

Group 14 heavier 1,4-dimetallabenzenes: Influence of Aromaticity, Open-Shell Character and Strain on Small Molecule Activation

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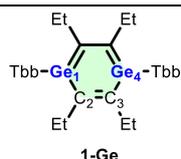
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1. X-Ray—DFT benchmark

Table S1. Comparison between X-Ray geometries and computed distances and angles using different functionals of **1-Ge**. All values are represented in angstroms and degrees.

Coordinates	X-Ray	B3LYP-D3	BP86-D3(BJ)	ω B97X-D
1-Ge				
Ge ₁ -C ₂	1.908	1.906	1.917	1.879
Ge ₁ -C ₂ -C ₃	123.4	121.8	123.3	121.4
Ge ₁ -C ₂ -C ₃ -Ge ₄	7.8	6.8	8.1	4.6
Tbb-Ge ₁ -C ₂ -C ₃	148.4	145.9	146.6	148.7



2. CAS-SCF electron density matrix and configuration coefficients

Table S2. CAS-SCF electron density matrix and configuration coefficients of **1-E**, corresponding to their ground state (S_0). All data was computed at the CAS-SCF[14,14]/def2-SVP//(u)B3LYP-D3/def2-SVP level of theory.

Si	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.94	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	0.00	1.94	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	0.00	0.00	1.94	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	0.00	0.00	0.00	1.94	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.00	0.00	0.00	0.00	1.93	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	0.00	0.00	0.00	0.00	0.00	1.89	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	0.00	0.00	0.00	0.00	0.00	0.00	1.77	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.23	0.00	0.00	0.00	0.00	0.00	0.00
9	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.11	0.00	0.00	0.00	0.00	0.00
10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06	0.00	0.00	0.00	0.00
11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06	0.00	0.00	0.00
12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06	0.00	0.00
13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06	0.00
14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06

Ge	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.94	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	0.00	1.94	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	0.00	0.00	1.94	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	0.00	0.00	0.00	1.94	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.00	0.00	0.00	0.00	1.92	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	0.00	0.00	0.00	0.00	0.00	1.90	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	0.00	0.00	0.00	0.00	0.00	0.00	1.65	0.00	0.00	0.00	0.00	0.00	0.00	0.00

8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.34	0.00	0.00	0.00	0.00	0.00	0.00
9	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.10	0.00	0.00	0.00	0.00	0.00
10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.07	0.00	0.00	0.00	0.00
11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06	0.00	0.00	0.00
12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06	0.00	0.00
13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06	0.00
14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06

Sn	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.94	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	0.00	1.94	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	0.00	0.00	1.94	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	0.00	0.00	0.00	1.94	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.00	0.00	0.00	0.00	1.92	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	0.00	0.00	0.00	0.00	0.00	1.91	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	0.00	0.00	0.00	0.00	0.00	0.00	1.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00
8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.60	0.00	0.00	0.00	0.00	0.00	0.00
9	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.09	0.00	0.00	0.00	0.00	0.00
10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.08	0.00	0.00	0.00	0.00
11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06	0.00	0.00	0.00
12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06	0.00	0.00
13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06	0.00
14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06

3. Cartesian coordinates of the DFT optimized structures

Cartesian coordinates (in Å) and total energies (in a.u., noncorrected ZVPE included) of all the stationary points discussed in the text. Unless otherwise mentioned, all calculations have been performed at the (u)B3LYP-D3/def2-SVP level.

G_{qh} denotes free energy values computed at the (u)B3LYP-D3/def2-SVP with quasi-harmonic corrections.

$G_{B3LYP-D3/TZVPP}$ denotes free energy values computed at the (u)B3LYP-D3/def2-TZVPP//(u)B3LYP-D3/def2-SVP with quasi-harmonic corrections.

SP denotes values computed at the DLPNO-CCSD(T)/def2-TZVP//(u)B3LYP-D3/def2-SVP.

G_{sp} denotes free energy values computed at the DLPNO-CCSD(T)/def2-TZVP//(u)B3LYP-D3/def2-SVP with quasi-harmonic corrections.

Acetylene

$G_{qh} = -77.264778$

$N_{imag} = 0$

$SP = -77.183645$

$G_{sp} = -77.175425$

C	0.000000000000	0.000000000000	0.604644000000
C	0.000000000000	0.000000000000	-0.604644000000
H	0.000000000000	0.000000000000	-1.679195000000
H	0.000000000000	0.000000000000	1.679195000000

Dihydrogen

$G_{qh} = -1.175360$

$N_{imag} = 0$

$SP = -1.168217$

$G_{sp} = -1.169790$

H	0.000000000000	0.000000000000	0.380307000000
H	0.000000000000	0.000000000000	-0.380307000000

1-C

$G_{qh} = -4746.368947$

$G_{B3LYP-D3/TZVPP} = -4749.892504$

$N_{imag} = 0$

C	3.645658000000	1.149379000000	0.010130000000
C	2.889710000000	-0.058946000000	-0.046346000000
C	3.596755000000	-1.303487000000	-0.023647000000
C	4.994222000000	-1.292580000000	0.101578000000
C	5.741342000000	-0.123343000000	0.260790000000
C	5.038309000000	1.077963000000	0.212645000000
C	1.370983000000	-0.054046000000	-0.033654000000
C	0.702975000000	-0.416419000000	1.171837000000
C	1.568663000000	-0.738091000000	2.388055000000
C	1.154406000000	-0.364535000000	3.823491000000
C	2.937650000000	-2.673539000000	-0.090218000000
Si	3.444462000000	-3.863239000000	1.355942000000
C	4.013276000000	-2.957530000000	2.929076000000
C	7.262957000000	-0.203569000000	0.463988000000
C	7.901556000000	1.187320000000	0.622730000000
C	3.067093000000	2.541896000000	-0.199183000000
Si	2.864141000000	3.579569000000	1.399744000000
C	4.456104000000	3.637916000000	2.417821000000
C	0.622369000000	0.242858000000	-1.200793000000
C	1.361875000000	0.619575000000	-2.478804000000

C	1.056648000000	1.983988000000	-3.112842000000
C	-0.792743000000	0.182408000000	-1.165319000000
C	-1.631536000000	0.524042000000	-2.392215000000
C	-1.438497000000	-0.274362000000	-3.691843000000
C	-1.457746000000	-0.158536000000	0.042775000000
C	-0.706851000000	-0.528092000000	1.187629000000
C	-1.426962000000	-1.118703000000	2.390459000000
C	-1.064066000000	-2.584416000000	2.677300000000
C	-2.967368000000	-0.009691000000	0.089037000000
C	-3.516046000000	1.309938000000	0.153051000000
C	-4.902624000000	1.479287000000	0.034026000000
C	-5.783332000000	0.421078000000	-0.207754000000
C	-5.231615000000	-0.858629000000	-0.243396000000
C	-3.858259000000	-1.109274000000	-0.050112000000
C	-2.680683000000	2.570792000000	0.299297000000
Si	-2.980454000000	3.905842000000	-1.066945000000
C	-3.689524000000	3.207067000000	-2.684014000000
C	-7.279545000000	0.705908000000	-0.419086000000
C	-8.084580000000	-0.576754000000	-0.688316000000
C	-3.422762000000	-2.565280000000	0.032824000000
Si	-3.098781000000	-3.405407000000	-1.666685000000
C	-4.050612000000	-2.493527000000	-3.019706000000
C	-4.218411000000	5.255984000000	-0.566605000000
C	-1.312992000000	4.729720000000	-1.414676000000
C	-1.216783000000	-3.406567000000	-1.885225000000
C	-3.597639000000	-5.232004000000	-1.779211000000
C	-7.449594000000	1.648678000000	-1.632179000000
C	-7.852514000000	1.384077000000	0.845595000000
Si	-2.808751000000	3.297446000000	2.076283000000
C	-2.188480000000	2.047345000000	3.340250000000
C	-4.588243000000	3.700343000000	2.579333000000
C	-1.722272000000	4.843954000000	2.222410000000
Si	-4.493580000000	-3.568054000000	1.276812000000
C	-6.198427000000	-4.066034000000	0.593782000000
C	-4.822073000000	-2.541701000000	2.833521000000
C	-3.597233000000	-5.163034000000	1.770624000000
C	4.898772000000	-5.011857000000	0.938463000000
C	1.948325000000	-4.944812000000	1.769827000000
C	1.530115000000	2.799869000000	2.472168000000
C	2.289900000000	5.337291000000	0.986050000000
C	7.562322000000	-1.025208000000	1.738240000000
C	7.903425000000	-0.897145000000	-0.759277000000
Si	3.178530000000	-3.515431000000	-1.807850000000
C	2.335466000000	-2.545250000000	-3.184977000000
C	4.999517000000	-3.634766000000	-2.310930000000
C	2.384191000000	-5.236720000000	-1.813526000000
Si	4.010062000000	3.523158000000	-1.575135000000
C	5.502304000000	4.503842000000	-0.924660000000
C	4.708449000000	2.360185000000	-2.895548000000
C	2.851258000000	4.806032000000	-2.374496000000
H	-1.492215000000	1.589492000000	-2.613900000000
H	-2.687077000000	0.434658000000	-2.118892000000
H	-0.496489000000	-0.058491000000	-4.211135000000
H	-2.253597000000	-0.025342000000	-4.389751000000
H	-1.478205000000	-1.355788000000	-3.518426000000
H	1.186897000000	-0.155522000000	-3.233710000000
H	2.436059000000	0.569380000000	-2.268751000000
H	0.116839000000	2.002767000000	-3.677741000000
H	1.852844000000	2.255432000000	-3.820564000000
H	1.000852000000	2.780434000000	-2.361612000000
H	-5.298356000000	2.493766000000	0.090167000000

H	-5.877376000000	-1.713518000000	-0.422775000000
H	-5.196377000000	2.782270000000	2.599641000000
H	-5.086237000000	4.425069000000	1.920409000000
H	-4.583452000000	4.119706000000	3.599789000000
H	-1.691743000000	5.168700000000	3.275973000000
H	-2.086620000000	5.692057000000	1.623780000000
H	-0.687503000000	4.629998000000	1.913362000000
H	-1.163272000000	1.723894000000	3.115859000000
H	-2.836634000000	1.159219000000	3.359211000000
H	-2.195219000000	2.497617000000	4.346929000000
H	-3.949754000000	5.795920000000	0.352585000000
H	-5.234186000000	4.847954000000	-0.437800000000
H	-4.265403000000	5.994094000000	-1.385046000000
H	-1.401646000000	5.481611000000	-2.215928000000
H	-0.573317000000	3.981344000000	-1.737236000000
H	-0.916027000000	5.233148000000	-0.520048000000
H	-4.373831000000	2.365209000000	-2.500564000000
H	-2.909480000000	2.865412000000	-3.378866000000
H	-4.261272000000	4.001928000000	-3.190846000000
H	-5.218475000000	-1.549274000000	2.567345000000
H	-3.919371000000	-2.395830000000	3.444728000000
H	-5.572595000000	-3.052055000000	3.460428000000
H	-2.531479000000	-5.002446000000	1.991243000000
H	-3.673025000000	-5.932956000000	0.988758000000
H	-4.067952000000	-5.570363000000	2.681475000000
H	-6.527716000000	-5.001333000000	1.076744000000
H	-6.199754000000	-4.235984000000	-0.493459000000
H	-6.956948000000	-3.299116000000	0.813678000000
H	-0.900501000000	-3.744325000000	-2.885186000000
H	-0.793641000000	-4.110067000000	-1.147457000000
H	-0.771495000000	-2.422052000000	-1.685511000000
H	-3.401982000000	-5.573354000000	-2.810309000000
H	-4.660282000000	-5.419121000000	-1.564874000000
H	-2.995108000000	-5.861567000000	-1.106806000000
H	-3.918668000000	-1.404589000000	-2.960410000000
H	-5.128656000000	-2.698814000000	-2.909422000000
H	-3.742210000000	-2.831368000000	-4.022374000000
H	-7.038500000000	1.189213000000	-2.545262000000
H	-6.933403000000	2.608723000000	-1.480611000000
H	-8.516236000000	1.865982000000	-1.807315000000
H	-8.926053000000	1.600041000000	0.716758000000
H	-7.344258000000	2.334849000000	1.066770000000
H	-7.737349000000	0.730515000000	1.725144000000
H	-7.725807000000	-1.103470000000	-1.586404000000
H	-9.145207000000	-0.327546000000	-0.849331000000
H	-8.033733000000	-1.275604000000	0.160573000000
H	-1.610777000000	2.320025000000	0.207260000000
H	-2.416859000000	-2.601748000000	0.468724000000
H	1.773408000000	-1.816714000000	2.365223000000
H	2.546915000000	-0.278495000000	2.210713000000
H	0.517594000000	-1.115915000000	4.308336000000
H	2.062856000000	-0.279306000000	4.440592000000
H	0.632523000000	0.598650000000	3.879504000000
H	-1.238738000000	-0.529490000000	3.293444000000
H	-2.506685000000	-1.041299000000	2.223307000000
H	-0.054865000000	-2.693573000000	3.092275000000
H	-1.761625000000	-3.024025000000	3.406024000000
H	-1.101005000000	-3.198957000000	1.766804000000
H	5.512163000000	-2.251312000000	0.109396000000
H	5.577893000000	2.015405000000	0.309466000000
H	5.433794000000	-2.628001000000	-2.414957000000

H	5.622945000000	-4.202533000000	-1.606445000000
H	5.064650000000	-4.130405000000	-3.294413000000
H	2.447569000000	-5.654586000000	-2.832222000000
H	2.861327000000	-5.953488000000	-1.129586000000
H	1.316263000000	-5.170884000000	-1.550622000000
H	1.280561000000	-2.338692000000	-2.956088000000
H	2.850260000000	-1.591817000000	-3.367800000000
H	2.374887000000	-3.135330000000	-4.116095000000
H	4.738529000000	-5.645252000000	0.054585000000
H	5.835140000000	-4.449991000000	0.790442000000
H	5.054564000000	-5.679827000000	1.802496000000
H	2.176825000000	-5.604314000000	2.623606000000
H	1.079341000000	-4.328121000000	2.043813000000
H	1.653435000000	-5.579904000000	0.921019000000
H	4.477172000000	-1.986919000000	2.699201000000
H	3.190864000000	-2.782669000000	3.638374000000
H	4.766773000000	-3.577775000000	3.441912000000
H	5.469149000000	1.692528000000	-2.463056000000
H	3.940770000000	1.728607000000	-3.364536000000
H	5.187245000000	2.957545000000	-3.689682000000
H	1.886460000000	4.893730000000	-1.854731000000
H	3.322982000000	5.801918000000	-2.362469000000
H	2.639547000000	4.549762000000	-3.423704000000
H	5.971745000000	5.010404000000	-1.785203000000
H	5.214396000000	5.284174000000	-0.203722000000
H	6.272975000000	3.873836000000	-0.455290000000
H	1.154039000000	3.509284000000	3.226633000000
H	0.680246000000	2.443603000000	1.871171000000
H	1.947681000000	1.936991000000	3.003414000000
H	2.123644000000	5.887504000000	1.927315000000
H	3.007607000000	5.913016000000	0.383017000000
H	1.332029000000	5.319918000000	0.441580000000
H	4.773847000000	2.618542000000	2.689423000000
H	5.289259000000	4.121792000000	1.887428000000
H	4.278465000000	4.196670000000	3.352182000000
H	7.108980000000	-0.552656000000	2.624226000000
H	7.165160000000	-2.049166000000	1.667107000000
H	8.649580000000	-1.097992000000	1.906200000000
H	8.997062000000	-0.965852000000	-0.637188000000
H	7.517354000000	-1.918012000000	-0.900183000000
H	7.696294000000	-0.331397000000	-1.681877000000
H	7.489157000000	1.730259000000	1.487578000000
H	8.987072000000	1.086462000000	0.779169000000
H	7.752784000000	1.808777000000	-0.274175000000
H	1.842244000000	-2.569516000000	-0.010258000000
H	2.028450000000	2.459931000000	-0.553482000000

1-C(T₁)

$G_{qh} = -4746.253395$

$G_{B3LYP-D3/TZVPP} = -4749.775381$

$N_{imag} = 0$

C	4.019400000000	0.862260000000	-0.331294000000
C	2.959753000000	-0.021443000000	0.065055000000
C	3.285475000000	-1.424775000000	0.104207000000
C	4.529311000000	-1.866346000000	-0.375915000000
C	5.509987000000	-1.018564000000	-0.890679000000
C	5.223755000000	0.340460000000	-0.840280000000
C	1.544920000000	0.434828000000	0.325634000000
C	0.770015000000	0.104893000000	1.457412000000
C	1.482299000000	-0.125810000000	2.782321000000
C	1.308592000000	1.034165000000	3.776209000000

C	2.390618000000	-2.525273000000	0.645176000000
Si	3.220342000000	-3.485877000000	2.094883000000
C	4.440179000000	-2.389369000000	3.038260000000
C	6.846893000000	-1.581048000000	-1.396707000000
C	7.745478000000	-0.484354000000	-1.995993000000
C	4.040436000000	2.364418000000	-0.121299000000
Si	5.216578000000	2.790026000000	1.341004000000
C	7.036861000000	2.350678000000	1.061142000000
C	0.741285000000	1.165439000000	-0.704200000000
C	0.818884000000	2.685569000000	-0.759348000000
C	0.720616000000	3.405732000000	0.593212000000
C	-0.638627000000	0.675414000000	-0.982142000000
C	-1.240056000000	1.001251000000	-2.324646000000
C	-0.299987000000	0.826842000000	-3.519383000000
C	-1.373289000000	0.216849000000	0.086758000000
C	-0.657397000000	-0.003164000000	1.362450000000
C	-1.421260000000	-0.595340000000	2.525218000000
C	-1.229824000000	-2.114779000000	2.639858000000
C	-2.898806000000	0.154260000000	0.002635000000
C	-3.623893000000	1.386230000000	0.163633000000
C	-5.026428000000	1.376310000000	0.182094000000
C	-5.788252000000	0.227639000000	-0.028947000000
C	-5.076729000000	-0.941636000000	-0.262188000000
C	-3.667546000000	-1.024541000000	-0.238698000000
C	-2.990851000000	2.766124000000	0.243280000000
Si	-3.607871000000	3.917429000000	-1.186064000000
C	-4.288943000000	2.949916000000	-2.664201000000
C	-7.323139000000	0.296514000000	-0.018425000000
C	-7.966773000000	-1.080112000000	-0.261173000000
C	-3.133733000000	-2.431951000000	-0.471995000000
Si	-3.362087000000	-3.029085000000	-2.296815000000
C	-5.160101000000	-3.030906000000	-2.896302000000
C	-5.032868000000	5.072400000000	-0.694801000000
C	-2.157858000000	4.997093000000	-1.755061000000
C	-2.497637000000	-1.943927000000	-3.575601000000
C	-2.629506000000	-4.769676000000	-2.442474000000
C	-7.798266000000	1.259632000000	-1.129519000000
C	-7.796859000000	0.821284000000	1.355293000000
Si	-3.128220000000	3.595650000000	1.973084000000
C	-2.189232000000	2.602440000000	3.272632000000
C	-4.906693000000	3.725232000000	2.606436000000
C	-2.355490000000	5.326847000000	1.923676000000
Si	-3.944865000000	-3.684908000000	0.789158000000
C	-5.473930000000	-4.607236000000	0.138485000000
C	-4.564322000000	-2.782020000000	2.339049000000
C	-2.759704000000	-5.077929000000	1.282923000000
C	4.196991000000	-5.010772000000	1.523469000000
C	1.909460000000	-4.110985000000	3.311356000000
C	4.689342000000	1.811788000000	2.864277000000
C	5.076588000000	4.642799000000	1.709276000000
C	7.592944000000	-2.231952000000	-0.209405000000
C	6.587393000000	-2.645342000000	-2.485113000000
Si	1.720062000000	-3.613078000000	-0.779711000000
C	0.730786000000	-2.479939000000	-1.907977000000
C	3.039588000000	-4.432699000000	-1.859636000000
C	0.615219000000	-4.960977000000	-0.054269000000
Si	4.341407000000	3.382737000000	-1.729972000000
C	6.163911000000	3.764885000000	-2.088331000000
C	3.683001000000	2.412087000000	-3.213311000000
C	3.485928000000	5.070541000000	-1.599904000000
H	-1.575666000000	2.051489000000	-2.307150000000

H	-2.156630000000	0.416017000000	-2.456799000000
H	0.551186000000	1.522143000000	-3.465385000000
H	-0.834417000000	1.021098000000	-4.462470000000
H	0.113324000000	-0.190218000000	-3.566495000000
H	0.025663000000	3.067530000000	-1.414530000000
H	1.754087000000	2.974563000000	-1.249898000000
H	-0.213428000000	3.152335000000	1.106863000000
H	0.757101000000	4.497981000000	0.454247000000
H	1.536866000000	3.121470000000	1.271172000000
H	-5.538868000000	2.326299000000	0.328564000000
H	-5.624792000000	-1.858313000000	-0.456797000000
H	-5.341270000000	2.723745000000	2.750224000000
H	-5.572792000000	4.296757000000	1.944698000000
H	-4.895254000000	4.228006000000	3.588416000000
H	-2.392240000000	5.765282000000	2.935024000000
H	-2.875350000000	6.017721000000	1.243476000000
H	-1.298547000000	5.285041000000	1.618888000000
H	-1.175382000000	2.338581000000	2.942835000000
H	-2.721757000000	1.670543000000	3.510033000000
H	-2.106529000000	3.190844000000	4.201730000000
H	-4.793778000000	5.755660000000	0.133070000000
H	-5.938060000000	4.507833000000	-0.419821000000
H	-5.288834000000	5.689670000000	-1.572476000000
H	-2.520721000000	5.813979000000	-2.400585000000
H	-1.426846000000	4.415947000000	-2.338990000000
H	-1.625211000000	5.448735000000	-0.904191000000
H	-5.216692000000	2.425580000000	-2.390347000000
H	-3.590785000000	2.201963000000	-3.062023000000
H	-4.526099000000	3.661644000000	-3.473194000000
H	-5.605364000000	-2.454604000000	2.194643000000
H	-3.977002000000	-1.888895000000	2.585566000000
H	-4.539511000000	-3.465860000000	3.203787000000
H	-1.932765000000	-4.745771000000	1.925189000000
H	-2.328948000000	-5.583569000000	0.406559000000
H	-3.337455000000	-5.827439000000	1.849848000000
H	-5.829120000000	-5.245613000000	0.965589000000
H	-5.261502000000	-5.266443000000	-0.716551000000
H	-6.304889000000	-3.940752000000	-0.136459000000
H	-2.528168000000	-2.472324000000	-4.543683000000
H	-1.450100000000	-1.730412000000	-3.339364000000
H	-3.028770000000	-0.989051000000	-3.706238000000
H	-2.654496000000	-5.096968000000	-3.494997000000
H	-3.173085000000	-5.518408000000	-1.846547000000
H	-1.578528000000	-4.774637000000	-2.113828000000
H	-5.560693000000	-2.004851000000	-2.899839000000
H	-5.846984000000	-3.666367000000	-2.323950000000
H	-5.161776000000	-3.387987000000	-3.940458000000
H	-7.461803000000	0.912413000000	-2.119437000000
H	-7.408168000000	2.278126000000	-0.981134000000
H	-8.898862000000	1.322623000000	-1.143646000000
H	-8.897506000000	0.875813000000	1.390458000000
H	-7.405273000000	1.828049000000	1.565349000000
H	-7.460003000000	0.154872000000	2.165428000000
H	-7.683195000000	-1.498361000000	-1.239462000000
H	-9.064233000000	-0.989906000000	-0.243384000000
H	-7.680562000000	-1.805539000000	0.516457000000
H	-1.907887000000	2.684503000000	0.082203000000
H	-2.043513000000	-2.464810000000	-0.311654000000
H	1.170763000000	-1.058707000000	3.271732000000
H	2.551959000000	-0.234846000000	2.569564000000
H	0.281605000000	1.108924000000	4.159199000000

H	1.978152000000	0.904291000000	4.641216000000
H	1.547942000000	1.997993000000	3.304079000000
H	-1.121519000000	-0.129831000000	3.473053000000
H	-2.491350000000	-0.377380000000	2.403363000000
H	-0.190586000000	-2.380846000000	2.860445000000
H	-1.860004000000	-2.543112000000	3.433556000000
H	-1.487817000000	-2.606015000000	1.697133000000
H	4.733130000000	-2.934503000000	-0.340502000000
H	5.978746000000	1.053720000000	-1.159094000000
H	3.608627000000	-3.682237000000	-2.428208000000
H	3.752432000000	-5.050471000000	-1.294185000000
H	2.531013000000	-5.088575000000	-2.586978000000
H	0.119966000000	-5.536076000000	-0.852722000000
H	1.184887000000	-5.674457000000	0.561410000000
H	-0.167699000000	-4.522511000000	0.579027000000
H	-0.099535000000	-1.992803000000	-1.376880000000
H	1.388075000000	-1.679820000000	-2.283657000000
H	0.325707000000	-3.028964000000	-2.772226000000
H	3.563519000000	-5.752570000000	1.012735000000
H	5.030158000000	-4.755294000000	0.850284000000
H	4.630622000000	-5.501250000000	2.411175000000
H	2.364840000000	-4.846189000000	3.995812000000
H	1.507209000000	-3.292973000000	3.928454000000
H	1.065091000000	-4.601570000000	2.804286000000
H	5.191825000000	-1.955285000000	2.361037000000
H	3.934795000000	-1.561883000000	3.557995000000
H	4.968550000000	-2.990714000000	3.796910000000
H	4.317009000000	1.530628000000	-3.397952000000
H	2.659645000000	2.043321000000	-3.049765000000
H	3.688140000000	3.037179000000	-4.121646000000
H	2.391520000000	4.998436000000	-1.515297000000
H	3.852554000000	5.634845000000	-0.728482000000
H	3.712217000000	5.664549000000	-2.501354000000
H	6.219636000000	4.312586000000	-3.044293000000
H	6.616419000000	4.405087000000	-1.314797000000
H	6.783190000000	2.860313000000	-2.190958000000
H	5.388123000000	2.001979000000	3.695950000000
H	3.680444000000	2.082203000000	3.202242000000
H	4.702010000000	0.731719000000	2.650297000000
H	5.590750000000	4.881971000000	2.654992000000
H	5.535329000000	5.256241000000	0.917326000000
H	4.023540000000	4.953394000000	1.810489000000
H	7.170406000000	1.258519000000	1.025506000000
H	7.466908000000	2.779427000000	0.145587000000
H	7.620024000000	2.729895000000	1.917738000000
H	7.787480000000	-1.491840000000	0.583354000000
H	7.008770000000	-3.052312000000	0.235257000000
H	8.560740000000	-2.646085000000	-0.537665000000
H	7.540684000000	-3.048001000000	-2.865117000000
H	5.999524000000	-3.491516000000	-2.100538000000
H	6.035643000000	-2.211738000000	-3.334435000000
H	8.018330000000	0.277161000000	-1.249360000000
H	8.680842000000	-0.928837000000	-2.370817000000
H	7.254340000000	0.024809000000	-2.840331000000
H	1.465817000000	-2.103300000000	1.062998000000
H	3.078434000000	2.705318000000	0.273339000000

1-Si

$G_{qh} = -5249.021657$

$G_{B3LYP-D3/TZVPP} = -5252.673647$

$N_{imag} = 0$

SP = -5243.703389

G_{sp} = -5242.202193

C	4.553407000000	0.833641000000	-0.094993000000
C	3.483185000000	-0.096291000000	0.075592000000
C	3.761234000000	-1.488207000000	-0.140792000000
C	5.022529000000	-1.868756000000	-0.624026000000
C	6.060225000000	-0.960859000000	-0.852702000000
C	5.802624000000	0.375847000000	-0.558455000000
Si	1.670613000000	0.430126000000	0.340712000000
C	0.632843000000	-0.381433000000	1.592207000000
C	1.293526000000	-0.706103000000	2.929035000000
C	0.993722000000	0.324328000000	4.030286000000
C	2.795168000000	-2.616177000000	0.181724000000
Si	3.530230000000	-3.782548000000	1.526557000000
C	4.696502000000	-2.814535000000	2.658212000000
C	7.423613000000	-1.459330000000	-1.357572000000
C	8.417962000000	-0.305755000000	-1.579226000000
C	4.481502000000	2.303839000000	0.282096000000
Si	5.255952000000	2.496440000000	2.040592000000
C	7.033270000000	1.854266000000	2.127896000000
C	0.793032000000	1.007667000000	-1.145508000000
C	1.609871000000	1.860876000000	-2.104719000000
C	1.390063000000	3.362115000000	-1.860271000000
C	-0.584391000000	0.812982000000	-1.343562000000
C	-1.280703000000	1.275275000000	-2.623224000000
C	-0.902543000000	0.526173000000	-3.913446000000
Si	-1.595923000000	-0.070146000000	-0.121179000000
C	-0.746823000000	-0.578014000000	1.399121000000
C	-1.579811000000	-1.320251000000	2.437005000000
C	-1.333456000000	-2.835036000000	2.414985000000
C	-3.478504000000	0.182819000000	-0.069591000000
C	-3.995687000000	1.517746000000	0.035315000000
C	-5.378056000000	1.708055000000	0.177537000000
C	-6.300046000000	0.658637000000	0.167263000000
C	-5.787312000000	-0.629229000000	0.030320000000
C	-4.408770000000	-0.901632000000	-0.067743000000
C	-3.144775000000	2.776606000000	0.002547000000
Si	-3.728699000000	4.040993000000	-1.330176000000
C	-4.564765000000	3.164885000000	-2.783686000000
C	-7.803069000000	0.955041000000	0.291022000000
C	-8.652695000000	-0.327687000000	0.263627000000
C	-4.025701000000	-2.368077000000	-0.195245000000
Si	-4.268124000000	-2.966213000000	-2.007980000000
C	-6.012689000000	-2.611667000000	-2.644398000000
C	-4.975200000000	5.315812000000	-0.677886000000
C	-2.242712000000	5.012519000000	-1.988208000000
C	-3.053677000000	-2.030090000000	-3.095184000000
C	-3.888803000000	-4.814235000000	-2.163208000000
C	-8.239993000000	1.854269000000	-0.887714000000
C	-8.068658000000	1.687486000000	1.625394000000
Si	-2.895687000000	3.513766000000	1.759712000000
C	-1.985886000000	2.272291000000	2.847490000000
C	-4.536667000000	3.910954000000	2.612938000000
C	-1.829866000000	5.075302000000	1.648499000000
Si	-4.853467000000	-3.534091000000	1.102540000000
C	-6.588150000000	-4.129642000000	0.606218000000
C	-5.050493000000	-2.659084000000	2.767961000000
C	-3.833057000000	-5.120569000000	1.306193000000
C	4.504191000000	-5.245053000000	0.812335000000
C	2.151859000000	-4.513903000000	2.597590000000
C	4.260688000000	1.466050000000	3.260708000000

