-0.65326500	C	3.18311200	3.22121300	0.84197700
C	-4.49697200	1.13256800	0.43055700	O	4.34262300	3.39325100	1.18070200
H	-5.51507000	1.26448200	-1.46972100	C	1.00334800	3.68952500	0.14949600
N	-4.87019300	-0.70923800	-1.17981200	H	0.37483600	4.09118400	0.96008200
H	-3.91721000	1.98718600	0.06905300	H	0.54597100	3.99019100	-0.80063500
H	-5.03788200	1.41864100	1.33846700	C	2.72945400	5.52884600	0.12176200
N	-3.50188300	0.06860700	0.82232800	H	2.50026900	5.88697000	-0.88945300
C	-4.88332400	-1.72508300	-0.12974900	H	2.18452300	6.15170500	0.84608800
C	-3.48791400	-0.47675000	-1.58924000	H	3.80313600	5.62531700	0.30447000
C	-4.25655500	-1.19168900	1.17099500	N	2.36803800	4.14205400	0.25575800
C	-2.60170800	0.52701300	1.91522700	C	1.14900500	2.16103900	0.28273500
C	-2.59231500	-0.22227000	-0.36995300	H	0.32730700	1.76878600	0.89154900
H	-5.91517800	-2.04527400	0.05924900	C	1.15292400	1.54410900	-1.09796600
H	-4.31841100	-2.59710100	-0.48431700	H	1.99844200	1.90694400	-1.69877200
H	-3.11829700	-1.34949800	-2.14084500	H	0.19446300	1.67503000	-1.61320600
H	-3.45482100	0.38894100	-2.26148900	Au	1.37003500	-0.56433800	-1.18406400
H	-3.54586100	-1.88660200	1.62631600	P	1.31481300	-3.04570300	-1.53879700
H	-5.00711800	-0.90761800	1.91570000	N	2.43438200	2.03773200	0.96818700
Cl	-3.45462600	0.77296100	3.45719800	F	-0.45562400	-0.52585700	-2.07234400
H	-2.17018100	1.47872500	1.59325900	C	1.84737200	-4.24966200	-0.27656600
H	-1.84993600	-0.25185800	2.07179900	H	2.89342000	-4.08368900	0.00822400
H	-1.98446700	-1.08530800	-0.08307100	H	1.21128900	-4.15026500	0.61133600
H	-1.94810700	0.65006200	-0.51249800	H	1.74626300	-5.26547800	-0.68179600
B	-2.12990300	3.24279600	-1.42039700	C	2.25229200	-3.53323000	-3.03382400
F	-1.81290800	2.20925600	-2.30750000	H	1.95715700	-2.90036900	-3.87933700
F	-3.50873500	3.43806200	-1.40106600	H	3.33031700	-3.41873300	-2.86689700
F	-1.46420200	4.40536000	-1.77561100	H	2.04847800	-4.58264700	-3.28496000
F	-1.71103400	2.85084100	-0.11613500	C	-0.39314000	-3.53756000	-1.93555800
B	-1.05546700	-2.91397800	1.81781700	H	-1.01177500	-3.47304300	-1.03273300
F	-0.13099600	-3.83400200	2.29515400	H	-0.79250800	-2.84874700	-2.68596500
F	-0.37338600	-1.94950300	1.03160000	H	-0.40645700	-4.56667500	-2.31680000
F	-2.00998800	-3.52965300	1.00590000	C	4.05030600	0.22928300	-2.70469900
F	-1.68854100	-2.25438100	2.87132000	O	3.67413900	-0.24043200	-1.38596700
C	2.43282300	-1.51982200	2.00165700	C	4.61673600	-1.25889100	-0.95200000
C	2.01076600	-0.28096100	1.49408000	C	5.59307400	-1.43589900	-2.10084600
C	2.89119300	0.82505100	1.46971800	C	5.52539600	-0.08303500	-2.80081100
C	4.18949700	0.65686800	1.98419000	H	3.46575500	-0.31911100	-3.46004800
C	4.58149800	-0.57684200	2.47968400	H	3.80319200	1.29427600	-2.76019800
C	3.71890100	-1.67930700	2.48329300	H	5.09586700	-0.87508300	-0.04350100
H	1.70839800	-2.33179700	2.04476100	H	4.05626100	-2.16555200	-0.69059600
H	0.94497500	-0.15386300	1.31530500	H	6.59592800	-1.69517600	-1.74698400
H	4.87205700	1.49820000	1.98726500	H	5.26084600	-2.22877800	-2.78538500
H	5.59094600	-0.68109300	2.87571700	H	6.10846600	0.66943100	-2.25391400

H	5.87703000	-0.11099300	-3.83705200
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Num. Imaginary Frequencies: 0			
O	4.87461300	0.71616400	0.60088900
H	4.80034700	0.03880800	1.29263400
H	4.87780300	0.21158200	-0.22783700
N	2.13476000	-1.17509300	0.27959400
C	1.35594700	-2.89681400	2.30694300
C	1.73314500	-2.78351100	-1.78461700
O	3.65422000	-1.54261400	2.35065100
O	1.46426800	-0.29428500	2.49555400
O	3.79131400	-1.12942800	-1.65746700
O	3.79084200	-3.13859900	-0.13635800
S	2.28337400	-1.34373600	1.90313400
S	3.08113600	-2.04106400	-0.76685000
F	1.93621000	-3.96169100	1.80273100
F	1.29561600	-2.99404400	3.62113800
F	0.12763200	-2.78619100	1.81431800
F	0.99945500	-1.82243400	-2.31725100
F	2.28401500	-3.51038800	-2.73603600
F	0.98076700	-3.54471600	-1.01106700
Au	1.93674900	0.96328800	-0.33071100
P	2.31511700	3.13503100	-1.01278900
H	-3.10739900	-2.31206700	-0.02437200
C	-2.89190000	-1.58176500	0.76134300
C	-4.15015300	-0.78799900	1.14640900
H	-2.39559600	-2.05798000	1.61190500
N	-1.90943800	-0.61079700	0.18619400
H	-4.45998800	-1.00459200	2.17364400
H	-4.96690900	-1.00169300	0.45259100
N	-3.83662000	0.68654300	1.05913800
C	-2.49758100	0.14110900	-0.96309100
C	-1.38775500	0.31848700	1.22674800
C	-3.58721300	1.04870400	-0.39166600
C	-4.92423400	1.55520800	1.63361300
C	-2.60250400	0.95540600	1.89609200
H	-2.88671600	-0.61453700	-1.65317500
H	-1.68220600	0.72453700	-1.39982300
H	-0.75823400	1.05637400	0.71762600
H	-0.78348300	-0.27255300	1.92010800
H	-3.29645900	2.10116500	-0.40521700
H	-4.52176300	0.87918900	-0.93041700
Cl	-6.48894600	1.27265000	0.88179100
H	-4.99114100	1.33227800	2.70192300

H	-4.60975600	2.59024600	1.46774800
H	-2.46137400	2.03589800	1.97629400
H	-2.79735100	0.52726100	2.88423700
F	-0.84238000	-1.33040600	-0.29876900
B	-1.31920500	3.74216300	0.44049800
F	-0.65787600	3.28353100	1.58405600
F	-1.10913400	2.79727800	-0.59422700
F	-2.70375600	3.78902600	0.71059500
F	-0.84865100	4.97454000	0.05167500
B	-5.06241700	-2.36137800	-1.77848300
F	-3.67868000	-2.44511400	-2.06644200
F	-5.28382900	-2.99071100	-0.54974800
F	-5.38591600	-0.99190200	-1.63238600
F	-5.80231400	-2.93109500	-2.78215700
C	4.01890000	3.15091700	-1.66200700
H	4.08183300	2.49998600	-2.54220800
H	4.31464100	4.17108400	-1.93959000
H	4.69339700	2.76246000	-0.88930300
C	1.29948300	3.88193200	-2.32006500
H	0.28852200	4.04507300	-1.93874500
H	1.74519800	4.84170900	-2.61248400
H	1.26280300	3.21664500	-3.18933300
C	2.32999000	4.33069800	0.35557900
H	2.68892100	5.30103800	-0.01191100
H	1.32042100	4.44537800	0.76206500
H	3.00240500	3.96546900	1.14035400

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Num. Imaginary Frequencies: 1			
N	2.23669500	-0.89198300	-0.16355700
C	4.93475000	-1.41422700	0.07027000
C	2.02336900	-1.74430700	-2.68756800
O	3.15527100	-2.27006100	1.84647300
O	3.60329700	0.20463100	1.60083400
O	0.10140900	-2.05445200	-0.92569800
O	2.19006300	-3.43490800	-0.66277600
S	3.36617600	-1.10869600	1.00785100
S	1.55243300	-2.16319300	-0.95037500
F	4.88423700	-2.52914500	-0.62777500
F	5.91785200	-1.47984800	0.94769300
F	5.14495200	-0.38968800	-0.75059700
F	1.55034800	-2.69098200	-3.47688000
F	3.33975100	-1.69352300	-2.78905600

F	1.50890000	-0.57679100	-3.04015800
Au	1.18935200	1.10746800	-0.13646300
P	0.21124900	3.22026700	-0.18282000
H	-1.18852500	-2.06818700	1.08939200
C	-2.05015300	-1.50342800	1.45773700
C	-3.31057700	-2.38668000	1.56879200
H	-1.77821000	-1.00125800	2.39005800
N	-2.37659600	-0.46837000	0.48394800
H	-3.57834500	-2.59209800	2.61071200
H	-3.20172600	-3.33498100	1.03563200
N	-4.47748100	-1.65160100	0.93177300
C	-2.82409400	-1.01542200	-0.79344200
C	-3.29269100	0.52063400	1.03649600
C	-4.25404100	-1.53109100	-0.56591500
C	-5.79091900	-2.30287500	1.23524500
C	-4.53341900	-0.24930700	1.51447600
H	-2.12231000	-1.80023300	-1.08669800
H	-2.82309900	-0.21624500	-1.53822100
H	-3.54788300	1.22280300	0.24182900
H	-2.77773100	1.01607300	1.86291800
H	-4.99979900	-0.82156700	-0.94167500
H	-4.41008400	-2.51801000	-1.01044200
Cl	-5.84169600	-3.99707700	0.74315200
H	-5.95472400	-2.23824200	2.31428400
H	-6.56458900	-1.75025800	0.69518800
H	-5.44717500	0.22735400	1.14612000
H	-4.57487300	-0.36550400	2.60216100
F	-0.90085500	0.37329700	0.15198400
B	-4.54396600	1.69172600	-2.12555400
F	-5.33195100	1.39782900	-0.98910000
F	-3.23657100	2.01460500	-1.67332400
F	-4.45845500	0.54058600	-2.90840000
F	-5.08148200	2.74473300	-2.82480400
O	3.50376700	2.16852600	-0.44866100
H	3.90211700	1.67758400	-1.18406000
H	3.84206400	1.72153600	0.35182700
B	0.23405700	0.91959800	3.19494200
F	0.63541900	0.77936300	4.50646800
F	0.57338700	-0.21642100	2.44707000
F	-1.16876300	1.08970200	3.14045200
F	0.83882800	2.05575400	2.62367300
C	-0.11481300	3.78787800	-1.87761200
H	-0.44522400	4.83494500	-1.85954900
H	0.79342500	3.70440300	-2.48464500

H	-0.90694600	3.17105200	-2.31713100
C	1.38627000	4.38884700	0.55509000
H	0.97379800	5.40521600	0.51549500
H	1.55610900	4.09136000	1.59512700
H	2.33458700	4.34241000	0.01014800
C	-1.35612000	3.41147100	0.70231100
H	-1.57060400	4.48295400	0.80833900
H	-2.14977400	2.94479500	0.10875200
H	-1.28191700	2.94367200	1.69011900

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Num. Imaginary Frequencies: 0

N	2.17241500	-0.10751400	-0.76262900
C	4.91160400	-0.25015400	-0.45731900
C	2.54173700	2.46362300	0.31610800
O	3.73757600	-0.60333500	-2.80879300
O	3.34160800	-2.27379500	-0.96621500
O	0.35356400	1.59198800	-0.95914500
O	2.45934900	1.94761700	-2.31108800
S	3.46295300	-0.88140800	-1.41554000
S	1.79184500	1.47309700	-1.11400000
F	5.02758900	1.05529300	-0.62967800
F	5.99117700	-0.86105600	-0.89811000
F	4.73249600	-0.52370800	0.82214800
F	1.58699600	3.18109100	0.87326800
F	3.45886200	3.27252500	-0.17918400
F	3.09680000	1.66940300	1.20709100
Au	0.50366400	-1.50468900	-0.10247800
P	-1.23280000	-3.01803500	0.40765000
H	-2.29198500	0.50656900	-1.49957000
C	-3.08480200	1.16870900	-1.13500800
C	-2.63363500	2.63809700	-1.24629200
H	-3.99437200	0.96909900	-1.71094300
N	-3.36185900	0.82428500	0.25518100
H	-3.21562400	3.22326400	-1.96810300
H	-1.56913300	2.72949900	-1.47922600
N	-2.83488000	3.29914400	0.10517100
C	-2.20466500	1.12532400	1.07724600
C	-4.51497000	1.57301200	0.72141200
C	-1.93638800	2.63808500	1.13110600
C	-2.60835600	4.76972400	0.04441800
C	-4.28029000	3.08793900	0.52651900
H	-1.33025100	0.62200900	0.65270600

H	-2.35964900	0.73939000	2.09345900	C	-5.38497700	0.52635500	1.62419100
H	-4.67867100	1.34746600	1.78246800	H	-7.51064000	0.31944800	1.14283200
H	-5.39155700	1.24128300	0.15565500	N	-6.39438300	-0.81234300	-0.20460200
H	-2.19287500	3.09458700	2.09490000	H	-5.71574900	0.68526100	2.65738700
H	-0.89912100	2.87730800	0.88071100	H	-4.68753900	1.31818900	1.32757000
Cl	-0.97793900	5.19960800	-0.49874500	N	-4.59996300	-0.76556600	1.59993500
H	-3.33394700	5.19511400	-0.65511000	C	-5.07410300	-0.80877800	-0.82490900
H	-2.75758000	5.17821600	1.04790100	C	-6.52301300	-1.99766300	0.62962600
H	-4.43329500	3.67050900	1.44195400	C	-3.95739900	-0.89779900	0.23671100
H	-4.89610100	3.51660400	-0.27231600	C	-3.58851200	-0.86373900	2.69273500
F	-0.81354500	-0.97920500	-1.45359500	C	-5.54972800	-1.93185500	1.81897000
B	0.59571700	0.01971100	2.96952400	H	-4.95954300	0.11048400	-1.40512200
F	0.56219300	0.84133000	1.83983500	H	-5.00195800	-1.66883100	-1.50184300
F	-0.25522100	-1.08192800	2.73615200	H	-6.29417000	-2.88041600	0.02156800
F	1.91697200	-0.51176200	3.08549600	H	-7.55437100	-2.08033900	0.99303600
F	0.24217700	0.68986600	4.10201100	H	-3.45860100	-1.87186200	0.25109400
O	1.83156000	-2.35772200	1.28764100	H	-3.22789800	-0.08354400	0.13825100
H	1.97402200	-1.69698700	2.02968100	Cl	-2.39883500	0.44357600	2.67151000
H	2.66854400	-2.44865300	0.77442700	H	-4.12489400	-0.83248300	3.64536400
B	-5.40189700	-1.53321600	-1.06450400	H	-3.07761500	-1.82320000	2.56784900
F	-6.22496500	-2.50900300	-1.61227300	H	-4.92700600	-2.82750300	1.89981300
F	-5.83786200	-0.26138000	-1.47549300	H	-6.04803500	-1.73869000	2.77634100
F	-5.43077000	-1.60415600	0.32923400	F	-0.79625900	0.39334900	-0.77915300
F	-4.08143800	-1.73263600	-1.51749700	B	-3.52601700	2.42074100	-1.14119800
C	-1.70656600	-3.77899900	-1.15043900	F	-3.09162500	1.33459900	-1.92495000
H	-0.82309800	-4.05665900	-1.73392600	F	-3.03596100	2.27566500	0.16368200
H	-2.28778000	-4.68024300	-0.91262100	F	-3.05560600	3.61056500	-1.69321500
H	-2.33669900	-3.07054400	-1.69688200	F	-4.92497100	2.42958500	-1.11096300
C	-0.52322900	-4.23354900	1.53088500	O	2.55883600	-0.81437000	-2.75874600
H	-0.17830500	-3.73475500	2.44132700	H	2.82382900	-1.73321700	-2.47017900
H	-1.31325500	-4.95429700	1.78202500	H	3.28207700	-0.28908600	-2.34313700
H	0.31219300	-4.75498300	1.05282400	B	-3.15950700	-4.59643900	0.36608900
C	-2.62469800	-2.18485700	1.14996700	F	-4.11093400	-3.94457800	-0.43320600
H	-3.43482000	-2.92530200	1.21393000	F	-3.55370400	-5.87059900	0.67544900
H	-2.34106800	-1.82635300	2.14289400	F	-1.93067800	-4.60722000	-0.32677500
H	-2.99051800	-1.36725000	0.50953900	F	-2.97791600	-3.82855800	1.54364000

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Num. Imaginary Frequencies: 0

Au	0.79365800	-0.16062100	-1.77747400	C	0.61562100	-3.67172200	-1.65535000
P	-0.28701700	-2.21979600	-1.10396500	H	1.58268700	-3.75333000	-1.14770400
H	-6.55782800	1.26411600	-0.03017900	H	-0.02147200	-4.52489400	-1.38350200
C	-6.54906700	0.38357400	0.61870800	H	0.75430500	-3.65216100	-2.74159900

C	-0.37991100	-2.12845300	0.68400400
H	-1.07308700	-2.90875100	1.02782300
H	0.62742200	-2.29708400	1.08636900
H	-0.72712000	-1.12897200	0.96654500
C	-1.30452600	3.56684600	2.70630600
C	-0.66251000	4.11369800	1.60064900
C	0.73352300	4.16023400	1.56441400
C	1.46651400	3.67186800	2.65092200
C	0.81429400	3.14729700	3.75810400
C	-0.57715400	3.09069700	3.79356200
H	-2.39239600	3.51393900	2.70588600
H	-1.24677900	4.49605200	0.76657000
H	2.55511100	3.70265600	2.61179200
H	1.40059600	2.77336300	4.59616600
H	-1.08942300	2.67325900	4.65876200
C	1.03091600	5.21764300	-0.72771400
O	1.54524400	6.22769000	-1.19048100
C	-0.06355300	3.05594200	-1.28329600
H	-0.17871100	2.73077800	-0.24393200
H	-0.97835100	2.75081300	-1.80277900
C	-0.39606900	5.07292900	-2.65898800
H	0.30344100	4.84924400	-3.47962900
H	-1.38072500	4.65615800	-2.88549500
H	-0.47106400	6.15834100	-2.56577900
N	0.04787900	4.51253900	-1.38967800
C	1.16315000	2.46903400	-1.90624900
H	2.10549900	2.62563900	-1.37209000
C	1.17423700	1.87199200	-3.12969500
H	2.10448200	1.61125800	-3.63319400
H	0.25673400	1.79464000	-3.71895100
H	2.32576100	5.16864800	0.76614900
N	1.46585800	4.70581900	0.48997000
N	4.05628800	-0.60709000	-0.21000800
C	4.13318800	0.43851000	2.36048500
C	5.54562000	-2.77156400	0.40908400
O	1.88922300	0.14054000	0.97730100
O	3.60070800	1.79344900	0.16756700
O	3.65686500	-2.78173800	-1.38493800
O	2.95946000	-2.64406300	1.01598400
S	3.28643400	0.48145000	0.71542600
S	3.85353100	-2.19437000	-0.04326500
F	3.98975000	-0.74980200	2.91653100
F	3.58289300	1.35727400	3.13279800
F	5.41483100	0.70523400	2.19683600

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Num. Imaginary Frequencies: 1

Au	0.60492800	-0.14979900	-1.32911400
P	-0.53341800	-2.13559700	-0.52840800
H	-5.61041200	2.62819700	2.13142300
C	-5.55698100	1.71799200	2.73801800
C	-4.15231700	1.61905600	3.36920400
H	-6.32979600	1.76925200	3.51508700
N	-5.83562700	0.56304000	1.88722800
H	-4.15627200	1.75559400	4.45715600
H	-3.44790500	2.32125400	2.91628100
N	-3.62925600	0.22226000	3.11346500
C	-4.75060200	0.41457200	0.92187400
C	-5.90942100	-0.64038900	2.70527100
C	-3.44750900	-0.00018000	1.62563500
C	-2.37061700	-0.06036900	3.85776600
C	-4.66978900	-0.76727900	3.61021500
H	-4.61443900	1.37516700	0.41279700
H	-5.02687200	-0.34919100	0.18293700
H	-5.96644600	-1.51090300	2.04089400
H	-6.81688800	-0.61411500	3.32049300
H	-3.23652100	-1.07137700	1.52582700
H	-2.59764900	0.60288500	1.29313600
Cl	-1.04772400	1.03458200	3.40832400
H	-2.57541400	0.06319000	4.92502000
H	-2.08641100	-1.09433600	3.63783000
H	-4.21216800	-1.75977900	3.56158200
H	-4.86813100	-0.49952800	4.65470300
F	-1.08290600	0.62709900	-0.67296400
B	-3.46943400	4.02135700	0.84598400
F	-2.66412900	2.86313400	0.91465800
F	-3.65571900	4.50592700	2.14280800
F	-2.83177700	4.98073100	0.05694600
F	-4.70196200	3.68225000	0.28473400
O	2.42142700	-1.00900400	-1.96090900
H	2.45679600	-1.97440900	-1.75718400
H	3.11744000	-0.68076700	-1.31895300
B	-3.28753300	-3.91863500	1.89408400
F	-2.68112100	-3.13872300	2.91073800

F	-2.28168400	-4.30985700	0.99166000
F	-3.91296900	-5.01165000	2.43513200
F	-4.20437400	-3.09662700	1.21398500
C	-2.23833700	-1.98709900	-1.09110400
H	-2.30260800	-2.34960100	-2.12279000
H	-2.86993900	-2.60534100	-0.43751200
H	-2.54507200	-0.93870300	-1.04485400
C	0.13269100	-3.71588900	-1.07662600
H	1.13601300	-3.88128600	-0.67072100
H	-0.55484300	-4.47618200	-0.67908100
H	0.14405900	-3.77386800	-2.17033200
C	-0.30851400	-1.90881400	1.23993000
H	-0.91454900	-2.65600900	1.77040800
H	0.75331700	-2.02799500	1.49424700
H	-0.61891900	-0.89236000	1.51281300
C	-0.46513800	4.47743700	2.93758400
C	-0.04827200	4.73998200	1.63687000
C	1.28283000	4.50645600	1.28043800
C	2.17985300	4.00537600	2.23152200
C	1.75108200	3.75385900	3.52831000
C	0.42682200	3.99224200	3.88988500
H	-1.51181300	4.64503200	3.18652300
H	-0.77386200	5.11048000	0.91419600
H	3.20855400	3.79151600	1.94028700
H	2.45806300	3.35927500	4.25676700
H	0.09015400	3.78899700	4.90491300
C	1.06233900	5.34661500	-1.07980500
O	1.46103600	6.39121700	-1.57102100
C	-0.29764400	3.26878500	-1.14033500
H	-0.94446100	3.19782100	-0.25793800
H	-0.84617000	2.82174700	-1.98107000
C	-0.94199600	5.26746700	-2.45589000
H	-0.86709100	4.78753200	-3.44169100
H	-1.96425000	5.17134900	-2.07489000
H	-0.68386200	6.32361700	-2.55572700
N	-0.02237300	4.65292400	-1.51576600
C	0.97871600	2.50255600	-0.94026200
H	1.33216700	2.32529600	0.07460200
C	1.64854300	1.90722800	-1.98068400
H	2.67082700	1.56565800	-1.82205800
H	1.33182800	2.08046300	-3.01164600
H	2.74814800	5.00150100	-0.05266900
N	1.77414800	4.70972500	-0.03264900
N	3.89253000	-0.76862700	0.40340700

C	4.75146400	0.69989200	2.60822200
C	5.39102900	-2.91432400	1.00242900
O	2.19056800	0.33298500	2.01716100
O	3.63904100	1.67142700	0.44801500
O	3.14014300	-3.03315800	-0.32484600
O	3.01919800	-2.52954000	2.13375000
S	3.45192700	0.51051800	1.30995700
S	3.65944900	-2.30632500	0.84684900
F	4.71679500	-0.31157000	3.45472500
F	4.50420100	1.82941300	3.25241300
F	5.93715500	0.76655600	2.03446900
F	5.35403000	-4.18677200	1.34806600
F	6.01326200	-2.21289400	1.93116300
F	6.01069600	-2.78004100	-0.15321300

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Num. Imaginary Frequencies: 0

C	0.68891900	-4.48008100	1.24134400
C	0.09937600	-3.80017200	0.18025100
C	-0.26136200	-2.47008600	0.35920200
C	-0.01565000	-1.79630100	1.54628400
C	0.56437900	-2.49225900	2.60273400
C	0.90567500	-3.83399600	2.45577500
H	0.96775400	-5.52352300	1.11587400
H	-0.08622700	-4.31988200	-0.75795300
H	-0.25236300	-0.73781600	1.65048700
H	0.75761100	-1.96248000	3.53277800
H	1.35587700	-4.37542900	3.28582600
C	-1.74960200	-2.66029600	-1.62718400
O	-2.74135500	-3.18921100	-1.21181800
C	0.20392900	-2.05601600	-2.77950700
H	1.00760000	-2.77179700	-2.56343700
H	0.40585700	-1.59876100	-3.75300300
C	-1.49894400	-3.59634400	-3.86128600
H	-1.55531000	-3.02880900	-4.79627400
H	-0.77443200	-4.41151300	-3.97844200
H	-2.48173700	-4.01018200	-3.62325500
N	-1.09087100	-2.71861300	-2.78260100
C	0.05725700	-1.00451300	-1.67187100
H	1.00752900	-0.88312700	-1.14172300
C	-0.47523600	0.31082900	-2.19189700
H	-1.55768800	0.31151700	-2.36280200
H	0.05038300	0.55187500	-3.12240800

