

Electronic Supplementary Information

Detection of catechins using a fluorescent molecule and its application toward the evaluation of astringent intensity

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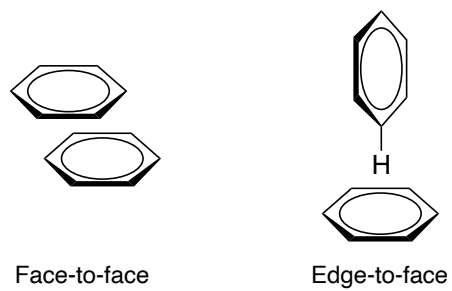


Fig. S1. Two modes of aromatic/aromatic interactions.

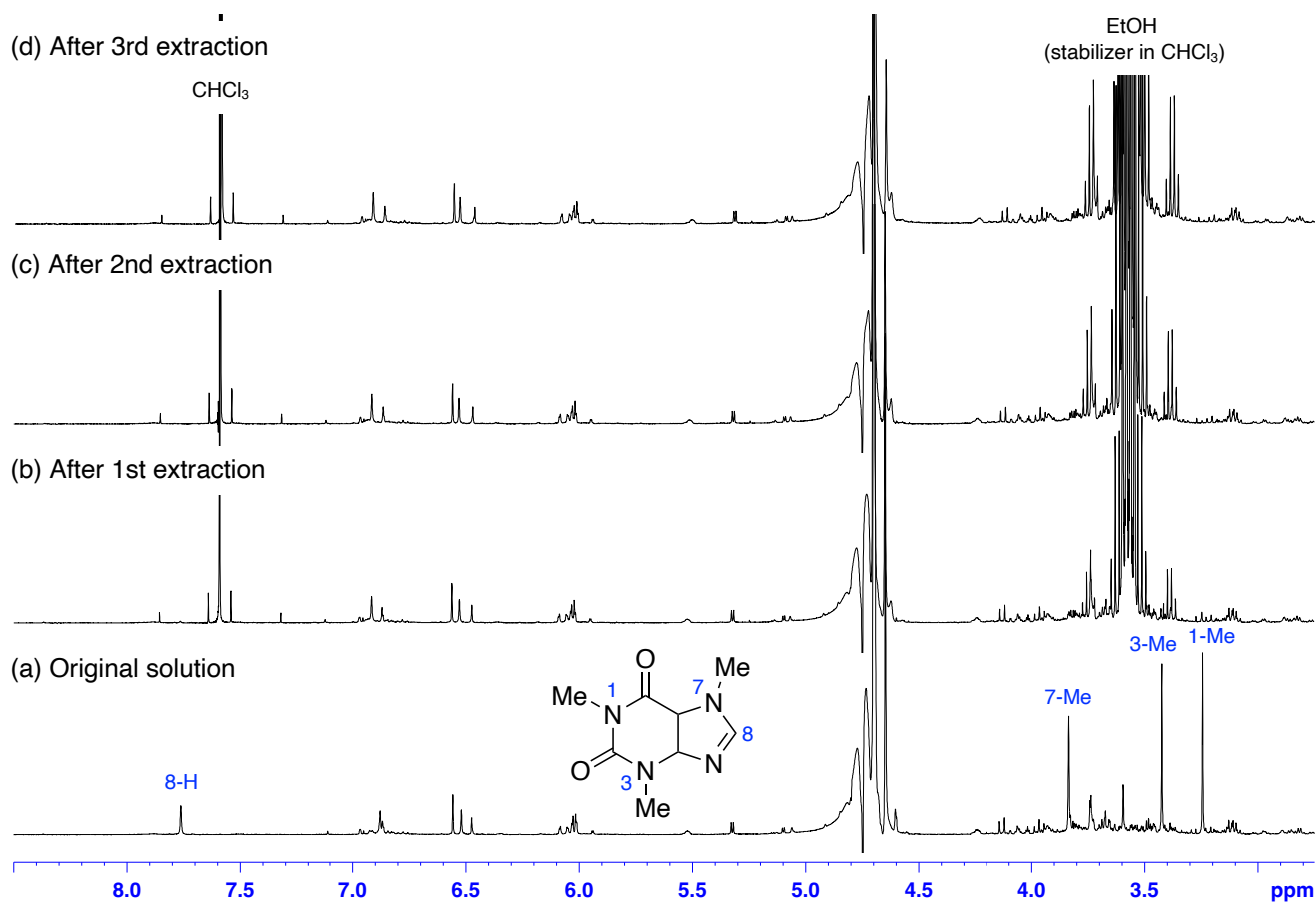


Fig. S2. ¹H NMR spectra of green tea samples.[†]

(a) Original solution, (b) aqueous layer after the first extraction with chloroform, (c) aqueous layer after the second extraction with chloroform, and (d) aqueous layer after the third extraction with chloroform.

[†] The NMR samples were prepared by adding an equal volume of deuterium oxide to the tea samples. ¹H NMR spectra were measured on an Avance 400 spectrometer (400 MHz, Bruker Biospin, Rheinstetten, Germany) with a CPBBO BB-1 H/19 F/D cryogenic probe at 298 K. The solvent signal was suppressed by presaturation.

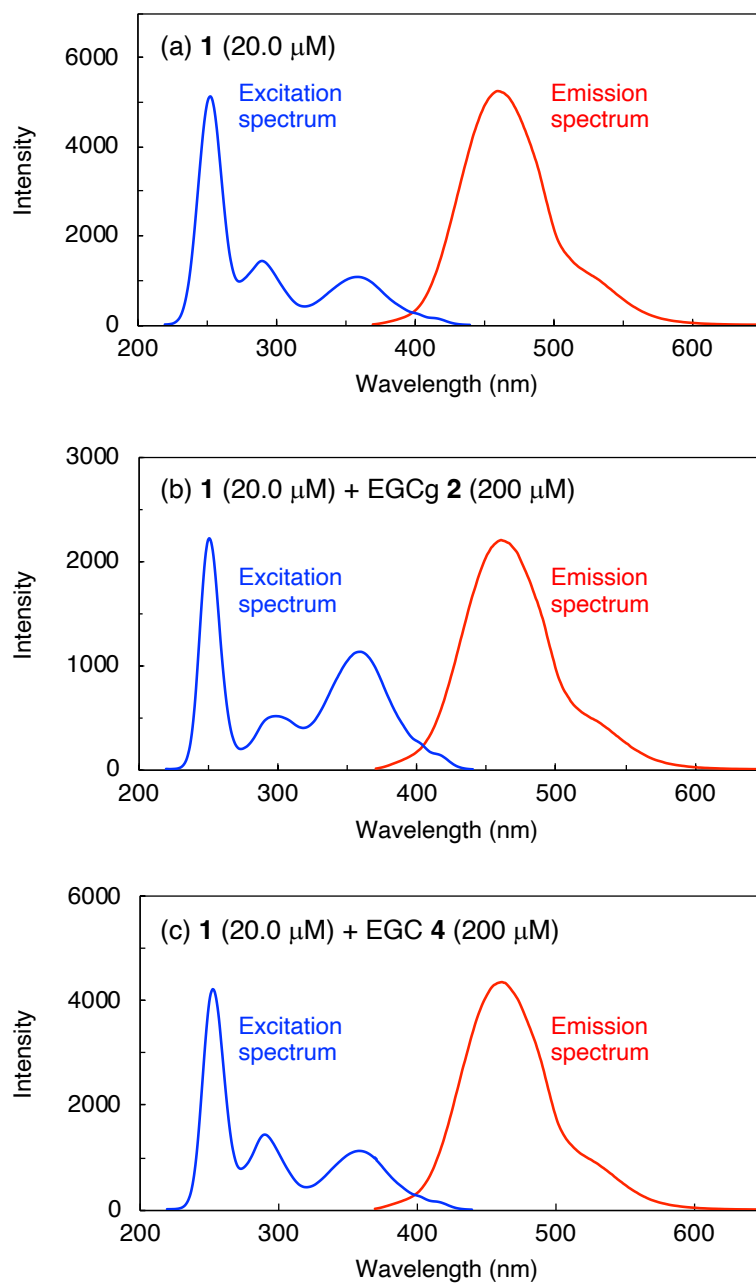


Fig. S3. Excitation and Emission spectra of sensor molecule **1** solution (a), mixed solutions of **1** + EGCg **2** (b), and **1** + EGC **4** (c) at pH 4.7 and 298 K (fluorescence spectrometer: FP-8300, JASCO; temperature control unit: EHC-813, JASCO).

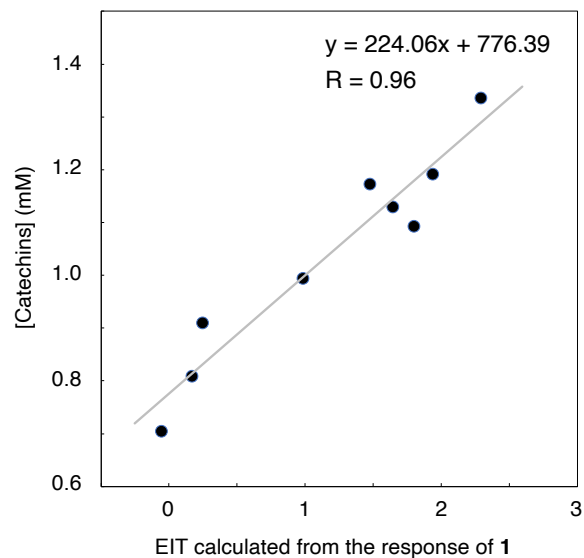


Fig. S4. Relation between the EIT values of green tea infusions calculated from the response of sensor molecule **1** and the catechin concentrations.

$$[\text{Catechins}] = [\text{EGCg}] + 1.004[\text{ECg}] + 0.306[\text{EGC}] + 0.184[\text{EC}] + 1.055[\text{GCg}] + 1.041[\text{Cg}] + 0.336[\text{GC}] + 0.170[\text{C}].^{\S}$$

The linear approximation formula and linear correlation coefficient (R) are provided in the graph area.

[§] The concentration of each catechin was corrected by multiplying the relative response intensity of sensor **1** for each catechin based on Fig. 4.

Table S1. Concentrations (μM) of catechins (2–9) in the green tea infusions.^a

Samples	EGCg 2	ECg 3	EGC 4	EC 5	GCg 6	Cg 7	GC 8	C 9
A	416 \pm 10	71.0 \pm 2.0	538 \pm 8	174 \pm 7	9.09 \pm 0.28	ND ^b	28.6 \pm 1.5	16.3 \pm 1.0
B	505 \pm 10	96.6 \pm 1.9	749 \pm 5	230 \pm 7	13.6 \pm 0.1	ND ^b	54.0 \pm 2.1	27.0 \pm 0.7
C	458 \pm 3	88.2 \pm 1.1	624 \pm 2	220 \pm 5	12.7 \pm 0.1	ND ^b	43.0 \pm 0.9	23.9 \pm 1.3
D	568 \pm 2	98.8 \pm 2.8	801 \pm 5	251 \pm 1	12.6 \pm 0.4	ND ^b	55.1 \pm 2.1	27.1 \pm 0.8
E	681 \pm 17	131 \pm 5	758 \pm 7	289 \pm 13	10.0 \pm 1.0	ND ^b	48.3 \pm 2.2	30.2 \pm 1.0
F	842 \pm 11	164 \pm 1	752 \pm 7	299 \pm 4	19.2 \pm 0.0	ND ^b	57.7 \pm 0.3	32.8 \pm 1.6
G	718 \pm 2	142 \pm 3	773 \pm 3	281 \pm 7	17.8 \pm 0.2	ND ^b	56.7 \pm 1.4	31.7 \pm 0.4
H	644 \pm 5	123 \pm 1	753 \pm 4	264 \pm 8	19.7 \pm 0.5	ND ^b	61.5 \pm 0.6	30.1 \pm 1.2
I	771 \pm 13	131 \pm 3	639 \pm 2	223 \pm 9	14.9 \pm 0.3	ND ^b	42.7 \pm 1.8	26.3 \pm 1.1

^aMeans and standard divisions (n = 3). ^bNot detected.

HPLC analysis of catechin concentrations of green tea infusions.

The analysis was conducted according to the procedure reported by Mizukami et al.^{R1} However, on advice from the original author, the following conditions were changed: HPLC column, Cadenza CD-C18 column (4.6 mm \times 150 mm, 3 μm ; Imtakt, Kyoto, Japan); guard column, Cadenza CD-C18 (2.0 mm \times 5.0 mm, 3 μm ; Imtakt, Kyoto, Japan); mobile phase, (A) 0.2% phosphoric acid aqueous solution, (B) methanol/acetonitrile (3:2 v/v).^{R2,R3} A gradient was established as follows: 0–15 min, 15% B; 15–25 min, linear gradient of B from 15 to 50%; and 25–30 min, 50% B. The HPLC system was consisted of a binary pump to generate gradients (G1312A; Agilent Technologies, Santa Clara, CA, USA), temperature-controlled column chamber (CO-8020; TOSOH, Tokyo, Japan), and UV-vis detector (SPD-10Avp; Shimadzu, Kyoto, Japan). The flow rate was 1.0 mL/min, and the injection volume was 10 μL . UV detection was performed at 210 nm. Under these conditions, GC, EGC, C, internal standard substance (catechol), EGCg, EC, GCg, ECg, and Cg were eluted at 3.5, 5.8, 7.1, 7.7, 13.1, 13.8, 18.9, 22.1, and 22.8 min, respectively.

References

- (R1) Y. Mizukami, Y. Sawai and Y. Yamaguchi, *J. Agric. Food Chem.*, 2007, **55**, 4957–4964.
- (R2) Y. Mizukami, *Tea Res. J.*, 2019, **127**, 19–25, and a reference therein.
- (R3) H. Hirono, S. Goto, S. Aiba, *Nippon Shokuhin Kagaku Kogaku Kaishi*, 2020, **67**, 264–270.

Cartesian coordinates, number of imaginary frequencies, and energies
(M06-2X/6-31G(d) level)

(1) Complexes of sensor molecule **1** and EGCg **2**

1: EGCg 2 = 1:1 complex

Number of imaginary frequency = 0

Sum of electronic and zero-point Energies = -6805.071796 au

Sum of electronic and thermal Energies = -6804.961564 au

Sum of electronic and thermal Enthalpies = -6804.960620 au

Sum of electronic and thermal Free Energies = -6805.223521 au

O	-3.76848400	-2.74551200	-2.06862000
H	-4.50789800	-2.97175700	-1.44499400
C	-2.59374100	-3.31501600	-1.66997900
C	-2.57227700	-4.52170000	-0.95849700
O	-3.72872500	-5.21424100	-0.74975000
H	-3.62036900	-5.87051900	-0.02156500
C	-1.34861600	-5.02512400	-0.50821900
O	-1.42567700	-6.18464600	0.21352700
H	-0.66429100	-6.24228300	0.81309500
C	-0.15560400	-4.38160900	-0.81606800
H	0.78634900	-4.79811400	-0.46072800
C	-0.17897500	-3.21522100	-1.58286800
C	1.11885200	-2.48000700	-1.80796800
H	1.96771400	-3.18120400	-1.82799600
C	2.09875100	-0.92965000	-3.30730100
C	2.31515500	-0.58827100	-4.64387100
H	1.68396900	-0.99067900	-5.42613000
C	3.37307200	0.26233800	-4.94719600
C	4.21408100	0.76925200	-3.95448900
H	5.05034500	1.42149800	-4.19474400
C	3.97170500	0.41751600	-2.62499900
C	2.90437500	-0.42937200	-2.28646200
C	1.38432800	-1.50638300	-0.66048700
H	1.34767800	-2.04007100	0.29283700
C	-0.09402100	-0.00248000	0.42418400
C	-1.21740000	0.92622000	0.23739400
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C	2.70924600	-0.80284800	-0.84777600
H	2.76091900	0.07952600	-0.20275200
H	3.51689500	-1.47531500	-0.53743700

O	1.05817900	-1.78376500	-3.04883900
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H	5.48838000	1.39841900	-1.89910000
C	-1.39540800	-2.68067700	-1.99984400
H	-1.43373100	-1.77120600	-2.59028000
O	0.31267400	-0.55331700	-0.71353100
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O	-3.42920000	2.03870800	-2.43538400
H	-4.42878300	2.01897500	-2.42175900
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O	-4.34726500	3.59747200	-0.21859300
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C	-0.98294200	-6.41684900	3.54334500
H	1.15956200	-6.70880900	3.41851100
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O	2.79223500	-5.26830000	2.07593500
N	2.29474800	-3.06701800	2.52870000
H	1.58686800	-2.47194100	2.96143500
C	-2.90215500	-3.34231100	2.46453700
O	-3.99479900	-3.76531700	2.06502400
N	-2.63165300	-2.03220400	2.64865500
H	-1.78336500	-1.78426700	3.16569900
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H	-5.10875800	1.58953400	3.91778900
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O	-5.65993200	3.98065700	2.96477000
O	7.02712100	3.86373600	2.46760300
O	7.03173300	-1.55227700	-1.69128000
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O	6.85556800	2.30822100	-2.13646000
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H	7.54730900	1.66435200	-1.87766200
O	-3.57141600	-0.45005300	-3.86163100
H	-3.47962900	0.37211400	-3.34657000
H	-3.73141100	-1.16154800	-3.21670300
O	-4.57943600	4.58485100	-2.66541000
H	-5.47234000	4.52964900	-3.10450600
H	-4.04398700	3.91305900	-3.11501100
O	8.40034500	6.27501900	1.69093800
H	7.72842300	6.57756800	1.03128900
H	8.20873600	5.32212500	1.76408500
O	4.60467900	6.87030400	2.20633600
H	5.31114500	6.81637200	2.89374200
H	4.34392900	5.93444300	2.11640200
O	6.72864400	6.33965700	3.85122000
H	6.63114100	5.37710500	3.73426400
H	7.42446700	6.52684200	3.17706800

1: EGCg 2 = 1:2 complex

Number of imaginary frequency = 0

Sum of electronic and zero-point Energies = -8633.508846 au

Sum of electronic and thermal Energies = -8633.364510 au

Sum of electronic and thermal Enthalpies = -8633.363566 au

Sum of electronic and thermal Free Energies = -8633.691581 au

O	-1.62590000	2.50110000	-2.99310000
H	-0.79570000	2.15280000	-3.36530000
C	-1.30080000	3.63760000	-2.32620000
C	0.05200000	4.01220000	-2.26040000
O	0.91730000	3.22520000	-2.97500000
H	1.72930000	2.96470000	-2.48520000
C	0.39100000	5.18290000	-1.57300000
O	1.66080000	5.61740000	-1.37780000
H	2.33670000	4.94210000	-1.63850000
C	-0.61830000	5.95890000	-1.00050000
H	-0.32050000	6.86930000	-0.48620000
C	-1.95160000	5.57880000	-1.08250000
C	-2.96210000	6.44310000	-0.37620000
H	-2.67050000	7.50060000	-0.47610000
C	-5.29000000	6.86470000	-0.35790000
C	-6.45450000	6.98230000	-1.12080000
H	-6.46000000	6.60580000	-2.13880000
C	-7.56490000	7.59040000	-0.55100000
C	-7.52600000	8.08380000	0.75340000
H	-8.40290000	8.56130000	1.17420000
C	-6.35430000	7.94600000	1.49280000
C	-5.21470000	7.32780000	0.95340000
C	-3.04510000	6.13730000	1.12550000
H	-2.04650000	6.14310000	1.57020000
C	-2.84250000	3.77760000	1.50200000
C	-3.62970000	2.51960000	1.46830000
C	-4.85910000	2.50440000	0.80530000
H	-5.24930000	3.39350000	0.32480000
C	-3.12030000	1.38770000	2.11060000
H	-2.17050000	1.42560000	2.63270000
C	-3.98020000	7.13160000	1.79480000
H	-4.25460000	6.76810000	2.78970000
H	-3.44960000	8.08050000	1.94310000
O	-4.23430000	6.25780000	-0.97700000
O	-8.73550000	7.74650000	-1.23210000
H	-8.63690000	7.36140000	-2.11430000
O	-6.24420000	8.38880000	2.76490000
H	-7.09480000	8.77760000	3.05840000

C	-2.30550000	4.39740000	-1.73050000
H	-3.33810000	4.07520000	-1.79810000
O	-3.62710000	4.84150000	1.26170000
O	-1.65370000	3.85800000	1.74200000
C	-3.85780000	0.20350000	2.07180000
O	-3.41170000	-0.90590000	2.70850000
H	-3.98110000	-1.71110000	2.55640000
C	-5.07980000	0.18120000	1.39000000
O	-5.79010000	-0.98870000	1.35420000
H	-6.00750000	-1.16410000	0.39420000
C	-5.59830000	1.32660000	0.77260000
O	-6.79910000	1.31640000	0.15860000
H	-7.25810000	0.45530000	0.26730000
O	-4.29690000	-1.70420000	-3.76540000
H	-4.86090000	-0.96740000	-3.44770000
C	-3.08840000	-1.74720000	-3.16280000
C	-2.22210000	-2.76760000	-3.57860000
O	-2.61180000	-3.60810000	-4.56670000
H	-2.06680000	-4.42120000	-4.50310000
C	-0.97720000	-2.90880000	-2.95480000
O	-0.18410000	-3.90440000	-3.46830000
H	0.19940000	-4.48220000	-2.78260000
C	-0.58580000	-2.04990000	-1.93200000
H	0.37700000	-2.19540000	-1.45440000
C	-1.43800000	-1.01090000	-1.54040000
C	-1.03790000	-0.01030000	-0.48160000
H	-1.83560000	0.74150000	-0.38520000
C	-0.25850000	-0.07140000	1.78890000
C	-0.34060000	-0.73280000	3.01160000
H	-0.96550000	-1.61180000	3.08150000
C	0.28730000	-0.19320000	4.13310000
C	1.06130000	0.96440000	4.00030000
H	1.55070000	1.40220000	4.86300000
C	1.11480000	1.62610000	2.76910000
C	0.44620000	1.13070000	1.63670000
C	0.24870000	0.75430000	-0.78100000
H	0.21060000	1.18490000	-1.78110000
C	2.44460000	0.07050000	-1.38100000
C	3.55670000	-0.80680000	-0.94500000
C	3.43370000	-1.61580000	0.18800000
H	2.49830000	-1.65680000	0.73870000
C	4.77150000	-0.70310000	-1.61670000
H	4.86200000	-0.04270000	-2.47310000
C	0.49150000	1.80910000	0.29020000
H	1.46050000	2.29430000	0.10680000