C	5.202681000000	4.303900000000	2.602330000000
C	8.024099000000	-2.425884000000	-0.311257000000
C	7.232401000000	-2.203238000000	-2.697980000000
Si	2.070763000000	-3.477226000000	-1.370784000000
C	1.127192000000	-2.221008000000	-2.409009000000
C	3.395322000000	-4.243698000000	-2.484013000000
C	0.842494000000	-4.811705000000	-0.821307000000
Si	5.206842000000	3.550821000000	-1.002542000000
C	7.068949000000	3.868841000000	-0.797978000000
C	4.989879000000	2.946041000000	-2.783394000000
C	4.372329000000	5.235237000000	-0.784120000000
H	-1.105378000000	2.351271000000	-2.777923000000
H	-2.367705000000	1.176551000000	-2.482253000000
H	0.116101000000	0.758445000000	-4.252903000000
H	-1.592648000000	0.801271000000	-4.727948000000
H	-0.956801000000	-0.559675000000	-3.776380000000
H	1.373701000000	1.626428000000	-3.151782000000
H	2.678541000000	1.629811000000	-1.984559000000
H	0.337319000000	3.644105000000	-1.993176000000
H	1.991840000000	3.979873000000	-2.545039000000
H	1.663134000000	3.626723000000	-0.827417000000
H	-5.744391000000	2.727903000000	0.285716000000
H	-6.471082000000	-1.471371000000	-0.003320000000
H	-5.130197000000	2.994510000000	2.756968000000
H	-5.152489000000	4.631569000000	2.055373000000
H	-4.333939000000	4.339061000000	3.609192000000
H	-1.599897000000	5.440274000000	2.663451000000
H	-2.322466000000	5.894867000000	1.102634000000
H	-0.871857000000	4.858881000000	1.147071000000
H	-0.993682000000	2.023045000000	2.443072000000
H	-2.552351000000	1.333020000000	2.938601000000
H	-1.850524000000	2.687509000000	3.860530000000
H	-4.557354000000	5.942231000000	0.125452000000
H	-5.900996000000	4.853951000000	-0.300293000000
H	-5.256955000000	5.985589000000	-1.507787000000
H	-2.593953000000	5.897453000000	-2.544695000000
H	-1.646232000000	4.402673000000	-2.683063000000
H	-1.576212000000	5.361433000000	-1.185834000000
H	-5.470988000000	2.628881000000	-2.463201000000
H	-3.896066000000	2.436265000000	-3.265984000000
H	-4.856955000000	3.909888000000	-3.542837000000
H	-5.576074000000	-1.699287000000	2.645550000000
H	-4.088783000000	-2.455747000000	3.259395000000
H	-5.647768000000	-3.292504000000	3.445060000000
H	-2.748643000000	-4.957619000000	1.242806000000
H	-4.105809000000	-5.863220000000	0.541650000000
H	-4.045732000000	-5.566603000000	2.292319000000
H	-6.948983000000	-4.813343000000	1.393489000000
H	-6.579309000000	-4.695391000000	-0.338243000000
H	-7.327902000000	-3.320015000000	0.511932000000
H	-3.147307000000	-2.327508000000	-4.152735000000
H	-2.016735000000	-2.218643000000	-2.777537000000
H	-3.234556000000	-0.947254000000	-3.029552000000
H	-3.837500000000	-5.086118000000	-3.230840000000
H	-4.657445000000	-5.448053000000	-1.695319000000
H	-2.917503000000	-5.064459000000	-1.705984000000
H	-6.209878000000	-1.528256000000	-2.648546000000
H	-6.797231000000	-3.096753000000	-2.045280000000
H	-6.103832000000	-2.976846000000	-3.681321000000
H	-8.049772000000	1.356085000000	-1.851815000000
H	-7.698589000000	2.812519000000	-0.893561000000

H	-9.317478000000	2.078797000000	-0.824212000000
H	-9.142528000000	1.911206000000	1.735789000000
H	-7.520525000000	2.639665000000	1.687174000000
H	-7.758179000000	1.066461000000	2.480876000000
H	-8.521449000000	-0.885214000000	-0.676950000000
H	-9.720268000000	-0.072235000000	0.352439000000
H	-8.401531000000	-1.000219000000	1.098771000000
H	-2.112617000000	2.527571000000	-0.296896000000
H	-2.937958000000	-2.483982000000	-0.036971000000
H	0.993156000000	-1.702258000000	3.284848000000
H	2.383951000000	-0.756659000000	2.790107000000
H	-0.069892000000	0.332141000000	4.307777000000
H	1.584417000000	0.114145000000	4.936682000000
H	1.239309000000	1.341116000000	3.690557000000
H	-1.381220000000	-0.933629000000	3.448271000000
H	-2.648437000000	-1.130362000000	2.253327000000
H	-0.301784000000	-3.086829000000	2.687743000000
H	-2.002540000000	-3.368160000000	3.107691000000
H	-1.499725000000	-3.236365000000	1.405488000000
H	5.201671000000	-2.927940000000	-0.802712000000
H	6.598348000000	1.106755000000	-0.668981000000
H	4.040825000000	-3.460905000000	-2.912605000000
H	4.037047000000	-4.969114000000	-1.963136000000
H	2.904867000000	-4.766498000000	-3.322560000000
H	0.309409000000	-5.214261000000	-1.698945000000
H	1.329470000000	-5.656455000000	-0.309072000000
H	0.089205000000	-4.386519000000	-0.137434000000
H	0.280659000000	-1.793186000000	-1.851640000000
H	1.770268000000	-1.382360000000	-2.717414000000
H	0.729565000000	-2.701023000000	-3.319135000000
H	3.864314000000	-5.914286000000	0.215472000000
H	5.349238000000	-4.929654000000	0.180796000000
H	4.917384000000	-5.837779000000	1.645767000000
H	2.562169000000	-5.325241000000	3.221939000000
H	1.736365000000	-3.754043000000	3.276148000000
H	1.325244000000	-4.930055000000	2.003662000000
H	5.546548000000	-2.394698000000	2.099172000000
H	4.174328000000	-1.980561000000	3.152043000000
H	5.093045000000	-3.477280000000	3.445496000000
H	5.285497000000	1.890245000000	-2.884005000000
H	3.957397000000	3.044044000000	-3.145657000000
H	5.635856000000	3.545128000000	-3.446808000000
H	3.276157000000	5.173579000000	-0.831216000000
H	4.645075000000	5.697459000000	0.176302000000
H	4.704779000000	5.914259000000	-1.587392000000
H	7.369045000000	4.609339000000	-1.558730000000
H	7.324789000000	4.288543000000	0.186781000000
H	7.685591000000	2.970256000000	-0.956194000000
H	4.674804000000	1.564171000000	4.277955000000
H	3.208373000000	1.779601000000	3.290009000000
H	4.293273000000	0.403317000000	2.978429000000
H	5.487818000000	4.364913000000	3.665941000000
H	5.895279000000	4.944943000000	2.035452000000
H	4.189508000000	4.726334000000	2.502378000000
H	7.061039000000	0.772361000000	1.925513000000
H	7.720571000000	2.350115000000	1.428505000000
H	7.416218000000	2.015383000000	3.150026000000
H	8.160342000000	-1.918352000000	0.657187000000
H	7.375611000000	-3.299100000000	-0.142991000000
H	9.007099000000	-2.796813000000	-0.645579000000
H	8.200702000000	-2.568440000000	-3.077943000000

H	6.565996000000	-3.072578000000	-2.593202000000
H	6.795737000000	-1.535293000000	-3.457549000000
H	8.628373000000	0.238099000000	-0.645078000000
H	9.374649000000	-0.702335000000	-1.953822000000
H	8.043310000000	0.417841000000	-2.320207000000
H	1.890536000000	-2.205674000000	0.659921000000
H	3.426333000000	2.604106000000	0.426971000000

1-Ge

$G_{qh} = -8823.745132$

$G_{B3LYP-D3/TZVPP} = -8827.720462$

$N_{imag} = 0$

$SP = -8816.812384$

$G_{sp} = -8815.315842$

C	4.584564000000	0.822073000000	-0.041951000000
C	3.559757000000	-0.160165000000	0.075103000000
C	3.903311000000	-1.535196000000	-0.116133000000
C	5.211271000000	-1.859158000000	-0.511688000000
C	6.222122000000	-0.907472000000	-0.668526000000
C	5.884167000000	0.418147000000	-0.407593000000
Ge	1.654040000000	0.352057000000	0.326712000000
C	0.568694000000	-0.651129000000	1.530448000000
C	1.208114000000	-1.033903000000	2.859466000000
C	0.865305000000	-0.087585000000	4.020787000000
C	2.965703000000	-2.704087000000	0.132186000000
Si	3.664344000000	-3.874450000000	1.492552000000
C	4.726734000000	-2.887632000000	2.708456000000
C	7.638935000000	-1.347133000000	-1.071222000000
C	8.599217000000	-0.152782000000	-1.212544000000
C	4.407779000000	2.296896000000	0.283814000000
Si	4.995461000000	2.587945000000	2.097360000000
C	6.752908000000	1.950540000000	2.378133000000
C	0.783736000000	0.863857000000	-1.292143000000
C	1.630734000000	1.694186000000	-2.242959000000
C	1.404040000000	3.201625000000	-2.050207000000
C	-0.568556000000	0.652148000000	-1.529762000000
C	-1.208100000000	1.035421000000	-2.858577000000
C	-0.864656000000	0.090325000000	-4.020702000000
Ge	-1.653771000000	-0.351023000000	-0.325980000000
C	-0.783642000000	-0.862741000000	1.292921000000
C	-1.630834000000	-1.692448000000	2.244108000000
C	-1.404351000000	-3.200036000000	2.052315000000
C	-3.559779000000	0.160335000000	-0.075229000000
C	-3.904029000000	1.535280000000	0.115449000000
C	-5.212421000000	1.858805000000	0.509909000000
C	-6.223038000000	0.906772000000	0.666092000000
C	-5.884311000000	-0.418789000000	0.405882000000
C	-4.584226000000	-0.822319000000	0.041530000000
C	-2.966667000000	2.704545000000	-0.132066000000
Si	-3.664805000000	3.875200000000	-1.492464000000
C	-4.726089000000	2.888574000000	-2.709489000000
C	-7.640366000000	1.345998000000	1.067436000000
C	-8.600321000000	0.151323000000	1.208221000000
C	-4.406465000000	-2.297300000000	-0.283027000000
Si	-4.992127000000	-2.590236000000	-2.096894000000
C	-6.749226000000	-1.953016000000	-2.380128000000
C	-4.739822000000	5.279733000000	-0.806639000000
C	-2.254388000000	4.694978000000	-2.452559000000
C	-3.844963000000	-1.646101000000	-3.253387000000
C	-4.895064000000	-4.422933000000	-2.563216000000
C	-8.200220000000	2.295071000000	-0.016594000000

C	-7.581895000000	2.086785000000	2.421917000000
Si	-2.380447000000	3.551246000000	1.484736000000
C	-1.438439000000	2.302246000000	2.533675000000
C	-3.809062000000	4.210286000000	2.536095000000
C	-1.199110000000	4.966804000000	1.051359000000
Si	-5.179627000000	-3.532529000000	0.980749000000
C	-7.011073000000	-3.917308000000	0.651679000000
C	-5.097539000000	-2.864724000000	2.749453000000
C	-4.276233000000	-5.192887000000	0.879831000000
C	4.738449000000	-5.279604000000	0.806599000000
C	2.254240000000	-4.693240000000	2.453935000000
C	3.849980000000	1.642236000000	3.254235000000
C	4.898749000000	4.420147000000	2.565691000000
C	8.199395000000	-2.296687000000	0.012071000000
C	7.578992000000	-2.087553000000	-2.425840000000
Si	2.378112000000	-3.551128000000	-1.483927000000
C	1.436055000000	-2.302085000000	-2.532761000000
C	3.805685000000	-4.211340000000	-2.535971000000
C	1.196359000000	-4.965920000000	-1.049173000000
Si	5.180281000000	3.532791000000	-0.979711000000
C	7.012096000000	3.916811000000	-0.651808000000
C	5.096586000000	2.866391000000	-2.748874000000
C	4.277353000000	5.193258000000	-0.876872000000
H	-0.917245000000	2.059476000000	-3.136387000000
H	-2.302365000000	1.060698000000	-2.742103000000
H	0.210140000000	0.100103000000	-4.252249000000
H	-1.415438000000	0.375856000000	-4.931735000000
H	-1.128770000000	-0.946204000000	-3.774803000000
H	1.422223000000	1.426320000000	-3.290021000000
H	2.695764000000	1.465563000000	-2.084559000000
H	0.359449000000	3.480811000000	-2.242212000000
H	2.041359000000	3.799487000000	-2.719990000000
H	1.627591000000	3.493840000000	-1.012912000000
H	-5.449241000000	2.908719000000	0.674873000000
H	-6.651228000000	-1.184730000000	0.467768000000
H	-4.443095000000	3.382940000000	2.891740000000
H	-4.449597000000	4.925971000000	2.000039000000
H	-3.399399000000	4.722073000000	3.423355000000
H	-0.747453000000	5.374026000000	1.971300000000
H	-1.703501000000	5.796689000000	0.531657000000
H	-0.380234000000	4.606701000000	0.406652000000
H	-0.528484000000	1.951659000000	2.024262000000
H	-2.054220000000	1.416058000000	2.752338000000
H	-1.138062000000	2.754989000000	3.493503000000
H	-4.167215000000	5.955001000000	-0.151225000000
H	-5.611683000000	4.915770000000	-0.241239000000
H	-5.120312000000	5.880291000000	-1.649972000000
H	-2.661591000000	5.497853000000	-3.089730000000
H	-1.748681000000	3.974601000000	-3.112123000000
H	-1.498105000000	5.141544000000	-1.790615000000
H	-5.612196000000	2.465173000000	-2.212298000000
H	-4.164068000000	2.053127000000	-3.155345000000
H	-5.068470000000	3.541860000000	-3.529412000000
H	-5.501613000000	-1.842200000000	2.806297000000
H	-4.074590000000	-2.845463000000	3.150339000000
H	-5.704101000000	-3.508622000000	3.408211000000
H	-3.185351000000	-5.087438000000	0.961193000000
H	-4.496570000000	-5.716267000000	-0.062372000000
H	-4.612240000000	-5.840621000000	1.707115000000
H	-7.343086000000	-4.659800000000	1.397055000000
H	-7.180120000000	-4.354469000000	-0.344243000000

H	-7.666829000000	-3.038395000000	0.752178000000
H	-4.147109000000	-1.778496000000	-4.305441000000
H	-2.810179000000	-2.004725000000	-3.148582000000
H	-3.854369000000	-0.569668000000	-3.026375000000
H	-5.082266000000	-4.531731000000	-3.644696000000
H	-5.637649000000	-5.039489000000	-2.034086000000
H	-3.895891000000	-4.838403000000	-2.353714000000
H	-6.794024000000	-0.863796000000	-2.226107000000
H	-7.490290000000	-2.420732000000	-1.715657000000
H	-7.047653000000	-2.161801000000	-3.421394000000
H	-8.241537000000	1.790267000000	-0.995087000000
H	-7.578553000000	3.196054000000	-0.130980000000
H	-9.220311000000	2.622243000000	0.244070000000
H	-8.590161000000	2.410289000000	2.728819000000
H	-6.944706000000	2.982544000000	2.372376000000
H	-7.177678000000	1.430914000000	3.209480000000
H	-8.713027000000	-0.396710000000	0.259667000000
H	-9.599375000000	0.506119000000	1.506313000000
H	-8.256018000000	-0.559434000000	1.975862000000
H	-2.017202000000	2.338628000000	-0.556005000000
H	-3.329443000000	-2.547254000000	-0.315566000000
H	0.916609000000	-2.057531000000	3.138148000000
H	2.302349000000	-1.059961000000	2.742944000000
H	-0.209467000000	-0.096663000000	4.252481000000
H	1.416122000000	-0.372446000000	4.932006000000
H	1.129792000000	0.948614000000	3.773806000000
H	-1.422418000000	-1.423940000000	3.291033000000
H	-2.695817000000	-1.463781000000	2.085449000000
H	-0.359920000000	-3.479350000000	2.244963000000
H	-2.042137000000	-3.797401000000	2.722094000000
H	-1.627452000000	-3.492784000000	1.015079000000
H	5.447572000000	-2.909137000000	-0.676990000000
H	6.651364000000	1.183790000000	-0.469829000000
H	4.439805000000	-3.384453000000	-2.892526000000
H	4.446304000000	-4.927028000000	-2.000017000000
H	3.395145000000	-4.723401000000	-3.422667000000
H	0.743765000000	-5.373235000000	-1.968611000000
H	1.700715000000	-5.795884000000	-0.529557000000
H	0.378188000000	-4.605143000000	-0.403948000000
H	0.526486000000	-1.951048000000	-2.022960000000
H	2.052026000000	-1.416153000000	-2.751928000000
H	1.135033000000	-2.754944000000	-3.492331000000
H	4.165189000000	-5.955001000000	0.151886000000
H	5.609990000000	-4.916091000000	0.240418000000
H	5.119394000000	-5.879900000000	1.649913000000
H	2.661519000000	-5.495850000000	3.091391000000
H	1.749176000000	-3.972248000000	3.113320000000
H	1.497420000000	-5.139946000000	1.792696000000
H	5.613077000000	-2.465410000000	2.210679000000
H	4.165523000000	-2.051303000000	3.153675000000
H	5.068744000000	-3.540460000000	3.528897000000
H	5.499067000000	1.843294000000	-2.806697000000
H	4.073455000000	2.849069000000	-3.149389000000
H	5.703893000000	3.509888000000	-3.407338000000
H	3.186545000000	5.088200000000	-0.959740000000
H	4.496679000000	5.714893000000	0.066530000000
H	4.614522000000	5.842376000000	-1.702597000000
H	7.343817000000	4.659534000000	-1.397082000000
H	7.182045000000	4.353435000000	0.344197000000
H	7.667455000000	3.037705000000	-0.753219000000
H	4.154459000000	1.772199000000	4.305920000000

H	2.815191000000	2.001642000000	3.152427000000
H	3.858350000000	0.566295000000	3.024861000000
H	5.087245000000	4.527879000000	3.647052000000
H	5.640615000000	5.037329000000	2.036277000000
H	3.899265000000	4.835695000000	2.357825000000
H	6.797489000000	0.861410000000	2.223403000000
H	7.493341000000	2.418630000000	1.713240000000
H	7.052381000000	2.158642000000	3.419239000000
H	8.241758000000	-1.792148000000	0.990655000000
H	7.577503000000	-3.197475000000	0.126774000000
H	9.219135000000	-2.624168000000	-0.249575000000
H	8.586871000000	-2.411320000000	-2.733737000000
H	6.941549000000	-2.983111000000	-2.375938000000
H	7.174281000000	-1.431347000000	-3.212868000000
H	8.712989000000	0.394944000000	-0.263940000000
H	9.597864000000	-0.507876000000	-1.511639000000
H	8.254491000000	0.558321000000	-1.979676000000
H	2.016657000000	-2.337723000000	0.556672000000
H	3.330887000000	2.547279000000	0.317651000000

1-Si (T₁)

$G_{qh} = -5248.986290$

$N_{imag} = 0$

$G_{B3LYP-D3/TZVPP} = -5252.638809$

C	4.532103000000	0.752385000000	-0.138930000000
C	3.416889000000	-0.117427000000	0.084295000000
C	3.607150000000	-1.515777000000	-0.161231000000
C	4.814848000000	-1.960046000000	-0.724388000000
C	5.881303000000	-1.107349000000	-1.021269000000
C	5.716446000000	0.237910000000	-0.699708000000
Si	1.711137000000	0.638714000000	0.552554000000
C	0.591564000000	-0.307122000000	1.744280000000
C	1.211975000000	-0.581870000000	3.111696000000
C	0.969699000000	0.545254000000	4.128020000000
C	2.614081000000	-2.597678000000	0.231287000000
Si	3.378448000000	-3.731831000000	1.591921000000
C	4.598350000000	-2.748279000000	2.651080000000
C	7.182534000000	-1.671807000000	-1.613481000000
C	8.210437000000	-0.566385000000	-1.914030000000
C	4.583578000000	2.210092000000	0.295528000000
Si	5.450554000000	2.273445000000	2.019854000000
C	7.163666000000	1.471428000000	1.985728000000
C	0.784322000000	1.198856000000	-1.002970000000
C	1.571484000000	2.174525000000	-1.862902000000
C	1.342465000000	3.624389000000	-1.409304000000
C	-0.496976000000	0.838770000000	-1.315408000000
C	-1.146528000000	1.272519000000	-2.628699000000
C	-0.671531000000	0.505091000000	-3.872149000000
Si	-1.538155000000	-0.259334000000	-0.193876000000
C	-0.720202000000	-0.591050000000	1.476122000000
C	-1.601380000000	-1.291923000000	2.502937000000
C	-1.400833000000	-2.811960000000	2.492944000000
C	-3.400806000000	0.182429000000	-0.069946000000
C	-3.873248000000	1.532398000000	0.038606000000
C	-5.242794000000	1.766606000000	0.241301000000
C	-6.200224000000	0.750860000000	0.275761000000
C	-5.737565000000	-0.551935000000	0.109391000000
C	-4.374449000000	-0.866766000000	-0.046427000000
C	-3.002801000000	2.774731000000	-0.078259000000
Si	-3.642761000000	3.972992000000	-1.451779000000
C	-4.516373000000	3.016998000000	-2.831013000000

C	-7.685957000000	1.097086000000	0.461938000000
C	-8.575351000000	-0.158543000000	0.489199000000
C	-4.054790000000	-2.343997000000	-0.232634000000
Si	-4.361832000000	-2.844443000000	-2.066859000000
C	-6.112757000000	-2.410170000000	-2.632344000000
C	-4.878302000000	5.268407000000	-0.817686000000
C	-2.216685000000	4.956631000000	-2.215706000000
C	-3.156374000000	-1.901771000000	-3.163289000000
C	-4.037521000000	-4.692423000000	-2.322715000000
C	-8.146271000000	1.994758000000	-0.709125000000
C	-7.869720000000	1.854471000000	1.795973000000
Si	-2.688721000000	3.603849000000	1.623757000000
C	-1.754809000000	2.402103000000	2.730575000000
C	-4.284492000000	4.071799000000	2.525372000000
C	-1.607248000000	5.140512000000	1.387225000000
Si	-4.897654000000	-3.529304000000	1.034937000000
C	-6.639422000000	-4.092399000000	0.524643000000
C	-5.096029000000	-2.699575000000	2.723505000000
C	-3.888393000000	-5.123667000000	1.205428000000
C	4.308092000000	-5.231771000000	0.897266000000
C	2.037463000000	-4.414899000000	2.737787000000
C	4.423840000000	1.298371000000	3.261195000000
C	5.594691000000	4.055213000000	2.644783000000
C	7.808771000000	-2.656561000000	-0.599679000000
C	6.869483000000	-2.416738000000	-2.929946000000
Si	1.839646000000	-3.508213000000	-1.268680000000
C	0.960689000000	-2.257070000000	-2.364863000000
C	3.093568000000	-4.398963000000	-2.373333000000
C	0.563687000000	-4.760013000000	-0.641202000000
Si	5.317105000000	3.469522000000	-0.966942000000
C	7.207423000000	3.637012000000	-0.877867000000
C	4.921789000000	2.997735000000	-2.758702000000
C	4.618617000000	5.190722000000	-0.602647000000
H	-0.978300000000	2.347899000000	-2.788892000000
H	-2.237713000000	1.157450000000	-2.545759000000
H	0.409984000000	0.620521000000	-4.034839000000
H	-1.193293000000	0.872013000000	-4.771283000000
H	-0.871605000000	-0.568424000000	-3.781452000000
H	1.314388000000	2.084092000000	-2.927546000000
H	2.642249000000	1.935799000000	-1.799453000000
H	0.281757000000	3.898481000000	-1.487872000000
H	1.922038000000	4.334102000000	-2.019860000000
H	1.635796000000	3.760027000000	-0.356110000000
H	-5.572028000000	2.798100000000	0.353432000000
H	-6.450183000000	-1.370889000000	0.092389000000
H	-4.876870000000	3.172462000000	2.755719000000
H	-4.921879000000	4.763411000000	1.955751000000
H	-4.028433000000	4.558399000000	3.481761000000
H	-1.302934000000	5.536665000000	2.370365000000
H	-2.125796000000	5.948787000000	0.848342000000
H	-0.690144000000	4.890813000000	0.828472000000
H	-0.784289000000	2.126016000000	2.295342000000
H	-2.325297000000	1.472505000000	2.879065000000
H	-1.571923000000	2.852221000000	3.720527000000
H	-4.432278000000	5.939817000000	-0.067362000000
H	-5.786128000000	4.825467000000	-0.379805000000
H	-5.195414000000	5.891191000000	-1.671107000000
H	-2.633566000000	5.730136000000	-2.882426000000
H	-1.554872000000	4.321695000000	-2.822867000000
H	-1.602308000000	5.464336000000	-1.457979000000
H	-5.394834000000	2.475826000000	-2.448297000000

H	-3.852065000000	2.282746000000	-3.310821000000
H	-4.858024000000	3.721711000000	-3.607654000000
H	-5.688982000000	-1.776044000000	2.637412000000
H	-4.136116000000	-2.437280000000	3.188878000000
H	-5.626854000000	-3.384462000000	3.405888000000
H	-2.814777000000	-4.946093000000	1.356178000000
H	-4.001976000000	-5.763947000000	0.318164000000
H	-4.258140000000	-5.693123000000	2.074880000000
H	-7.014908000000	-4.783008000000	1.298804000000
H	-6.642308000000	-4.639059000000	-0.430911000000
H	-7.362593000000	-3.265934000000	0.445633000000
H	-3.313009000000	-2.151952000000	-4.225814000000
H	-2.116486000000	-2.149980000000	-2.902759000000
H	-3.285246000000	-0.815535000000	-3.046863000000
H	-4.042556000000	-4.917076000000	-3.402457000000
H	-4.796989000000	-5.331201000000	-1.846627000000
H	-3.050863000000	-4.981762000000	-1.924742000000
H	-6.275311000000	-1.322356000000	-2.578856000000
H	-6.893945000000	-2.900004000000	-2.033012000000
H	-6.244959000000	-2.721734000000	-3.682235000000
H	-8.014368000000	1.478465000000	-1.673469000000
H	-7.575360000000	2.934689000000	-0.752221000000
H	-9.212362000000	2.254599000000	-0.602058000000
H	-8.930236000000	2.113286000000	1.950088000000
H	-7.290503000000	2.789758000000	1.819722000000
H	-7.540826000000	1.235347000000	2.645917000000
H	-8.510097000000	-0.726247000000	-0.452186000000
H	-9.628622000000	0.130818000000	0.629780000000
H	-8.302206000000	-0.833336000000	1.315651000000
H	-1.982960000000	2.499560000000	-0.392714000000
H	-2.967573000000	-2.508415000000	-0.111624000000
H	0.839143000000	-1.527650000000	3.530910000000
H	2.297651000000	-0.719155000000	2.993085000000
H	-0.096860000000	0.638298000000	4.378566000000
H	1.531672000000	0.363570000000	5.058199000000
H	1.288168000000	1.517983000000	3.723491000000
H	-1.407673000000	-0.900640000000	3.513615000000
H	-2.658757000000	-1.065085000000	2.294646000000
H	-0.374557000000	-3.083294000000	2.766170000000
H	-2.083442000000	-3.320587000000	3.190384000000
H	-1.581791000000	-3.217831000000	1.488226000000
H	4.929870000000	-3.026528000000	-0.910049000000
H	6.542965000000	0.925786000000	-0.852435000000
H	3.735574000000	-3.672827000000	-2.895922000000
H	3.740806000000	-5.106095000000	-1.835615000000
H	2.541164000000	-4.965188000000	-3.142546000000
H	-0.015018000000	-5.164183000000	-1.488772000000
H	1.029546000000	-5.610731000000	-0.118759000000
H	-0.146131000000	-4.282278000000	0.052786000000
H	0.081422000000	-1.836759000000	-1.854845000000
H	1.619750000000	-1.415591000000	-2.628165000000
H	0.618653000000	-2.732760000000	-3.299032000000
H	3.638575000000	-5.917565000000	0.354380000000
H	5.132368000000	-4.953162000000	0.222978000000
H	4.745365000000	-5.793737000000	1.739659000000
H	2.477816000000	-5.179700000000	3.399336000000
H	1.625260000000	-3.621779000000	3.379036000000
H	1.205719000000	-4.881043000000	2.189705000000
H	5.385632000000	-2.283226000000	2.038462000000
H	4.088947000000	-1.948965000000	3.210247000000
H	5.079434000000	-3.415668000000	3.385478000000

H	5.050790000000	1.917598000000	-2.929448000000
H	3.895759000000	3.267997000000	-3.047605000000
H	5.610241000000	3.533713000000	-3.433210000000
H	3.522538000000	5.185700000000	-0.518027000000
H	5.027705000000	5.606761000000	0.329848000000
H	4.888979000000	5.877838000000	-1.422151000000
H	7.515155000000	4.404521000000	-1.608197000000
H	7.559712000000	3.965743000000	0.111683000000
H	7.739365000000	2.708054000000	-1.136792000000
H	4.909412000000	1.303521000000	4.251295000000
H	3.413457000000	1.716568000000	3.372382000000
H	4.328799000000	0.253671000000	2.932528000000
H	5.937968000000	4.045144000000	3.692850000000
H	6.314271000000	4.653664000000	2.065295000000
H	4.621445000000	4.571722000000	2.616390000000
H	7.080444000000	0.398735000000	1.751941000000
H	7.847138000000	1.926489000000	1.254845000000
H	7.623283000000	1.565523000000	2.984237000000
H	8.034865000000	-2.147995000000	0.351254000000
H	7.133299000000	-3.496627000000	-0.377559000000
H	8.748087000000	-3.076119000000	-0.996345000000
H	7.794054000000	-2.823023000000	-3.372032000000
H	6.179369000000	-3.258682000000	-2.770780000000
H	6.407838000000	-1.737575000000	-3.664338000000
H	8.513303000000	-0.030026000000	-1.001245000000
H	9.118305000000	-1.008129000000	-2.353906000000
H	7.816223000000	0.171478000000	-2.630394000000
H	1.734723000000	-2.144274000000	0.718763000000
H	3.561482000000	2.572762000000	0.516755000000

1-Ge (T₁)

$G_{qh} = -8823.718938$

$N_{imag} = 0$

$G_{B3LYP-D3/TZVPP} = -8827.695514$

C	4.575969000000	0.783357000000	-0.069952000000
C	3.521074000000	-0.166622000000	0.071215000000
C	3.822385000000	-1.548039000000	-0.129675000000
C	5.107324000000	-1.908792000000	-0.570079000000
C	6.137483000000	-0.986332000000	-0.768312000000
C	5.847519000000	0.347440000000	-0.490500000000
Ge	1.656918000000	0.492601000000	0.427722000000
C	0.520768000000	-0.626769000000	1.588321000000
C	1.138095000000	-0.980142000000	2.936192000000
C	0.789672000000	0.013098000000	4.054735000000
C	2.869905000000	-2.693854000000	0.170281000000
Si	3.595711000000	-3.829798000000	1.548487000000
C	4.675044000000	-2.813404000000	2.723927000000
C	7.526406000000	-1.464185000000	-1.221651000000
C	8.506845000000	-0.294180000000	-1.418112000000
C	4.463462000000	2.254575000000	0.300742000000
Si	5.115076000000	2.460595000000	2.104876000000
C	6.870301000000	1.784800000000	2.302182000000
C	0.764495000000	0.952334000000	-1.276716000000
C	1.619724000000	1.808733000000	-2.195879000000
C	1.404547000000	3.306032000000	-1.932945000000
C	-0.520311000000	0.629036000000	-1.586250000000
C	-1.137784000000	0.983208000000	-2.933848000000
C	-0.788417000000	-0.008435000000	-4.053505000000
Ge	-1.656056000000	-0.491073000000	-0.426017000000
C	-0.764177000000	-0.949721000000	1.278974000000
C	-1.619881000000	-1.804851000000	2.198898000000