H	-1.61879200	-1.07986900	-0.29978900	F	2.99669500	-2.82130100	-3.91539200
N	-0.91198600	-1.71502200	-0.73320700	F	3.11416800	-2.88684600	-1.63241900
N	-3.35285000	-0.47886200	0.34272700	B	1.24410800	1.53375300	2.78183900
C	-3.83538600	-1.51230000	2.73331800	F	0.62107600	1.34010800	1.50977700
C	-5.87913600	-0.36599200	-0.84892200	F	1.64987400	0.27898300	3.24579300
O	-4.62434300	0.94052900	2.13304400	F	2.36761900	2.34765700	2.59283000
O	-2.15788000	0.49866000	2.31843900	F	0.34899200	2.13839900	3.63170700
O	-3.59659400	-0.47095800	-2.11866100	Au	0.07441200	2.07532100	-1.12692600
O	-4.10834500	1.64201600	-0.86678000	P	0.86364400	4.24286100	-0.19848500
S	-3.48771200	0.07524200	1.86399800	F	1.58978100	2.15441200	-2.37875300
S	-4.10988900	0.17070700	-0.91548200	O	-1.56320200	2.21674900	0.17861800
F	-5.01062300	-1.96153400	2.33398100	H	-2.45919400	2.06274600	-0.21205200
F	-3.86405900	-1.26965000	4.03054900	H	-1.45134300	1.66777600	0.99507900
F	-2.89753000	-2.39866900	2.46361900	C	0.08104000	4.75124600	1.36072800
F	-6.46013800	0.03733600	-1.96335300	H	-0.99582000	4.87811900	1.20428900
F	-6.49674600	0.15320800	0.19035200	H	0.23662500	3.97787200	2.12302100
F	-5.90298100	-1.68321500	-0.77815700	H	0.51355900	5.69997500	1.70306600
H	6.62338200	0.49951400	-0.74296900	C	0.48606900	5.54360100	-1.41665200
C	5.56799900	0.20743700	-0.68305000	H	0.99475900	5.30699600	-2.35888700
C	5.43990700	-1.13767300	0.05806700	H	-0.59352100	5.58636000	-1.59983400
H	5.18025600	0.09897000	-1.70217500	H	0.83077700	6.52131000	-1.05603500
N	4.81048600	1.25475000	-0.00571000	C	2.65904400	4.35214600	0.06669600
H	5.15862300	-1.95532900	-0.61298400	H	2.91066400	3.80117000	0.97893100
H	6.34542200	-1.40978200	0.60984200	H	3.19155400	3.91585800	-0.78634800
N	4.33937000	-0.99912900	1.08601700	H	2.94960600	5.40400600	0.18408800
C	5.18477700	1.29292600	1.40538500	TS8_{H2O}			
C	3.38828000	0.94589900	-0.11576900	Num. Imaginary Frequencies: 1			
C	4.75762800	0.00165300	2.13562000	C	-0.05814700	-4.56640800	1.21652100
C	3.94351800	-2.30830700	1.66769100	C	-0.56790100	-3.82604400	0.15368300
C	3.09257500	-0.46915600	0.39791500	C	-0.59504100	-2.43529600	0.23731500
H	6.27060500	1.43444900	1.47143600	C	-0.07914700	-1.78931600	1.35616300
H	4.69505700	2.14660600	1.88674900	C	0.41439400	-2.53676400	2.42021300
H	2.82929000	1.66955400	0.48425800	C	0.42037100	-3.92751100	2.35640600
H	3.06588600	1.03195600	-1.16039300	H	-0.04348400	-5.65218900	1.14905700
H	3.88329200	0.14843600	2.77982500	H	-0.95957800	-4.34100600	-0.72142100
H	5.56713400	-0.45377900	2.71472800	H	-0.07947900	-0.70181500	1.41058400
Cl	5.28274300	-3.16112900	2.46029600	H	0.78870800	-2.01189000	3.29718300
H	3.56188600	-2.92725200	0.84792200	H	0.80158200	-4.51303100	3.19101100
H	3.16374800	-2.11671200	2.41113700	C	-1.98932000	-2.40329600	-1.74951600
H	2.29091000	-0.47983600	1.14614900	O	-3.04076700	-2.90422400	-1.41682800
H	2.88491900	-1.18078100	-0.40660000	C	-0.00360400	-1.89991300	-2.85218200
B	3.46647500	-2.15540000	-2.79897000	H	0.72988600	-2.69315100	-2.65365600
F	2.85579800	-0.88819100	-2.69885000				
F	4.84796900	-2.00814900	-2.84300500				

H	0.28038500	-1.40176100	-3.78447600
C	-1.82389600	-3.20166400	-4.05872900
H	-1.82710500	-2.57801400	-4.96023500
H	-1.18065200	-4.07399200	-4.23394000
H	-2.84167300	-3.53901100	-3.84521600
N	-1.34976800	-2.43898800	-2.92878200
C	-0.11841800	-0.92502800	-1.67025600
H	0.82715600	-0.90821700	-1.11807300
C	-0.50838000	0.45935900	-2.14290300
H	-1.58660900	0.60179200	-2.26981300
H	0.01312800	0.68896800	-3.07853300
H	-2.25810500	-0.84153500	-0.16546100
N	-1.16521700	-1.60448300	-0.81917200
N	-3.20870700	-0.31180800	0.27787900
C	-3.75990100	-1.62634500	2.56171400
C	-5.87858600	-0.08567600	-0.65533600
O	-4.41459200	0.92914300	2.16645200
O	-1.96308000	0.35842400	2.38294400
O	-3.69272700	-0.06661000	-2.14774400
O	-4.04989600	1.91641400	-0.62533400
S	-3.30062900	0.04363400	1.90539800
S	-4.10948400	0.47770800	-0.87106800
F	-4.98202100	-1.89150600	2.15068100
F	-3.71861000	-1.56514100	3.87470800
F	-2.91878700	-2.53022200	2.11312700
F	-6.48055400	0.19219900	-1.79241600
F	-6.46254300	0.54612800	0.33205000
F	-5.87437400	-1.38154700	-0.44087400
H	6.62204100	0.10648600	-0.81660800
C	5.54925500	-0.10915800	-0.74397800
C	5.33551200	-1.46309900	-0.03973600
H	5.13764600	-0.16194300	-1.75804000
N	4.88491900	0.97092300	-0.02147700
H	4.98444900	-2.23625100	-0.73010400
H	6.22712100	-1.81663600	0.48801400
N	4.26468300	-1.27634900	1.01150400
C	5.28428700	0.93696700	1.38215700
C	3.44134500	0.77478900	-0.10762700
C	4.77731400	-0.34353100	2.08188800
C	3.78237400	-2.57216800	1.55900800
C	3.04933100	-0.63036400	0.36655900
H	6.37826600	0.99939400	1.43376700
H	4.86279200	1.80688800	1.89756300
H	2.95339300	1.51623800	0.53207100

H	3.10286000	0.91996900	-1.14130400
H	3.92925400	-0.15160500	2.74947200
H	5.56299400	-0.87429200	2.62912900
Cl	5.07286100	-3.54675300	2.29126300
H	3.33791000	-3.13162900	0.72815200
H	3.03401600	-2.35191600	2.32619000
H	2.26622200	-0.60603200	1.13247000
H	2.76620200	-1.29677500	-0.45386700
B	3.25119500	-2.21654300	-2.87641200
F	2.72296000	-0.92072200	-2.72269000
F	4.64007800	-2.14901800	-2.95008400
F	2.72387900	-2.81767600	-4.00372200
F	2.88451500	-2.96425900	-1.72547800
B	1.40082900	1.43058700	2.86426100
F	0.77207000	1.34986100	1.57853400
F	1.71566100	0.12912000	3.26145600
F	2.57510700	2.17401400	2.71642600
F	0.53426700	2.04326600	3.73697300
Au	0.21752800	2.13890100	-1.05127100
P	1.18155200	4.23604900	-0.07801600
F	1.67615700	2.17468100	-2.37204600
O	-1.35095700	2.31251500	0.34797000
H	-2.27301900	2.19801300	0.02587800
H	-1.16758100	1.73132200	1.12330300
C	0.47068600	4.77945500	1.50644500
H	-0.59863600	4.98172000	1.38141000
H	0.59449700	3.98860700	2.25594200
H	0.97517800	5.69207400	1.84877900
C	0.89212700	5.60060700	-1.25203300
H	1.37765600	5.36141300	-2.20563000
H	-0.18285700	5.72504100	-1.42584100
H	1.30532300	6.54009400	-0.86291800
C	2.98343700	4.21263100	0.17441700
H	3.19876400	3.63941900	1.08239700
H	3.47712100	3.74003300	-0.68266100
H	3.35533800	5.23811700	0.29578300

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Num. Imaginary Frequencies: 0

C	-0.83397400	-3.77665900	1.56980900
C	-0.97742200	-3.46209000	0.22557200
C	-0.65310400	-2.17720500	-0.22971300
C	-0.17893800	-1.23214400	0.67897100

C	-0.03710400	-1.55716800	2.02493100	H	4.76273000	-2.70043100	-0.44181500
C	-0.36239800	-2.83104500	2.47805900	H	6.00062100	-2.37971700	0.80685700
H	-1.08538400	-4.78141100	1.90606200	N	4.13610700	-1.48953000	1.18113500
H	-1.32836700	-4.21013100	-0.47982300	C	5.52369400	0.52761300	1.46074600
H	0.10623800	-0.23731800	0.33799300	C	3.73279600	0.59869000	-0.09202600
H	0.35180700	-0.80443400	2.70916400	C	4.76503500	-0.58653700	2.21445600
H	-0.24927200	-3.08564900	3.53029600	C	3.40423000	-2.63568600	1.78425300
C	-1.66628700	-2.39549300	-2.47354700	C	3.08301900	-0.68547000	0.43314000
O	-2.67536700	-3.04359600	-2.15323000	H	6.60832800	0.39555000	1.55979800
C	-0.02725000	-1.34495600	-3.71721400	H	5.24741100	1.49469600	1.89714800
H	0.80468500	-2.03974500	-3.90000500	H	3.36377700	1.44828700	0.48997000
H	-0.01135700	-0.54873800	-4.47063900	H	3.44836100	0.74875700	-1.13990200
C	-2.04612900	-2.40037500	-4.90404100	H	3.94002900	-0.19899100	2.82286100
H	-2.17309100	-1.52336900	-5.55089000	H	5.41818000	-1.20671600	2.83668900
H	-1.53686200	-3.18941500	-5.47392100	Cl	4.47379700	-3.76647400	2.64136700
H	-3.03096800	-2.76136500	-4.59183500	H	2.90146600	-3.16745900	0.96863700
N	-1.30744500	-2.03959700	-3.72380800	H	2.67889400	-2.23271700	2.49829700
C	0.01137100	-0.80139800	-2.28162200	H	2.28839100	-0.47687300	1.15516300
H	1.05046600	-0.75346300	-1.92855200	H	2.71854700	-1.34638000	-0.35944200
C	-0.74081700	0.51968400	-2.16927100	B	3.16958500	-2.76232600	-2.61282600
H	-1.70876400	0.40479800	-1.66948400	F	3.08144700	-1.36121500	-2.71290100
H	-0.87493000	1.02259900	-3.13682700	F	4.51201700	-3.13437100	-2.56310300
H	-3.52336900	-2.07638200	-1.08934300	F	2.53627900	-3.35560600	-3.69597400
N	-0.74183600	-1.86022100	-1.59427600	F	2.53853200	-3.16054900	-1.41407000
N	-4.17696000	-1.36086600	-0.65179400	B	1.79407600	1.70942900	2.89115400
C	-5.15731200	-3.31621700	0.92517800	F	1.19276800	1.54690500	1.61683700
C	-6.25276900	-1.17502600	-2.41376900	F	1.97378900	0.44420700	3.46289400
O	-5.74133400	-0.72623300	1.26852000	F	3.04225200	2.31633700	2.72131800
O	-3.39074700	-1.52885300	1.76616600	F	0.96284600	2.49396400	3.67362600
O	-3.84905000	-0.15618700	-2.81925900	Au	0.13989100	2.09145500	-1.07394200
O	-5.28880300	0.91554800	-1.03520300	P	1.15697500	4.18726200	-0.13635100
S	-4.59451400	-1.55272500	0.96789800	F	1.75458400	1.88197600	-2.18610300
S	-4.80210600	-0.25289400	-1.73357400	C	0.56564800	4.89125800	1.43667500
F	-6.19762700	-3.42669700	0.12586100	H	-0.49699300	5.15234500	1.35864700
F	-5.48552800	-3.65492100	2.15329700	H	0.69896800	4.15702800	2.24131700
F	-4.16731300	-4.06824800	0.48884400	H	1.13368700	5.80069700	1.67410500
F	-6.78983400	-0.44976300	-3.37171800	C	0.89721300	5.50577600	-1.37479400
F	-7.12651500	-1.38323600	-1.45112800	H	1.31842300	5.18231400	-2.33456800
F	-5.81946700	-2.32293900	-2.89482700	H	-0.17373900	5.69857400	-1.51077700
H	6.75198900	-0.68037700	-0.65145100	H	1.39027700	6.43553100	-1.06271400
C	5.65740800	-0.69729500	-0.58527800	C	2.96605500	4.09829800	0.03353500
C	5.20010900	-1.93571400	0.20626700	H	3.20962600	3.55273400	0.95217100
H	5.24788200	-0.75014900	-1.60049700	H	3.38638700	3.57297900	-0.83202700
N	5.18535600	0.53497500	0.04052400	H	3.38232700	5.11230100	0.09179700

C	-2.72399800	3.06945700	-0.51917100
O	-1.68353400	2.16935300	-0.02512100
C	-1.83649200	1.90321400	1.40378200
C	-3.30480100	2.17857600	1.62188200
C	-3.58765000	3.35791400	0.69433500
H	-2.23928200	3.95803300	-0.94213900
H	-3.25188800	2.52484800	-1.31290500
H	-1.54547000	0.85971500	1.56175900
H	-1.16266800	2.56382300	1.96643300
H	-3.90090600	1.30880600	1.31677100
H	-3.52672500	2.39699000	2.67106900
H	-4.64506200	3.42827800	0.41979100
H	-3.28597700	4.30199200	1.16554400

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Num. Imaginary Frequencies: 0

H	-6.32538900	-0.65547300	-0.57366200
C	-5.32611000	-0.31951600	-0.87808300
C	-4.66946900	0.53229000	0.22510700
H	-5.43317700	0.29249900	-1.78204900
N	-4.51697800	-1.49329200	-1.18713400
H	-4.21798700	1.44839400	-0.16730900
H	-5.35825500	0.78329000	1.03801600
N	-3.54841600	-0.27792600	0.83005200
C	-4.48817500	-2.38140100	-0.02843000
C	-3.15469600	-1.05887400	-1.48381300
C	-4.08609400	-1.62332700	1.25232700
C	-2.87543300	0.44815700	1.94064300
C	-2.46941200	-0.50899300	-0.22521900
H	-5.47564400	-2.84013600	0.10419700
H	-3.76447300	-3.18181300	-0.22425300
H	-2.57530800	-1.90450900	-1.87131000
H	-3.18499700	-0.28194100	-2.25735800
H	-3.29083800	-2.12593400	1.81180300
H	-4.93456300	-1.42751300	1.91599700
Cl	-3.94461800	0.72540400	3.33716000
H	-2.55470000	1.41628700	1.54522600
H	-2.03835700	-0.17332900	2.27272300
H	-1.75363700	-1.20885600	0.21484800
H	-1.98443900	0.45215300	-0.41140000
B	-2.53532200	2.82050100	-1.70658600
F	-1.95286300	1.81464200	-2.48331300
F	-3.92092700	2.76323600	-1.82652100

F	-2.04927000	4.06355000	-2.07853100
F	-2.19056100	2.58422800	-0.34284400
B	-0.56891800	-2.87364200	1.81718200
F	0.35065400	-3.70873100	2.43773000
F	0.09856100	-2.10395900	0.83557600
F	-1.57317900	-3.60427100	1.18715600
F	-1.13176300	-1.99092300	2.74834200
C	2.39275300	-1.02545800	2.48755600
C	1.79675700	0.10229000	1.93125300
C	2.54826600	1.26529000	1.69119700
C	3.91908100	1.25866600	2.02092800
C	4.49428900	0.12362800	2.59033000
C	3.74286200	-1.02363600	2.82426600
H	1.78347100	-1.91341200	2.64395900
H	0.73877600	0.05443900	1.68538700
H	4.50834300	2.15318700	1.85115800
H	5.55358800	0.14456800	2.84068600
H	4.20405900	-1.90824800	3.25847200
C	2.47192800	3.66430600	1.03513800
O	3.51024600	4.04671900	1.55112800
C	0.35385100	3.74594700	0.07579300
H	-0.39639400	4.03590200	0.82938900
H	-0.06517800	3.96982100	-0.91205500
C	1.69357200	5.86274500	0.27820800
H	1.46450300	6.24191000	-0.72478200
H	0.98686400	6.31271400	0.99241500
H	2.71094000	6.15579500	0.55168800
N	1.61045600	4.42490500	0.29629400
C	0.74692800	2.26526600	0.23062800
H	-0.05837100	1.72333000	0.74084300
C	1.02154600	1.66906800	-1.13497100
H	1.85618500	2.17663900	-1.64225500
H	0.11249100	1.67410400	-1.74850400
Au	1.50892600	-0.39633900	-1.20347000
P	1.93997500	-2.85374000	-1.41612000
N	1.94278600	2.36765500	1.07645500
F	-0.32298000	-0.65928100	-1.86557700
O	3.60273600	-0.09734200	-0.79213200
H	3.98651200	0.53860400	-1.42260400
H	3.75217600	0.28546300	0.10747400
C	2.71538800	-3.66757900	0.01710000
H	3.59875800	-3.09696400	0.33050200
H	1.99812600	-3.70095100	0.84427500
H	3.01961800	-4.68790100	-0.25144600

C	3.07686000	-3.21071300	-2.80086900
H	2.67018100	-2.80381500	-3.73385000
H	4.04985800	-2.74261600	-2.60760800
H	3.22019000	-4.29304800	-2.91509300
C	0.43085400	-3.79902100	-1.78529500
H	-0.27012300	-3.68256600	-0.95223400
H	-0.03012500	-3.40430600	-2.69754200
H	0.67114000	-4.86067700	-1.92504700

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Num. Imaginary Frequencies: 1

C	-0.10247400	-4.49535800	1.24076900
C	-0.46165100	-3.83901500	0.06802700
C	-0.59157300	-2.45146200	0.06887500
C	-0.34846200	-1.73318600	1.23887100
C	0.00444800	-2.39971500	2.40896300
C	0.11945400	-3.78632300	2.41820500
H	0.00207100	-5.57857300	1.22661600
H	-0.63718900	-4.40661000	-0.83869000
H	-0.41783700	-0.64786500	1.25721800
H	0.20887500	-1.80989300	3.30061300
H	0.39301600	-4.31087200	3.33220200
C	-1.17673400	-2.45546600	-2.36317900
O	-1.87451900	-3.44387100	-2.45329200
C	0.30846500	-0.70376000	-2.83577300
H	1.37492000	-0.96757300	-2.82788900
H	0.17249000	0.17567200	-3.47694900
C	-0.40187100	-2.28883600	-4.67061300
H	-0.59772800	-1.46847600	-5.37185100
H	0.59827300	-2.70202900	-4.85062100
H	-1.15273200	-3.07145600	-4.80929100
N	-0.49394100	-1.80686800	-3.31358900
C	-0.24695400	-0.45155600	-1.42985100
H	0.56307800	-0.38557100	-0.69651700
C	-1.13384700	0.77082400	-1.34746300
H	-1.81061400	0.74397000	-0.48289500
H	-1.69861900	0.95579100	-2.27068700
H	-2.39118300	-1.42189900	-0.81859400
N	-1.03040400	-1.70410200	-1.10749300
N	-3.56487200	-1.20439100	-0.63160200
C	-4.34440700	-2.78948700	1.38328700
C	-5.72123600	-1.74745800	-2.26090000
O	-5.41534800	-0.39848000	0.97701500

O	-3.00882900	-0.51415300	1.74067400
O	-3.41615700	-0.72640400	-3.05900200
O	-4.93925900	0.73002000	-1.66383000
S	-4.10463700	-1.01338900	0.92988800
S	-4.33834400	-0.55816500	-1.95078700
F	-5.25680400	-3.31491000	0.58838800
F	-4.75525700	-2.83406700	2.63555500
F	-3.20460100	-3.43491200	1.25506600
F	-6.32157000	-1.36639500	-3.37277100
F	-6.57373400	-1.72135100	-1.25671700
F	-5.22556100	-2.95710200	-2.40434900
H	6.67518400	-0.39486300	-0.58254500
C	5.58811400	-0.52011800	-0.65626700
C	5.16976500	-1.86385700	-0.03357700
H	5.30736900	-0.50634600	-1.71549000
N	4.92652300	0.59748700	0.00969700
H	4.83224500	-2.59640300	-0.77411400
H	5.95814500	-2.30964500	0.58152700
N	4.00869700	-1.60471500	0.90264200
C	5.14935800	0.50918500	1.45051800
C	3.49665300	0.52181000	-0.26837200
C	4.48288200	-0.75005800	2.05169900
C	3.36223600	-2.87344700	1.33750600
C	2.91908900	-0.82751500	0.18329500
H	6.23108400	0.49508400	1.63209800
H	4.72651500	1.39741800	1.93200700
H	2.98000600	1.32815600	0.26232000
H	3.32349000	0.65969000	-1.34133200
H	3.59282000	-0.51087200	2.64623400
H	5.17025200	-1.35600200	2.65012700
Cl	4.45928200	-3.94993400	2.22714100
H	3.01288500	-3.38786000	0.43500800
H	2.52106400	-2.61762200	1.99024000
H	2.10766600	-0.70682500	0.91212900
H	2.58970000	-1.46126300	-0.64426100
B	2.88691100	-3.16123500	-2.57722900
F	3.44223700	-1.87062500	-2.68647300
F	3.85074800	-4.02427900	-2.05422100
F	2.44013600	-3.59052800	-3.81302600
F	1.80913300	-3.09435100	-1.66513200
B	1.35406200	1.50894900	2.59205300
F	0.76423400	1.30699200	1.30997000
F	1.55414300	0.25611000	3.16792100
F	2.57891000	2.15926900	2.40704300

F	0.50790900	2.29735700	3.35163300	N	-5.09574900	-0.30710400	1.18383100
Au	0.00669400	2.50246100	-0.96657600	C	-4.33107000	-0.63840600	-1.15835600
P	1.39588800	4.46011400	-0.31128400	C	-6.19507900	-1.98186800	-0.28239900
F	1.43818700	1.79677300	-2.12196200	C	-3.87952700	-0.45460100	0.29035800
C	0.89417300	5.04788800	1.33767000	C	-4.66324900	-0.10629900	2.61328700
H	-0.12008000	5.46298400	1.27918900	C	-5.91827100	-1.57789600	1.16625700
H	0.88947800	4.20121500	2.03752600	H	-4.13758300	0.23855600	-1.78639500
H	1.58222000	5.82218100	1.69995500	H	-3.91657800	-1.55285300	-1.58982400
C	1.27780000	5.90365300	-1.41750700	H	-5.57922800	-2.83011700	-0.59217100
H	1.63360600	5.63032100	-2.41711600	H	-7.25348200	-2.18287300	-0.46629800
H	0.23510800	6.23280400	-1.49252900	H	-3.33318600	-1.32680200	0.65566300
H	1.88865200	6.73016600	-1.03194800	H	-3.26822700	0.44644400	0.39135700
C	3.17107000	4.07721500	-0.19936400	Cl	-3.84310000	1.42879500	2.86560100
H	3.33223000	3.39372200	0.64275200	H	-5.56346000	-0.13887900	3.23328300
H	3.50643700	3.59656400	-1.12564400	H	-3.99141400	-0.93788800	2.84707600
H	3.74207700	4.99991600	-0.03486100	H	-5.35079600	-2.36273600	1.67359300
C	-2.70411900	3.82796500	-0.51278900	H	-6.83897000	-1.36447400	1.71822900
O	-1.56723600	3.25544200	0.20015500	F	-6.22113100	-1.09448800	-2.41995000
C	-2.00467300	2.63664500	1.46502700	B	-3.49010700	-3.97880400	0.99039100
C	-3.50739700	2.81570000	1.44994300	F	-3.38793500	-3.34769200	-0.27139700
C	-3.70718600	4.06057000	0.58986900	F	-3.33585200	-2.97819600	1.98605600
H	-2.33357200	4.72464200	-1.02147500	F	-4.77284000	-4.50600800	1.10581800
H	-3.06473800	3.09666500	-1.25123900	F	-2.51115200	-4.93690100	1.12248900
H	-1.66575900	1.59738100	1.48455700	Au	1.13094300	-0.34813000	-1.10419900
H	-1.49053800	3.18550600	2.26091300	P	0.63213700	-2.49467800	-0.25557700
H	-3.99529100	1.95388500	0.97238000	C	0.83478000	4.45538300	2.68259600
H	-3.91219500	2.91597600	2.46170400	C	0.88039300	3.23122400	2.01954100
H	-4.72557800	4.15468900	0.20065800	C	2.06607400	2.81087300	1.41851100
H	-3.45670500	4.97204000	1.14875500	C	3.19008600	3.63021300	1.44262700

3.3 Cycle III and Cycle IIIa

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Num. Imaginary Frequencies: 0

H	-6.27356700	1.20395300	-1.45361300
C	-6.50443600	0.43523000	-0.70875000
C	-5.95277800	0.82206000	0.67037600
H	-7.57526100	0.21321700	-0.70642000
N	-5.81312800	-0.81986400	-1.13663700
H	-6.75628500	0.98784500	1.39463700
H	-5.32099900	1.71058000	0.59943000

H	-0.37999300	1.75258500	2.74963000
N	-0.73322700	2.58253500	-0.31883900
C	-0.74635700	1.81110600	0.81233100
O	-1.16010500	0.64748400	0.82029600
C	-1.04433700	1.93575100	-1.57433600
H	-1.60711700	2.63978500	-2.20403100
H	-1.71680000	1.08806600	-1.39751400

C	0.15842300	1.47238800	-2.34191800
H	-0.06011000	0.97813000	-3.29201500
C	1.45761800	1.76440900	-2.03173000
H	1.70358200	2.39221700	-1.17381700
H	2.26469600	1.55289900	-2.73066500
C	-0.75147400	4.03898500	-0.29106700
H	0.23173300	4.47825800	-0.51530700
H	-1.48903100	4.38766500	-1.02167000
H	-1.07352100	4.38761600	0.69342700
B	-4.25634800	3.00718600	-1.58603100
F	-3.58329900	4.13528000	-2.01209300
F	-5.59396000	3.27595700	-1.29448000
F	-4.20675600	2.01444900	-2.58553000
F	-3.64475400	2.48839400	-0.42174100
N	3.74605200	-0.22701100	-0.01863000
C	4.82638500	-0.58733900	-2.38883900
C	5.08376100	-1.84720900	1.81645100
O	6.26876700	0.23065200	-0.34187100
O	4.57361400	1.80044600	-1.33748100
O	2.60193200	-0.97391600	2.02800200
O	4.47464500	0.68691900	2.28758600
S	4.92819900	0.46184400	-0.87268400
S	3.88042000	-0.43494900	1.57146000
F	5.00960100	-1.86177600	-2.09567500
F	5.77435900	-0.18642000	-3.22092400
F	3.64510100	-0.44774100	-2.98528100
F	4.71036500	-2.52904700	2.88978400
F	6.30860700	-1.39814600	1.99379900
F	5.05830400	-2.65610700	0.76636200
C	2.06214100	-3.59361900	0.00680600
H	2.63516800	-3.22134000	0.86102900
H	1.71490600	-4.61336500	0.21738400
H	2.70948500	-3.59842800	-0.87792800
C	-0.23667900	-2.46008400	1.34089600
H	-0.58904100	-3.46846100	1.59274100
H	0.44710200	-2.07715100	2.10698000
H	-1.09243400	-1.78068100	1.26794800
C	-0.47045000	-3.44824500	-1.35169000
H	-0.77205200	-4.37727900	-0.84992700
H	-1.37597100	-2.86973600	-1.56113200
H	0.04352600	-3.67519100	-2.29270200

