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Supporting Information

Dithiafulvenyl-Extended *N*-Heterotriangulenes and Their Interaction with C₆₀: Cooperative Fluorescence

Bettina D. Gliemann,^[a] Volker Strauss,^[b] Jakob F. Hitzengerger,^[b] Pavlo O. Dral,^[c]
Frank Hampel,^[a] Jean-Paul Gisselbrecht,^[d] Thomas Drewello,^[b] Walter Thiel,^[c]
Dirk M. Guldi,^{*[b]} and Milan Kivala^{*[a]}

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Table of Contents

1. Experimental Section	3
2. ^1H and ^{13}C NMR Spectra	4
3. X-ray Crystallography	9
4. (Spectro-)Electrochemistry	15
5. Mass Spectrometry Experiments with 1 , 2 , and C_{60}	20
6. Photophysical Characterization.....	23
7. Theoretical Calculations.....	24
8. References	28

1. Experimental Section

Elemental analyses were carried out by the Microanalytic Laboratory (Institute of Organic Chemistry, University of Erlangen-Nürnberg) on a CHNS He (varioMICRO) system. Basic UV/vis absorption spectra were recorded in a quartz cuvette (1 cm) at room temperature. The absorption maxima (λ_{\max}) are reported in nanometers with the extinction coefficient (ϵ) in $M^{-1} \text{ cm}^{-1}$; shoulders are indicated as sh. The ^1H NMR illumination experiment was carried out by using a Herolab GmbH Laborgeräte UV lamp.

4,4,8,8,12,12-Hexamethyl-4*H*,8*H*,12*H*-benzo[1,9]quinolizino[3,4,5,6,7-*defg*]acridine-2,6-dicarbaldehyde (5). A degassed solution of **4** (44 mg, 1.1 mmol) in dry DMF (6.7 mL, 12 mmol) was cooled to 0 °C. To this mixture POCl_3 (1.8 mL, 12 mmol) was added dropwise under nitrogen atmosphere. After stirring at 100 °C for 20 h the reaction mixture was diluted with H_2O (40 mL) and its pH was adjusted to 8 with aqueous NaOH (2.8 M). The obtained mixture was extracted with CH_2Cl_2 (3×30 mL). The combined organic layers were washed with H_2O (2×30 mL), dried (MgSO_4), and the solvents evaporated under reduced pressure. Purification by column chromatography (SiO_2 , hexanes/EtOAc 4:1) yielded **5** as a yellow solid (308 mg, 67%). $R_f = 0.79$ (SiO_2 , hexanes/EtOAc 4:1). ^1H NMR (300 MHz, CDCl_3) δ 9.95 (s, 2H), 7.92 (dd, $^4J_{\text{H,H}} = 4.9$ Hz, $^4J_{\text{H,H}} = 2.0$ Hz, 4H), 7.47 (d, $^3J_{\text{H,H}} = 7.7$ Hz, 2H), 7.26 (dd, $^3J_{\text{H,H}} = 8.2$ Hz, $^3J_{\text{H,H}} = 7.3$ Hz, 1H), 1.68 (s, 18H) ppm. ^{13}C NMR (100 MHz, CD_2Cl_2) δ 191.4, 136.8, 132.7, 131.5, 131.3, 130.9, 126.2, 125.4, 125.3, 124.6, 36.1, 35.9, 33.5, 32.4 ppm (14 signals out of 15 expected). ESI HRMS (ACN-MeOH) m/z calcd. for $\text{C}_{29}\text{H}_{28}\text{NO}_2$ $[\text{M}+\text{H}]^+$ 422.2115, found 422.2117.