C	-1.404874000000	-3.302512000000	1.937949000000
C	-3.521004000000	0.166791000000	-0.071226000000
C	-3.823578000000	1.548040000000	0.128954000000
C	-5.109309000000	1.907964000000	0.567720000000
C	-6.139062000000	0.984826000000	0.764859000000
C	-5.847754000000	-0.348811000000	0.487829000000
C	-4.575339000000	-0.783942000000	0.069097000000
C	-2.871549000000	2.694540000000	-0.169846000000
Si	-3.596735000000	3.830609000000	-1.548276000000
C	-4.674400000000	2.814016000000	-2.725091000000
C	-7.528894000000	1.461797000000	1.216326000000
C	-8.508866000000	0.291174000000	1.411430000000
C	-4.461186000000	-2.255332000000	-0.300441000000
Si	-5.110337000000	-2.463390000000	-2.105208000000
C	-6.865369000000	-1.787968000000	-2.305358000000
C	-4.665291000000	5.247375000000	-0.877115000000
C	-2.216985000000	4.643872000000	-2.556022000000
C	-4.000470000000	-1.483323000000	-3.270670000000
C	-5.058923000000	-4.278282000000	-2.643319000000
C	-8.109758000000	2.408728000000	0.141525000000
C	-7.401371000000	2.219192000000	2.556632000000
Si	-2.259824000000	3.590729000000	1.410306000000
C	-1.314252000000	2.360598000000	2.475939000000
C	-3.658820000000	4.291908000000	2.475154000000
C	-1.084002000000	4.992524000000	0.923282000000
Si	-5.230701000000	-3.508402000000	0.944990000000
C	-7.080242000000	-3.835719000000	0.659969000000
C	-5.076168000000	-2.906362000000	2.732853000000
C	-4.370017000000	-5.184371000000	0.760458000000
C	4.662743000000	-5.247466000000	0.876842000000
C	2.216401000000	-4.641503000000	2.558072000000
C	4.006861000000	1.479158000000	3.270755000000
C	5.064539000000	4.274947000000	2.644873000000
C	8.108115000000	-2.411443000000	-0.147594000000
C	7.396611000000	-2.221547000000	-2.561757000000
Si	2.256143000000	-3.590347000000	-1.408914000000
C	1.309821000000	-2.360313000000	-2.473999000000
C	3.653684000000	-4.292469000000	-2.475068000000
C	1.080339000000	-4.991572000000	-0.920209000000
Si	5.232362000000	3.508105000000	-0.944610000000
C	7.082453000000	3.833946000000	-0.661503000000
C	5.075271000000	2.907684000000	-2.732810000000
C	4.372977000000	5.184463000000	-0.757660000000
H	-0.830652000000	1.993604000000	-3.242546000000
H	-2.232786000000	1.027513000000	-2.832297000000
H	0.292739000000	-0.020398000000	-4.256102000000
H	-1.314178000000	0.253195000000	-4.985972000000
H	-1.073851000000	-1.033261000000	-3.780077000000
H	1.412295000000	1.588604000000	-3.254428000000
H	2.681484000000	1.559915000000	-2.046595000000
H	0.360921000000	3.594426000000	-2.115215000000
H	2.046077000000	3.929342000000	-2.574455000000
H	1.630426000000	3.553474000000	-0.884367000000
H	-5.314227000000	2.964071000000	0.733387000000
H	-6.633962000000	-1.093313000000	0.571448000000
H	-4.275874000000	3.481563000000	2.893472000000
H	-4.320906000000	4.981159000000	1.930885000000
H	-3.217815000000	4.845864000000	3.321258000000
H	-0.606217000000	5.411160000000	1.824740000000
H	-1.602084000000	5.816542000000	0.407536000000
H	-0.285301000000	4.623219000000	0.260206000000

H	-0.384098000000	2.041134000000	1.984501000000
H	-1.910048000000	1.454609000000	2.666992000000
H	-1.048821000000	2.807927000000	3.448103000000
H	-4.084284000000	5.938787000000	-0.246469000000
H	-5.529100000000	4.896703000000	-0.291834000000
H	-5.057603000000	5.827410000000	-1.729348000000
H	-2.660156000000	5.377623000000	-3.250132000000
H	-1.669272000000	3.906453000000	-3.160615000000
H	-1.491823000000	5.176207000000	-1.923301000000
H	-5.520190000000	2.351626000000	-2.193602000000
H	-4.101716000000	2.007327000000	-3.208075000000
H	-5.078368000000	3.462563000000	-3.520337000000
H	-5.412830000000	-1.862944000000	2.832855000000
H	-4.046792000000	-2.966853000000	3.112893000000
H	-5.709965000000	-3.533298000000	3.382204000000
H	-3.275081000000	-5.103978000000	0.814812000000
H	-4.626546000000	-5.666981000000	-0.194246000000
H	-4.697276000000	-5.855811000000	1.572174000000
H	-7.411815000000	-4.589548000000	1.394066000000
H	-7.288793000000	-4.239915000000	-0.342424000000
H	-7.707814000000	-2.942161000000	0.802981000000
H	-4.357991000000	-1.566380000000	-4.310450000000
H	-2.964439000000	-1.851048000000	-3.234735000000
H	-3.993800000000	-0.418489000000	-2.994528000000
H	-5.280414000000	-4.344938000000	-3.721689000000
H	-5.795883000000	-4.901294000000	-2.113618000000
H	-4.061296000000	-4.717212000000	-2.479019000000
H	-6.884644000000	-0.703824000000	-2.113908000000
H	-7.593842000000	-2.264487000000	-1.633553000000
H	-7.200796000000	-1.955260000000	-3.342905000000
H	-8.201185000000	1.891695000000	-0.827119000000
H	-7.472286000000	3.292936000000	-0.010228000000
H	-9.110995000000	2.763336000000	0.437220000000
H	-8.389958000000	2.566927000000	2.898983000000
H	-6.749754000000	3.101396000000	2.468723000000
H	-6.978480000000	1.566097000000	3.336660000000
H	-8.675870000000	-0.263006000000	0.474568000000
H	-9.485573000000	0.672060000000	1.748853000000
H	-8.147198000000	-0.420138000000	2.170541000000
H	-1.933062000000	2.305065000000	-0.598096000000
H	-3.394898000000	-2.539973000000	-0.381556000000
H	0.830104000000	-1.989915000000	3.246087000000
H	2.233051000000	-1.025492000000	2.834563000000
H	-0.291420000000	0.025971000000	4.257601000000
H	1.315572000000	-0.247626000000	4.987375000000
H	1.075590000000	1.037439000000	3.779889000000
H	-1.412759000000	-1.583361000000	3.257230000000
H	-2.681561000000	-1.556059000000	2.048916000000
H	-0.361409000000	-3.590901000000	2.121082000000
H	-2.046869000000	-3.924928000000	2.579862000000
H	-1.630260000000	-3.551174000000	0.889568000000
H	5.311322000000	-2.965012000000	-0.736151000000
H	6.634172000000	1.091397000000	-0.574857000000
H	4.270428000000	-3.482531000000	-2.894627000000
H	4.316262000000	-4.981591000000	-1.931237000000
H	3.211477000000	-4.846783000000	-3.320311000000
H	0.601397000000	-5.410234000000	-1.821042000000
H	1.598652000000	-5.815671000000	-0.404825000000
H	0.282520000000	-4.621779000000	-0.256353000000
H	0.379710000000	-2.041301000000	-1.982132000000
H	1.905176000000	-1.454057000000	-2.665128000000

H	1.044153000000	-2.807575000000	-3.446130000000
H	4.080769000000	-5.938700000000	0.246897000000
H	5.526247000000	-4.897461000000	0.290712000000
H	5.055455000000	-5.827495000000	1.728894000000
H	2.659715000000	-5.374963000000	3.252397000000
H	1.669787000000	-3.903166000000	3.162546000000
H	1.490273000000	-5.173859000000	1.926480000000
H	5.519874000000	-2.350525000000	2.191342000000
H	4.102831000000	-2.007158000000	3.208197000000
H	5.080425000000	-3.462188000000	3.518261000000
H	5.409551000000	1.863599000000	-2.833842000000
H	4.045751000000	2.970765000000	-3.112048000000
H	5.709972000000	3.533702000000	-3.382162000000
H	3.277942000000	5.104789000000	-0.811128000000
H	4.630649000000	5.665949000000	0.197303000000
H	4.699944000000	5.856504000000	-1.568996000000
H	7.413716000000	4.587964000000	-1.395544000000
H	7.292414000000	4.237425000000	0.340885000000
H	7.709239000000	2.940032000000	-0.805734000000
H	4.365639000000	1.561381000000	4.310168000000
H	2.970623000000	1.846419000000	3.236454000000
H	4.000399000000	0.414597000000	2.993577000000
H	5.287358000000	4.340552000000	3.723033000000
H	5.800947000000	4.898347000000	2.114856000000
H	4.066781000000	4.714181000000	2.482193000000
H	6.889215000000	0.700833000000	2.109694000000
H	7.598080000000	2.261866000000	1.630020000000
H	7.206934000000	1.951044000000	3.339509000000
H	8.201139000000	-1.894435000000	0.820911000000
H	7.470292000000	-3.295249000000	0.005029000000
H	9.108741000000	-2.766678000000	-0.444603000000
H	8.384521000000	-2.569912000000	-2.905420000000
H	6.744567000000	-3.103344000000	-2.472937000000
H	6.973081000000	-1.568219000000	-3.341242000000
H	8.675501000000	0.259890000000	-0.481481000000
H	9.482842000000	-0.675684000000	-1.756886000000
H	8.144569000000	0.417363000000	-2.176717000000
H	1.932094000000	-2.303640000000	0.599348000000
H	3.397497000000	2.539978000000	0.383506000000

1-Sn (CSS)

$G_{qh} = -5098.868593$

$N_{imag} = 0$

$G_{B3LYP-D3/TZVP} = -5102.341811$

C	-4.854495000000	0.757553000000	0.070872000000
C	-3.791915000000	-0.175589000000	-0.055997000000
C	-4.061458000000	-1.558710000000	0.141572000000
C	-5.348891000000	-1.948175000000	0.550160000000
C	-6.400963000000	-1.042661000000	0.721224000000
C	-6.130268000000	0.299491000000	0.458669000000
Sn	-1.735388000000	0.576038000000	-0.443253000000
C	-0.517931000000	-0.646185000000	-1.757021000000
C	-1.136087000000	-0.896257000000	-3.126353000000
C	-0.835781000000	0.201138000000	-4.157705000000
C	-3.060345000000	-2.666668000000	-0.132776000000
Si	-3.675170000000	-3.804071000000	-1.558678000000
C	-4.738485000000	-2.796444000000	-2.754933000000
C	-7.791817000000	-1.548831000000	1.138338000000
C	-8.803182000000	-0.400239000000	1.301550000000
C	-4.735994000000	2.232525000000	-0.278263000000
Si	-5.364809000000	2.481647000000	-2.082746000000

C	-7.139755000000	1.867240000000	-2.298006000000
C	-0.786955000000	0.914539000000	1.480268000000
C	-1.687266000000	1.693044000000	2.427305000000
C	-1.539579000000	3.213073000000	2.271817000000
C	0.517891000000	0.646570000000	1.756992000000
C	1.136067000000	0.896728000000	3.126302000000
C	0.835619000000	-0.200536000000	4.157754000000
Sn	1.735305000000	-0.575854000000	0.443331000000
C	0.786915000000	-0.914143000000	-1.480271000000
C	1.687230000000	-1.692644000000	-2.427310000000
C	1.539541000000	-3.212676000000	-2.271827000000
C	3.791911000000	0.175578000000	0.056085000000
C	4.061580000000	1.558665000000	-0.141552000000
C	5.349050000000	1.947998000000	-0.550152000000
C	6.401047000000	1.042384000000	-0.721149000000
C	6.130228000000	-0.299730000000	-0.458538000000
C	4.854407000000	-0.757667000000	-0.070745000000
C	3.060534000000	2.666725000000	0.132655000000
Si	3.675387000000	3.804212000000	1.558483000000
C	4.738586000000	2.796630000000	2.754874000000
C	7.791950000000	1.548411000000	-1.138274000000
C	8.803200000000	0.399716000000	-1.301480000000
C	4.735776000000	-2.232626000000	0.278395000000
Si	5.364558000000	-2.481783000000	2.082875000000
C	7.139562000000	-1.867545000000	2.298138000000
C	4.711553000000	5.277144000000	0.966496000000
C	2.202181000000	4.509887000000	2.510626000000
C	4.280779000000	-1.474077000000	3.254739000000
C	5.250539000000	-4.302001000000	2.590515000000
C	8.323664000000	2.513530000000	-0.054284000000
C	7.683079000000	2.296032000000	-2.485809000000
Si	2.462049000000	3.548061000000	-1.459285000000
C	1.693408000000	2.270834000000	-2.610256000000
C	3.851359000000	4.393693000000	-2.428037000000
C	1.143687000000	4.826396000000	-0.997785000000
Si	5.475184000000	-3.461541000000	-1.004858000000
C	7.310001000000	-3.854711000000	-0.719422000000
C	5.338978000000	-2.775743000000	-2.761395000000
C	4.536769000000	-5.099960000000	-0.887804000000
C	-4.711199000000	-5.277136000000	-0.966790000000
C	-2.201946000000	-4.509546000000	-2.510943000000
C	-4.280938000000	1.474055000000	-3.254625000000
C	-5.250965000000	4.301879000000	-2.590373000000
C	-8.323425000000	-2.513993000000	0.054335000000
C	-7.682883000000	-2.296454000000	2.485867000000
Si	-2.461710000000	-3.548101000000	1.459055000000
C	-1.693002000000	-2.270941000000	2.610054000000
C	-3.850932000000	-4.393828000000	2.427854000000
C	-1.143369000000	-4.826380000000	0.997360000000
Si	-5.475484000000	3.461380000000	1.004995000000
C	-7.310392000000	3.854235000000	0.719714000000
C	-5.338983000000	2.775698000000	2.761556000000
C	-4.537368000000	5.099956000000	0.887764000000
H	0.779696000000	1.861511000000	3.522399000000
H	2.229053000000	0.999326000000	3.029405000000
H	-0.243908000000	-0.285567000000	4.351676000000
H	1.347457000000	0.005782000000	5.111717000000
H	1.174688000000	-1.183375000000	3.797362000000
H	-1.476313000000	1.410381000000	3.471851000000
H	-2.738507000000	1.411172000000	2.249357000000
H	-0.515769000000	3.541473000000	2.498475000000

H	-2.229845000000	3.757886000000	2.935009000000
H	-1.754109000000	3.517649000000	1.234993000000
H	5.536301000000	3.008990000000	-0.710944000000
H	6.930555000000	-1.031369000000	-0.532740000000
H	4.552251000000	3.647423000000	-2.833833000000
H	4.427076000000	5.116757000000	-1.832469000000
H	3.411522000000	4.934853000000	-3.283012000000
H	0.666341000000	5.224836000000	-1.908507000000
H	1.565756000000	5.679163000000	-0.442287000000
H	0.355105000000	4.370157000000	-0.376438000000
H	0.779626000000	1.837382000000	-2.180930000000
H	2.392205000000	1.441832000000	-2.805364000000
H	1.427991000000	2.730362000000	-3.576891000000
H	4.124509000000	5.967093000000	0.339717000000
H	5.601864000000	4.970497000000	0.395787000000
H	5.060773000000	5.843738000000	1.846099000000
H	2.554078000000	5.244159000000	3.254432000000
H	1.671816000000	3.714149000000	3.052842000000
H	1.479648000000	5.013946000000	1.852195000000
H	5.634044000000	2.399683000000	2.252473000000
H	4.180374000000	1.940843000000	3.165008000000
H	5.063891000000	3.424860000000	3.600775000000
H	5.839437000000	-1.798727000000	-2.844725000000
H	4.294967000000	-2.644189000000	-3.078863000000
H	5.822213000000	-3.470876000000	-3.468298000000
H	3.456488000000	-4.965073000000	-1.044944000000
H	4.679168000000	-5.581709000000	0.091306000000
H	4.902971000000	-5.796533000000	-1.660594000000
H	7.636795000000	-4.575886000000	-1.487576000000
H	7.495039000000	-4.314109000000	0.263879000000
H	7.956669000000	-2.967396000000	-0.806377000000
H	4.652954000000	-1.553644000000	4.289687000000
H	3.237224000000	-1.824294000000	3.244168000000
H	4.288125000000	-0.411058000000	2.969508000000
H	5.485736000000	-4.401524000000	3.663393000000
H	5.954573000000	-4.940638000000	2.034858000000
H	4.234235000000	-4.698712000000	2.432673000000
H	7.197944000000	-0.784440000000	2.109011000000
H	7.853611000000	-2.368938000000	1.628747000000
H	7.463658000000	-2.048614000000	3.336920000000
H	8.402685000000	2.003097000000	0.918973000000
H	7.662335000000	3.383458000000	0.077043000000
H	9.323586000000	2.890009000000	-0.326586000000
H	8.672364000000	2.663717000000	-2.804642000000
H	7.010444000000	3.164320000000	-2.419345000000
H	7.294630000000	1.629932000000	-3.272711000000
H	8.954649000000	-0.149034000000	-0.358777000000
H	9.780649000000	0.801764000000	-1.611188000000
H	8.480373000000	-0.320910000000	-2.069309000000
H	2.127580000000	2.232013000000	0.534462000000
H	3.665970000000	-2.515535000000	0.339195000000
H	-0.779628000000	-1.860970000000	-3.522542000000
H	-2.229060000000	-0.998975000000	-3.029448000000
H	0.243731000000	0.286316000000	-4.351646000000
H	-1.347615000000	-0.005158000000	-5.111675000000
H	-1.174967000000	1.183902000000	-3.797224000000
H	1.476295000000	-1.409980000000	-3.471857000000
H	2.738470000000	-1.410776000000	-2.249344000000
H	0.515733000000	-3.541069000000	-2.498503000000
H	2.229817000000	-3.757496000000	-2.935005000000
H	1.754056000000	-3.517247000000	-1.235001000000

H	-5.536052000000	-3.009194000000	0.710889000000
H	-6.930661000000	1.031052000000	0.532907000000
H	-4.551804000000	-3.647599000000	2.833757000000
H	-4.426684000000	-5.116854000000	1.832273000000
H	-3.411027000000	-4.935048000000	3.282756000000
H	-0.665981000000	-5.224907000000	1.908023000000
H	-1.565466000000	-5.679095000000	0.441802000000
H	-0.354818000000	-4.370081000000	0.376019000000
H	-0.779262000000	-1.837440000000	2.180689000000
H	-2.391800000000	-1.441970000000	2.805285000000
H	-1.427487000000	-2.730535000000	3.576632000000
H	-4.124087000000	-5.967092000000	-0.340083000000
H	-5.601523000000	-4.970609000000	-0.396036000000
H	-5.060392000000	-5.843683000000	-1.846435000000
H	-2.553814000000	-5.243794000000	-3.254786000000
H	-1.671683000000	-3.713718000000	-3.053130000000
H	-1.479329000000	-5.013587000000	-1.852590000000
H	-5.633941000000	-2.399583000000	-2.252463000000
H	-4.180334000000	-1.940596000000	-3.165024000000
H	-5.063797000000	-3.424621000000	-3.600872000000
H	-5.839141000000	1.798534000000	2.844959000000
H	-4.294915000000	2.644481000000	3.078982000000
H	-5.822395000000	3.470718000000	3.468448000000
H	-3.457037000000	4.965263000000	1.044727000000
H	-4.680017000000	5.581673000000	-0.091326000000
H	-4.903568000000	5.796469000000	1.660609000000
H	-7.637226000000	4.575397000000	1.487863000000
H	-7.495595000000	4.313557000000	-0.263592000000
H	-7.956919000000	2.966827000000	0.806773000000
H	-4.653132000000	1.553591000000	-4.289569000000
H	-3.237418000000	1.824375000000	-3.244062000000
H	-4.288175000000	0.411030000000	-2.969404000000
H	-5.486136000000	4.401382000000	-3.663258000000
H	-5.955087000000	4.940436000000	-2.034736000000
H	-4.234709000000	4.698703000000	-2.432494000000
H	-7.198033000000	0.784129000000	-2.108888000000
H	-7.853850000000	2.368559000000	-1.628611000000
H	-7.463871000000	2.048288000000	-3.336785000000
H	-8.402494000000	-2.003558000000	-0.918918000000
H	-7.662003000000	-3.383850000000	-0.076998000000
H	-9.323309000000	-2.890580000000	0.326627000000
H	-8.672135000000	-2.664233000000	2.804691000000
H	-7.010169000000	-3.164681000000	2.419400000000
H	-7.294501000000	-1.630325000000	3.272777000000
H	-8.954707000000	0.148484000000	0.358844000000
H	-9.780583000000	-0.802384000000	1.611282000000
H	-8.480412000000	0.320431000000	2.069364000000
H	-2.127446000000	-2.231850000000	-0.534597000000
H	-3.666210000000	2.515513000000	-0.339069000000

1-Sn (T₁)

G_{qh} = -5098.859156

N_{imag} = 0

G_{B3LYP-D3/TZVPP} = -5102.333019

C	-4.877968000000	0.717588000000	0.068472000000
C	-3.790522000000	-0.186454000000	-0.060949000000
C	-4.023966000000	-1.576004000000	0.134322000000
C	-5.298939000000	-2.001733000000	0.545215000000
C	-6.374751000000	-1.125068000000	0.719517000000
C	-6.140379000000	0.223841000000	0.456958000000
Sn	-1.751350000000	0.627270000000	-0.456548000000

C	-0.500286000000	-0.589713000000	-1.791080000000
C	-1.119793000000	-0.830188000000	-3.162616000000
C	-0.854991000000	0.299486000000	-4.168665000000
C	-2.993595000000	-2.655662000000	-0.142722000000
Si	-3.574307000000	-3.785744000000	-1.590351000000
C	-4.637574000000	-2.776969000000	-2.785741000000
C	-7.750712000000	-1.667948000000	1.139641000000
C	-8.790386000000	-0.546082000000	1.310891000000
C	-4.800412000000	2.196597000000	-0.271969000000
Si	-5.442306000000	2.444435000000	-2.070917000000
C	-7.205103000000	1.794588000000	-2.282997000000
C	-0.774779000000	0.933534000000	1.494340000000
C	-1.680221000000	1.669688000000	2.469646000000
C	-1.627025000000	3.192351000000	2.283800000000
C	0.500588000000	0.588429000000	1.792189000000
C	1.120032000000	0.828568000000	3.163812000000
C	0.855938000000	-0.301776000000	4.169307000000
Sn	1.752003000000	-0.628012000000	0.457431000000
C	0.774966000000	-0.935161000000	-1.493118000000
C	1.680070000000	-1.672275000000	-2.467993000000
C	1.626194000000	-3.194797000000	-2.281107000000
C	3.790630000000	0.186549000000	0.060812000000
C	4.023378000000	1.576186000000	-0.134670000000
C	5.297969000000	2.002464000000	-0.546135000000
C	6.374075000000	1.126240000000	-0.720924000000
C	6.140401000000	-0.222755000000	-0.458204000000
C	4.878392000000	-0.717028000000	-0.069052000000
C	2.992648000000	2.655363000000	0.142863000000
Si	3.573324000000	3.785354000000	1.590536000000
C	4.637049000000	2.776657000000	2.785595000000
C	7.749639000000	1.669699000000	-1.141597000000
C	8.789694000000	0.548267000000	-1.313374000000
C	4.801637000000	-2.196023000000	0.271649000000
Si	5.444565000000	-2.443149000000	2.070362000000
C	7.207143000000	-1.792366000000	2.281414000000
C	4.600291000000	5.282446000000	1.045822000000
C	2.077601000000	4.463320000000	2.525782000000
C	4.343871000000	-1.469059000000	3.255204000000
C	5.373764000000	-4.269937000000	2.562150000000
C	8.260265000000	2.644137000000	-0.055799000000
C	7.616221000000	2.419248000000	-2.485823000000
Si	2.380674000000	3.528681000000	-1.449689000000
C	1.851519000000	2.215425000000	-2.691104000000
C	3.694511000000	4.576941000000	-2.321018000000
C	0.894466000000	4.613243000000	-1.003330000000
Si	5.559234000000	-3.393717000000	-1.028571000000
C	7.404006000000	-3.750364000000	-0.760499000000
C	5.393260000000	-2.686046000000	-2.773538000000
C	4.656942000000	-5.053254000000	-0.923849000000
C	-4.601750000000	-5.282485000000	-1.045533000000
C	-2.078648000000	-4.464373000000	-2.525219000000
C	-4.341453000000	1.470105000000	-3.255415000000
C	-5.370311000000	4.271298000000	-2.562231000000
C	-8.261313000000	-2.642279000000	0.053742000000
C	-7.618115000000	-2.417425000000	2.483993000000
Si	-2.382756000000	-3.529199000000	1.450146000000
C	-1.851496000000	-2.216286000000	2.691017000000
C	-3.698268000000	-4.574975000000	2.321947000000
C	-0.898235000000	-4.616232000000	1.004172000000
Si	-5.558080000000	3.394327000000	1.028165000000
C	-7.402411000000	3.752426000000	0.759045000000

C	-5.393841000000	2.685729000000	2.772915000000
C	-4.654592000000	5.053291000000	0.924661000000
H	0.752481000000	1.776179000000	3.589672000000
H	2.208768000000	0.958291000000	3.055875000000
H	-0.216700000000	-0.390229000000	4.396872000000
H	1.399557000000	-0.125429000000	5.111454000000
H	1.180926000000	-1.275095000000	3.770500000000
H	-1.426611000000	1.418695000000	3.512273000000
H	-2.717273000000	1.320083000000	2.328519000000
H	-0.619030000000	3.579656000000	2.485390000000
H	-2.333721000000	3.708169000000	2.952489000000
H	-1.878945000000	3.471603000000	1.248118000000
H	5.454353000000	3.068902000000	-0.705387000000
H	6.959932000000	-0.932540000000	-0.535360000000
H	4.511377000000	3.941733000000	-2.698596000000
H	4.132901000000	5.361170000000	-1.688493000000
H	3.230129000000	5.067028000000	-3.193762000000
H	0.386813000000	4.963740000000	-1.917324000000
H	1.190749000000	5.503006000000	-0.424724000000
H	0.161128000000	4.046922000000	-0.405185000000
H	1.002165000000	1.624887000000	-2.325190000000
H	2.678968000000	1.515385000000	-2.890859000000
H	1.557896000000	2.681321000000	-3.646349000000
H	3.999381000000	6.004913000000	0.471172000000
H	5.477442000000	5.007707000000	0.439950000000
H	4.968762000000	5.801426000000	1.946830000000
H	2.409679000000	5.180239000000	3.295129000000
H	1.533417000000	3.654941000000	3.034083000000
H	1.372279000000	4.982787000000	1.860190000000
H	5.540263000000	2.395737000000	2.284480000000
H	4.088275000000	1.910597000000	3.185615000000
H	4.950085000000	3.401745000000	3.638404000000
H	5.915822000000	-1.720867000000	-2.859049000000
H	4.344464000000	-2.522469000000	-3.058727000000
H	5.838153000000	-3.383927000000	-3.502520000000
H	3.573121000000	-4.940875000000	-1.074577000000
H	4.814588000000	-5.540416000000	0.050312000000
H	5.034770000000	-5.734713000000	-1.704475000000
H	7.742842000000	-4.453048000000	-1.540484000000
H	7.604657000000	-4.219189000000	0.215348000000
H	8.029852000000	-2.847369000000	-0.838058000000
H	4.726542000000	-1.542102000000	4.286803000000
H	3.309967000000	-1.847121000000	3.250784000000
H	4.320916000000	-0.405202000000	2.973956000000
H	5.616973000000	-4.374768000000	3.632733000000
H	6.088511000000	-4.887534000000	1.996388000000
H	4.365503000000	-4.687197000000	2.405649000000
H	7.242250000000	-0.706944000000	2.099661000000
H	7.927670000000	-2.274321000000	1.604595000000
H	7.540797000000	-1.973832000000	3.317092000000
H	8.357010000000	2.131852000000	0.914877000000
H	7.576487000000	3.495504000000	0.082027000000
H	9.248664000000	3.048131000000	-0.330733000000
H	8.594431000000	2.813354000000	-2.807159000000
H	6.922375000000	3.270238000000	-2.412897000000
H	7.241385000000	1.746669000000	-3.273768000000
H	8.959761000000	0.000555000000	-0.373280000000
H	9.754879000000	0.976727000000	-1.626113000000
H	8.482188000000	-0.177999000000	-2.082187000000
H	2.067234000000	2.194779000000	0.533298000000
H	3.739910000000	-2.505283000000	0.339207000000

H	-0.752743000000	-1.778223000000	-3.587949000000
H	-2.208616000000	-0.959243000000	-3.054701000000
H	0.217695000000	0.387150000000	-4.396317000000
H	-1.398746000000	0.123011000000	-5.110710000000
H	-1.179344000000	1.273202000000	-3.770326000000
H	1.426493000000	-1.421937000000	-3.510787000000
H	2.717281000000	-1.323014000000	-2.327193000000
H	0.617953000000	-3.581729000000	-2.482180000000
H	2.332428000000	-3.711398000000	-2.949680000000
H	1.878275000000	-3.473508000000	-1.245312000000
H	-5.455845000000	-3.068096000000	0.704435000000
H	-6.959636000000	0.933984000000	0.533783000000
H	-4.513503000000	-3.938078000000	2.700200000000
H	-4.138777000000	-5.358062000000	1.689477000000
H	-3.234393000000	-5.066336000000	3.194246000000
H	-0.391257000000	-4.967486000000	1.918248000000
H	-1.195946000000	-5.505571000000	0.425646000000
H	-0.163891000000	-4.051196000000	0.406033000000
H	-1.000711000000	-1.627748000000	2.325217000000
H	-2.677601000000	-1.514398000000	2.889851000000
H	-1.559415000000	-2.682184000000	3.646733000000
H	-4.001283000000	-6.004693000000	-0.470086000000
H	-5.479297000000	-5.007356000000	-0.440413000000
H	-4.969662000000	-5.801911000000	-1.946510000000
H	-2.410783000000	-5.181270000000	-3.294559000000
H	-1.534028000000	-3.656278000000	-3.033496000000
H	-1.373706000000	-4.984028000000	-1.859384000000
H	-5.541180000000	-2.396449000000	-2.285029000000
H	-4.088821000000	-1.910612000000	-3.185156000000
H	-4.949938000000	-3.401894000000	-3.638917000000
H	-5.920041000000	1.722529000000	2.858448000000
H	-4.345537000000	2.517986000000	3.057467000000
H	-5.835667000000	3.385115000000	3.502318000000
H	-3.571013000000	4.940284000000	1.076639000000
H	-4.810819000000	5.540627000000	-0.049646000000
H	-5.032933000000	5.734910000000	1.704901000000
H	-7.741280000000	4.454877000000	1.539227000000
H	-7.602093000000	4.221972000000	-0.216654000000
H	-8.028918000000	2.849809000000	0.835656000000
H	-4.723619000000	1.543454000000	-4.287181000000
H	-3.307434000000	1.847844000000	-3.250449000000
H	-4.318949000000	0.406190000000	-2.974345000000
H	-5.613046000000	4.376485000000	-3.632889000000
H	-6.084930000000	4.889179000000	-1.996617000000
H	-4.361873000000	4.687954000000	-2.405255000000
H	-7.240860000000	0.709172000000	-2.101344000000
H	-7.925730000000	2.276867000000	-1.606514000000
H	-7.538131000000	1.976299000000	-3.318833000000
H	-8.357460000000	-2.130057000000	-0.917028000000
H	-7.577860000000	-3.493961000000	-0.083727000000
H	-9.249992000000	-3.045821000000	0.328329000000
H	-8.596604000000	-2.811119000000	2.804988000000
H	-6.924559000000	-3.268679000000	2.411409000000
H	-7.243326000000	-1.744913000000	3.272018000000
H	-8.959755000000	0.001689000000	0.370705000000
H	-9.755901000000	-0.974132000000	1.623174000000
H	-8.482962000000	0.180069000000	2.079847000000
H	-2.067824000000	-2.195545000000	-0.532842000000
H	-3.738521000000	2.505436000000	-0.338876000000

1-Sn (OSS)

G_{qh} = -5098.869845

N_{imag} = 0

G_{B3LYP-D3/TZVPP} = -5102.343152

SP = -5092.882047

G_{sp} = -5091.393968

C	-4.858638000000	-0.750356000000	-0.071784000000
C	-3.790899000000	0.177021000000	0.056522000000
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C	-5.338152000000	1.958058000000	-0.551256000000
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Si	2.446909000000	-3.547234000000	1.455663000000
C	1.696803000000	-2.267095000000	2.615514000000
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H	-2.904237000000	-1.686311000000	2.947259000000
H	-1.611303000000	-2.702983000000	3.644456000000
H	-3.871174000000	-6.039867000000	-0.677707000000
H	-5.364968000000	-5.071159000000	-0.584425000000
H	-4.849337000000	-5.768103000000	-2.136592000000
H	-2.226645000000	-4.940771000000	-3.460245000000
H	-1.351436000000	-3.481263000000	-2.934069000000
H	-1.296717000000	-4.956122000000	-1.940731000000
H	-5.465501000000	-2.371237000000	-2.336878000000
H	-4.007224000000	-1.829243000000	-3.193734000000
H	-4.837882000000	-3.314327000000	-3.720251000000
H	-5.989306000000	1.547810000000	2.918094000000
H	-4.461118000000	2.433394000000	3.097077000000
H	-5.990712000000	3.205083000000	3.583873000000
H	-3.845087000000	4.900927000000	1.094444000000
H	-5.172740000000	5.469668000000	0.056015000000
H	-5.307956000000	5.600386000000	1.824577000000
H	-7.984503000000	4.208811000000	1.640767000000