Num. Imaginary Frequencies: 1

C	4.10228100	-1.54767100	-3.10756000
C	3.63190500	-0.28067600	-2.73001100
C	4.13034200	0.32946700	-1.54920000
C	5.05221600	-0.38428300	-0.76485900
C	5.49244300	-1.63579400	-1.15759200
C	5.02454200	-2.23202400	-2.33743400
H	3.75687700	-1.96312300	-4.05362600
H	3.06135500	0.30823600	-3.44028400
H	5.43139600	0.06999100	0.14877200
H	6.21599900	-2.15898800	-0.53469700
H	5.39756200	-3.20522900	-2.64858000
C	2.85122900	2.37962500	-1.80894000
O	2.76637900	2.29335300	-3.03258700
C	0.80626200	3.54640400	-1.87559400
H	0.26690300	4.32866800	-1.33189000
H	1.08525300	3.92274300	-2.86369400
C	2.02686800	3.56294500	0.29128700
H	2.33146700	4.61330300	0.39411900
H	1.01971800	3.45123200	0.70998800
H	2.70202300	2.93905000	0.88071300
N	1.99895100	3.18891700	-1.11253600
C	-0.07926600	2.33537100	-1.97503200
H	-0.65473800	2.10563700	-1.07773900
C	-0.20337600	1.56013000	-3.08635700
H	0.34246100	1.80775200	-3.99626600
H	-1.03042000	0.85384900	-3.17432600
Au	0.84305100	-0.32306500	-1.90553900
P	0.98418900	-2.62248700	-1.28900400
H	-2.27716600	-0.50621800	1.44479600
C	-3.05031700	-0.86690200	0.75843000
C	-4.46547800	-0.64719500	1.32961500
H	-2.88726600	-1.92661600	0.54598900
N	-2.97209800	-0.11254300	-0.47845900
H	-4.94486600	-1.60266500	1.56342700
H	-4.46825600	0.00717500	2.20512800
N	-5.30620200	0.03676700	0.26679900
C	-3.25073500	1.30029100	-0.29597100
C	-3.77016100	-0.69153800	-1.54289700
C	-4.76024000	1.42659400	0.01251700
C	-6.75311100	0.05060900	0.65347900
C	-5.21829800	-0.76542700	-1.02183300
H	-2.64085500	1.68968300	0.52212600
H	-2.99434400	1.85711300	-1.20483000

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H	-3.67658800	-0.05737400	-2.42995800
H	-3.41436800	-1.70201200	-1.75656100
H	-5.32495700	1.84578500	-0.82664000
H	-4.93487100	2.03830100	0.89982500
Cl	-7.04511200	0.88778700	2.18044600
H	-7.06851400	-0.99267200	0.74551400
H	-7.30692800	0.55972700	-0.13993500
H	-5.93257400	-0.33148900	-1.72876100
H	-5.49964700	-1.79271000	-0.76896600
F	-1.18969100	-0.31549700	-1.08188500
B	-2.46833800	4.37771400	-0.46074200
F	-3.71717500	4.00887100	0.06246900
F	-2.37726000	3.89009200	-1.77897900
F	-1.45879200	3.76729000	0.30999800
F	-2.31197700	5.74711700	-0.44720500
B	-4.57328300	-4.05462100	0.38421900
F	-4.82847300	-5.40182300	0.29731500
F	-3.72996400	-3.75956600	1.45603900
F	-3.96577300	-3.58801400	-0.80250800
F	-5.78524900	-3.33525300	0.55762400
N	3.74147600	1.58755400	-1.09663900
H	3.80540200	1.69269500	-0.08555800
N	2.20818900	-0.48487000	2.80735000
C	0.12762000	1.22637300	2.76884700
C	4.74316900	-1.12138900	3.01544600
O	0.11193900	-1.15594400	1.66565100
O	1.46494100	0.65650400	0.59712900
O	3.70218200	0.89991300	4.32808300
O	4.02040100	1.13201300	1.85953700
S	1.04852200	-0.04633200	1.81327000
S	3.59146500	0.31627900	2.99959500
F	-0.36655000	0.70330100	3.87335900
F	-0.86371700	1.69067400	2.01966300
F	0.94801800	2.22217000	3.07237000
F	5.98032900	-0.64791100	3.02074800
F	4.57197000	-1.87017700	1.93695300
F	4.54167800	-1.85279900	4.09429800
C	1.30973700	-3.65679700	-2.74872900
H	2.29589700	-3.43049300	-3.16710700
H	1.27948900	-4.71189700	-2.44606500
H	0.54216000	-3.47867200	-3.50986500
C	-0.57244200	-3.25715800	-0.60860500
H	-1.38289200	-3.15438800	-1.33687300
H	-0.43526400	-4.32200000	-0.37739100

H	-0.81865400	-2.71640200	0.31016300
C	2.27338200	-3.01816400	-0.07739200
H	2.32772000	-4.11036400	0.02726400
H	3.24197700	-2.63893100	-0.42020800
H	2.02416100	-2.57670600	0.89371100

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Num. Imaginary Frequencies: 0

C	3.36655800	-3.14524700	-1.72272900
C	2.94565700	-1.78943000	-2.01433100
C	3.70765900	-0.70533200	-1.38757800
C	4.62732200	-1.01959000	-0.36274200
C	4.93933000	-2.32908300	-0.10494000
C	4.32365600	-3.41398200	-0.79602700
H	2.90180500	-3.94169300	-2.30243600
H	2.72826100	-1.62350500	-3.07339700
H	5.12714400	-0.20730200	0.15966500
H	5.69792300	-2.54569200	0.64577800
H	4.63936900	-4.43362600	-0.59021000
C	2.75388700	0.93395700	-2.87902500
O	2.81931600	0.25551900	-3.89172700
C	0.67529700	1.82790000	-3.53974900
H	0.10123000	2.75242500	-3.43900100
H	0.97556400	1.68888600	-4.58281400
C	1.91797200	2.86151800	-1.57260300
H	2.77809200	3.53595300	-1.67385300
H	1.00755200	3.46723900	-1.57274700
H	2.00125900	2.32249800	-0.62812100
N	1.87022000	1.93512200	-2.69663700
C	-0.14173600	0.65996600	-3.04446000
H	-0.83669100	0.85628400	-2.22148800
C	-0.07564900	-0.59021800	-3.58521700
H	0.57304400	-0.79674500	-4.43570000
H	-0.84381400	-1.32381200	-3.33930300
Au	0.82676000	-1.53629500	-1.42096900
P	0.75760500	-3.00761600	0.49295500
H	-2.25105000	0.52022800	1.50353600
C	-2.99565100	0.13773500	0.79236000
C	-4.36362200	0.04912600	1.48493500
H	-2.67674900	-0.85150900	0.44945200
N	-3.06112900	1.00673400	-0.37599000
H	-4.64277000	-0.97519200	1.74744500
H	-4.43508200	0.68575800	2.37303000

N	-5.39978200	0.57131400	0.50820800
C	-3.69239200	2.27070100	-0.02634600
C	-3.84342100	0.34565000	-1.40594500
C	-5.18164300	2.05483100	0.32097300
C	-6.78046000	0.23197000	0.94669400
C	-5.19778000	-0.11695600	-0.83702400
H	-3.14487200	2.70460500	0.81906200
H	-3.59303000	2.96638900	-0.86502500
H	-3.97691700	1.04924400	-2.23723000
H	-3.28312200	-0.52357100	-1.76725300
H	-5.85994600	2.36363300	-0.48416800
H	-5.48720800	2.55142900	1.24721000
Cl	-7.18679900	0.89955300	2.54145000
H	-6.83989000	-0.85886000	0.99489500
H	-7.48252700	0.64181900	0.21548300
H	-6.05115500	0.16406300	-1.46520300
H	-5.22783200	-1.19021300	-0.62646500
F	-1.15043400	-1.42985300	-1.05867300
B	-1.54505700	4.29172500	-1.82356700
F	-2.69737000	5.04248900	-2.02792400
F	-1.78679200	2.96323400	-2.21455100
F	-1.17583300	4.32990800	-0.47848500
F	-0.48912300	4.78776600	-2.60692400
B	-4.43191500	-3.40132600	0.82648200
F	-4.58628100	-4.77066300	0.74678900
F	-3.77422900	-3.03635000	2.00292000
F	-3.68648200	-2.92675900	-0.27052700
F	-5.69832900	-2.77043500	0.80298000
N	3.54603900	0.58399200	-1.74094300
H	3.81913800	1.28008900	-1.03948600
N	2.24966300	1.54282400	2.85625200
C	0.09830600	2.20118100	1.31876400
C	4.74020600	0.60940800	3.00646400
O	0.29529300	-0.01223200	2.77744600
O	1.70225400	0.17332100	0.72301900
O	4.13678300	3.16671600	3.07499200
O	3.93548100	1.94109500	0.89906800
S	1.16987300	0.80513600	1.93989900
S	3.70549500	1.98624600	2.34713200
F	-0.86830800	2.45113500	2.18660100
F	-0.42178500	1.81527800	0.17311500
F	0.82905100	3.28928100	1.15696100
F	5.97630300	0.73791900	2.54582200
F	4.24795600	-0.55468400	2.59011400

F	4.75288100	0.62986600	4.32333600
C	0.79941700	-4.70552700	-0.13581200
H	1.80365700	-4.99182000	-0.45962900
H	0.48828000	-5.36252800	0.68817100
H	0.09001100	-4.81562900	-0.96288100
C	-0.82736900	-2.78869000	1.31338700
H	-1.66367700	-2.99582600	0.64064200
H	-0.82771600	-3.49494000	2.15676600
H	-0.90283200	-1.76658000	1.70008200
C	2.04135900	-2.78579100	1.74521400
H	2.21263500	-3.75977600	2.22203500
H	2.97819500	-2.41568000	1.32405300
H	1.66962900	-2.06405900	2.48145700

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Num. Imaginary Frequencies: 0

N	-3.93786100	1.24104700	0.00079500
C	-5.34163700	0.31330100	-2.08341100
C	-4.16096000	2.16756600	2.55055400
O	-4.50570400	2.79360500	-1.87066300
O	-6.39377100	2.02644600	-0.39642600
O	-3.09541000	-0.11624600	1.88975500
O	-5.58188300	0.11188600	1.68583400
S	-5.09011900	1.78529100	-0.99998500
S	-4.25769800	0.67755200	1.46651200
F	-4.23034900	0.03278400	-2.74999900
F	-6.31076400	0.57179300	-2.94509600
F	-5.67899900	-0.73838600	-1.34733100
F	-4.42855400	1.80432800	3.79476200
F	-5.03105100	3.08072800	2.15863200
F	-2.93856100	2.67681300	2.49790000
C	-2.95105900	-2.16191300	-0.64430400
C	-1.93618300	-1.23059600	-1.09096500
C	-1.02267100	-1.68825000	-2.14035000
C	-1.00201000	-3.05970400	-2.47769800
C	-1.99194200	-3.88565900	-2.01129800
C	-3.00039400	-3.43720600	-1.11190900
H	-3.69175600	-1.79055900	0.06197000
H	-2.31884900	-0.20648800	-1.18836900
H	-0.25172200	-3.42190300	-3.17482500
H	-2.01040900	-4.92006800	-2.34999400
H	-3.78912300	-4.11841600	-0.80249300
C	-0.22158100	0.54799800	-2.58185000

O	-1.29978700	1.10305300	-2.47540300
C	0.87785700	2.35850500	-1.54639600
H	1.85617600	2.84789200	-1.54233000
H	0.12577300	3.04920600	-1.94086200
C	2.25832100	0.62137300	-2.79533300
H	2.22795000	0.28939800	-3.84016000
H	3.00312600	1.41716400	-2.71272900
H	2.55436300	-0.21821200	-2.15963500
N	0.96782700	1.17496900	-2.40814900
C	0.53289100	1.91516600	-0.14789100
H	1.36930500	1.62143900	0.49117300
C	-0.72230800	1.88715900	0.37340400
H	-1.59244300	2.20005500	-0.20317000
H	-0.85652100	1.74562400	1.44683400
Au	-0.63715100	-0.66044400	0.58793200
P	-0.34217700	-2.71087500	1.79866800
H	4.11864600	-2.17304900	1.40213500
C	4.97915300	-1.61719400	1.79549000
C	5.91121700	-1.22526900	0.63322800
H	5.51458000	-2.26826200	2.49634000
N	4.48515600	-0.43481900	2.50054700
H	6.97319100	-1.31429700	0.88247200
H	5.69657800	-1.79491600	-0.27625200
N	5.64937500	0.23076000	0.32938100
C	3.55750400	0.28575900	1.62702300
C	5.61567600	0.44818400	2.78380000
C	4.14123900	0.39733300	0.21896100
C	6.21755500	0.67932100	-0.97293700
C	6.15314000	1.07245100	1.48361600
H	2.58721800	-0.22474900	1.58321200
H	3.38615400	1.28466900	2.04947800
H	5.29680900	1.24400700	3.46691000
H	6.39294100	-0.13520000	3.29273300
H	3.94596100	1.36616500	-0.24977900
H	3.80644400	-0.41740200	-0.43040700
H	6.02914400	1.75420900	-1.05918200
H	5.78655600	2.08661600	1.29208000
H	7.24635800	1.07494600	1.42941700
F	0.40354000	-0.10785600	2.25713300
B	2.39092700	-2.70840400	-1.25142800
F	1.91663100	-3.89442300	-0.70742400
F	3.77467500	-2.63279900	-1.16703300
F	1.99126300	-2.59566000	-2.59516600
F	1.83991000	-1.62516900	-0.52118500

N	-0.15825300	-0.85922200	-2.76678600
H	0.70802100	-1.30732600	-3.08176500
C	-0.74122600	-4.29950400	1.05118800
H	-1.79616100	-4.36903200	0.77461900
H	-0.08525600	-4.47090000	0.19029800
H	-0.52664600	-5.05390300	1.82188500
C	-1.40250200	-2.44332600	3.23295000
H	-1.09551100	-1.50855600	3.71243100
H	-2.44622600	-2.35714200	2.91212400
H	-1.28485500	-3.28748400	3.92496900
C	1.38248200	-2.84015500	2.31439700
H	1.98655300	-3.11355500	1.44385000
H	1.70906200	-1.89367900	2.75120500
H	1.43153300	-3.64117900	3.06477800
F	3.33724200	3.38164700	0.41643200
F	4.03715300	3.11259600	-1.73106400
F	5.54380500	3.65801200	-0.11549400
F	4.00020200	5.20674700	-0.79888500
B	4.22432300	3.87503300	-0.55300700
Cl	7.96326000	0.38083800	-1.09497300
H	5.71208600	0.11868100	-1.76583700

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Num. Imaginary Frequencies: 1

N	3.71320600	0.90332300	0.11631000
C	5.05195900	0.07198200	2.32331800
C	4.35541900	2.34082700	-2.20661700
O	3.89424200	2.43988200	2.14876900
O	5.95804000	1.99459700	0.77657600
O	3.24002600	-0.01376300	-2.13389000
O	5.65978800	0.13661300	-1.45819500
S	4.67691500	1.56198700	1.30634600
S	4.30956800	0.66563500	-1.40206000
F	3.93218800	-0.44388100	2.80226400
F	5.83424900	0.43910300	3.31993400
F	5.67009200	-0.82174300	1.57202300
F	4.69205300	2.13296100	-3.46719400
F	5.22622800	3.14183200	-1.63697400
F	3.15047100	2.87994200	-2.15271600
C	3.03687000	-2.13822500	0.13459700
C	2.02205200	-1.23593500	0.58690000
C	1.40238400	-1.56366800	1.84830600
C	1.78621900	-2.71285200	2.54986100

C	2.82371800	-3.50163300	2.09269100	H	-6.01681500	1.79169300	-1.14800100
C	3.48578800	-3.19440000	0.89267600	H	-7.40487500	0.67845900	-1.05052800
H	3.52392000	-1.92857500	-0.81584700	F	-0.61604600	0.04380700	-2.39561400
H	2.74318500	-0.05468300	0.46166400	B	-2.31273300	-2.62160100	1.22693700
H	1.27893000	-2.94528800	3.48420200	F	-2.54654200	-3.70141100	0.38505600
H	3.13548200	-4.36391500	2.67877400	F	-3.51685000	-2.15334700	1.76238000
H	4.32339000	-3.79921200	0.55426100	F	-1.43655100	-2.96761400	2.25851400
C	0.34160800	0.56611300	2.10319100	F	-1.71671400	-1.58609700	0.46769500
O	1.37078600	1.16422800	1.82126400	N	0.39474000	-0.79352900	2.39663800
C	-0.87897200	2.39823900	1.26117800	H	-0.40502600	-1.30544200	2.76606200
H	-1.87531300	2.84514700	1.33763600	C	0.46146300	-4.06387500	-0.63085400
H	-0.13452100	3.10182700	1.65132000	H	1.47478200	-4.15613100	-0.23185700
C	-2.06201800	0.68601500	2.74971200	H	-0.27002300	-3.97549500	0.17873300
H	-1.88146400	0.65308900	3.83249500	H	0.22288300	-4.95714900	-1.22451400
H	-2.87399500	1.39551100	2.56439100	C	1.50614800	-2.80062300	-3.09720900
H	-2.38480600	-0.30369200	2.40820200	H	1.38038600	-1.94663600	-3.77255300
N	-0.88069800	1.16201200	2.04661900	H	2.53455100	-2.81703600	-2.72350100
C	-0.59475900	2.04006100	-0.17276300	H	1.30338000	-3.73139400	-3.64365700
H	-1.44326200	1.70481700	-0.77359800	C	-1.34197400	-2.72670500	-2.45783100
C	0.62820100	2.10106600	-0.76231000	H	-2.05973700	-2.83014300	-1.63834600
H	1.49631500	2.45758400	-0.21121500	H	-1.52983700	-1.81671300	-3.03290000
H	0.71349600	1.98265100	-1.84305200	H	-1.38064100	-3.61467700	-3.10325500
Au	0.65267700	-0.46694900	-0.87507200	F	-3.60622800	3.27669600	-0.62931500
P	0.31360500	-2.65356100	-1.74523900	F	-4.01080800	3.12241700	1.60806400
H	-4.08243900	-2.37399300	-1.12913300	F	-5.73807500	3.47580600	0.16961900
C	-5.00819600	-1.88678000	-1.46242500	F	-4.21528400	5.14524600	0.54859100
C	-5.83549600	-1.45488400	-0.23739500	B	-4.38847600	3.78894200	0.41683000
H	-5.57580900	-2.61636200	-2.05209000	Cl	-7.79679000	0.14687600	1.58854900
N	-4.66917500	-0.73803400	-2.30229900	H	-5.47307200	0.06367400	2.01276700
H	-6.90920700	-1.62563800	-0.36483600				
H	-5.49523300	-1.93025300	0.68761900				
N	-5.64349600	0.03402100	-0.07422100	19			
C	-3.70792900	0.11278800	-1.59605500	Num. Imaginary Frequencies: 0			
C	-5.88226700	0.04850300	-2.52341300	N	4.54596500	0.75052900	0.34258000
C	-4.14685100	0.30707900	-0.14529700	C	6.51320500	-0.40693000	1.88193700
C	-6.09755000	0.54034700	1.25017000	C	4.45930300	2.74597600	-1.57534600
C	-6.32573800	0.74360500	-1.22255300	O	4.67674200	1.33216400	2.76169000
H	-2.70039100	-0.31996000	-1.62409600	O	6.52112600	2.15639000	1.21370100
H	-3.65868200	1.08007400	-2.11284500	O	3.83785500	0.23788000	-1.99958700
H	-5.69380400	0.80402500	-3.29503200	O	6.28050700	0.77798900	-1.52632700
H	-6.66646200	-0.62093100	-2.89899600	S	5.54949200	1.16674700	1.62008500
H	-3.97199900	1.32289200	0.22014800	S	4.86818100	0.96085200	-1.28460100
H	-3.68943800	-0.42232700	0.52719800	F	5.82960800	-1.21190600	2.67088900
H	-5.97685200	1.62837000	1.24513300	F	7.64977500	-0.07719900	2.45929500

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N	4.54596500	0.75052900	0.34258000
C	6.51320500	-0.40693000	1.88193700
C	4.45930300	2.74597600	-1.57534600
O	4.67674200	1.33216400	2.76169000
O	6.52112600	2.15639000	1.21370100
O	3.83785500	0.23788000	-1.99958700
O	6.28050700	0.77798900	-1.52632700
S	5.54949200	1.16674700	1.62008500
S	4.86818100	0.96085200	-1.28460100
F	5.82960800	-1.21190600	2.67088900
F	7.64977500	-0.07719900	2.45929500

F	6.74451600	-0.99398400	0.72690300	C	-6.77650600	1.15487400	-0.29691400
F	4.50153000	2.94790200	-2.87750600	H	-3.87509200	-1.06691800	-1.36453500
F	5.31841800	3.52892700	-0.96536200	H	-4.64904300	0.34859500	-2.08128900
F	3.23895900	2.96981100	-1.12135500	H	-7.03082100	0.44406600	-2.32866600
C	2.51412500	-2.35152500	-0.95825100	H	-8.00428500	-0.44340200	-1.14584700
C	1.54120200	-1.62561000	-0.27889200	H	-3.99445700	1.37909000	-0.05703400
C	1.70193600	-1.36987000	1.08922900	H	-3.89039400	-0.18208500	0.79821600
C	2.79810500	-1.88679100	1.76960700	H	-5.25784500	2.53202400	1.40167500
C	3.73936900	-2.66305900	1.09586100	H	-6.29324400	2.04074100	-0.72559800
C	3.61281400	-2.87090600	-0.27185700	H	-7.68584200	1.46457000	0.22841200
H	2.43842000	-2.50279700	-2.03459300	F	-1.87226200	-0.68290800	-2.36739700
H	3.51609200	0.74922700	0.58651700	B	-2.57921200	-2.09149300	1.95039500
H	2.91170400	-1.65231800	2.82733700	F	-3.20837000	-3.30237400	1.73282600
H	4.58714700	-3.07739100	1.63607400	F	-3.42852600	-1.19598300	2.60015200
H	4.36850800	-3.43539100	-0.81479000	F	-1.39447000	-2.24742300	2.68187900
C	0.92225500	0.82741000	1.32931600	F	-2.21048900	-1.54841700	0.68663400
O	1.96108900	1.23918700	0.79409200	N	0.80272900	-0.47286400	1.74757600
C	-0.26804700	2.57281800	0.29425900	H	-0.11035000	-0.84767100	2.01015700
H	-1.05124100	3.30440200	0.50739500	C	-0.24691200	-4.19901700	0.30880900
H	0.68767900	3.08613200	0.16386100	H	0.83464800	-4.36795600	0.34368000
C	-1.38836800	1.23701800	2.08562000	H	-0.55624900	-3.60521300	1.17574000
H	-1.16818300	0.83500800	3.08140900	H	-0.77352600	-5.16239500	0.31874100
H	-2.03404100	2.11213900	2.20081800	C	0.13580400	-4.16590500	-2.60645000
H	-1.92808200	0.47517800	1.50976900	H	-0.08674000	-3.62919500	-3.53546300
N	-0.15713800	1.66307200	1.44146600	H	1.21756500	-4.21497700	-2.45679900
C	-0.63504000	1.79845800	-0.94797400	H	-0.25880900	-5.18788900	-2.67830700
H	-1.70247000	1.66167900	-1.15411300	C	-2.45880800	-3.52195400	-1.52860100
C	0.27432000	1.30505400	-1.83702200	H	-3.00482000	-3.30751200	-0.60609200
H	1.33991500	1.48535500	-1.70307500	H	-2.74026300	-2.81166000	-2.31275300
H	-0.07032900	0.96529100	-2.81616400	H	-2.64475100	-4.55438700	-1.85109500
Au	-0.16840000	-1.03398500	-1.27034800	F	-3.27994500	4.97149900	-1.08338800
P	-0.68819600	-3.34158700	-1.21974300	F	-3.21790100	3.28649100	0.46605900
H	-5.27530900	-2.35674000	0.20481000	F	-3.65459100	2.80413300	-1.71879000
C	-6.15250600	-1.71361000	0.04880400	F	-5.20713100	3.89811600	-0.44837400
C	-6.30046100	-0.72474700	1.22196500	B	-3.83609800	3.76839500	-0.71716500
H	-7.03597700	-2.36177900	0.00230100	Cl	-7.02909800	1.86305400	2.83490000
N	-5.99504000	-1.00457300	-1.21935400	H	-4.79867000	1.15560500	2.48574700
H	-7.33975700	-0.59253700	1.53931700				
H	-5.68473600	-0.99832200	2.08534900				
N	-5.81485200	0.62168500	0.73779000				
C	-4.68807700	-0.34599200	-1.23328300				
C	-7.02703700	0.02616400	-1.31513700				
C	-4.46174600	0.40250000	0.07804000				
C	-5.57787600	1.58497800	1.84697800				

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H	-1.41290500	-0.40323500	1.11618800
C	-2.03152200	0.05057500	0.33642800
C	-3.49013600	-0.39889700	0.48779300

H	-1.99830300	1.14036600	0.44220200
N	-1.48498100	-0.35497500	-0.95917500
H	-4.19443300	0.43047200	0.36137400
H	-3.67108300	-0.91464400	1.43517900
N	-3.78592700	-1.38608600	-0.62369600
C	-1.38051000	-1.80976400	-1.00601600
C	-2.36659200	0.07495400	-2.03746200
C	-2.72288500	-2.46563300	-0.62918700
C	-5.16010000	-1.94050100	-0.50393100
C	-3.72531700	-0.64664400	-1.94972300
H	-0.62053700	-2.13665900	-0.29333100
H	-1.04588300	-2.09009200	-2.01069300
H	-1.88084700	-0.15166400	-2.99513300
H	-2.52180200	1.15594700	-1.96442100
H	-3.05506000	-3.23415000	-1.33748700
H	-2.69167200	-2.88418700	0.38156700
Cl	-5.38235700	-2.94664400	0.93831000
H	-5.85612000	-1.09856400	-0.45273900
H	-5.35904900	-2.55227000	-1.38808500
H	-3.86784300	-1.40623300	-2.72747500
H	-4.55766000	0.06371300	-1.95845800
B	-0.32984100	-2.78785900	2.22290800
F	0.44602600	-1.72318600	1.64988200
F	-1.63078900	-2.32955500	2.41262400
F	-0.34111600	-3.83695000	1.29655700
F	0.26026400	-3.17493600	3.40339000
B	-3.68202600	3.13476900	-0.44254100
F	-2.37921100	3.10824500	-0.99698900
F	-3.60446000	2.76357600	0.89811300
F	-4.47788900	2.19653300	-1.12893900
F	-4.21181700	4.40391400	-0.57772300
C	4.35315200	1.19396600	0.13915600
C	3.00843000	0.89862900	0.33610300
C	2.32978100	1.36661600	1.46196600
C	3.01760400	2.15388700	2.38890900
C	4.35755800	2.46654200	2.18889900
C	5.02761300	1.98788700	1.06712500
H	4.87657500	0.84110200	-0.75049200
H	2.48405300	2.51856400	3.26631000
H	4.88224500	3.08225600	2.91639100
H	6.07495600	2.23465300	0.90425400
C	0.00309000	2.05798300	1.94855900
O	-0.83633200	1.86200200	2.81538900
C	0.77839200	3.28267500	-0.07520100