H	-0.27700000	2.58890000	0.21030000
O	-0.90490000	-0.69690000	0.76560000
O	0.17220000	-0.76130000	5.35480000
H	-0.61650000	-1.35920000	5.34160000
O	1.91250000	2.72030000	2.70570000
H	1.55260000	3.42850000	2.11030000
C	-2.68400000	-0.86890000	-2.15560000
H	-3.36700000	-0.08410000	-1.83650000
O	1.32010000	-0.19200000	-0.70140000
O	2.53730000	0.93530000	-2.22510000
C	5.87620000	-1.40720000	-1.16060000
O	7.07290000	-1.29910000	-1.83220000
H	7.78230000	-1.01920000	-1.18370000
C	5.77150000	-2.23030000	-0.02940000
O	6.78370000	-2.94180000	0.51500000
H	7.57730000	-3.01010000	-0.07550000
C	4.54010000	-2.31390000	0.64180000
O	4.44290000	-3.08540000	1.76180000
H	5.34560000	-3.35400000	2.00800000
C	2.67330000	-3.43760000	6.26710000
C	2.85720000	-2.87180000	5.00640000
C	1.89760000	-3.04530000	4.01360000
C	0.74220000	-3.77600000	4.28680000
C	0.53220000	-4.28930000	5.56780000
C	1.49860000	-4.12390000	6.55490000
H	3.45390000	-3.32150000	7.01270000
H	2.06100000	-2.59540000	3.03810000
H	-0.38810000	-4.82890000	5.76600000
H	1.33850000	-4.53930000	7.54460000
C	4.13740000	-2.15570000	4.69340000
O	5.21800000	-2.61260000	5.03450000
N	3.96070000	-0.99230000	4.00040000
H	3.00050000	-0.67320000	3.88290000
C	-0.30790000	-4.04060000	3.25930000
O	-1.46370000	-4.31600000	3.59940000
N	0.07450000	-3.98220000	1.96190000
H	1.06370000	-3.91400000	1.75680000
C	4.89890000	-0.34080000	3.18300000
C	4.41830000	0.61780000	2.32200000
C	6.27740000	-0.67830000	3.15610000
C	5.25570000	1.19420000	1.34810000
H	3.36680000	0.88640000	2.32510000
C	7.11240000	-0.11060000	2.22430000
H	6.66060000	-1.40130000	3.86230000
C	4.70640000	2.09140000	0.39590000

C	6.62420000	0.81400000	1.26410000
H	8.15550000	-0.40290000	2.22570000
C	5.48110000	2.56020000	-0.62470000
H	3.66150000	2.37770000	0.47650000
C	7.39510000	1.35240000	0.18590000
C	6.84590000	2.19260000	-0.74780000
H	7.45130000	2.55660000	-1.57520000
C	-0.81240000	-4.24840000	0.88220000
C	-2.01200000	-3.59320000	0.77480000
C	-0.44500000	-5.23070000	-0.06650000
C	-2.91850000	-3.94980000	-0.25540000
H	-2.27820000	-2.80030000	1.46690000
C	-1.31120000	-5.58520000	-1.06460000
H	0.51990000	-5.72620000	0.01050000
C	-4.15490000	-3.27660000	-0.39100000
C	-2.58770000	-4.98160000	-1.17310000
H	-1.01640000	-6.34440000	-1.76740000
C	-5.02460000	-3.64100000	-1.38540000
H	-4.38310000	-2.47350000	0.30150000
C	-3.54050000	-5.34440000	-2.17110000
C	-4.73280000	-4.68240000	-2.29090000
H	-5.42700000	-4.93890000	-3.08310000
S	4.76970000	3.62970000	-1.85120000
S	9.09970000	0.85080000	-0.04070000
S	-6.55140000	-2.74580000	-1.50910000
S	-3.19300000	-6.68890000	-3.30530000
O	8.99410000	-0.65600000	-0.16680000
O	9.55170000	1.47720000	-1.28620000
O	5.33950000	4.97530000	-1.64950000
O	3.30200000	3.60030000	-1.58670000
O	-4.37160000	-6.84170000	-4.15620000
O	-2.94960000	-7.86470000	-2.40540000
O	-6.19770000	-1.32410000	-1.22850000
O	-7.44770000	-3.26410000	-0.42580000
O	-7.11990000	-2.96330000	-2.85070000
O	-1.94710000	-6.31140000	-4.02470000
O	5.14460000	3.03350000	-3.15710000
O	9.84050000	1.22240000	1.17490000
O	-4.51280000	-3.32000000	2.80450000
H	-4.17490000	-4.18180000	2.47540000
H	-5.48850000	-3.37580000	2.75510000
O	-8.97820000	-0.64820000	-2.47200000
H	-8.91470000	-0.56580000	-1.50390000
H	-8.68350000	-1.55710000	-2.65070000
O	-8.57890000	-0.87800000	0.38790000

H	-8.25590000	-1.78700000	0.19160000
H	-9.11360000	-0.96050000	1.18950000
O	7.97320000	5.53230000	-2.46380000
H	8.36050000	4.64900000	-2.62940000
H	7.14150000	5.34780000	-1.98780000
O	-7.30730000	-3.02890000	2.37870000
H	-7.29350000	-3.37630000	1.46670000
H	-6.98220000	-2.11890000	2.25380000
O	-6.59800000	-0.36530000	-4.01520000
H	-7.23820000	-0.15460000	-3.30830000
H	-6.68390000	-1.33270000	-4.06170000
O	11.29690000	2.60850000	-3.30350000
H	10.44530000	2.92000000	-3.66080000
H	10.99760000	2.16350000	-2.49570000
O	-3.46420000	-5.88210000	2.30880000
H	-2.64910000	-5.51190000	2.69210000
H	-3.17390000	-6.34670000	1.50010000
O	-0.39470000	-8.60380000	-1.56220000
H	-1.19170000	-8.52860000	-2.12500000
H	-0.75930000	-8.34840000	-0.69560000
O	0.82030000	-6.48520000	-3.09930000
H	0.62980000	-7.24900000	-2.51950000
H	-0.00020000	-6.40900000	-3.62190000
O	6.65740000	4.81370000	-4.81240000
H	7.04180000	5.34180000	-4.07930000
H	5.96010000	4.29990000	-4.36280000
O	6.94370000	0.92610000	-3.71260000
H	7.03010000	0.23880000	-3.02810000
H	6.21550000	1.51140000	-3.42810000
O	-2.57770000	-7.83010000	0.31680000
H	-3.06440000	-8.60010000	0.64300000
H	-2.87110000	-7.72760000	-0.61780000
O	-2.22940000	-2.05980000	5.12810000
H	-2.20610000	-2.94260000	4.71320000
H	-2.67760000	-1.50800000	4.45890000
O	0.99170000	4.84400000	1.41150000
H	0.04460000	4.68670000	1.24640000
H	1.37870000	5.11300000	0.55970000
O	8.96840000	-3.22430000	-1.10650000
H	9.44130000	-2.41170000	-0.84580000
H	8.48450000	-2.94410000	-1.90140000
O	10.31450000	-1.35170000	2.33330000
H	10.40090000	-0.39770000	2.15850000
H	9.79280000	-1.61400000	1.55900000
O	8.57240000	3.14050000	-3.76240000

H	8.19600000	2.23880000	-3.65510000
H	7.95230000	3.59880000	-4.37340000
O	-8.66240000	9.48300000	3.58970000
H	-8.96590000	10.29320000	3.15760000
H	-9.43220000	8.89790000	3.61180000

1: EGCg 2 = 1:3 complex

Number of imaginary frequency = 0

Sum of electronic and zero-point Energies =	-10232.851327 au
Sum of electronic and thermal Energies =	-10232.682808 au
Sum of electronic and thermal Enthalpies =	-10232.681864 au
Sum of electronic and thermal Free Energies =	-10233.049701 au

O	6.08975500	5.96356300	-2.82397900
H	6.64239200	6.26198100	-2.05453000
C	4.99234300	5.40487500	-2.22992500
C	4.96450200	4.03581400	-1.95067500
O	6.01569300	3.22556300	-2.29290200
H	6.58332300	3.16725400	-1.48543900
C	3.86177500	3.48557100	-1.27171400
O	3.83950200	2.16708400	-0.98454100
H	4.66117900	1.73881900	-1.30647700
C	2.79850400	4.29992400	-0.87436300
H	1.95437000	3.86320900	-0.35111200
C	2.83024200	5.65764500	-1.17498100
C	1.83047900	6.61647000	-0.59064100
H	1.69533500	7.47456300	-1.26697100
C	-0.37990000	6.71598300	0.21544600
C	-1.70406100	6.35033300	-0.03015800
H	-1.91321700	5.53492200	-0.71314100
C	-2.73150800	7.04993200	0.59901000
C	-2.43065500	8.13379500	1.43431400
H	-3.24282600	8.67490700	1.91083000
C	-1.10453700	8.48057800	1.64463000
C	-0.04637900	7.77969500	1.05423300
C	2.35640400	7.16055400	0.75068600
H	3.34888100	7.59340200	0.60470500
C	3.64260600	5.43535100	1.79624200
C	3.53991900	4.23153500	2.65197700
C	4.69578800	3.48358000	2.86278800
H	5.64491400	3.80398600	2.44630500
C	2.33168300	3.83150100	3.23265300
H	1.42259900	4.40340000	3.07310700
C	1.38111500	8.17545200	1.32706900

H	1.55772300	8.27899000	2.40262300
H	1.59354200	9.15705700	0.88451500
O	0.58341000	5.97167900	-0.41024600
O	-4.03681800	6.76167100	0.41950500
H	-4.16305400	5.86025100	0.04290700
O	-0.74716100	9.52484900	2.45119500
H	-1.54983800	9.92177900	2.81770900
C	3.90973200	6.20729700	-1.86644600
H	3.97454900	7.27767200	-2.05403600
O	2.46082000	6.06328100	1.66593800
O	4.67761000	5.81865900	1.28150800
C	2.28613300	2.68005000	4.00929200
O	1.14078300	2.24464400	4.59935200
H	0.44556100	2.14883100	3.91389500
C	3.45500000	1.92788000	4.24404200
O	3.33386000	0.86949100	5.07103100
H	4.07310300	0.23951700	4.98534000
C	4.65695100	2.33190000	3.63664300
O	5.83508300	1.65461600	3.81954300
H	5.68265500	0.70460300	4.00537600
O	0.71842700	6.13200000	-3.66962400
H	1.33172000	6.61055700	-4.25270800
C	1.13573500	4.83675400	-3.65946300
C	2.33140300	4.50290200	-4.28870400
O	3.10722000	5.49142000	-4.88419300
H	3.65844300	5.87323000	-4.17084400
C	2.79085500	3.18931700	-4.25623200
O	3.98625700	2.88083500	-4.84568400
H	4.37735500	3.71771600	-5.15129400
C	2.09297500	2.21869600	-3.55639900
H	2.52039500	1.22814300	-3.45838200
C	0.94234300	2.58331100	-2.84922900
C	0.43453500	1.61067000	-1.79584200
H	1.30972900	1.34625300	-1.20118600
C	-1.77753700	2.29435100	-1.27764300
C	-2.58619600	3.11460300	-0.49138100
H	-2.17413700	3.59786900	0.38710100
C	-3.90647100	3.30228300	-0.88200500
C	-4.43639900	2.64433800	-1.98540300
H	-5.48615800	2.77662900	-2.20953700
C	-3.62374200	1.78151200	-2.71971600
C	-2.26975600	1.60595800	-2.38997000
C	-0.21382800	0.32103500	-2.29695200
H	-0.53535900	-0.24521700	-1.41535400
C	0.69613200	-1.74242200	-3.02407400

C	1.91966100	-2.38775900	-3.54188900
C	3.13978900	-1.71530600	-3.50219200
H	3.22621300	-0.72580600	-3.06786300
C	1.83103300	-3.68137600	-4.06425800
H	0.86918000	-4.18104700	-4.09557900
C	-1.40728800	0.64442700	-3.17031900
H	-1.05977000	1.08506500	-4.11423900
H	-1.97820900	-0.25797700	-3.41115900
O	-0.46431800	2.22501600	-0.88748900
O	-4.72694100	4.16550300	-0.19378300
H	-4.71031800	3.87417800	0.75789900
O	-4.08770800	1.07104500	-3.77019700
H	-5.05502300	1.23151100	-3.87188000
C	0.43004500	3.87621200	-2.93842000
H	-0.42520700	4.19096300	-2.35219400
O	0.81206200	-0.41323600	-2.96502900
O	-0.32087800	-2.33065900	-2.69210000
C	2.97812600	-4.33296000	-4.52320000
O	2.96687900	-5.55874000	-5.08581600
H	2.03993800	-5.85633900	-5.16920500
C	4.22916400	-3.69792000	-4.40541600
O	5.35111200	-4.35554300	-4.76374500
H	6.08260200	-4.06322600	-4.16340100
C	4.27964700	-2.35805400	-3.98399800
O	5.49165400	-1.76746700	-4.03777500
H	5.42483500	-0.82355700	-3.73961700
O	0.55545200	-1.75376900	5.42716000
H	1.30292700	-1.43034200	4.89178500
C	-0.03929400	-2.84248700	4.83578100
C	0.64946400	-4.05640500	4.75501300
O	1.92585200	-4.20246700	5.23514000
H	2.38215400	-3.33550600	5.16997500
C	0.03680900	-5.17523400	4.16863000
O	0.67391300	-6.35149900	4.00799100
H	1.67218500	-6.27887300	4.01706600
C	-1.28969600	-5.07423900	3.75588000
H	-1.74530700	-5.95433600	3.30884300
C	-1.99092200	-3.87452800	3.87267600
C	-3.37658100	-3.80057000	3.27603700
H	-3.98293500	-4.66227600	3.60181900
C	-5.23281300	-2.34195100	3.14131800
C	-6.06145200	-1.45900400	3.83234300
H	-5.70819700	-0.95971500	4.72450000
C	-7.32707000	-1.18901200	3.31920800
C	-7.76983900	-1.82146400	2.15654900

H	-8.75822900	-1.62310200	1.76157700
C	-6.89896600	-2.65214900	1.45723400
C	-5.61386000	-2.92860200	1.93274900
C	-3.29655500	-3.84811300	1.74421200
H	-2.75900200	-4.74152600	1.42258600
C	-1.27495000	-2.89378900	0.92779600
C	-0.44414300	-1.67460600	1.03559600
C	0.79315300	-1.63568400	0.38481500
H	1.13712900	-2.47483500	-0.20998300
C	-0.91566700	-0.58263000	1.77553300
H	-1.86041900	-0.63540500	2.30335700
C	-4.68585900	-3.79955400	1.13179800
H	-4.62822500	-3.44551700	0.09649600
H	-5.07552500	-4.82461400	1.08239500
O	-4.00631800	-2.60288000	3.69908100
O	-8.13338300	-0.31013000	3.98141900
H	-9.02841800	-0.32704300	3.56608700
O	-7.25568600	-3.23712100	0.28520600
H	-7.95614600	-2.69059900	-0.12637900
C	-1.36131500	-2.75155800	4.39967800
H	-1.87781000	-1.80159700	4.46987200
O	-2.52868100	-2.69679300	1.36885600
O	-0.90074200	-3.95657500	0.46365100
C	-0.16020600	0.58084500	1.80629600
O	-0.53627100	1.74037500	2.42893700
H	-1.52019700	1.71249900	2.59111900
C	1.06859900	0.63042200	1.15027800
O	1.79739000	1.77031900	1.09921600
H	1.24032000	2.49806400	1.42734000
C	1.55691700	-0.47592400	0.44812900
O	2.72623700	-0.37497400	-0.22954700
H	3.06323400	0.54340100	-0.16499900
C	-0.21472800	-7.43259800	-3.53489300
C	-0.05784600	-6.31515800	-2.71715300
C	-1.06355300	-5.34595800	-2.65547200
C	-2.22021100	-5.48262900	-3.42491700
C	-2.38688900	-6.62651200	-4.21396500
C	-1.38983600	-7.59862600	-4.26658700
H	0.59626600	-8.15191400	-3.59339600
H	-0.91673300	-4.47350600	-2.02706000
H	-3.30971700	-6.73172400	-4.77517100
H	-1.52083600	-8.47527500	-4.89292000
C	1.25153200	-6.12481000	-1.99368100
O	2.29221200	-6.58900800	-2.42744900
N	1.14759500	-5.40265300	-0.84460300

H	0.22590700	-5.16708700	-0.48693300
C	-3.36712100	-4.49872000	-3.38534000
O	-4.47852800	-4.84699600	-3.75626900
N	-3.06844600	-3.25638500	-2.90289100
H	-2.09347800	-3.03542100	-2.71252100
C	2.18543200	-4.77001800	-0.13090100
C	3.21372600	-4.08540900	-0.74705600
C	2.04391200	-4.73035000	1.27802600
C	4.03380600	-3.21636800	0.01894600
H	3.34377700	-4.13640200	-1.82470100
C	2.84826500	-3.92459600	2.03818600
H	1.28025000	-5.34194200	1.75115700
C	5.02029400	-2.40371800	-0.61333300
C	3.81652800	-3.09188500	1.42234300
H	2.73303500	-3.94078400	3.11354800
C	5.68032000	-1.44932100	0.10701600
H	5.25144000	-2.55045400	-1.66465200
C	4.58064500	-2.11259400	2.13129500
C	5.46551200	-1.28982500	1.49566800
H	6.03918900	-0.55460900	2.05021800
C	-3.99724100	-2.32226100	-2.39243600
C	-3.56879000	-1.46445800	-1.40262000
C	-5.34770800	-2.26708100	-2.82381600
C	-4.48510400	-0.63069900	-0.72000500
H	-2.52809200	-1.47439900	-1.08162700
C	-6.24565900	-1.43539300	-2.20178900
H	-5.67394200	-2.91145700	-3.62735200
C	-4.05641700	0.13116400	0.39965000
C	-5.85768200	-0.62598800	-1.09977900
H	-7.27216200	-1.44772900	-2.55829500
C	-4.95923200	0.83723000	1.14632200
H	-3.00551600	0.12433700	0.66924100
C	-6.75536000	0.14783700	-0.29780300
C	-6.33180400	0.85072400	0.80178800
H	-7.04349300	1.38252600	1.42448700
S	6.89901900	-0.37797800	-0.62890200
S	4.57203600	-2.10384800	3.90818800
S	-4.40933600	1.75643600	2.58609500
S	-8.50492100	0.13536900	-0.65298700
O	5.39521200	-0.94630900	4.35088000
O	3.17998400	-1.98156200	4.39341600
O	7.15640000	-0.85827600	-1.99421700
O	8.07243300	-0.49985500	0.28239200
O	-8.97149800	-1.27356800	-0.68361600
O	-8.66088100	0.77485500	-1.99083900

O	-5.38746800	1.49463900	3.65562900
O	-4.37968000	3.19254200	2.20560200
O	-3.05877700	1.22691300	2.89848000
O	-9.16930100	0.92804100	0.41167200
O	6.31886800	0.98686600	-0.59067800
O	5.19518200	-3.40522200	4.27227000
O	4.30679600	-5.37308600	6.08773000
H	3.36384800	-5.14294600	6.14974500
H	4.68889500	-4.60798500	5.61821400
O	7.25339500	-3.56336100	-2.91803600
H	7.51316100	-3.71063900	-1.98493800
H	7.09895100	-2.60253400	-2.95131500
O	-6.80546000	1.53212300	-3.89615700
H	-7.11917100	0.89540000	-3.22468500
H	-6.99374900	2.38658600	-3.44240500
O	-8.19304000	3.58679000	0.63020800
H	-8.76162700	2.81138500	0.48770200
H	-7.89853200	3.43661500	1.55098600
O	7.92190300	1.91604200	1.82513400
H	8.00738500	1.08705900	1.31019400
H	7.22597100	1.75480300	2.48842500
O	-7.75561000	3.42702300	-2.11540000
H	-8.35460000	2.68057900	-1.93792800
H	-7.46245900	3.67857100	-1.21471300
O	-9.46948200	0.81817300	-4.65811200
H	-8.53675800	1.09366200	-4.73501100
H	-9.64703400	0.99583100	-3.71999400
O	6.90598900	3.78251800	0.20250700
H	5.97167900	3.84788500	0.46157600
H	7.29241400	3.04734300	0.75934400
O	-10.48201000	-0.06479300	2.60716300
H	-10.91143500	-0.88252900	2.32088100
H	-10.09075500	0.30627600	1.78482700
O	-9.28922100	-1.86610200	-3.59155200
H	-9.37364400	-1.65184300	-2.64812000
H	-9.33358700	-1.00034400	-4.04054400
O	-7.82923000	2.62649400	3.28001200
H	-8.15926100	1.71957600	3.40610400
H	-6.88527900	2.49542900	3.50627000
O	6.64919000	-4.42945900	2.09861700
H	7.47754000	-4.80772100	2.42561200
H	6.20460100	-4.04134600	2.88439100
O	8.11179100	-3.46666300	-0.17777100
H	8.34975100	-2.52916200	-0.05871600
H	7.41331900	-3.61696200	0.48549900

O	3.27798900	-6.64333700	3.83158800
H	3.81244600	-6.24712000	4.54940800
H	3.77102100	-6.51237900	2.99233600
O	0.36559500	-5.66443100	-6.07067000
H	-0.44016600	-5.76091500	-5.53890600
H	0.44189500	-4.71464200	-6.24480000
O	5.13846000	0.76626500	-3.26227700
H	4.92526100	1.53685600	-3.82125800
H	5.90678700	1.04026800	-2.73211400
O	7.01894300	6.46068000	-0.34925200
H	7.23577100	5.54048700	-0.08361600
H	6.15460300	6.58681800	0.07949500
O	4.78501600	-6.41536600	1.47416300
H	4.20711900	-6.06000600	0.78151100
H	5.45660200	-5.71647900	1.61514600