2. ^1H and ^{13}C NMR Spectra

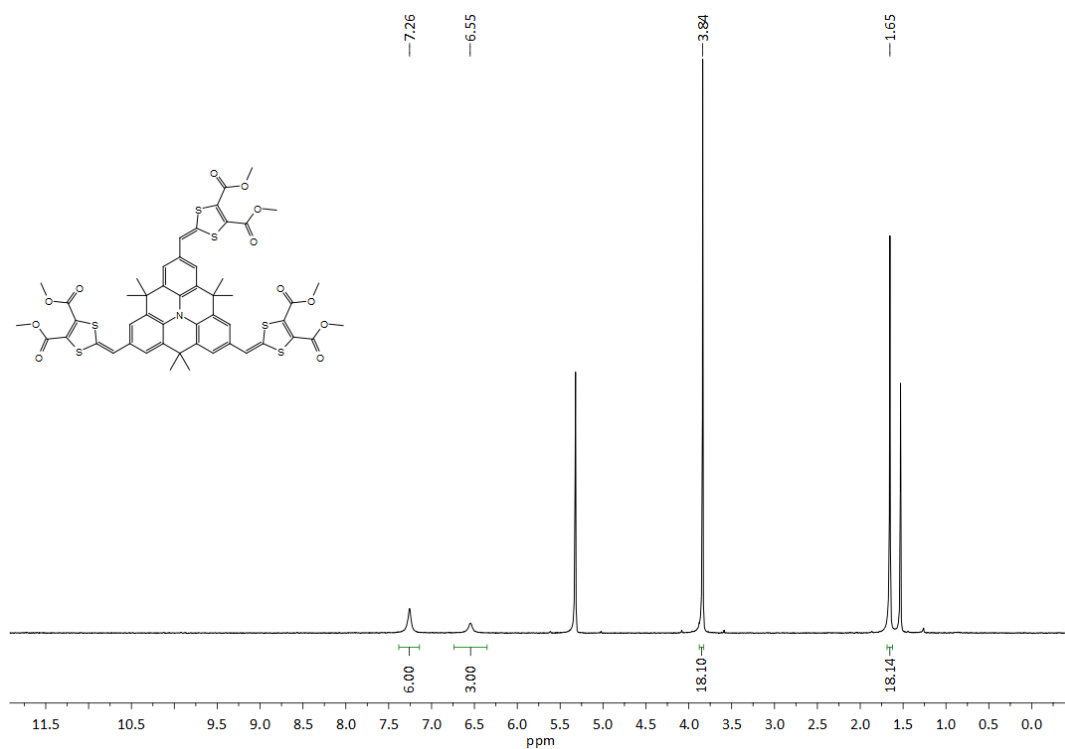


Figure S1. ^1H NMR (400 MHz, CD_2Cl_2) spectrum of **1**; * = water.

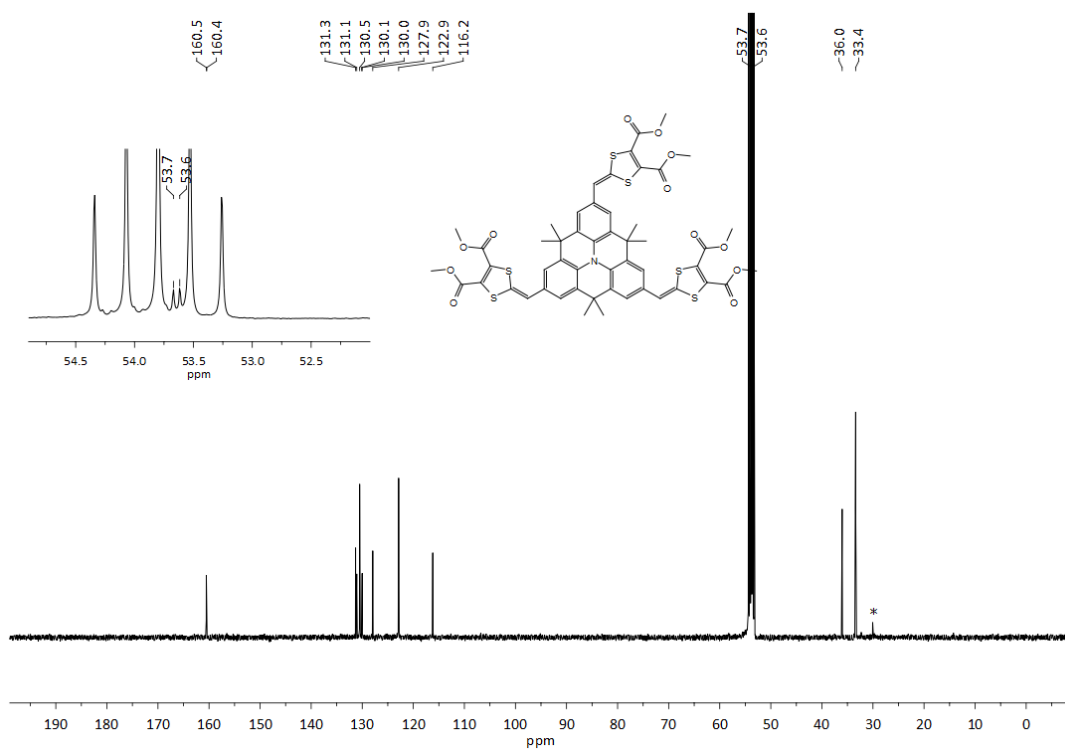


Figure S2. ^{13}C NMR (100 MHz, CD_2Cl_2) spectrum of **1**; * = grease.