H	-7.848701000000	3.989495000000	-0.117060000000
H	-8.200514000000	2.594298000000	0.932713000000
H	-4.807822000000	1.540032000000	-4.237243000000
H	-3.415841000000	1.911056000000	-3.194639000000
H	-4.346906000000	0.409849000000	-2.937525000000
H	-5.853293000000	4.307598000000	-3.541370000000
H	-6.376654000000	4.762020000000	-1.903694000000
H	-4.639644000000	4.671246000000	-2.290788000000
H	-7.291688000000	0.530973000000	-2.087432000000
H	-8.059411000000	2.047722000000	-1.558590000000
H	-7.658228000000	1.807572000000	-3.277828000000
H	-8.363306000000	-2.343341000000	-0.901189000000
H	-7.529271000000	-3.687838000000	-0.089590000000
H	-9.215079000000	-3.308174000000	0.335924000000
H	-8.557925000000	-3.083855000000	2.810919000000
H	-6.869816000000	-3.468094000000	2.406285000000
H	-7.246849000000	-1.970009000000	3.287811000000
H	-9.038367000000	-0.252906000000	0.416831000000
H	-9.791289000000	-1.274297000000	1.659833000000
H	-8.560258000000	-0.079005000000	2.126036000000
H	-2.068115000000	-2.146896000000	-0.538029000000
H	-3.906765000000	2.461879000000	-0.257776000000

1-Pb (T₁)

$G_{qh} = -5055.949049$

$N_{imag} = 1$, -5 cm^{-1} (inverted frequency gives less than $0.1 \text{ kcal mol}^{-1}$ deviation)

$G_{B3LYP-D3/TZVPP} = -5059.423454$

C	-5.070273000000	0.605593000000	0.063308000000
C	-3.936874000000	-0.234317000000	-0.023824000000
C	-4.083808000000	-1.635616000000	0.121831000000
C	-5.355147000000	-2.151978000000	0.429097000000
C	-6.491552000000	-1.344989000000	0.554958000000
C	-6.323626000000	0.025164000000	0.355322000000
Pb	-1.807519000000	0.756941000000	-0.344303000000
C	-0.547364000000	-0.414331000000	-1.929421000000
C	-1.260650000000	-0.431538000000	-3.274986000000
C	-0.962772000000	0.796818000000	-4.145911000000
C	-2.958184000000	-2.627884000000	-0.094475000000
Si	-3.309078000000	-3.732902000000	-1.629078000000
C	-4.373793000000	-2.772415000000	-2.860736000000
C	-7.856162000000	-1.982842000000	0.865953000000
C	-8.976769000000	-0.933843000000	0.978405000000
C	-5.047778000000	2.102007000000	-0.194453000000
Si	-5.684733000000	2.459553000000	-1.970225000000
C	-7.445016000000	1.825902000000	-2.242140000000
C	-0.713712000000	0.831539000000	1.731261000000
C	-1.589832000000	1.450676000000	2.804545000000
C	-1.925658000000	2.926673000000	2.563201000000
C	0.545863000000	0.400421000000	1.922585000000
C	1.261309000000	0.418316000000	3.266799000000
C	0.967275000000	-0.811086000000	4.137478000000
Pb	1.806994000000	-0.769031000000	0.336923000000
C	0.715546000000	-0.836857000000	-1.740616000000
C	1.597913000000	-1.438306000000	-2.818895000000
C	1.947214000000	-2.913663000000	-2.593538000000
C	3.932689000000	0.233482000000	0.022892000000
C	4.076151000000	1.636938000000	-0.106779000000
C	5.342934000000	2.158470000000	-0.424054000000
C	6.479498000000	1.355227000000	-0.570360000000
C	6.316774000000	-0.016847000000	-0.380377000000
C	5.067456000000	-0.602795000000	-0.082273000000

C	2.953744000000	2.626330000000	0.139735000000
Si	3.333644000000	3.712553000000	1.681254000000
C	4.403488000000	2.729248000000	2.890444000000
C	7.839186000000	1.998931000000	-0.890599000000
C	8.959735000000	0.953068000000	-1.029727000000
C	5.051696000000	-2.101139000000	0.164989000000
Si	5.692278000000	-2.465889000000	1.938254000000
C	7.448365000000	-1.821246000000	2.210878000000
C	4.257656000000	5.321946000000	1.298631000000
C	1.702922000000	4.170512000000	2.515316000000
C	4.567007000000	-1.582437000000	3.171047000000
C	5.639045000000	-4.326312000000	2.282857000000
C	8.220080000000	2.969987000000	0.250095000000
C	7.735901000000	2.779806000000	-2.219672000000
Si	2.387046000000	3.514938000000	-1.459502000000
C	2.171744000000	2.218076000000	-2.807644000000
C	3.615286000000	4.786420000000	-2.136605000000
C	0.732046000000	4.365764000000	-1.109100000000
Si	5.823811000000	-3.146921000000	-1.248527000000
C	7.680662000000	-3.470240000000	-1.038296000000
C	5.581712000000	-2.247736000000	-2.892873000000
C	4.971626000000	-4.836207000000	-1.292556000000
C	-4.221211000000	-5.347535000000	-1.241114000000
C	-1.660742000000	-4.176529000000	-2.434957000000
C	-4.563939000000	1.560349000000	-3.195626000000
C	-5.618825000000	4.317471000000	-2.325823000000
C	-8.224391000000	-2.967031000000	-0.267643000000
C	-7.770640000000	-2.747799000000	2.205495000000
Si	-2.418278000000	-3.495725000000	1.525184000000
C	-2.221268000000	-2.179959000000	2.857665000000
C	-3.658719000000	-4.756256000000	2.200349000000
C	-0.759048000000	-4.352783000000	1.212140000000
Si	-5.814231000000	3.159480000000	1.213294000000
C	-7.670031000000	3.487784000000	1.002672000000
C	-5.571799000000	2.269346000000	2.862312000000
C	-4.955122000000	4.845488000000	1.246574000000
H	0.998761000000	1.329979000000	3.830749000000
H	2.347797000000	0.480816000000	3.100890000000
H	-0.087158000000	-0.834546000000	4.449649000000
H	1.598212000000	-0.814345000000	5.040758000000
H	1.161943000000	-1.746206000000	3.587324000000
H	-1.122238000000	1.344640000000	3.798135000000
H	-2.528186000000	0.869218000000	2.859361000000
H	-1.017689000000	3.544252000000	2.535446000000
H	-2.586689000000	3.320012000000	3.350867000000
H	-2.444486000000	3.063211000000	1.601667000000
H	5.439454000000	3.239249000000	-0.530621000000
H	7.179640000000	-0.674787000000	-0.449381000000
H	4.565567000000	4.304829000000	-2.416919000000
H	3.837502000000	5.606110000000	-1.439435000000
H	3.190457000000	5.228997000000	-3.053776000000
H	0.268542000000	4.713618000000	-2.047276000000
H	0.851943000000	5.241802000000	-0.451446000000
H	0.027469000000	3.671896000000	-0.620417000000
H	1.411748000000	1.476375000000	-2.528836000000
H	3.121571000000	1.686002000000	-2.976992000000
H	1.864084000000	2.686380000000	-3.757083000000
H	3.629548000000	6.035893000000	0.743109000000
H	5.180518000000	5.156288000000	0.721104000000
H	4.542707000000	5.801734000000	2.250215000000
H	1.882882000000	4.739949000000	3.442176000000

H	1.139961000000	3.262439000000	2.773712000000
H	1.067300000000	4.783443000000	1.857875000000
H	5.376739000000	2.480382000000	2.439852000000
H	3.920076000000	1.785182000000	3.181069000000
H	4.583811000000	3.315988000000	3.806518000000
H	6.216040000000	-1.349133000000	-2.940095000000
H	4.540233000000	-1.919897000000	-3.022871000000
H	5.845921000000	-2.903422000000	-3.739147000000
H	3.883366000000	-4.747603000000	-1.429540000000
H	5.150212000000	-5.400276000000	-0.364256000000
H	5.366475000000	-5.435453000000	-2.130112000000
H	8.039401000000	-4.066539000000	-1.894280000000
H	7.901720000000	-4.040806000000	-0.122362000000
H	8.273467000000	-2.542361000000	-1.011966000000
H	4.928243000000	-1.723198000000	4.203275000000
H	3.532615000000	-1.957239000000	3.122660000000
H	4.548524000000	-0.502197000000	2.959518000000
H	5.874762000000	-4.519296000000	3.342749000000
H	6.368234000000	-4.882789000000	1.672986000000
H	4.638896000000	-4.743448000000	2.080299000000
H	7.478344000000	-0.724725000000	2.116165000000
H	8.172961000000	-2.245065000000	1.499899000000
H	7.780574000000	-2.082519000000	3.229819000000
H	8.292092000000	2.435326000000	1.210826000000
H	7.475694000000	3.772048000000	0.368800000000
H	9.194675000000	3.444025000000	0.047072000000
H	8.702158000000	3.248495000000	-2.469220000000
H	6.981643000000	3.579442000000	-2.166522000000
H	7.455797000000	2.108703000000	-3.047235000000
H	9.106495000000	0.384171000000	-0.098332000000
H	9.912062000000	1.453131000000	-1.266466000000
H	8.749708000000	0.236377000000	-1.839280000000
H	2.043754000000	2.080231000000	0.448748000000
H	4.003460000000	-2.454375000000	0.207052000000
H	-0.998624000000	-1.344586000000	-3.837182000000
H	-2.347624000000	-0.491771000000	-3.111476000000
H	0.093616000000	0.821777000000	-4.451451000000
H	-1.588214000000	0.797868000000	-5.053022000000
H	-1.162022000000	1.732465000000	-3.598395000000
H	1.130624000000	-1.326229000000	-3.811895000000
H	2.530915000000	-0.847446000000	-2.866356000000
H	1.045638000000	-3.540925000000	-2.578895000000
H	2.616783000000	-3.290474000000	-3.381988000000
H	2.461658000000	-3.056816000000	-1.630650000000
H	-5.454828000000	-3.231571000000	0.545505000000
H	-7.185296000000	0.685877000000	0.411629000000
H	-4.611528000000	-4.269142000000	2.461789000000
H	-3.873225000000	-5.583691000000	1.509966000000
H	-3.247588000000	-5.188768000000	3.128500000000
H	-0.311622000000	-4.690221000000	2.161851000000
H	-0.868920000000	-5.236157000000	0.562556000000
H	-0.045516000000	-3.665139000000	0.727591000000
H	-1.454934000000	-1.445303000000	2.577673000000
H	-3.172047000000	-1.642990000000	3.004524000000
H	-1.928814000000	-2.634471000000	3.818540000000
H	-3.595217000000	-6.047293000000	-0.665446000000
H	-5.155404000000	-5.183675000000	-0.681382000000
H	-4.485284000000	-5.842905000000	-2.190764000000
H	-1.816491000000	-4.755520000000	-3.360232000000
H	-1.107872000000	-3.261303000000	-2.689915000000
H	-1.026274000000	-4.773919000000	-1.762166000000

H	-5.359497000000	-2.539910000000	-2.428875000000
H	-3.902076000000	-1.820285000000	-3.144200000000
H	-4.526608000000	-3.364278000000	-3.778516000000
H	-6.198485000000	1.365412000000	2.910411000000
H	-4.527895000000	1.951439000000	2.997886000000
H	-5.845093000000	2.926166000000	3.704804000000
H	-3.866935000000	4.752624000000	1.381606000000
H	-5.133196000000	5.405854000000	0.315951000000
H	-5.345319000000	5.450550000000	2.082134000000
H	-8.026483000000	4.090311000000	1.855232000000
H	-7.889383000000	4.053688000000	0.083415000000
H	-8.265828000000	2.561673000000	0.981925000000
H	-4.922353000000	1.696898000000	-4.229396000000
H	-3.527124000000	1.928287000000	-3.147772000000
H	-4.553191000000	0.481319000000	-2.977169000000
H	-5.851176000000	4.505816000000	-3.387290000000
H	-6.345988000000	4.881750000000	-1.720665000000
H	-4.616630000000	4.729724000000	-2.123400000000
H	-7.482728000000	0.729926000000	-2.144108000000
H	-8.167461000000	2.256995000000	-1.533344000000
H	-7.774349000000	2.086207000000	-3.262270000000
H	-8.283359000000	-2.443951000000	-1.235618000000
H	-7.480130000000	-3.771815000000	-0.367264000000
H	-9.202328000000	-3.436925000000	-0.071176000000
H	-8.740672000000	-3.211999000000	2.448728000000
H	-7.017070000000	-3.549092000000	2.171241000000
H	-7.499643000000	-2.067191000000	3.028317000000
H	-9.109946000000	-0.375042000000	0.038901000000
H	-9.932996000000	-1.429852000000	1.207839000000
H	-8.776590000000	-0.208574000000	1.782787000000
H	-2.043141000000	-2.085159000000	-0.394674000000
H	-3.997838000000	2.450118000000	-0.237432000000

TS-Si_{H2}

G_{qh} = -5250.180283

N_{imag} = 1, -344 cm⁻¹

SP = -5244.867858

G_{sp} = -5243.351877

Si	-1.554568000000	0.385945000000	-0.069050000000
H	-0.482480000000	2.020846000000	-0.020585000000
Si	1.554472000000	0.385902000000	0.068933000000
H	0.482392000000	2.020874000000	0.020485000000
C	-0.616112000000	0.092578000000	-1.623840000000
C	0.756348000000	-0.030463000000	-1.545256000000
C	0.616004000000	0.092515000000	1.623700000000
C	-0.756452000000	-0.030535000000	1.545108000000
C	-1.388059000000	0.290207000000	-2.924970000000
H	-2.454822000000	0.398584000000	-2.683946000000
H	-1.323980000000	-0.607124000000	-3.555453000000
C	-0.962800000000	1.514933000000	-3.748506000000
H	-0.941931000000	2.421384000000	-3.128038000000
H	-1.674738000000	1.688001000000	-4.572189000000
H	0.033496000000	1.395593000000	-4.196560000000
C	1.685366000000	-0.182165000000	-2.746012000000
H	2.678937000000	-0.467462000000	-2.369841000000
H	1.838676000000	0.807499000000	-3.208234000000
C	1.287198000000	-1.180455000000	-3.844152000000
H	0.900674000000	-2.116557000000	-3.416605000000
H	2.166727000000	-1.431927000000	-4.458764000000
H	0.523733000000	-0.783601000000	-4.526839000000
C	1.387925000000	0.290108000000	2.924844000000

H	1.323792000000	-0.607242000000	3.555283000000
H	2.454704000000	0.398460000000	2.683873000000
C	0.962657000000	1.514815000000	3.748399000000
H	0.941905000000	2.421299000000	3.127975000000
H	1.674523000000	1.687799000000	4.572162000000
H	-0.033692000000	1.395514000000	4.196343000000
C	-1.685462000000	-0.182346000000	2.745854000000
H	-2.679001000000	-0.467745000000	2.369671000000
H	-1.838886000000	0.807298000000	3.208079000000
C	-1.287186000000	-1.180612000000	3.843985000000
H	-0.900306000000	-2.116569000000	3.416440000000
H	-2.166739000000	-1.432382000000	4.458439000000
H	-0.523950000000	-0.783577000000	4.526828000000
C	-3.431306000000	0.121456000000	-0.122324000000
C	-4.296492000000	1.069671000000	0.505811000000
C	-5.679401000000	0.840649000000	0.520665000000
H	-6.320270000000	1.591126000000	0.984182000000
C	-6.260741000000	-0.311250000000	-0.019664000000
C	-5.403131000000	-1.239271000000	-0.609542000000
H	-5.814990000000	-2.151036000000	-1.033275000000
C	-4.008620000000	-1.053041000000	-0.696364000000
C	-3.792504000000	2.344307000000	1.155376000000
H	-2.691975000000	2.296608000000	1.252238000000
Si	-4.036878000000	3.832357000000	-0.038178000000
C	-3.060421000000	3.502151000000	-1.616597000000
H	-3.225409000000	4.304728000000	-2.354621000000
H	-3.362356000000	2.548706000000	-2.076565000000
H	-1.982272000000	3.445903000000	-1.403865000000
C	-3.359595000000	5.417273000000	0.744868000000
H	-2.308673000000	5.284127000000	1.050463000000
H	-3.931935000000	5.738387000000	1.628593000000
H	-3.391824000000	6.238531000000	0.009491000000
C	-5.848955000000	4.065448000000	-0.524705000000
H	-5.935776000000	4.930014000000	-1.204301000000
H	-6.508263000000	4.246170000000	0.336714000000
H	-6.222295000000	3.178600000000	-1.060242000000
Si	-4.397978000000	2.647797000000	2.958069000000
C	-3.001280000000	3.524605000000	3.886969000000
H	-2.069861000000	2.935867000000	3.866399000000
H	-3.277266000000	3.680809000000	4.943099000000
H	-2.780952000000	4.509392000000	3.446830000000
C	-5.949608000000	3.735613000000	3.061125000000
H	-6.206965000000	3.884377000000	4.123341000000
H	-6.818431000000	3.260840000000	2.577119000000
H	-5.813038000000	4.730181000000	2.610301000000
C	-4.849182000000	1.043436000000	3.855794000000
H	-3.975396000000	0.415731000000	4.077648000000
H	-5.557246000000	0.440587000000	3.266745000000
H	-5.333679000000	1.296075000000	4.814029000000
C	-7.783495000000	-0.509415000000	0.055842000000
C	-8.482587000000	0.650148000000	-0.688935000000
H	-9.577833000000	0.530457000000	-0.648942000000
H	-8.178850000000	0.674006000000	-1.747779000000
H	-8.236327000000	1.628046000000	-0.248349000000
C	-8.222473000000	-0.510798000000	1.537743000000
H	-9.312385000000	-0.656075000000	1.617837000000
H	-7.974430000000	0.436898000000	2.039400000000
H	-7.726551000000	-1.323435000000	2.092258000000
C	-8.230453000000	-1.836244000000	-0.582789000000
H	-7.776045000000	-2.705003000000	-0.081383000000
H	-7.969303000000	-1.882745000000	-1.651668000000

H	-9.323978000000	-1.940428000000	-0.503733000000
C	-3.227335000000	-2.142532000000	-1.415807000000
H	-2.181817000000	-1.824935000000	-1.556509000000
Si	-3.004336000000	-3.730343000000	-0.357606000000
C	-1.978796000000	-3.323549000000	1.167751000000
H	-2.545823000000	-2.663340000000	1.838226000000
H	-1.036935000000	-2.813330000000	0.913615000000
H	-1.736744000000	-4.243818000000	1.725319000000
C	-4.652331000000	-4.435937000000	0.245596000000
H	-4.467284000000	-5.344175000000	0.843659000000
H	-5.332712000000	-4.704493000000	-0.575772000000
H	-5.169290000000	-3.707807000000	0.890570000000
C	-2.056053000000	-5.041482000000	-1.341118000000
H	-1.780256000000	-5.868316000000	-0.665341000000
H	-1.123296000000	-4.625012000000	-1.755724000000
H	-2.639390000000	-5.469148000000	-2.170685000000
Si	-3.862459000000	-2.490804000000	-3.204838000000
C	-4.593696000000	-0.933033000000	-3.994814000000
H	-3.822830000000	-0.198827000000	-4.270504000000
H	-5.306062000000	-0.439132000000	-3.315827000000
H	-5.135438000000	-1.212194000000	-4.914069000000
C	-5.223032000000	-3.812364000000	-3.281211000000
H	-6.131830000000	-3.525622000000	-2.729054000000
H	-4.884577000000	-4.786864000000	-2.896851000000
H	-5.511114000000	-3.955987000000	-4.336363000000
C	-2.433616000000	-3.128578000000	-4.275167000000
H	-2.208509000000	-4.184274000000	-4.063980000000
H	-1.505070000000	-2.556576000000	-4.128755000000
H	-2.708972000000	-3.052593000000	-5.340541000000
C	3.431212000000	0.121449000000	0.122332000000
C	4.008558000000	-1.052964000000	0.696524000000
C	5.403106000000	-1.239028000000	0.609943000000
H	5.815010000000	-2.150717000000	1.033793000000
C	6.260710000000	-0.310965000000	0.020125000000
C	5.679332000000	0.840830000000	-0.520380000000
H	6.320192000000	1.591334000000	-0.983864000000
C	4.296400000000	1.069719000000	-0.505727000000
C	3.227292000000	-2.142605000000	1.415807000000
H	2.181718000000	-1.825145000000	1.556422000000
Si	3.862371000000	-2.491040000000	3.204846000000
C	4.593497000000	-0.933317000000	3.995029000000
H	3.822531000000	-0.199277000000	4.270891000000
H	5.305744000000	-0.439186000000	3.316086000000
H	5.135341000000	-1.212548000000	4.914202000000
C	5.222942000000	-3.812611000000	3.281097000000
H	5.510989000000	-3.956355000000	4.336241000000
H	6.131757000000	-3.525799000000	2.729007000000
H	4.884519000000	-4.787071000000	2.896606000000
C	2.433677000000	-3.128947000000	4.275222000000
H	2.205933000000	-4.183525000000	4.061328000000
H	1.506185000000	-2.554468000000	4.131872000000
H	2.710804000000	-3.056666000000	5.340396000000
Si	3.004740000000	-3.730246000000	0.357215000000
C	4.652962000000	-4.435412000000	-0.245877000000
H	5.169885000000	-3.707068000000	-0.890635000000
H	4.468146000000	-5.343563000000	-0.844143000000
H	5.333276000000	-4.704021000000	0.575530000000
C	1.979431000000	-3.323251000000	-1.168237000000
H	1.037482000000	-2.813161000000	-0.914168000000
H	1.737546000000	-4.243435000000	-1.726017000000
H	2.546524000000	-2.662873000000	-1.838487000000

C	2.056508000000	-5.041916000000	1.340065000000
H	2.639581000000	-5.469477000000	2.169872000000
H	1.781438000000	-5.868753000000	0.663995000000
H	1.123333000000	-4.625919000000	1.754208000000
C	7.783494000000	-0.508985000000	-0.055139000000
C	8.222686000000	-0.510456000000	-1.536978000000
H	7.974609000000	0.437165000000	-2.038758000000
H	7.726934000000	-1.323200000000	-2.091488000000
H	9.312626000000	-0.655620000000	-1.616901000000
C	8.482364000000	0.650714000000	0.689634000000
H	9.577627000000	0.531128000000	0.649811000000
H	8.178471000000	0.674638000000	1.748432000000
H	8.236073000000	1.628549000000	0.248924000000
C	8.230492000000	-1.835712000000	0.583674000000
H	9.324038000000	-1.939793000000	0.504789000000
H	7.776245000000	-2.704561000000	0.082278000000
H	7.969188000000	-1.882144000000	1.652519000000
C	3.792396000000	2.344287000000	-1.155418000000
H	2.691878000000	2.296529000000	-1.252372000000
Si	4.398019000000	2.647690000000	-2.958077000000
C	3.001423000000	3.524465000000	-3.887161000000
H	3.277477000000	3.680502000000	-4.943298000000
H	2.781146000000	4.509331000000	-3.447173000000
H	2.069957000000	2.935802000000	-3.866561000000
C	4.849296000000	1.043273000000	-3.855662000000
H	3.975512000000	0.415607000000	-4.077635000000
H	5.557232000000	0.440415000000	-3.266467000000
H	5.333964000000	1.295846000000	-4.813828000000
C	5.949656000000	3.735503000000	-3.061058000000
H	6.818450000000	3.260756000000	-2.576975000000
H	5.813044000000	4.730087000000	-2.610281000000
H	6.207085000000	3.884233000000	-4.123262000000
Si	4.036601000000	3.832429000000	0.038060000000
C	5.848625000000	4.065672000000	0.524715000000
H	5.935343000000	4.930372000000	1.204155000000
H	6.508020000000	4.246254000000	-0.336666000000
H	6.221942000000	3.178941000000	1.060463000000
C	3.359291000000	5.417255000000	-0.745142000000
H	2.308412000000	5.284024000000	-1.050849000000
H	3.931711000000	5.738358000000	-1.628819000000
H	3.391385000000	6.238555000000	-0.009805000000
C	3.060069000000	3.502263000000	1.616442000000
H	3.361991000000	2.548829000000	2.076443000000
H	1.981929000000	3.446004000000	1.403672000000
H	3.225030000000	4.304857000000	2.354454000000

TS-Ge_{H2}

G_{qh} = -8824.903144

N_{imag} = 1, 422 cm⁻¹

SP = -8817.974949

G_{sp} = -8816.465812

Ge	1.577305000000	0.447888000000	0.079468000000
H	0.503204000000	2.052701000000	0.016830000000
Ge	-1.577339000000	0.447887000000	-0.079455000000
H	-0.503242000000	2.052697000000	-0.016737000000
C	0.600272000000	0.086652000000	1.697794000000
C	-0.762174000000	-0.027416000000	1.609515000000
C	-0.600304000000	0.086725000000	-1.697803000000
C	0.762146000000	-0.027305000000	-1.609535000000
C	1.379499000000	0.265452000000	2.994199000000
H	2.449420000000	0.338560000000	2.753670000000

H	1.284777000000	-0.623893000000	3.632558000000
C	0.988316000000	1.512081000000	3.801307000000
H	1.043594000000	2.416684000000	3.179729000000
H	1.671906000000	1.648496000000	4.655384000000
H	-0.032969000000	1.446641000000	4.202921000000
C	-1.718343000000	-0.167967000000	2.787066000000
H	-2.700637000000	-0.466073000000	2.390047000000
H	-1.889466000000	0.829902000000	3.227221000000
C	-1.342270000000	-1.144798000000	3.910961000000
H	-0.964651000000	-2.094921000000	3.506365000000
H	-2.230346000000	-1.371070000000	4.523036000000
H	-0.579012000000	-0.742099000000	4.590378000000
C	-1.379552000000	0.265536000000	-2.994195000000
H	-1.284837000000	-0.623801000000	-3.632570000000
H	-2.449468000000	0.338633000000	-2.753638000000
C	-0.988411000000	1.512183000000	-3.801298000000
H	-1.043653000000	2.416773000000	-3.179697000000
H	-1.672052000000	1.648618000000	-4.655332000000
H	0.032850000000	1.446752000000	-4.202976000000
C	1.718315000000	-0.167734000000	-2.787101000000
H	2.700649000000	-0.465750000000	-2.390111000000
H	1.889329000000	0.830164000000	-3.227232000000
C	1.342322000000	-1.144569000000	-3.911017000000
H	0.964911000000	-2.094783000000	-3.506439000000
H	2.230387000000	-1.370647000000	-4.523182000000
H	0.578928000000	-0.741977000000	-4.590342000000
C	3.525488000000	0.116110000000	0.132367000000
C	4.409594000000	1.049647000000	-0.481122000000
C	5.785740000000	0.779937000000	-0.500066000000
H	6.448483000000	1.518542000000	-0.952198000000
C	6.332076000000	-0.397140000000	0.023053000000
C	5.447336000000	-1.308319000000	0.599354000000
H	5.831336000000	-2.237895000000	1.010565000000
C	4.057964000000	-1.082379000000	0.689317000000
C	3.936767000000	2.347270000000	-1.106428000000
H	2.835515000000	2.325028000000	-1.202408000000
Si	4.212480000000	3.804051000000	0.117117000000
C	3.227855000000	3.458201000000	1.688452000000
H	3.410860000000	4.237872000000	2.446418000000
H	3.505702000000	2.486155000000	2.124679000000
H	2.148702000000	3.434229000000	1.473336000000
C	3.567411000000	5.418048000000	-0.632877000000
H	2.512255000000	5.314066000000	-0.935240000000
H	4.142580000000	5.740834000000	-1.514229000000
H	3.621985000000	6.225897000000	0.115900000000
C	6.030168000000	3.988135000000	0.602367000000
H	6.139037000000	4.833707000000	1.302329000000
H	6.687887000000	4.176306000000	-0.258870000000
H	6.387842000000	3.080519000000	1.113279000000
Si	4.540131000000	2.663567000000	-2.905743000000
C	3.151689000000	3.574130000000	-3.814067000000
H	2.216345000000	2.990866000000	-3.806307000000
H	3.427323000000	3.754118000000	-4.866447000000
H	2.938653000000	4.549290000000	-3.349289000000
C	6.111030000000	3.723342000000	-3.000822000000
H	6.371775000000	3.879405000000	-4.061149000000
H	6.970294000000	3.226738000000	-2.521613000000
H	5.992879000000	4.714998000000	-2.538307000000
C	4.953839000000	1.060592000000	-3.822381000000
H	4.072686000000	0.428527000000	-3.997841000000
H	5.691957000000	0.461904000000	-3.266984000000

H	5.389275000000	1.312060000000	-4.804207000000
C	7.848618000000	-0.639070000000	-0.054941000000
C	8.581240000000	0.486337000000	0.709738000000
H	9.672553000000	0.335118000000	0.668188000000
H	8.277366000000	0.501165000000	1.768711000000
H	8.364376000000	1.478483000000	0.285748000000
C	8.289521000000	-0.628728000000	-1.536192000000
H	9.374573000000	-0.806023000000	-1.617981000000
H	8.071619000000	0.334689000000	-2.021688000000
H	7.769487000000	-1.416027000000	-2.104977000000
C	8.255346000000	-1.989138000000	0.561500000000
H	7.775290000000	-2.835403000000	0.045736000000
H	7.992406000000	-2.045645000000	1.629462000000
H	9.345316000000	-2.124735000000	0.480804000000
C	3.240925000000	-2.153048000000	1.396375000000
H	2.206243000000	-1.802563000000	1.538844000000
Si	2.969154000000	-3.730523000000	0.334771000000
C	1.958067000000	-3.297089000000	-1.193090000000
H	2.540945000000	-2.646285000000	-1.859128000000
H	1.024727000000	-2.770198000000	-0.942450000000
H	1.701215000000	-4.211238000000	-1.754047000000
C	4.596029000000	-4.484778000000	-0.267060000000
H	4.385311000000	-5.389072000000	-0.862603000000
H	5.269351000000	-4.769992000000	0.554493000000
H	5.132917000000	-3.773245000000	-0.914359000000
C	1.980648000000	-5.009499000000	1.321184000000
H	1.668119000000	-5.823139000000	0.645368000000
H	1.068018000000	-4.559769000000	1.745415000000
H	2.554273000000	-5.461162000000	2.144782000000
Si	3.855868000000	-2.530928000000	3.185459000000
C	4.619553000000	-0.996041000000	3.989035000000
H	3.869544000000	-0.233967000000	4.245819000000
H	5.363246000000	-0.529975000000	3.323967000000
H	5.131278000000	-1.290861000000	4.920554000000
C	5.186816000000	-3.881988000000	3.262395000000
H	6.106173000000	-3.611199000000	2.719717000000
H	4.829255000000	-4.845540000000	2.867881000000
H	5.462802000000	-4.040149000000	4.318763000000
C	2.398366000000	-3.147328000000	4.233220000000
H	2.589069000000	-2.940417000000	5.299490000000
H	2.257807000000	-4.233057000000	4.124638000000
H	1.447653000000	-2.663434000000	3.963370000000
C	-3.525523000000	0.116089000000	-0.132332000000
C	-4.057977000000	-1.082407000000	-0.689281000000
C	-5.447345000000	-1.308375000000	-0.599330000000
H	-5.831324000000	-2.237956000000	-1.010555000000
C	-6.332103000000	-0.397206000000	-0.023038000000
C	-5.785788000000	0.779877000000	0.500089000000
H	-6.448544000000	1.518473000000	0.952217000000
C	-4.409645000000	1.049607000000	0.481160000000
C	-3.240910000000	-2.153035000000	-1.396348000000
H	-2.206224000000	-1.802536000000	-1.538767000000
Si	-3.855728000000	-2.530823000000	-3.185492000000
C	-4.619478000000	-0.995933000000	-3.989008000000
H	-3.869502000000	-0.233842000000	-4.245837000000
H	-5.363140000000	-0.529889000000	-3.323889000000
H	-5.131262000000	-1.290756000000	-4.920494000000
C	-5.186606000000	-3.881938000000	-3.262615000000
H	-5.462571000000	-4.039972000000	-4.319008000000
H	-6.105981000000	-3.611257000000	-2.719913000000
H	-4.829003000000	-4.845525000000	-2.868224000000