1: EGCg 2 = 1:4 complex

Number of imaginary frequency = 0

Sum of electronic and zero-point Energies = -11984.859804 au

Sum of electronic and thermal Energies = -11984.658080 au

Sum of electronic and thermal Enthalpies = -11984.657136 au

Sum of electronic and thermal Free Energies = -11985.101641 au

O	-4.39310400	-1.65208400	1.83497500
H	-4.79014800	-0.85580700	1.41623400
C	-5.25170800	-2.70621000	1.62635300
C	-4.71067000	-3.91076000	1.17535500
O	-3.39913900	-4.10344200	0.87274800
H	-2.79007400	-3.54483900	1.40205700
C	-5.57640500	-4.97869800	0.89392700
O	-5.09094600	-6.12212500	0.35686800
H	-4.20906500	-5.94938200	-0.03670200
C	-6.94262900	-4.85473100	1.13069700
H	-7.58228300	-5.70468900	0.90713400
C	-7.46907000	-3.64968900	1.59825400
C	-8.96514100	-3.51693000	1.75417500
H	-9.38843200	-4.49466700	2.03469600
C	-10.54193000	-2.20513200	2.95715900
C	-10.82371900	-1.52970400	4.13921400
H	-10.03675000	-1.34422700	4.85976000
C	-12.12900900	-1.10758300	4.38762300
C	-13.14529100	-1.36863900	3.46464000
H	-14.16746800	-1.05696700	3.65006300
C	-12.83006300	-2.04125200	2.29016800

C	-11.52811500	-2.46813300	1.99723600
C	-9.67764200	-3.08840600	0.46727400
H	-9.38184900	-3.73031100	-0.36631500
C	-9.36387700	-1.29667500	-1.05907700
C	-8.87184000	0.10378300	-1.17074800
C	-8.46492900	0.56240700	-2.42336100
H	-8.57172200	-0.06366100	-3.30196200
C	-8.73219300	0.89348900	-0.02866100
H	-9.06351700	0.52174900	0.93628800
C	-11.18554500	-3.12508800	0.68169500
H	-11.65623500	-2.60963200	-0.16627100
H	-11.51587400	-4.17280400	0.64404000
O	-9.23809600	-2.57990600	2.78478400
O	-12.36560900	-0.45693600	5.54763400
H	-13.31516700	-0.22136200	5.60367900
O	-13.85670400	-2.26115000	1.41877800
H	-13.54250900	-2.79277000	0.67459600
C	-6.62293700	-2.57317300	1.84657200
H	-7.02213900	-1.62517900	2.19209100
O	-9.26212500	-1.74621600	0.20741100
O	-9.74587400	-1.98221600	-1.98048700
C	-8.16684600	2.15749300	-0.14261300
O	-8.04713900	3.02165400	0.89751200
H	-8.18273100	2.54055300	1.72602600
C	-7.67403600	2.59558600	-1.37753900
O	-7.00772700	3.78453400	-1.49655300
H	-6.34078900	3.78667300	-0.76356300
C	-7.85646300	1.81075300	-2.52054400
O	-7.40760500	2.25085900	-3.72533700
H	-7.01551000	3.13264700	-3.59660800
O	10.75839400	3.59624500	1.78012100
H	11.49603800	3.37605700	2.37592700
C	10.40812900	2.43421400	1.17508700
C	11.10541500	1.26769100	1.51714600
O	12.05685200	1.39689200	2.48924800
H	12.84187700	0.83081400	2.28843600
C	10.75243400	0.07703200	0.88864500
O	11.44974900	-1.06210000	1.23904300
H	11.03429000	-1.81847500	0.79935900
C	9.74384100	0.04530600	-0.07126000
H	9.50936200	-0.89212200	-0.56839900
C	9.04522700	1.20832800	-0.38968900
C	7.92350900	1.18213100	-1.41332900
H	8.00261900	2.06653400	-2.05587700
C	7.48610300	-1.12335500	-1.92366900

C	7.85180100	-2.21460900	-2.70530800
H	8.48438800	-2.07904200	-3.57345600
C	7.28663600	-3.45697000	-2.43492100
C	6.41654900	-3.62074000	-1.34947300
H	5.99453500	-4.59568900	-1.13526800
C	6.09091000	-2.51531100	-0.56847800
C	6.61576200	-1.24467200	-0.84101500
C	6.52223000	1.19878000	-0.77719100
H	5.79047900	1.29760500	-1.58078300
C	5.91957200	3.46952000	-0.38973400
C	5.83892300	4.52890500	0.64601900
C	5.05986400	5.66374200	0.37528000
H	4.53442800	5.74587000	-0.57076600
C	6.52468200	4.37637500	1.85769200
H	7.13937600	3.50601800	2.05823400
C	6.25490400	-0.06222500	0.01187000
H	6.83600500	-0.04993300	0.94315100
H	5.19955700	-0.10639900	0.30272600
O	8.04383800	0.07641200	-2.29230000
O	7.61386500	-4.48254400	-3.25491000
H	7.03697100	-5.25677600	-3.06794300
O	5.25773200	-2.58376300	0.50247200
H	5.00878100	-3.49809200	0.73282700
C	9.38645500	2.40993800	0.23425800
H	8.87344400	3.33786700	0.00119800
O	6.41787500	2.31859000	0.10505700
O	5.59140000	3.60556300	-1.55261000
C	6.42933400	5.38054900	2.81248100
O	7.08324600	5.27717400	4.00139500
H	6.80594000	6.03464000	4.54168900
C	5.64815600	6.50162700	2.55419800
O	5.55662600	7.45463100	3.52322200
H	4.89362400	8.09060000	3.19766100
C	4.94539600	6.65018800	1.35237800
O	4.23974800	7.80017500	1.29449400
H	3.50264400	7.84814100	0.61579800
O	3.09378600	2.88797300	5.02975800
H	3.07002700	3.48571900	4.23508800
C	1.82949700	2.50250000	5.34515800
C	1.64370700	1.67615600	6.45581200
O	2.63330200	1.23961300	7.28436500
H	3.49858300	1.13064300	6.79224400
C	0.34331800	1.28379000	6.80395500
O	0.18934800	0.48400900	7.89654600
H	1.09461900	0.30894700	8.21038000

C	-0.75806100	1.69460000	6.06675800
H	-1.74614800	1.34821900	6.35629900
C	-0.55861600	2.49901800	4.94312100
C	-1.72859000	2.81970500	4.04211500
H	-2.59592600	3.16122100	4.63149900
C	-2.22902900	4.23157200	2.21755400
C	-2.06897200	5.51313400	1.69793300
H	-1.21360200	6.10858300	2.00125200
C	-2.99657500	5.98561100	0.77733300
C	-4.08314200	5.19494800	0.39494500
H	-4.77847200	5.56568300	-0.35118700
C	-4.17633500	3.89926900	0.88496900
C	-3.25093000	3.37739200	1.80074600
C	-2.17342800	1.59913400	3.22311100
H	-2.46605700	0.78522700	3.88791700
C	-0.29710000	0.19379200	3.06252700
C	1.15341800	0.26720300	2.77987900
C	1.70957000	1.22762700	1.93073500
H	1.08268900	1.89925400	1.35476800
C	1.96988000	-0.56492300	3.54363700
H	1.51489200	-1.29448400	4.20247100
C	-3.32477400	1.95171100	2.28726100
H	-3.29991000	1.24069200	1.45098100
H	-4.27289700	1.77818900	2.81454500
O	-1.32503900	3.85892500	3.16530400
O	-2.87653600	7.22433100	0.24211100
H	-1.97077100	7.56315100	0.42529300
O	-5.23492200	3.14077800	0.45863000
H	-5.02957200	2.17981500	0.39506900
C	0.72422100	2.90224000	4.58840200
H	0.88342100	3.50647500	3.70245000
O	-1.02103100	1.18131400	2.47545500
O	-0.80460200	-0.62162400	3.80595500
C	3.35187000	-0.42102000	3.50780900
O	4.19260200	-1.17210800	4.27556000
H	3.72208200	-2.00574800	4.52420500
C	3.91515600	0.57985000	2.71395300
O	5.24770100	0.82164300	2.76883700
H	5.45354200	1.48952800	2.08512100
C	3.09048600	1.35780700	1.88935200
O	3.77377000	2.23785300	1.10683900
H	3.16385800	2.80886600	0.56422300
O	-2.21076900	-0.89503600	0.39115700
H	-2.65580300	-1.36199100	1.12835800
C	-0.90001500	-1.25364800	0.32525200

C	-0.39972000	-2.25043400	1.16579700
O	-1.26447200	-2.86942800	2.02484600
H	-0.80398400	-3.03754400	2.89709800
C	0.96072400	-2.57308400	1.10991000
O	1.41831800	-3.52342700	1.96715300
H	2.36786300	-3.67792600	1.79041200
C	1.80257800	-1.89847700	0.23946600
H	2.86943000	-2.12098400	0.23566400
C	1.29037900	-0.91134000	-0.60007500
C	2.30061700	-0.22065300	-1.47160300
H	3.16316200	0.05115300	-0.83953300
C	3.77983000	-0.80242900	-3.20585400
C	4.47244300	-1.82531000	-3.83443300
H	4.18816200	-2.85835200	-3.66638700
C	5.55722900	-1.49409900	-4.63609800
C	5.96449400	-0.15986000	-4.75876600
H	6.87556400	0.09014200	-5.28927200
C	5.24924400	0.83574200	-4.10104000
C	4.08569000	0.54920600	-3.36707000
C	1.91177400	1.05231400	-2.21161100
H	1.45654500	1.79010700	-1.54463000
C	0.08395300	1.61674900	-3.63952800
C	-1.15243300	1.04089500	-4.24776900
C	-2.09545800	1.93059700	-4.78319500
H	-1.89938100	2.99973900	-4.77155400
C	-1.38641600	-0.33784400	-4.20284000
H	-0.64201600	-1.02860800	-3.82215800
C	3.18469700	1.63751400	-2.81970500
H	2.91514200	2.35910000	-3.59843900
H	3.66518100	2.22197700	-2.02308900
O	2.73615600	-1.19796400	-2.41345700
O	6.27430600	-2.45547900	-5.27210400
H	6.01050200	-3.32663900	-4.91462400
O	5.70857000	2.12200100	-4.18409700
H	5.43815200	2.61995500	-3.38949000
C	-0.06419600	-0.60416700	-0.58524300
H	-0.48575800	0.13628900	-1.25532000
O	0.93266700	0.65793900	-3.19935400
O	0.29843500	2.79859700	-3.51658000
C	-2.58151600	-0.82682800	-4.71718300
O	-2.84120100	-2.17287800	-4.71357800
H	-3.77136100	-2.29852000	-4.96904500
C	-3.54300200	0.04822400	-5.21024100
O	-4.72873800	-0.46631300	-5.63420000
H	-5.30625700	0.29943100	-5.81318900

C	-3.30866000	1.43224100	-5.25327200
O	-4.35460700	2.12192200	-5.74429300
H	-4.32992400	3.12863500	-5.65347200
C	-6.23243400	-2.10505300	-1.35970000
C	-4.92801800	-1.61399600	-1.36355400
C	-3.87204200	-2.43445500	-1.74249200
C	-4.12386500	-3.76914400	-2.06833200
C	-5.43070700	-4.25067200	-2.10104700
C	-6.49056400	-3.40455600	-1.77742700
H	-7.01752600	-1.45534500	-0.99907700
H	-2.85118300	-2.06450700	-1.68679600
H	-5.60415700	-5.29855100	-2.32689500
H	-7.51361300	-3.76564500	-1.81398000
C	-4.68260800	-0.19129200	-0.97781400
O	-5.17472800	0.33148400	0.04026900
N	-3.91994200	0.46498300	-1.85418800
H	-3.60125700	-0.04143500	-2.67485500
C	-2.96075200	-4.70279100	-2.16099200
O	-2.98080000	-5.80668900	-1.61595000
N	-1.88366400	-4.20326300	-2.82334600
H	-2.04293600	-3.40230900	-3.43327600
C	-3.49050600	1.81939100	-1.76560500
C	-2.35488800	2.14540400	-1.07665000
C	-4.17047900	2.77951600	-2.54516700
C	-1.77286300	3.42410300	-1.26215100
H	-1.86990800	1.41470000	-0.43452900
C	-3.64236600	4.02948900	-2.70502100
H	-5.07674500	2.47894700	-3.06221000
C	-0.51252700	3.71306500	-0.69880000
C	-2.39232900	4.36633900	-2.12421400
H	-4.15410200	4.74062200	-3.32977900
C	0.12597600	4.87648400	-1.02332800
H	-0.03422500	2.96996400	-0.06711900
C	-1.71592200	5.59044200	-2.38605500
C	-0.47570300	5.84142500	-1.85991200
H	0.05423300	6.75169600	-2.12040300
C	-0.55667300	-4.64425200	-2.64477200
C	-0.12216500	-5.05578300	-1.40980800
C	0.34940200	-4.56778000	-3.73129600
C	1.22729800	-5.42207400	-1.22490800
H	-0.80132500	-5.07837300	-0.56262100
C	1.66970400	-4.91483900	-3.57060900
H	0.00571100	-4.18188900	-4.68575200
C	1.68345500	-5.75763400	0.07346300
C	2.14321200	-5.37974100	-2.31323900

H	2.35006500	-4.82757300	-4.41062700
C	3.00582700	-6.03545100	0.27164700
H	0.99365400	-5.72351700	0.90948500
C	3.48394500	-5.81411500	-2.07282800
C	3.91278000	-6.12946100	-0.81055700
H	4.92891300	-6.47377500	-0.64618600
S	1.80315600	5.09596900	-0.48377700
S	-2.43395300	6.76360200	-3.53085600
S	3.63279500	-6.00824200	1.92889300
S	4.58348200	-6.15920500	-3.44849600
O	-2.51583300	6.04704800	-4.82507100
O	-3.76832400	7.11238600	-2.97354300
O	2.34241800	3.70903100	-0.44688200
O	1.78701000	5.74263400	0.84856100
O	4.71406400	-4.93496800	-4.26346800
O	3.88124300	-7.25795300	-4.16384900
O	2.51106500	-6.33947300	2.83957700
O	4.04324500	-4.56736600	2.09108400
O	4.77410200	-6.93181800	2.01644200
O	5.86239400	-6.57874700	-2.82745700
O	2.43515800	5.92674000	-1.53260900
O	-1.50897200	7.91648700	-3.57082400
O	-0.47394000	8.56029800	0.29839800
H	-0.49706400	9.20908000	1.01640500
H	-1.01004800	8.97886700	-0.43625400
O	-15.06275400	0.19346100	5.66470900
H	-15.56202000	-0.19481000	6.39633000
H	-15.26829500	1.13826000	5.68500900
O	2.90713500	-3.56106300	4.41666000
H	1.96781300	-3.42348300	4.16281000
H	3.35229600	-3.85674400	3.59306600
O	3.25581300	4.42216200	2.86601900
H	2.64870200	4.91184300	2.27217600
H	3.83325300	3.92270900	2.26326300
O	2.34649500	8.40544100	-0.44352000
H	2.37762800	7.62239200	-1.03224300
H	1.45222900	8.34578200	-0.05234600
O	3.27828900	-5.96392800	5.87267700
H	3.09029600	-6.79196100	5.37281000
H	3.19270800	-5.21182900	5.25172800
O	1.99787700	-6.92892300	-6.25831800
H	2.83101800	-6.84501200	-5.75976200
H	1.62241300	-7.73437900	-5.87269200
O	4.88309900	0.98345700	5.92763500
H	4.85141800	0.15800200	5.40590900

H	4.62813700	1.68138500	5.29634200
O	14.02942800	-0.31966300	1.79245400
H	13.32809700	-0.88772300	1.42246400
H	14.35511100	-0.79651600	2.56850200
O	0.59518100	-5.66565000	4.97539600
H	1.03733500	-5.81605900	4.11871800
H	1.32749300	-5.75470500	5.61459400
O	-0.85380500	-8.02711700	-1.47953500
H	-1.46484900	-7.29277400	-1.65035500
H	-0.19472500	-7.98138700	-2.19483500
O	-4.68235200	4.67568200	-5.71694500
H	-3.90147500	5.22844100	-5.48492800
H	-5.36580200	4.95453900	-5.07283600
O	1.07897100	-7.97441300	-3.76599400
H	2.04167800	-7.90232600	-3.61414900
H	0.87262800	-7.09492800	-4.12340700
O	0.02527800	-3.16139800	4.33535900
H	-0.35899200	-2.45220100	4.87259600
H	0.01767500	-4.03477300	4.79817000
O	-2.30113600	9.39586100	-1.43093800
H	-2.97443800	8.72732100	-1.20525700
H	-2.01131700	9.08864400	-2.31751300
O	1.23763900	-1.95479800	-4.69053400
H	1.60330100	-2.21361400	-3.82883000
H	1.38222100	-0.99577100	-4.67201500
O	-6.21178200	5.74901000	-3.59875300
H	-6.47233200	5.27372800	-2.79169800
H	-5.44552100	6.30680500	-3.34107600
O	5.64728900	-7.22351600	4.73414500
H	5.10154600	-6.58491400	5.23075800
H	5.56482200	-6.95822800	3.79941800
O	3.15544200	-8.43356500	4.60096000
H	2.87327300	-8.04625500	3.75453000
H	4.12940500	-8.31839100	4.59194500

(2) Complexes of sensor molecule **1** and EGC **4**

1: EGC **4** = 1:1 complex

Number of imaginary frequency = 0

Sum of electronic and zero-point Energies = -6693.556871 au

Sum of electronic and thermal Energies = -6693.439081 au

Sum of electronic and thermal Enthalpies = -6693.438137 au

Sum of electronic and thermal Free Energies = -6693.716302 au

C	5.14268800	-1.34973900	-1.92622400
C	4.34011500	-2.35146200	-1.37525900
C	3.00991700	-2.11206200	-1.00162800
C	2.54089700	-0.80765300	-1.16759500
C	3.30444000	0.20651900	-1.73548000
C	4.61418200	-0.06957000	-2.12099200
H	6.16462800	-1.57629800	-2.21449100
H	2.90469300	1.21070900	-1.82996200
O	1.28685900	-0.42965200	-0.75839600
C	0.35925200	-1.43047900	-0.31685500
H	-0.08175500	-1.92361900	-1.19487700
C	-0.74757500	-0.72149300	0.42651900
C	-1.88679900	-1.44680000	0.76634700
C	-0.69740000	0.64586300	0.69530400
C	-2.98902900	-0.81582300	1.34339100
H	-1.95694100	-2.50194400	0.51966500
C	-1.80287700	1.27417200	1.25897900
H	0.18325000	1.22556600	0.44077300
C	-2.96038500	0.56120900	1.58555100
C	2.12000500	-3.17522800	-0.40493900
H	2.70800500	-3.89641500	0.16969100
H	1.59236200	-3.73529200	-1.18796200
O	1.68295500	-1.93155700	1.63580300
C	1.08201500	-2.50800400	0.49329500
H	0.32906100	-3.24119700	0.80858100
H	2.64988700	-2.03884900	1.54490300
O	4.82556600	-3.60979800	-1.21892600
H	5.81668000	-3.57258800	-1.14953600
O	5.33260900	0.94001900	-2.65878500
H	6.18819200	0.59048400	-3.01182600
O	-4.13157700	-1.48830400	1.65731600
H	-4.18497400	-2.27332400	1.07152200
O	-3.98619300	1.28656900	2.09251500
H	-4.84158800	0.77229700	2.13364100
O	-1.78815600	2.62550500	1.46412000
H	-2.70322700	2.87268000	1.69248400
C	-1.22263300	6.30600200	-0.98196600
C	-1.18553500	4.91589200	-0.87695100
C	0.01713800	4.27636400	-0.59330500
C	1.18639900	5.01679000	-0.43577900
C	1.15748900	6.40262100	-0.59658600
C	-0.04852900	7.04554600	-0.85924300
H	-2.17675400	6.79036500	-1.16437200
H	0.03419500	3.19640900	-0.51345100
H	2.08579600	6.95721100	-0.50174000

H	-0.07530800	8.12561500	-0.96337700
C	-2.46588100	4.14207400	-0.99355600
O	-3.51693300	4.63161600	-0.59530100
N	-2.34725300	2.91093000	-1.57008800
H	-1.41494400	2.60632500	-1.85812500
C	2.49647300	4.35191400	-0.13228900
O	3.56092000	4.83249900	-0.48525600
N	2.37665200	3.18058600	0.57176400
H	1.45906300	2.97048700	0.94513000
C	-3.31563500	1.89276500	-1.54117000
C	-4.63271800	2.09740000	-1.20377300
C	-2.87100700	0.57585600	-1.84562900
C	-5.50319800	0.99061100	-1.06324200
H	-5.03439900	3.08343400	-1.02824000
C	-3.69893700	-0.50554800	-1.70216900
H	-1.83238800	0.42998500	-2.12989700
C	-6.84641700	1.22411700	-0.67289600
C	-5.04547500	-0.33913600	-1.27465100
H	-3.28366600	-1.49553700	-1.84863500
C	-7.69282100	0.16518200	-0.49518200
H	-7.17181400	2.24798800	-0.49889800
C	-5.96405900	-1.40647900	-1.03136600
C	-7.26069400	-1.17274500	-0.65654600
H	-7.93747800	-2.00191400	-0.47666700
C	3.37669800	2.24175600	0.87569800
C	4.65245300	2.27808400	0.35702700
C	2.99229200	1.18166200	1.73798300
C	5.54707600	1.21410200	0.62833700
H	4.96162400	3.08190300	-0.29704300
C	3.85375700	0.16345500	2.03618800
H	1.98854500	1.16324000	2.15630700
C	6.84223800	1.20650300	0.04040700
C	5.14356500	0.12044600	1.44790100
H	3.54198700	-0.59338100	2.74713900
C	7.69477100	0.16997900	0.30215800
H	7.13971000	2.01695300	-0.61790100
C	6.05237000	-0.96219000	1.63011300
C	7.31313400	-0.92385700	1.10832200
H	8.01297300	-1.72612500	1.31984200
S	-9.31578700	0.46434500	0.14747500
S	-5.45630600	-3.10879400	-1.23405700
S	9.28688600	0.03659300	-0.45840200
S	5.59871300	-2.46109000	2.49661200
O	-5.24989700	-3.28573700	-2.70134100
O	-4.18695800	-3.25457500	-0.47345700