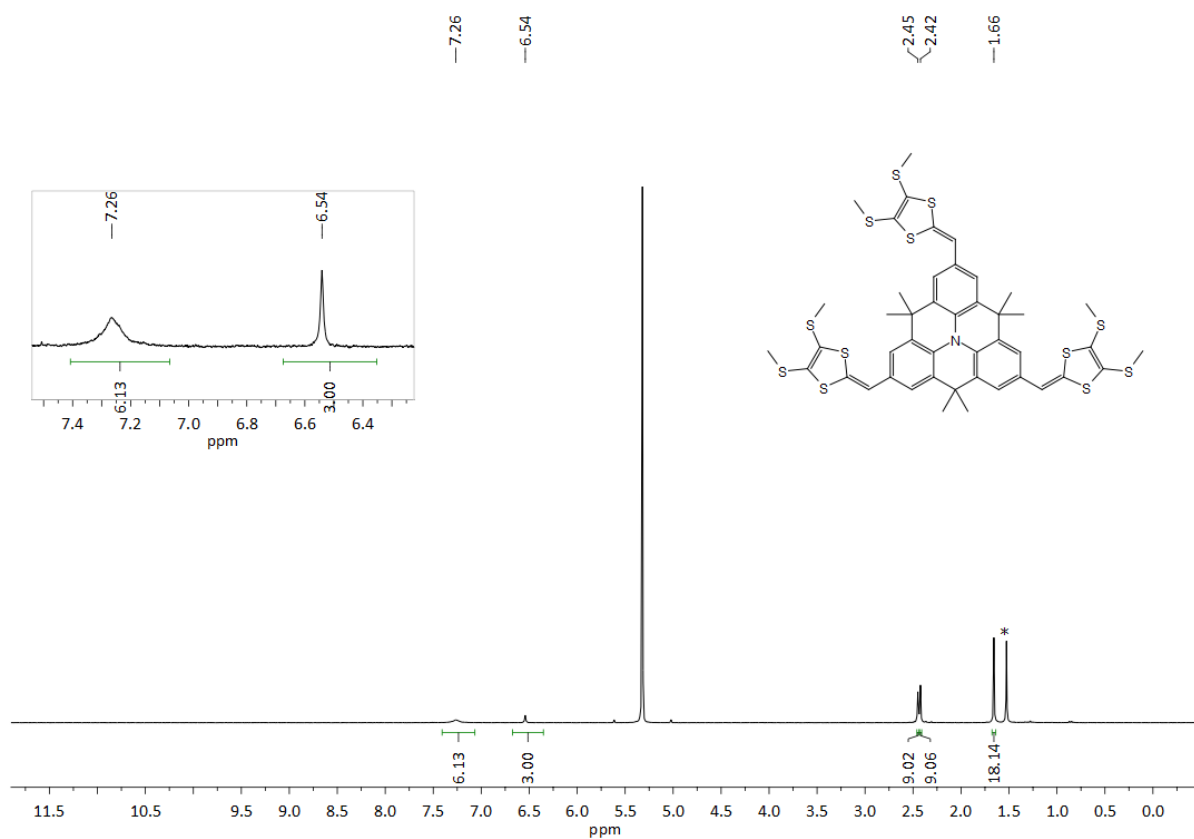


Figure S3. ¹H NMR (300 MHz, CD₂Cl₂) spectrum of **2**; * = water.

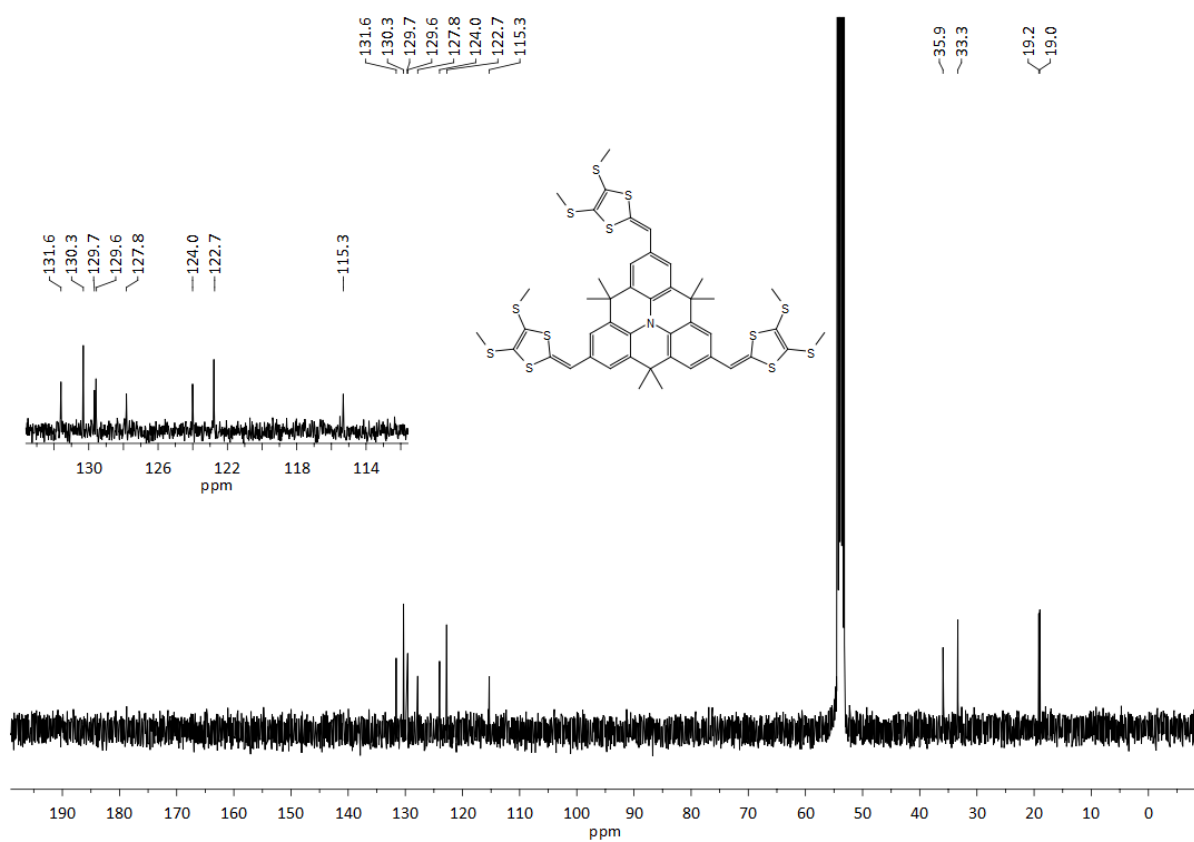


Figure S4. ¹³C NMR (100 MHz, CD₂Cl₂) spectrum of **2**.