H	0.46319300	4.22525700	-0.55107700
H	1.86875600	3.37708900	0.05565600
C	-0.83108000	4.30477000	1.50473400
H	-1.39888800	4.03817600	2.39674700
H	-0.25101900	5.21820200	1.69308600
H	-1.53717400	4.47481400	0.68379800
N	0.05584400	3.19761700	1.17981500
C	0.45391000	2.22841700	-1.07771000
H	-0.52641700	1.76208200	-1.00041600
C	1.25459400	1.91628700	-2.14109000
H	2.19708600	2.44592300	-2.30170300
H	0.84217200	1.34978000	-2.97751400
Au	1.93479800	-0.06768400	-1.10046100
P	2.97777700	-2.08469700	-0.45954300
F	1.07059400	-1.10649400	-2.66738200
N	0.94909800	1.08712300	1.61235300
H	0.71163300	0.15839700	1.96598600
C	4.45660600	-2.22400800	-1.49816100
H	4.94691400	-3.18507600	-1.29484700
H	4.16083200	-2.18373600	-2.55262600
H	5.16114500	-1.41297000	-1.28628200
C	3.49106500	-2.24650700	1.26641400
H	3.97943200	-3.22229800	1.38603500
H	4.19279700	-1.44807100	1.53038000
H	2.60373700	-2.19504300	1.90671300
C	1.89955000	-3.46063500	-0.90846400
H	1.41649100	-3.19213700	-1.85477200
H	2.51300300	-4.36305500	-1.02663900
H	1.14412800	-3.62251200	-0.13005300

TS12

Num. Imaginary Frequencies: 1

H	-2.02100900	0.31051400	1.99334700
C	-1.79692200	1.08348000	1.24530200
C	-3.05833300	1.86065500	0.85443400
H	-1.06862200	1.78239200	1.67360100
N	-1.23105600	0.40541700	0.06783000
H	-2.83767100	2.91063600	0.62387600
H	-3.84878400	1.79897900	1.60844500
N	-3.58973600	1.25338100	-0.42801600
C	-2.10866900	-0.71155600	-0.29014400
C	-1.21400100	1.31942600	-1.07924700
C	-3.57508200	-0.25973000	-0.31495000

C	-4.93068900	1.79046500	-0.78346600	H	1.16460100	2.26966400	-1.01493100
C	-2.64050900	1.64850200	-1.54256600	C	2.54736400	0.87917500	-1.89882200
H	-2.02799400	-1.51031000	0.44717300	H	3.61668200	0.69944100	-2.03457900
H	-1.78073100	-1.08495900	-1.26800900	H	1.93448000	0.83975500	-2.80433600
H	-0.66282900	0.83141700	-1.89441800	Au	1.68814600	-1.07802800	-1.18037700
H	-0.71704000	2.24267300	-0.78029600	P	0.77074400	-3.11455500	-0.31685900
H	-4.13842500	-0.65895900	-1.16439600	F	0.27415800	-0.99494000	-2.68807500
H	-4.09539700	-0.52239000	0.61067500	N	1.72282300	0.94134500	1.04581600
Cl	-6.19451800	1.31110900	0.36113300	H	0.77660600	0.54422800	0.95603800
H	-4.86232800	2.88196800	-0.79670700	C	1.93796100	-4.50484000	-0.30106800
H	-5.19323200	1.40698100	-1.77343300	H	1.39400500	-5.40784200	0.00445300
H	-2.95448800	1.08659600	-2.42984600	H	2.35837700	-4.65774200	-1.30099400
H	-2.76029700	2.72354300	-1.71457300	H	2.74669700	-4.31884100	0.41308100
B	-3.40898600	-3.57782300	1.27480100	C	0.24492400	-2.87711400	1.40353500
F	-3.00073300	-2.49872300	2.07695100	H	-0.44024300	-3.68384300	1.69046900
F	-3.67185900	-3.09759500	-0.02399400	H	1.13594900	-2.86484700	2.04221500
F	-2.35994300	-4.51007500	1.19518000	H	-0.28099500	-1.92136100	1.51068300
F	-4.54017800	-4.17070700	1.80050100	C	-0.61925100	-3.59076200	-1.39009300
B	-0.48490900	4.66180100	-0.33786100	H	-0.69532600	-2.84170000	-2.18811700
F	0.36432000	4.22739300	-1.36835800	H	-0.40553800	-4.57291600	-1.82723200
F	-0.31806900	3.79801200	0.75910300	H	-1.54982500	-3.64748300	-0.81112000
F	-1.82073400	4.57082500	-0.76688000				
F	-0.16851500	5.95611500	0.02585400				
C	4.04714000	-1.89963600	0.55499900	21			
C	2.98150000	-1.02422000	0.38095200	Num. Imaginary Frequencies: 0			
C	2.76246200	0.01276600	1.29923600	C	-2.38876700	-2.13077100	2.19675000
C	3.63293700	0.16499300	2.38310600	C	-1.39696500	-1.94444000	1.23311200
C	4.70236900	-0.70706200	2.54386100	C	-0.09576900	-2.33859300	1.56462800
C	4.91760500	-1.73529300	1.63116600	C	0.20685200	-2.90010900	2.80124300
H	4.23033700	-2.68935400	-0.17352500	C	-0.80416100	-3.07831700	3.73904800
H	3.45063600	0.94998300	3.11556200	C	-2.10236500	-2.68901700	3.43988900
H	5.36873100	-0.58361300	3.39478800	H	-3.41870200	-1.85815100	1.97157900
H	5.76525200	-2.40725000	1.74799000	H	1.22652400	-3.17688300	3.05149300
C	1.74385500	2.19828200	1.75849100	H	-0.56666500	-3.51898900	4.70448700
O	1.12844100	2.38826200	2.78817800	H	-2.89943900	-2.82420200	4.16817700
C	3.11434300	2.67731400	-0.16887900	C	2.36253700	-2.53817000	0.97911300
H	3.30808500	3.58466600	-0.76303800	O	2.92455800	-2.05859000	1.93295600
H	4.08232800	2.16690400	-0.03258900	C	1.75637000	-3.76360000	-0.92368300
C	2.64289000	4.45285600	1.54654700	H	2.24445800	-3.78868600	-1.90457900
H	2.28169800	4.51026500	2.57549100	H	1.27480400	-4.73573000	-0.73855300
H	3.68938500	4.77576300	1.51011700	C	4.07728300	-4.00450700	0.06376300
H	2.02366500	5.10771700	0.91850000	H	4.63992000	-3.59735500	0.90603600
N	2.52930900	3.07829800	1.09736100	H	4.04901500	-5.09814400	0.12322200
C	2.16675600	1.84649100	-0.95982200	H	4.56365600	-3.69251600	-0.86860100

N	2.73252400	-3.46968000	0.10535300
C	0.77108700	-2.59902100	-0.84674000
H	1.15222700	-1.79077100	-1.47695400
C	-0.64795200	-2.92425900	-1.18958100
H	-0.99801700	-3.85017600	-0.71759600
H	-0.77291100	-2.98458000	-2.27622500
Au	-1.94713600	-1.37189900	-0.64713600
P	-3.73228900	0.28131100	-0.17013600
F	-2.52726700	-1.08659200	-2.59083400
N	0.97442300	-2.08223500	0.57923500
H	1.07430700	-1.00250200	0.54062800
C	-4.12923400	1.31905900	-1.61099200
H	-3.89410400	0.72185200	-2.49854400
H	-5.19201800	1.59036900	-1.59728300
H	-3.51451400	2.22295000	-1.60178600
C	-3.71350100	1.36365400	1.29703100
H	-4.70673200	1.80770400	1.44379200
H	-3.44491200	0.78359000	2.18854200
H	-2.98211900	2.16866900	1.15770700
C	-5.24362000	-0.73529100	0.01576500
H	-6.12139900	-0.08761900	0.13989600
H	-5.37262300	-1.34010300	-0.89032300
H	-5.17925600	-1.40927500	0.87750900
H	2.67799500	0.68549300	2.14763200
C	2.73050200	0.86949300	1.06868900
C	3.19670800	2.29885100	0.76698200
H	3.44071700	0.15260100	0.64539100
N	1.38014700	0.64070000	0.51912700
H	3.89449700	2.31745600	-0.07764700
H	3.64924200	2.79025900	1.63341000
N	1.98565000	3.10168300	0.35669400
C	0.41762600	1.42997700	1.29812900
C	1.31140000	1.06928600	-0.88785300
C	0.88977700	2.88805100	1.38455700
C	2.28001000	4.55256600	0.16931400
C	1.54375100	2.58028300	-1.00209200
H	0.32477900	0.99592900	2.30117200
H	-0.55554400	1.37213300	0.79723600
H	0.31210900	0.82338200	-1.27188300
H	2.06688300	0.51422300	-1.45135600
H	0.08413500	3.60067500	1.18365000
H	1.33909200	3.12129500	2.35481600
Cl	2.78572300	5.35329000	1.66900200
H	3.09013400	4.64092300	-0.55956100

H	1.35895100	5.01843800	-0.19403400
H	0.64470200	3.13641000	-1.27496900
H	2.35792300	2.81181600	-1.69773800
B	-1.78343300	4.05514100	-0.48410700
F	-1.94435200	4.17524000	0.90084100
F	-0.67250900	4.82157000	-0.88034900
F	-1.50465100	2.69739900	-0.77459900
F	-2.91834900	4.45156900	-1.15705000
B	4.47595400	-0.74271600	-1.53994600
F	5.33451100	-1.21035100	-2.51213500
F	4.92062000	-1.10887000	-0.26530800
F	3.19022600	-1.30112500	-1.72989000
F	4.35576500	0.65632300	-1.60675400

TS13

Num. Imaginary Frequencies: 1

C	-3.65849800	-1.67162000	0.42693900
C	-2.34815200	-1.37441200	0.07360100
C	-1.28813100	-2.01069900	0.72114100
C	-1.54911600	-2.89382400	1.76684200
C	-2.86250900	-3.17142900	2.12830100
C	-3.91957500	-2.57815900	1.45036500
H	-4.48525500	-1.19682100	-0.10137700
H	-0.73576500	-3.36258400	2.31547400
H	-3.05336200	-3.86571900	2.94390400
H	-4.94814200	-2.81109100	1.71972800
C	1.04715000	-2.70213700	0.90243900
O	1.57126600	-2.44724600	1.96104400
C	0.44328500	-3.69659100	-1.12559700
H	1.06436800	-4.07389600	-1.94761200
H	-0.50115400	-4.26324600	-1.10187900
C	2.13978200	-4.82512600	0.39083800
H	2.53986600	-4.67637900	1.39697800
H	1.68272000	-5.81848700	0.32199400
H	2.95781500	-4.74117100	-0.33626100
N	1.15352400	-3.80080100	0.13644400
C	0.22556000	-2.19588400	-1.23421600
H	1.19273500	-1.77066600	-1.51643200
C	-0.85765300	-1.68012800	-2.14033100
H	-1.62857900	-2.43229100	-2.34337200
H	-0.44618000	-1.30973400	-3.08648300
Au	-1.85690900	-0.00280600	-1.32329500
P	-3.25746100	1.88642200	-0.58148700

F	-0.97805700	1.41632300	-2.59578300
N	0.07663800	-1.79080400	0.22605100
H	0.55795500	-0.55671900	0.23844000
C	-2.38278500	3.46503100	-0.32709200
H	-1.69463800	3.62017700	-1.16643400
H	-3.11025900	4.28638500	-0.29387300
H	-1.83396100	3.42552400	0.61925300
C	-4.39112500	1.70050500	0.83167500
H	-4.89511600	2.65639700	1.02518400
H	-5.14694500	0.94233200	0.59566300
H	-3.82640600	1.38363400	1.71533500
C	-4.34685400	2.23547100	-2.00572100
H	-4.98594000	3.10439000	-1.80083900
H	-3.72637100	2.43828200	-2.88646800
H	-4.98020500	1.36453700	-2.21417600
H	1.86092900	0.60327100	2.05235100
C	2.35997400	0.43715200	1.09277700
C	3.47793700	1.43520700	0.80881400
H	2.77606300	-0.57380000	1.09140800
N	1.30632700	0.53853000	0.04803000
H	4.32276300	0.96075600	0.29794900
H	3.82436200	1.93773600	1.71666300
N	2.94187700	2.49483300	-0.12828500
C	0.58519700	1.82925200	0.18966300
C	1.92166300	0.56553700	-1.30522900
C	1.59716200	2.96034000	0.38417200
C	3.91128000	3.61459100	-0.31211200
C	2.73609200	1.85134900	-1.48289400
H	-0.09481300	1.77694000	1.04153300
H	0.01210800	1.96845000	-0.73676100
H	1.10846400	0.55634100	-2.04178600
H	2.57118800	-0.30417300	-1.41292900
H	1.31934300	3.86232900	-0.17403000
H	1.73855300	3.22757600	1.43572100
Cl	4.14384000	4.56658100	1.15906400
H	4.86933100	3.17808700	-0.60796900
H	3.52459700	4.26851900	-1.09868700
H	2.23071500	2.59563000	-2.10853800
H	3.72560100	1.62805900	-1.89475100
B	-1.41438700	0.76525000	3.05018300
F	-1.04173600	1.11434600	4.33632900
F	-1.65257200	1.94490100	2.29495100
F	-0.36598300	0.05959700	2.42410200
F	-2.57193400	0.00416900	3.05163100

B	4.65500800	-1.68981800	-0.58319200
F	5.52431800	-2.66169100	-1.02520200
F	4.87566200	-1.37727500	0.75662500
F	3.31754900	-2.14329200	-0.72719600
F	4.79943900	-0.51187500	-1.34919400

18a

Num. Imaginary Frequencies: 0

C	0.53088400	-0.78088100	1.66988400
C	0.45989600	0.51287300	1.02717800
C	-0.58043300	1.42806000	1.49132100
C	-1.67288400	0.91484000	2.21903600
C	-1.61578900	-0.38327400	2.66821600
C	-0.49733300	-1.22959400	2.43812500
H	1.44117600	-1.36550900	1.54284600
H	1.42219600	1.00202300	0.82976100
H	-2.49320700	1.56476800	2.51786600
H	-2.43560500	-0.75122600	3.28131600
H	-0.46449100	-2.21234600	2.90135900
Au	-0.12115200	0.27223500	-1.10256200
H	3.54931600	-1.16703500	-0.31512700
C	3.97135500	-0.16023100	-0.40735700
C	4.73305700	0.17000400	0.88650000
H	3.16498000	0.56314400	-0.57033700
N	4.84762600	-0.11220100	-1.57381600
H	4.26323400	0.97864100	1.45635300
H	4.86853200	-0.71225400	1.51481100
N	6.11391500	0.65470800	0.49867200
C	5.99359900	-0.98773700	-1.34869400
C	5.31081800	1.25585600	-1.76851000
C	6.86393700	-0.46781100	-0.18654400
C	6.86421900	1.18383200	1.67189300
C	5.95465600	1.80498800	-0.47965900
H	5.61617300	-1.98875400	-1.11432300
H	6.59106300	-1.04093500	-2.26655000
H	6.03198200	1.26395900	-2.59473100
H	4.46205100	1.89215300	-2.04277800
H	7.81854000	-0.03863600	-0.51363200
H	7.04241500	-1.24152700	0.56448800
Cl	7.06716900	-0.00803100	2.96518600
H	6.30744500	2.03865500	2.06544100
H	7.85411500	1.49502900	1.32670400
H	6.95127800	2.23105200	-0.64318600

H	5.31934000	2.55223500	0.00810600
F	-0.31688800	0.10710200	-3.12356600
B	4.21852300	-3.41153700	0.95688400
F	3.26015500	-2.56005000	1.56290900
F	5.48764900	-2.86482100	1.17098100
F	3.95155300	-3.43388100	-0.42745500
F	4.12711300	-4.67683900	1.48600300
B	2.51106800	3.27034500	-0.49381800
F	2.09439500	2.29915600	-1.42709600
F	2.73641200	2.61667400	0.73901100
F	3.66237000	3.89089800	-0.92137800
F	1.47200600	4.19129700	-0.29243700
N	-2.51717500	3.62701700	0.63821900
C	-1.34294900	3.81584500	1.28942000
O	-0.99863800	4.83291400	1.85734300
C	-3.52068600	4.68272000	0.72807400
H	-3.17089600	5.44602000	1.42409900
H	-4.46748500	4.26137200	1.08758700
H	-3.68135200	5.13690300	-0.25716300
N	-0.41513600	2.72729800	1.20469300
H	0.52339500	3.05430400	0.95214100
P	0.57398700	-1.98185300	-1.66806700
C	-2.87765800	2.48549700	-0.19157200
H	-3.00660600	1.56794200	0.40152900
H	-3.88904600	2.67985200	-0.57494000
C	-2.05444800	2.13429300	-1.38071700
H	-2.56179200	1.41124400	-2.02722200
C	-0.84902800	2.62118600	-1.77284000
H	-0.30409200	3.38549400	-1.22417900
H	-0.46456500	2.35726300	-2.75549900
N	-4.10126700	-0.47973500	-0.13902400
C	-6.13455200	0.56591700	1.15524900
C	-4.22450100	-2.96803100	1.02910000
O	-6.53691200	-1.05126900	-0.88312500
O	-5.54128800	1.21849600	-1.31189000
O	-2.11290600	-1.93299500	-0.09071800
O	-4.00782900	-2.64139200	-1.57104900
S	-5.59723800	-0.00273300	-0.51321700
S	-3.55226700	-1.96029100	-0.36534100
F	-6.12416600	-0.45096800	2.00104400
F	-7.36024300	1.05292600	1.06465200
F	-5.32206200	1.51674600	1.60695600
F	-3.73499000	-4.19404900	0.93657200
F	-5.54305400	-3.01217400	0.97355700

F	-3.85210700	-2.43992200	2.18759600
C	2.11986600	-1.78846400	-2.60108500
H	2.85478500	-2.49721000	-2.19594300
H	1.91492000	-2.00134100	-3.65608800
H	2.53633600	-0.77847800	-2.52174700
C	0.80481600	-3.20363500	-0.36219900
H	-0.11528300	-3.29025900	0.22353500
H	0.98662500	-4.15114700	-0.89148100
H	1.67427300	-2.99343700	0.26580200
C	-0.67483700	-2.67496500	-2.77459200
H	-0.90952700	-1.95043700	-3.55610700
H	-0.22444000	-3.57633800	-3.21435600
H	-1.57275600	-2.94533700	-2.21468100

TS11a

Num. Imaginary Frequencies: 1

C	-0.03895800	-0.25044700	1.30166400
C	0.18488900	0.49773800	0.10541700
C	-0.09925800	1.91048200	0.16653100
C	-0.51007500	2.49507100	1.34734200
C	-0.74918700	1.70980900	2.47830500
C	-0.50071700	0.34053000	2.46232000
H	0.18196600	-1.31073200	1.31768400
H	1.41029100	0.48243100	-0.17957500
H	-0.61874100	3.57698700	1.39247000
H	-1.09557400	2.18715600	3.39256000
H	-0.66352900	-0.26140300	3.35202200
Au	-0.31875900	-0.55506400	-1.69396400
H	2.90847000	-0.35540000	1.59220600
C	3.31674200	0.56418700	1.16233100
C	4.84448000	0.55654600	1.30965800
H	2.87147100	1.43247300	1.66077900
N	2.94925100	0.59737600	-0.26137600
H	5.19731500	1.41882700	1.88447600
H	5.21036700	-0.38097100	1.74089900
N	5.46834300	0.66904700	-0.06941700
C	3.51549600	-0.56618000	-0.94584300
C	3.43831600	1.82829200	-0.89542700
C	5.05387500	-0.51598800	-0.91100200
C	6.95804700	0.79685700	0.01224600
C	4.96297100	1.92984900	-0.73764900
H	3.17577300	-1.46912100	-0.42930500
H	3.14155200	-0.57533100	-1.97863500

H	3.13989400	1.81414300	-1.95035500
H	2.98687600	2.69022600	-0.39928000
H	5.49866700	-0.36459600	-1.90089400
H	5.47586400	-1.41261400	-0.44619400
Cl	7.73330100	-0.58754900	0.78049700
H	7.17848900	1.69812100	0.59105700
H	7.33929700	0.89454100	-1.00786400
H	5.48390400	2.01652300	-1.69681900
H	5.23135500	2.76849000	-0.08803100
F	-0.65259900	-1.61981000	-3.40789000
B	4.25880000	-3.32432000	1.21669700
F	3.37112600	-2.40718800	1.82989300
F	5.53695400	-2.76204500	1.22699600
F	3.84881800	-3.48779100	-0.12360200
F	4.22797700	-4.52845600	1.87695900
B	2.72486700	4.09151900	1.86331100
F	2.04106400	4.25969300	0.62999100
F	2.01659300	3.17311600	2.63972500
F	4.00015200	3.55414000	1.58379000
F	2.84364400	5.30298200	2.50011200
N	-1.92452800	3.48339600	-1.57113500
C	-0.57948600	3.72724500	-1.49526300
O	-0.05804400	4.74012900	-1.93872400
C	-2.73318400	4.45172000	-2.30048100
H	-2.20211100	5.40297800	-2.33980100
H	-3.69120400	4.58816100	-1.78696700
H	-2.92750100	4.10827400	-3.32791800
N	0.24702100	2.73051200	-0.94394000
H	1.12462500	3.21281100	-0.73422100
P	0.34575100	-2.86227300	-1.30256200
C	-2.55745500	2.20007300	-1.34768500
H	-2.40824900	1.82251200	-0.32537000
H	-3.64435800	2.34774000	-1.40922000
C	-2.22585800	1.12492600	-2.32515100
H	-2.91879300	0.27812700	-2.31466900
C	-1.22724500	1.17137800	-3.25085200
H	-0.57064500	2.03422100	-3.33716900
H	-1.15646500	0.40719800	-4.02156100
N	-3.81169600	-0.42770600	0.28527200
C	-5.45310100	1.32503600	1.38404100
C	-3.88975600	-2.24140900	2.37264700
O	-6.38689200	-0.86846800	0.26693100
O	-5.36148200	0.89279300	-1.20297800
O	-2.02719600	-2.10328600	0.56874900

O	-4.27384700	-2.94494300	-0.14328500
S	-5.32254900	0.09363200	0.01920300
S	-3.48573500	-1.96260200	0.59044100
F	-5.36776000	0.70594200	2.54954800
F	-6.62409800	1.93370100	1.29351600
F	-4.48421000	2.22545700	1.29313700
F	-3.54084400	-3.47950900	2.68697000
F	-5.18099400	-2.07881500	2.59499500
F	-3.20413400	-1.39110600	3.12234300
C	1.70603300	-3.23469100	-2.43690200
H	1.63688000	-4.30499800	-2.67571100
H	1.58888700	-2.65782600	-3.35793700
H	2.66800600	-3.05159500	-1.95072100
C	0.82544800	-3.41291600	0.34808000
H	-0.06388600	-3.45200600	0.98340800
H	1.22384200	-4.42979300	0.21150700
H	1.62208400	-2.81750200	0.80613000
C	-1.06410100	-3.88900200	-1.78282000
H	-1.27002900	-3.74930800	-2.84458200
H	-0.77047800	-4.92841200	-1.57942500
H	-1.94229500	-3.63587100	-1.18302500

19a

Num. Imaginary Frequencies: 0

C	1.08546400	0.87544600	-1.79860200
C	0.14267100	0.66886400	-0.78854800
C	-0.32943100	-0.62373600	-0.55157300
C	0.07955900	-1.68134200	-1.36425900
C	0.98963700	-1.46771400	-2.39003500
C	1.51359900	-0.19187600	-2.58609200
H	1.53058300	1.85925800	-1.94365900
H	2.20489800	-1.39445000	2.03756000
H	-0.31189400	-2.67521000	-1.14832900
H	1.33640200	-2.29520800	-3.00224100
H	2.27397400	-0.03216500	-3.34904600
Au	-0.53368400	2.24923300	0.33478400
H	2.49229900	0.00887400	0.23393200
C	3.06000000	-0.92587100	0.24911800
C	4.44790800	-0.75005700	-0.35421100
H	2.50490400	-1.71964700	-0.25565900
N	3.18860600	-1.32209100	1.68505300
H	4.58585500	-1.36448800	-1.24888100
H	4.64382600	0.30157100	-0.57743100