C	-2.398035000000	-3.147048000000	-4.233122000000
H	-2.258143000000	-4.232960000000	-4.125491000000
H	-1.447199000000	-2.663950000000	-3.962273000000
H	-2.588017000000	-2.939013000000	-5.299301000000
Si	-2.969113000000	-3.730587000000	-0.334877000000
C	-4.595973000000	-4.485079000000	0.266697000000
H	-5.132980000000	-3.773674000000	0.914039000000
H	-4.385227000000	-5.389425000000	0.862151000000
H	-5.269198000000	-4.770250000000	-0.554947000000
C	-1.958228000000	-3.297260000000	1.193153000000
H	-1.024983000000	-2.770121000000	0.942680000000
H	-1.701214000000	-4.211480000000	1.753919000000
H	-2.541276000000	-2.646729000000	1.859312000000
C	-1.980358000000	-5.009279000000	-1.321410000000
H	-2.553873000000	-5.460903000000	-2.145107000000
H	-1.667722000000	-5.822973000000	-0.645710000000
H	-1.067790000000	-4.559333000000	-1.745540000000
C	-7.848644000000	-0.639151000000	0.054928000000
C	-8.289585000000	-0.628776000000	1.536168000000
H	-8.071719000000	0.334661000000	2.021642000000
H	-7.769550000000	-1.416047000000	2.104989000000
H	-9.374636000000	-0.806090000000	1.617933000000
C	-8.581258000000	0.486231000000	-0.709797000000
H	-9.672571000000	0.335005000000	-0.668267000000
H	-8.277359000000	0.501033000000	-1.768763000000
H	-8.364410000000	1.478389000000	-0.285827000000
C	-8.255344000000	-1.989238000000	-0.561489000000
H	-9.345314000000	-2.124844000000	-0.480815000000
H	-7.775290000000	-2.835485000000	-0.045692000000
H	-7.992379000000	-2.045770000000	-1.629443000000
C	-3.936834000000	2.347226000000	1.106486000000
H	-2.835581000000	2.324989000000	1.202465000000
Si	-4.540186000000	2.663471000000	2.905810000000
C	-3.151699000000	3.573940000000	3.814159000000
H	-3.427322000000	3.753925000000	4.866543000000
H	-2.938614000000	4.549097000000	3.349395000000
H	-2.216385000000	2.990629000000	3.806386000000
C	-4.953964000000	1.060473000000	3.822372000000
H	-4.072918000000	0.428143000000	3.997407000000
H	-5.692443000000	0.462064000000	3.267156000000
H	-5.388973000000	1.311913000000	4.804395000000
C	-6.111049000000	3.723294000000	3.000945000000
H	-6.970325000000	3.226738000000	2.521707000000
H	-5.992868000000	4.714971000000	2.538481000000
H	-6.371794000000	3.879311000000	4.061279000000
Si	-4.212550000000	3.804031000000	-0.117025000000
C	-6.030243000000	3.988144000000	-0.602244000000
H	-6.139119000000	4.833740000000	-1.302177000000
H	-6.687948000000	4.176291000000	0.259009000000
H	-6.387929000000	3.080547000000	-1.113181000000
C	-3.567449000000	5.418000000000	0.633001000000
H	-2.512287000000	5.313996000000	0.935338000000
H	-4.142594000000	5.740766000000	1.514377000000
H	-3.622030000000	6.225874000000	-0.115748000000
C	-3.227949000000	3.458201000000	-1.688379000000
H	-3.505803000000	2.486161000000	-2.124614000000
H	-2.148792000000	3.434223000000	-1.473276000000
H	-3.410960000000	4.237882000000	-2.446333000000

TS-SnH₂

G_{qh} = -5100.015056

$N_{imag} = 1, -62 \text{ cm}^{-1}$

$SP = -5094.034160$

$G_{sp} = -5092.531690$

Sn	-1.724313000000	0.556511000000	-0.108882000000
H	-0.235937000000	2.005896000000	0.052254000000
Sn	1.697601000000	0.007646000000	0.081208000000
H	0.687509000000	1.851550000000	0.078456000000
C	-0.617400000000	-0.022941000000	-1.873492000000
C	0.713328000000	-0.322798000000	-1.792025000000
C	0.530653000000	-0.355745000000	1.829315000000
C	-0.825569000000	-0.274241000000	1.686979000000
C	-1.298962000000	0.248495000000	-3.207879000000
H	-2.374342000000	0.031338000000	-3.137419000000
H	-0.908765000000	-0.417106000000	-3.990872000000
C	-1.134440000000	1.702257000000	-3.677078000000
H	-1.567786000000	2.406038000000	-2.952055000000
H	-1.638297000000	1.862312000000	-4.644414000000
H	-0.073813000000	1.965914000000	-3.797571000000
C	1.575250000000	-0.636578000000	-3.010245000000
H	2.638314000000	-0.621597000000	-2.720968000000
H	1.466248000000	0.155294000000	-3.773184000000
C	1.270480000000	-1.999879000000	-3.653828000000
H	1.364277000000	-2.811807000000	-2.920888000000
H	1.968841000000	-2.206314000000	-4.481479000000
H	0.248895000000	-2.043882000000	-4.057928000000
C	1.270998000000	-0.475359000000	3.152879000000
H	0.927577000000	-1.368808000000	3.696103000000
H	2.338178000000	-0.643816000000	2.964739000000
C	1.147945000000	0.761002000000	4.053976000000
H	1.536659000000	1.654679000000	3.542881000000
H	1.724762000000	0.625336000000	4.983777000000
H	0.103700000000	0.965815000000	4.333025000000
C	-1.836372000000	-0.385162000000	2.829296000000
H	-2.828238000000	-0.544143000000	2.377983000000
H	-1.913928000000	0.599583000000	3.326604000000
C	-1.642703000000	-1.467150000000	3.903383000000
H	-1.344163000000	-2.426042000000	3.455193000000
H	-2.591416000000	-1.631065000000	4.439906000000
H	-0.892317000000	-1.195025000000	4.658377000000
C	-3.872079000000	0.035539000000	-0.086921000000
C	-4.756349000000	0.898568000000	0.620278000000
C	-6.111058000000	0.548457000000	0.734567000000
H	-6.776523000000	1.232985000000	1.262500000000
C	-6.632018000000	-0.638044000000	0.207991000000
C	-5.747865000000	-1.468445000000	-0.479681000000
H	-6.114405000000	-2.394751000000	-0.913036000000
C	-4.383831000000	-1.155144000000	-0.666181000000
C	-4.325377000000	2.215523000000	1.236852000000
H	-3.219618000000	2.268704000000	1.246771000000
Si	-4.792679000000	3.665552000000	0.064468000000
C	-3.942133000000	3.394707000000	-1.599895000000
H	-4.261653000000	4.156566000000	-2.330286000000
H	-4.181601000000	2.401667000000	-2.012591000000
H	-2.848434000000	3.464534000000	-1.492271000000
C	-4.165085000000	5.301959000000	0.781229000000
H	-3.081237000000	5.250513000000	0.977385000000
H	-4.666276000000	5.576298000000	1.722221000000
H	-4.335669000000	6.119376000000	0.060830000000
C	-6.653792000000	3.757297000000	-0.252303000000
H	-6.869564000000	4.606904000000	-0.921965000000
H	-7.240563000000	3.894949000000	0.667651000000

H	-7.006156000000	2.839727000000	-0.748730000000
Si	-4.796291000000	2.462537000000	3.084920000000
C	-3.365950000000	3.395727000000	3.899725000000
H	-2.425642000000	2.825572000000	3.819183000000
H	-3.565883000000	3.567750000000	4.970327000000
H	-3.203165000000	4.375564000000	3.423817000000
C	-6.390496000000	3.460014000000	3.336168000000
H	-6.567749000000	3.583826000000	4.417803000000
H	-7.266208000000	2.937554000000	2.917967000000
H	-6.350463000000	4.464456000000	2.888325000000
C	-5.079005000000	0.823113000000	3.983751000000
H	-4.181719000000	0.190685000000	4.004356000000
H	-5.886274000000	0.242946000000	3.511475000000
H	-5.372238000000	1.030005000000	5.026838000000
C	-8.122638000000	-0.969377000000	0.390814000000
C	-8.972626000000	0.134448000000	-0.277934000000
H	-10.047796000000	-0.080868000000	-0.162164000000
H	-8.750106000000	0.199850000000	-1.355088000000
H	-8.779699000000	1.123806000000	0.163716000000
C	-8.450586000000	-1.029387000000	1.899795000000
H	-9.515092000000	-1.270725000000	2.055310000000
H	-8.250078000000	-0.070030000000	2.400612000000
H	-7.846646000000	-1.802227000000	2.401445000000
C	-8.500621000000	-2.321110000000	-0.240094000000
H	-7.932173000000	-3.153147000000	0.203898000000
H	-8.323191000000	-2.327951000000	-1.326934000000
H	-9.570948000000	-2.524268000000	-0.078231000000
C	-3.576315000000	-2.119472000000	-1.520229000000
H	-2.563311000000	-1.712668000000	-1.680355000000
Si	-3.198670000000	-3.774900000000	-0.630379000000
C	-2.215079000000	-3.413071000000	0.933842000000
H	-2.819515000000	-2.797859000000	1.616638000000
H	-1.284353000000	-2.862561000000	0.728398000000
H	-1.959068000000	-4.348689000000	1.458735000000
C	-4.756939000000	-4.707692000000	-0.096834000000
H	-4.465540000000	-5.663165000000	0.371441000000
H	-5.434500000000	-4.934373000000	-0.932865000000
H	-5.319885000000	-4.127025000000	0.650855000000
C	-2.158301000000	-4.880905000000	-1.761523000000
H	-1.790491000000	-5.751898000000	-1.193762000000
H	-1.281015000000	-4.337599000000	-2.150245000000
H	-2.732760000000	-5.262248000000	-2.620523000000
Si	-4.316414000000	-2.281534000000	-3.292156000000
C	-5.123293000000	-0.641537000000	-3.785454000000
H	-4.424850000000	0.205953000000	-3.701905000000
H	-5.984454000000	-0.421957000000	-3.135407000000
H	-5.478636000000	-0.687339000000	-4.828407000000
C	-5.634809000000	-3.636413000000	-3.447849000000
H	-6.486241000000	-3.495673000000	-2.764524000000
H	-5.213425000000	-4.638018000000	-3.266609000000
H	-6.031119000000	-3.626656000000	-4.477277000000
C	-2.970117000000	-2.721695000000	-4.548413000000
H	-2.458677000000	-3.661485000000	-4.293616000000
H	-2.208345000000	-1.934910000000	-4.632494000000
H	-3.431078000000	-2.849603000000	-5.542422000000
C	3.886477000000	0.046758000000	0.042924000000
C	4.675468000000	-0.988075000000	0.607844000000
C	6.077368000000	-0.928302000000	0.459090000000
H	6.662774000000	-1.739581000000	0.880934000000
C	6.728793000000	0.123336000000	-0.183817000000
C	5.928692000000	1.151331000000	-0.692357000000

H	6.404948000000	2.002204000000	-1.180140000000
C	4.527849000000	1.139670000000	-0.607056000000
C	4.125013000000	-2.157758000000	1.404811000000
H	3.036094000000	-2.030558000000	1.546206000000
Si	4.834788000000	-2.195741000000	3.197796000000
C	5.123701000000	-0.420493000000	3.784853000000
H	4.203088000000	0.182775000000	3.747829000000
H	5.873188000000	0.080845000000	3.152763000000
H	5.489448000000	-0.415632000000	4.825110000000
C	6.476386000000	-3.134761000000	3.331318000000
H	6.813989000000	-3.112998000000	4.381194000000
H	7.278240000000	-2.696057000000	2.717989000000
H	6.366097000000	-4.192336000000	3.043126000000
C	3.627791000000	-3.064288000000	4.367743000000
H	3.519447000000	-4.131482000000	4.123466000000
H	2.626989000000	-2.610221000000	4.351952000000
H	4.011211000000	-2.995615000000	5.399807000000
Si	4.215201000000	-3.807505000000	0.430809000000
C	5.957269000000	-4.211700000000	-0.182287000000
H	6.307396000000	-3.457053000000	-0.903390000000
H	5.945286000000	-5.188718000000	-0.694247000000
H	6.691613000000	-4.269070000000	0.635510000000
C	3.087825000000	-3.617858000000	-1.066030000000
H	2.047372000000	-3.429626000000	-0.755426000000
H	3.095151000000	-4.517590000000	-1.702771000000
H	3.414039000000	-2.764686000000	-1.680768000000
C	3.585759000000	-5.238549000000	1.495743000000
H	4.276807000000	-5.480555000000	2.318597000000
H	3.479018000000	-6.143152000000	0.873982000000
H	2.599520000000	-5.013839000000	1.933325000000
C	8.256767000000	0.192074000000	-0.340843000000
C	8.608978000000	0.247186000000	-1.844677000000
H	8.170953000000	1.129736000000	-2.335294000000
H	8.234918000000	-0.647421000000	-2.367642000000
H	9.701492000000	0.294809000000	-1.984447000000
C	8.783283000000	1.464844000000	0.359687000000
H	9.879403000000	1.533312000000	0.263675000000
H	8.533336000000	1.452294000000	1.432707000000
H	8.352101000000	2.379925000000	-0.073431000000
C	8.961370000000	-1.028359000000	0.277165000000
H	10.050122000000	-0.944512000000	0.134253000000
H	8.635402000000	-1.970078000000	-0.191225000000
H	8.774752000000	-1.101988000000	1.360038000000
C	3.789175000000	2.333035000000	-1.175743000000
H	2.707483000000	2.112013000000	-1.224045000000
Si	4.220424000000	2.759749000000	-3.000046000000
C	2.644580000000	3.409085000000	-3.813712000000
H	2.825829000000	3.672840000000	-4.868697000000
H	2.255175000000	4.302381000000	-3.301544000000
H	1.857138000000	2.639937000000	-3.788504000000
C	4.812082000000	1.224245000000	-3.929580000000
H	4.057892000000	0.424068000000	-3.914105000000
H	5.738331000000	0.820856000000	-3.492551000000
H	5.012763000000	1.481727000000	-4.983112000000
C	5.575037000000	4.072953000000	-3.185506000000
H	6.534476000000	3.747657000000	-2.752253000000
H	5.300610000000	5.032472000000	-2.720343000000
H	5.745264000000	4.260552000000	-4.259060000000
Si	3.865594000000	3.795305000000	0.073130000000
C	5.641972000000	4.350272000000	0.407532000000
H	5.630093000000	5.202294000000	1.108111000000

H	6.176514000000	4.666945000000	-0.499679000000
H	6.217724000000	3.538108000000	0.878186000000
C	2.837709000000	5.241461000000	-0.582945000000
H	1.808103000000	4.917905000000	-0.808390000000
H	3.264621000000	5.679654000000	-1.498767000000
H	2.779949000000	6.040467000000	0.174851000000
C	3.145161000000	3.241280000000	1.730453000000
H	3.628756000000	2.314574000000	2.079013000000
H	2.062599000000	3.057049000000	1.660975000000
H	3.310714000000	4.018264000000	2.495464000000

TS-Pb_{H2}

$G_{qh} = -5057.084136$

$N_{imag} = 1, -1080 \text{ cm}^{-1}$

$SP = -5051.056598$

$G_{sp} = -5049.559449$

Pb	-1.714194000000	0.358645000000	-0.277186000000
H	-0.336579000000	1.699009000000	-0.040786000000
Pb	1.736499000000	-0.234626000000	0.100594000000
H	0.806115000000	1.509609000000	0.062775000000
C	-0.526864000000	-0.463232000000	-2.064166000000
C	0.788437000000	-0.736050000000	-1.888555000000
C	0.431327000000	-0.794253000000	1.841089000000
C	-0.897055000000	-0.671438000000	1.624405000000
C	-1.176897000000	-0.401115000000	-3.435065000000
H	-2.127231000000	-0.952747000000	-3.428102000000
H	-0.554903000000	-0.904446000000	-4.191196000000
C	-1.451271000000	1.035322000000	-3.903542000000
H	-2.133196000000	1.562584000000	-3.218678000000
H	-1.915397000000	1.040879000000	-4.903031000000
H	-0.521529000000	1.621040000000	-3.954977000000
C	1.720508000000	-1.194421000000	-3.002407000000
H	2.766164000000	-1.113895000000	-2.664083000000
H	1.640750000000	-0.515619000000	-3.871304000000
C	1.462267000000	-2.638922000000	-3.456810000000
H	1.523896000000	-3.334457000000	-2.608741000000
H	2.202167000000	-2.954832000000	-4.210463000000
H	0.459234000000	-2.751021000000	-3.894931000000
C	1.133705000000	-0.997309000000	3.169429000000
H	0.700303000000	-1.856149000000	3.704784000000
H	2.183877000000	-1.263227000000	3.000737000000
C	1.091266000000	0.252508000000	4.060028000000
H	1.548586000000	1.113435000000	3.546076000000
H	1.640560000000	0.087810000000	5.001262000000
H	0.056802000000	0.531336000000	4.313242000000
C	-1.975703000000	-0.780148000000	2.699107000000
H	-2.943302000000	-0.919368000000	2.193462000000
H	-2.054180000000	0.210256000000	3.184555000000
C	-1.871899000000	-1.857463000000	3.788688000000
H	-1.612992000000	-2.837052000000	3.359743000000
H	-2.845560000000	-1.964529000000	4.293949000000
H	-1.132481000000	-1.616513000000	4.565166000000
C	-3.986453000000	0.038777000000	-0.048326000000
C	-4.709849000000	0.954713000000	0.754918000000
C	-6.052650000000	0.664724000000	1.052753000000
H	-6.618145000000	1.396184000000	1.632675000000
C	-6.675027000000	-0.526992000000	0.661717000000
C	-5.929430000000	-1.410732000000	-0.121854000000
H	-6.374156000000	-2.345141000000	-0.456953000000
C	-4.611790000000	-1.127943000000	-0.539915000000
C	-4.125301000000	2.250532000000	1.278709000000

H	-3.024416000000	2.209642000000	1.190850000000
Si	-4.568783000000	3.696797000000	0.094232000000
C	-3.911000000000	3.304155000000	-1.633386000000
H	-4.234399000000	4.075376000000	-2.352304000000
H	-4.278091000000	2.329699000000	-1.990760000000
H	-2.809496000000	3.278548000000	-1.640869000000
C	-3.724779000000	5.286462000000	0.682052000000
H	-2.634406000000	5.138138000000	0.754992000000
H	-4.085266000000	5.628518000000	1.664106000000
H	-3.902408000000	6.099094000000	-0.042004000000
C	-6.438749000000	3.933638000000	-0.037190000000
H	-6.664160000000	4.743688000000	-0.750931000000
H	-6.902580000000	4.192458000000	0.926039000000
H	-6.916010000000	3.013393000000	-0.410144000000
Si	-4.386488000000	2.595495000000	3.152654000000
C	-2.762043000000	3.333876000000	3.782571000000
H	-1.930015000000	2.621906000000	3.649876000000
H	-2.825193000000	3.585125000000	4.854190000000
H	-2.503307000000	4.253046000000	3.232890000000
C	-5.801908000000	3.802432000000	3.522102000000
H	-5.859781000000	3.964198000000	4.611712000000
H	-6.771904000000	3.389924000000	3.199762000000
H	-5.677590000000	4.785990000000	3.044845000000
C	-4.799268000000	1.032822000000	4.136190000000
H	-4.122201000000	0.197043000000	3.919017000000
H	-5.823344000000	0.689772000000	3.927312000000
H	-4.731272000000	1.258693000000	5.213978000000
C	-8.135096000000	-0.797703000000	1.064981000000
C	-9.042316000000	0.242358000000	0.368998000000
H	-10.098599000000	0.081890000000	0.642052000000
H	-8.955560000000	0.165077000000	-0.726630000000
H	-8.772514000000	1.270919000000	0.654190000000
C	-8.288067000000	-0.669358000000	2.596988000000
H	-9.325347000000	-0.887296000000	2.899805000000
H	-8.048349000000	0.344354000000	2.951254000000
H	-7.622148000000	-1.374455000000	3.119220000000
C	-8.601408000000	-2.205418000000	0.653229000000
H	-7.980415000000	-2.989339000000	1.114711000000
H	-8.573446000000	-2.346024000000	-0.437992000000
H	-9.641015000000	-2.366053000000	0.979526000000
C	-3.969137000000	-2.055410000000	-1.549018000000
H	-2.980816000000	-1.645469000000	-1.808802000000
Si	-3.476428000000	-3.792574000000	-0.909819000000
C	-3.027311000000	-3.666226000000	0.914918000000
H	-3.847662000000	-3.233288000000	1.508344000000
H	-2.144705000000	-3.018873000000	1.030760000000
H	-2.782233000000	-4.657073000000	1.331839000000
C	-4.842249000000	-5.085233000000	-1.127305000000
H	-4.521230000000	-6.046049000000	-0.691283000000
H	-5.077246000000	-5.262452000000	-2.189009000000
H	-5.772145000000	-4.782517000000	-0.618455000000
C	-1.930172000000	-4.320699000000	-1.863226000000
H	-1.537805000000	-5.275440000000	-1.474870000000
H	-1.141420000000	-3.557962000000	-1.748928000000
H	-2.121857000000	-4.447752000000	-2.939658000000
Si	-4.921363000000	-1.964422000000	-3.214142000000
C	-5.068771000000	-0.144347000000	-3.703682000000
H	-4.092734000000	0.343582000000	-3.834068000000
H	-5.614841000000	0.403853000000	-2.918980000000
H	-5.630356000000	-0.039107000000	-4.646907000000
C	-6.688866000000	-2.642207000000	-3.142686000000

H	-7.353934000000	-1.960982000000	-2.590658000000
H	-6.753433000000	-3.637417000000	-2.678913000000
H	-7.076984000000	-2.724557000000	-4.172223000000
C	-3.995996000000	-2.941117000000	-4.547725000000
H	-4.048597000000	-4.024780000000	-4.354104000000
H	-2.933411000000	-2.662597000000	-4.618389000000
H	-4.459344000000	-2.757023000000	-5.531435000000
C	4.006311000000	0.048597000000	0.013811000000
C	4.899587000000	-0.871340000000	0.606809000000
C	6.285335000000	-0.654906000000	0.440574000000
H	6.963659000000	-1.377014000000	0.884487000000
C	6.805213000000	0.440767000000	-0.249292000000
C	5.889067000000	1.352773000000	-0.783220000000
H	6.257493000000	2.234209000000	-1.310315000000
C	4.498591000000	1.184664000000	-0.678782000000
C	4.480303000000	-2.057137000000	1.456979000000
H	3.380085000000	-2.054180000000	1.564453000000
Si	5.111176000000	-1.870268000000	3.266460000000
C	4.965043000000	-0.047577000000	3.744260000000
H	3.928219000000	0.311879000000	3.655953000000
H	5.589859000000	0.576066000000	3.085784000000
H	5.291157000000	0.112456000000	4.785285000000
C	6.909028000000	-2.423390000000	3.489554000000
H	7.181219000000	-2.342274000000	4.555375000000
H	7.621110000000	-1.808787000000	2.918488000000
H	7.048489000000	-3.475349000000	3.192554000000
C	4.080062000000	-2.922627000000	4.457176000000
H	4.302831000000	-3.994519000000	4.349929000000
H	2.996822000000	-2.788632000000	4.323677000000
H	4.326276000000	-2.633982000000	5.493139000000
Si	4.791999000000	-3.735239000000	0.585841000000
C	6.575354000000	-3.950344000000	-0.003876000000
H	6.833675000000	-3.206878000000	-0.773517000000
H	6.692860000000	-4.953109000000	-0.448243000000
H	7.303984000000	-3.859092000000	0.816717000000
C	3.647178000000	-3.782839000000	-0.910610000000
H	2.593601000000	-3.716608000000	-0.593927000000
H	3.767585000000	-4.709666000000	-1.494852000000
H	3.849848000000	-2.931376000000	-1.578696000000
C	4.356483000000	-5.170668000000	1.737945000000
H	5.088723000000	-5.280795000000	2.553635000000
H	4.349693000000	-6.114463000000	1.167395000000
H	3.359699000000	-5.043422000000	2.190120000000
C	8.314062000000	0.674437000000	-0.434973000000
C	8.637963000000	0.707706000000	-1.945922000000
H	8.097859000000	1.515951000000	-2.462113000000
H	8.358595000000	-0.242990000000	-2.427389000000
H	9.716449000000	0.870312000000	-2.106862000000
C	8.704138000000	2.025284000000	0.205961000000
H	9.784043000000	2.212303000000	0.086343000000
H	8.473024000000	2.028251000000	1.283221000000
H	8.166556000000	2.868064000000	-0.254156000000
C	9.160516000000	-0.433262000000	0.216356000000
H	10.230764000000	-0.232979000000	0.051070000000
H	8.937112000000	-1.423750000000	-0.209524000000
H	8.998282000000	-0.484287000000	1.304344000000
C	3.616069000000	2.257841000000	-1.273812000000
H	2.568383000000	1.916832000000	-1.265822000000
Si	3.902957000000	2.603740000000	-3.138625000000
C	2.195689000000	2.899882000000	-3.891900000000
H	2.256886000000	3.098022000000	-4.974560000000

H	1.681899000000	3.750232000000	-3.416547000000
H	1.568815000000	2.006226000000	-3.742563000000
C	4.695683000000	1.105126000000	-3.973555000000
H	4.106870000000	0.192555000000	-3.799255000000
H	5.712786000000	0.922797000000	-3.594071000000
H	4.758401000000	1.268589000000	-5.062510000000
C	5.010721000000	4.099262000000	-3.491525000000
H	6.023535000000	3.965117000000	-3.078197000000
H	4.598205000000	5.034583000000	-3.081834000000
H	5.112618000000	4.228395000000	-4.582193000000
Si	3.543674000000	3.774383000000	-0.096405000000
C	5.223839000000	4.625886000000	0.076902000000
H	5.123206000000	5.500730000000	0.741329000000
H	5.633220000000	4.975664000000	-0.881959000000
H	5.957054000000	3.943134000000	0.534546000000
C	2.249933000000	4.989840000000	-0.750098000000
H	1.277197000000	4.485630000000	-0.874877000000
H	2.536170000000	5.421660000000	-1.722324000000
H	2.109167000000	5.822782000000	-0.041397000000
C	3.038703000000	3.205261000000	1.635734000000
H	3.674649000000	2.372276000000	1.976535000000
H	1.991679000000	2.867229000000	1.663502000000
H	3.151109000000	4.034404000000	2.354346000000

TS-Si_{ace}

$G_{qh} = -5326.276060$

$N_{imag} = 1, -261 \text{ cm}^{-1}$

$SP = -5320.892679$

$G_{sp} = -5319.364214$

Si	-1.610424000000	0.494702000000	-0.080077000000
Si	1.610417000000	0.494730000000	0.080064000000
C	-0.608815000000	0.384558000000	-1.597082000000
C	0.778682000000	0.272305000000	-1.527794000000
C	0.608806000000	0.384548000000	1.597068000000
C	-0.778696000000	0.272288000000	1.527783000000
C	-1.370778000000	0.606674000000	-2.900733000000
H	-2.443984000000	0.666022000000	-2.670862000000
H	-1.267803000000	-0.263473000000	-3.564899000000
C	-0.973039000000	1.880418000000	-3.663016000000
H	-0.907821000000	2.742127000000	-2.982243000000
H	-1.716460000000	2.113183000000	-4.442316000000
H	0.004366000000	1.785028000000	-4.156791000000
C	1.696329000000	0.191967000000	-2.745738000000
H	2.701556000000	-0.075489000000	-2.388971000000
H	1.811394000000	1.201368000000	-3.175958000000
C	1.330840000000	-0.785427000000	-3.873891000000
H	0.989395000000	-1.750734000000	-3.475939000000
H	2.215299000000	-0.979481000000	-4.502181000000
H	0.546814000000	-0.398929000000	-4.538964000000
C	1.370770000000	0.606668000000	2.900717000000
H	1.267784000000	-0.263468000000	3.564895000000
H	2.443977000000	0.666004000000	2.670848000000
C	0.973040000000	1.880431000000	3.662971000000
H	0.907896000000	2.742140000000	2.982187000000
H	1.716424000000	2.113170000000	4.442314000000
H	-0.004400000000	1.785084000000	4.156686000000
C	-1.696348000000	0.191947000000	2.745725000000
H	-2.701579000000	-0.075506000000	2.388961000000
H	-1.811406000000	1.201347000000	3.175950000000
C	-1.330858000000	-0.785452000000	3.873874000000
H	-0.989439000000	-1.750768000000	3.475917000000

H	-2.215309000000	-0.979487000000	4.502180000000
H	-0.546809000000	-0.398968000000	4.538928000000
C	-3.466237000000	0.075069000000	-0.159096000000
C	-4.441388000000	0.934029000000	0.439771000000
C	-5.783551000000	0.532913000000	0.496973000000
H	-6.501440000000	1.206880000000	0.966482000000
C	-6.233213000000	-0.682973000000	-0.028746000000
C	-5.281208000000	-1.496889000000	-0.640060000000
H	-5.589336000000	-2.445357000000	-1.071044000000
C	-3.915158000000	-1.158471000000	-0.722256000000
C	-4.109768000000	2.311383000000	0.975376000000
H	-3.011913000000	2.423483000000	1.020182000000
Si	-4.658786000000	3.619401000000	-0.328768000000
C	-3.900484000000	3.176046000000	-1.999707000000
H	-4.210411000000	3.911776000000	-2.760458000000
H	-4.255825000000	2.184224000000	-2.320889000000
H	-2.803051000000	3.148046000000	-1.990858000000
C	-4.064821000000	5.338159000000	0.201491000000
H	-2.981090000000	5.358343000000	0.401559000000
H	-4.576963000000	5.688080000000	1.111549000000
H	-4.269154000000	6.069043000000	-0.598479000000
C	-6.526131000000	3.651232000000	-0.622012000000
H	-6.750782000000	4.441598000000	-1.358326000000
H	-7.119285000000	3.853552000000	0.280043000000
H	-6.863124000000	2.694469000000	-1.049356000000
Si	-4.659815000000	2.697542000000	2.782169000000
C	-3.319999000000	3.798373000000	3.538440000000
H	-2.332528000000	3.310235000000	3.510734000000
H	-3.553124000000	4.033725000000	4.590141000000
H	-3.233176000000	4.750007000000	2.990619000000
C	-6.309359000000	3.627355000000	2.898467000000
H	-6.515637000000	3.836377000000	3.961724000000
H	-7.149518000000	3.027058000000	2.513336000000
H	-6.306283000000	4.590481000000	2.366035000000
C	-4.896132000000	1.134654000000	3.824829000000
H	-3.945565000000	0.706684000000	4.170589000000
H	-5.435021000000	0.355405000000	3.263650000000
H	-5.494354000000	1.385275000000	4.716715000000
C	-7.716170000000	-1.071298000000	0.086402000000
C	-8.583896000000	0.002914000000	-0.606707000000
H	-9.651647000000	-0.263797000000	-0.542845000000
H	-8.316925000000	0.094809000000	-1.671718000000
H	-8.459957000000	0.993059000000	-0.143268000000
C	-8.097204000000	-1.156064000000	1.581939000000
H	-9.158307000000	-1.432899000000	1.695733000000
H	-7.944250000000	-0.195482000000	2.097159000000
H	-7.487474000000	-1.914322000000	2.098710000000
C	-8.014003000000	-2.431774000000	-0.568458000000
H	-7.440555000000	-3.246316000000	-0.099459000000
H	-7.781461000000	-2.425555000000	-1.644995000000
H	-9.083208000000	-2.672932000000	-0.461059000000
C	-3.015149000000	-2.169397000000	-1.411145000000
H	-2.001161000000	-1.750532000000	-1.527684000000
Si	-2.706313000000	-3.702635000000	-0.295380000000
C	-1.868412000000	-3.115089000000	1.285073000000
H	-2.530382000000	-2.410445000000	1.809406000000
H	-0.921005000000	-2.591449000000	1.087693000000
H	-1.668956000000	-3.960404000000	1.963855000000
C	-4.301939000000	-4.576706000000	0.226364000000
H	-4.042979000000	-5.466757000000	0.824717000000
H	-4.912952000000	-4.910055000000	-0.625165000000