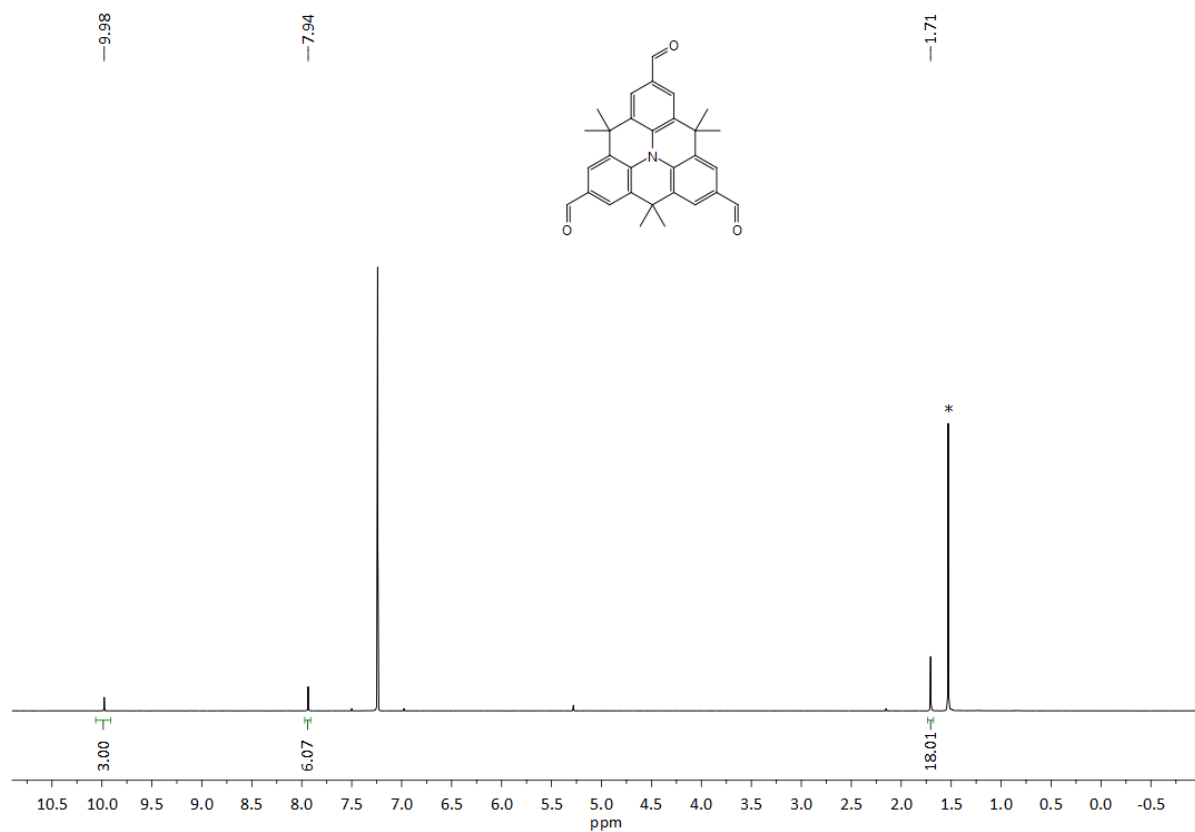


Figure S5. ¹H NMR (400 MHz, CDCl₃) spectrum of trialdehyde **3**; * = water.