N	5.48138000	-1.17384700	0.66856800	H	0.59352500	0.72153800	2.62446200
C	3.97522800	-0.29771600	2.43069000	H	0.39227200	2.55966400	2.74675600
C	3.82718000	-2.66227800	1.78876000	N	-4.12512500	-0.88472800	0.49329300
C	5.39691900	-0.24845800	1.85475400	C	-4.01501200	-3.52216400	0.55460300
C	6.85061500	-1.19714000	0.05150300	C	-4.30897500	-0.71402500	-2.22417800
C	5.20786200	-2.59205900	1.13414700	O	-6.33324600	-2.26616600	0.48224900
H	3.46212500	0.65939800	2.29179000	O	-4.90811700	-2.07859900	2.55044900
H	3.97374600	-0.57446600	3.48846700	O	-3.46976200	1.17435700	-0.64610300
H	3.88228200	-2.92521600	2.84874300	O	-5.92718700	0.62089500	-0.62254100
H	3.18404000	-3.37266000	1.26234400	S	-5.02752500	-2.08075500	1.09922500
H	6.15334200	-0.57903500	2.57383500	S	-4.54310400	0.17516400	-0.62630700
H	5.62921100	0.75940000	1.50085800	F	-3.84650800	-3.49077000	-0.75811200
Cl	7.35377000	0.38532000	-0.54603400	F	-4.64677200	-4.63419000	0.89270600
H	6.79988700	-1.90780200	-0.77925900	F	-2.83139200	-3.49578500	1.14680100
H	7.55789200	-1.52696800	0.81766400	F	-4.44879900	0.15296000	-3.21780000
H	6.00608300	-2.84998300	1.83710000	F	-5.19702200	-1.68060200	-2.35700000
H	5.26567900	-3.22840200	0.24683900	F	-3.08628200	-1.22491800	-2.26155600
F	-1.15973800	3.97368500	1.28805000	C	0.03525900	4.62331700	-1.98247800
B	3.17924600	2.94319900	0.57522800	H	-0.27077000	5.18336500	-2.87563400
F	2.53679100	3.35771000	-0.59162300	H	0.09414200	5.29887100	-1.12123000
F	4.34030300	2.21428700	0.25736200	H	1.01946700	4.17067400	-2.13596900
F	2.31011600	2.05883000	1.27406000	C	-1.51585600	2.35809600	-3.08773700
F	3.48661000	4.01682400	1.37797400	H	-2.20271500	1.55059600	-2.81609300
B	4.15614900	-3.61698100	-2.18796900	H	-1.98575100	3.00275400	-3.84165200
F	3.36194100	-3.72001700	-1.02694100	H	-0.58852800	1.93691000	-3.48513100
F	3.77974300	-2.46689700	-2.88544000	C	-2.74718500	4.21377400	-1.20122400
F	5.50442900	-3.45366900	-1.77288600	H	-2.59293300	4.72186400	-0.24487900
F	4.03196900	-4.74355800	-2.96352100	H	-2.98349600	4.92942700	-1.99915500
N	-1.33670200	-1.03172400	2.87151000	H	-3.54520700	3.47182700	-1.10098200
C	-0.58516100	-1.27642900	1.74921700				
O	0.53918400	-1.80067500	1.80543100				
C	-0.82405400	-1.51471600	4.14268900	20a			
H	-0.32745500	-2.47522800	3.99114900	Num. Imaginary Frequencies: 0			
H	-1.66069400	-1.65316900	4.83529800	C	3.98642000	1.10387700	0.39845400
H	-0.10399500	-0.81316800	4.59367700	C	2.61460400	0.88062000	0.45528200
N	-1.15194600	-0.88215800	0.57502400	C	1.81752700	1.56314600	1.37911800
H	-2.16293200	-0.74096500	0.52209400	C	2.41723500	2.48582700	2.24028800
P	-1.20957400	3.36494100	-1.61933500	C	3.78513900	2.72343000	2.17493800
C	-2.16766500	0.16180900	2.91751200	C	4.57218100	2.03454400	1.25627700
H	-2.96949300	0.13245900	2.16442000	H	4.60432200	0.58645000	-0.33621600
H	-2.70713100	0.16475500	3.87597000	H	1.79118400	3.01810500	2.95531300
C	-1.41669200	1.44451300	2.80564500	H	4.23915100	3.44655100	2.84932600
H	-2.01703900	2.35500200	2.86250300	H	5.64237800	2.22304300	1.19809600
C	-0.07382600	1.58189500	2.64410600	C	-0.53394000	2.36958300	1.27751800

Num. Imaginary Frequencies: 0

C	3.98642000	1.10387700	0.39845400
C	2.61460400	0.88062000	0.45528200
C	1.81752700	1.56314600	1.37911800
C	2.41723500	2.48582700	2.24028800
C	3.78513900	2.72343000	2.17493800
C	4.57218100	2.03454400	1.25627700
H	4.60432200	0.58645000	-0.33621600
H	1.79118400	3.01810500	2.95531300
H	4.23915100	3.44655100	2.84932600
H	5.64237800	2.22304300	1.19809600
C	-0.53394000	2.36958300	1.27751800

O	-1.61674600	2.30166200	1.83599600
C	0.68911700	3.21546400	-0.69936900
H	0.54427400	4.08126300	-1.36506700
H	1.76213400	3.22208100	-0.44796800
C	-1.05845600	4.57110100	0.40326000
H	-1.59168600	4.65405000	1.35206000
H	-0.47298000	5.48354300	0.23957600
H	-1.80078100	4.47661000	-0.40238600
N	-0.16665000	3.42518900	0.45760400
C	0.34329500	2.01868400	-1.51996800
H	-0.68499600	1.65724400	-1.46404500
C	1.19061300	1.42875500	-2.41283800
H	2.19089100	1.83597600	-2.58183400
H	0.79115100	0.72303000	-3.14211700
Au	1.68571400	-0.31498600	-0.90960900
P	2.59015000	-2.18927700	0.19558600
F	0.92824900	-1.60423800	-2.31240600
N	0.42005100	1.36951300	1.38615200
H	0.05213600	0.45329500	1.64887200
N	-1.73199600	-0.41446500	-0.17972800
C	-3.78134800	1.15295500	-0.76086700
C	-2.93789600	-1.66969900	1.96790400
O	-3.76013300	-1.37585100	-1.51170300
O	-2.14168300	0.23861300	-2.57072400
O	-0.36818800	-1.50245600	1.55467800
O	-1.71195800	-2.99889100	0.05776700
S	-2.80401200	-0.28480900	-1.37875300
S	-1.56833700	-1.71287100	0.72776600
F	-4.26191900	0.90680200	0.44437000
F	-4.78678800	1.36428200	-1.59823300
F	-3.01854800	2.23591400	-0.72382800
F	-2.81238200	-2.72172400	2.76440500
F	-4.10756900	-1.72137100	1.35262100
F	-2.86369400	-0.56661900	2.68836500
C	4.20234100	-2.52235900	-0.56033400
H	4.61879900	-3.43669000	-0.11769200
H	4.07319900	-2.66785100	-1.63861900
H	4.89865300	-1.69616000	-0.38474800
C	2.82758100	-2.02251500	1.97959600
H	3.22000100	-2.97218900	2.36625500
H	3.53575000	-1.21494500	2.19359700
H	1.86224300	-1.80543800	2.44881900
C	1.54661500	-3.61876900	-0.15428600
H	1.22544400	-3.53881800	-1.19854400

H	2.12695900	-4.53409600	0.01464500
H	0.66317100	-3.60069100	0.48999800

TS12a

Num. Imaginary Frequencies: 1

C	2.33036800	1.50910000	2.12102400
C	1.41413500	1.43712700	1.07442900
C	0.18320900	2.08793000	1.20284800
C	-0.12193700	2.78950400	2.36824400
C	0.79859900	2.83982200	3.40957700
C	2.02635900	2.20195700	3.29060700
H	3.30653900	1.03171000	2.02311400
H	-1.08941600	3.27058400	2.48492800
H	0.54644000	3.38511100	4.31679200
H	2.75245000	2.24561400	4.10023900
C	-2.04238400	2.65996000	0.30737200
O	-2.84645300	2.34261500	1.15977300
C	-0.94656400	3.71919200	-1.45876200
H	-1.21934400	3.90206800	-2.50513500
H	-0.28760100	4.53613500	-1.12017400
C	-3.26524000	4.50605500	-0.74988900
H	-4.01715000	4.20196400	-0.01697700
H	-2.97116100	5.54564400	-0.55783000
H	-3.69241300	4.43639100	-1.75772000
N	-2.12918100	3.62528700	-0.62518500
C	-0.30238800	2.34678900	-1.27160100
H	-0.79822200	1.63240900	-1.94419800
C	1.18243900	2.28981600	-1.48168900
H	1.70591500	3.14634500	-1.04039400
H	1.41981100	2.21605400	-2.54927000
Au	1.94873000	0.52297900	-0.65667800
P	2.88945200	-1.58743600	0.15175500
F	2.59991000	-0.26836600	-2.45370500
N	-0.77208700	1.96206800	0.11715000
H	-1.21413000	0.58408900	0.16950200
N	-1.68998100	-0.49902300	0.20023300
C	-1.50390100	-2.85641700	1.61058000
C	-1.59271100	-1.73433300	-2.16437600
O	-3.36921300	-1.05838600	2.11389400
O	-0.94535500	-0.46486600	2.57104000
O	-2.92440500	0.50065100	-1.76219700
O	-3.82530600	-1.63748300	-0.73030400
S	-1.97059100	-1.07012100	1.74532700

S	-2.72562900	-0.76346800	-1.07607300
F	-2.36039600	-3.50777300	0.85373800
F	-1.51236200	-3.35173100	2.83285300
F	-0.28690900	-2.96134900	1.09735200
F	-2.24965900	-2.05123700	-3.26151100
F	-1.20608800	-2.83100700	-1.53715700
F	-0.53871200	-0.99654000	-2.46450600
C	2.71968800	-2.12454100	1.88723700
H	3.05621800	-3.16278200	2.00143800
H	3.33079300	-1.48252800	2.53209000
H	1.67633100	-2.03794700	2.20823000
C	2.28997700	-2.94014100	-0.90859000
H	2.93060300	-3.82616000	-0.81745700
H	1.26077900	-3.20762500	-0.65367500
H	2.31558000	-2.54918600	-1.93211500
C	4.68358700	-1.53895300	-0.16783300
H	5.16025100	-0.78186100	0.46625400
H	5.14570300	-2.51599200	0.02228100
H	4.82325300	-1.26018400	-1.21843600

21a

Num. Imaginary Frequencies: 0

C	2.62797900	1.08274700	2.18544200
C	1.73257200	1.13104600	1.11922400
C	0.60045200	1.93087800	1.25616800
C	0.34530100	2.66903200	2.40400400
C	1.25380900	2.60729900	3.45523300
C	2.39005000	1.81396700	3.34760600
H	3.53125000	0.47675600	2.10797900
H	-0.56055900	3.26284600	2.50206500
H	1.06218200	3.17584000	4.36218900
H	3.09999400	1.76283200	4.17080600
C	-1.58786500	2.76653900	0.35037200
O	-2.47576100	2.42309700	1.08550400
C	-0.17840100	3.86856500	-1.16104400
H	-0.33685700	4.28179100	-2.16334800
H	0.58545100	4.47302400	-0.64679400
C	-2.36106100	4.95701800	-0.41471100
H	-3.20472900	4.69795100	0.22962600
H	-1.87975300	5.86738500	-0.03840200
H	-2.72145500	5.13505200	-1.43411800
N	-1.42091900	3.85631500	-0.40664000
C	0.20023000	2.39493700	-1.21467500

H	-0.43367500	1.87858600	-1.94747900
C	1.64751500	2.06951900	-1.44939300
H	2.31970800	2.82656300	-1.02907700
H	1.84250500	1.94560600	-2.51988200
Au	2.15068900	0.19421300	-0.63190400
P	2.67836200	-2.05815100	0.12878400
F	2.74663100	-0.62493600	-2.41807400
N	-0.35563900	1.91523300	0.13323300
H	-0.70327400	0.91970600	0.05359200
N	-1.39250800	-0.68577800	0.01719300
C	-3.14575400	-0.35081500	-1.92833500
C	-3.18883600	-1.71205600	1.82218600
O	-1.92835700	-2.68602600	-1.56198000
O	-0.60615100	-0.68878300	-2.35567100
O	-0.86084300	-0.66292000	2.42434200
O	-0.90635200	-2.89656300	1.26287300
S	-1.61444600	-1.26877000	-1.47449100
S	-1.40384400	-1.53248400	1.39119600
F	-4.15290700	-0.69954100	-1.15064700
F	-3.44417900	-0.61561800	-3.18745700
F	-2.92057200	0.95467500	-1.79611600
F	-3.27229100	-2.27361400	3.01795300
F	-3.79429200	-2.48056800	0.93261600
F	-3.76905900	-0.52636400	1.85131900
C	1.71281000	-3.21212700	-0.88987700
H	1.76980700	-2.84978500	-1.92281700
H	2.11929100	-4.22872600	-0.81446500
H	0.66818100	-3.21253700	-0.55465300
C	2.43541300	-2.55781000	1.86226600
H	2.61763500	-3.63494400	1.96941400
H	3.12770700	-2.01254200	2.51363700
H	1.40738100	-2.33648100	2.16873000
C	4.42307000	-2.41765700	-0.24467000
H	4.64860200	-3.47610400	-0.06253400
H	4.60078000	-2.17248900	-1.29727300
H	5.07213100	-1.79441200	0.38198600

TS13a

Num. Imaginary Frequencies: 1

C	2.33036800	1.50910000	2.12102400
C	1.41413500	1.43712700	1.07442900
C	0.18320900	2.08793000	1.20284800
C	-0.12193700	2.78950400	2.36824400

C	0.79859900	2.83982200	3.40957700
C	2.02635900	2.20195700	3.29060700
H	3.30653900	1.03171000	2.02311400
H	-1.08941600	3.27058400	2.48492800
H	0.54644000	3.38511100	4.31679200
H	2.75245000	2.24561400	4.10023900
C	-2.04238400	2.65996000	0.30737200
O	-2.84645300	2.34261500	1.15977300
C	-0.94656400	3.71919200	-1.45876200
H	-1.21934400	3.90206800	-2.50513500
H	-0.28760100	4.53613500	-1.12017400
C	-3.26524000	4.50605500	-0.74988900
H	-4.01715000	4.20196400	-0.01697700
H	-2.97116100	5.54564400	-0.55783000
H	-3.69241300	4.43639100	-1.75772000
N	-2.12918100	3.62528700	-0.62518500
C	-0.30238800	2.34678900	-1.27160100
H	-0.79822200	1.63240900	-1.94419800
C	1.18243900	2.28981600	-1.48168900
H	1.70591500	3.14634500	-1.04039400
H	1.41981100	2.21605400	-2.54927000
Au	1.94873000	0.52297900	-0.65667800
P	2.88945200	-1.58743600	0.15175500
F	2.59991000	-0.26836600	-2.45370500
N	-0.77208700	1.96206800	0.11715000
H	-1.21413000	0.58408900	0.16950200
N	-1.68998100	-0.49902300	0.20023300
C	-1.50390100	-2.85641700	1.61058000
C	-1.59271100	-1.73433300	-2.16437600
O	-3.36921300	-1.05838600	2.11389400
O	-0.94535500	-0.46486600	2.57104000
O	-2.92440500	0.50065100	-1.76219700
O	-3.82530600	-1.63748300	-0.73030400
S	-1.97059100	-1.07012100	1.74532700
S	-2.72562900	-0.76346800	-1.07607300
F	-2.36039600	-3.50777300	0.85373800
F	-1.51236200	-3.35173100	2.83285300
F	-0.28690900	-2.96134900	1.09735200
F	-2.24965900	-2.05123700	-3.26151100
F	-1.20608800	-2.83100700	-1.53715700
F	-0.53871200	-0.99654000	-2.46450600
C	2.71968800	-2.12454100	1.88723700
H	3.05621800	-3.16278200	2.00143800
H	3.33079300	-1.48252800	2.53209000

H	1.67633100	-2.03794700	2.20823000
C	2.28997700	-2.94014100	-0.90859000
H	2.93060300	-3.82616000	-0.81745700
H	1.26077900	-3.20762500	-0.65367500
H	2.31558000	-2.54918600	-1.93211500
C	4.68358700	-1.53895300	-0.16783300
H	5.16025100	-0.78186100	0.46625400
H	5.14570300	-2.51599200	0.02228100
H	4.82325300	-1.26018400	-1.21843600

3.4 Cycle IV

22

Num. Imaginary Frequencies: 0

N	1.82106200	-0.28054500	-0.63120500
C	4.08413500	-1.49719300	0.32265600
C	2.57263000	2.16504200	0.06487200
O	3.12088200	-1.99547800	-2.08798000
O	1.79076800	-2.66495200	-0.06265900
O	0.95164700	1.67998800	-1.92581300
O	3.37984800	1.10798600	-2.20192500
S	2.60378500	-1.66960700	-0.76748300
S	2.17486900	1.09243100	-1.38365300
F	4.92434500	-0.60936700	-0.18003500
F	4.68483600	-2.67190000	0.41176900
F	3.70305400	-1.10550800	1.52970600
F	1.59851000	2.14383400	0.97025200
F	2.72183500	3.40695600	-0.36992700
F	3.69359700	1.75518900	0.63348200
C	-0.00272300	0.05978600	3.19094700
C	-1.12815600	-1.65808900	1.84284900
C	-2.12407200	-1.73827700	2.82861500
C	-2.04410900	-0.93464600	3.95792400
C	-1.00038900	-0.02547300	4.14883300
H	0.84479600	0.73078300	3.32145000
H	-2.93841500	-2.44144100	2.70141500
H	-2.81948000	-1.02621600	4.71666200
H	-0.96326800	0.59145400	5.04326300
C	-2.28616200	-2.67105200	-0.04835600
O	-3.39901700	-2.58984700	0.45796400
C	-3.30341500	-3.09824300	-2.17932900

H	-3.09685800	-3.80799200	-2.99172800	F	5.19505400	-2.03931400	0.23262900
H	-4.09404500	-3.51956900	-1.55199600	F	4.40712600	-0.12475300	0.85365800
C	-0.84360300	-2.73238000	-2.06429400	F	2.04990800	3.05956200	-1.93362500
H	-0.57507000	-1.66182800	-2.04447600	F	3.56440200	1.96460600	-0.84197300
H	-0.00998900	-3.31441400	-1.65398100	F	1.71631500	2.50928200	0.12744100
H	-0.96349500	-3.03248600	-3.10959600	C	0.49351900	-0.37521600	3.00426200
N	-2.09057400	-3.00220200	-1.36395100	C	-0.72419500	-1.77519100	1.45640100
C	-3.72617000	-1.76540100	-2.72445200	C	-0.67488200	-2.82571100	2.37732200
H	-3.11952400	-1.35620400	-3.53800800	C	-0.04234600	-2.63049000	3.59813400
C	-4.76552600	-1.07629000	-2.25683400	C	0.55791800	-1.41346400	3.92157100
H	-5.37868400	-1.46568600	-1.44373500	H	0.96059700	0.58118400	3.24736200
H	-5.04803500	-0.10782100	-2.66958300	H	-1.12279100	-3.78227100	2.13145400
Au	-1.17173800	0.81735700	0.70259400	H	-0.00393800	-3.45752100	4.30624900
P	-2.12275400	2.34285000	-0.77103700	H	1.06094700	-1.28318700	4.87809500
N	-1.12035000	-2.44037800	0.68665400	C	-2.13323500	-2.90675400	-0.27362200
H	-0.21897400	-2.45976500	0.20756900	O	-2.66222500	-3.72093900	0.47437800
C	-0.05838400	-0.73577900	2.02379800	C	-3.49414800	-3.65955100	-2.12611200
H	0.81131500	-0.79589700	1.36501500	H	-3.23670600	-4.01328400	-3.13474900
C	-2.16018000	1.76400700	-2.49349000	H	-3.60844000	-4.53425800	-1.47874500
H	-2.65680400	2.51264400	-3.12444800	C	-1.75347600	-1.91469100	-2.51983600
H	-1.13303100	1.60275900	-2.83877100	H	-2.12919400	-0.88887900	-2.36519500
H	-2.70982200	0.81605600	-2.54048100	H	-0.66045800	-1.90964200	-2.41264800
C	-3.84845700	2.76150900	-0.37020300	H	-1.98043100	-2.19869200	-3.55238300
H	-3.90426200	3.19094200	0.63626500	N	-2.35904300	-2.88470100	-1.62940900
H	-4.23804200	3.48624700	-1.09699100	C	-4.75525900	-2.84993500	-2.14162900
H	-4.46003500	1.85258000	-0.39804200	H	-4.76506700	-1.98016700	-2.80538700
C	-1.23117200	3.92847800	-0.79889600	C	-5.81202400	-3.11914500	-1.37978400
H	-0.19026000	3.74441400	-1.08620500	H	-5.81593300	-3.97627500	-0.70516100
H	-1.69693200	4.60848600	-1.52375000	H	-6.71030500	-2.50435900	-1.39683700
H	-1.25601200	4.38531700	0.19669900	Au	-1.08704300	1.23462400	0.97576800

TS14

Num. Imaginary Frequencies: 1

N	1.71680300	-0.39318700	-0.27500800	H	0.90141800	-0.31410300	0.60427800
C	4.38584400	-1.04830300	-0.08904200	C	-1.10041800	4.28537800	-0.78094500
C	2.26965800	2.13787700	-1.01295800	H	-1.68274500	5.10255200	-1.22640300
O	2.63799800	-2.50911900	-1.45766500	H	-0.40850900	4.69578200	-0.03726600
O	2.40767800	-2.36770300	1.06018300	H	-0.52115900	3.78898400	-1.56826500
O	0.10844700	0.83246600	-1.80507700	C	-3.25368600	2.49957100	-1.39524500
O	2.35959000	0.11690600	-2.71410300	H	-4.01512000	1.80186400	-1.02820400
S	2.67867900	-1.75529900	-0.22266100	H	-3.74461000	3.35167800	-1.88341900
S	1.52449300	0.55568900	-1.61639100	H	-2.62073800	1.97674000	-2.12293600
F	4.75365600	-0.52120700	-1.23931300	C	-3.33268900	4.05334600	1.03582100

H	-2.76752900	4.52318500	1.84847900
H	-3.82039100	4.83231200	0.43561500
H	-4.09690200	3.40197000	1.47418800

23

Num. Imaginary Frequencies: 0

N	1.88597700	-0.59914100	-0.38917800
C	4.49737600	-1.27792400	0.06477100
C	2.37734400	1.95038300	-1.17532300
O	2.91701800	-2.68504800	-1.54350400
O	2.38734700	-2.63164100	0.94444900
O	0.21814900	0.59477200	-1.89717800
O	2.47410400	-0.12647500	-2.82467900
S	2.82795000	-2.00153600	-0.27655900
S	1.63824100	0.34829500	-1.74877000
F	4.92911900	-0.64427800	-1.00554700
F	5.30204100	-2.27820900	0.35825800
F	4.41230800	-0.44738000	1.08281200
F	2.12343500	2.85005000	-2.10697300
F	3.67474700	1.79967200	-1.02590700
F	1.83374400	2.32585700	-0.03233800
C	0.20507700	-0.87006000	2.97196000
C	-1.01376500	-1.88017300	1.16194600
C	-0.87480700	-3.13051200	1.77171700
C	-0.21115500	-3.23170000	2.98982500
C	0.34150300	-2.10868900	3.59496100
H	0.63401600	0.01114700	3.45329500
H	-1.29427200	-4.00819200	1.29148900
H	-0.11341500	-4.21029200	3.45883100
H	0.87195300	-2.19498700	4.54241300
C	-2.60168400	-2.53556400	-0.66344400
O	-2.88952000	-3.64891800	-0.23517200
C	-4.33214000	-2.74053200	-2.33922300
H	-4.34544000	-2.57122400	-3.42584000
H	-4.15615300	-3.80618400	-2.16352000
C	-3.05411800	-0.61274000	-2.17302700
H	-3.44714400	0.07665800	-1.40515600
H	-2.00942600	-0.34727900	-2.38418900
H	-3.61849500	-0.44307400	-3.09575600
N	-3.18939300	-2.00802100	-1.79717800
C	-5.62904400	-2.31916000	-1.71607000
H	-5.94127500	-1.28607600	-1.89594600
C	-6.37785400	-3.11608900	-0.95885500

H	-6.07873300	-4.14530300	-0.75689400
H	-7.31047100	-2.77879000	-0.50962000
Au	-0.96328500	1.19909600	1.06534600
P	-1.64347300	3.34814400	0.28448600
N	-1.65095100	-1.71886100	-0.08692100
H	-1.53933300	-0.78337400	-0.46396000
C	-0.48459000	-0.71249000	1.76082200
H	1.15578700	-0.54152000	0.35923800
C	-0.72469800	4.77823600	0.95230100
H	-1.10507500	5.71589900	0.52643300
H	-0.83120800	4.80713300	2.04256900
H	0.33933200	4.67678700	0.71082600
C	-1.52812100	3.55790100	-1.52670900
H	-2.11209100	2.77532000	-2.02546400
H	-1.91181800	4.54285800	-1.82393600
H	-0.48633300	3.46447000	-1.85181200
C	-3.39119600	3.73750900	0.64430800
H	-3.55721800	3.72335100	1.72741000
H	-3.65937100	4.72562600	0.24807900
H	-4.03482800	2.97700000	0.18624600

24

Num. Imaginary Frequencies: 0

H	3.77656100	1.07297600	1.50698300
C	3.56692500	0.07405400	1.90440100
C	4.44929600	-0.99910600	1.25533900
H	3.62184400	0.06422300	2.99551600
N	2.14360900	-0.21256000	1.54228600
H	4.93593300	-1.64010600	1.99649900
H	5.19290100	-0.52178500	0.61473800
N	3.58486300	-1.88475800	0.39825500
C	1.92040200	-0.05939600	0.07492900
C	1.69441000	-1.55739400	1.99586400
C	2.85720100	-1.04139500	-0.63144700
C	4.36828700	-2.97576300	-0.28563200
C	2.59219800	-2.58634700	1.29935100
H	2.15508800	0.98038100	-0.16473200
H	0.86552200	-0.29141700	-0.11171400
H	0.64364800	-1.66902200	1.69552500
H	1.78305300	-1.57435600	3.08573500
H	2.28895500	-1.73083100	-1.26247400
H	3.61329200	-0.50237100	-1.20780400
Cl	5.61369000	-2.34181900	-1.35533500

H	4.83692600	-3.58425400	0.49249200
H	3.64100000	-3.55638700	-0.86069400
H	1.98721400	-3.25461800	0.68235900
H	3.17242700	-3.16622500	2.02277300
B	4.22376300	2.21313700	-1.01970100
F	4.94406800	3.27017400	-1.51006900
F	5.07509600	1.16760000	-0.61027800
F	3.45837600	2.61098700	0.11041200
F	3.33559300	1.70082800	-1.97268700
B	0.09323200	-3.27559300	-1.00293900
F	-0.00768600	-1.88286900	-1.23983600
F	1.40027900	-3.67005200	-1.39181900
F	-0.85806600	-3.95637700	-1.71194200
F	-0.02654200	-3.50038600	0.37338300
C	-1.70506300	-0.77825900	2.65025500
C	-1.90537100	-0.46507200	1.29598400
C	-2.59860300	-1.41259500	0.52432400
C	-3.08316100	-2.59702700	1.08351800
C	-2.89168100	-2.86284600	2.43422700
C	-2.19089700	-1.95459100	3.22203800
H	-1.16453300	-0.07317100	3.28729500
H	-3.59872600	-3.31629800	0.44747200
H	-3.27239300	-3.78868900	2.86364500
H	-2.02906800	-2.15760100	4.28073800
C	-3.85585100	-1.49594300	-1.64997200
O	-3.72119700	-1.86151300	-2.81477600
C	-5.38269100	-0.29614900	-0.10190500
H	-6.35164000	-0.53876400	0.36116600
H	-4.64104400	-0.30536000	0.70603500
C	-6.22265200	-1.73470700	-1.91383100
H	-6.00878700	-2.68354700	-2.41213700
H	-7.11688700	-1.85055600	-1.29055800
H	-6.43071100	-0.98713800	-2.69595500
N	-5.10520000	-1.36542500	-1.06395200
C	-5.44086200	1.06175800	-0.73483200
H	-6.05516600	1.14816500	-1.63554200
C	-4.81445100	2.13519300	-0.25752600
H	-4.19198500	2.08099200	0.63975200
H	-4.90384000	3.11132100	-0.73234800
Au	-1.27218100	1.34286600	0.48858100
P	-0.48799000	3.46554000	-0.28326800
F	1.37500400	0.72792700	2.19010500
N	-2.76381200	-1.16986000	-0.87341500
H	-1.89541300	-1.26221000	-1.39840100