O	-9.13292300	0.36188200	1.63909700
O	-10.20111500	-0.59232500	-0.37724800
O	5.52488500	-2.10598500	3.93501000
O	6.65890800	-3.43329800	2.16582100
O	9.13032500	-1.10824800	-1.41600500
O	10.24872300	-0.26027300	0.61839900
O	9.53659300	1.32058600	-1.15938900
O	4.27351000	-2.85992800	1.95826400
O	-9.73681500	1.81206500	-0.27965300
O	-6.53881100	-3.95148100	-0.71069900
O	2.58917000	-2.00341200	4.42022500
H	2.18655900	-2.21334300	3.56093700
H	3.53541700	-2.18884900	4.29292300
O	-11.51565400	-1.04802000	2.36922500
H	-11.37452900	-1.86761400	1.86222400
H	-10.63985900	-0.62291800	2.33970800
O	9.90231200	1.46837800	-3.94879000
H	10.32447400	0.59310800	-4.07714500
H	9.96361600	1.60779900	-2.98556700
O	10.25964500	-1.28968500	-4.01442600
H	9.32604700	-1.25251900	-4.28499800
H	10.18339300	-1.39370600	-3.04759700
O	11.60687500	1.82485900	2.06178000
H	11.46799400	1.07010000	1.46157000
H	11.03873500	2.51510200	1.65661400
O	-6.33052600	0.11711300	2.46616200
H	-6.33106100	-0.81858600	2.19162000
H	-7.15284300	0.47896200	2.09622000
O	-12.21506700	1.48680700	1.31351300
H	-11.68413800	1.57819500	0.50505500
H	-12.13214400	0.53977300	1.55772700
O	9.38775100	3.15243900	1.05833000
H	9.38827700	2.70308100	0.19397800
H	8.96317700	2.51006400	1.66358500
O	-10.19915100	2.66493400	2.89406700
H	-11.01292500	2.42072100	2.40051400
H	-9.64428100	1.88645700	2.71496600
O	8.31603500	-1.29328700	4.29982200
H	8.32045600	-0.32876400	4.20010200
H	7.37827600	-1.55209800	4.31963000
O	-7.78770500	-4.18446700	-3.61351100
H	-7.57423200	-5.08701400	-3.33671400
H	-6.95898700	-3.70738900	-3.40769000
O	7.67889900	-0.06052400	-3.59079100
H	8.05203500	-0.44520800	-2.77216600

H	8.32319300	0.65985900	-3.80628100
O	-1.68349600	-3.44677900	-1.93537100
H	-1.98748900	-3.14051900	-2.81186800
H	-2.51149500	-3.52603700	-1.42913800
O	7.41161900	-3.53806600	-0.60142400
H	7.22978700	-3.54339300	0.36236600
H	7.94227600	-2.74084500	-0.77991300
O	-6.48153000	4.81058400	-0.56214800
H	-5.56301800	4.83827200	-0.25414500
H	-7.03699500	4.59401100	0.21215500
O	-10.12098100	-3.03964700	0.77208900
H	-10.14552000	-2.20096500	0.26583400
H	-9.96212000	-3.71893900	0.07695300
O	-7.90216600	-2.19225400	2.27020100
H	-8.53393400	-2.71229400	1.73306700
H	-8.38125700	-1.35854600	2.39458500
O	-8.56416600	3.97792900	1.05999600
H	-8.94826000	3.41559200	0.36666900
H	-9.08511000	3.69684400	1.84291100
O	0.24072900	1.64733400	-2.27486900
H	0.54979200	0.90128400	-1.71805200
H	0.76950300	1.59068200	-3.08223300
O	4.27276500	-5.52857400	0.87614400
H	4.43374400	-5.05852800	0.04128000
H	4.36564500	-4.79466600	1.50696000
O	-3.05730600	-2.43448500	-4.21680200
H	-3.87071400	-2.76578400	-3.78310400
H	-3.09672200	-1.47959600	-4.06289500
O	9.12153100	1.09838500	2.98996200
H	9.12300200	0.27186800	2.47708700
H	10.07756300	1.33139800	2.99397600
O	-9.16341900	-4.63844200	-1.22244100
H	-8.26411000	-4.58365800	-0.85048400
H	-9.01817100	-4.22133500	-2.09380400

1: EGC 4 = 1:2 complex

Number of imaginary frequency = 0

Sum of electronic and zero-point Energies = -7188.449560 au

Sum of electronic and thermal Energies = -7188.330956 au

Sum of electronic and thermal Enthalpies = -7188.330012 au

Sum of electronic and thermal Free Energies = -7188.611512 au

C	0.78455800	-3.17055700	-2.03225400
C	-0.41658300	-2.74156300	-1.46983900

C	-0.88533500	-1.42588100	-1.64117100
C	-0.09455300	-0.57960300	-2.43098900
C	1.09455800	-0.98566600	-3.01939300
C	1.53889300	-2.29011000	-2.81061300
H	1.12856800	-4.17996700	-1.83518900
H	1.68980500	-0.28280700	-3.58975500
O	-0.41511000	0.74323900	-2.62117400
C	-1.73768800	1.16274700	-2.32861500
H	-2.42803800	0.74319300	-3.07682600
C	-1.75262300	2.67868700	-2.40706400
C	-2.96004300	3.38191000	-2.29117900
C	-0.55922400	3.37073600	-2.61050700
C	-2.95480200	4.77224900	-2.39246800
H	-3.90625100	2.86777200	-2.13329200
C	-0.55780000	4.76125400	-2.66761300
H	0.38213700	2.84385000	-2.70947300
C	-1.75626200	5.45905400	-2.58548300
C	-2.17255700	-0.92453100	-1.02292300
H	-2.28727700	-1.30964900	-0.00082700
H	-3.04068600	-1.28379900	-1.58900300
O	-1.19053700	1.02804200	0.02743400
C	-2.14306700	0.59921400	-0.96099500
H	-3.10708300	1.01013100	-0.65139700
H	-0.37648600	0.52296400	-0.15518600
O	-1.10605300	-3.67177100	-0.76079000
H	-1.96662000	-3.35923800	-0.41683700
O	2.69983500	-2.65027100	-3.39855400
H	3.09594000	-3.42000000	-2.93378400
O	-4.06241800	5.57019800	-2.29749400
H	-4.56307800	5.31773300	-1.48703200
O	-1.71928200	6.82099300	-2.64716600
H	-2.62260600	7.12120500	-2.44067600
O	0.61992500	5.43589800	-2.76088600
H	0.41215900	6.38456800	-2.72728700
C	-0.19000700	3.47487700	3.29878100
C	1.11459400	3.94669300	3.38722300
C	2.22487200	3.10516200	3.25335100
C	1.98356800	1.75908900	2.97834100
C	0.68222100	1.26218800	2.85143300
C	-0.38808300	2.13612800	2.97762600
H	-1.02025600	4.16906400	3.35006200
H	0.53283300	0.21032500	2.62509200
O	2.98695400	0.86909500	2.77767400
C	4.27518900	1.41274100	2.45587000
H	4.23287600	1.86599400	1.45334400

C	5.23429300	0.25292300	2.45624500
C	5.17202700	-0.70274000	3.47570300
C	6.17655500	0.12071000	1.44054000
C	6.03374900	-1.80128200	3.46401700
H	4.41360200	-0.65116000	4.25224400
C	7.02458200	-0.98993200	1.41075000
H	6.25054100	0.86119100	0.64833200
C	6.95457200	-1.96435400	2.41841100
C	3.62487400	3.64590400	3.36985400
H	3.71364800	4.26928300	4.26647100
H	3.87061400	4.27241800	2.50451100
O	4.67217900	2.04485500	4.77682300
C	4.65002700	2.52285400	3.44738000
H	5.63507100	2.90893600	3.14630000
H	5.24211600	1.25866000	4.78456800
O	1.30094000	5.29575000	3.54249200
H	1.91924200	5.56969700	2.84031000
O	-1.66818800	1.70801200	2.68018300
H	-1.58068900	1.18027600	1.85826600
O	5.97310500	-2.70732600	4.46874500
H	5.98797600	-3.60734400	4.04396000
O	7.76297400	-3.05032400	2.45183900
H	8.08770200	-3.27227100	1.54359700
O	7.93536300	-1.19777400	0.42715300
H	7.90482000	-0.45510000	-0.22111600
C	-2.70946400	6.43365600	0.64712000
C	-2.67588100	5.03761500	0.72256600
C	-1.46053100	4.36342800	0.65081200
C	-0.26850400	5.08096100	0.53065800
C	-0.30396700	6.47331600	0.49848900
C	-1.52229300	7.14836400	0.55293200
H	-3.67092400	6.93792000	0.66495700
H	-1.45606900	3.27762200	0.67437800
H	0.63378400	7.01322100	0.41563700
H	-1.54221300	8.23234000	0.50871800
C	-3.97390100	4.29262700	0.72198900
O	-4.95153100	4.73954800	0.11367800
N	-3.99492100	3.11138200	1.38862300
H	-3.15622200	2.84222600	1.90744600
C	1.07503000	4.41897700	0.40803900
O	2.10710700	5.04456300	0.67821100
N	1.05677700	3.14033000	-0.02451500
H	0.15314900	2.71961800	-0.22330600
C	-4.94499100	2.08003200	1.20064100
C	-4.53964900	0.78950300	1.45573600

C	-6.26075600	2.30935400	0.71368400
C	-5.35203500	-0.30965400	1.10083100
H	-3.55924600	0.59112100	1.87886500
C	-7.08436600	1.25061200	0.41248200
H	-6.60736600	3.32137300	0.56294900
C	-4.83081600	-1.62661700	1.17397500
C	-6.64222900	-0.09320700	0.54681100
H	-8.07842200	1.46583500	0.03673100
C	-5.54754200	-2.67241000	0.67164500
H	-3.83404000	-1.79499900	1.56924400
C	-7.38917800	-1.23200300	0.11123800
C	-6.85656800	-2.49249500	0.15828900
H	-7.42327400	-3.34354800	-0.20965800
C	2.17791000	2.35932900	-0.40218600
C	2.17724400	1.01129400	-0.13768000
C	3.25290600	2.92383500	-1.12991700
C	3.22806800	0.17798900	-0.58060100
H	1.40332000	0.57348900	0.48407800
C	4.29585000	2.13808300	-1.55650900
H	3.23700100	3.98274900	-1.36241900
C	3.20087200	-1.21085000	-0.28670500
C	4.31057500	0.73513800	-1.31764500
H	5.10908900	2.58682900	-2.11146100
C	4.20560400	-2.01536500	-0.73811500
H	2.36493100	-1.63324200	0.26526600
C	5.33595400	-0.15785100	-1.77371400
C	5.28646200	-1.49741700	-1.49239800
H	6.08008700	-2.15828600	-1.83490100
S	-4.77795200	-4.27725100	0.58312900
S	-9.02803400	-1.00803100	-0.58901800
S	4.13417800	-3.76958100	-0.44744400
S	6.83903800	0.43824300	-2.56055500
O	-9.50510600	-2.37492400	-0.90494600
O	-9.81362900	-0.33524400	0.46484100
O	-3.32330000	-4.00297000	0.75990200
O	-5.13655900	-4.80040600	-0.74662700
O	7.70396900	0.83927300	-1.42102700
O	6.47524000	1.55529500	-3.44974900
O	5.37170800	-4.11183900	0.29548300
O	4.12404500	-4.38606000	-1.80638500
O	2.89688900	-4.02758100	0.30753800
O	7.37685300	-0.72859100	-3.30446500
O	-5.33633300	-5.08653900	1.69508700
O	-8.82799900	-0.17411400	-1.79320900
O	-8.78919000	-4.90611500	-1.94630700

H	-8.75956500	-3.93431800	-1.95919800
H	-9.53170000	-5.05486000	-1.32419600
O	6.84717100	-5.05809300	-2.41297600
H	5.89552900	-4.89042300	-2.27153600
H	7.21659300	-5.13410300	-1.51496200
O	8.08131300	-4.08119500	-0.00725000
H	8.43716600	-3.48077800	-0.70704300
H	7.12521300	-3.87599900	0.01178600
O	-10.33861300	-4.76573600	0.36989100
H	-9.47401100	-5.10543000	0.68509200
H	-10.17526700	-3.82053200	0.19746400
O	3.05691500	-3.08916700	2.90857900
H	2.86179600	-3.37065800	1.99220200
H	3.56850100	-2.26778100	2.81525400
O	-7.82621700	-5.86437200	0.48451900
H	-6.96958600	-5.72168700	0.92534900
H	-7.69467500	-5.62303100	-0.45274900
O	-2.41004900	-6.81367600	0.29018600
H	-2.55003700	-6.68035700	1.24578900
H	-2.39174800	-5.90244800	-0.03705100
O	-8.77477700	0.36886400	3.03611900
H	-9.20231700	0.08187800	2.20785400
H	-8.00723100	0.86396300	2.72199200
O	-3.40692100	-3.43660500	-2.51272700
H	-4.11652900	-3.91478300	-2.04305100
H	-2.61399100	-3.95196400	-2.30581900
O	7.67037300	0.56386700	-5.87738400
H	7.21279800	1.20662100	-5.31137700
H	7.74584100	-0.17157800	-5.24857500
O	5.23070100	-4.82690200	3.09673300
H	5.53387900	-4.68396200	2.18200500
H	4.37800300	-4.33650500	3.11732600
O	-2.90831800	-5.81717800	2.93794200
H	-3.86615900	-5.79648100	2.75481400
H	-2.63105100	-5.01582400	2.46273200
O	4.95537700	4.90456400	0.53091100
H	3.99173400	4.77433000	0.47721100
H	5.03911800	5.82227000	0.82384600
O	-9.08263200	2.61410600	-1.74098100
H	-8.14922900	2.67805200	-1.98466300
H	-9.23414500	1.64865000	-1.76965700
O	8.68698400	-2.98787400	-2.39911300
H	8.01537700	-3.63284000	-2.70273800
H	8.33173400	-2.11467100	-2.65392000

1: EGC 4 = 1:3 complex

Number of imaginary frequency = 0

Sum of electronic and zero-point Energies = -8828.990549 au

Sum of electronic and thermal Energies = -8828.838954 au

Sum of electronic and thermal Enthalpies = -8828.838009 au

Sum of electronic and thermal Free Energies = -8829.184299 au

C	2.79469200	4.98904900	-4.33503200
C	1.45501900	5.26528500	-4.58912300
C	0.66762400	6.00119100	-3.69664300
C	1.26294700	6.40116900	-2.49781500
C	2.59220900	6.09671100	-2.19407700
C	3.34306300	5.36763900	-3.11226800
H	3.38209100	4.41353000	-5.04252200
H	3.00893600	6.37729900	-1.23371900
O	0.57492000	7.06922900	-1.51794000
C	-0.84687300	7.16385300	-1.60867700
H	-1.10223800	8.06967900	-1.04942100
C	-1.54711700	5.98749300	-0.94854300
C	-2.87963100	6.12661800	-0.55075100
C	-0.88396000	4.77000100	-0.75507200
C	-3.56674100	5.04917000	0.01528600
H	-3.40419600	7.06545400	-0.69482400
C	-1.59316600	3.69301700	-0.22632100
H	0.17318700	4.67577800	-0.99047000
C	-2.93127100	3.81117500	0.14506100
C	-0.78771900	6.26723000	-3.96625800
H	-1.39159700	5.36703200	-3.78570600
H	-0.94757400	6.53231700	-5.01573100
O	-2.66333500	7.61211300	-3.16812500
C	-1.28442400	7.39740100	-3.07445300
H	-0.78550500	8.32638700	-3.38330500
H	-3.10273600	6.72937100	-3.23127700
O	0.84655700	4.77848500	-5.70756200
H	1.32905600	3.96913800	-5.96760700
O	4.60839700	4.99537500	-2.76834200
H	4.84496200	4.20634600	-3.29458100
O	-4.85203000	5.20693800	0.42329800
H	-5.16148700	4.41831000	0.92817700
O	-3.55359700	2.73500800	0.70193700
H	-4.32836200	2.49057200	0.13062100
O	-1.07021500	2.43994300	-0.03702300
H	-0.10554200	2.43248500	-0.15596300
C	2.72979800	2.71096200	-1.04517800

C	1.58648700	2.30011600	-1.72154600
C	1.01259200	1.03752000	-1.55491100
C	1.62130700	0.18599900	-0.62330000
C	2.78784500	0.54358000	0.05194500
C	3.34910600	1.80300200	-0.16921500
H	3.13733300	3.70633400	-1.18643100
H	3.22570800	-0.14368200	0.77125500
O	1.14734500	-1.06339900	-0.37429900
C	-0.14570900	-1.38831300	-0.89769500
H	-0.90741300	-0.86098500	-0.30325600
C	-0.32360800	-2.87765100	-0.79454300
C	0.72134000	-3.69411300	-1.21421800
C	-1.54370300	-3.42847700	-0.40641200
C	0.55509800	-5.07108000	-1.28037400
H	1.65985200	-3.26480100	-1.53202600
C	-1.67696200	-4.81588500	-0.40112300
H	-2.37376100	-2.80441200	-0.08438100
C	-0.62528500	-5.64212700	-0.79847400
C	-0.16926700	0.60346200	-2.38270400
H	-0.04790200	0.93160600	-3.42242800
H	-1.10559000	1.03114200	-2.00123000
O	0.83235500	-1.47561800	-3.07231600
C	-0.24507700	-0.91659800	-2.35601400
H	-1.20548100	-1.26192900	-2.76199300
H	0.83266300	-1.07580300	-3.98914400
O	1.02827000	3.17169200	-2.63066800
H	0.05746000	3.12372000	-2.59120600
O	4.46142500	2.21107400	0.46435400
H	4.84594500	1.44709100	0.97828100
O	1.51348100	-5.88209100	-1.79544800
H	2.09820800	-5.32508300	-2.37652100
O	-0.79153200	-7.00023600	-0.67968200
H	-0.00656900	-7.32184600	-0.18913100
O	-2.83853300	-5.39608300	0.02629700
H	-2.65637200	-6.35160100	0.10004400
C	-0.42333600	-0.76484500	3.03685300
C	-0.51934700	0.56199400	2.61452000
C	0.59458500	1.41105000	2.60680800
C	1.81669900	0.86696000	3.02290400
C	1.93864400	-0.45271800	3.44720700
C	0.80526900	-1.25841700	3.47157400
H	-1.31728200	-1.38075100	3.05546600
H	2.89615200	-0.80546700	3.80934500
O	2.96236900	1.60240200	3.05715100
C	2.91349600	3.03661000	3.08563500

H	3.20443800	3.38243200	2.08519500
C	3.95257000	3.50352600	4.09399600
C	5.13310000	2.76665800	4.23985500
C	3.75460900	4.66997700	4.84152200
C	6.10411700	3.19567000	5.14302100
H	5.29069200	1.86284900	3.65855200
C	4.72787700	5.08984000	5.74754200
H	2.86693500	5.28643900	4.73996900
C	5.89128000	4.35068200	5.89967200
C	0.53850500	2.90095000	2.38545100
H	-0.47359800	3.28625200	2.54646900
H	0.86274900	3.19960400	1.37938400
O	1.06981000	3.25181100	4.67502000
C	1.50578700	3.55745300	3.36320700
H	1.50619200	4.64343800	3.19530300
H	1.81229200	3.39208500	5.28414400
O	-1.77786500	1.00206600	2.29897000
H	-1.76735500	1.61945300	1.53882800
O	0.90990200	-2.53994100	3.95882000
H	0.13832400	-2.68847800	4.57792700
O	7.28088800	2.57297300	5.39262700
H	7.57344200	2.05722800	4.58420400
O	6.83019600	4.78942800	6.79225200
H	7.58675700	4.18408500	6.69751700
O	4.54009800	6.22362200	6.47863500
H	5.33213800	6.34237400	7.02789900
C	-3.12607900	-6.09131500	3.08333100
C	-2.50899200	-4.84882200	2.93590900
C	-1.14824400	-4.76534700	2.65356700
C	-0.41811400	-5.93534800	2.43472300
C	-1.04060000	-7.17824800	2.55976600
C	-2.38233100	-7.25730400	2.92132400
H	-4.18877800	-6.14383800	3.30285000
H	-0.69383000	-3.78956300	2.49634600
H	-0.46100300	-8.07505100	2.36409500
H	-2.85696200	-8.22543700	3.04273500
C	-3.30906900	-3.57902000	2.93341100
O	-3.13991100	-2.67782500	3.75571300
N	-4.20493700	-3.50560600	1.92505700
H	-4.17231300	-4.25898900	1.24056800
C	0.98815300	-5.89466200	1.91157900
O	1.39897000	-6.78856400	1.16389100
N	1.71633000	-4.83031000	2.30867300
H	1.29133300	-4.18732300	2.97995600
C	-5.03161400	-2.37902200	1.64394000

C	-6.32873400	-2.59563700	1.25562200
C	-4.51841900	-1.05737400	1.71241400
C	-7.15758900	-1.50826200	0.88389100
H	-6.74372600	-3.60041300	1.22783000
C	-5.30661100	0.00929500	1.35873100
H	-3.50248400	-0.87992600	2.04860500
C	-8.50279300	-1.74918600	0.50030100
C	-6.64034700	-0.18144900	0.90466900
H	-4.90203300	1.01000000	1.45829600
C	-9.30155200	-0.70181700	0.13583900
H	-8.88069600	-2.76995300	0.51597500
C	-7.50285000	0.86881400	0.45734900
C	-8.80027800	0.61970100	0.09207000
H	-9.44155300	1.43177800	-0.23224900
C	2.92633300	-4.33794800	1.77839700
C	3.48915700	-4.72732900	0.58550800
C	3.52332600	-3.29935800	2.53875600
C	4.57341800	-3.97860100	0.05316300
H	3.10436800	-5.56623600	0.01975300
C	4.55823400	-2.56201000	2.04027700
H	3.10838500	-3.07361000	3.51482200
C	5.12819900	-4.32673400	-1.21098000
C	5.06928000	-2.83202300	0.74266800
H	4.96630900	-1.74313400	2.61881100
C	6.04787900	-3.50365200	-1.80323000
H	4.80413300	-5.23776900	-1.71055100
C	6.02300000	-2.00334200	0.07734200
C	6.48619900	-2.31572800	-1.17301100
H	7.19150600	-1.65761900	-1.67050300
S	-10.97823000	-1.00192700	-0.39829500
S	-6.89718300	2.53852000	0.21161000
S	6.70012700	-3.86565700	-3.42536800
S	6.69699100	-0.53337400	0.85111200
O	-8.02598500	3.29625800	-0.35739000
O	-6.39835800	3.05407000	1.50230400
O	-11.43432900	-2.20379500	0.36441200
O	-10.89134600	-1.28451800	-1.85460100
O	5.56658300	0.12970700	1.56988000
O	7.22943000	0.28383100	-0.25703800
O	6.14683800	-5.18192600	-3.80151200
O	8.16530200	-3.82031800	-3.28107400
O	6.17105900	-2.77746200	-4.30255400
O	7.72416800	-0.98733200	1.81293600
O	-11.73301700	0.21886600	-0.07592500
O	-5.76800300	2.38724900	-0.76835200