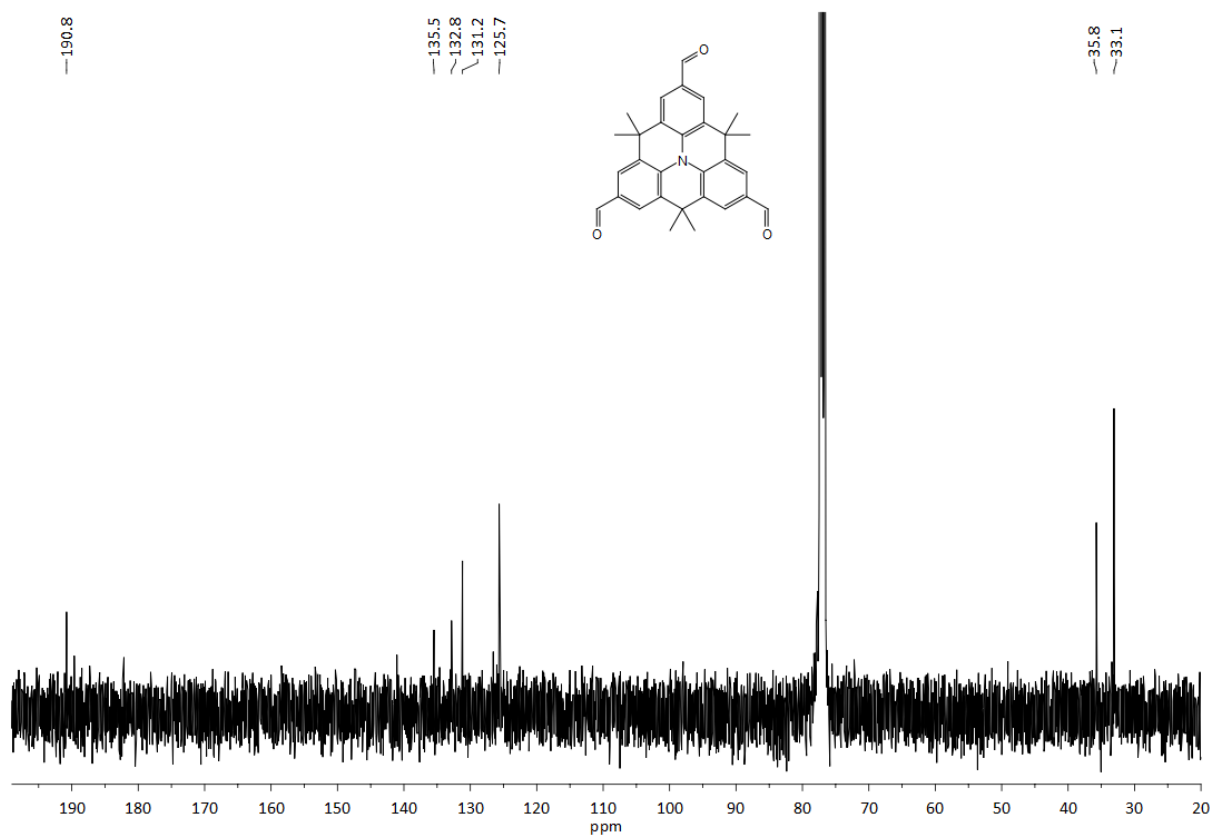


Figure S6. ¹³C NMR (100 MHz, CDCl₃) spectrum of trialdehyde **3**.

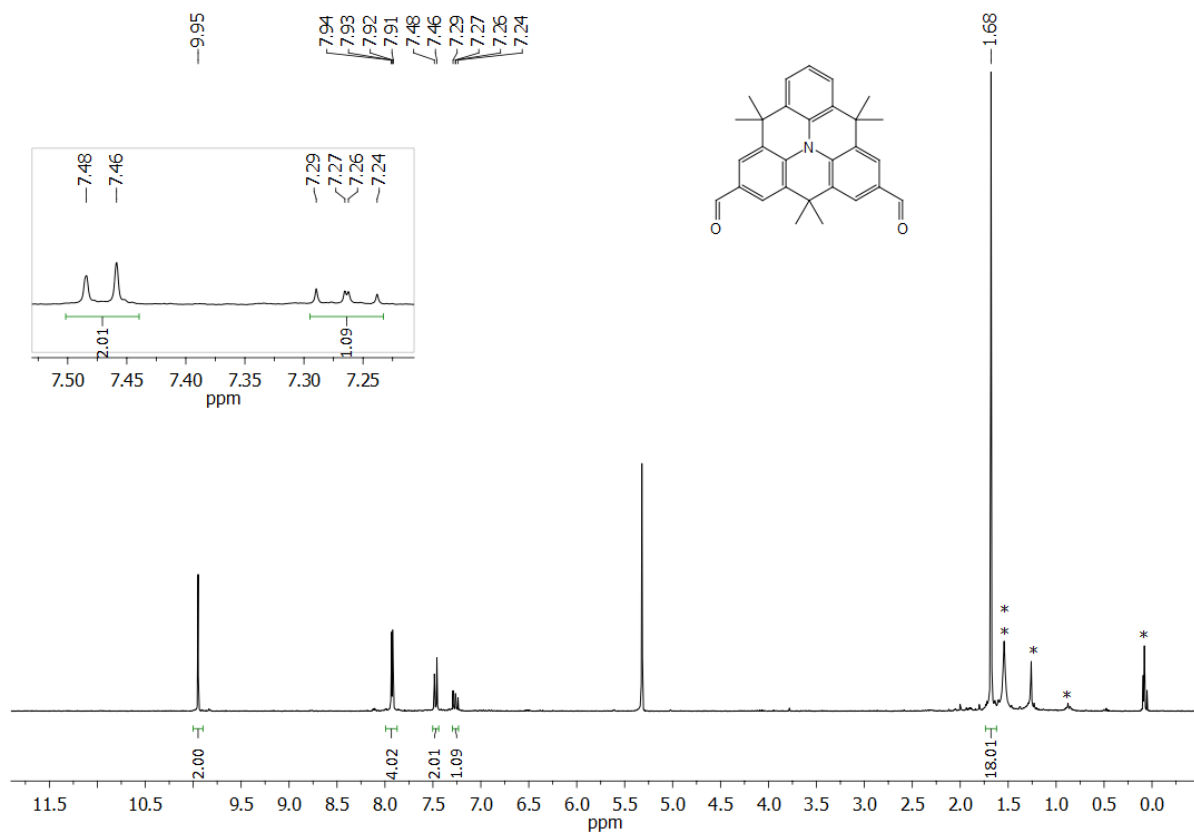


Figure S7. ^1H NMR (300 MHz, CD_2Cl_2) spectrum of dialdehyde **5**; * = grease/hexanes, ** = water.