C	0.50234700	3.48574600	-1.81644400
H	0.76856700	4.51901600	-2.07673700
H	1.42374400	2.90470200	-1.68190200
H	-0.07436700	3.04398900	-2.63690800
C	-1.79781600	4.70205600	-0.59572900
H	-1.35538800	5.67935800	-0.83020200
H	-2.41396800	4.37492300	-1.44123500
H	-2.43963900	4.79639400	0.28825200
C	0.60807400	4.27897200	0.93143700
H	1.51660900	3.67587100	1.04604400
H	0.88996700	5.28212200	0.58483100
H	0.10276500	4.35665700	1.90094300

TS15

Num. Imaginary Frequencies: 1

H	2.03189800	-1.94314500	-0.80717700
C	2.43455000	-1.13188800	-1.42015300
C	3.96928700	-1.23739300	-1.56168000
H	1.94156000	-1.12505800	-2.39655300
N	2.17129200	0.14307200	-0.75984100
H	4.30512200	-1.13317400	-2.59888000
H	4.32627600	-2.17987800	-1.13419000
N	4.61297200	-0.10791500	-0.78063100
C	2.60131600	0.14510600	0.64058400
C	2.68715500	1.27395200	-1.52233300
C	4.10972500	-0.15298400	0.64969100
C	6.11126900	-0.17655700	-0.84839800
C	4.21725100	1.22712700	-1.38653100
H	2.06414700	-0.65423200	1.15724000
H	2.36438500	1.12607200	1.05633100
H	2.29908300	2.20517200	-1.10134100
H	2.35238400	1.16454700	-2.55788600
H	4.65446100	0.61170400	1.21234000
H	4.32075900	-1.15881700	1.02620500
Cl	6.77205400	-1.61197600	-0.07524900
H	6.39083900	-0.17748000	-1.90557100
H	6.49998700	0.71680300	-0.35117200
H	4.56700000	2.00247000	-0.69693000
H	4.71622300	1.31912700	-2.35614400
B	2.93786700	-3.76492200	0.82309400
F	2.84898700	-4.91023300	1.58038900
F	2.47231600	-3.98487100	-0.47730400
F	2.16175700	-2.73694400	1.40492700

F	4.26993500	-3.30695100	0.75012900
B	2.71088100	3.76019100	0.91098900
F	1.53933500	2.99435600	1.12614800
F	3.82534400	2.92130900	1.13014700
F	2.74095600	4.84197200	1.75426800
F	2.71542600	4.15535800	-0.43399600
C	-0.76455100	-2.23154700	0.41163200
C	-1.78157100	-1.43791300	-0.12056200
C	-2.92636200	-2.07795700	-0.61060300
C	-3.06102700	-3.46654300	-0.53541700
C	-2.04770300	-4.23378400	0.03136200
C	-0.88880500	-3.61724600	0.49661800
H	0.14842300	-1.77821100	0.79438500
H	-3.96391200	-3.93830600	-0.92384000
H	-2.15783700	-5.31557400	0.08915900
H	-0.07298300	-4.20026600	0.92405700
C	-5.31613500	-1.35980000	-1.05442700
O	-6.07704100	-1.08468100	-1.97792200
C	-5.02660400	-1.32771100	1.40209900
H	-5.63710800	-1.65431200	2.25645300
H	-4.07959300	-1.87820500	1.48276300
C	-7.21265800	-1.75729500	0.35711200
H	-7.66577100	-2.16900300	-0.54678400
H	-7.46289300	-2.39856300	1.20959600
H	-7.64300500	-0.75714700	0.52969100
N	-5.76804200	-1.71568400	0.20282700
C	-4.77649700	0.14724100	1.50513900
H	-5.53107000	0.79754600	1.05155600
C	-3.72286900	0.67946000	2.13259300
H	-2.96824700	0.05224100	2.61077600
H	-3.61417600	1.75572900	2.25792700
Au	-1.72935600	0.63440400	-0.09466800
P	-1.75550300	3.05360000	-0.20146000
F	0.51463300	0.34972500	-0.67873200
N	-3.94792300	-1.28744200	-1.22481500
H	-3.71726900	-0.90414100	-2.13583500
C	-1.52078900	4.02966000	1.32154500
H	-1.65503900	5.09737200	1.10377400
H	-2.24355200	3.72801400	2.08792000
H	-0.50506900	3.85876400	1.69275200
C	-0.55113900	3.77857600	-1.36498200
H	-0.80411100	4.82757300	-1.56871400
H	0.44990400	3.73816700	-0.91903300
H	-0.55498800	3.21568000	-2.30597100

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Num. Imaginary Frequencies: 0

H	-2.24927800	-2.27422200	1.18384900
C	-2.42827800	-1.24588900	1.52186100
C	-3.87903200	-0.83884800	1.18625300
H	-2.27198600	-1.20055500	2.60697900
N	-1.46757600	-0.37340300	0.85712600
H	-4.40537500	-0.35942500	2.02131000
H	-4.45282300	-1.69021000	0.81103900
N	-3.82740700	0.18980500	0.07974900
C	-1.57315600	-0.56974400	-0.58709100
C	-1.76563300	1.01456500	1.17869200
C	-3.01638200	-0.36750000	-1.07700100
C	-5.18271800	0.61799600	-0.35407600
C	-3.13401000	1.43291000	0.60605600
H	-1.25438900	-1.58832100	-0.84160900
H	-0.92459400	0.14476300	-1.10337300
H	-0.99625000	1.66901100	0.75330500
H	-1.75275000	1.13138000	2.26970900
H	-3.07314400	0.36861000	-1.88504400
H	-3.48848700	-1.30961100	-1.36485100
Cl	-6.14075000	-0.68672600	-1.07480400
H	-5.71710000	0.99446100	0.52259000
H	-5.05583700	1.40927800	-1.09849700
H	-3.03063500	2.11911900	-0.23991900
H	-3.79864600	1.87093400	1.35987900
B	-3.01999800	-4.07453000	-0.96916800
F	-3.44319500	-5.30743500	-1.44402100
F	-2.09052500	-4.24759800	0.06320200
F	-2.44061300	-3.33186400	-2.00608400
F	-4.12531300	-3.35542300	-0.46741700
B	-0.88765600	3.09404600	-1.65720900
F	0.18153500	2.19092700	-1.39874400
F	-1.97136600	2.36837800	-2.17336700
F	-0.46375700	4.03544900	-2.58147800
F	-1.26031800	3.69244000	-0.45873500
C	0.79980400	-3.05549500	-2.24239100
C	1.24422400	-1.76373800	-2.04007300

C	1.61107700	-1.29153700	-0.78304900	B	-3.18635200	-2.97940000	-1.59632400
C	1.57128500	-2.16097800	0.30457000	F	-2.04251300	-2.48261000	-2.22400400
C	1.13819800	-3.47039200	0.11819400	F	-3.86236900	-3.85242600	-2.43309700
C	0.73980200	-3.91176700	-1.14056300	F	-4.03111700	-1.88989700	-1.27270800
H	0.47927700	-3.39825800	-3.22496600	F	-2.81873500	-3.63203200	-0.41046900
H	1.84938500	-1.79083700	1.29073500	C	1.70872600	-2.36562800	-2.25821500
H	1.08105400	-4.14544000	0.96961400	C	1.61029500	-1.74988900	-1.02092000
H	0.35393900	-4.92084600	-1.26535400	C	0.97142700	-2.37399600	0.04987300
C	3.17877600	0.66074800	-0.36749400	C	0.44122100	-3.65407700	-0.12986200
O	3.25559100	1.76940700	0.14260500	C	0.56467800	-4.29067700	-1.35873000
C	4.29791400	-0.97029900	-1.86218000	C	1.19586100	-3.65266100	-2.42138800
H	5.34597200	-1.24951600	-2.05869900	H	2.18502700	-1.85676100	-3.09583800
H	3.78441500	-1.91624400	-1.64887200	H	-0.10315600	-4.12453100	0.68886500
C	5.58748800	0.55008700	-0.41694200	H	0.13538700	-5.28139600	-1.49401300
H	5.50259800	1.09283700	0.52566100	H	1.28289500	-4.14897300	-3.38629300
H	6.34580000	-0.23372700	-0.31246300	C	0.99983100	-2.35978300	2.49822700
H	5.91092400	1.25993500	-1.19437700	O	0.12800700	-2.43525200	3.35048700
N	4.30558900	-0.06467900	-0.73154900	C	3.31309000	-2.42056700	1.75092600
C	3.82792000	-0.38266100	-3.15580000	H	4.29120900	-2.62357100	2.22582100
H	4.07802600	0.66789300	-3.33281000	H	3.33161700	-2.97887200	0.79933500
C	3.33812200	-1.14797600	-4.19573700	C	2.61613900	-3.69715500	3.77581200
H	3.23013300	-2.22689700	-4.07049300	H	1.70167300	-3.90822600	4.33353700
H	3.33642100	-0.77165900	-5.21818300	H	3.05136800	-4.64181200	3.42606600
Au	1.39491600	-0.27139800	-3.46456000	H	3.33262500	-3.20155000	4.44429700
P	1.44492400	1.85505500	-4.76749100	N	2.27471300	-2.84524500	2.65383000
F	-0.58382100	-0.05602500	-3.34602300	C	3.33973900	-0.96175800	1.49609000
N	1.95483900	0.08653100	-0.64060200	H	2.96897100	-0.30376400	2.28552500
H	1.19026000	0.75485900	-0.54206600	C	4.01390600	-0.40532900	0.40771100
C	2.35465400	1.97598000	-6.34515800	H	4.54993100	-1.08900700	-0.25606200
H	2.22219600	2.97961700	-6.76938900	H	4.49364000	0.55903500	0.57590200
H	3.42583400	1.80537100	-6.18304300	N	0.83558100	-1.67643800	1.28764800
H	1.97866800	1.23437300	-7.05894700	H	-0.04582200	-1.11516200	1.31560500
C	-0.26251200	2.34817900	-5.13605300	H	-2.57003900	-1.36246900	2.66766300
H	-0.31748600	3.42704000	-5.32130000	C	-2.71119200	-1.13895900	1.60318000
H	-0.60156000	1.79746100	-6.02129200	C	-4.06246200	-0.44374500	1.34702700
H	-0.89404200	2.07905900	-4.28433800	H	-2.67756500	-2.07736100	1.03652500
C	2.18789000	3.13319300	-3.70026200	N	-1.60671800	-0.28448000	1.16898500
H	3.27685300	3.00470600	-3.67584200	H	-4.60646600	-0.93362700	0.53664600
H	1.95204000	4.13109700	-4.09051800	H	-4.69551600	-0.37328000	2.23947100
H	1.77585200	3.04178300	-2.69020400	N	-3.77898000	0.97366500	0.90033800
				C	-1.55715400	0.92008500	1.98753400
				C	-1.77250400	0.07807000	-0.24155100
				C	-2.91670800	1.63830200	1.95844500
				C	-5.01106900	1.80097400	0.78915400

TS16

Num. Imaginary Frequencies: 1

C	-3.01967500	0.95497400	-0.41601400
H	-1.29677300	0.64149100	3.01685000
H	-0.77937300	1.58145300	1.58996700
H	-0.88777300	0.62614000	-0.58555600
H	-1.86086700	-0.84016800	-0.83308600
H	-2.82446100	2.69301100	1.68685700
H	-3.46889000	1.54590100	2.90089900
Cl	-6.20829600	1.11886100	-0.32486100
H	-4.70855900	2.78835900	0.42731500
H	-5.46273300	1.87307700	1.78255200
H	-2.77849900	2.00197900	-0.62880100
H	-3.70021000	0.54481400	-1.16635000
B	-1.02669200	4.08201600	0.34622800
F	-0.48707100	2.92975600	-0.25859800
F	-2.40749100	4.12374100	0.08398800
F	-0.40096900	5.21499700	-0.15027000
F	-0.82747100	3.98314200	1.72958500
Au	2.24390200	0.20307500	-0.74261200
P	2.78248500	2.63048800	-0.53543900
F	0.80928500	0.74346700	-2.03560300
C	4.55011100	3.03987200	-0.76453000
H	4.67600400	4.13015800	-0.76035600
H	4.90744300	2.64223000	-1.72117700
H	5.16159000	2.62018200	0.04308200
C	2.39424100	3.32037000	1.10651000
H	2.71979100	4.36767000	1.15578500
H	2.92431800	2.74472200	1.87651100
H	1.31640400	3.27449300	1.29388600
C	1.89950900	3.58903800	-1.80996700
H	1.17071500	2.91861600	-2.27505700
H	2.61596800	3.94803600	-2.55722000
H	1.36263500	4.42667200	-1.35284700

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Num. Imaginary Frequencies: 0

H	2.08490600	-5.16193200	-1.63122700
N	0.77670300	-4.17700100	-0.34154500
C	-0.50675300	-2.29816300	-0.84863900
H	0.26239100	-1.72091700	-1.37145500
C	-1.87255600	-1.73135200	-1.11475300
H	-2.66743800	-2.44691100	-0.86625600
H	-1.94016600	-1.50767600	-2.18650800
Au	-2.33430700	-0.03231000	0.00465600

P	-2.87902200	1.35882200	-1.91777700
F	-3.03611000	1.46140500	1.21653800
N	-0.05727100	-2.27547000	0.60469200
H	0.49937700	-1.37080300	0.75851100
C	-1.57306000	1.58381700	-3.16755800
H	-1.14800200	0.61295300	-3.45066300
H	-1.98245000	2.07320400	-4.06045500
H	-0.78864000	2.21108300	-2.73222600
C	-3.47068900	3.01694800	-1.47312100
H	-3.93910800	3.49033100	-2.34520900
H	-4.19681600	2.91829500	-0.66002800
H	-2.63337900	3.62840100	-1.12004500
C	-4.27273500	0.60084000	-2.82164400
H	-4.54268100	1.21298000	-3.69191800
H	-4.00942100	-0.40689800	-3.16294800
H	-5.13815100	0.52692200	-2.15270200
H	2.94836600	-0.72068300	2.10617400
C	2.92979600	-0.45459000	1.04295400
C	3.95299000	0.64633700	0.71884100
H	3.17549400	-1.35169800	0.46308200
N	1.56455400	-0.00491200	0.71888000
H	4.49888100	0.41994600	-0.20395700
H	4.66007900	0.82518500	1.53420300
N	3.19524000	1.92941200	0.48022600
C	1.17749100	1.07974200	1.63197000
C	1.52620000	0.50053100	-0.66080100
C	2.25986300	2.16751000	1.64935800
C	4.08398900	3.10441200	0.24976800
C	2.38906800	1.75913600	-0.79753100
H	1.03540100	0.66776100	2.63766600
H	0.22639800	1.50983100	1.29608700
H	0.48392000	0.74154600	-0.90924100
H	1.89540700	-0.28504900	-1.32596500
H	1.83723800	3.16950100	1.53870200
H	2.88236500	2.13120100	2.54864100
Cl	5.09727200	3.49222300	1.65131700
H	4.73705800	2.87183500	-0.59559400
H	3.43226400	3.95607900	0.03148900
H	1.79651200	2.66919300	-0.91499700
H	3.11532900	1.66588000	-1.61216600
B	-0.15529800	4.17172800	0.11894800
F	1.17211900	4.59306800	-0.12074600
F	-0.30737400	3.90398900	1.47472600
F	-1.04997300	5.12996600	-0.31344400

F	-0.35968300	2.97278400	-0.60924500
B	3.50524500	-2.37186800	-1.97939000
F	4.15615500	-3.02501400	-3.00475400
F	3.74322200	-3.00433800	-0.75521100
F	2.11323200	-2.37357200	-2.21738200
F	3.93687900	-1.03365500	-1.89449800

TS17

Num. Imaginary Frequencies: 1

C	-2.22701400	-1.73306400	2.91638600
C	-1.43015100	-1.65848900	1.77639900
C	-0.19477100	-2.30540400	1.78209200
C	0.22636700	-3.04588900	2.88444100
C	-0.59905500	-3.13516100	4.00125800
C	-1.81865100	-2.46965000	4.02616700
H	-3.17257700	-1.19347600	2.92693100
H	1.19938000	-3.52874200	2.89849100
H	-0.27177900	-3.71855100	4.85948300
H	-2.45440900	-2.52204300	4.90837000
C	1.98022200	-2.86375000	0.68519800
O	2.84388600	-2.60398800	1.49108800
C	0.72303600	-3.76640700	-1.06378300
H	0.96650500	-3.86296000	-2.12855000
H	0.04200000	-4.58390000	-0.77890700
C	3.05412700	-4.64792600	-0.58879000
H	3.82785400	-4.50202900	0.16837300
H	2.74210900	-5.69842500	-0.59646200
H	3.45440800	-4.37648400	-1.57367300
N	1.93029900	-3.79919700	-0.26554300
C	0.14281700	-2.38816600	-0.75329300
H	0.64786100	-1.66589300	-1.40448300
C	-1.34935600	-2.28485500	-0.90506800
H	-1.85650500	-3.17886200	-0.51834400
H	-1.57443200	-2.20510600	-1.97563700
Au	-2.24516400	-0.71444500	0.12889900
P	-3.30350200	0.27587100	-1.82743200
F	-3.31842700	0.58400200	1.30370500
N	0.69799800	-2.09867400	0.62707800
H	1.03638100	-0.94565100	0.66221400
C	-2.16442400	0.76318800	-3.16363900
H	-1.49865200	-0.07162700	-3.41537700
H	-2.72823700	1.05733000	-4.05810800
H	-1.56800800	1.60958800	-2.80802900

C	-4.31508200	1.73783300	-1.46111400
H	-4.89570000	2.01880000	-2.34908600
H	-4.98975400	1.50265100	-0.63221900
H	-3.66941900	2.57089500	-1.16161800
C	-4.45541400	-0.90802600	-2.60492400
H	-4.93672400	-0.45423900	-3.48094800
H	-3.91818700	-1.80959700	-2.92149200
H	-5.22637000	-1.19676200	-1.88119800
H	3.01310300	0.22169400	2.02443800
C	2.94629700	0.41068100	0.94734900
C	3.57681900	1.75547200	0.56589400
H	3.46485900	-0.40426000	0.43193900
N	1.50814200	0.39891100	0.58915300
H	4.15785500	1.67228400	-0.35901100
H	4.20079100	2.16809000	1.36395700
N	2.46125600	2.73450600	0.29560500
C	0.78627100	1.33588200	1.47246600
C	1.32447100	0.83583500	-0.81116500
C	1.48764200	2.69909900	1.45553500
C	2.94541200	4.12358200	0.03825700
C	1.76538900	2.28988800	-0.97880600
H	0.76581700	0.92518600	2.48764900
H	-0.24432600	1.43824900	1.11450800
H	0.25848100	0.74655200	-1.05237100
H	1.91281000	0.17585100	-1.45242400
H	0.77286500	3.51493100	1.32261000
H	2.08054000	2.87729100	2.35736500
Cl	3.77120600	4.83513800	1.43365200
H	3.64754500	4.08419500	-0.79874500
H	2.06370100	4.72479200	-0.20494500
H	0.92720700	2.97351800	-1.13341200
H	2.49987100	2.39061700	-1.78491100
B	-1.37737300	3.85500700	-0.15924600
F	-0.24332500	4.62862100	-0.48908600
F	-1.39765300	3.65372700	1.21772900
F	-2.52838800	4.47380100	-0.60087200
F	-1.23933000	2.59645300	-0.79967700
B	4.10520800	-1.19128600	-2.04069300
F	4.80846000	-1.68725700	-3.11777100
F	4.70038100	-1.56257300	-0.83510400
F	2.78178500	-1.69309000	-2.06058700
F	4.03913400	0.21686400	-2.10171100

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Num. Imaginary Frequencies: 0

C	0.30792400	-2.73107200	1.03375500
C	0.85854300	-1.46856200	1.26662100
C	0.25740100	-0.63775600	2.22568200
C	-0.81882500	-1.12414900	2.98710900
C	-1.34446100	-2.38536700	2.73707400
C	-0.79760800	-3.19007400	1.74365900
H	0.74990400	-3.34413400	0.24915000
H	-1.25520500	-0.49859700	3.75977900
H	-2.20606900	-2.72448600	3.30887800
H	-1.22969700	-4.16408300	1.52110400
C	-0.07238500	1.73931600	2.87147300
O	-1.27396800	1.70159800	3.17785300
C	2.04629900	2.57609700	2.43549400
H	2.42367100	3.36472300	1.77338200
H	2.72488200	2.46490600	3.29799500
C	0.19846100	4.17731600	3.16849200
H	-0.85453200	4.09619300	3.45266800
H	0.75913500	4.62320400	4.00032200
H	0.28723600	4.83261900	2.29030800
N	0.68918600	2.86128900	2.86094200
C	1.83613300	1.27396900	1.67727000
H	1.45838500	1.54866600	0.68553000
C	3.01409300	0.36953800	1.51450500
H	3.29654900	-0.13898100	2.44550900
H	3.87195000	0.93592000	1.13141900
Au	2.50227800	-1.03120900	0.07720000
P	4.32324800	-0.64891600	-1.48273000
F	2.06817600	-2.49004400	-1.35708800
N	0.71206100	0.68551900	2.42934200
H	-2.22418400	1.07471800	1.83896000
C	3.62357900	-0.52119000	-3.15505100
H	3.05653700	0.41317600	-3.21726900
H	4.41190600	-0.54011700	-3.91807200
H	2.93906000	-1.36647600	-3.27800400
C	5.46292000	-2.06938400	-1.55554300
H	6.20551300	-1.93227400	-2.35199500
H	5.97771400	-2.18967200	-0.59566600
H	4.87396000	-2.97172600	-1.75516900
C	5.38257000	0.82044200	-1.28464300
H	6.10034400	0.88756200	-2.11207200
H	4.74430100	1.71197300	-1.28373600
H	5.93469500	0.76919500	-0.33883700

H	-4.42374700	0.17110200	1.25361300
C	-4.08979300	1.14314700	0.87612200
C	-4.58958600	1.38634000	-0.55025900
H	-4.40307700	1.93981300	1.55624500
N	-2.59822900	1.11635600	0.85729600
H	-5.03783100	2.37702400	-0.68489100
H	-5.30007600	0.60626100	-0.83007200
N	-3.42317500	1.30822400	-1.50912700
C	-2.12078400	-0.07541600	0.08690000
C	-2.07057400	2.38117700	0.26921500
C	-2.69367100	-0.00719500	-1.32743800
C	-3.87012600	1.48817500	-2.92965400
C	-2.46451800	2.43984900	-1.20648800
H	-2.46798900	-0.97227600	0.60755100
H	-1.02856200	-0.04852500	0.07912400
H	-0.98013700	2.40055800	0.36812300
H	-2.49714200	3.20701100	0.84789300
H	-1.89877200	-0.03439300	-2.07957700
H	-3.41743100	-0.80736600	-1.50153300
Cl	-4.95816700	0.21298500	-3.47411400
H	-4.38577800	2.45013000	-2.99592000
H	-2.97363500	1.48901100	-3.55560500
H	-1.59683200	2.31740100	-1.86397400
H	-2.97747900	3.37536100	-1.45035600
B	-4.66904800	-2.44054600	0.39693900
F	-5.28943200	-1.46945900	-0.42558200
F	-5.51637000	-3.50765400	0.59502900
F	-3.48222300	-2.84052400	-0.21965000
F	-4.35498000	-1.82623700	1.62798500
B	0.98690100	2.32225400	-1.59188700
F	0.46432800	2.81477200	-2.77814300
F	0.75501800	3.24092100	-0.55298600
F	2.34990400	2.05989400	-1.69234600
F	0.30697500	1.12087500	-1.27230500

TS18

Num. Imaginary Frequencies: 1

C	1.12586400	-2.76613300	2.18607200
C	1.44561900	-1.47753800	1.76304800
C	0.88789800	-0.36845200	2.41502500
C	-0.08159400	-0.54484200	3.40264100
C	-0.45271000	-1.83946300	3.75695400
C	0.15690400	-2.94565600	3.17234900

H	1.59357200	-3.63032200	1.71557800	C	-3.00712600	1.03780500	1.50102200
H	-0.51610400	0.32047900	3.90024700	C	-1.10241100	0.47880600	0.08771100
H	-1.21270900	-1.98110500	4.52278100	C	-4.01036000	1.00247800	0.35016600
H	-0.12827500	-3.95168000	3.47207400	C	-4.14751200	0.74071600	-2.10910500
C	1.18735200	2.10769200	2.55547900	C	-2.10100200	0.10954600	-0.99891400
O	0.07062200	2.52636000	2.88697000	H	-3.33423000	1.71087000	2.29855300
C	3.47592900	1.94088900	2.13324200	H	-2.83331400	0.03397800	1.90202300
H	4.13865100	2.52327400	1.48294000	H	-0.90774800	-0.40035800	0.70341800
H	4.05867300	1.55944500	2.98719900	H	-0.17182500	0.88401500	-0.32151600
C	2.45543500	4.20602600	2.72154400	H	-4.57504600	0.06680400	0.35769300
H	1.50035800	4.58101200	3.10015700	H	-4.70582200	1.84649100	0.37759400
H	3.25024700	4.47954200	3.42488900	Cl	-5.57822000	1.77727700	-2.23334200
H	2.66044000	4.66578500	1.74427800	H	-3.56389000	0.83861400	-3.02800000
N	2.36304900	2.77347400	2.59531800	H	-4.46117200	-0.29365700	-1.94037300
C	2.74344000	0.83683800	1.36574400	H	-2.52205400	-0.88674100	-0.85177400
H	2.59491700	1.18032200	0.33317300	H	-1.65152800	0.19352000	-1.99245000
C	3.26541700	-0.57727500	1.34918500	B	-4.03358400	-2.36105900	0.87926800
H	3.57619900	-0.97243500	2.32003300	F	-4.24422000	-2.04747700	-0.48808200
H	4.10122500	-0.70340900	0.65086000	F	-4.92479200	-1.59200900	1.63754800
Au	1.87347600	-1.40401000	-0.29764700	F	-4.23026900	-3.70510000	1.09274300
P	2.28602300	-1.34185100	-2.68512000	F	-2.71952300	-1.98627300	1.21808300
F	-0.24376700	-1.78229000	-1.06587200	B	1.35164400	2.84465000	-1.50308800
N	1.43646100	0.85223900	2.04202300	F	1.75302900	4.03540300	-2.06389900
H	-1.05649700	1.77115200	1.75298800	F	1.14046900	3.00165000	-0.11449100
C	0.88642100	-0.52752000	-3.51614700	F	2.31479900	1.84847500	-1.70260300
H	0.86545200	0.53190600	-3.23846300	F	0.13436700	2.41345000	-2.07289800
H	0.95066400	-0.63872100	-4.60629200				
H	-0.00592200	-1.01568900	-3.10791600				
C	2.27633400	-3.02379600	-3.40044800				
H	2.32024800	-2.98095200	-4.49681500				
H	3.12963300	-3.60225600	-3.02833900				
H	1.35121800	-3.52592000	-3.09373900				
C	3.78372300	-0.56156200	-3.38085400				
H	3.78387800	-0.63446000	-4.47644000				
H	3.79241700	0.49317300	-3.08566100				
H	4.68247500	-1.05083600	-2.98789200				
H	-2.48322400	3.48466900	0.86624200				
C	-1.92776900	2.81139200	0.20604600				
C	-2.68841400	2.49333900	-1.08015200				
H	-0.94299100	3.23398800	-0.00609300				
N	-1.71042600	1.54078200	0.96280300				
H	-2.01721000	2.49477700	-1.94425000				
H	-3.51330200	3.19179100	-1.24693400				
N	-3.26299200	1.10675400	-0.96115400				