H	-4.921377000000	-3.918674000000	0.855403000000
C	-1.580484000000	-4.943877000000	-1.173320000000
H	-1.275129000000	-5.728098000000	-0.460960000000
H	-0.666006000000	-4.459212000000	-1.547004000000
H	-2.079841000000	-5.437112000000	-2.021642000000
Si	-3.555843000000	-2.580105000000	-3.212818000000
C	-4.439883000000	-1.106539000000	-4.004088000000
H	-3.780101000000	-0.234517000000	-4.119107000000
H	-5.303845000000	-0.797080000000	-3.395175000000
H	-4.808875000000	-1.387834000000	-5.004610000000
C	-4.751104000000	-4.049385000000	-3.331889000000
H	-5.697255000000	-3.872697000000	-2.796303000000
H	-4.311105000000	-4.982067000000	-2.946047000000
H	-5.000403000000	-4.215936000000	-4.393473000000
C	-2.024490000000	-3.032508000000	-4.227457000000
H	-2.305852000000	-3.192976000000	-5.281685000000
H	-1.555615000000	-3.958024000000	-3.860855000000
H	-1.261016000000	-2.241232000000	-4.200593000000
C	3.466227000000	0.075061000000	0.159067000000
C	3.915130000000	-1.158471000000	0.722261000000
C	5.281183000000	-1.496890000000	0.640061000000
H	5.589297000000	-2.445349000000	1.071128000000
C	6.233208000000	-0.682989000000	0.028814000000
C	5.783560000000	0.532882000000	-0.496952000000
H	6.501464000000	1.206837000000	-0.966453000000
C	4.441397000000	0.934003000000	-0.439791000000
C	3.015101000000	-2.169396000000	1.411128000000
H	2.001115000000	-1.750527000000	1.527657000000
Si	3.555763000000	-2.580145000000	3.212801000000
C	4.439820000000	-1.106613000000	4.004117000000
H	3.780053000000	-0.234577000000	4.119123000000
H	5.303811000000	-0.797166000000	3.395240000000
H	4.808767000000	-1.387929000000	5.004649000000
C	4.750993000000	-4.049452000000	3.331865000000
H	5.000271000000	-4.216023000000	4.393452000000
H	5.697157000000	-3.872770000000	2.796300000000
H	4.310987000000	-4.982121000000	2.946001000000
C	2.024378000000	-3.032522000000	4.227405000000
H	1.555364000000	-3.957908000000	3.860653000000
H	1.261013000000	-2.241136000000	4.200698000000
H	2.305745000000	-3.193211000000	5.281598000000
Si	2.706281000000	-3.702622000000	0.295338000000
C	4.301919000000	-4.576665000000	-0.226414000000
H	4.921369000000	-3.918606000000	-0.855413000000
H	4.042969000000	-5.466689000000	-0.824812000000
H	4.912916000000	-4.910053000000	0.625110000000
C	1.868380000000	-3.115065000000	-1.285110000000
H	0.921002000000	-2.591375000000	-1.087726000000
H	1.668872000000	-3.960381000000	-1.963872000000
H	2.530378000000	-2.410463000000	-1.809465000000
C	1.580464000000	-4.943906000000	1.173239000000
H	2.079753000000	-5.437030000000	2.021664000000
H	1.275282000000	-5.728211000000	0.460896000000
H	0.665887000000	-4.459304000000	1.546764000000
C	7.716168000000	-1.071320000000	-0.086277000000
C	8.097232000000	-1.156180000000	-1.581802000000
H	7.944316000000	-0.195620000000	-2.097075000000
H	7.487490000000	-1.914448000000	-2.098544000000
H	9.158329000000	-1.433051000000	-1.695559000000
C	8.583885000000	0.002933000000	0.606780000000
H	9.651636000000	-0.263786000000	0.542954000000

H	8.316895000000	0.094896000000	1.671781000000
H	8.459959000000	0.993049000000	0.143276000000
C	8.013987000000	-2.431755000000	0.568676000000
H	9.083200000000	-2.672907000000	0.461340000000
H	7.440570000000	-3.246331000000	0.099700000000
H	7.781396000000	-2.425475000000	1.645203000000
C	4.109807000000	2.311356000000	-0.975413000000
H	3.011956000000	2.423508000000	-1.020225000000
Si	4.659891000000	2.697466000000	-2.782202000000
C	3.320126000000	3.798333000000	-3.538512000000
H	3.553276000000	4.033655000000	-4.590214000000
H	3.233352000000	4.749983000000	-2.990708000000
H	2.332629000000	3.310250000000	-3.510806000000
C	4.896201000000	1.134552000000	-3.824821000000
H	3.945624000000	0.706253000000	-4.170137000000
H	5.435548000000	0.355518000000	-3.263782000000
H	5.493989000000	1.385258000000	-4.716975000000
C	6.309459000000	3.627233000000	-2.898522000000
H	7.149598000000	3.026946000000	-2.513335000000
H	6.306387000000	4.590393000000	-2.366153000000
H	6.515764000000	3.836184000000	-3.961788000000
Si	4.658826000000	3.619379000000	0.328729000000
C	6.526171000000	3.651273000000	0.621969000000
H	6.750803000000	4.441690000000	1.358235000000
H	7.119323000000	3.853551000000	-0.280096000000
H	6.863185000000	2.694544000000	1.049374000000
C	4.064818000000	5.338109000000	-0.201562000000
H	2.981136000000	5.358208000000	-0.401912000000
H	4.577153000000	5.688097000000	-1.111487000000
H	4.268899000000	6.068989000000	0.598476000000
C	3.900588000000	3.175983000000	1.999692000000
H	4.255962000000	2.184154000000	2.320818000000
H	2.803157000000	3.147950000000	1.990909000000
H	4.210546000000	3.911692000000	2.760451000000
C	-0.612130000000	3.199524000000	-0.066677000000
C	0.612152000000	3.199575000000	0.066989000000
H	1.613922000000	3.561498000000	0.193865000000
H	-1.613956000000	3.561313000000	-0.193455000000

TS-Ge_{ace}

G_{qh} = -8900.998910

N_{imag} = 1, -198 cm⁻¹

SP = -8894.001705

G_{sp} = -8892.478580

Ge	-1.643413000000	-0.523954000000	0.081131000000
Ge	1.643418000000	-0.523912000000	-0.081052000000
C	-0.606344000000	-0.388633000000	1.662432000000
C	0.774917000000	-0.283654000000	1.590931000000
C	0.606341000000	-0.388627000000	-1.662345000000
C	-0.774903000000	-0.283665000000	-1.590844000000
C	-1.380107000000	-0.597378000000	2.957791000000
H	-2.453246000000	-0.633795000000	2.722304000000
H	-1.261978000000	0.270095000000	3.623584000000
C	-1.010021000000	-1.879154000000	3.719814000000
H	-0.990230000000	-2.746566000000	3.043475000000
H	-1.742901000000	-2.081985000000	4.517399000000
H	-0.018326000000	-1.812617000000	4.189751000000
C	1.707636000000	-0.213147000000	2.795360000000
H	2.708679000000	0.054396000000	2.425693000000
H	1.826621000000	-1.225026000000	3.220730000000
C	1.357014000000	0.761005000000	3.930442000000

H	1.038954000000	1.736793000000	3.538159000000
H	2.241961000000	0.929745000000	4.565341000000
H	0.560732000000	0.385027000000	4.586849000000
C	1.380107000000	-0.597351000000	-2.957707000000
H	1.261972000000	0.270131000000	-3.623489000000
H	2.453246000000	-0.633761000000	-2.722218000000
C	1.010036000000	-1.879118000000	-3.719748000000
H	0.990264000000	-2.746541000000	-3.043422000000
H	1.742913000000	-2.081924000000	-4.517342000000
H	0.018336000000	-1.812590000000	-4.189677000000
C	-1.707620000000	-0.213168000000	-2.795275000000
H	-2.708672000000	0.054352000000	-2.425614000000
H	-1.826580000000	-1.225047000000	-3.220653000000
C	-1.357005000000	0.761001000000	-3.930346000000
H	-1.038951000000	1.736785000000	-3.538050000000
H	-2.241952000000	0.929747000000	-4.565244000000
H	-0.560720000000	0.385036000000	-4.586757000000
C	-3.562909000000	-0.040132000000	0.154506000000
C	-4.543024000000	-0.896001000000	-0.429301000000
C	-5.882287000000	-0.481252000000	-0.471999000000
H	-6.613527000000	-1.151636000000	-0.925708000000
C	-6.311631000000	0.744588000000	0.048609000000
C	-5.343971000000	1.555626000000	0.639760000000
H	-5.636113000000	2.512261000000	1.064216000000
C	-3.980771000000	1.201293000000	0.711881000000
C	-4.222762000000	-2.277146000000	-0.962781000000
H	-3.124795000000	-2.389289000000	-1.021049000000
Si	-4.746533000000	-3.581055000000	0.353426000000
C	-3.923477000000	-3.147388000000	1.995535000000
H	-4.202207000000	-3.882762000000	2.768459000000
H	-4.258066000000	-2.153981000000	2.333386000000
H	-2.827035000000	-3.124498000000	1.935262000000
C	-4.188990000000	-5.306577000000	-0.194662000000
H	-3.111814000000	-5.341164000000	-0.426158000000
H	-4.731820000000	-5.650195000000	-1.089166000000
H	-4.378599000000	-6.035062000000	0.611105000000
C	-6.605680000000	-3.590278000000	0.693555000000
H	-6.824497000000	-4.373017000000	1.439628000000
H	-7.219186000000	-3.791522000000	-0.195470000000
H	-6.922696000000	-2.626271000000	1.120053000000
Si	-4.797668000000	-2.659332000000	-2.760436000000
C	-3.485241000000	-3.781977000000	-3.532375000000
H	-2.490355000000	-3.308544000000	-3.516024000000
H	-3.733949000000	-4.011915000000	-4.581687000000
H	-3.406594000000	-4.735858000000	-2.987407000000
C	-6.464834000000	-3.559570000000	-2.852341000000
H	-6.695833000000	-3.762616000000	-3.911634000000
H	-7.287284000000	-2.947157000000	-2.448601000000
H	-6.466860000000	-4.524014000000	-2.322004000000
C	-5.012387000000	-1.092460000000	-3.799310000000
H	-4.054273000000	-0.638688000000	-4.086415000000
H	-5.598952000000	-0.332446000000	-3.260016000000
H	-5.554360000000	-1.346200000000	-4.725690000000
C	-7.792873000000	1.145305000000	-0.048695000000
C	-8.658061000000	0.090327000000	0.676477000000
H	-9.724764000000	0.363885000000	0.624439000000
H	-8.375107000000	0.015128000000	1.738676000000
H	-8.548170000000	-0.908800000000	0.228856000000
C	-8.199385000000	1.210194000000	-1.538439000000
H	-9.259415000000	1.496387000000	-1.638314000000
H	-8.065793000000	0.239928000000	-2.040751000000

H	-7.590984000000	1.953501000000	-2.077994000000
C	-8.067226000000	2.518727000000	0.589165000000
H	-7.493164000000	3.319964000000	0.098405000000
H	-7.817900000000	2.527144000000	1.661914000000
H	-9.135616000000	2.768839000000	0.494711000000
C	-3.054094000000	2.198923000000	1.383818000000
H	-2.049654000000	1.756042000000	1.496240000000
Si	-2.719612000000	3.714183000000	0.251974000000
C	-1.892376000000	3.099895000000	-1.324761000000
H	-2.561639000000	2.395719000000	-1.840739000000
H	-0.949208000000	2.569816000000	-1.124000000000
H	-1.685554000000	3.935988000000	-2.012829000000
C	-4.304331000000	4.607100000000	-0.270525000000
H	-4.037217000000	5.486300000000	-0.881156000000
H	-4.903644000000	4.959042000000	0.582032000000
H	-4.938565000000	3.950838000000	-0.886591000000
C	-1.571189000000	4.945199000000	1.114958000000
H	-1.263518000000	5.723242000000	0.397077000000
H	-0.658658000000	4.451336000000	1.481785000000
H	-2.056931000000	5.447113000000	1.966038000000
Si	-3.565602000000	2.633749000000	3.187037000000
C	-4.461912000000	1.179222000000	3.999203000000
H	-3.816431000000	0.295262000000	4.104127000000
H	-5.342406000000	0.884354000000	3.406952000000
H	-4.807018000000	1.469191000000	5.005757000000
C	-4.736323000000	4.122318000000	3.307314000000
H	-5.691294000000	3.954261000000	2.784724000000
H	-4.286833000000	5.043762000000	2.905694000000
H	-4.970365000000	4.304329000000	4.369833000000
C	-2.012646000000	3.068537000000	4.176887000000
H	-2.269682000000	3.207742000000	5.240301000000
H	-1.553256000000	4.001782000000	3.818054000000
H	-1.248831000000	2.279281000000	4.116445000000
C	3.562918000000	-0.040119000000	-0.154486000000
C	3.980774000000	1.201297000000	-0.711886000000
C	5.343984000000	1.555607000000	-0.639829000000
H	5.636123000000	2.512235000000	-1.064302000000
C	6.311658000000	0.744553000000	-0.048721000000
C	5.882315000000	-0.481274000000	0.471917000000
H	6.613564000000	-1.151670000000	0.925594000000
C	4.543042000000	-0.895995000000	0.429283000000
C	3.054084000000	2.198941000000	-1.383784000000
H	2.049631000000	1.756076000000	-1.496162000000
Si	3.565515000000	2.633768000000	-3.187025000000
C	4.461766000000	1.179234000000	-3.999245000000
H	3.816252000000	0.295303000000	-4.104202000000
H	5.342251000000	0.884309000000	-3.407008000000
H	4.806881000000	1.469228000000	-5.005788000000
C	4.736250000000	4.122321000000	-3.307351000000
H	4.970241000000	4.304335000000	-4.369880000000
H	5.691245000000	3.954250000000	-2.784808000000
H	4.286791000000	5.043770000000	-2.905703000000
C	2.012517000000	3.068580000000	-4.176799000000
H	1.553171000000	4.001844000000	-3.817959000000
H	1.248684000000	2.279346000000	-4.116302000000
H	2.269500000000	3.207759000000	-5.240229000000
Si	2.719677000000	3.714203000000	-0.251920000000
C	4.304433000000	4.607102000000	0.270503000000
H	4.938688000000	3.950832000000	0.886539000000
H	4.037358000000	5.486305000000	0.881146000000
H	4.903709000000	4.959037000000	-0.582083000000

C	1.892512000000	3.099922000000	1.324856000000
H	0.949334000000	2.569846000000	1.124139000000
H	1.685724000000	3.936019000000	2.012929000000
H	2.561797000000	2.395747000000	1.840808000000
C	1.571225000000	4.945233000000	-1.114847000000
H	2.056934000000	5.447144000000	-1.965947000000
H	1.263594000000	5.723277000000	-0.396950000000
H	0.658674000000	4.451379000000	-1.481634000000
C	7.792914000000	1.145238000000	0.048500000000
C	8.199521000000	1.210096000000	1.538220000000
H	8.065950000000	0.239825000000	2.040525000000
H	7.591163000000	1.953403000000	2.077826000000
H	9.259561000000	1.496274000000	1.638033000000
C	8.658033000000	0.090251000000	-0.676740000000
H	9.724746000000	0.363780000000	-0.624760000000
H	8.375015000000	0.015078000000	-1.738924000000
H	8.548141000000	-0.908881000000	-0.229130000000
C	8.067258000000	2.518663000000	-0.589356000000
H	9.135659000000	2.768752000000	-0.494960000000
H	7.493240000000	3.319905000000	-0.098553000000
H	7.817872000000	2.527100000000	-1.662091000000
C	4.222762000000	-2.277125000000	0.962787000000
H	3.124799000000	-2.389214000000	1.021149000000
Si	4.797766000000	-2.659295000000	2.760412000000
C	3.485347000000	-3.781887000000	3.532443000000
H	3.734140000000	-4.011866000000	4.581726000000
H	3.406599000000	-4.735750000000	2.987458000000
H	2.490484000000	-3.308402000000	3.516197000000
C	5.012577000000	-1.092398000000	3.799227000000
H	4.054488000000	-0.638462000000	4.086158000000
H	5.599324000000	-0.332505000000	3.259962000000
H	5.554385000000	-1.346152000000	4.725699000000
C	6.464909000000	-3.559582000000	2.852258000000
H	7.287353000000	-2.947215000000	2.448438000000
H	6.466871000000	-4.524051000000	2.321968000000
H	6.695966000000	-3.762583000000	3.911547000000
Si	4.746402000000	-3.581085000000	-0.353430000000
C	6.605530000000	-3.590364000000	-0.693657000000
H	6.824292000000	-4.373131000000	-1.439716000000
H	7.219076000000	-3.791594000000	0.195344000000
H	6.922547000000	-2.626378000000	-1.120201000000
C	4.188839000000	-5.306573000000	0.194742000000
H	3.111673000000	-5.341127000000	0.426291000000
H	4.731704000000	-5.650177000000	1.089231000000
H	4.378390000000	-6.035089000000	-0.611012000000
C	3.923283000000	-3.147458000000	-1.995528000000
H	4.257818000000	-2.154037000000	-2.333391000000
H	2.826838000000	-3.124624000000	-1.935257000000
H	4.202054000000	-3.882823000000	-2.768446000000
C	-0.613200000000	-3.294481000000	0.034111000000
C	0.613179000000	-3.294490000000	-0.033962000000
H	1.636921000000	-3.606435000000	-0.095761000000
H	-1.636921000000	-3.606497000000	0.095952000000

TS-Sn_{ace}

G_{qh} = -5176.110403

N_{imag} = 1, -170 cm⁻¹

SP = -5170.053789

G_{sp} = -5168.538780

Sn	-1.894976000000	-1.107156000000	0.017128000000
Sn	1.634963000000	-0.300714000000	-0.258130000000

C	-0.611063000000	-0.805445000000	1.735486000000
C	0.724455000000	-0.513409000000	1.640898000000
C	0.367574000000	-0.092095000000	-1.937121000000
C	-0.981445000000	-0.232793000000	-1.736664000000
C	-1.213013000000	-1.296846000000	3.046255000000
H	-2.291624000000	-1.069528000000	3.076059000000
H	-0.770257000000	-0.770483000000	3.904796000000
C	-1.029783000000	-2.809775000000	3.252019000000
H	-1.502871000000	-3.378440000000	2.437532000000
H	-1.479588000000	-3.135536000000	4.204116000000
H	0.035477000000	-3.086401000000	3.260312000000
C	1.654488000000	-0.424521000000	2.843328000000
H	2.698647000000	-0.425242000000	2.498794000000
H	1.547655000000	-1.325003000000	3.472640000000
C	1.447253000000	0.826376000000	3.711257000000
H	1.591520000000	1.739796000000	3.120840000000
H	2.167509000000	0.845882000000	4.545893000000
H	0.435250000000	0.869655000000	4.138499000000
C	0.985738000000	0.185075000000	-3.296873000000
H	0.348251000000	0.890402000000	-3.855947000000
H	1.947242000000	0.698411000000	-3.174985000000
C	1.217906000000	-1.073860000000	-4.143186000000
H	1.925255000000	-1.752767000000	-3.646701000000
H	1.635438000000	-0.814975000000	-5.130208000000
H	0.282416000000	-1.632378000000	-4.298930000000
C	-1.963431000000	-0.049996000000	-2.892622000000
H	-2.837743000000	-0.695394000000	-2.727162000000
H	-1.532511000000	-0.386398000000	-3.850717000000
C	-2.470477000000	1.391735000000	-3.045096000000
H	-3.012776000000	1.709043000000	-2.141677000000
H	-3.162767000000	1.472973000000	-3.897381000000
H	-1.639851000000	2.094917000000	-3.214051000000
C	-3.822446000000	0.007789000000	0.166038000000
C	-4.934642000000	-0.518256000000	-0.549736000000
C	-6.096255000000	0.259675000000	-0.682154000000
H	-6.944359000000	-0.165509000000	-1.220403000000
C	-6.207645000000	1.547780000000	-0.148224000000
C	-5.128559000000	2.019810000000	0.599494000000
H	-5.195420000000	2.994665000000	1.073554000000
C	-3.951843000000	1.267118000000	0.807356000000
C	-4.972440000000	-1.929265000000	-1.115782000000
H	-3.938449000000	-2.321052000000	-1.178526000000
Si	-5.778141000000	-3.089758000000	0.191489000000
C	-4.727311000000	-3.085261000000	1.761154000000
H	-5.214377000000	-3.680623000000	2.551432000000
H	-4.596224000000	-2.059325000000	2.135140000000
H	-3.727593000000	-3.511117000000	1.581472000000
C	-5.845209000000	-4.875123000000	-0.441231000000
H	-4.840292000000	-5.231676000000	-0.722329000000
H	-6.503755000000	-5.000388000000	-1.314258000000
H	-6.220245000000	-5.536110000000	0.358079000000
C	-7.510532000000	-2.499697000000	0.662727000000
H	-7.943056000000	-3.180825000000	1.414810000000
H	-8.197240000000	-2.462392000000	-0.195798000000
H	-7.464597000000	-1.491886000000	1.104027000000
Si	-5.650520000000	-2.138094000000	-2.900554000000
C	-4.715254000000	-3.583245000000	-3.687259000000
H	-3.631733000000	-3.376903000000	-3.697009000000
H	-5.037603000000	-3.734346000000	-4.731020000000
H	-4.874856000000	-4.527223000000	-3.143993000000
C	-7.511663000000	-2.502922000000	-2.966338000000

H	-7.808280000000	-2.652184000000	-4.018190000000
H	-8.108037000000	-1.663682000000	-2.573008000000
H	-7.796209000000	-3.407882000000	-2.408694000000
C	-5.375374000000	-0.600660000000	-3.972048000000
H	-4.353335000000	-0.567548000000	-4.376781000000
H	-5.550142000000	0.330014000000	-3.411643000000
H	-6.071583000000	-0.622025000000	-4.827028000000
C	-7.494182000000	2.360199000000	-0.371850000000
C	-8.688938000000	1.602944000000	0.250447000000
H	-9.625530000000	2.165392000000	0.100683000000
H	-8.541421000000	1.464419000000	1.333530000000
H	-8.820629000000	0.606554000000	-0.197930000000
C	-7.727172000000	2.533867000000	-1.889745000000
H	-8.645016000000	3.115521000000	-2.077179000000
H	-7.834973000000	1.565054000000	-2.400690000000
H	-6.882419000000	3.065452000000	-2.356245000000
C	-7.420108000000	3.757780000000	0.267712000000
H	-6.584650000000	4.349028000000	-0.138226000000
H	-7.297788000000	3.701082000000	1.360599000000
H	-8.350987000000	4.311674000000	0.067862000000
C	-2.948955000000	1.820322000000	1.810007000000
H	-2.119025000000	1.102031000000	1.922360000000
Si	-2.029978000000	3.409938000000	1.269932000000
C	-0.843152000000	2.997282000000	-0.132180000000
H	-1.375091000000	2.691438000000	-1.039903000000
H	-0.183252000000	2.163539000000	0.150321000000
H	-0.216798000000	3.870886000000	-0.371861000000
C	-3.191704000000	4.779960000000	0.673846000000
H	-2.598914000000	5.673371000000	0.414175000000
H	-3.927276000000	5.074000000000	1.438558000000
H	-3.742736000000	4.467710000000	-0.226977000000
C	-0.979367000000	4.088928000000	2.693706000000
H	-0.357453000000	4.918476000000	2.317893000000
H	-0.299378000000	3.318899000000	3.090412000000
H	-1.584897000000	4.475974000000	3.527808000000
Si	-3.751640000000	1.888552000000	3.557895000000
C	-4.965047000000	0.450856000000	3.754788000000
H	-4.441582000000	-0.517474000000	3.725739000000
H	-5.720218000000	0.448694000000	2.953800000000
H	-5.485340000000	0.520748000000	4.724658000000
C	-4.697456000000	3.502357000000	3.872198000000
H	-5.529402000000	3.644865000000	3.165443000000
H	-4.041813000000	4.385184000000	3.807781000000
H	-5.125627000000	3.480308000000	4.888458000000
C	-2.446824000000	1.726887000000	4.920953000000
H	-2.941369000000	1.794086000000	5.904833000000
H	-1.679232000000	2.512341000000	4.876785000000
H	-1.940545000000	0.752059000000	4.870704000000
C	3.813121000000	0.004660000000	-0.206649000000
C	4.360620000000	1.237053000000	-0.652280000000
C	5.738051000000	1.477778000000	-0.464565000000
H	6.135154000000	2.425250000000	-0.815592000000
C	6.593232000000	0.560745000000	0.144601000000
C	6.034494000000	-0.656265000000	0.547445000000
H	6.678860000000	-1.410100000000	1.000924000000
C	4.676213000000	-0.967543000000	0.376825000000
C	3.573316000000	2.327954000000	-1.354529000000
H	2.516748000000	2.016538000000	-1.465985000000
Si	4.177758000000	2.578317000000	-3.169222000000
C	4.725943000000	0.905971000000	-3.864154000000
H	3.919542000000	0.157465000000	-3.852302000000

H	5.562249000000	0.502259000000	-3.271746000000
H	5.065978000000	1.019027000000	-4.906975000000
C	5.646403000000	3.765266000000	-3.321251000000
H	5.955053000000	3.809510000000	-4.379367000000
H	6.521976000000	3.447526000000	-2.734568000000
H	5.378466000000	4.788371000000	-3.013687000000
C	2.787946000000	3.311863000000	-4.223885000000
H	2.607943000000	4.366655000000	-3.967370000000
H	1.837052000000	2.771372000000	-4.113015000000
H	3.075105000000	3.272041000000	-5.288202000000
Si	3.417263000000	3.919681000000	-0.288660000000
C	5.072539000000	4.726534000000	0.149541000000
H	5.648909000000	4.094552000000	0.842629000000
H	4.870777000000	5.682903000000	0.661523000000
H	5.703354000000	4.941095000000	-0.725235000000
C	2.611907000000	3.430843000000	1.341757000000
H	1.613387000000	2.998445000000	1.192486000000
H	2.505894000000	4.297403000000	2.014751000000
H	3.237933000000	2.680726000000	1.849933000000
C	2.354550000000	5.185914000000	-1.207548000000
H	2.923821000000	5.682216000000	-2.009816000000
H	2.011879000000	5.967952000000	-0.509774000000
H	1.464430000000	4.722423000000	-1.660370000000
C	8.087970000000	0.835510000000	0.378133000000
C	8.374681000000	0.788096000000	1.896166000000
H	8.126668000000	-0.193632000000	2.327834000000
H	7.783033000000	1.548400000000	2.430511000000
H	9.441748000000	0.981589000000	2.094325000000
C	8.928083000000	-0.245039000000	-0.338891000000
H	10.004109000000	-0.058232000000	-0.189345000000
H	8.727692000000	-0.242353000000	-1.422318000000
H	8.709805000000	-1.254710000000	0.039474000000
C	8.517017000000	2.213936000000	-0.154600000000
H	9.590169000000	2.371260000000	0.035871000000
H	7.968908000000	3.032773000000	0.336258000000
H	8.357476000000	2.299135000000	-1.241012000000
C	4.240761000000	-2.367351000000	0.753810000000
H	3.136943000000	-2.419600000000	0.753132000000
Si	4.698888000000	-2.969222000000	2.530499000000
C	3.275564000000	-4.071516000000	3.102845000000
H	3.438338000000	-4.425119000000	4.134204000000
H	3.168453000000	-4.955031000000	2.454186000000
H	2.320441000000	-3.523629000000	3.077139000000
C	4.956941000000	-1.538458000000	3.742648000000
H	4.017818000000	-1.052901000000	4.040956000000
H	5.617293000000	-0.766540000000	3.317795000000
H	5.436698000000	-1.929163000000	4.655665000000
C	6.305976000000	-3.974172000000	2.607982000000
H	7.185612000000	-3.366322000000	2.340938000000
H	6.299914000000	-4.865881000000	1.963646000000
H	6.448805000000	-4.316425000000	3.646816000000
Si	4.793448000000	-3.566436000000	-0.657514000000
C	6.666325000000	-3.589162000000	-0.903711000000
H	6.907152000000	-4.335053000000	-1.679982000000
H	7.230639000000	-3.851638000000	0.001623000000
H	7.021509000000	-2.610079000000	-1.258777000000
C	4.170921000000	-5.320414000000	-0.310892000000
H	3.081470000000	-5.350324000000	-0.150186000000
H	4.652673000000	-5.764929000000	0.573572000000
H	4.396365000000	-5.968125000000	-1.174478000000
C	4.071320000000	-2.964545000000	-2.297905000000

H	4.311218000000	-1.902094000000	-2.459789000000
H	2.980073000000	-3.080177000000	-2.365589000000
H	4.511575000000	-3.541659000000	-3.128041000000
C	-0.386864000000	-3.643296000000	-0.515707000000
C	0.811014000000	-3.385222000000	-0.557600000000
H	1.876564000000	-3.425794000000	-0.629857000000
H	-1.341035000000	-4.133686000000	-0.526601000000

TS-Pb_{ace}

G_{qh} = -5133.194874

N_{imag} = 1, -260 cm⁻¹

SP = -5127.090376

G_{sp} = -5125.579154

Pb	-1.928157000000	-1.237406000000	0.014299000000
Pb	1.628473000000	-0.197936000000	-0.282627000000
C	-0.567708000000	-0.757164000000	1.850590000000
C	0.732462000000	-0.408500000000	1.765384000000
C	0.274112000000	0.126430000000	-2.041269000000
C	-1.033593000000	-0.067719000000	-1.795114000000
C	-1.172294000000	-1.237460000000	3.161974000000
H	-2.237782000000	-0.957714000000	3.210614000000
H	-0.691843000000	-0.758080000000	4.029416000000
C	-1.058818000000	-2.762022000000	3.327035000000
H	-1.574279000000	-3.291937000000	2.511232000000
H	-1.508683000000	-3.088984000000	4.278499000000
H	-0.006389000000	-3.085053000000	3.313629000000
C	1.704159000000	-0.243517000000	2.921352000000
H	2.732763000000	-0.177171000000	2.534833000000
H	1.681206000000	-1.153351000000	3.547859000000
C	1.440598000000	0.985294000000	3.804376000000
H	1.483495000000	1.909250000000	3.214631000000
H	2.196240000000	1.059492000000	4.603760000000
H	0.449909000000	0.945037000000	4.278368000000
C	0.923893000000	0.493837000000	-3.355728000000
H	0.241548000000	1.148366000000	-3.925566000000
H	1.826194000000	1.094216000000	-3.183480000000
C	1.297314000000	-0.727386000000	-4.205631000000
H	2.019115000000	-1.367796000000	-3.676016000000
H	1.755072000000	-0.423135000000	-5.160925000000
H	0.410745000000	-1.342479000000	-4.423571000000
C	-2.070783000000	0.143294000000	-2.892861000000
H	-2.902349000000	-0.560589000000	-2.735628000000
H	-1.663818000000	-0.098279000000	-3.891742000000
C	-2.654983000000	1.563018000000	-2.913601000000
H	-3.131666000000	1.801897000000	-1.951294000000
H	-3.419292000000	1.656792000000	-3.700568000000
H	-1.872720000000	2.313813000000	-3.109302000000
C	-3.898744000000	0.074540000000	0.182010000000
C	-5.024999000000	-0.415867000000	-0.530826000000
C	-6.150053000000	0.412181000000	-0.685699000000
H	-7.015667000000	0.014864000000	-1.217242000000
C	-6.204149000000	1.715169000000	-0.181443000000
C	-5.106499000000	2.153832000000	0.559571000000
H	-5.131023000000	3.141084000000	1.010802000000
C	-3.965691000000	1.351861000000	0.788783000000
C	-5.130283000000	-1.835712000000	-1.072746000000
H	-4.118708000000	-2.273330000000	-1.156176000000
Si	-5.964669000000	-2.937889000000	0.265636000000
C	-4.865420000000	-2.997606000000	1.801873000000
H	-5.376606000000	-3.532387000000	2.619724000000
H	-4.631518000000	-1.980868000000	2.149425000000