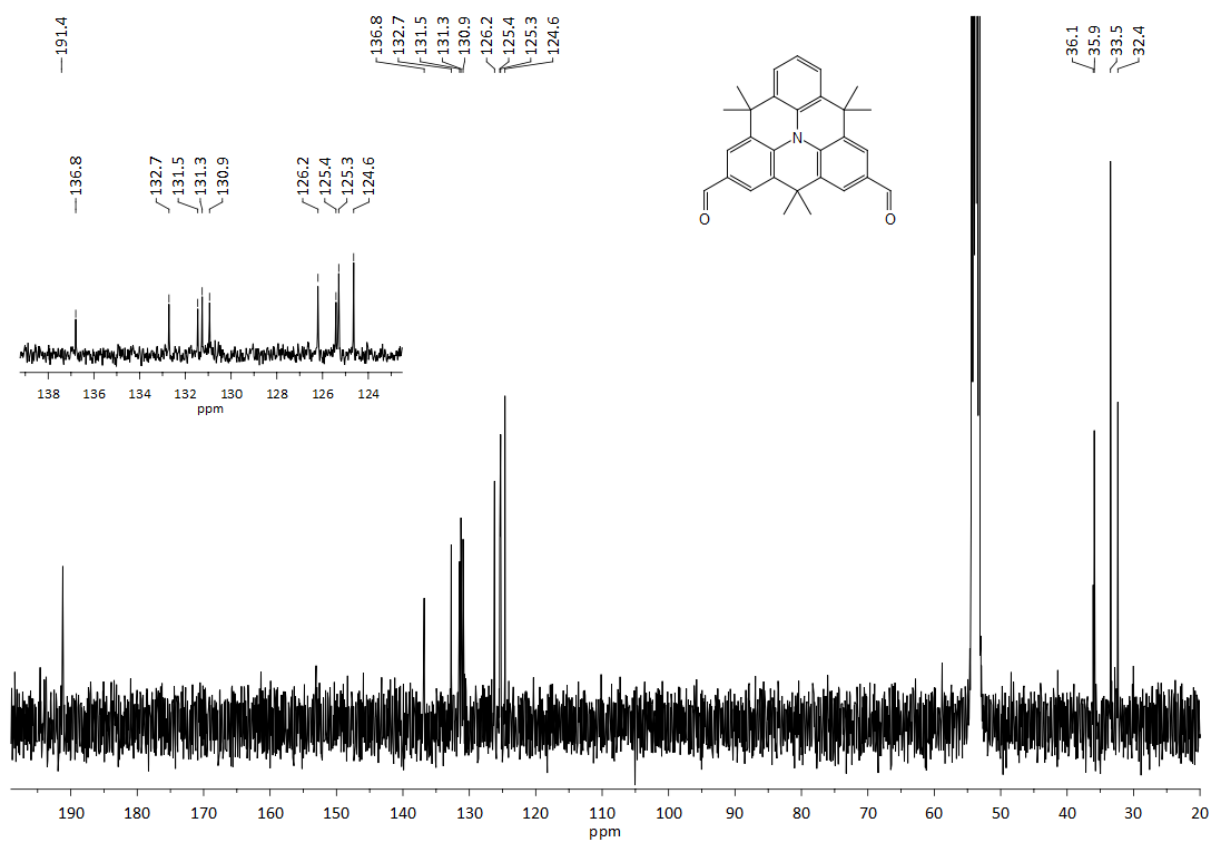


Figure S8. ^{13}C NMR (100 MHz, CD_2Cl_2) spectrum of **5**.

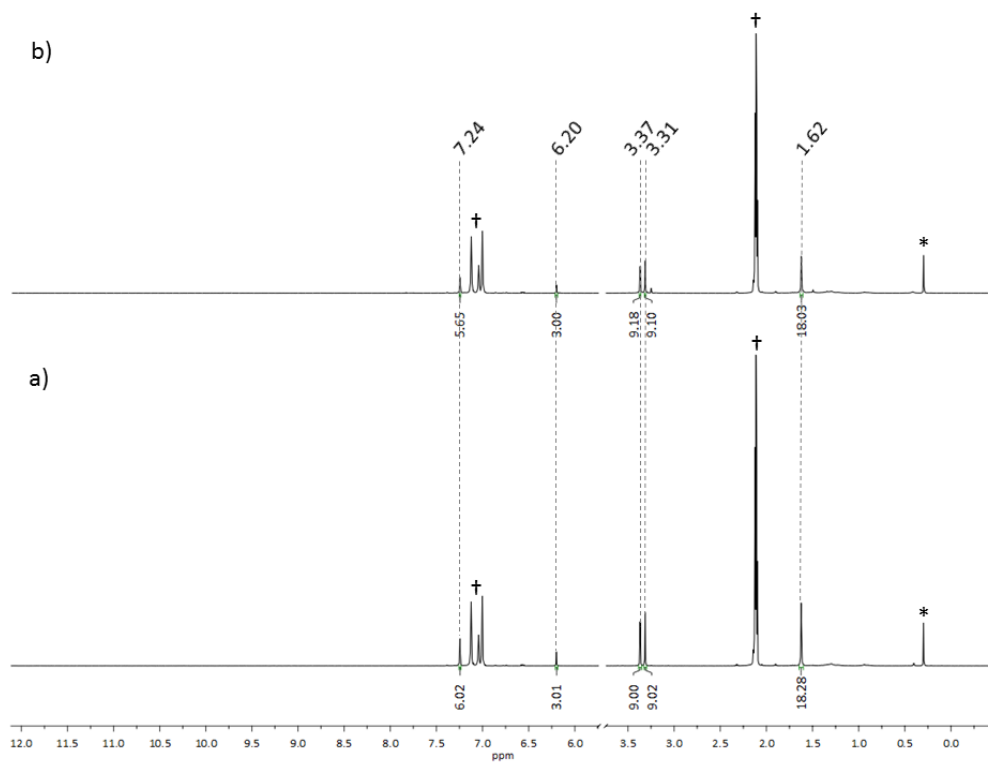


Figure S9A. ^1H NMR spectrum (300 MHz, toluene- d_8 , r.t.) of a deoxygenated 1:1 mixture of **1**: C_{60} ; a) spectrum before illumination; b) spectrum after illumination at 366 nm for 12h; † = toluene- d_8 , * = solvent impurity.