O	3.39782000	-1.79667900	-2.14514600
H	3.39680700	-1.71394700	-1.17749200
H	2.47116300	-1.58612500	-2.42337400
O	0.88614700	-0.38272900	-5.49812700
H	1.26559300	0.52069500	-5.45186800
H	1.64711400	-0.97432200	-5.69639400
O	-12.69609400	-3.47239700	-1.88461100
H	-12.50438300	-3.33631500	-0.93864300
H	-12.39231500	-2.61685400	-2.23843700
O	-6.14701000	5.50918200	-2.15376500
H	-5.98089200	5.35175800	-1.20765800
H	-6.65683900	4.72896200	-2.46684100
O	2.95703400	-2.04057600	-5.16950800
H	3.64537500	-1.45790600	-4.78465600
H	3.45846500	-2.76402100	-5.62568700
O	7.19255500	3.03122500	1.10983100
H	6.44929600	2.75277400	0.55076400
H	7.99982400	2.68645800	0.67169200
O	8.68476700	-6.53473500	-4.12165200
H	7.71660500	-6.46322100	-4.12571100
H	8.90951300	-5.63481300	-3.83429000
O	-1.82382200	2.81495400	4.64116900
H	-0.86056900	2.77682800	4.75800200
H	-2.01240400	2.18314200	3.92902700
O	4.35408600	2.29899600	-3.76358200
H	4.78507800	1.41448300	-3.85339500
H	3.93628000	2.26303600	-2.88388300
O	8.01480800	1.47781600	3.14251400
H	7.79234700	0.54750800	2.93393600
H	7.51335200	2.02402100	2.47897600
O	4.89794700	-0.38078100	-3.86924800
H	4.46278800	-0.74775300	-3.06491900
H	5.61471500	-1.02799800	-4.03678500
O	-7.30062600	3.14339500	-3.03769600
H	-7.93971400	3.14193200	-2.30159400
H	-6.54721300	2.69425300	-2.61265600
O	2.96069700	-4.23871700	-3.42229200
H	2.45662600	-3.57817400	-3.94207600
H	3.52314300	-3.63733700	-2.89259700
O	9.53063300	1.61080300	0.65920200
H	8.98268800	0.92794300	0.22892400
H	9.38337400	1.44171100	1.60766400
O	1.93145200	2.21340300	-5.15647500
H	2.86596800	2.17210100	-4.84721300
H	1.48620100	2.58044800	-4.36770100

O	-1.15653400	-2.63439700	5.58841300
H	-1.94098000	-2.76864100	5.00774300
H	-1.20536600	-1.69754900	5.83021800
O	3.26633000	-7.86185000	-0.69309500
H	2.96657800	-7.69840100	0.21373200
H	2.59564700	-7.37490400	-1.19936400
O	-9.89385800	-4.67780000	0.47741500
H	-10.51999400	-3.96390200	0.68458100
H	-9.78970400	-4.56596800	-0.49189500
O	-3.77458500	5.09026800	-3.31365600
H	-3.32147700	4.63423700	-2.58862500
H	-4.68163700	5.25879100	-2.93725900
O	-9.97082500	-3.97254100	-2.22258100
H	-10.94409800	-4.08370400	-2.23235500
H	-9.90353200	-3.00126500	-2.17958000
O	4.37105400	-4.19652100	-5.94035000
H	4.11012300	-4.65877200	-5.12091500
H	5.23176800	-3.82871500	-5.66474200
O	-12.87850600	-0.71338600	2.40803700
H	-12.50071000	-1.50810200	1.99958900
H	-12.68802900	-0.06591400	1.71021700

(3) Complexes of sensor molecule **1** and GCg **6**

1: GCg **6** = 1:1 complex

Number of imaginary frequency = 0

Sum of electronic and zero-point Energies = -6881.453479 au

Sum of electronic and thermal Energies = -6881.339943 au

Sum of electronic and thermal Enthalpies = -6881.338998 au

Sum of electronic and thermal Free Energies = -6881.607351 au

C	-5.56364100	-1.30065700	-2.86952100
C	-4.83721500	-2.45142500	-2.55931300
H	-5.23146700	-3.41394500	-2.84204000
C	-3.59670400	-2.36160900	-1.93560500
C	-5.05466400	-0.04670800	-2.53329900
H	-5.56532200	0.87301100	-2.79243800
O	-6.72188700	-1.47090500	-3.54485800
H	-7.31258700	-0.67334800	-3.39808200
O	-2.87980800	-3.47180700	-1.63809300
H	-3.43156200	-4.26310700	-1.85629100
C	-3.80190400	0.01221500	-1.92333200
C	-3.04315500	-1.11481600	-1.61005800
C	-1.67343100	-1.00943900	-0.99453900

H	-1.59482200	-1.64693300	-0.10372800
H	-0.91830800	-1.36477700	-1.70863600
C	-1.31660200	0.42847800	-0.62699900
H	-1.64435000	0.69051900	0.37746900
C	-1.93362300	1.43972600	-1.60437700
H	-1.51852600	1.24230600	-2.60573600
O	-3.34108800	1.27072300	-1.63516800
C	-1.65746100	2.86643700	-1.18352100
O	0.09630000	0.59243900	-0.73093400
C	-0.40967200	3.45396100	-1.40529800
H	0.39199100	2.92191200	-1.90770800
C	-0.17950400	4.75510300	-0.96638100
C	-1.18364000	5.45883100	-0.30392800
C	-2.42232000	4.86655400	-0.08577500
C	-2.66358000	3.57041300	-0.52446800
H	-3.63569300	3.12346700	-0.36724800
O	-3.34314100	5.63929900	0.56856700
H	-4.23238500	5.20185800	0.50033100
O	-0.91252700	6.74124800	0.10012300
H	-1.73987700	7.10235000	0.45867100
O	1.02180300	5.35746400	-1.19069000
H	0.96647700	6.25179300	-0.81712000
C	0.85118200	0.73372600	0.36407500
C	2.26848000	0.95163600	0.01276400
O	0.41275400	0.70411300	1.50314200
C	3.17529700	1.34764400	0.99764400
H	2.83486500	1.47076600	2.02258500
C	4.50179800	1.57794900	0.65352400
C	4.94638500	1.41306300	-0.66904300
C	4.03269900	0.93481200	-1.62243500
C	2.69964500	0.74880300	-1.29809500
H	2.00984400	0.40792800	-2.06094000
O	4.43948600	0.62344300	-2.88040400
H	5.42041300	0.53161000	-2.94053500
O	6.19929900	1.62359500	-1.08215700
H	6.78237400	2.10188500	-0.41071700
O	5.45535700	1.96655200	1.55740900
H	5.07970400	1.92890800	2.44785000
C	1.96663200	-3.56413400	4.74358400
C	1.99154200	-2.69965300	3.64616500
C	0.79928100	-2.21308900	3.10256100
C	-0.41840400	-2.60878200	3.65998800
C	-0.43825700	-3.51435800	4.72299600
C	0.74960100	-3.98300300	5.26890500
H	2.90368600	-3.90068300	5.17831800

H	0.82644200	-1.52064100	2.26231900
H	-1.40273200	-3.82432900	5.11097000
H	0.73012400	-4.67033900	6.10875100
C	3.34232100	-2.32125100	3.11547100
O	4.32492600	-2.27876200	3.85714500
N	3.41120100	-2.07866800	1.78558500
H	2.57842800	-2.20176600	1.20379600
C	-1.76172600	-2.11586500	3.19706800
O	-2.76950000	-2.77406800	3.40247000
N	-1.77149500	-0.88501400	2.60182300
H	-0.90658900	-0.35436100	2.51802100
C	4.59143800	-1.81134500	1.06124700
C	5.72694800	-1.24395000	1.59462800
C	4.55093600	-2.13456300	-0.31591600
C	6.83268700	-0.95539200	0.75542100
H	5.77892600	-0.98962700	2.64501400
C	5.60403000	-1.85598700	-1.14007000
H	3.65821400	-2.58927800	-0.72415800
C	7.99500600	-0.33419900	1.28590200
C	6.78231600	-1.25636800	-0.63437900
H	5.51989400	-2.08483600	-2.19174900
C	9.03199000	0.00118600	0.46150400
H	8.06063400	-0.13296300	2.35090000
C	7.89283300	-0.89594100	-1.45293600
C	8.97492300	-0.24281000	-0.93132000
H	9.77676800	0.10230500	-1.57747400
C	-2.94712800	-0.20816300	2.21531700
C	-4.02241800	-0.85680000	1.66103100
C	-2.98474400	1.20277100	2.38065400
C	-5.17558500	-0.12375000	1.28552800
H	-4.00370800	-1.93024400	1.51302300
C	-4.08197100	1.93268100	2.01007900
H	-2.11886800	1.70955300	2.79870600
C	-6.29218800	-0.80279300	0.74039100
C	-5.22416900	1.29112900	1.45699200
H	-4.06689400	3.00367700	2.17053800
C	-7.42225800	-0.11150400	0.39677400
H	-6.23860500	-1.88093700	0.61665300
C	-6.42272200	1.96677800	1.07429000
C	-7.49569900	1.28839400	0.55224600
H	-8.39303800	1.82150000	0.25911300
S	10.51628800	0.74510700	1.11964600
S	7.85870700	-1.19046500	-3.22139200
S	-8.83508500	-1.00961100	-0.21569800
S	-6.58009700	3.74558300	1.22497100

O	7.45091700	-2.60584700	-3.40386200
O	6.86863200	-0.23763300	-3.76939100
O	10.45793500	0.52344100	2.58264600
O	10.43673400	2.18972200	0.76355600
O	-5.62439800	4.29204900	0.19569900
O	-6.18804100	4.11146000	2.59536000
O	-9.44480600	-1.67287200	0.96861100
O	-8.26686900	-1.98652900	-1.17749900
O	-9.72516200	-0.01146500	-0.84011100
O	-7.97750500	4.06438200	0.88170500
O	11.62079900	0.03843300	0.44271600
O	9.24779500	-0.94309800	-3.67540700
O	2.85572400	-1.86260800	-2.92178400
H	3.44499300	-2.55846500	-3.28151200
H	3.40212800	-1.05709000	-2.99419800
O	7.80281400	3.00561700	0.43004200
H	7.64442300	2.76605800	1.36302800
H	8.73670500	2.74187300	0.29473200
O	11.81526800	-1.21739600	-2.16599800
H	10.92191800	-1.39135300	-2.51270800
H	11.68638600	-0.87947000	-1.25798800
O	-6.67036500	2.81445900	-2.24845600
H	-6.01139000	2.76880500	-1.53802000
H	-7.07508500	3.70386800	-2.13967100
O	-3.54294200	4.93477900	3.39118000
H	-4.48576700	4.71779700	3.28261100
H	-3.30690200	5.30600400	2.52569700
O	-6.55201600	-4.18376400	-0.46332000
H	-6.41982000	-3.31625100	-0.89143900
H	-7.42922800	-4.45799500	-0.83495500
O	5.06342700	-3.80612400	6.08923100
H	5.52074700	-4.43278100	5.51307500
H	4.80793600	-3.09716400	5.47021500
O	-10.24120300	-4.41240400	0.82255400
H	-9.41675600	-4.46196900	1.35862400
H	-10.35260800	-3.44409200	0.77121000
O	1.42639500	-2.08405800	-0.41263500
H	1.87227300	-1.90877500	-1.27325500
H	0.63803900	-2.59891600	-0.63412600
O	-9.02226600	-4.54538100	-1.56761500
H	-8.99051600	-3.56416600	-1.59276700
H	-9.57231800	-4.71216100	-0.75938100
O	-7.84676500	-3.79120100	2.00099200
H	-7.25332000	-3.93667200	1.23553900
H	-8.22304700	-2.90499300	1.83936100

O	-8.20554200	0.68205400	-3.10552300
H	-8.84814700	0.46173000	-2.40261900
H	-7.67698300	1.42988100	-2.74527900
O	8.73533300	2.69061200	3.08581200
H	9.18034000	1.83185900	3.22098300
H	9.37109100	3.10055200	2.47541400
O	-7.58015500	5.34543400	-1.56787500
H	-8.08226900	4.99427200	-0.80717400
H	-6.70297100	5.43034800	-1.15525200
O	-7.05234000	-4.49813300	-3.57604500
H	-7.80649300	-4.75057600	-3.01301100
H	-7.10350900	-3.52448000	-3.63251800
O	11.17070700	1.15725300	-3.57566200
H	11.66238600	0.46801700	-3.09207100
H	10.36161000	0.67499500	-3.81351700
O	4.90960900	-3.61374100	-3.84884700
H	5.09197900	-4.21556800	-3.11300900
H	5.76151700	-3.12839000	-3.92729200
O	-4.73185400	-5.53175800	-2.04756700
H	-5.32844200	-5.37860900	-2.80594400
H	-5.29347100	-5.19917300	-1.31279200

1: GCg 6 = 1:2 complex

Number of imaginary frequency = 0

Sum of electronic and zero-point Energies = -8251.588575 au

Sum of electronic and thermal Energies = -8251.455657 au

Sum of electronic and thermal Enthalpies = -8251.454713 au

Sum of electronic and thermal Free Energies = -8251.763063 au

C	4.98765900	-4.58728700	-0.31231900
C	4.43459200	-5.22609300	-1.43274300
H	5.07546900	-5.75536900	-2.12868300
C	3.05751400	-5.20003100	-1.63792500
C	4.15124100	-3.86944900	0.55140100
H	4.55451500	-3.34245200	1.41051200
O	6.31401700	-4.64475700	-0.14317500
H	6.56039000	-4.40008700	0.79616300
O	2.56807300	-5.82519800	-2.74667000
H	1.92289300	-5.22517500	-3.16859600
C	2.77575900	-3.88191100	0.32964800
C	2.18584900	-4.56412400	-0.73782000
C	0.68682800	-4.71523300	-0.84775200
H	0.40337500	-5.71334300	-0.50329900
H	0.34078000	-4.61177600	-1.87795000

C	0.00465400	-3.65933100	0.01438400
H	0.11219900	-2.67670900	-0.45417600
C	0.66619900	-3.56827400	1.39782100
H	0.70909000	-4.56455300	1.85123800
O	2.01998400	-3.11870200	1.19592100
C	-0.05602300	-2.61489900	2.30940700
O	-1.41621300	-3.82070700	0.12048900
C	-0.96505000	-3.14653500	3.22183300
H	-1.11847900	-4.21878100	3.30696600
C	-1.73119400	-2.29598000	4.02041500
C	-1.52244600	-0.91122100	3.96634800
C	-0.62645000	-0.38343000	3.02706900
C	0.08754000	-1.23379200	2.17860700
H	0.75147400	-0.78587600	1.44498300
O	-0.41098400	0.95076800	2.94334100
H	-0.98312400	1.44330200	3.57371300
O	-2.10338200	-0.11334500	4.91176500
H	-2.76682200	0.50639500	4.52752500
O	-2.64501800	-2.81993900	4.86664800
H	-3.40409000	-2.18437800	4.88997500
C	-1.91544500	-4.91612800	0.72106200
C	-3.39529700	-4.83716200	0.86728800
O	-1.25247000	-5.86895800	1.06728000
C	-4.01074300	-3.68835800	1.36894800
H	-3.43246400	-2.82786900	1.69630600
C	-5.39829200	-3.65463000	1.44609300
C	-6.15349700	-4.75217600	1.03398100
C	-5.52238700	-5.89712400	0.55394400
C	-4.13784000	-5.95595900	0.48855200
H	-3.64342500	-6.84743500	0.11635500
O	-6.35337300	-6.90566400	0.13192800
H	-6.10858800	-7.10478800	-0.79090800
O	-7.50918500	-4.64507200	1.07878000
H	-7.87113000	-5.35596400	0.51531600
O	-6.04239500	-2.54005600	1.89604700
H	-6.99938500	-2.69604800	1.82480700
C	0.71999500	-2.53959700	-3.35850100
C	1.07283600	-1.36717600	-2.69252200
H	2.08908200	-0.99640800	-2.70853200
C	0.10148800	-0.67314500	-1.97755900
C	-0.60951600	-2.93782500	-3.43047400
H	-0.89619500	-3.84424900	-3.95162600
O	1.67535800	-3.34570400	-3.90762600
H	2.55158800	-2.99935200	-3.62070700
O	0.45950500	0.37678200	-1.19045100

H	1.39727200	0.25873000	-0.93815700
C	-1.57176300	-2.18841900	-2.75189800
C	-1.24524600	-1.05359500	-2.00292000
C	-2.28211400	-0.34977200	-1.17693400
H	-2.62045000	0.56871200	-1.66928800
H	-1.86945700	-0.06025400	-0.20337000
C	-3.50312100	-1.22723300	-0.98030600
H	-3.33154700	-1.99288000	-0.22311800
C	-3.90914400	-1.89804700	-2.30192300
H	-4.12905300	-1.09371800	-3.02257100
O	-2.84025400	-2.68462500	-2.80669500
C	-5.12308900	-2.80355500	-2.17295300
O	-4.60774300	-0.40271600	-0.62461300
C	-6.35753900	-2.25095000	-1.80321700
H	-6.45631700	-1.18989700	-1.60681600
C	-7.46314700	-3.06899100	-1.64496100
C	-7.37141400	-4.43413500	-1.90336000
C	-6.16363100	-4.96824400	-2.32567600
C	-5.02988100	-4.16751400	-2.44119100
H	-4.09133700	-4.61565200	-2.74076400
O	-6.08652900	-6.32145700	-2.57522100
H	-6.99460900	-6.62651800	-2.74817400
O	-8.43043200	-5.28506200	-1.69899000
H	-9.23022800	-4.73837400	-1.61537600
O	-8.69394900	-2.63711300	-1.23943200
H	-8.65484600	-1.68838900	-1.04339200
C	-4.81555300	-0.10512000	0.67735600
C	-6.04785600	0.70105400	0.84328000
O	-4.06784000	-0.46224800	1.56077200
C	-6.49115800	0.97990500	2.13831700
H	-5.97506200	0.57983400	3.00067300
C	-7.56497200	1.84034400	2.35123500
C	-8.22943900	2.37414700	1.23792400
C	-7.79994600	2.07555100	-0.06003700
C	-6.70429400	1.25134400	-0.26740000
H	-6.33580600	1.09778300	-1.27601700
O	-8.51992100	2.65704800	-1.07575400
H	-7.92439500	3.32147500	-1.50314700
O	-9.26638200	3.22428700	1.41353500
H	-9.42851600	3.60004600	0.52758500
O	-7.95762100	2.16668600	3.60377200
H	-8.07037100	3.15725900	3.61836800
C	3.84338100	1.05899000	-5.36567100
C	4.05234800	1.22146100	-3.99488400
C	3.02553900	1.70735100	-3.18913000

C	1.78874300	2.03948000	-3.74502200
C	1.57447200	1.84146400	-5.10864400
C	2.59870000	1.34472100	-5.91419700
H	4.66238400	0.71796000	-5.99142100
H	3.18820800	1.88866800	-2.13018400
H	0.62876600	2.12273700	-5.56393000
H	2.43033800	1.21043900	-6.97774100
C	5.42573700	1.03633100	-3.40846800
O	6.38930000	1.62918900	-3.86007400
N	5.45171800	0.21267400	-2.31328200
H	4.71729000	-0.49233200	-2.27480000
C	0.78281400	2.67913100	-2.83059500
O	1.14366900	3.34025200	-1.86764800
N	-0.52510800	2.47480200	-3.14904800
H	-0.74150700	1.86926800	-3.92864600
C	6.52611300	0.02677300	-1.42530300
C	7.57278500	0.91122600	-1.29427100
C	6.46202700	-1.11409100	-0.57788700
C	8.54875300	0.70970600	-0.28288000
H	7.66053300	1.76955000	-1.94870400
C	7.40058900	-1.33121100	0.39327900
H	5.65476800	-1.83004900	-0.71599800
C	9.60825300	1.64652700	-0.12615400
C	8.46528400	-0.41040400	0.59362300
H	7.33543500	-2.21866700	1.00881400
C	10.53376400	1.46576500	0.86821800
H	9.67042200	2.50214000	-0.79828800
C	9.44056600	-0.53995000	1.62772900
C	10.45178700	0.37398200	1.76353000
H	11.17043400	0.27069000	2.56886800
C	-1.60093300	2.88361300	-2.32551000
C	-1.53691800	2.75581100	-0.96063500
C	-2.78009400	3.37216000	-2.93170100
C	-2.65560400	3.09023400	-0.16308800
H	-0.65367100	2.33896100	-0.49237400
C	-3.86217200	3.73700200	-2.17226100
H	-2.80789300	3.49018400	-4.01099000
C	-2.60774600	2.85916500	1.23437200
C	-3.83083900	3.63138700	-0.75411500
H	-4.74514200	4.11758400	-2.66453600
C	-3.67432100	3.18506600	2.02367000
H	-1.71335700	2.41910800	1.66710900
C	-4.88944100	4.03385900	0.12582400
C	-4.82572900	3.80988200	1.47930500
H	-5.64228900	4.11989100	2.12743200

S	11.92480300	2.58192400	1.00386900
S	9.36575400	-1.89575800	2.80989900
S	-3.52067200	2.85555400	3.77487400
S	-6.19839500	5.09410600	-0.48776500
O	7.99413600	-1.83236600	3.37850500
O	9.56320900	-3.12314600	1.98979100
O	12.97958400	2.01784800	0.13149300
O	12.30187400	2.57791900	2.43643400
O	-6.70793400	4.49106600	-1.76261800
O	-5.50653200	6.37854800	-0.75901500
O	-4.07152700	1.49459700	4.00985500
O	-4.29713000	3.90769100	4.45539500
O	-2.06877600	2.89535200	4.05444200
O	-7.24136600	5.16512100	0.54369500
O	11.42789700	3.90404100	0.54076800
O	10.43795300	-1.64102600	3.77657700
O	-5.74096300	6.18603300	4.32035800
H	-5.08144600	5.46737200	4.21839800
H	-5.93612200	6.16424800	5.26726900
O	14.57787800	4.40486300	2.47102200
H	13.79585800	4.96734700	2.61808600
H	14.16614800	3.52889100	2.40668900
O	-0.56749100	5.66434100	-3.03373300
H	-1.45797400	5.94750700	-2.75244900
H	-0.23627300	5.10118100	-2.31800600
O	-3.25893800	6.74103700	-2.47908400
H	-3.68478000	6.47895300	-1.64135200
H	-3.87467600	6.33728400	-3.13154000
O	-7.94305200	4.82298900	3.32868300
H	-7.94495300	4.90866700	2.35938500
H	-7.15904300	5.33000900	3.63534800
O	-5.44525900	8.53915500	-2.52725700
H	-4.50252300	8.28388100	-2.54355700
H	-5.76224000	8.02840600	-1.75991500
O	2.88635600	-0.84312000	-0.28164500
H	3.64465300	-0.46323200	0.19014300
H	2.47246600	-1.46365800	0.35552100
O	7.11659200	-4.23263700	2.32660500
H	6.99018900	-3.40080900	2.82721700
H	8.08341800	-4.14064100	2.15438900
O	11.90477700	5.34803300	2.92493200
H	11.66400900	5.19895700	1.99143300
H	11.90910900	4.42529700	3.23455700
O	10.60073200	4.02542000	-2.20766400
H	11.07335300	3.20791300	-2.45828300