3.5 Cycle V

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Num. Imaginary Frequencies: 0

C	6.96632100	0.86754400	-1.59634500
C	5.96759400	-0.02628400	-1.22482600
C	6.14230900	-0.83630300	-0.09907400
C	7.33254500	-0.74326900	0.63044400
C	8.32788800	0.14255300	0.24134000
C	8.15039000	0.95917100	-0.87235100
H	6.81341700	1.49303200	-2.47416000
H	5.05365800	-0.10075500	-1.80978500
H	7.46848300	-1.37444600	1.50849000
H	9.24848600	0.19694800	0.81991900

H	8.92781900	1.65823500	-1.17326400
C	3.93639600	-2.08501400	-0.19655900
O	3.58912900	-3.25374400	-0.32248100
C	3.11548600	0.21544300	0.23198300
H	4.14397600	0.52061400	0.46188300
H	2.70937700	1.00637600	-0.41245900
C	1.87654900	-1.37766700	-1.18834900
H	1.46517000	-0.47514100	-1.65018200
H	2.06277300	-2.13291100	-1.95552900
H	1.13534600	-1.78682000	-0.48209000
N	3.12447700	-1.02879800	-0.53051800
C	2.32006200	0.15180800	1.50159300
H	2.09252100	1.12762200	1.93862800
C	1.89866400	-0.96119500	2.09878100
H	1.34981400	-0.92904300	3.03901000
H	2.08962500	-1.95267700	1.68617700
H	5.59832300	-2.62448100	0.72953600
N	5.19030300	-1.78386800	0.33359600
H	-3.69796400	-1.86538900	1.30515900
C	-3.36111400	-0.89962400	1.69445200
C	-4.18876700	0.25483400	1.10721200
H	-3.33179900	-0.90664900	2.78733600
N	-1.95122200	-0.72021500	1.22727200
H	-4.78418500	0.75035700	1.87967600
H	-4.83878000	-0.10122200	0.30438500
N	-3.24722000	1.27836700	0.52198600
C	-1.89329900	-0.64978500	-0.26388200
C	-1.30825700	0.47469400	1.84670800
C	-2.54381200	0.67109800	-0.67564800
C	-3.94151100	2.55481000	0.12603300
C	-2.23910900	1.65791400	1.58758300
H	-2.43089500	-1.53100200	-0.62788100
H	-0.83413700	-0.67382200	-0.53300000
H	-0.32658200	0.59181400	1.37408100
H	-1.19955200	0.26299100	2.91371700
H	-1.80716500	1.40391500	-1.01170000
H	-3.30359100	0.48343400	-1.43653300
Cl	-5.26345000	2.28077700	-1.00310000
H	-4.33495500	3.00951800	1.03933900
H	-3.17689500	3.18930700	-0.33293300
H	-1.66427200	2.51836400	1.23669600
H	-2.81474800	1.93272800	2.47696500
F	-1.23576500	-1.82830800	1.61840300
F	1.42002200	3.36582200	-0.93073600

F	-0.85749000	3.30628400	-0.62984500
F	0.53076100	2.86820700	1.12240200
F	0.35199500	1.37392400	-0.58811800
B	0.39190800	2.75409500	-0.26429400
F	-4.70703700	-1.20069000	-1.53947000
F	-3.83868100	-3.02607700	-0.48026600
F	-5.72380300	-3.24173100	-1.76678900
F	-5.80165700	-2.12298000	0.23046600
B	-5.04333900	-2.41949500	-0.90656600

TS19

Num. Imaginary Frequencies: 1

C	6.09803300	-1.10915200	2.44100500
C	5.76176700	-0.56316200	1.20646200
C	5.45080300	-1.40496400	0.13629800
C	5.49341200	-2.79079200	0.31609800
C	5.85015700	-3.32521400	1.54729000
C	6.14853700	-2.48799100	2.61920900
H	6.33773800	-0.44293500	3.26776100
H	5.74718100	0.51685000	1.06871800
H	5.24430900	-3.44185900	-0.52175600
H	5.88602600	-4.40613100	1.67026400
H	6.42058000	-2.90778700	3.58528900
C	4.85306900	0.41644400	-1.50201900
O	5.41814500	0.92781900	-2.45765400
C	2.91085300	0.31551900	0.02633600
H	3.31874100	0.02064600	1.00236500
H	2.07812300	1.00967700	0.21079800
C	3.65031000	2.46312000	-1.02593300
H	3.28521000	2.93984400	-0.11163500
H	4.58219200	2.93367700	-1.34579700
H	2.88925900	2.60146400	-1.80503400
N	3.89785700	1.05276300	-0.75843100
C	2.37865800	-0.87774100	-0.70458600
H	2.52770500	-1.86886600	-0.27711400
C	1.66558800	-0.74693400	-1.86526500
H	1.33814100	-1.61325900	-2.43141200
H	1.50544500	0.23807700	-2.30127500
H	5.57559100	-1.39511300	-1.90908100
N	5.10547500	-0.91784200	-1.14548200
H	-2.40837500	-2.02439000	-0.17678200
C	-2.10281200	-1.46216300	0.70893100
C	-3.33820300	-0.92244800	1.47577700

H	-1.47857600	-2.08586100	1.35537200
N	-1.33710200	-0.29300500	0.29201800
H	-3.28663800	-1.12508200	2.55072500
H	-4.25657800	-1.34297700	1.05372700
N	-3.39889100	0.58536200	1.31491800
C	-2.03540000	0.46455400	-0.74732900
C	-0.92676000	0.50694100	1.43830400
C	-3.39070400	0.90945800	-0.16739300
C	-4.58363000	1.17936500	2.01989100
C	-2.17765300	1.22550400	1.95260600
H	-2.19576500	-0.21029700	-1.59141700
H	-1.40144700	1.30486500	-1.03073100
H	-0.16670400	1.23340700	1.13675000
H	-0.50174300	-0.17285300	2.18320900
H	-3.54031900	1.98937600	-0.26500500
H	-4.22158300	0.35703500	-0.61962900
Cl	-6.13200500	0.66249800	1.36673600
H	-4.52213000	0.87907600	3.06916300
H	-4.49822100	2.26577200	1.92784700
H	-2.16974900	2.27754100	1.64882700
H	-2.28167000	1.14526000	3.03896900
F	0.20313800	-0.68663400	-0.48185800
F	0.72259300	4.45514600	-0.83069800
F	-1.05318600	3.27584900	0.00746300
F	1.04413700	2.90098200	0.82334300
F	0.50798200	2.22116000	-1.28302900
B	0.31433800	3.24155200	-0.33358700
F	-5.46957200	-1.28000800	-0.93589400
F	-3.55269600	-1.88337900	-2.01493300
F	-5.46736900	-3.09501800	-2.33316100
F	-4.37168700	-3.17655300	-0.32560300
B	-4.73141800	-2.37696600	-1.41887600

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Num. Imaginary Frequencies: 0

C	-6.16085200	0.95935000	0.89060600
C	-4.80587300	1.23740000	0.76862000
C	-3.99230500	0.30053000	0.14472200
C	-4.48157300	-0.89953900	-0.34952900
C	-5.84172300	-1.16242000	-0.21813400
C	-6.67759900	-0.23630400	0.39612900
H	-6.81447800	1.67808100	1.37872700
H	-4.39299700	2.16291100	1.16776000

H	-3.81208500	-1.62314300	-0.81521800
H	-6.24418500	-2.09847900	-0.59781100
H	-7.73985000	-0.44780900	0.49620900
C	-1.79622100	0.84987200	1.30439700
O	-2.16955000	0.41252300	2.35247900
C	-0.74475600	1.96740300	-0.47566300
H	-0.41548300	3.00001700	-0.61617400
H	-0.05170900	1.31469400	-1.03034200
C	0.15499600	2.18004300	1.91095200
H	1.18900500	2.01870400	1.59444800
H	-0.01505700	3.25997700	1.99902500
H	-0.02908300	1.70106900	2.87573800
N	-0.76939400	1.61929100	0.93928400
C	-2.18690100	1.73800000	-0.89104300
H	-2.81040800	2.58739800	-0.58257100
C	-2.39458000	1.44534300	-2.35933600
H	-3.45721500	1.28943600	-2.58727100
H	-1.82354200	0.56088900	-2.66694700
H	-2.10720100	-0.26375100	-0.42336000
N	-2.56756500	0.57905800	-0.01784900
H	2.21642100	-3.53407100	-1.47729100
C	3.08131200	-3.01751900	-1.05203400
C	2.81471400	-2.71758800	0.43960000
H	3.95885800	-3.66599500	-1.15891600
N	3.31970300	-1.79348100	-1.80725100
H	3.52458800	-3.20552000	1.11737200
H	1.79326300	-2.97308800	0.73454200
N	2.96936700	-1.23040700	0.65004000
C	2.17717500	-0.89520200	-1.67136300
C	4.51371600	-1.13908300	-1.29127500
C	1.94708200	-0.50357000	-0.19814600
C	2.85707000	-0.83964600	2.08572300
C	4.36449500	-0.81744700	0.20817300
H	1.28435000	-1.39385500	-2.06261300
H	2.36941700	0.00858200	-2.26313300
H	4.67584800	-0.20819500	-1.84321600
H	5.37639500	-1.79549900	-1.45488700
H	2.09990000	0.56316500	-0.00841000
H	0.96144500	-0.80976500	0.17176200
Cl	1.28390400	-1.24574600	2.79522700
H	3.63599300	-1.37166500	2.63821200
H	3.00598000	0.24302300	2.13488000
H	4.44891300	0.25306400	0.41166600
H	5.06152100	-1.37840400	0.84136000

F	-1.93630000	2.54857400	-3.03812300
F	3.85645000	4.01866600	-0.05845600
F	3.39417700	2.09919900	1.09828000
F	4.08635500	1.97888600	-1.07234000
F	2.00742100	2.77081800	-0.57822100
B	3.34819400	2.74636600	-0.16909100
F	-1.20242000	-1.87181200	0.64249200
F	-1.21093500	-1.28978100	-1.53236900
F	-2.24694800	-3.22484800	-0.88394600
F	0.03473500	-3.09070700	-0.84896700
B	-1.15523800	-2.41920200	-0.64517800

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Num. Imaginary Frequencies: 1

H	-0.77436600	-2.08566500	0.82511200
C	-0.85073900	-1.09266000	1.28068200
C	-2.33782100	-0.73659000	1.45739500
H	-0.31237800	-1.09401400	2.23477900
N	-0.19215500	-0.10282100	0.40002500
H	-2.65624600	-0.76378300	2.50569900
H	-2.97758600	-1.39044300	0.85907200
N	-2.54595000	0.67571800	0.96023400
C	-0.98731300	0.03476600	-0.83903400
C	-0.13576000	1.19269200	1.10830800
C	-2.32719600	0.70518900	-0.53775500
C	-3.88462300	1.23511600	1.30937600
C	-1.52254100	1.56934100	1.63111900
H	-1.13725100	-0.96952000	-1.24869400
H	-0.43840400	0.65414600	-1.55549900
H	0.22373900	1.95853100	0.41715900
H	0.57493000	1.10004800	1.93739000
H	-2.34427300	1.76122500	-0.82580700
H	-3.15376900	0.15694600	-0.99575900
Cl	-5.22504500	0.22732400	0.75021500
H	-3.94193600	1.32084400	2.39801500
H	-3.95181100	2.22020800	0.83752400
H	-1.76630700	2.60624700	1.38281500
H	-1.63374400	1.40386800	2.70861400
F	2.12058500	-3.22999100	-2.50394000
F	-0.79113300	5.25325600	-1.52529400
F	-2.20894300	3.80034400	-0.46174200
F	-0.13970300	4.20712400	0.40446700
F	-0.34214500	3.00974800	-1.52674000
B	-0.86180400	4.09352200	-0.78505500

F	-3.24576700	-2.23744900	-1.12088400
F	-1.17225800	-3.19480200	-1.13124000
F	-3.02548700	-4.48321000	-1.51323000
F	-2.62179300	-3.62949800	0.57300900
B	-2.53015900	-3.40914500	-0.80485400
C	4.68427900	2.32441000	0.56539500
C	4.14696600	1.04508900	0.67449600
C	3.01343700	0.73321600	-0.06585200
C	2.42190300	1.65902300	-0.91754000
C	2.96033100	2.93682100	-1.00636500
C	4.09193300	3.26909100	-0.26709600
H	5.56874900	2.58175300	1.14366000
H	4.60538500	0.31567900	1.34102100
H	1.53871000	1.40919600	-1.50487800
H	2.47875700	3.66805000	-1.65088200
H	4.51167800	4.27012500	-0.33635600
C	2.70909200	-1.31543100	1.30216500
O	2.25193200	-0.93338500	2.35188600
C	3.88763900	-2.41061500	-0.40102900
H	4.90964800	-2.02838100	-0.53308100
H	3.84881400	-3.44082400	-0.77313000
C	4.02802400	-3.25464500	1.99487600
H	3.77046300	-4.28744300	1.73655400
H	5.11860600	-3.15646000	2.04797500
H	3.59066000	-2.99900700	2.96302700
N	3.49527500	-2.35043800	0.99634900
C	2.83744100	-1.53606100	-1.08158900
H	3.25739800	-0.94464400	-1.90063700
C	1.64797700	-2.33559900	-1.57992700
H	0.91173600	-1.67784000	-2.06246000
H	1.14894800	-2.88404900	-0.76751600
H	1.24285200	-0.44377600	0.09010700
N	2.39979300	-0.60516800	0.01361800

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Num. Imaginary Frequencies: 0

H	-0.58673100	1.68684500	1.34351500
C	0.41017600	1.38365400	1.66778800
C	1.48102000	2.30091800	1.08427100
H	0.43299000	1.34192000	2.76128200
N	0.65406000	-0.00956500	1.17873700
H	1.87530600	2.99977100	1.82907400
H	1.09300400	2.85238600	0.22268400

N	2.62460300	1.43724900	0.60200600
C	0.86700000	-0.04298800	-0.30317000
C	1.85813100	-0.56933000	1.85167800
C	2.16688200	0.68024600	-0.62695900
C	3.87053700	2.21386200	0.30711500
C	2.98386300	0.45370700	1.70370100
H	-0.00106000	0.43181400	-0.76093700
H	0.94137100	-1.09327400	-0.59816600
H	2.11494500	-1.51189700	1.36046100
H	1.62381700	-0.75032300	2.90427100
H	2.97717200	-0.00617300	-0.88637200
H	2.00698700	1.41762800	-1.41732000
Cl	3.59678400	3.51941700	-0.84990900
H	4.22910500	2.64264800	1.24733100
H	4.59220700	1.50050300	-0.10250700
H	3.91723800	-0.04453800	1.42850400
H	3.13418300	1.05205400	2.60889100
F	-5.72730500	0.30083300	-1.68678700
F	5.19165800	-3.07128000	-0.69334200
F	4.84824300	-0.82075100	-0.42447600
F	4.39622200	-2.24852500	1.29265200
F	3.06018600	-2.24536300	-0.55283000
B	4.38945900	-2.12636200	-0.10031300
F	-0.16299900	2.54989500	-1.56274400
F	-1.79869600	1.35568000	-0.49412100
F	-2.37392100	3.10458100	-1.84409700
F	-1.31831200	3.48670400	0.15885000
B	-1.43101000	2.64908100	-0.95163200
C	-0.04136400	-3.48379100	-0.40665400
C	-1.06712600	-2.78864000	0.22340500
C	-1.93183400	-1.97763700	-0.52568400
C	-1.78184700	-1.92218300	-1.91297300
C	-0.76393700	-2.63908500	-2.53516100
C	0.12208200	-3.40850300	-1.78801200
H	0.63326700	-4.09537100	0.18998600
H	-1.20498800	-2.87628500	1.29858000
H	-2.44677700	-1.30510100	-2.51256200
H	-0.65719800	-2.57694500	-3.61642800
H	0.93566700	-3.94279900	-2.27336000
C	-2.86358800	-0.73194200	1.38545600
O	-1.83112800	-0.61653000	2.05434900
C	-5.11557300	-0.86534800	0.87311600
H	-5.52614300	-1.81573800	1.25075700
H	-5.93925000	-0.15415700	0.74050600

C	-4.41445300	0.05121000	3.12856000
H	-5.06232300	0.93548700	3.12693500
H	-4.92422400	-0.75885000	3.67096800
H	-3.48013600	0.29201800	3.64271500
N	-4.10539200	-0.34653600	1.77899900
C	-4.30844800	-1.04166900	-0.41464300
H	-4.63674100	-1.90852500	-1.00185200
C	-4.41615800	0.22131100	-1.25913900
H	-3.75901100	0.21240700	-2.13635700
H	-4.17423000	1.10807200	-0.66179500
H	-0.22395500	-0.53796600	1.41712100
N	-2.96483100	-1.26912000	0.11788000

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Num. Imaginary Frequencies: 0

N	1.33898900	-1.25180400	-1.60149800
C	3.67083900	-1.89950000	-2.85730600
C	0.88894000	-3.58233100	-0.43663400
O	1.62072300	-0.87755900	-4.15278000
O	2.81135600	0.53449200	-2.44789600
O	-1.02251100	-1.94309100	-1.10786200
O	0.17835200	-3.17802800	-2.93410400
S	2.23282600	-0.74700100	-2.83764300
S	0.23411800	-2.41034000	-1.69729700
F	3.27371900	-3.12836500	-3.14796100
F	4.53201300	-1.48798800	-3.77508500
F	4.26298100	-1.90017000	-1.67243300
F	0.01769400	-4.57203000	-0.29610400
F	2.05298100	-4.07157600	-0.82420100
F	1.04256000	-2.97807300	0.73631300
C	2.19646600	0.39003100	1.55984900
C	1.18198100	2.51084900	0.87233600
C	1.41804600	3.01126500	2.15209500
C	2.03292200	2.21423700	3.12044000
C	2.40556500	0.90519200	2.84849500
H	2.57836400	-0.59065600	1.27410300
H	1.13360800	4.03131300	2.39176500
H	2.20612100	2.63125800	4.11041500
H	2.88355800	0.29304800	3.60920300
Au	-0.20803600	-0.12370400	1.42825700
P	-2.36222500	-0.97420900	1.68401200
C	1.59269000	1.19276500	0.56745700
H	1.59342400	0.84416200	-0.46329300

C	0.63750300	4.67188200	-0.13773800	F	2.55183700	-2.97822900	0.72846600
O	1.52416300	5.32491800	0.38247900	F	-1.73936700	-3.99086100	-1.36779100
C	-1.18396400	4.10127700	-1.47196500	F	0.13857500	-4.02937600	-0.29343300
H	-0.93028000	4.04211600	-2.54534100	F	-1.44453300	-2.70230600	0.33614300
H	-2.26553900	4.26164200	-1.39161300	C	0.50935400	-0.83324400	2.27188400
C	-0.49033700	6.51124500	-1.30630700	C	1.39541400	1.27681400	1.49617200
H	-1.49972300	6.91980600	-1.17676300	C	2.33457400	1.21281800	2.53955200
H	-0.22176200	6.56873100	-2.37197900	C	2.36714300	0.13274600	3.40447200
H	0.21749400	7.10923100	-0.72591100	C	1.46103600	-0.91750800	3.27145800
N	-0.43683500	5.15344800	-0.82746400	H	-0.19486500	-1.65850000	2.15575800
C	-0.72861300	2.84139600	-0.72628400	H	3.05922500	2.00933900	2.65927400
N	0.54417300	3.26807000	-0.13063100	H	3.11644900	0.11395400	4.19477500
F	-1.90620400	1.54177300	-2.24158700	H	1.49720100	-1.77680000	3.93839200
H	-1.43787200	2.58925800	0.08402900	Au	-1.59446600	0.49794000	0.67284100
C	-0.64872200	1.66859400	-1.68429400	P	-3.78160500	0.67007200	-0.18609900
H	-0.40066800	0.71521100	-1.19902800	C	0.42465600	0.24520400	1.35227400
H	0.08837700	1.86556900	-2.47887700	H	0.58679200	-0.52409400	0.01075200
C	-3.18962300	-0.49052500	3.23287300	C	2.61207200	3.17297200	0.42784000
H	-3.24675700	0.60136600	3.30031700	O	3.74550600	2.93714200	0.80486500
H	-4.20420200	-0.90894100	3.25823200	C	0.78672700	4.38064200	-0.35442100
H	-2.62220700	-0.86784000	4.09054500	H	0.44505500	4.78678800	-1.31459800
C	-3.45629900	-0.37782200	0.35753400	H	0.40220800	5.02358100	0.45549900
H	-4.43532500	-0.86907000	0.42958800	C	3.07800200	5.42588200	-0.42779600
H	-3.58798600	0.70563700	0.45983200	H	2.82656700	6.19524900	0.31907200
H	-3.00086300	-0.58907500	-0.61607700	H	2.97605800	5.86293800	-1.42826700
C	-2.46451400	-2.79006800	1.65417900	H	4.11398300	5.11056800	-0.27693900
H	-3.51459000	-3.09714800	1.74543500	N	2.22639400	4.27207400	-0.29827200
H	-2.05149700	-3.16305300	0.71124400	C	0.37267300	2.92300500	-0.18500700
H	-1.89311300	-3.20480300	2.49227700	N	1.46197900	2.38171600	0.62462200

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Num. Imaginary Frequencies: 1

N	0.92114400	-1.22814500	-0.92430300
C	3.08567600	-2.85792300	-0.47207800
C	-0.85605700	-3.26857400	-0.70533400
O	2.87470500	-1.31738900	-2.62658800
O	3.11312300	-0.21800800	-0.36121600
O	-1.33971900	-1.06906100	-2.05915200
O	0.37133600	-2.69415800	-2.97022000
S	2.56044500	-1.24692600	-1.21626000
S	-0.21986500	-1.97362100	-1.86275800
F	2.69489100	-3.85785700	-1.23894100
F	4.40182600	-2.84990100	-0.38282100

H	0.08905300	1.17025600	-1.45569200
H	1.22950300	2.39291700	-2.09696300
C	-5.02239200	1.57847100	0.79547800
H	-4.67623400	2.60448900	0.96357500
H	-5.98472900	1.60325400	0.26797000
H	-5.15597700	1.09208400	1.76814700
C	-3.76643900	1.50991300	-1.80464800
H	-4.77760600	1.56260000	-2.22865500
H	-3.35843700	2.52035000	-1.69099500
H	-3.10816600	0.95289300	-2.48162400
C	-4.56043700	-0.94471200	-0.52658600
H	-5.54135900	-0.80425100	-0.99902700

H	-3.91279600	-1.52097000	-1.19752800
H	-4.68534500	-1.50293500	0.40814300

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Num. Imaginary Frequencies: 0

N	0.82725500	-1.81137300	-0.60848100
C	2.88631900	-3.37188800	0.26617600
C	-1.19638600	-3.47777200	0.07839300
O	2.74466600	-2.44481500	-2.22105500
O	3.07874400	-0.78129900	-0.32856700
O	-1.40598300	-1.66708600	-1.82676400
O	0.12950100	-3.65322900	-2.22287500
S	2.48691400	-1.97548400	-0.88182700
S	-0.42241300	-2.62704400	-1.37185600
F	2.30431400	-4.47053100	-0.17156600
F	4.19474100	-3.51843700	0.27090500
F	2.45364300	-3.08221900	1.47417500
F	-2.30391300	-4.05054800	-0.34886500
F	-0.36589200	-4.37858800	0.55430700
F	-1.48324300	-2.58674200	1.00932100
C	0.63461300	-0.30137800	2.51379900
C	1.54789800	1.54291300	1.27428600
C	2.69650900	1.46640300	2.07754500
C	2.81645400	0.50064600	3.06528900
C	1.78503400	-0.40311500	3.28728100
H	-0.17349900	-1.01056000	2.70357300
H	3.51264600	2.16091200	1.91035100
H	3.72407900	0.46595400	3.66669600
H	1.87033800	-1.17109400	4.05515600
Au	-1.44840400	0.68392900	0.63894200
P	-3.59415100	0.69792800	-0.39253900
C	0.46364100	0.65973500	1.49632200
H	0.57471300	-0.97016400	-0.04342000
C	2.62775300	3.25434800	-0.19913600
O	3.79683100	2.91510800	-0.13259200
C	0.78757700	4.65143400	-0.43724700
H	0.23888200	5.14272100	-1.25186200
H	0.70555000	5.27647600	0.46839800
C	3.06518100	5.48879300	-1.12128400
H	3.09669400	6.24697300	-0.32288900
H	2.74956300	5.97468000	-2.05246000
H	4.06790400	5.07314300	-1.25460500
N	2.16960600	4.41204800	-0.78906300

C	0.30322700	3.22360200	-0.21192000
N	1.50856400	2.55372500	0.27115700
F	-1.41316600	3.17706700	-1.81589300
H	-0.50431900	3.16247800	0.52933500
C	-0.16710000	2.63376000	-1.53383800
H	-0.26268800	1.53860100	-1.49315300
H	0.52153100	2.90316100	-2.34719600
C	-4.63624800	-0.76351400	-0.05356700
H	-4.77504700	-0.88630100	1.02637500
H	-5.61648300	-0.65770200	-0.53681700
H	-4.13850800	-1.65695000	-0.44909800
C	-4.63862800	2.12145400	0.07559600
H	-5.61140500	2.07371700	-0.43105800
H	-4.79397300	2.13063700	1.16030200
H	-4.12646100	3.04787900	-0.21112200
C	-3.55538800	0.77534700	-2.21653100
H	-4.57615600	0.85310100	-2.61339900
H	-2.96994000	1.64741700	-2.52671900
H	-3.07762000	-0.12948500	-2.60794600

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Num. Imaginary Frequencies: 0

H	0.61382200	0.01405000	-0.87652600
H	1.94071900	1.10121200	0.74246900
C	2.26324300	0.12145100	0.37989800
C	3.77796300	0.00510600	0.25965800
H	1.86790500	-0.66966100	1.02417500
N	1.66151400	-0.05965200	-0.97444800
H	4.16114200	-0.93268300	0.66767100
H	4.26817900	0.86546900	0.72223600
N	4.15955100	0.01467500	-1.20578400
C	2.04464700	1.06696800	-1.88088200
C	2.11494200	-1.35929100	-1.53927100
C	3.56146900	1.24435700	-1.84326900
C	5.64662200	-0.07015200	-1.36085900
C	3.59079800	-1.20840200	-1.90510200
H	1.54127900	1.97320600	-1.53005900
H	1.67197400	0.81233800	-2.87805900
H	1.50926300	-1.59511600	-2.41874600
H	1.97532000	-2.13105000	-0.77490600
H	3.99313200	1.35098300	-2.84414600
H	3.83799200	2.10246900	-1.22496100
Cl	6.47583100	1.36173900	-0.74306600