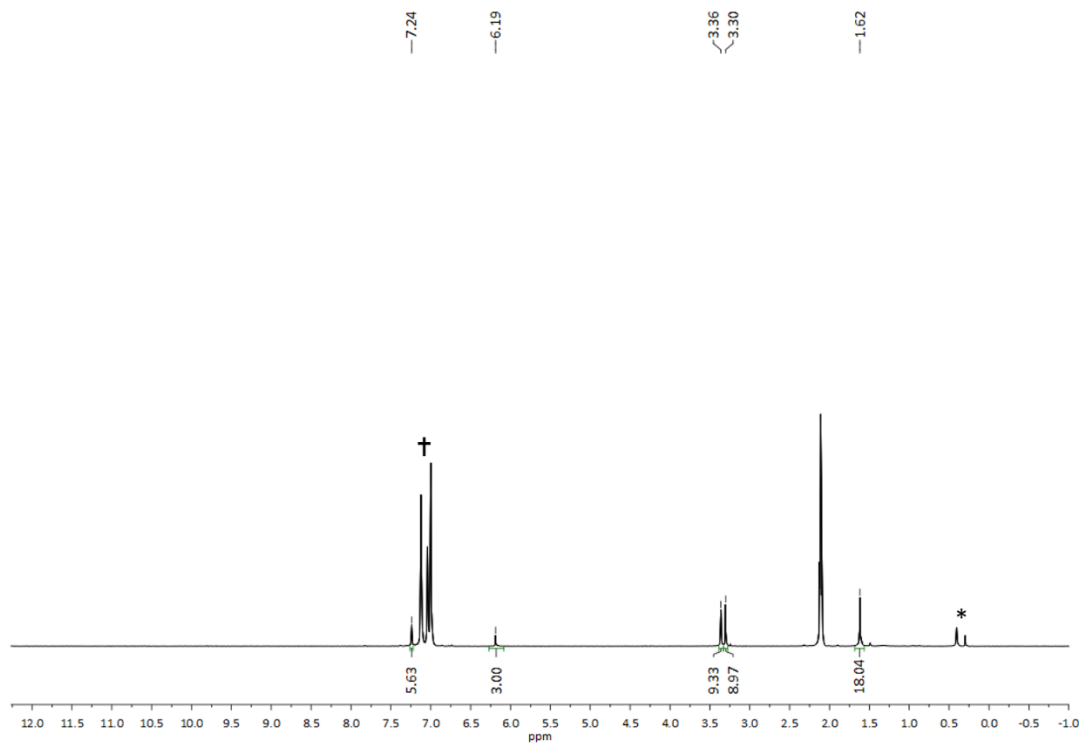


Figure S9B. ^1H NMR spectrum (300 MHz, toluene- d_8 , r.t.) of pristine **1**. † = toluene- d_8 , * = solvent impurity.

3. X-ray Crystallography

Experimental. Single crystals suitable for X-ray crystallographic analysis were mounted on a loop on a SuperNova, Dual, Cu at zero, Atlas diffractometer. Diffraction intensity was collected using $\text{Cu}_{K\alpha}$ radiation ($\lambda = 1.5413 \text{ \AA}$). The crystal was kept at 173.0(2) K during data collection. Using Olex2,^[1] the structure was solved and refined with the ShelX program, using Direct Methods for structure solution and Least Squares minimization for refinement.^[2] Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed according to a riding model refinement routine.

Crystal data of compound 3. Single crystals of **3** were grown by slow liquid diffusion of *n*-hexanes into a CH_2Cl_2 solution of the compound at room temperature within one week under light exclusion. One molecule of **3** forms the asymmetric unit. The disorder of one aldehyde (O1:O1a) group was refined to 63:37 % occupancy. The *N*-heterotriangulene core is planarized with angles between the planes of the phenyl rings of 17.29, 19.13, and 23.31°. The central nitrogen atom shows only a negligible deviation from the plane defined by the adjacent C-atoms (C1-C2-C3) of 0.04 Å.