H	10.92482500	4.18139200	-1.30269100
O	3.89535800	-2.33029700	-2.51813800
H	4.45772300	-3.10199400	-2.32231600
H	3.43055900	-2.15206900	-1.67396200
O	-5.59689400	6.10897600	-3.89410800
H	-6.10662800	5.58065500	-3.25060400
H	-5.74834200	7.03282500	-3.60203600
O	11.91505700	1.50773600	-2.37942700
H	12.43354100	1.67640000	-1.56253000
H	11.18894000	0.95102700	-2.06298500
O	-4.78169100	-1.28102700	4.23361000
H	-4.47457700	-0.39859900	3.96192300
H	-5.07814900	-1.67487000	3.39455500

1: GCg 6 = 1:3 complex

Number of imaginary frequency = 0

Sum of electronic and zero-point Energies = -10614.666793 au

Sum of electronic and thermal Energies = -10614.486372 au

Sum of electronic and thermal Enthalpies = -10614.485427 au

Sum of electronic and thermal Free Energies = -10614.884182 au

C	-6.75032900	-2.20793100	-2.31502600
C	-5.40057200	-2.43674700	-2.59882300
H	-5.04435700	-3.43879800	-2.79686200
C	-4.50398300	-1.37761900	-2.56467700
C	-7.19817300	-0.91450100	-2.04615400
H	-8.23081700	-0.71859800	-1.78272600
O	-7.64504100	-3.21735100	-2.31840400
H	-7.15462000	-4.08117600	-2.36167400
O	-3.17781000	-1.57135800	-2.83574400
H	-2.94153400	-2.51127200	-2.67607900
C	-6.27567400	0.12618200	-2.06001100
C	-4.91666100	-0.06462800	-2.31441600
C	-3.95361400	1.09276700	-2.27207800
H	-3.83726700	1.55449200	-3.26257800
H	-2.96569400	0.74821800	-1.95032000
C	-4.50614400	2.10684700	-1.28849200
H	-4.49739900	1.69799200	-0.27764300
C	-5.94400000	2.50933400	-1.65467900
H	-5.90177800	3.05341100	-2.61202500
O	-6.79327600	1.37602200	-1.79960100
C	-6.53300300	3.37471500	-0.56917900
O	-3.70910700	3.30902200	-1.31786600
C	-6.53707800	4.75915400	-0.66759800

H	-6.20000600	5.26799700	-1.56645000
C	-6.96211400	5.54796000	0.41064700
C	-7.37290500	4.90725500	1.57804800
C	-7.36446200	3.50940200	1.67075800
C	-6.95406900	2.73561000	0.59805200
H	-6.96936700	1.65170100	0.66842400
O	-7.78915600	3.01525700	2.86074300
H	-7.51677300	2.06263600	2.93742200
O	-7.80476300	5.61853100	2.68068400
H	-7.95963300	4.94509300	3.36807700
O	-6.96338600	6.89243900	0.24952800
H	-7.16977000	7.37228000	1.08090400
C	-3.50970300	3.98025000	-0.14221400
C	-2.88047700	5.31497000	-0.34462000
O	-3.79200600	3.51954300	0.93415000
C	-2.30237000	5.91426500	0.77733400
H	-2.29373100	5.40895200	1.73664600
C	-1.71560700	7.15986000	0.63065300
C	-1.70522100	7.82278300	-0.59961300
C	-2.29072200	7.21739500	-1.71570000
C	-2.88722200	5.96262000	-1.58347500
H	-3.36673900	5.50895800	-2.44428800
O	-2.25331700	7.90850000	-2.88837200
H	-2.36025500	7.28959000	-3.66289000
O	-1.03409900	9.00746100	-0.62348400
H	-1.43683800	9.63463100	-1.27722000
O	-1.08928800	7.77615100	1.68052600
H	-0.84002000	8.66076900	1.35489000
C	4.02505000	2.29016500	5.73172600
C	3.45370600	1.01797300	5.78443300
H	2.80566700	0.72945700	6.60810900
C	3.72776500	0.10022500	4.76985800
C	4.89388800	2.62604100	4.70044600
H	5.32452700	3.61764700	4.64059400
O	3.76295000	3.23996400	6.67216800
H	2.95298000	2.98619800	7.14770500
O	3.18831600	-1.14647400	4.78589900
H	2.27482500	-1.10941600	5.13397700
C	5.17580400	1.67647100	3.72293000
C	4.60154200	0.39877500	3.71875400
C	4.95474400	-0.64250900	2.67516800
H	4.19645000	-0.72563100	1.88714500
H	5.03698400	-1.63214400	3.13117900
C	6.27784500	-0.19907100	2.09300900
H	7.02185500	-0.20329000	2.88863300

C	6.12205000	1.26155200	1.58905800
H	5.16148000	1.35116700	1.06105200
O	6.08915300	2.06843100	2.76919400
C	7.24748400	1.71913300	0.69296100
O	6.73320300	-1.05296100	1.04507700
C	8.39949800	2.30819400	1.22617200
H	8.44274900	2.61302100	2.26336500
C	9.52046500	2.48374200	0.42143900
C	9.47588600	2.08510000	-0.91592300
C	8.30055200	1.60158100	-1.46996300
C	7.17801800	1.40693300	-0.66547800
H	6.28920100	0.95576100	-1.10218600
O	8.26030500	1.25434100	-2.79156000
H	9.16686000	1.20898200	-3.14065600
O	10.62304200	2.11974900	-1.67823000
H	11.29652100	2.52182000	-1.09712700
O	10.69617800	3.02761600	0.81745200
H	10.83053900	2.85887000	1.79906200
C	8.05748600	-1.13243600	0.88529500
C	8.45410000	-1.55036300	-0.47027000
O	8.85355300	-0.81382200	1.76614400
C	7.52052200	-2.10975500	-1.34351300
H	6.54149700	-2.42094200	-0.99518800
C	7.84646800	-2.21959600	-2.68638400
C	9.06944100	-1.73527300	-3.17023100
C	9.98614400	-1.15389300	-2.28980600
C	9.70055700	-1.11364100	-0.93209400
H	10.39918800	-0.61990800	-0.26256500
O	11.07998300	-0.53623700	-2.83193700
H	11.28990700	0.22976200	-2.26804000
O	9.30505700	-1.73047500	-4.50087200
H	8.48383400	-2.07108600	-4.90191500
O	6.99534300	-2.69688500	-3.63868600
H	6.09789900	-2.34083300	-3.42178500
C	-4.75801500	-5.69277800	4.13753900
C	-5.33653300	-4.43843300	4.33001600
H	-6.41576700	-4.33285600	4.34708900
C	-4.50978300	-3.31801300	4.41494700
C	-3.37204800	-5.84316400	4.10833000
H	-2.91088600	-6.81858600	3.99420900
O	-5.57645200	-6.77515100	3.98038100
H	-5.19385000	-7.28458600	3.23103500
O	-4.99778800	-2.07247300	4.61112000
H	-5.93135700	-2.03047100	4.29446200
C	-2.56996200	-4.70538600	4.17074900

C	-3.12007200	-3.43222700	4.28877600
C	-2.24808400	-2.22919300	4.07472400
H	-1.84695500	-1.81285000	5.00369100
H	-2.82902600	-1.44688600	3.57382500
C	-1.11784600	-2.69319100	3.16745900
H	-1.53614500	-3.08362600	2.23565500
C	-0.32282000	-3.84436100	3.80509400
H	0.13615800	-3.49600400	4.73678000
O	-1.22049200	-4.91451700	4.11768300
C	0.72045000	-4.37525900	2.84668900
O	-0.28809900	-1.60179400	2.72920900
C	1.90120300	-3.67198400	2.60795800
H	2.17915200	-2.78176400	3.16745800
C	2.75796200	-4.09580500	1.59469400
C	2.47504600	-5.24983700	0.84500400
C	1.32017600	-5.97949000	1.14591900
C	0.43715000	-5.52595200	2.12266100
H	-0.47102800	-6.07812500	2.32539500
O	1.07789500	-7.15298400	0.47734100
H	0.13621200	-7.41626900	0.65925600
O	3.38721900	-5.62449400	-0.10339000
H	2.91121300	-5.92182100	-0.91176400
O	3.89340300	-3.39209000	1.35555800
H	4.14033300	-3.50902600	0.41477500
C	0.36919600	-0.87405700	3.61515000
C	1.01168900	0.32542900	3.03720200
O	0.41794200	-1.12618900	4.81684600
C	1.58949600	0.38250800	1.76733400
H	1.61685000	-0.49950300	1.13092100
C	2.14307200	1.58147200	1.32164800
C	2.08913500	2.74173600	2.12511400
C	1.56797300	2.63205800	3.41694000
C	1.00412900	1.44702100	3.85499700
H	0.56191400	1.38888100	4.84203500
O	1.57479600	3.75536500	4.21316400
H	1.68630800	3.46963700	5.13942500
O	2.56472900	3.90085900	1.63522800
H	2.14736400	4.65922900	2.10844900
O	2.70501100	1.72472600	0.09447000
H	2.99896300	0.85025600	-0.24194200
C	0.76495400	5.81008100	-2.98676000
C	0.35507300	4.55378500	-3.43242400
C	-0.00651000	3.57696900	-2.49894700
C	0.12736300	3.82160700	-1.13849700
C	0.57276400	5.06984800	-0.69361900

C	0.87341800	6.06300600	-1.61943700
H	0.99575900	6.57842100	-3.71862000
H	-0.43807300	2.64339000	-2.83947200
H	0.65794400	5.24531200	0.37495500
H	1.17555800	7.04824400	-1.27661000
C	0.27773700	4.30957900	-4.90484200
O	0.00436000	5.21088500	-5.70454200
N	0.52079200	3.05708800	-5.37077700
H	0.30551100	2.94797800	-6.35525200
C	-0.34675200	2.81259900	-0.13913200
O	-0.79955300	3.16611700	0.94257400
N	-0.31895500	1.51040200	-0.55246600
H	0.32846200	1.28360700	-1.30030700
C	0.98755500	1.91774300	-4.65778400
C	0.24237500	0.76648400	-4.65762600
C	2.20296300	1.98474900	-3.93466800
C	0.70035200	-0.37267900	-3.95173100
H	-0.71270100	0.71884100	-5.17511200
C	2.64604400	0.90751200	-3.21157800
H	2.78864000	2.89767400	-3.95126700
C	-0.05383300	-1.57307700	-3.98370800
C	1.92289400	-0.31668000	-3.22385100
H	3.57730300	1.00114900	-2.66684800
C	0.41121900	-2.68280900	-3.33992500
H	-0.98580900	-1.59756200	-4.54087900
C	2.37126000	-1.51636200	-2.58451600
C	1.64119900	-2.67407300	-2.63451400
H	2.01373900	-3.56981100	-2.14410300
C	-1.10576000	0.45296400	-0.05353000
C	-2.23303800	0.66782600	0.70432000
C	-0.78426400	-0.86256700	-0.47736100
C	-3.14771300	-0.39131600	0.91835900
H	-2.48578000	1.65490200	1.06985800
C	-1.62483100	-1.91583600	-0.22726200
H	0.14145000	-1.02851700	-1.02472200
C	-4.39722000	-0.11436100	1.54197900
C	-2.86961800	-1.69978700	0.43190300
H	-1.34521600	-2.91250400	-0.56197900
C	-5.34310500	-1.09474600	1.65584600
H	-4.60325500	0.89110100	1.90369800
C	-3.87927600	-2.69643600	0.61282800
C	-5.08708100	-2.40970100	1.19571600
H	-5.83431400	-3.18811700	1.30711500
S	-0.49277200	-4.20887200	-3.48381900
S	3.98329400	-1.55818000	-1.80476000

S	-6.95062600	-0.70499500	2.34412600
S	-3.60755500	-4.35629900	0.00645200
O	4.92220500	-1.16915400	-2.90003000
O	3.95510000	-0.56202900	-0.70918500
O	0.21375000	-5.01753000	-4.49884000
O	-1.86357400	-3.82764500	-3.91692300
O	-4.89097000	-5.09248900	0.21994400
O	-2.50145800	-4.93375000	0.80589200
O	-7.28477300	-1.84593300	3.23445300
O	-7.87437900	-0.57143400	1.20511400
O	-6.75380900	0.56524500	3.09257700
O	-3.27267000	-4.22224700	-1.42971100
O	-0.43688000	-4.80962800	-2.12960700
O	4.20275800	-2.94702400	-1.37136100
O	-3.92513900	-5.76699000	-3.84855000
H	-3.46698200	-6.28631200	-3.13758600
H	-3.47614200	-4.90520500	-3.74558400
O	-7.67509500	8.32963900	2.52416700
H	-8.59507600	8.56312500	2.33796500
H	-7.73260200	7.45848400	2.95830100
O	-4.41565300	4.73790000	-5.75172300
H	-4.00176000	4.07857900	-5.15010600
H	-5.24243500	4.99153000	-5.31991700
O	-2.85371700	-1.78762800	-5.67720300
H	-2.52456300	-2.67944300	-5.47541100
H	-3.11149100	-1.49082900	-4.78588600
O	-0.43812300	-7.86301400	-3.51354200
H	-0.85793400	-7.49828700	-4.32683700
H	0.37307400	-7.34042700	-3.37129800
O	8.71600500	0.99883500	4.09578600
H	7.89030400	1.48437300	3.92653300
H	8.78465500	0.39190200	3.33396900
O	-2.38312600	10.53980500	-2.37399900
H	-2.53358800	9.71079600	-2.87200000
H	-3.23561900	10.75308400	-1.97017400
O	-2.33818400	6.21367100	-4.84525800
H	-3.08758400	5.88370200	-5.39429500
H	-1.48832600	6.04714400	-5.31048200
O	5.56054300	1.50646000	-3.74087000
H	6.51137400	1.57506200	-3.56521100
H	5.36913800	0.56996700	-3.55718700
O	1.69387700	-6.55366800	-2.08535900
H	1.40100600	-7.06319900	-1.30011400
H	1.02693800	-5.83300100	-2.10597200
O	-3.41257400	-8.95032500	-0.51279300

H	-4.01547800	-8.56449200	0.15361900
H	-3.27198500	-8.22290600	-1.15260800
O	1.05252900	2.75197200	6.93685300
H	0.68714600	1.85499000	6.93122200
H	0.38701400	3.30466200	7.37226500
O	-1.83183100	-6.63705500	-5.57323300
H	-2.63990600	-6.34642600	-5.09964900
H	-1.21631100	-5.88772300	-5.47585400
O	11.50915200	-0.05078600	1.83002800
H	10.58575700	-0.37077400	1.75920900
H	12.02966200	-0.83716100	2.04303500
O	-9.47818100	0.96531700	-0.58897300
H	-9.05801200	0.44625300	0.12004800
H	-8.70650900	1.36642900	-1.01880500
O	0.93447900	5.94317600	2.54201500
H	0.50787400	6.71033700	2.12644100
H	0.17134900	5.42762300	2.88480400
O	-2.68696000	3.58550600	-4.00004400
H	-2.84857500	3.43608900	-3.05093400
H	-2.31495700	4.48905600	-4.04421900
O	-1.55118200	-7.54367300	0.93263400
H	-1.80900000	-6.64114500	0.63996400
H	-2.03677700	-8.16078100	0.33316300
O	-4.36238200	-7.43460100	1.62511500
H	-3.40389400	-7.31951800	1.77869800
H	-4.62528600	-6.57571500	1.21721800
O	11.07928200	2.23444300	3.27434100
H	10.24568300	1.97002300	3.71851500
H	11.42956000	1.38598100	2.92699800
O	-2.35862700	-6.86450800	-1.95773500
H	-2.08664800	-5.96088400	-1.69714000
H	-1.57402300	-7.25131400	-2.43958900
O	-6.23667500	-5.51679000	-2.24290500
H	-5.77790600	-5.40051300	-1.38495100
H	-5.50564900	-5.59874700	-2.89310500
O	-1.10828100	4.28799600	3.49508600
H	-0.36198400	3.95885800	4.02368600
H	-1.13042900	3.70126100	2.71584400

1: GCg **6** = 1:4 complex

Number of imaginary frequency = 0

Sum of electronic and zero-point Energies = -12443.115199 au

Sum of electronic and thermal Energies = -12442.901602 au

Sum of electronic and thermal Enthalpies = -12442.900657 au

Sum of electronic and thermal Free Energies = -12443.364058 au

C	-3.48709300	-6.27683700	3.48109400
C	-2.13989400	-6.29372600	3.85113800
H	-1.86005600	-6.21621600	4.89562300
C	-1.17661400	-6.39859700	2.85766300
C	-3.86627000	-6.38781700	2.14627000
H	-4.91051500	-6.35935600	1.85136300
O	-4.39446500	-6.09378200	4.47523400
H	-5.32199300	-6.14393400	4.13542000
O	0.15835300	-6.40181600	3.18222400
H	0.45776600	-5.52651800	3.52329400
C	-2.87841900	-6.50643400	1.16623700
C	-1.51692200	-6.51811900	1.50423200
C	-0.44996200	-6.46097300	0.44007200
H	-0.01184000	-7.44078700	0.21114300
H	0.36013400	-5.80569300	0.75959700
C	-1.13970800	-5.90183600	-0.78262400
H	-1.59108400	-4.93854300	-0.53133500
C	-2.33260900	-6.81309900	-1.13272400
H	-2.03088300	-7.86533900	-1.05134100
O	-3.32207300	-6.55308700	-0.12706700
C	-2.84549500	-6.55186100	-2.52170800
O	-0.28353500	-5.54637000	-1.86498700
C	-3.20560900	-5.26909800	-2.94252900
H	-3.33085100	-4.45930700	-2.22735300
C	-3.34428400	-4.99988800	-4.30595100
C	-3.09763200	-6.00672600	-5.24841700
C	-2.80448600	-7.29902300	-4.81430300
C	-2.69567200	-7.57360200	-3.45473600
H	-2.40393600	-8.56921900	-3.13721400
O	-2.54633700	-8.21880600	-5.78756600
H	-1.92407700	-8.88173600	-5.41790100
O	-3.08693000	-5.69835300	-6.57333000
H	-2.56269100	-6.39758100	-7.00943400
O	-3.66200300	-3.77744300	-4.79890500
H	-3.72316500	-3.11944400	-4.06447100
C	0.14460000	-6.41308600	-2.77420900
C	0.37732500	-5.73562000	-4.07061500
O	0.24312300	-7.61921400	-2.55747700
C	0.15777700	-6.47413600	-5.24090300
H	-0.00337700	-7.54606600	-5.22900000
C	-0.03565300	-5.77731700	-6.42636800
C	0.04435600	-4.38429000	-6.46601800
C	0.39402600	-3.66466300	-5.31319900

C	0.53170900	-4.34696100	-4.10843200
H	0.75285900	-3.79655500	-3.20012700
O	0.49629900	-2.32887200	-5.43301900
H	0.81431100	-1.93211300	-4.58535000
O	-0.25276200	-3.77973000	-7.64390300
H	-0.92932100	-3.07090900	-7.40730500
O	-0.41593100	-6.42531800	-7.56492200
H	-0.53543600	-5.71378100	-8.22338300
C	-1.66233000	8.28299300	-2.46346200
C	-1.39779900	8.32013200	-1.08738900
H	-0.61986800	8.96472800	-0.68790100
C	-2.15158300	7.52196400	-0.22968300
C	-2.68298700	7.47966000	-2.96859400
H	-2.87835300	7.42618100	-4.03369600
O	-0.97576300	9.06113700	-3.33000600
H	-0.09882300	9.30960300	-2.92232700
O	-1.94776200	7.50378500	1.11296600
H	-1.00159400	7.66680800	1.30711500
C	-3.42782500	6.71056300	-2.08120000
C	-3.17883600	6.70035200	-0.70674200
C	-3.91174300	5.77938300	0.22941000
H	-4.68386900	6.30724500	0.80610500
H	-3.22120900	5.34682200	0.95932900
C	-4.57619400	4.69890600	-0.59041500
H	-3.85168800	4.00741100	-1.02602800
C	-5.35659100	5.33429100	-1.75794700
H	-6.02953000	6.10697700	-1.35461100
O	-4.41763200	5.93291100	-2.64009600
C	-6.13044000	4.26899800	-2.48114000
O	-5.46725100	3.98524100	0.26830200
C	-7.42016200	3.98122100	-2.03761600
H	-7.93030300	4.61681600	-1.32013600
C	-8.01187900	2.78478600	-2.43352200
C	-7.33467900	1.90707700	-3.27793200
C	-6.05967400	2.22560200	-3.76299100
C	-5.46065100	3.42542800	-3.36655400
H	-4.44834700	3.66327400	-3.68231500
O	-5.46446900	1.30982100	-4.55110100
H	-4.49720400	1.51748400	-4.63628600
O	-7.92935100	0.69473700	-3.53372600
H	-7.28982800	0.04039000	-3.15740900
O	-9.23572900	2.42329700	-1.96693200
H	-9.36725800	1.51619000	-2.29931200
C	-5.64410100	2.67059200	0.08426700
C	-6.69339800	2.12915400	0.98465300