H	-3.914798000000	-3.516802000000	1.599504000000
C	-6.172001000000	-4.720833000000	-0.344461000000
H	-5.202572000000	-5.149521000000	-0.648087000000
H	-6.862523000000	-4.809403000000	-1.196937000000
H	-6.569207000000	-5.345073000000	0.473566000000
C	-7.640572000000	-2.231014000000	0.777964000000
H	-8.102741000000	-2.878786000000	1.541713000000
H	-8.340839000000	-2.148978000000	-0.066811000000
H	-7.516186000000	-1.226843000000	1.212252000000
Si	-5.846296000000	-2.038618000000	-2.842161000000
C	-5.012580000000	-3.552739000000	-3.614868000000
H	-3.918817000000	-3.412760000000	-3.645894000000
H	-5.360570000000	-3.702085000000	-4.650648000000
H	-5.219734000000	-4.475829000000	-3.052305000000
C	-7.727157000000	-2.291700000000	-2.878029000000
H	-8.047700000000	-2.447598000000	-3.921872000000
H	-8.267692000000	-1.410183000000	-2.496830000000
H	-8.056553000000	-3.164892000000	-2.294867000000
C	-5.490261000000	-0.546277000000	-3.950918000000
H	-4.445149000000	-0.534470000000	-4.293332000000
H	-5.690226000000	0.405436000000	-3.436325000000
H	-6.134143000000	-0.595700000000	-4.845047000000
C	-7.450445000000	2.581284000000	-0.431513000000
C	-8.681948000000	1.897890000000	0.204291000000
H	-9.590991000000	2.498657000000	0.034320000000
H	-8.545395000000	1.781936000000	1.291442000000
H	-8.857389000000	0.896665000000	-0.217681000000
C	-7.670200000000	2.726953000000	-1.954345000000
H	-8.557261000000	3.348574000000	-2.161073000000
H	-7.824963000000	1.751737000000	-2.440475000000
H	-6.798258000000	3.203050000000	-2.430654000000
C	-7.312724000000	3.990158000000	0.171701000000
H	-6.448418000000	4.530106000000	-0.245069000000
H	-7.197320000000	3.956797000000	1.266230000000
H	-8.215562000000	4.582119000000	-0.047108000000
C	-2.942341000000	1.879530000000	1.787659000000
H	-2.133473000000	1.137144000000	1.898024000000
Si	-1.989796000000	3.455716000000	1.263124000000
C	-0.717552000000	3.014679000000	-0.053515000000
H	-1.176734000000	2.628183000000	-0.969694000000
H	-0.053909000000	2.225889000000	0.330834000000
H	-0.104047000000	3.894043000000	-0.306468000000
C	-3.104101000000	4.822688000000	0.576110000000
H	-2.484372000000	5.699007000000	0.321001000000
H	-3.867850000000	5.149944000000	1.298990000000
H	-3.619749000000	4.494780000000	-0.339785000000
C	-1.004263000000	4.173459000000	2.715502000000
H	-0.368206000000	4.993852000000	2.342575000000
H	-0.341007000000	3.415932000000	3.161048000000
H	-1.643090000000	4.582207000000	3.513551000000
Si	-3.757894000000	1.960489000000	3.529306000000
C	-4.963110000000	0.516451000000	3.728990000000
H	-4.433346000000	-0.448835000000	3.724289000000
H	-5.703507000000	0.497037000000	2.914604000000
H	-5.500898000000	0.598227000000	4.688362000000
C	-4.722996000000	3.568835000000	3.812912000000
H	-5.578541000000	3.665393000000	3.127116000000
H	-4.088876000000	4.461571000000	3.693683000000
H	-5.119949000000	3.578225000000	4.841981000000
C	-2.472120000000	1.824689000000	4.913713000000
H	-2.991856000000	1.834549000000	5.886888000000

H	-1.747980000000	2.651352000000	4.912190000000
H	-1.912528000000	0.880788000000	4.847003000000
C	3.947322000000	0.015820000000	-0.206601000000
C	4.510442000000	1.253525000000	-0.600251000000
C	5.891341000000	1.461550000000	-0.391230000000
H	6.308872000000	2.414567000000	-0.701157000000
C	6.723940000000	0.505438000000	0.190077000000
C	6.139646000000	-0.714625000000	0.544863000000
H	6.763799000000	-1.497190000000	0.979170000000
C	4.775675000000	-0.991789000000	0.352478000000
C	3.745251000000	2.384259000000	-1.267406000000
H	2.684824000000	2.095191000000	-1.399425000000
Si	4.351969000000	2.671961000000	-3.074260000000
C	4.763112000000	0.988700000000	-3.829488000000
H	3.904415000000	0.301624000000	-3.809520000000
H	5.582875000000	0.511206000000	-3.269849000000
H	5.082199000000	1.101720000000	-4.878841000000
C	5.898359000000	3.758209000000	-3.193715000000
H	6.195170000000	3.833698000000	-4.253479000000
H	6.756339000000	3.349979000000	-2.638318000000
H	5.707872000000	4.780986000000	-2.831981000000
C	3.011107000000	3.542728000000	-4.089080000000
H	2.926103000000	4.603822000000	-3.810733000000
H	2.017407000000	3.085503000000	-3.975133000000
H	3.278256000000	3.499570000000	-5.158509000000
Si	3.609530000000	3.938618000000	-0.146583000000
C	5.277111000000	4.698405000000	0.324729000000
H	5.837949000000	4.034922000000	1.000824000000
H	5.093618000000	5.644231000000	0.862331000000
H	5.915317000000	4.923595000000	-0.542403000000
C	2.776308000000	3.395604000000	1.452405000000
H	1.749415000000	3.048885000000	1.272393000000
H	2.726497000000	4.217926000000	2.184607000000
H	3.343544000000	2.568598000000	1.907577000000
C	2.568082000000	5.256249000000	-1.015570000000
H	3.145215000000	5.779232000000	-1.794772000000
H	2.233548000000	6.011877000000	-0.285434000000
H	1.672727000000	4.824370000000	-1.489358000000
C	8.221736000000	0.743896000000	0.445797000000
C	8.495639000000	0.634569000000	1.962961000000
H	8.229859000000	-0.359157000000	2.354837000000
H	7.911173000000	1.382760000000	2.521660000000
H	9.563915000000	0.803612000000	2.176393000000
C	9.048601000000	-0.324025000000	-0.304726000000
H	10.126643000000	-0.161767000000	-0.141415000000
H	8.855929000000	-0.278527000000	-1.388588000000
H	8.810558000000	-1.342697000000	0.035902000000
C	8.680604000000	2.133166000000	-0.031015000000
H	9.754674000000	2.263385000000	0.174262000000
H	8.143090000000	2.943096000000	0.485662000000
H	8.532731000000	2.262046000000	-1.114728000000
C	4.299808000000	-2.389522000000	0.677834000000
H	3.197832000000	-2.415313000000	0.647174000000
Si	4.671182000000	-3.034082000000	2.456903000000
C	3.142145000000	-4.014189000000	2.977578000000
H	3.238197000000	-4.396551000000	4.006918000000
H	2.980858000000	-4.874716000000	2.308523000000
H	2.239700000000	-3.384504000000	2.927635000000
C	5.016101000000	-1.630006000000	3.675111000000
H	4.169651000000	-0.940790000000	3.791996000000
H	5.889192000000	-1.037675000000	3.360418000000

H	5.239182000000	-2.063134000000	4.664748000000
C	6.186171000000	-4.168101000000	2.574699000000
H	7.117591000000	-3.630824000000	2.333162000000
H	6.124609000000	-5.053467000000	1.924294000000
H	6.274321000000	-4.524998000000	3.614694000000
Si	4.852462000000	-3.564632000000	-0.748919000000
C	6.731032000000	-3.700813000000	-0.899966000000
H	6.967024000000	-4.434633000000	-1.689125000000
H	7.228951000000	-4.027556000000	0.023144000000
H	7.163769000000	-2.735203000000	-1.202633000000
C	4.094570000000	-5.279971000000	-0.491014000000
H	2.999160000000	-5.229330000000	-0.382918000000
H	4.496138000000	-5.777107000000	0.405801000000
H	4.316061000000	-5.924470000000	-1.357930000000
C	4.274299000000	-2.858634000000	-2.409776000000
H	4.539225000000	-1.792742000000	-2.488789000000
H	3.193379000000	-2.951289000000	-2.591449000000
H	4.783840000000	-3.395480000000	-3.227160000000
C	-0.159502000000	-3.396842000000	-0.659706000000
C	0.991614000000	-2.943413000000	-0.756430000000
H	2.017766000000	-3.161475000000	-1.003584000000
H	-0.994706000000	-4.073241000000	-0.652847000000

2-Si

$G_{qh} = -5250.242712$

$N_{imag} = 0$

$SP = -5244.938809$

$G_{sp} = -5243.416321$

Si	-1.653697000000	0.887902000000	-0.083523000000
H	-1.790916000000	2.374710000000	-0.059264000000
Si	1.653619000000	0.887762000000	0.082992000000
H	1.791070000000	2.374536000000	0.058742000000
C	-0.589975000000	0.602592000000	-1.622999000000
C	0.764449000000	0.515966000000	-1.556875000000
C	0.589854000000	0.602516000000	1.622413000000
C	-0.764573000000	0.515904000000	1.556306000000
C	-1.377479000000	0.744371000000	-2.923492000000
H	-2.454059000000	0.681463000000	-2.705656000000
H	-1.169138000000	-0.096781000000	-3.597822000000
C	-1.112778000000	2.068119000000	-3.654554000000
H	-1.319958000000	2.926167000000	-2.999221000000
H	-1.760897000000	2.159277000000	-4.541561000000
H	-0.069201000000	2.152245000000	-3.991581000000
C	1.720934000000	0.448102000000	-2.746210000000
H	2.693873000000	0.107627000000	-2.362316000000
H	1.911245000000	1.482848000000	-3.085265000000
C	1.382903000000	-0.420275000000	-3.964508000000
H	1.039734000000	-1.417672000000	-3.658070000000
H	2.284652000000	-0.556808000000	-4.582994000000
H	0.615961000000	0.021314000000	-4.614415000000
C	1.377368000000	0.744101000000	2.922911000000
H	1.169002000000	-0.097137000000	3.597125000000
H	2.453947000000	0.681165000000	2.705052000000
C	1.112708000000	2.067757000000	3.654150000000
H	1.319852000000	2.925882000000	2.998900000000
H	1.760884000000	2.158810000000	4.541125000000
H	0.069152000000	2.151819000000	3.991260000000
C	-1.720970000000	0.448074000000	2.745699000000
H	-2.693904000000	0.107460000000	2.361930000000
H	-1.911331000000	1.482829000000	3.084670000000
C	-1.382656000000	-0.420114000000	3.964062000000

H	-1.039091000000	-1.417394000000	3.657704000000
H	-2.284362000000	-0.556946000000	4.582546000000
H	-0.615895000000	0.021827000000	4.613957000000
C	-3.449372000000	0.213291000000	-0.191895000000
C	-4.522668000000	1.001822000000	0.347058000000
C	-5.846986000000	0.553916000000	0.225332000000
H	-6.637986000000	1.179400000000	0.638520000000
C	-6.192822000000	-0.653444000000	-0.384529000000
C	-5.145445000000	-1.419137000000	-0.887076000000
H	-5.366130000000	-2.372538000000	-1.356657000000
C	-3.793492000000	-1.027182000000	-0.809938000000
C	-4.352314000000	2.332463000000	1.064729000000
H	-3.290742000000	2.527291000000	1.273250000000
Si	-4.832972000000	3.786927000000	-0.099778000000
C	-3.760676000000	3.747926000000	-1.653942000000
H	-4.148886000000	4.461965000000	-2.399488000000
H	-3.765655000000	2.745173000000	-2.109143000000
H	-2.716188000000	4.014616000000	-1.435114000000
C	-4.542138000000	5.436564000000	0.783261000000
H	-3.507239000000	5.507381000000	1.156750000000
H	-5.221519000000	5.585847000000	1.636878000000
H	-4.701487000000	6.271008000000	0.080035000000
C	-6.627859000000	3.687368000000	-0.690046000000
H	-6.850520000000	4.575692000000	-1.305232000000
H	-7.359365000000	3.653884000000	0.129892000000
H	-6.779742000000	2.797700000000	-1.320580000000
Si	-5.152011000000	2.400225000000	2.815966000000
C	-4.066087000000	3.503363000000	3.905656000000
H	-3.046378000000	3.096980000000	4.001205000000
H	-4.491664000000	3.580034000000	4.920071000000
H	-3.983649000000	4.522251000000	3.496721000000
C	-6.908129000000	3.118605000000	2.843714000000
H	-7.261930000000	3.140291000000	3.888278000000
H	-7.619556000000	2.503446000000	2.269736000000
H	-6.958504000000	4.147214000000	2.455198000000
C	-5.285810000000	0.682978000000	3.597788000000
H	-4.304244000000	0.220095000000	3.770393000000
H	-5.871490000000	0.001017000000	2.962548000000
H	-5.795828000000	0.765513000000	4.572220000000
C	-7.664410000000	-1.090325000000	-0.458021000000
C	-8.478008000000	-0.021999000000	-1.221809000000
H	-9.537998000000	-0.317871000000	-1.287498000000
H	-8.093325000000	0.104125000000	-2.246542000000
H	-8.435140000000	0.958936000000	-0.725337000000
C	-8.219184000000	-1.232658000000	0.977578000000
H	-9.274727000000	-1.550243000000	0.955133000000
H	-8.167377000000	-0.282836000000	1.531420000000
H	-7.647115000000	-1.983676000000	1.545593000000
C	-7.834334000000	-2.438736000000	-1.179919000000
H	-7.296008000000	-3.249227000000	-0.664442000000
H	-7.471251000000	-2.392711000000	-2.218689000000
H	-8.899905000000	-2.715163000000	-1.212202000000
C	-2.802002000000	-2.020561000000	-1.397716000000
H	-1.792916000000	-1.578564000000	-1.459576000000
Si	-2.563468000000	-3.496189000000	-0.185872000000
C	-1.759613000000	-2.824347000000	1.380070000000
H	-2.444563000000	-2.101595000000	1.846335000000
H	-0.812441000000	-2.300104000000	1.181727000000
H	-1.569069000000	-3.625433000000	2.112433000000
C	-4.199961000000	-4.289389000000	0.337042000000
H	-3.984777000000	-5.135468000000	1.011722000000

H	-4.780020000000	-4.677654000000	-0.513285000000
H	-4.832219000000	-3.572796000000	0.883109000000
C	-1.475883000000	-4.843057000000	-0.948163000000
H	-1.284382000000	-5.624823000000	-0.195912000000
H	-0.503352000000	-4.447853000000	-1.272368000000
H	-1.957172000000	-5.323179000000	-1.813106000000
Si	-3.215749000000	-2.568741000000	-3.202533000000
C	-4.092698000000	-1.204054000000	-4.179372000000
H	-3.415413000000	-0.387292000000	-4.466413000000
H	-4.922629000000	-0.769996000000	-3.600588000000
H	-4.511450000000	-1.634200000000	-5.104633000000
C	-4.361781000000	-4.081678000000	-3.299770000000
H	-5.364756000000	-3.884348000000	-2.889948000000
H	-3.956666000000	-4.968015000000	-2.789200000000
H	-4.490458000000	-4.344290000000	-4.363469000000
C	-1.610324000000	-3.036107000000	-4.085942000000
H	-1.831347000000	-3.358879000000	-5.117044000000
H	-1.086261000000	-3.860514000000	-3.579940000000
H	-0.916212000000	-2.185583000000	-4.144257000000
C	3.449229000000	0.212941000000	0.191425000000
C	3.793325000000	-1.027530000000	0.809487000000
C	5.145278000000	-1.419442000000	0.886803000000
H	5.365932000000	-2.372785000000	1.356512000000
C	6.192696000000	-0.653709000000	0.384410000000
C	5.846901000000	0.553666000000	-0.225440000000
H	6.637960000000	1.179252000000	-0.638357000000
C	4.522588000000	1.001519000000	-0.347374000000
C	2.801839000000	-2.020752000000	1.397549000000
H	1.792821000000	-1.578619000000	1.459588000000
Si	3.216107000000	-2.568802000000	3.202285000000
C	4.093544000000	-1.204061000000	4.178595000000
H	3.416613000000	-0.386781000000	4.464988000000
H	4.923834000000	-0.770760000000	3.599755000000
H	4.511855000000	-1.633873000000	5.104213000000
C	4.362029000000	-4.081829000000	3.299214000000
H	4.491235000000	-4.344320000000	4.362878000000
H	5.364812000000	-3.884648000000	2.888850000000
H	3.956580000000	-4.968198000000	2.788959000000
C	1.611004000000	-3.035836000000	4.086437000000
H	1.085949000000	-3.859432000000	3.580142000000
H	0.917596000000	-2.184828000000	4.145993000000
H	1.832550000000	-3.359635000000	5.117104000000
Si	2.562823000000	-3.496528000000	0.185943000000
C	4.199076000000	-4.290215000000	-0.336970000000
H	4.831490000000	-3.573881000000	-0.883195000000
H	3.983644000000	-5.136358000000	-1.011491000000
H	4.779066000000	-4.678478000000	0.513401000000
C	1.758935000000	-2.824814000000	-1.380034000000
H	0.811757000000	-2.300560000000	-1.181772000000
H	1.568439000000	-3.625941000000	-2.112366000000
H	2.443893000000	-2.102078000000	-1.846313000000
C	1.475002000000	-4.842995000000	0.948644000000
H	1.956613000000	-5.323549000000	1.813173000000
H	1.282504000000	-5.624471000000	0.196360000000
H	0.502914000000	-4.447305000000	1.273614000000
C	7.664310000000	-1.090447000000	0.458241000000
C	8.219455000000	-1.232717000000	-0.977221000000
H	8.167703000000	-0.282899000000	-1.531073000000
H	7.647602000000	-1.983788000000	-1.545385000000
H	9.275023000000	-1.550199000000	-0.954514000000
C	8.477592000000	-0.022021000000	1.222223000000

H	9.537616000000	-0.317725000000	1.288107000000
H	8.092690000000	0.104004000000	2.246887000000
H	8.434650000000	0.958928000000	0.725781000000
C	7.834213000000	-2.438840000000	1.180181000000
H	8.899809000000	-2.715140000000	1.212726000000
H	7.296109000000	-3.249393000000	0.664570000000
H	7.470874000000	-2.392857000000	2.218862000000
C	4.352366000000	2.332364000000	-1.064710000000
H	3.290839000000	2.527286000000	-1.273326000000
Si	5.152316000000	2.400755000000	-2.815805000000
C	4.066637000000	3.504487000000	-3.905132000000
H	4.492339000000	3.581558000000	-4.919464000000
H	3.984246000000	4.523202000000	-3.495761000000
H	3.046899000000	3.098239000000	-4.000979000000
C	5.286004000000	0.683834000000	-3.598356000000
H	4.304391000000	0.221252000000	-3.771494000000
H	5.871323000000	0.001457000000	-2.963234000000
H	5.796362000000	0.766700000000	-4.572582000000
C	6.908528000000	3.118939000000	-2.843059000000
H	7.619842000000	2.503433000000	-2.269313000000
H	6.959034000000	4.147371000000	-2.454089000000
H	7.262395000000	3.141030000000	-3.887593000000
Si	4.833063000000	3.786401000000	0.100314000000
C	6.627912000000	3.686336000000	0.690605000000
H	6.850664000000	4.574367000000	1.306181000000
H	7.359470000000	3.653091000000	-0.129301000000
H	6.779626000000	2.796366000000	1.320755000000
C	4.542463000000	5.436420000000	-0.782083000000
H	3.507564000000	5.507524000000	-1.155521000000
H	5.221844000000	5.585962000000	-1.635654000000
H	4.701932000000	6.270553000000	-0.078518000000
C	3.760741000000	3.746981000000	1.654463000000
H	3.765619000000	2.744065000000	2.109306000000
H	2.716274000000	4.013876000000	1.435781000000
H	4.149072000000	4.460703000000	2.400248000000

2-Ge

$G_{qh} = -8824.956440$

$N_{imag} = 0$

$SP = -8818.036105$

$G_{sp} = -8816.51982$

Ge	1.684119000000	-0.882729000000	-0.086982000000
H	1.820284000000	-2.424819000000	-0.059428000000
Ge	-1.684168000000	-0.882658000000	0.086854000000
H	-1.820342000000	-2.424753000000	0.059358000000
C	0.585966000000	-0.575982000000	-1.694009000000
C	-0.763143000000	-0.499304000000	-1.623930000000
C	-0.585994000000	-0.575837000000	1.693883000000
C	0.763125000000	-0.499247000000	1.623787000000
C	1.387016000000	-0.689930000000	-2.985327000000
H	2.459495000000	-0.599564000000	-2.757588000000
H	1.161730000000	0.145881000000	-3.661246000000
C	1.160334000000	-2.019343000000	-3.718984000000
H	1.397306000000	-2.872463000000	-3.066758000000
H	1.805123000000	-2.088785000000	-4.610366000000
H	0.116566000000	-2.132509000000	-4.048236000000
C	-1.736539000000	-0.424800000000	-2.795356000000
H	-2.701647000000	-0.076468000000	-2.397294000000
H	-1.939877000000	-1.459483000000	-3.129164000000
C	-1.406718000000	0.439544000000	-4.018411000000
H	-1.066457000000	1.439697000000	-3.715985000000

H	-2.311066000000	0.569540000000	-4.634552000000
H	-0.639127000000	-0.002250000000	-4.667606000000
C	-1.387031000000	-0.689654000000	2.985225000000
H	-1.161636000000	0.146164000000	3.661105000000
H	-2.459510000000	-0.599164000000	2.757520000000
C	-1.160509000000	-2.019062000000	3.718930000000
H	-1.397657000000	-2.872178000000	3.066759000000
H	-1.805266000000	-2.088353000000	4.610347000000
H	-0.116745000000	-2.132390000000	4.048136000000
C	1.736516000000	-0.424674000000	2.795213000000
H	2.701600000000	-0.076267000000	2.397156000000
H	1.939928000000	-1.459339000000	3.129032000000
C	1.406588000000	0.439657000000	4.018256000000
H	1.066144000000	1.439736000000	3.715803000000
H	2.310927000000	0.569833000000	4.634370000000
H	0.639087000000	-0.002245000000	4.667489000000
C	3.545690000000	-0.166039000000	-0.190815000000
C	4.619888000000	-0.945234000000	0.347610000000
C	5.938142000000	-0.475470000000	0.239037000000
H	6.735949000000	-1.092394000000	0.652469000000
C	6.267876000000	0.741733000000	-0.361012000000
C	5.212096000000	1.494230000000	-0.866995000000
H	5.420689000000	2.453726000000	-1.329806000000
C	3.865176000000	1.081299000000	-0.800240000000
C	4.455947000000	-2.287409000000	1.042253000000
H	3.393620000000	-2.490885000000	1.239383000000
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H	3.261099000000	-3.885100000000	-1.808776000000
H	4.729108000000	-4.369998000000	-2.702789000000

2-Pb $G_{qh} = -5057.119676$ $N_{imag} = 0$ $SP = -5051.098097$ $G_{sp} = -5049.595708$

Pb	-1.961969000000	-1.199739000000	-0.048617000000
H	-2.338986000000	-2.924257000000	-0.384975000000
Pb	1.802675000000	-0.899788000000	-0.128916000000
H	2.063065000000	-2.668808000000	-0.336620000000
C	-0.676742000000	-1.265962000000	1.829862000000
C	0.645642000000	-1.017131000000	1.840809000000
C	0.499217000000	-0.399425000000	-1.919927000000
C	-0.839473000000	-0.508448000000	-1.895770000000
C	-1.441860000000	-1.800191000000	3.032483000000
H	-2.476800000000	-1.419762000000	3.026314000000
H	-0.998202000000	-1.439446000000	3.973017000000
C	-1.476287000000	-3.337232000000	3.059894000000
H	-1.923420000000	-3.745490000000	2.141227000000
H	-2.068027000000	-3.702395000000	3.914629000000
H	-0.459281000000	-3.751807000000	3.141602000000
C	1.505053000000	-1.169917000000	3.091881000000
H	2.561911000000	-1.264951000000	2.804979000000
H	1.254033000000	-2.123285000000	3.590407000000
C	1.389050000000	-0.025906000000	4.109288000000
H	1.712520000000	0.926361000000	3.672907000000
H	2.022801000000	-0.226150000000	4.988482000000
H	0.355543000000	0.106647000000	4.459971000000
C	1.304835000000	-0.094679000000	-3.168686000000
H	0.768502000000	0.623239000000	-3.812437000000
H	2.242913000000	0.401014000000	-2.885570000000
C	1.654154000000	-1.352123000000	-3.979410000000
H	2.228695000000	-2.068761000000	-3.373034000000
H	2.264307000000	-1.094003000000	-4.860444000000
H	0.745390000000	-1.867555000000	-4.327573000000
C	-1.723735000000	-0.250004000000	-3.106708000000
H	-2.576692000000	-0.949981000000	-3.098903000000
H	-1.171877000000	-0.474700000000	-4.034699000000
C	-2.262612000000	1.187081000000	-3.176922000000
H	-2.925244000000	1.406409000000	-2.325321000000
H	-2.843168000000	1.347587000000	-4.098041000000
H	-1.437456000000	1.914934000000	-3.165763000000
C	-3.909885000000	-0.004194000000	0.131641000000
C	-5.043614000000	-0.401522000000	-0.630154000000
C	-6.140949000000	0.471555000000	-0.706454000000
H	-7.012776000000	0.150302000000	-1.277344000000
C	-6.166224000000	1.719790000000	-0.075217000000
C	-5.066272000000	2.053512000000	0.714201000000
H	-5.067086000000	2.990290000000	1.263836000000
C	-3.948254000000	1.204760000000	0.867048000000
C	-5.191296000000	-1.765027000000	-1.281053000000
H	-4.205118000000	-2.244514000000	-1.381009000000
Si	-6.101864000000	-2.923690000000	-0.038142000000
C	-5.079041000000	-3.072620000000	1.542922000000
H	-5.643266000000	-3.626478000000	2.311548000000
H	-4.842206000000	-2.076339000000	1.945175000000
H	-4.133557000000	-3.606248000000	1.363981000000
C	-6.302670000000	-4.659880000000	-0.766006000000
H	-5.326158000000	-5.075923000000	-1.063762000000
H	-6.964448000000	-4.683466000000	-1.645363000000
H	-6.733643000000	-5.332117000000	-0.005271000000

C	-7.787971000000	-2.220457000000	0.447771000000
H	-8.287306000000	-2.912486000000	1.146677000000
H	-8.455228000000	-2.069818000000	-0.413463000000
H	-7.668773000000	-1.252110000000	0.958160000000
Si	-5.881352000000	-1.812370000000	-3.071933000000
C	-5.072443000000	-3.285144000000	-3.941235000000
H	-3.975040000000	-3.174622000000	-3.946724000000
H	-5.408169000000	-3.350212000000	-4.989636000000
H	-5.311208000000	-4.240382000000	-3.449355000000
C	-7.765918000000	-2.007728000000	-3.167253000000
H	-8.064075000000	-2.064193000000	-4.227704000000
H	-8.294416000000	-1.148644000000	-2.723240000000
H	-8.129884000000	-2.920000000000	-2.670670000000
C	-5.450234000000	-0.247113000000	-4.040435000000
H	-4.389140000000	-0.236675000000	-4.325901000000
H	-5.655528000000	0.668931000000	-3.466289000000
H	-6.045605000000	-0.213016000000	-4.968171000000
C	-7.389921000000	2.636357000000	-0.240155000000
C	-8.637891000000	1.923201000000	0.327514000000
H	-9.530985000000	2.560780000000	0.219983000000
H	-8.505038000000	1.696722000000	1.397593000000
H	-8.838809000000	0.973801000000	-0.191456000000
C	-7.603278000000	2.934073000000	-1.741489000000
H	-8.476305000000	3.591864000000	-1.885221000000
H	-7.779097000000	2.014780000000	-2.320536000000
H	-6.721180000000	3.436058000000	-2.170065000000
C	-7.218213000000	3.975430000000	0.498143000000
H	-6.338911000000	4.531271000000	0.137093000000
H	-7.108996000000	3.832216000000	1.584506000000
H	-8.104544000000	4.609000000000	0.336800000000
C	-2.911447000000	1.610236000000	1.903015000000
H	-2.153164000000	0.814622000000	1.999046000000
Si	-1.849785000000	3.119355000000	1.393360000000
C	-0.794458000000	2.560930000000	-0.062135000000
H	-1.425818000000	2.095435000000	-0.827650000000
H	-0.056553000000	1.808687000000	0.251589000000
H	-0.255421000000	3.388286000000	-0.543150000000
C	-2.883264000000	4.605598000000	0.847914000000
H	-2.211070000000	5.443865000000	0.598115000000
H	-3.573533000000	4.950151000000	1.633672000000
H	-3.476704000000	4.369095000000	-0.048849000000
C	-0.727144000000	3.651321000000	2.820902000000
H	0.004010000000	4.394073000000	2.463809000000
H	-0.162604000000	2.798560000000	3.227802000000
H	-1.296436000000	4.109391000000	3.644946000000
Si	-3.705366000000	1.680113000000	3.654055000000
C	-5.044592000000	0.351495000000	3.785810000000
H	-4.612683000000	-0.657592000000	3.694199000000
H	-5.802121000000	0.464436000000	2.995073000000
H	-5.550406000000	0.411331000000	4.763896000000
C	-4.487506000000	3.362071000000	4.044959000000
H	-5.314046000000	3.611623000000	3.361938000000
H	-3.750288000000	4.179306000000	3.998833000000
H	-4.898039000000	3.343238000000	5.068492000000
C	-2.407584000000	1.329483000000	4.984988000000
H	-1.581542000000	2.054733000000	4.978477000000
H	-1.979983000000	0.323996000000	4.860686000000
H	-2.883217000000	1.368395000000	5.979459000000
C	3.911476000000	0.026467000000	-0.293638000000
C	4.142456000000	1.316412000000	-0.837499000000
C	5.471453000000	1.705310000000	-1.111590000000