H	5.96638300	-0.95570100	-0.80347400
H	5.86541100	-0.17353700	-2.42724700
H	3.74250700	-1.03995800	-2.97688900
H	4.15618600	-2.08740200	-1.58503000
B	2.05145500	3.76260900	0.39766900
F	1.95333600	4.00536200	-0.98011100
F	3.23532400	3.03285500	0.63615000
F	2.05786100	4.93963000	1.11057900
F	0.95478000	2.95995800	0.78126500
B	4.05386100	-3.60414900	0.50313700
F	3.03847700	-2.83948600	1.10586800
F	3.61408600	-4.00472200	-0.76385100
F	4.38464300	-4.68467400	1.28478700
F	5.18567600	-2.76571500	0.32592600
C	-0.51877500	-2.26745800	1.93264100
C	-0.85010800	0.08920500	1.77066300
C	0.09211500	0.30113100	2.78018600
C	0.72430700	-0.78375200	3.37671400
C	0.43304500	-2.07178500	2.93340900
H	-0.74194300	-3.28850600	1.61968300
H	0.35666200	1.32250300	3.05814000
H	1.46450400	-0.62214400	4.15861400
H	0.95491300	-2.92664500	3.36159400
Au	-2.77280100	-1.33313900	-0.02396200
P	-4.61288800	-0.93927300	-1.47949200
C	-1.21244100	-1.20086000	1.34055900
C	-1.31274100	1.61850800	-0.12230200
O	-0.76560300	0.97134100	-1.02583100
C	-2.19275200	3.44438200	0.97739900
H	-3.15624800	3.97051000	0.96954900
H	-1.39500400	4.15989500	1.23084400
C	-1.49944100	3.66364300	-1.41606100
H	-0.50586900	4.10292900	-1.23145200
H	-2.23413300	4.46266600	-1.56340800
H	-1.45368500	3.05574700	-2.32469800
N	-1.91608600	2.83167400	-0.30954300
C	-2.19025600	2.24874000	1.93879400
N	-1.44204400	1.24989600	1.18406900
F	-4.29985000	1.50502300	1.13695200
H	-1.67332100	2.49389100	2.87758000
C	-3.57130100	1.74177600	2.29154200
H	-4.11242700	2.48609300	2.89162000
H	-3.50357600	0.80046000	2.85436500
C	-5.05539000	-2.05034900	-2.86167800

H	-4.19216200	-2.17924400	-3.52406100
H	-5.89006500	-1.62637300	-3.43532900
H	-5.34759800	-3.03258200	-2.47408700
C	-6.18871500	-0.68468500	-0.59028700
H	-6.51458500	-1.62229700	-0.12643800
H	-6.96783400	-0.32796900	-1.27694300
H	-6.02356900	0.05891900	0.19780600
C	-4.32606800	0.67770700	-2.28519800
H	-4.13953400	1.42764100	-1.50508000
H	-5.19283300	0.97669700	-2.88947400
H	-3.43569500	0.62003900	-2.92264800

TS22

Num. Imaginary Frequencies: 1

H	1.25408900	0.55890300	1.14759700
H	1.96418000	-0.18193300	-0.91341200
C	2.67171100	0.45622700	-0.37739600
C	4.09571900	-0.07146500	-0.51998600
H	2.59480400	1.49568700	-0.70826500
N	2.29547400	0.43499500	1.07595500
H	4.68630500	0.58343900	-1.16756700
H	4.11837100	-1.10585100	-0.88152300
N	4.74821500	-0.06710800	0.84879700
C	2.57613400	-0.90157800	1.67730500
C	3.05398900	1.48392500	1.80995600
C	4.08818200	-1.13370500	1.68858300
C	6.23382400	-0.25961500	0.76741300
C	4.53663100	1.29374600	1.48919500
H	2.06504100	-1.65129600	1.07242600
H	2.15651500	-0.90384700	2.68737500
H	2.83785800	1.36414800	2.87548200
H	2.71158500	2.46381000	1.46861900
H	4.52493400	-1.06601800	2.69126200
H	4.32437200	-2.10696200	1.24452900
Cl	6.70212500	-1.73335300	-0.07290000
H	6.64149000	0.60399300	0.23467400
H	6.61475500	-0.29534000	1.79181100
H	5.15236000	1.33168400	2.39333000
H	4.88544100	2.03919100	0.76819800
B	2.55988300	-3.50344700	-0.66134700
F	2.49278800	-3.74995100	0.71933500
F	3.88750500	-3.21740600	-0.99861600
F	2.06635300	-4.57281900	-1.37492200

F	1.78230500	-2.35151100	-0.93909900
B	3.63527300	4.01558900	-0.49954900
F	2.28540300	3.61999800	-0.35959100
F	4.16241000	4.22648400	0.77819600
F	3.73123700	5.14409300	-1.27770100
F	4.34081900	2.94336100	-1.09322300
C	-3.19928100	2.19225000	-2.00129500
C	-1.24715900	1.02053700	-1.30939700
C	-0.55383100	2.20452800	-1.10343400
C	-1.21007800	3.41128700	-1.34932100
C	-2.52414000	3.40367500	-1.80936800
H	-4.23427700	2.21719400	-2.35121200
H	0.48237300	2.20852000	-0.76736900
H	-0.67818300	4.34962400	-1.19876400
H	-3.02846500	4.34657500	-2.02349500
Au	-3.86130700	-0.23598400	-0.13860700
P	-3.96224800	0.44701200	2.06349200
C	-2.57516800	0.96626700	-1.73644900
C	-0.60783100	-0.79825500	0.15767300
O	-0.33134900	-0.15233900	1.18685400
C	-1.14343400	-2.58335200	-1.23781200
H	-2.13900900	-3.03890200	-1.32616200
H	-0.37056100	-3.31647900	-1.50357100
C	-0.72015600	-3.02396100	1.20542200
H	0.11313600	-3.70785600	0.99031300
H	-1.63516700	-3.60455000	1.38140500
H	-0.48224400	-2.45022100	2.10661200
N	-0.91399500	-2.10745700	0.11194200
C	-1.03255400	-1.30315800	-2.08312100
N	-0.62473700	-0.26409900	-1.12098400
F	-3.84290200	-1.46560800	-1.97631800
H	-0.22225300	-1.42505800	-2.82505900
C	-2.24254300	-0.98306500	-2.90419000
H	-2.59063600	-1.87610300	-3.42820900
H	-2.14752400	-0.16245800	-3.60911600
C	-3.11993900	2.06247900	2.17451000
H	-2.10355100	1.94217400	1.77693600
H	-3.07634700	2.41805100	3.21260300
H	-3.64650300	2.79711900	1.55395700
C	-5.57795000	0.70393300	2.86940500
H	-6.18833100	1.38361700	2.26465300
H	-5.43642200	1.13521100	3.86921700
H	-6.10359100	-0.25319300	2.95839700
C	-3.01428400	-0.60125100	3.21485100

H	-3.44052000	-1.61007300	3.24987900
H	-3.02003500	-0.16514500	4.22282300
H	-1.98317400	-0.65593400	2.84034300

3.6 Cycle VI

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Num. Imaginary Frequencies: 0

C	-7.10140900	-0.70128200	-0.81647700
C	-5.82423800	-0.82082200	-0.28150300
C	-5.08725100	-2.00539000	-0.44052300
C	-5.67525900	-3.06358300	-1.15208300
C	-6.95392000	-2.92770000	-1.67859600
C	-7.68084900	-1.75154800	-1.52005700
H	-7.64509500	0.23204300	-0.67645800
H	-5.40321900	0.02186900	0.26151200
H	-5.12289600	-3.98667200	-1.28093700
H	-7.38598600	-3.76491900	-2.22566900
H	-8.68047000	-1.65429400	-1.93936000
N	-3.80507800	-2.09970400	0.12591100
C	-2.98867900	-3.22226600	0.12220500
O	-3.24277300	-4.33340800	-0.32165500
C	-1.91835700	-1.59027100	1.38513600
H	-2.14371400	-1.73384900	2.45670300
H	-0.99098600	-1.00552800	1.30647800
C	-0.89124500	-3.87100700	1.21042400
H	-1.06803700	-4.79960500	0.66022400
H	0.15638500	-3.56987100	1.06870500
H	-1.04547600	-4.05987800	2.28510100
N	-1.79724400	-2.86659700	0.71769900
C	-3.06653500	-0.91431500	0.63151300
H	-3.70770000	-0.38020200	1.34444700
C	-2.60905300	0.00500700	-0.49021900
H	-3.47806400	0.30844700	-1.09312900
H	-1.95238800	-0.56147700	-1.16698000
Au	-1.68674800	1.78070300	0.17564600
P	-0.93013400	3.95547300	0.87017400
H	1.91289900	-2.52399600	-2.54703900
C	2.22575500	-2.43293600	-1.50323700
C	3.72557000	-2.19553300	-1.32158300
H	1.89672500	-3.29572000	-0.91893100

N	1.51118400	-1.23957200	-0.95188500
H	4.13199000	-2.78496100	-0.49323100
H	4.27383400	-2.40776500	-2.24340700
N	3.93950700	-0.74350200	-0.97466900
C	1.71801400	-0.02923200	-1.80592500
C	1.91242600	-0.95516300	0.45602200
C	3.23068900	0.11000900	-2.00294300
C	5.40109600	-0.40006100	-0.87349600
C	3.36417800	-0.47776700	0.40829500
H	1.18864100	-0.20398300	-2.74640300
H	1.28409200	0.82349100	-1.27165100
H	1.24111000	-0.16932400	0.81989500
H	1.79996000	-1.88380000	1.02280700
H	3.54068700	1.14819900	-1.86336600
H	3.55167100	-0.24388700	-2.98609000
Cl	6.24170700	-0.57749000	-2.41352800
H	5.83566100	-1.08271400	-0.13734900
H	5.45137300	0.64263800	-0.54727200
H	3.44510700	0.59747500	0.57595000
H	3.96619300	-1.04263300	1.12408400
F	0.17067500	-1.54672900	-0.94821400
B	3.60917400	-3.48860600	2.06859900
F	2.64649400	-3.83507800	1.08262200
F	4.77450200	-3.05308200	1.38733400
F	3.88786700	-4.56540100	2.86591700
F	3.10653900	-2.41160600	2.79896100
B	2.78060900	3.01530600	-0.25819500
F	4.06827200	2.43275700	-0.21712000
F	1.89650900	2.16078500	0.44721100
F	2.79384800	4.26320700	0.31125400
F	2.35521400	3.05444200	-1.59005800
C	-2.36219700	4.97030200	1.39565200
H	-2.83820900	4.51129800	2.27029500
H	-2.04318500	5.98901700	1.65371900
H	-3.09990000	5.01843400	0.58592000
C	-0.19650500	4.95704400	-0.46971900
H	0.14224000	5.92766000	-0.08389100
H	0.65235300	4.43004400	-0.91614600
H	-0.96068900	5.11921000	-1.23974500
C	0.21444500	4.13056900	2.28156900
H	1.15819900	3.63454400	2.04524700
H	0.40021700	5.19421900	2.48196000
H	-0.23186600	3.66756200	3.16926100

TS23

Num. Imaginary Frequencies: 1

C	-7.29952600	0.18107900	-0.21697900
C	-5.98136700	-0.16191700	0.06098200
C	-5.52128000	-1.47013100	-0.15690300
C	-6.42073100	-2.41950700	-0.66730200
C	-7.73479000	-2.05888700	-0.93843700
C	-8.18962300	-0.76202700	-0.71795100
H	-7.62739100	1.20370800	-0.03619600
H	-5.31358700	0.60298500	0.45104300
H	-6.07866200	-3.43293900	-0.84211200
H	-8.41403100	-2.81366100	-1.33272400
H	-9.22085500	-0.49107500	-0.93568900
N	-4.19022100	-1.79549800	0.15789300
C	-3.59235500	-3.05047200	0.04536800
O	-4.11613500	-4.09212700	-0.31815900
C	-2.06394400	-1.64888000	1.08878400
H	-2.15457500	-1.76611200	2.18283700
H	-1.07222400	-1.23830500	0.86054600
C	-1.50839900	-4.07366700	0.80773100
H	-1.80675200	-4.91890200	0.18160500
H	-0.43726800	-3.88224100	0.67509100
H	-1.68384100	-4.33693600	1.86385300
N	-2.27565700	-2.91411000	0.41993500
C	-3.18058000	-0.77782400	0.51263500
H	-3.58729400	-0.11974000	1.29068700
C	-2.75706200	0.00077000	-0.71980500
H	-3.61480500	0.44441100	-1.24509300
H	-2.20014500	-0.64084600	-1.41225400
Au	-1.60248700	1.70053300	-0.19137900
P	-0.67142500	3.84101200	0.50895000
H	1.39305400	-1.48982000	-2.59012400
C	1.71744800	-1.68539100	-1.56430000
C	3.18931200	-2.15470300	-1.48637200
H	1.05849400	-2.42071400	-1.09272800
N	1.65258000	-0.43989800	-0.81405000
H	3.29932200	-3.04102100	-0.85733600
H	3.60818200	-2.33599800	-2.47985400
N	4.01900800	-1.06136300	-0.84400800
C	2.36206200	0.65196000	-1.47260000
C	2.03949800	-0.60849900	0.58330200
C	3.83531200	0.22192300	-1.62015000
C	5.45803200	-1.46577800	-0.73806700

C	3.55985100	-0.81757900	0.58920900
H	1.89203400	0.83015300	-2.44375100
H	2.27218800	1.53898800	-0.84318300
H	1.77646400	0.30617400	1.12156800
H	1.51527000	-1.47907300	0.98842100
H	4.50655900	0.97254300	-1.19149600
H	4.10916100	0.01881400	-2.65884400
Cl	6.22177200	-1.68894600	-2.31697900
H	5.47682400	-2.40849400	-0.18379300
H	5.97905900	-0.66849700	-0.19950400
H	4.08850000	0.08049000	0.92532500
H	3.83224100	-1.68796100	1.19125100
F	0.02522200	0.18055400	-0.71249200
B	2.92683800	-4.03474300	1.58904600
F	1.86153100	-3.74464900	0.69820100
F	4.13169000	-3.92970000	0.85024300
F	2.79083300	-5.29729900	2.10719700
F	2.93937400	-3.06066100	2.58594100
B	3.94646000	2.90676100	0.67830200
F	4.97181600	1.93833400	0.71488400
F	2.75737800	2.30287600	1.16351400
F	4.27512200	3.99687000	1.44193100
F	3.72359000	3.26254000	-0.65819300
C	-1.97685800	5.11882500	0.57315700
H	-2.76479800	4.80521000	1.26755100
H	-1.55774000	6.07532300	0.91224300
H	-2.41992700	5.25084400	-0.42058300
C	0.61207300	4.58527800	-0.55332100
H	0.83699900	5.59976600	-0.19740100
H	1.53328700	3.99043000	-0.52135600
H	0.25412100	4.63938800	-1.58774800
C	0.05757200	3.88061300	2.18022600
H	0.97126700	3.27663900	2.18778300
H	0.30888500	4.91501300	2.44987900
H	-0.65452900	3.47834500	2.90930300

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Num. Imaginary Frequencies: 0

C	2.14614100	-0.35538100	2.70605800
C	1.24233600	0.25781700	1.81566400
C	1.17219400	1.66709100	1.74477700
C	1.96115000	2.43456700	2.59135600
C	2.83884600	1.81747800	3.48827800

C	2.95607500	0.43577400	3.53409900
H	2.14230600	-1.44146200	2.78732100
H	0.48712300	-0.33143300	1.29832600
H	1.88807200	3.51971700	2.54340000
H	3.44948700	2.43479800	4.14402700
H	3.64756200	-0.03592900	4.22811800
N	0.30506600	2.26516100	0.80905000
C	-0.72570000	3.12668900	1.17736800
O	-1.08129400	3.35524100	2.32123600
C	-0.72068600	2.99015200	-1.15828200
H	-0.45411600	3.71759700	-1.93830300
H	-1.47440600	2.31044200	-1.58253900
C	-2.53081300	4.30202200	-0.00500000
H	-2.75790000	4.65067200	1.00675700
H	-3.32312000	3.61386600	-0.33716900
H	-2.50173400	5.16505600	-0.68167700
N	-1.24375400	3.64900700	0.02316300
C	0.52541900	2.26029000	-0.63275300
H	0.59134900	1.23160200	-1.02671800
Au	2.93713000	-0.31033600	0.28968900
P	4.00747800	-0.66544200	-1.74070300
H	-3.19091800	0.65514900	2.46410200
C	-3.12914400	0.35901200	1.41028000
C	-4.31113600	-0.55485800	1.04446000
H	-3.16886600	1.26845200	0.79482300
N	-1.85985800	-0.31804200	1.17092500
H	-5.02212300	-0.07226000	0.36968200
H	-4.84092800	-0.93603900	1.92287900
N	-3.76574700	-1.77627500	0.32747900
C	-1.85092900	-1.60472200	1.86537400
C	-1.71085800	-0.52406300	-0.26428600
C	-2.91220800	-2.56635900	1.28842100
C	-4.86499800	-2.57719400	-0.27815500
C	-2.87525400	-1.35129200	-0.83192000
H	-2.03641400	-1.41768000	2.93034600
H	-0.86062600	-2.06469800	1.76174300
H	-0.75858400	-1.02271200	-0.47053500
H	-1.70654100	0.45613700	-0.75333300
H	-2.45528900	-3.37901300	0.71228900
H	-3.57676600	-2.98284900	2.05140300
Cl	-6.02633900	-3.18452000	0.91977200
H	-5.38831200	-1.92001300	-0.97899300
H	-4.41729800	-3.43410100	-0.78872300
H	-2.52477900	-2.27645000	-1.30211300

H	-3.50607000	-0.77842400	-1.51575300	O	1.99260600	-3.62348200	1.30645900
B	0.85133400	-3.06887000	-0.44619400	C	0.38966800	-3.08574400	-1.76249700
F	1.03007700	-1.97230000	-1.31723500	H	-0.10667900	-3.75874300	-2.47557400
F	-0.48776300	-3.46484000	-0.49276800	H	0.93024900	-2.31190900	-2.32775800
F	1.69425200	-4.09907300	-0.82112200	C	2.54334400	-4.33487400	-1.42455700
F	1.15897300	-2.64602900	0.86478200	H	3.25584300	-4.42843000	-0.59963900
B	-4.91133100	1.54007300	-1.73152500	H	2.97013100	-3.65077700	-2.16955000
F	-5.14531900	2.06346700	-0.45477800	H	2.37988900	-5.31849100	-1.88274200
F	-3.52069000	1.45889400	-1.92986400	N	1.30990000	-3.79601500	-0.89806000
F	-5.49527400	2.32134400	-2.70505700	C	-0.61909900	-2.48591100	-0.77985100
F	-5.44171200	0.22856100	-1.78501500	H	-0.87385900	-1.45493800	-1.06994800
C	4.40047300	-2.41947100	-2.00871100	Au	-2.24458100	0.09674700	0.42237600
H	5.17040800	-2.73829200	-1.29720100	P	-3.86224600	0.58061600	-1.21420700
H	3.49461300	-3.01544100	-1.84160000	H	2.33230800	-0.36809400	2.25823100
H	4.76660900	-2.56863300	-3.03268900	C	2.37369000	-0.03685000	1.21344700
C	2.92809700	-0.18456700	-3.12236100	C	3.57714800	0.87613300	0.96031100
H	2.00825600	-0.77526300	-3.05977000	H	2.43071900	-0.91845000	0.56627800
H	2.67735800	0.87967700	-3.04374200	N	1.13840000	0.70062500	0.90127400
H	3.43389900	-0.37644400	-4.07774200	H	4.33003000	0.38534700	0.33852100
C	5.55441000	0.25866100	-1.99245200	H	4.04141900	1.23583900	1.88309400
H	5.34851200	1.33296700	-1.91705400	N	3.10139900	2.11270900	0.21976400
H	6.28520500	-0.01520700	-1.22389000	C	1.09901600	1.97639100	1.64227900
H	5.96875100	0.03762400	-2.98445200	C	1.05997900	0.92658700	-0.54941200
C	1.80428200	3.00447900	-0.97117700	C	2.20615000	2.91127000	1.13488400
H	2.68122900	2.53938000	-0.49322200	C	4.26108700	2.89781900	-0.30237400
H	1.73183500	4.05369400	-0.64598500	C	2.28209600	1.72586200	-1.00379900
F	1.98620500	2.97185500	-2.34059000	H	1.22220100	1.74187100	2.70644300

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C	-1.28592900	-0.37056300	3.19121500	H	1.79047500	3.73282600	0.54307800
C	-0.88739600	-0.76699400	1.89297600	H	2.82726500	3.30727800	1.94290400
C	-0.41784400	-2.09878300	1.73871100	Cl	5.34531000	3.46098600	0.97926000
C	-0.38897500	-2.97484800	2.82604400	H	4.81334900	2.23448300	-0.97520500
C	-0.81279000	-2.54563300	4.07832500	H	3.86789600	3.76855500	-0.83380500
C	-1.25826100	-1.23980200	4.27301300	H	1.98696100	2.66377400	-1.48476600
H	-1.61927500	0.65778600	3.34419000	H	2.94287700	1.13911200	-1.64597200
H	0.04726500	0.03650900	1.28802100	B	-1.35312900	3.56855600	-0.64425300
H	-0.02204200	-3.98866900	2.69229500	F	-1.52483300	2.48811200	-1.53606200
H	-0.78829400	-3.24264000	4.91444900	F	0.00094400	3.93832400	-0.66705000
H	-1.57813100	-0.90798700	5.25887700	F	-2.16566800	4.61602000	-1.02642000
N	0.10028200	-2.52733700	0.49175900	F	-1.68964200	3.13894400	0.65131800
C	1.22748700	-3.35954900	0.39461400	B	4.20265600	-1.30502200	-1.67641500
				F	4.46877000	-1.81062000	-0.40622700

F	2.80095800	-1.20583500	-1.83207700	N	1.10315900	-3.87111100	-0.87090700
F	4.73007800	-2.10920600	-2.66473500	C	-0.84122400	-2.61298900	-0.59733500
F	4.74207200	0.00118700	-1.77311700	H	-1.15266900	-1.61191000	-0.93008500
C	-4.66549200	2.21483200	-1.17093600	Au	-2.31308100	0.05701300	0.45323300
H	-5.17543700	2.34283900	-0.20925100	P	-3.83671100	0.72490900	-1.24125900
H	-3.91399200	3.00378300	-1.28272300	H	2.38929400	-0.41631400	2.21019900
H	-5.40266000	2.28528700	-1.98164800	C	2.42406500	-0.11636000	1.15741000
C	-3.22157500	0.37942700	-2.90901500	C	3.63161400	0.76658600	0.84455600
H	-2.41136900	1.09688000	-3.06924300	H	2.42858700	-1.01745300	0.53588200
H	-2.83691400	-0.64142100	-3.02129700	N	1.18932800	0.66623700	0.86304300
H	-4.02262800	0.54739800	-3.64080400	H	4.32322000	0.25621200	0.16908900
C	-5.23975300	-0.61650500	-1.14495200	H	4.16447500	1.08561400	1.74457500
H	-4.83203800	-1.62548800	-1.28345600	N	3.16271400	2.02961100	0.15313700
H	-5.73560800	-0.56605400	-0.16901900	C	1.18657900	1.94813100	1.62989500
H	-5.97247900	-0.41073600	-1.93622400	C	1.07746600	0.90655100	-0.60366000
C	-1.90459300	-3.28436000	-0.69819300	C	2.32083400	2.83591100	1.11047600
H	-2.52968300	-2.94889800	0.14186400	C	4.32977900	2.80421800	-0.38195700
H	-1.68950200	-4.35732100	-0.58433800	C	2.30727200	1.68615700	-1.05686600
F	-2.60933000	-3.09082900	-1.87373600	H	1.30870600	1.68682800	2.68613400

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C	-1.33195900	-0.31988400	3.24808800	H	1.92268300	3.68777500	0.55138700
C	-1.13564800	-0.83530900	1.95030200	H	2.97280400	3.18325600	1.91612600
C	-0.34867200	-2.00883600	1.84748200	Cl	5.45818200	3.30481900	0.88228300
C	0.13177500	-2.64818200	3.00154800	H	4.84490700	2.14722900	-1.08869800
C	-0.09530100	-2.10523200	4.25816500	H	3.93846200	3.69573700	-0.87925900
C	-0.81597600	-0.92271700	4.38988100	H	2.01826100	2.63660700	-1.51396300
H	-1.91371800	0.59670000	3.36271000	H	2.93799200	1.09532300	-1.72579100
H	0.34078600	0.12474600	1.16964300	B	-1.16914400	3.66138600	-0.63614900
H	0.71072600	-3.56072900	2.90601500	F	-1.41386600	2.59120300	-1.52117200
H	0.29623100	-2.61493800	5.13730300	F	0.21363200	3.93372700	-0.66983200
H	-0.98697700	-0.48363400	5.37174300	F	-1.89837400	4.76471900	-1.01911900
N	0.02529100	-2.54085500	0.57675900	F	-1.51807800	3.26162500	0.66274300
C	1.18799500	-3.29867400	0.36947600	B	3.99063100	-1.42345200	-1.86230200
O	2.11982500	-3.41501000	1.14979100	F	4.30909400	-1.91855500	-0.60086100
C	0.05795400	-3.25408600	-1.65569500	F	2.58472200	-1.29162100	-1.94637600
H	-0.49428500	-3.98571200	-2.26167900	F	4.44969800	-2.24589700	-2.86705100
H	0.49539100	-2.50352000	-2.33193300	F	4.55716700	-0.13010000	-1.99621400
C	2.27973100	-4.40775000	-1.51463600	C	-4.55369800	2.40198100	-1.23354300
H	3.06199400	-4.50978400	-0.75706200	H	-5.08188000	2.56665000	-0.28729600
H	2.64327100	-3.72520100	-2.29465300	H	-3.75598600	3.14638900	-1.32862000
H	2.06418400	-5.38800000	-1.95761500	H	-5.26329800	2.51031900	-2.06447900
				C	-3.17394800	0.48568000	-2.92538300

H	-2.31501300	1.14802800	-3.07041700
H	-2.85266400	-0.55863700	-3.03033800
H	-3.94363100	0.70311700	-3.67764100
C	-5.28920000	-0.38740200	-1.22414700
H	-4.93604300	-1.42112300	-1.33027500
H	-5.81962400	-0.29579800	-0.26925700
H	-5.97784800	-0.15154900	-2.04617700
C	-2.10006800	-3.40904100	-0.32732000
H	-2.63388100	-3.02057100	0.55085700
H	-1.87011800	-4.47409500	-0.17676700
F	-2.91779800	-3.27650500	-1.43644000