O	-5.00064700	1.98861100	-0.68774800
C	-7.00962100	0.77531900	0.88714300
H	-6.54477800	0.14203400	0.13620900
C	-7.97029800	0.23358300	1.73191200
C	-8.62410900	1.03817900	2.66870700
C	-8.29389500	2.39904300	2.74057900
C	-7.33758100	2.95306500	1.91047800
H	-7.08317800	4.00306200	1.99999000
O	-8.88176800	3.16366500	3.70593300
H	-9.52392000	2.60027400	4.17170200
O	-9.52925200	0.61756700	3.58802000
H	-9.91444700	-0.26471000	3.37757000
O	-8.22792000	-1.12132800	1.65756400
H	-9.19164000	-1.28612200	1.62932600
C	1.91859400	0.24055000	-0.05170800
C	1.49166700	1.11269000	-1.05083800
H	0.43638900	1.31233900	-1.20520600
C	2.46719400	1.68688000	-1.86304000
C	3.25519400	-0.04308700	0.16261100
H	3.58687600	-0.72514400	0.93706000
O	0.95309900	-0.34698800	0.73845000
H	1.38720200	-1.08796600	1.21056100
O	2.16973900	2.60341400	-2.82813000
H	1.23164900	2.56712200	-3.09845100
C	4.19127000	0.51047600	-0.70432100
C	3.82668300	1.38847700	-1.72093800
C	4.87383500	1.99470300	-2.61200000
H	4.60825400	3.01956000	-2.87836800
H	4.97895200	1.41971500	-3.54067400
C	6.21126400	1.99568300	-1.89903400
H	7.02706600	2.26114800	-2.57487100
C	6.52893400	0.63016000	-1.26728000
H	7.36315800	0.76169000	-0.56936100
O	5.47267000	0.12662800	-0.47457600
C	6.98390800	-0.31214000	-2.34938100
O	6.14672300	2.95908000	-0.84427500
C	8.29604800	-0.10764800	-2.76267500
H	8.91560600	0.60204700	-2.22490600
C	8.80993200	-0.73328300	-3.89258300
C	8.01343400	-1.67043600	-4.55337100
C	6.71220600	-1.91854500	-4.09237800
C	6.17138800	-1.23142900	-3.00359700
H	5.15487300	-1.43466300	-2.67301100
O	6.04529400	-2.87912000	-4.79748000
H	5.04078500	-2.83545000	-4.62385700

O	8.48073800	-2.32938200	-5.65066800
H	7.73612100	-2.87680300	-5.95455800
O	10.05237300	-0.44190000	-4.36404700
H	10.32457500	0.39273600	-3.93387800
C	7.31177300	3.33223300	-0.31262900
C	7.12522800	3.92717700	1.03441500
O	8.39420100	3.13043000	-0.83876100
C	5.85282300	4.30024100	1.47646700
H	5.00842700	4.27492100	0.79441600
C	5.67785800	4.65665500	2.81140100
C	6.76257800	4.58599500	3.69340300
C	8.03858000	4.26890900	3.21228000
C	8.23444200	3.94479000	1.87735100
H	9.21131500	3.64944800	1.51372000
O	9.07470700	4.25461200	4.08759600
H	8.70210300	4.55705300	4.93554700
O	6.63460100	4.80914100	5.04038400
H	6.54370600	3.90323300	5.44884900
O	4.47907600	5.04446200	3.32756500
H	3.78377200	5.08879700	2.63734300
C	1.93492400	-3.25519200	9.95659300
C	2.80810700	-4.29831500	9.64310400
H	2.95790200	-5.10164200	10.35763300
C	3.46472100	-4.27560300	8.41896700
C	1.71547500	-2.21714500	9.06185000
H	1.03294100	-1.40217000	9.28114500
O	1.31415600	-3.31680300	11.16734200
H	0.74219300	-2.54253600	11.26598900
O	4.33620200	-5.25660100	8.05185200
H	4.40608800	-5.90131300	8.77008400
C	2.39017400	-2.22681000	7.83752600
C	3.28020300	-3.24205300	7.49173000
C	4.03277700	-3.21536800	6.18746100
H	3.58596600	-3.90823200	5.46336000
H	5.07234200	-3.52242100	6.33980800
C	3.97325500	-1.81752200	5.58968000
H	4.62412800	-1.11604000	6.11984300
C	2.53139500	-1.30289700	5.64275500
H	1.88582000	-2.04834300	5.15571900
O	2.14197300	-1.16918900	7.01534600
C	2.36682100	0.04641400	4.99879800
O	4.38182600	-1.91111200	4.22924200
C	1.53522900	0.21383800	3.89299700
H	0.96156500	-0.62275700	3.50192200
C	1.40530800	1.47643500	3.31291900

C	2.12172500	2.55504700	3.83063800
C	2.95899400	2.38227600	4.92883600
C	3.07141700	1.12907700	5.52031100
H	3.71177800	1.00727700	6.38903700
O	3.66851800	3.43234900	5.43900500
H	3.83398200	4.10606000	4.73758600
O	2.02345300	3.79319700	3.27182500
H	1.57528900	3.72784200	2.40639900
O	0.59698700	1.77943200	2.26890200
H	0.47037500	0.97674500	1.71705100
C	5.45256900	-1.20050900	3.80604900
C	5.94055800	-1.68917800	2.49863100
O	5.95742600	-0.30882600	4.46043600
C	7.10961000	-1.14098000	1.96211300
H	7.61461900	-0.31861700	2.45640900
C	7.61394800	-1.66452200	0.78292300
C	6.96573600	-2.71783600	0.11394800
C	5.76357600	-3.21402500	0.63410600
C	5.27564200	-2.72839900	1.83919000
H	4.37064100	-3.15098500	2.25698000
O	5.15615600	-4.21228000	-0.07412300
H	4.27383200	-4.38698900	0.29395400
O	7.57592000	-3.18608600	-0.98549000
H	6.99357900	-3.77844600	-1.56200000
O	8.75585400	-1.16408700	0.23089400
H	8.81206200	-1.54684900	-0.66559500
C	-6.81186100	-0.48909400	5.23638500
C	-5.73717000	-0.98000900	4.48399700
C	-4.85884400	-0.07430800	3.87457200
C	-5.08104500	1.29858700	3.98964900
C	-6.13889300	1.76741100	4.77348000
C	-7.00127900	0.87548800	5.39444100
H	-7.46857900	-1.19448600	5.73222000
H	-3.98027000	-0.43510100	3.35273700
H	-6.27651300	2.83715000	4.88707600
H	-7.83199000	1.24325500	5.98736700
C	-5.57193500	-2.47044100	4.51232700
O	-6.25898400	-3.12631400	5.31467300
N	-4.68236500	-3.12911300	3.73234100
H	-4.57056500	-4.10364000	4.02303400
C	-4.21102800	2.34790200	3.35046100
O	-4.29255200	3.51882900	3.69850400
N	-3.32267000	1.92460700	2.39978200
H	-3.51878700	1.04985900	1.92537400
C	-3.98129500	-2.74766200	2.55575800

C	-2.66710000	-3.11674200	2.42881800
C	-4.64277300	-2.09499900	1.48164600
C	-1.96287000	-2.87170900	1.22387900
H	-2.16202200	-3.62758900	3.24416200
C	-3.97718000	-1.82482000	0.31216100
H	-5.69146000	-1.82326900	1.58311900
C	-0.59977800	-3.24906400	1.10644400
C	-2.62004500	-2.22455400	0.13752500
H	-4.51101000	-1.33207500	-0.49357700
C	0.07332400	-3.02033500	-0.06287400
H	-0.10064900	-3.71158000	1.95693100
C	-1.87001300	-2.02265400	-1.06228600
C	-0.55809500	-2.40035700	-1.16268100
H	-0.00482400	-2.17947700	-2.06883700
C	-2.39399600	2.78948800	1.76283400
C	-2.16915500	2.66733900	0.41546300
C	-1.67277200	3.75379300	2.51601500
C	-1.29740700	3.57294500	-0.24232600
H	-2.71100600	1.93679300	-0.18277300
C	-0.77079700	4.58979400	1.91040300
H	-1.84216600	3.82806200	3.58272600
C	-1.26226000	3.59795200	-1.65949200
C	-0.56038000	4.53847400	0.50253600
H	-0.24500100	5.31374400	2.52481100
C	-0.53469100	4.55486200	-2.31587100
H	-1.86989800	2.88342500	-2.21006700
C	0.28552600	5.42747700	-0.23302600
C	0.28671500	5.45645100	-1.60556400
H	0.89392800	6.18247600	-2.13957100
S	1.83787100	-3.30485500	-0.12003500
S	-2.59880600	-1.22415800	-2.49142700
S	-0.61816800	4.62946000	-4.10010000
S	1.46228500	6.48828400	0.60235200
O	-3.83281500	-2.01902900	-2.77818100
O	-2.92137100	0.15681100	-2.07449900
O	2.29294400	-2.73831500	1.18018700
O	2.14319800	-4.76834500	-0.16848100
O	0.73008100	7.29743700	1.60885000
O	2.09474200	7.32558600	-0.43586100
O	-2.04918400	4.37001700	-4.41850400
O	0.25721600	3.53856500	-4.59474600
O	-0.16057500	5.97489000	-4.47995400
O	2.41110800	5.52506700	1.23200100
O	2.31830500	-2.62665600	-1.32864600
O	-1.60289000	-1.32358100	-3.57696000

O	-5.97738800	-0.41206900	-2.02185200
H	-5.29828500	-0.94640600	-2.47932100
H	-5.51498100	0.42324000	-1.81119800
O	-6.94679500	-5.57763600	4.14339500
H	-6.74313500	-4.88896200	4.80622900
H	-7.45481100	-5.08455200	3.47700800
O	2.17880200	7.44927400	-4.28112700
H	2.92497900	7.10052300	-3.72869400
H	1.47005100	6.77574000	-4.32103400
O	-4.12632500	5.96463500	-5.53854700
H	-4.55163500	5.94176000	-4.66723200
H	-3.28984900	5.50401200	-5.34803600
O	-8.38800400	-3.20842300	3.46808000
H	-7.97090600	-3.08525500	4.34031100
H	-7.97755100	-2.52680400	2.89671800
O	3.53554000	-2.95797100	-4.32094700
H	3.38438900	-3.64486000	-3.63109500
H	3.03367500	-2.16085800	-4.05954100
O	1.46911700	9.26723800	-2.39082900
H	1.51685500	8.68592900	-1.60915900
H	1.75034500	8.68180700	-3.13799000
O	1.74396900	-1.01088800	-3.45330600
H	1.30463100	-0.13212900	-3.56016600
H	1.86708300	-1.15611100	-2.49717200
O	10.00922800	2.36800200	-3.32126400
H	9.29268800	2.51408400	-3.95530000
H	9.61166300	2.62119900	-2.46679300
O	2.74585300	-6.32161500	2.10380200
H	2.56852600	-5.87960900	1.25183600
H	1.90295600	-6.75951700	2.31801000
O	1.05955500	6.34064900	4.29910000
H	1.06691800	6.80435600	3.44482500
H	1.48552400	5.49288200	4.09454200
O	6.30947300	-4.72798600	-2.65308600
H	5.36831200	-4.85655900	-2.40481700
H	6.27553200	-4.26229300	-3.50866400
O	3.55315700	-5.10230600	-2.62079600
H	3.34362200	-5.98593000	-2.99652200
H	3.04867000	-5.01249100	-1.79059900
O	6.16102100	2.31457400	5.89656400
H	6.21830000	1.56462600	5.27632100
H	5.21934600	2.57268300	5.88949800
O	-2.08895100	-2.25767100	-6.58123500
H	-2.67046400	-2.92200000	-6.15910400
H	-1.61168500	-1.85887300	-5.83035900

O	1.78012400	-4.23293800	3.56797100
H	1.88597500	-3.50345200	2.92931600
H	2.36321500	-4.92893900	3.17971100
O	2.87304400	-7.53742800	-3.81480000
H	2.08512200	-7.86873100	-3.34936400
H	2.50197300	-7.16983800	-4.63223100
O	-2.82092800	1.69919500	-4.44062700
H	-2.53517900	2.63874000	-4.42490500
H	-2.78001800	1.36078600	-3.52510500
O	-6.68332700	5.13594600	4.35735200
H	-5.90172000	4.66112600	4.02636500
H	-7.43664700	4.55153700	4.18229200
O	3.49844300	4.55622100	-1.29103100
H	3.11421900	4.69716100	-0.40728600
H	2.84391400	4.04877100	-1.80605500
O	-0.03151100	0.99660300	-3.72827100
H	-0.18605900	1.70546900	-4.37977600
H	-0.76127500	0.35576000	-3.82492200
O	0.56597400	9.26355000	-5.73833100
H	1.31473500	8.71097600	-5.46154300
H	-0.14444000	8.96563500	-5.14642700
O	4.05365100	6.93559400	-2.45360200
H	3.59808000	7.45882800	-1.77407700
H	3.96339700	6.02808500	-2.07744900
O	-0.53262400	-9.60659200	-4.44936500
H	-0.49712900	-10.50092600	-4.08503400
H	-0.26453900	-9.00544900	-3.72595800
O	-10.54337900	-1.78204500	2.83299900
H	-11.47430500	-2.04076900	2.85735700
H	-10.00152800	-2.50651000	3.22680300

(4) Complexes of sensor molecule **1** and GC **8**

1: GC **8** = 1:1 complex

Number of imaginary frequency = 0

Sum of electronic and zero-point Energies = -6388.007024 au

Sum of electronic and thermal Energies = -6387.896703 au

Sum of electronic and thermal Enthalpies = -6387.895758 au

Sum of electronic and thermal Free Energies = -6388.163810 au

C	0.05251000	-5.56744900	-0.04486400
C	1.39480100	-5.22791400	0.08344100
H	2.19012900	-5.91549100	-0.19338900
C	1.72065900	-3.94606900	0.53574900

C	-0.95868300	-4.68505200	0.29867100
H	-2.00437400	-4.94860700	0.19643400
O	-0.33591400	-6.78539300	-0.55607700
H	0.44867300	-7.26021900	-0.86780000
O	3.00643000	-3.54819300	0.62574600
H	3.59913400	-4.29318000	0.30688600
C	-0.59991000	-3.40667900	0.72283600
C	0.72886100	-3.00901600	0.86157400
C	1.07435800	-1.61091400	1.30249800
H	1.40466500	-1.00025200	0.44796400
H	1.90934200	-1.63795800	2.01347300
C	-0.14229300	-0.92865700	1.92201900
H	-0.36441200	-1.32910200	2.92214600
C	-1.36572700	-1.17132200	1.03099300
H	-1.11233900	-0.81031000	0.02226100
O	-1.63910200	-2.56796100	0.97427200
C	-2.62986000	-0.50554400	1.51156400
O	0.04234500	0.47984400	1.98766000
H	0.90748800	0.64371900	2.39190700
C	-3.54450100	-1.21517400	2.28617500
H	-3.38212800	-2.25741300	2.53150800
C	-4.72467600	-0.60470800	2.70609800
C	-4.98613900	0.71693500	2.35491200
C	-4.04696000	1.44308000	1.61258500
C	-2.87152200	0.83161500	1.18802800
H	-2.14214800	1.39403100	0.61584500
O	-4.39592300	2.73076900	1.37307400
H	-3.82903300	3.10681100	0.66238700
O	-6.16977000	1.28592200	2.71333000
H	-6.20229100	2.15727800	2.27797500
O	-5.63717900	-1.29661000	3.45692300
H	-6.47537100	-1.28601400	2.93325800
C	2.51732900	-4.65972200	-3.17850800
C	2.56706000	-3.40878700	-2.55927900
C	1.38007600	-2.74591600	-2.28568400
C	0.14878400	-3.27844600	-2.65627200
C	0.09644300	-4.52901000	-3.27107700
C	1.28700900	-5.21527200	-3.52260900
H	3.44698600	-5.18217500	-3.38202500
H	1.37607600	-1.80533200	-1.75208700
H	-0.85714900	-4.96535000	-3.55342600
H	1.25255000	-6.18321200	-4.01318500
C	3.88797500	-2.82631100	-2.15855500
O	4.91085200	-3.51412700	-2.16297000
N	3.87767300	-1.51485500	-1.80855900

H	3.04739200	-0.94189200	-1.96984300
C	-1.01347800	-2.37203200	-2.38915500
O	-0.80595700	-1.15276500	-2.34535100
N	-2.23259300	-2.92241100	-2.18964900
H	-2.29459800	-3.94067000	-2.10031600
C	4.96371500	-0.82476800	-1.23258800
C	5.07659600	0.52725500	-1.45588400
C	5.87826700	-1.48083000	-0.36811700
C	6.12602300	1.27404400	-0.86705300
H	4.35286400	1.03019000	-2.09317000
C	6.89933000	-0.77558300	0.21606000
H	5.75218800	-2.53400500	-0.15020400
C	6.24957000	2.67163100	-1.10678000
C	7.06948400	0.61527900	-0.02641100
H	7.58420200	-1.29638500	0.87592200
C	7.29296400	3.37030800	-0.57107100
H	5.50942900	3.19156500	-1.70860800
C	8.12884300	1.39612900	0.52786800
C	8.25527700	2.72615100	0.23912500
H	9.08246300	3.29554800	0.64450200
C	-3.36018200	-2.17478000	-1.78102800
C	-3.53366800	-0.85774800	-2.13742200
C	-4.33262600	-2.80860600	-0.96435600
C	-4.62351400	-0.12145400	-1.62449200
H	-2.85006900	-0.35685500	-2.81011500
C	-5.42350500	-2.11834800	-0.49551700
H	-4.18937600	-3.85375000	-0.70232600
C	-4.71523600	1.25889000	-1.93741500
C	-5.59664800	-0.73873700	-0.79524500
H	-6.14572000	-2.61538100	0.14248200
C	-5.73143300	2.00897300	-1.42309700
H	-3.96881900	1.69402400	-2.59572100
C	-6.66905000	0.08153100	-0.31802000
C	-6.72824900	1.42100900	-0.60608100
H	-7.54764000	2.01883900	-0.22032600
S	7.48685900	5.13070300	-0.84015600
S	9.30981400	0.69194500	1.67363300
S	-5.83296600	3.74078200	-1.84074600
S	-8.08719200	-0.63229000	0.51870200
O	9.96339300	-0.43337800	0.94238400
O	10.23211500	1.78059600	2.02975100
O	6.17681700	5.58805500	-1.35311800
O	8.60185000	5.27953900	-1.78402100
O	-8.88717500	0.51740900	1.00194800
O	-7.57496200	-1.46666200	1.64596100

O	-6.03545200	4.44873400	-0.55569800
O	-6.94623000	3.89260600	-2.79199000
O	-4.50001400	4.06615800	-2.44584000
O	-8.76014000	-1.44965100	-0.50386700
O	7.79057300	5.64783300	0.52479300
O	8.51538700	0.19080200	2.82625400
O	5.72781900	7.63116300	0.60356500
H	6.51346500	7.14914700	0.91278600
H	5.54315500	7.10942900	-0.19550100
O	5.63614500	-3.93452200	1.85912800
H	4.83052000	-3.39789000	1.90256200
H	6.35035100	-3.38607800	2.26726700
O	-7.29242900	0.08912100	5.37033200
H	-6.51897900	-0.18313000	4.84678300
H	-7.98687500	-0.53330100	5.06596700
O	-11.19408900	0.08454000	-0.71777100
H	-10.69290300	0.54440400	-0.02571900
H	-10.57158900	-0.63444800	-0.91423900
O	4.70039600	-5.39961300	-0.17807600
H	5.32026200	-5.06844500	0.51125000
H	4.95855600	-4.93775400	-1.00057200
O	-2.68098000	3.53530600	-0.61834600
H	-2.21143600	4.34690900	-0.37724500
H	-3.32508700	3.79771500	-1.33742700
O	-8.90363100	1.59403300	3.62729400
H	-8.14584600	1.31754300	4.18502000
H	-8.63693500	1.35997100	2.71942800
O	7.48956100	-2.40679000	3.10576600
H	8.44684700	-2.62075800	3.09209800
H	7.50977900	-1.43852000	2.98740900
O	9.38938100	-1.08342600	-1.79933900
H	9.67003900	-0.82415100	-0.90292500
H	8.42984700	-1.15924700	-1.71105600
O	1.56733100	0.37980500	-2.09616500
H	0.82885500	-0.08688700	-2.52840000
H	1.08260100	1.06324500	-1.60094100
O	-2.45642600	2.56376100	-4.02835700
H	-1.83044800	2.33613300	-3.31656800
H	-3.08466700	3.19035800	-3.63165000
O	-0.97446800	1.59490900	-1.71922900
H	-1.34498500	0.69486500	-1.69633500
H	-1.57669700	2.17049500	-1.20452500
O	10.23021400	-2.13281500	3.16663900
H	10.31854500	-1.77304700	2.26078800
H	9.91570900	-1.34000500	3.63332300

O	-2.59005400	-5.81734000	-2.01512000
H	-3.14344800	-6.43674200	-2.50864300
H	-1.86994700	-6.34251300	-1.61674800
O	-8.43020600	5.82205800	-1.33755600
H	-7.88460700	5.42158200	-0.63890400
H	-8.17936300	5.25142800	-2.08775600
O	-5.94169200	7.23373000	-1.46885800
H	-6.88154400	6.98793200	-1.54701800
H	-5.56836100	6.42123300	-1.09415900
O	-9.34194100	-1.12608500	3.92300900
H	-8.87813800	-1.38926800	3.10721000
H	-9.49726000	-0.16627000	3.78227400
O	9.86748000	4.73709500	2.42570400
H	9.86888500	3.76612000	2.41944900
H	9.14582300	5.00456200	1.82842500
O	-1.65289200	0.62806500	4.30880100
H	-2.52854100	0.33093900	4.02045300
H	-1.21362900	0.83857800	3.46754800

1: GC 8 = 1:2 complex

Number of imaginary frequency = 0

Sum of electronic and zero-point Energies = -7570.316981 au

Sum of electronic and thermal Energies = -7570.186043 au

Sum of electronic and thermal Enthalpies = -7570.185099 au

Sum of electronic and thermal Free Energies = -7570.489030 au

C	-1.70271300	-1.05405300	-3.95278200
C	-2.57425300	-1.71982700	-3.08107300
H	-3.63039400	-1.46515800	-3.07634000
C	-2.07018700	-2.69244200	-2.21671300
C	-0.34090700	-1.34528300	-3.93585600
H	0.34797900	-0.82036500	-4.58814600
O	-2.12186000	-0.12882300	-4.83897300
H	-3.08380100	0.05631700	-4.74174900
O	-2.89071200	-3.36483000	-1.35530700
H	-3.83890000	-3.21238900	-1.60211800
C	0.13048100	-2.31100200	-3.05491300
C	-0.70196300	-3.01202100	-2.17771400
C	-0.12714300	-4.04469000	-1.23844100
H	-0.24131100	-5.06247000	-1.63695500
H	-0.64004500	-4.02671100	-0.27306800
C	1.35392300	-3.77330700	-1.03377500
H	1.47870900	-2.82292300	-0.49396200
C	2.05499400	-3.61268100	-2.38709700