H	5.627157000000	2.693888000000	-1.534492000000
C	6.575953000000	0.910212000000	-0.816884000000
C	6.320504000000	-0.330784000000	-0.226484000000
H	7.160137000000	-0.965784000000	0.053707000000
C	5.021751000000	-0.798737000000	0.040018000000
C	3.083629000000	2.383349000000	-1.059182000000
H	2.072615000000	1.943263000000	-1.002775000000
Si	3.132203000000	3.294085000000	-2.756543000000
C	3.810735000000	2.206414000000	-4.153830000000
H	3.048262000000	1.539636000000	-4.581178000000
H	4.650380000000	1.584919000000	-3.805367000000
H	4.182609000000	2.852136000000	-4.966771000000
C	4.229403000000	4.844625000000	-2.757980000000
H	4.126828000000	5.337968000000	-3.739352000000
H	5.295895000000	4.600112000000	-2.627757000000
H	3.955680000000	5.580952000000	-1.988189000000
C	1.360337000000	3.823824000000	-3.149603000000
H	0.991686000000	4.564639000000	-2.423428000000
H	0.678638000000	2.959475000000	-3.121197000000
H	1.299549000000	4.275170000000	-4.153625000000
Si	3.155173000000	3.575686000000	0.458484000000
C	4.898743000000	4.238284000000	0.776276000000
H	5.591478000000	3.425862000000	1.041717000000
H	4.858343000000	4.943034000000	1.624194000000
H	5.317677000000	4.776031000000	-0.087204000000
C	2.647696000000	2.563965000000	1.960727000000
H	1.644302000000	2.137595000000	1.823806000000
H	2.635730000000	3.171506000000	2.879562000000
H	3.353768000000	1.732141000000	2.102679000000
C	2.007296000000	5.075061000000	0.294167000000
H	2.296242000000	5.741352000000	-0.532419000000
H	2.067172000000	5.660749000000	1.227057000000
H	0.956492000000	4.790772000000	0.149663000000
C	8.023179000000	1.366822000000	-1.064691000000
C	8.750270000000	1.478343000000	0.294911000000
H	8.771458000000	0.513787000000	0.825004000000
H	8.247296000000	2.209222000000	0.948268000000
H	9.793125000000	1.806476000000	0.151711000000
C	8.748520000000	0.332790000000	-1.953607000000
H	9.785272000000	0.652324000000	-2.149505000000
H	8.235705000000	0.219916000000	-2.922133000000
H	8.791197000000	-0.658341000000	-1.478134000000
C	8.088158000000	2.736869000000	-1.763161000000
H	9.138395000000	3.020636000000	-1.934413000000
H	7.626743000000	3.529192000000	-1.153488000000
H	7.583195000000	2.718706000000	-2.741852000000
C	4.917052000000	-2.150619000000	0.721624000000
H	3.860072000000	-2.395141000000	0.908479000000
Si	5.643130000000	-2.113905000000	2.499537000000
C	4.715345000000	-3.372781000000	3.565952000000
H	5.061396000000	-3.313539000000	4.611545000000
H	4.880031000000	-4.403022000000	3.215203000000
H	3.630083000000	-3.186422000000	3.560890000000
C	5.405796000000	-0.381636000000	3.221612000000
H	4.344391000000	-0.091822000000	3.251593000000
H	5.936725000000	0.368521000000	2.614747000000
H	5.797553000000	-0.335059000000	4.251301000000
C	7.487767000000	-2.532925000000	2.583923000000
H	8.100688000000	-1.850974000000	1.973507000000
H	7.687894000000	-3.563816000000	2.251201000000
H	7.834156000000	-2.446659000000	3.627510000000

Si	5.460232000000	-3.585402000000	-0.432633000000
C	7.287076000000	-3.520751000000	-0.926316000000
H	7.542619000000	-4.450748000000	-1.462216000000
H	7.970151000000	-3.427817000000	-0.069436000000
H	7.478574000000	-2.681010000000	-1.611841000000
C	5.120744000000	-5.233714000000	0.431517000000
H	4.089302000000	-5.280084000000	0.817358000000
H	5.808607000000	-5.401085000000	1.276084000000
H	5.254110000000	-6.068425000000	-0.276673000000
C	4.469647000000	-3.488593000000	-2.038517000000
H	4.535150000000	-2.474206000000	-2.464651000000
H	3.406161000000	-3.720083000000	-1.878101000000
H	4.870781000000	-4.196543000000	-2.782897000000

3-Si

$G_{qh} = -5326.354482$

$N_{imag} = 0$

$SP = -5320.984263$

$G_{sp} = -5319.449814$

Si	-1.497321000000	0.475257000000	-0.124729000000
Si	1.497307000000	0.475229000000	0.124652000000
C	-0.546011000000	-0.092998000000	-1.666395000000
C	0.791265000000	-0.241115000000	-1.508574000000
C	0.546001000000	-0.092906000000	1.666358000000
C	-0.791285000000	-0.240968000000	1.508566000000
C	-1.260629000000	0.074939000000	-3.001972000000
H	-2.338589000000	0.172980000000	-2.819517000000
H	-1.140955000000	-0.803239000000	-3.647982000000
C	-0.796219000000	1.331660000000	-3.754457000000
H	-0.862104000000	2.222361000000	-3.112650000000
H	-1.421195000000	1.506727000000	-4.645415000000
H	0.248410000000	1.248695000000	-4.087707000000
C	1.805575000000	-0.513548000000	-2.607448000000
H	2.703081000000	-0.946115000000	-2.139109000000
H	2.151358000000	0.465396000000	-2.987356000000
C	1.407257000000	-1.399363000000	-3.795440000000
H	0.852019000000	-2.288550000000	-3.462540000000
H	2.310764000000	-1.746654000000	-4.322054000000
H	0.786313000000	-0.875719000000	-4.534789000000
C	1.260722000000	0.074971000000	3.001887000000
H	1.141214000000	-0.803269000000	3.647854000000
H	2.338647000000	0.173117000000	2.819300000000
C	0.796298000000	1.331575000000	3.754550000000
H	0.861937000000	2.222329000000	3.112792000000
H	1.421438000000	1.506662000000	4.645390000000
H	-0.248244000000	1.248436000000	4.088027000000
C	-1.805548000000	-0.513399000000	2.607492000000
H	-2.703109000000	-0.945866000000	2.139159000000
H	-2.151220000000	0.465519000000	2.987568000000
C	-1.407190000000	-1.399384000000	3.795342000000
H	-0.852147000000	-2.288629000000	3.462271000000
H	-2.310669000000	-1.746571000000	4.322070000000
H	-0.786045000000	-0.875906000000	4.534637000000
C	-3.387469000000	0.164350000000	-0.150698000000
C	-4.291190000000	1.083296000000	0.470176000000
C	-5.650007000000	0.763969000000	0.596547000000
H	-6.309400000000	1.504960000000	1.051607000000
C	-6.181286000000	-0.458826000000	0.177125000000
C	-5.293759000000	-1.357023000000	-0.410649000000
H	-5.664804000000	-2.315366000000	-0.761621000000
C	-3.924350000000	-1.080475000000	-0.609092000000

C	-3.866899000000	2.445285000000	0.976921000000
H	-2.770711000000	2.494178000000	1.022248000000
Si	-4.296313000000	3.766547000000	-0.349721000000
C	-3.609411000000	3.204998000000	-2.018531000000
H	-3.912632000000	3.908464000000	-2.811783000000
H	-3.996622000000	2.207305000000	-2.279866000000
H	-2.511649000000	3.150092000000	-2.019979000000
C	-3.494228000000	5.412647000000	0.134002000000
H	-2.405891000000	5.298182000000	0.269142000000
H	-3.905709000000	5.815460000000	1.072795000000
H	-3.655258000000	6.167236000000	-0.653698000000
C	-6.159001000000	3.986716000000	-0.584770000000
H	-6.337501000000	4.744404000000	-1.366418000000
H	-6.678864000000	4.313825000000	0.326817000000
H	-6.617236000000	3.044671000000	-0.924648000000
Si	-4.338087000000	2.872006000000	2.792492000000
C	-2.798078000000	3.682174000000	3.536071000000
H	-1.937771000000	2.993140000000	3.507247000000
H	-2.961980000000	3.980379000000	4.584609000000
H	-2.517559000000	4.583321000000	2.966380000000
C	-5.799505000000	4.066343000000	2.967890000000
H	-5.953942000000	4.285109000000	4.037978000000
H	-6.731956000000	3.620577000000	2.585232000000
H	-5.644048000000	5.025423000000	2.450750000000
C	-4.816215000000	1.343718000000	3.800656000000
H	-4.080450000000	0.531879000000	3.726007000000
H	-5.785879000000	0.938947000000	3.473707000000
H	-4.908202000000	1.627221000000	4.862887000000
C	-7.678818000000	-0.755213000000	0.357711000000
C	-8.497342000000	0.281895000000	-0.444032000000
H	-9.577599000000	0.089573000000	-0.336032000000
H	-8.246015000000	0.234360000000	-1.515754000000
H	-8.304350000000	1.309273000000	-0.099765000000
C	-8.044501000000	-0.653534000000	1.855433000000
H	-9.113438000000	-0.875928000000	2.007814000000
H	-7.855208000000	0.354206000000	2.254990000000
H	-7.456117000000	-1.368040000000	2.452663000000
C	-8.057829000000	-2.161612000000	-0.138768000000
H	-7.507679000000	-2.948216000000	0.400670000000
H	-7.858185000000	-2.281944000000	-1.214963000000
H	-9.133437000000	-2.337581000000	0.019352000000
C	-3.155795000000	-2.148769000000	-1.374138000000
H	-2.119906000000	-1.825252000000	-1.556534000000
Si	-2.867173000000	-3.807852000000	-0.449625000000
C	-1.742152000000	-3.569707000000	1.044281000000
H	-2.313222000000	-3.173546000000	1.894668000000
H	-0.906802000000	-2.881677000000	0.846509000000
H	-1.325525000000	-4.544094000000	1.348489000000
C	-4.459465000000	-4.595617000000	0.203284000000
H	-4.209513000000	-5.545603000000	0.705541000000
H	-5.197514000000	-4.813100000000	-0.581966000000
H	-4.937294000000	-3.940021000000	0.948522000000
C	-1.985922000000	-5.013448000000	-1.615806000000
H	-1.762729000000	-5.944450000000	-1.068218000000
H	-1.026601000000	-4.591318000000	-1.955236000000
H	-2.572794000000	-5.281244000000	-2.507074000000
Si	-3.903929000000	-2.418481000000	-3.140010000000
C	-4.749265000000	-0.847967000000	-3.776126000000
H	-4.055711000000	-0.003112000000	-3.897575000000
H	-5.549654000000	-0.529813000000	-3.090120000000
H	-5.203306000000	-1.055452000000	-4.759791000000

C	-5.243153000000	-3.763386000000	-3.200103000000
H	-6.107865000000	-3.537643000000	-2.557283000000
H	-4.862403000000	-4.758577000000	-2.924706000000
H	-5.612749000000	-3.827634000000	-4.237684000000
C	-2.529431000000	-2.955584000000	-4.343049000000
H	-2.794336000000	-3.903302000000	-4.838774000000
H	-1.565554000000	-3.106882000000	-3.835337000000
H	-2.378394000000	-2.198962000000	-5.129241000000
C	3.387453000000	0.164274000000	0.150635000000
C	3.924293000000	-1.080552000000	0.609077000000
C	5.293733000000	-1.357079000000	0.410809000000
H	5.664750000000	-2.315418000000	0.761818000000
C	6.181315000000	-0.458867000000	-0.176857000000
C	5.650064000000	0.763911000000	-0.596361000000
H	6.309503000000	1.504912000000	-1.051338000000
C	4.291225000000	1.083214000000	-0.470179000000
C	3.155635000000	-2.148895000000	1.373946000000
H	2.119716000000	-1.825394000000	1.556223000000
Si	3.903439000000	-2.418821000000	3.139932000000
C	4.748350000000	-0.848304000000	3.776622000000
H	4.054352000000	-0.004043000000	3.899621000000
H	5.547827000000	-0.528973000000	3.090096000000
H	5.203557000000	-1.056422000000	4.759613000000
C	5.242929000000	-3.763460000000	3.200060000000
H	5.612119000000	-3.828012000000	4.237767000000
H	6.107854000000	-3.537293000000	2.557674000000
H	4.862502000000	-4.758629000000	2.924144000000
C	2.528696000000	-2.956557000000	4.342421000000
H	1.564492000000	-3.105816000000	3.834726000000
H	2.378774000000	-2.201179000000	5.130030000000
H	2.792614000000	-3.905487000000	4.836341000000
Si	2.867207000000	-3.807938000000	0.449288000000
C	4.459627000000	-4.595452000000	-0.203618000000
H	4.937384000000	-3.939752000000	-0.948811000000
H	4.209820000000	-5.545449000000	-0.705926000000
H	5.197687000000	-4.812867000000	0.581641000000
C	1.742178000000	-3.569874000000	-1.044628000000
H	0.906845000000	-2.881814000000	-0.846892000000
H	1.325525000000	-4.544281000000	-1.348735000000
H	2.313231000000	-3.173801000000	-1.895068000000
C	1.986072000000	-5.013737000000	1.615346000000
H	2.573038000000	-5.281718000000	2.506494000000
H	1.762818000000	-5.944629000000	1.067595000000
H	1.026795000000	-4.591670000000	1.954975000000
C	7.678862000000	-0.755237000000	-0.357331000000
C	8.044556000000	-0.653834000000	-1.855071000000
H	7.855177000000	0.353807000000	-2.254843000000
H	7.456238000000	-1.368519000000	-2.452155000000
H	9.113512000000	-0.876175000000	-2.007401000000
C	8.497345000000	0.282045000000	0.444227000000
H	9.577607000000	0.089714000000	0.336296000000
H	8.245989000000	0.234716000000	1.515952000000
H	8.304354000000	1.309354000000	0.099757000000
C	8.057901000000	-2.161529000000	0.139425000000
H	9.133530000000	-2.337475000000	-0.018576000000
H	7.507836000000	-2.948257000000	-0.399918000000
H	7.858169000000	-2.281675000000	1.215625000000
C	3.866987000000	2.445191000000	-0.977006000000
H	2.770807000000	2.494064000000	-1.022535000000
Si	4.338523000000	2.872137000000	-2.792445000000
C	2.798990000000	3.683285000000	-3.535945000000

H	2.963109000000	3.981541000000	-4.584436000000
H	2.518886000000	4.584497000000	-2.966160000000
H	1.938343000000	2.994661000000	-3.507281000000
C	4.815817000000	1.344007000000	-3.801215000000
H	4.077713000000	0.533985000000	-3.729929000000
H	5.783475000000	0.936250000000	-3.472056000000
H	4.911573000000	1.628807000000	-4.862766000000
C	5.800631000000	4.065710000000	-2.967352000000
H	6.732861000000	3.619232000000	-2.584979000000
H	5.645765000000	5.024626000000	-2.449735000000
H	5.955118000000	4.284910000000	-4.037342000000
Si	4.296240000000	3.766381000000	0.349792000000
C	6.158914000000	3.986000000000	0.585490000000
H	6.337377000000	4.744123000000	1.366725000000
H	6.679330000000	4.312291000000	-0.326071000000
H	6.616606000000	3.043982000000	0.926171000000
C	3.494728000000	5.412698000000	-0.134141000000
H	2.406447000000	5.298426000000	-0.269894000000
H	3.906793000000	5.815606000000	-1.072636000000
H	3.655447000000	6.167121000000	0.653782000000
C	3.608660000000	3.205076000000	2.018411000000
H	3.995001000000	2.207017000000	2.279632000000
H	2.510850000000	3.151119000000	2.019747000000
H	3.912413000000	3.908149000000	2.811808000000
C	-0.672557000000	2.234165000000	-0.053161000000
C	0.672585000000	2.234156000000	0.052885000000
H	1.203348000000	3.189931000000	0.110350000000
H	-1.203303000000	3.189943000000	-0.110765000000

3-Ge

$G_{qh} = -8901.067742$

$N_{imag} = 0$

$SP = -8894.084390$

$G_{sp} = -8892.555639$

Ge	-1.534793000000	0.474852000000	-0.131208000000
Ge	1.534767000000	0.474844000000	0.131201000000
C	-0.538786000000	-0.107801000000	-1.732711000000
C	0.795059000000	-0.243966000000	-1.575018000000
C	0.538785000000	-0.107657000000	1.732757000000
C	-0.795066000000	-0.243790000000	1.575081000000
C	-1.264761000000	0.033123000000	-3.062166000000
H	-2.345620000000	0.092196000000	-2.879521000000
H	-1.114225000000	-0.842876000000	-3.705140000000
C	-0.844399000000	1.303478000000	-3.817542000000
H	-0.961406000000	2.194836000000	-3.183734000000
H	-1.460413000000	1.444577000000	-4.720728000000
H	0.209382000000	1.263744000000	-4.130613000000
C	1.822642000000	-0.499356000000	-2.662988000000
H	2.723625000000	-0.917618000000	-2.187464000000
H	2.153479000000	0.485265000000	-3.042133000000
C	1.446174000000	-1.392406000000	-3.852863000000
H	0.913457000000	-2.296017000000	-3.521283000000
H	2.357640000000	-1.715038000000	-4.381412000000
H	0.811407000000	-0.881141000000	-4.589273000000
C	1.264837000000	0.033242000000	3.062167000000
H	1.114361000000	-0.842768000000	3.705143000000
H	2.345678000000	0.092328000000	2.879426000000
C	0.844529000000	1.303578000000	3.817607000000
H	0.961454000000	2.194949000000	3.183805000000
H	1.460633000000	1.444676000000	4.720732000000
H	-0.209217000000	1.263812000000	4.130793000000

C	-1.822620000000	-0.499153000000	2.663091000000
H	-2.723629000000	-0.917382000000	2.187583000000
H	-2.153420000000	0.485455000000	3.042301000000
C	-1.446136000000	-1.392254000000	3.852923000000
H	-0.913486000000	-2.295888000000	3.521293000000
H	-2.357591000000	-1.714841000000	4.381517000000
H	-0.811300000000	-0.881041000000	4.589308000000
C	-3.495109000000	0.128835000000	-0.146129000000
C	-4.393496000000	1.051078000000	0.466768000000
C	-5.750423000000	0.723471000000	0.596510000000
H	-6.415132000000	1.463507000000	1.045508000000
C	-6.271875000000	-0.507947000000	0.187605000000
C	-5.379958000000	-1.405995000000	-0.395337000000
H	-5.744565000000	-2.369821000000	-0.738497000000
C	-4.012559000000	-1.120465000000	-0.598218000000
C	-3.963302000000	2.416046000000	0.958429000000
H	-2.865753000000	2.459179000000	0.994642000000
Si	-4.389457000000	3.729893000000	-0.374711000000
C	-3.673476000000	3.165878000000	-2.030480000000
H	-3.969198000000	3.860405000000	-2.834253000000
H	-4.044568000000	2.161987000000	-2.291364000000
H	-2.574940000000	3.123375000000	-2.010411000000
C	-3.605797000000	5.384864000000	0.108654000000
H	-2.518110000000	5.279854000000	0.255920000000
H	-4.030459000000	5.790584000000	1.040215000000
H	-3.764119000000	6.133091000000	-0.685659000000
C	-6.252196000000	3.932149000000	-0.622410000000
H	-6.436238000000	4.686391000000	-1.406033000000
H	-6.777173000000	4.256183000000	0.287699000000
H	-6.700362000000	2.984522000000	-0.960284000000
Si	-4.422521000000	2.849580000000	2.774131000000
C	-2.881171000000	3.667973000000	3.506117000000
H	-2.017422000000	2.983129000000	3.471933000000
H	-3.039143000000	3.966361000000	4.555528000000
H	-2.608698000000	4.569875000000	2.933778000000
C	-5.889810000000	4.036450000000	2.949598000000
H	-6.045514000000	4.258571000000	4.018797000000
H	-6.819606000000	3.583505000000	2.568732000000
H	-5.740557000000	4.994283000000	2.428307000000
C	-4.885736000000	1.318225000000	3.784396000000
H	-4.159255000000	0.501328000000	3.679654000000
H	-5.867573000000	0.924848000000	3.480419000000
H	-4.945507000000	1.591161000000	4.851646000000
C	-7.767319000000	-0.813152000000	0.373297000000
C	-8.594331000000	0.209878000000	-0.437776000000
H	-9.673162000000	0.011997000000	-0.325434000000
H	-8.344867000000	0.152243000000	-1.509449000000
H	-8.406966000000	1.242202000000	-0.105304000000
C	-8.131900000000	-0.699372000000	1.870429000000
H	-9.199193000000	-0.927116000000	2.026505000000
H	-7.948386000000	0.313291000000	2.260175000000
H	-7.538095000000	-1.404322000000	2.473635000000
C	-8.137152000000	-2.227122000000	-0.108431000000
H	-7.580587000000	-3.004278000000	0.438137000000
H	-7.938321000000	-2.357055000000	-1.183680000000
H	-9.211252000000	-2.409124000000	0.053185000000
C	-3.225883000000	-2.175348000000	-1.362141000000
H	-2.198427000000	-1.827418000000	-1.548539000000
Si	-2.901697000000	-3.823476000000	-0.431611000000
C	-1.782449000000	-3.551048000000	1.060686000000
H	-2.354691000000	-3.125577000000	1.896054000000

H	-0.940811000000	-2.875132000000	0.847204000000
H	-1.373631000000	-4.518722000000	1.395921000000
C	-4.480914000000	-4.635641000000	0.222536000000
H	-4.218007000000	-5.579716000000	0.729193000000
H	-5.213437000000	-4.867200000000	-0.564026000000
H	-4.971074000000	-3.984278000000	0.963515000000
C	-1.995144000000	-5.017169000000	-1.590114000000
H	-1.757206000000	-5.942452000000	-1.039065000000
H	-1.042182000000	-4.579051000000	-1.927939000000
H	-2.574970000000	-5.297778000000	-2.482170000000
Si	-3.967737000000	-2.454723000000	-3.126937000000
C	-4.816332000000	-0.884943000000	-3.759907000000
H	-4.130298000000	-0.029320000000	-3.845469000000
H	-5.637955000000	-0.589150000000	-3.089136000000
H	-5.241350000000	-1.078008000000	-4.759312000000
C	-5.296728000000	-3.809027000000	-3.185774000000
H	-6.161002000000	-3.591823000000	-2.539430000000
H	-4.904437000000	-4.800286000000	-2.911589000000
H	-5.669318000000	-3.877296000000	-4.222027000000
C	-2.587226000000	-2.985468000000	-4.325873000000
H	-2.836322000000	-3.945355000000	-4.806114000000
H	-1.619537000000	-3.111498000000	-3.818455000000
H	-2.452236000000	-2.238345000000	-5.123941000000
C	3.495083000000	0.128823000000	0.146127000000
C	4.012490000000	-1.120481000000	0.598246000000
C	5.379889000000	-1.406047000000	0.395401000000
H	5.744471000000	-2.369880000000	0.738573000000
C	6.271846000000	-0.508018000000	-0.187505000000
C	5.750431000000	0.723410000000	-0.596435000000
H	6.415169000000	1.463437000000	-1.045405000000
C	4.393502000000	1.051033000000	-0.466765000000
C	3.225777000000	-2.175360000000	1.362163000000
H	2.198324000000	-1.827413000000	1.548550000000
Si	3.967627000000	-2.454743000000	3.126991000000
C	4.816008000000	-0.884920000000	3.760124000000
H	4.129620000000	-0.029699000000	3.846838000000
H	5.636912000000	-0.588329000000	3.088830000000
H	5.241986000000	-1.078403000000	4.759040000000
C	5.296686000000	-3.808974000000	3.185781000000
H	5.669062000000	-3.877448000000	4.222098000000
H	6.161087000000	-3.591673000000	2.539643000000
H	4.904421000000	-4.800174000000	2.911345000000
C	2.587060000000	-2.985727000000	4.325755000000
H	1.619253000000	-3.110881000000	3.818347000000
H	2.452557000000	-2.239117000000	5.124387000000
H	2.835684000000	-3.946090000000	4.805287000000
Si	2.901639000000	-3.823472000000	0.431574000000
C	4.480877000000	-4.635519000000	-0.222673000000
H	4.970858000000	-3.984061000000	-0.963692000000
H	4.218039000000	-5.579605000000	-0.729339000000
H	5.213525000000	-4.866995000000	0.563794000000
C	1.782356000000	-3.551161000000	-1.060729000000
H	0.940902000000	-2.874966000000	-0.847421000000
H	1.373254000000	-4.518846000000	-1.395592000000
H	2.354643000000	-3.126142000000	-1.896301000000
C	1.995131000000	-5.017160000000	1.590118000000
H	2.575092000000	-5.297933000000	2.482032000000
H	1.756911000000	-5.942360000000	1.039053000000
H	1.042318000000	-4.578888000000	1.928164000000
C	7.767286000000	-0.813248000000	-0.373165000000
C	8.131897000000	-0.699456000000	-1.870289000000

H	7.948371000000	0.313203000000	-2.260044000000
H	7.538124000000	-1.404423000000	-2.473507000000
H	9.199198000000	-0.927176000000	-2.026344000000
C	8.594296000000	0.209763000000	0.437939000000
H	9.673127000000	0.011865000000	0.325621000000
H	8.344805000000	0.152119000000	1.509604000000
H	8.406954000000	1.242092000000	0.105471000000
C	8.137081000000	-2.227230000000	0.108555000000
H	9.211188000000	-2.409240000000	-0.053007000000
H	7.580537000000	-3.004370000000	-0.438055000000
H	7.938193000000	-2.357179000000	1.183792000000
C	3.963349000000	2.415983000000	-0.958514000000
H	2.865804000000	2.459133000000	-0.994791000000
Si	4.422699000000	2.849509000000	-2.774189000000
C	2.881495000000	3.668156000000	-3.506199000000
H	3.039468000000	3.966376000000	-4.555657000000
H	2.609199000000	4.570175000000	-2.933965000000
H	2.017633000000	2.983456000000	-3.471892000000
C	4.885674000000	1.318218000000	-3.784639000000
H	4.157966000000	0.502180000000	-3.681688000000
H	5.866511000000	0.923375000000	-3.479338000000
H	4.947519000000	1.591831000000	-4.851597000000
C	5.890222000000	4.036122000000	-2.949469000000
H	6.819921000000	3.582963000000	-2.568618000000
H	5.741129000000	4.993919000000	-2.428067000000
H	6.046006000000	4.258339000000	-4.018635000000
Si	4.389499000000	3.729848000000	0.374610000000
C	6.252234000000	3.931851000000	0.622557000000
H	6.436262000000	4.686097000000	1.406178000000
H	6.777389000000	4.255775000000	-0.287488000000
H	6.700223000000	2.984175000000	0.960531000000
C	3.606129000000	5.384925000000	-0.108872000000
H	2.518377000000	5.280136000000	-0.255817000000
H	4.030627000000	5.790400000000	-1.040613000000
H	3.764839000000	6.133242000000	0.685279000000
C	3.673205000000	3.166064000000	2.030326000000
H	4.043965000000	2.162074000000	2.291305000000
H	2.574658000000	3.123900000000	2.010151000000
H	3.969059000000	3.860541000000	2.834094000000
C	-0.670055000000	2.297408000000	-0.048767000000
C	0.670038000000	2.297397000000	0.048508000000
H	1.219766000000	3.243578000000	0.097813000000
H	-1.219762000000	3.243597000000	-0.098162000000

3-Sn

$G_{qh} = -5176.182166$

$N_{imag} = 0$

$SP = -5170.148365$

$G_{sp} = -5168.626002$

Sn	1.623585000000	0.394897000000	0.193266000000
Sn	-1.642837000000	0.325087000000	-0.392163000000
C	0.383525000000	-0.277165000000	1.849446000000
C	-0.930606000000	-0.407078000000	1.564525000000
C	-0.379878000000	-0.449044000000	-2.011121000000
C	0.939784000000	-0.414068000000	-1.725319000000
C	0.983573000000	-0.246769000000	3.248282000000
H	2.080504000000	-0.285271000000	3.194649000000
H	0.685638000000	-1.134239000000	3.826544000000
C	0.598097000000	1.028454000000	4.013541000000
H	0.915268000000	1.925702000000	3.458441000000
H	1.078005000000	1.055545000000	5.005560000000

H	-0.490302000000	1.100686000000	4.160148000000
C	-2.059985000000	-0.655287000000	2.555210000000
H	-2.947621000000	-0.986115000000	1.997665000000
H	-2.354244000000	0.328524000000	2.958858000000
C	-1.851559000000	-1.633228000000	3.719055000000
H	-1.380516000000	-2.567472000000	3.376811000000
H	-2.826468000000	-1.895165000000	4.160805000000
H	-1.233572000000	-1.217110000000	4.527032000000
C	-0.917724000000	-0.657776000000	-3.414565000000
H	-0.247701000000	-1.318064000000	-3.990033000000
H	-1.882032000000	-1.180977000000	-3.388829000000
C	-1.103314000000	0.670473000000	-4.163675000000
H	-1.792656000000	1.339986000000	-3.624397000000
H	-1.516354000000	0.506992000000	-5.172382000000
H	-0.145049000000	1.204290000000	-4.262870000000
C	2.034417000000	-0.601715000000	-2.765786000000
H	2.811307000000	0.156281000000	-2.587192000000
H	1.648597000000	-0.394353000000	-3.777645000000
C	2.720911000000	-1.971019000000	-2.761619000000
H	3.203861000000	-2.159820000000	-1.794009000000
H	3.504143000000	-2.014110000000	-3.535700000000
H	2.003355000000	-2.784912000000	-2.951226000000
C	3.779824000000	0.058637000000	0.162856000000
C	4.608269000000	0.971681000000	-0.545439000000
C	5.934661000000	0.610497000000	-0.825069000000
H	6.568140000000	1.332865000000	-1.341049000000
C	6.463877000000	-0.640110000000	-0.484690000000
C	5.640697000000	-1.507659000000	0.234577000000
H	6.023560000000	-2.475627000000	0.544845000000
C	4.322645000000	-1.173973000000	0.610361000000
C	4.139434000000	2.354636000000	-0.955738000000
H	3.037785000000	2.377839000000	-0.973342000000
Si	4.573230000000	3.589705000000	0.456652000000
C	3.684981000000	3.067106000000	2.042065000000
H	3.993856000000	3.716509000000	2.878127000000
H	3.937081000000	2.030391000000	2.308362000000
H	2.590616000000	3.142996000000	1.945661000000
C	3.993858000000	5.339650000000	0.024781000000
H	2.913525000000	5.353750000000	-0.194888000000
H	4.520973000000	5.765463000000	-0.842601000000
H	4.167129000000	6.008953000000	0.883969000000
C	6.429478000000	3.575460000000	0.807940000000
H	6.662227000000	4.276997000000	1.626444000000
H	7.028060000000	3.865649000000	-0.068323000000
H	6.752431000000	2.570069000000	1.121066000000
Si	4.586230000000	2.947049000000	-2.728883000000
C	3.164538000000	4.053587000000	-3.304344000000
H	2.211951000000	3.498539000000	-3.266291000000
H	3.322277000000	4.384808000000	-4.344202000000
H	3.054915000000	4.950486000000	-2.675972000000
C	6.212615000000	3.919324000000	-2.811222000000
H	6.378405000000	4.256915000000	-3.848054000000
H	7.077474000000	3.298676000000	-2.525374000000
H	6.212036000000	4.811541000000	-2.166755000000
C	4.752594000000	1.514682000000	-3.956773000000
H	3.769932000000	1.124186000000	-4.260231000000
H	5.338067000000	0.678064000000	-3.546338000000
H	5.263285000000	1.875497000000	-4.865366000000
C	7.905584000000	-0.993350000000	-0.886917000000
C	8.877896000000	-0.016453000000	-0.188143000000
H	9.920973000000	-0.243817000000	-0.463913000000

H	8.788041000000	-0.093270000000	0.907293000000
H	8.676876000000	1.029228000000	-0.466981000000
C	8.054040000000	-0.862654000000	-2.419802000000
H	9.079337000000	-1.121194000000	-2.731703000000
H	7.848718000000	0.160999000000	-2.767460000000
H	7.356578000000	-1.538991000000	-2.939292000000
C	8.287020000000	-2.429850000000	-0.488612000000
H	7.621176000000	-3.172224000000	-0.955667000000
H	8.250371000000	-2.577107000000	0.601663000000
H	9.315464000000	-2.648732000000	-0.816268000000
C	3.612250000000	-2.114354000000	1.573995000000
H	2.638300000000	-1.679714000000	1.844497000000
Si	3.089692000000	-3.841576000000	0.903042000000
C	1.360301000000	-3.689421000000	0.157840000000
H	1.287548000000	-2.932963000000	-0.634319000000
H	0.643514000000	-3.398493000000	0.943562000000
H	1.029633000000	-4.654057000000	-0.260786000000
C	4.334146000000	-4.524399000000	-0.347008000000
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H	2.169233000000	-4.837034000000	3.025346000000
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C	-5.876594000000	4.063899000000	2.898446000000
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3-Pb

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$N_{imag} = 0$

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