H	1.90034200	-4.53893800	-2.96107200
O	1.48872100	-2.51532800	-3.10058400
C	3.53187600	-3.34225300	-2.22863400
O	1.92992900	-4.84357600	-0.31623000
H	2.81680400	-4.56416400	-0.02433900
C	4.44053600	-4.39970500	-2.22056000
H	4.11690200	-5.42346800	-2.38028200
C	5.80193500	-4.15188800	-2.04164300
C	6.26431900	-2.83812200	-1.84801200
C	5.34729300	-1.77973400	-1.86938100
C	3.98473300	-2.03877600	-2.03675100
H	3.29627200	-1.19948200	-2.04170800
O	5.71715400	-0.47476900	-1.75659100
H	6.67375600	-0.35950100	-1.56453500
O	7.60457600	-2.72275300	-1.62627100
H	7.96867600	-1.82591800	-1.78493100
O	6.66743700	-5.18303500	-2.06038600
H	7.60167500	-4.87087300	-2.18906300
C	-2.27618500	-3.00634700	5.13811900
C	-1.06680500	-2.38047600	5.43030600
H	-0.25344000	-2.93473000	5.88227500
C	-0.89747600	-1.04190300	5.09214900
C	-3.29879200	-2.32181300	4.49185700
H	-4.23552000	-2.80235300	4.22297900
O	-2.38736700	-4.32984600	5.45673300
H	-3.28067200	-4.62868400	5.23478700
O	0.28056400	-0.44644700	5.41115300
H	0.59968600	0.07173800	4.63276900
C	-3.10456000	-0.97948300	4.15642900
C	-1.93015500	-0.30081100	4.48743000
C	-1.84843900	1.19409400	4.31534600
H	-1.24951100	1.47640300	3.44109100
H	-1.36895700	1.63335400	5.20072700
C	-3.24609000	1.77728100	4.10542900
H	-3.84566400	1.68902000	5.02577400
C	-3.92783300	0.94542100	3.01249200
H	-3.21658400	0.89516800	2.17538400
O	-4.14216600	-0.37354200	3.51972800
C	-5.25082100	1.45179500	2.48692700
O	-3.18221900	3.11749200	3.66788800
H	-2.57830400	3.58731900	4.26029400
C	-5.26500100	2.56563900	1.64731100
H	-4.35188300	3.09778100	1.40055300
C	-6.45260600	2.96793800	1.04450700
C	-7.63996500	2.26898200	1.26715600

C	-7.62125100	1.16001400	2.12076900
C	-6.43719300	0.75688000	2.73316400
H	-6.43933100	-0.12767300	3.36065500
O	-8.80966800	0.51672000	2.28548300
H	-8.66347200	-0.45198300	2.37787900
O	-8.76299600	2.65881800	0.60776700
H	-9.39137400	1.90252300	0.56580100
O	-6.42895300	4.03982400	0.19614000
H	-7.11850500	3.95619800	-0.49249000
C	0.89990000	-4.28098400	2.67862100
C	1.48608800	-3.08530000	2.25954600
C	0.68557100	-2.04447700	1.80625500
C	-0.69533700	-2.17139900	1.77015200
C	-1.28497200	-3.36281100	2.19507600
C	-0.48521100	-4.40663900	2.65792700
H	1.52465000	-5.11519000	2.98142600
H	1.12819300	-1.13716400	1.41314600
H	-2.36495400	-3.47054600	2.19052200
H	-0.95001200	-5.32079400	3.01143400
C	2.96837900	-2.92417400	2.15282800
O	3.71096000	-3.85402300	1.82906500
N	3.38665300	-1.65343000	2.39374700
H	2.67606400	-0.99814600	2.72658300
C	-1.44854800	-0.99451100	1.24083800
O	-1.01058400	0.15518300	1.35651100
N	-2.60781700	-1.31069100	0.63078900
H	-2.75033800	-2.29078700	0.39572000
C	4.59926800	-1.04354600	2.02090400
C	4.66158800	0.32556600	2.13863000
C	5.70677000	-1.76326400	1.49882000
C	5.79657100	1.03504000	1.68907500
H	3.81758100	0.88951300	2.53006500
C	6.82318400	-1.08925100	1.07435000
H	5.65254000	-2.83992300	1.41677400
C	5.81444800	2.45058100	1.73336400
C	6.89830100	0.32943800	1.12834700
H	7.65200600	-1.65831900	0.66874000
C	6.88014000	3.14020400	1.22356700
H	4.95832000	2.97516100	2.15057900
C	7.98107000	1.10029900	0.61183900
C	7.97975300	2.47001900	0.65014700
H	8.78969700	3.03804700	0.20691600
C	-3.54470400	-0.43689100	0.03350400
C	-4.86104900	-0.80834100	0.08620900
C	-3.17692800	0.75864800	-0.63141600

C	-5.84953900	-0.05889700	-0.59200600
H	-5.15953400	-1.69083000	0.64737000
C	-4.12244200	1.50832200	-1.28400500
H	-2.14130400	1.07348400	-0.61209900
C	-7.19950800	-0.47744700	-0.52233000
C	-5.48688900	1.09630000	-1.34128900
H	-3.82890400	2.44705400	-1.73040800
C	-8.16343000	0.17177400	-1.24008800
H	-7.45325100	-1.30071100	0.13465200
C	-6.53315700	1.74103100	-2.07448600
C	-7.83236600	1.28840900	-2.03599000
H	-8.60745700	1.78503900	-2.61923300
S	6.80511700	4.92001800	1.22473300
S	9.21449000	0.30909000	-0.40026300
S	-9.85999700	-0.36843700	-1.13660000
S	-6.32329300	3.14555800	-3.18176500
O	10.20360800	1.35423100	-0.75940400
O	9.79498800	-0.83182200	0.32873500
O	5.54087600	5.27080400	0.52255300
O	8.01999100	5.38042700	0.51527600
O	-6.89058500	2.67905200	-4.47048300
O	-4.87257100	3.43732200	-3.30942900
O	-10.53998900	0.59731500	-0.24194000
O	-9.79333200	-1.73945300	-0.53134300
O	-10.37318800	-0.37815000	-2.51331300
O	-7.09319100	4.24150600	-2.55054200
O	6.75568500	5.32561100	2.65209800
O	8.43262200	-0.13321700	-1.60371000
O	-8.85496300	-2.18808800	2.01921400
H	-8.17568600	-2.74533700	1.60406200
H	-9.43586000	-1.97884800	1.25643100
O	-5.52143300	-2.96963200	-2.02474900
H	-6.24254000	-3.25229200	-1.42164200
H	-5.67470900	-2.01883100	-2.13549700
O	1.24691200	0.57582800	3.08861700
H	0.49323000	0.55305000	2.45982400
H	1.62027200	1.48518400	3.09389000
O	-13.08286400	0.12936500	-1.57360800
H	-12.40982900	-0.08833700	-2.23883400
H	-12.51132700	0.47641700	-0.86969700
O	5.44061300	4.70354900	-2.24878400
H	5.33095200	4.95306700	-1.31141400
H	6.36780000	4.98698000	-2.43869000
O	9.01956800	7.12871200	2.61116400
H	8.25423300	6.66843900	2.99161000

H	9.02632700	6.73120200	1.72641100
O	10.46300000	-2.33971700	-2.11393500
H	10.47197600	-1.51809500	-2.65153200
H	10.26270500	-2.03049900	-1.21262100
O	6.39798700	2.20540400	-1.96808700
H	5.75835600	1.48433800	-2.05750400
H	5.91489400	3.06261000	-2.07810300
O	2.78418100	-6.62967900	1.74339800
H	3.28666800	-5.80742500	1.87191600
H	2.14430200	-6.36410300	1.06312800
O	10.76501200	0.21306200	-3.33736200
H	11.05542900	0.58290000	-2.48622800
H	9.91446200	0.67764100	-3.45325500
O	-4.59205800	0.82460000	-4.39597500
H	-4.32069100	1.67531000	-4.00088300
H	-5.41947500	1.06881300	-4.84511800
O	3.09201400	-0.87129800	-4.88489800
H	2.58443800	-1.54942500	-4.40909400
H	3.85405800	-0.73846200	-4.30391600
O	3.91357900	5.16890800	2.79205100
H	4.81463300	5.26434100	3.15670000
H	4.11189600	5.26802800	1.84034100
O	9.27473000	-4.74602800	-2.70060300
H	9.87295600	-5.24365200	-2.12839300
H	9.53914300	-3.80702000	-2.54828900
O	2.74143600	2.82557000	3.48758200
H	3.08244100	3.70432500	3.18339800
H	3.13102500	2.69874400	4.36263000
O	-7.75154600	-3.53243900	-0.36237200
H	-8.10314300	-4.43045800	-0.44070800
H	-8.48661000	-2.93796400	-0.65024000
O	-9.52818200	3.65911300	-3.99529000
H	-9.00049100	4.10991100	-3.31581500
H	-8.81726000	3.21883200	-4.49074400
O	-3.93156400	4.87895900	-1.02039800
H	-4.16966400	4.59898800	-1.91997000
H	-4.74610200	4.68089600	-0.52680500
O	8.86402800	2.50895800	-2.97507700
H	9.39789200	2.28384800	-2.19028100
H	7.95230000	2.22183900	-2.71072900
O	8.12374100	5.14713200	-2.36561600
H	8.20577600	5.20188400	-1.39543600
H	8.46029300	4.25793700	-2.61647500

1: GC 8 = 1:3 complex

Number of imaginary frequency = 0

Sum of electronic and zero-point Energies = -9134.510493 au

Sum of electronic and thermal Energies = -9134.347284 au

Sum of electronic and thermal Enthalpies = -9134.346340 au

Sum of electronic and thermal Free Energies = -9134.715403 au

C	-1.42692300	-0.92366300	4.25051800
C	-1.34889500	-1.81281200	5.32478500
H	-2.25411900	-2.08221600	5.85524600
C	-0.11168100	-2.33977200	5.69013100
C	-0.27881600	-0.54068600	3.56590100
H	-0.29294800	0.21397500	2.78870800
O	-2.66459800	-0.49892200	3.86922800
H	-2.58962100	0.33073900	3.34094600
O	0.03284900	-3.22461300	6.70239600
H	-0.84750700	-3.46805100	7.06145700
C	0.94353800	-1.10349100	3.93950200
C	1.06198000	-2.00468400	4.99269200
C	2.39060400	-2.62482800	5.33639300
H	2.43369100	-3.66069800	4.96683500
H	2.51845200	-2.66796100	6.42489100
C	3.53592400	-1.85445600	4.68244600
H	3.71910800	-0.90193100	5.20030100
C	3.17405700	-1.55118000	3.22726500
H	2.95739100	-2.51932600	2.75386900
O	2.00996900	-0.73023600	3.18461600
C	4.23481800	-0.84141500	2.43251800
O	4.72228700	-2.64344700	4.65056600
H	4.90546800	-2.93812900	5.55464100
C	5.22669000	-1.57687900	1.79725000
H	5.23669100	-2.65699200	1.86416800
C	6.16771600	-0.93876300	0.99727000
C	6.15225300	0.45718500	0.83900900
C	5.16966900	1.18559700	1.52398500
C	4.20155600	0.53759800	2.28880400
H	3.39367900	1.11491500	2.71770700
O	5.13593100	2.55225800	1.50698600
H	5.71650500	2.96084300	0.79977600
O	7.01591700	1.12450300	0.03500900
H	7.78143600	0.55151600	-0.27548500
O	7.13132200	-1.63970200	0.34250600
H	6.98799300	-2.60225800	0.50798500
C	3.53976900	5.61449700	-0.69650300
C	3.59139100	6.86196500	-0.07422300

H	4.32536400	7.59470000	-0.38922400
C	2.70676300	7.13754400	0.97049200
C	2.60834600	4.66429200	-0.30136200
H	2.63408500	3.66252200	-0.69976100
O	4.43574900	5.34015900	-1.68799200
H	4.17018400	4.48941500	-2.10914200
O	2.72970300	8.30823200	1.64646200
H	3.43988800	8.88374000	1.29314100
C	1.71115700	4.98854100	0.70665900
C	1.73876600	6.20525700	1.38044900
C	0.84959800	6.45307300	2.57091700
H	0.42824500	7.46208300	2.54231500
H	1.43750000	6.37351400	3.49488400
C	-0.28757500	5.43902000	2.60414600
H	-0.80265100	5.45231900	3.56896900
C	0.21272900	4.01817400	2.31953000
H	-0.66255300	3.36583100	2.23127300
O	0.78308100	4.01212300	1.00213900
C	1.14122000	3.42496100	3.35412900
O	-1.28006700	5.76104400	1.62863300
H	-0.93158100	5.47982200	0.76594700
C	0.57349400	2.64580100	4.36341000
H	-0.49812400	2.46782700	4.39856800
C	1.38862600	2.00452700	5.29276100
C	2.77126400	2.15932000	5.21816900
C	3.33612300	2.94858800	4.21868700
C	2.52720800	3.58834400	3.28761000
H	3.00920800	4.13505500	2.48631600
O	4.69942800	2.98238400	4.18556200
H	4.98471800	2.99515400	3.23950800
O	3.56114100	1.45785500	6.08991800
H	4.46781200	1.53653300	5.74096700
O	0.83847600	1.19901600	6.23969500
H	1.55412700	0.66834800	6.62594800
C	-2.60726700	1.56826700	0.97613200
C	-3.43609800	2.33936600	0.15905100
H	-4.05476900	3.12793600	0.57707200
C	-3.44881200	2.08839400	-1.21437300
C	-1.78734800	0.58792300	0.42962400
H	-1.10952000	0.01080000	1.04377100
O	-2.57660400	1.76022600	2.33008300
H	-2.93976700	2.68095200	2.55756500
O	-4.27682000	2.78471500	-2.03706200
H	-4.97028000	3.23100800	-1.49366400
C	-1.76913700	0.41343400	-0.95293100

C	-2.61445700	1.13041400	-1.80278300
C	-2.62461900	0.89639100	-3.29357400
H	-2.26975600	1.79195700	-3.81963200
H	-3.64566700	0.71272900	-3.64387800
C	-1.69544400	-0.25008900	-3.68196800
H	-2.18400600	-1.22347100	-3.51188700
C	-0.45763300	-0.19506000	-2.77592800
H	-0.06924300	0.82884000	-2.78659600
O	-0.87399000	-0.49302600	-1.44164300
C	0.63334600	-1.14049900	-3.19643900
O	-1.34992000	-0.08499300	-5.04094300
H	-0.62269700	-0.70203500	-5.22356100
C	1.66665300	-0.63334800	-3.98928300
H	1.71751200	0.42719500	-4.22534800
C	2.67774400	-1.48220500	-4.43618300
C	2.64681400	-2.83838500	-4.10939000
C	1.62815900	-3.34475600	-3.29207100
C	0.61013100	-2.49287600	-2.85707000
H	-0.15992400	-2.89053700	-2.20375200
O	1.60275400	-4.64871400	-2.92264200
H	2.50306100	-5.04297100	-2.96018000
O	3.62758000	-3.67734600	-4.55684800
H	4.46977400	-3.18190400	-4.66899800
O	3.73934000	-1.07215400	-5.18151900
H	3.87480500	-0.11229800	-5.03303700
C	-0.40218800	-5.03436000	4.13199000
C	-0.45121200	-4.21708500	3.00121200
C	-1.68168900	-3.74333800	2.54406200
C	-2.85568200	-4.10994100	3.20249900
C	-2.80094400	-4.95927500	4.30861900
C	-1.57182500	-5.39860800	4.79107900
H	0.56450900	-5.38637300	4.47524900
H	-1.74949900	-3.14702600	1.63772400
H	-3.73821500	-5.28592400	4.75399200
H	-1.52345100	-6.03452400	5.66987700
C	0.84517000	-3.97559300	2.28592300
O	1.81931300	-4.68314100	2.54236500
N	0.86130400	-2.99556300	1.33916000
H	0.14377100	-2.28088500	1.39285300
C	-4.20344200	-3.72699000	2.67147900
O	-5.16224800	-4.47539600	2.79660700
N	-4.23680600	-2.52241400	2.02728200
H	-3.54088600	-1.83587400	2.31566600
C	1.94936200	-2.73375700	0.47168200
C	2.19430000	-1.45846300	0.02517400

C	2.75307000	-3.80253600	0.00707800
C	3.27849100	-1.20496200	-0.85260200
H	1.56608000	-0.62257200	0.32517200
C	3.82123900	-3.57274300	-0.81621400
H	2.50184000	-4.81817500	0.28438900
C	3.46864400	0.10838300	-1.34855300
C	4.14622300	-2.26370900	-1.26157200
H	4.37595800	-4.41978700	-1.18536500
C	4.48829700	0.35473600	-2.22743100
H	2.76184900	0.88277900	-1.06440100
C	5.23660000	-1.93101000	-2.12472900
C	5.39399500	-0.65555700	-2.60642000
H	6.19180000	-0.43778700	-3.31261800
C	-5.30547700	-2.05152000	1.24147300
C	-5.49407800	-0.69780200	1.11438900
C	-6.11907600	-2.95404400	0.50493100
C	-6.49726500	-0.19690700	0.25192800
H	-4.86511000	0.00533200	1.65674700
C	-7.10363300	-2.48333200	-0.32267700
H	-5.96479900	-4.02366800	0.58049900
C	-6.65768600	1.19937300	0.08713900
C	-7.32882900	-1.09054500	-0.47870100
H	-7.70207400	-3.20036700	-0.87066500
C	-7.57431500	1.68545300	-0.80342400
H	-6.03655300	1.87659300	0.66177000
C	-8.31805500	-0.52831900	-1.34158400
C	-8.43419600	0.82519300	-1.52263300
H	-9.16983700	1.22395800	-2.21240500
S	4.58326500	1.89726100	-3.09127200
S	6.48701700	-3.06120900	-2.75291400
S	-7.65895700	3.44746000	-1.01893800
S	-9.45438800	-1.59237400	-2.21948200
O	6.26640200	-4.40565500	-2.13748000
O	6.27291000	-3.08239500	-4.22296900
O	3.59848300	2.81952600	-2.47370600
O	4.23444500	1.57703500	-4.50407800
O	-8.62139200	-2.44647600	-3.11027900
O	-10.34622000	-0.68288700	-2.97748400
O	-7.88452100	3.69559000	-2.46481400
O	-6.29861400	3.91489700	-0.60142900
O	-8.73206000	3.97445400	-0.16143700
O	-10.16128000	-2.37662300	-1.17850500
O	5.98102500	2.39165200	-2.96171900
O	7.79322500	-2.48491700	-2.38589000
O	4.70092500	-4.75505100	2.61273300

H	4.78884400	-4.09858300	3.33078900
H	3.75006000	-4.73576300	2.39467100
O	-9.23051100	-5.22464800	-2.80698800
H	-8.85287600	-4.34299600	-2.98251900
H	-10.20054800	-5.04933700	-2.84909100
O	-2.50533500	-4.05258600	7.44624600
H	-2.92285700	-4.08951400	6.57185300
H	-3.08045300	-3.49396500	7.98839200
O	8.60742800	-6.17575800	-2.37060700
H	8.99982400	-5.57897100	-1.70443100
H	7.74301700	-5.76271600	-2.51352000
O	-5.48299100	5.01994100	-3.23537300
H	-4.70337900	4.44300700	-3.26093800
H	-6.23113500	4.40575600	-3.09477800
O	9.22793900	-4.13573000	-0.51082400
H	8.50148500	-4.31872800	0.11077000
H	8.83509600	-3.50624100	-1.14431300
O	-5.42154900	6.65305400	-0.65648900
H	-5.22133500	5.90916800	-1.25453500
H	-6.35477000	6.81059900	-0.90193000
O	7.86162200	3.13155600	-5.00910900
H	7.11978400	3.28564000	-4.39807900
H	8.36205300	2.44014600	-4.52576200
O	-5.50942900	5.17037400	1.66146000
H	-5.39541700	5.86017800	0.96161400
H	-5.88881800	4.44598900	1.12819500
O	6.65974600	-4.31703500	0.64933000
H	6.33703200	-4.51429400	-0.25057800
H	5.94632000	-4.54340600	1.29216200
O	-9.25501400	-4.93662700	-0.08207600
H	-9.19223000	-5.18941500	-1.03439800
H	-9.51431300	-4.00170000	-0.13146200
O	4.10804100	-6.01380700	-3.24110200
H	4.05169500	-5.46709000	-4.04410400
H	4.89118600	-5.63094000	-2.80471300
O	-11.78788700	-4.33337200	-2.52526100
H	-12.01312000	-3.72157300	-3.26302800
H	-11.40652000	-3.73358900	-1.85860000
O	6.48656800	3.78017100	-0.40547100
H	5.90304600	4.38329200	-0.89981200
H	6.62111300	3.01158900	-0.98757100
O	8.42766300	0.95271900	-3.40766700
H	7.57056000	1.25099500	-3.04771600
H	8.20085800	0.21578700	-4.04351400
O	7.68474200	-0.79669600	-5.25884800

H	7.07609000	-0.19218400	-5.75077500
H	7.18691400	-1.59780500	-5.00915600
O	9.03432600	-0.20991300	-1.00973600
H	8.57959900	-1.06948500	-1.05374500
H	8.99395200	0.13876400	-1.92748100
O	-3.25380800	4.21235700	2.79535200
H	-2.62804600	4.74981900	2.26576300
H	-4.13911300	4.54085200	2.49327300
O	0.92410600	2.00617200	-1.21601700
H	0.73199400	2.61435200	-0.48232200
H	1.56540600	2.46742800	-1.78129500
O	6.34003500	1.26414600	-6.36291900
H	5.54269500	1.42981600	-5.82857400
H	6.95805200	1.96480200	-6.05326000
O	4.75645600	9.93311900	0.64672100
H	4.67073700	10.24598600	-0.26441800
H	5.65972400	9.59488200	0.71877000
O	-12.17337500	-2.32703200	-4.36945600
H	-11.89663400	-1.64167900	-3.73465600
H	-11.41013200	-2.32210100	-4.98525600
O	-7.63239600	6.63970900	-2.37667600
H	-8.07540600	5.77327600	-2.35579900
H	-6.83965900	6.45755800	-2.91020500
O	-7.63306000	3.48930000	2.44271300
H	-7.16577300	4.33188400	2.55463400
H	-8.19852100	3.64911100	1.66601400
O	-9.74024200	-1.72120800	-5.58893400
H	-9.90250300	-0.90809500	-5.08146100
H	-9.19431300	-2.21115200	-4.94463200
O	-6.90950100	-6.04693400	1.03108800
H	-7.72710700	-5.59523300	0.73396300
H	-6.58713100	-5.52988300	1.78406900