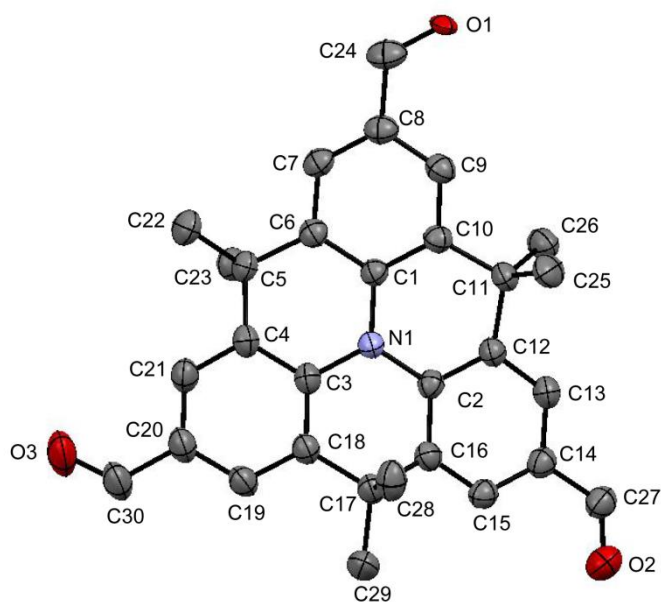


Table S1. Crystallographic data and structure refinement details for **3**

Empirical formula	$C_{30}H_{27}NO_3$	
Formula weight	449.53	
CCDC number	1537955	
Temperature/K	173.0(2)	
Wavelength	1.5413 Å	
Crystal system	triclinic	
Space group	<i>P</i> -1	
Unit cell dimensions	$a = 9.5120(7)$ Å	$\alpha = 110.271(7)^\circ$
	$b = 11.9676(10)$ Å	$\beta = 98.685(6)^\circ$
	$c = 12.3407(9)$ Å	$\gamma = 110.804(7)^\circ$
Volume	1170.17(15) Å ³	
Z	2	
Density calculated	1.276 mg/mm ³	
Absorption coefficient	0.649 mm ⁻¹	
F(000)	476.0	
Crystal size	0.1867 × 0.07 × 0.0418 mm ³	
2 Θ range for data collection	8.04 to 151.98°	
Index ranges	$-10 \leq h \leq 11$, $-14 \leq k \leq 14$, $-10 \leq l \leq 15$	
Reflections collected	8486	
Independent reflections	4737[R(int) = 0.0615]	
Data/restraints/parameters	4737/1/317	
Goodness-of-fit on F ²	1.156	
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0899$, $wR_2 = 0.2805$	
Final R indexes [all data]	$R_1 = 0.1113$, $wR_2 = 0.2967$	
Largest diff. peak and hole	0.71 and -0.34 eÅ ⁻³	

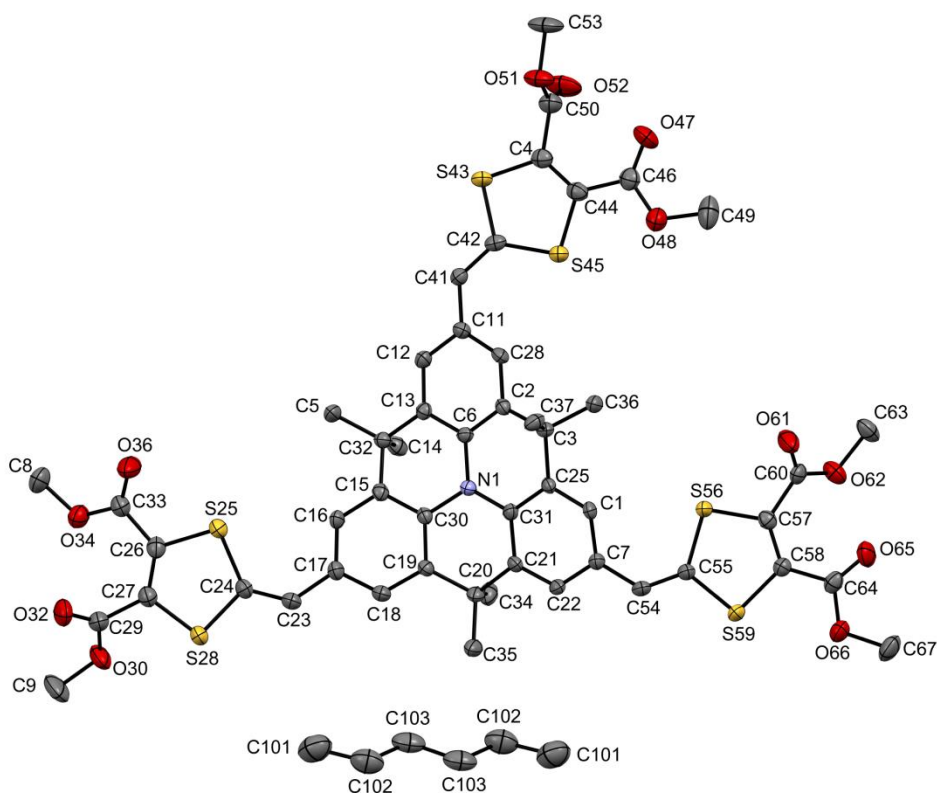


Table S2. Crystallographic data and structure refinement details for **1**

Empirical formula	$C_{54}H_{52}NO_{12}S_6$	
Formula weight	1099.33	
CCDC	1537954	
Temperature/K	173.00(10)	
Wavelength	1.5413 Å	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	$a = 12.7049(2)$ Å	$\alpha = 90.00^\circ$
	$b = 37.7415(4)$ Å	$\beta = 90.4134(14)^\circ$
	$c = 10.92040(12)$ Å	$\gamma = 90.00^\circ$
Volume	$5236.22(12)$ Å ³	
Z	4	
Density calculated	1.394 mg/mm ³	
Absorption coefficient	2.943 mm ⁻¹	
F(000)	2300.0	

Crystal size	$0.5326 \times 0.0958 \times 0.046 \text{ mm}^3$
2 θ range for data collection	6.96 to 108.48°
Index ranges	$-13 \leq h \leq 11, -39 \leq k \leq 35, -11 \leq l \leq 9$
Reflections collected	9327
Independent reflections	5357[R(int) = 0.0265]
Data/restraints/parameters	5357/0/671
Goodness-of-fit on F ²	1.023
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0503, wR_2 = 0.1375$
Final R indexes [all data]	$R_1 = 0.0552, wR_2 = 0.1441$
Largest diff. peak and hole	0.46 and -0.32 eÅ ⁻³

Crystal data of compound S1. Single crystals of **S1** suitable for X-ray crystallographic analysis were grown by slow liquid diffusion of *n*-hexanes into a CH₂Cl₂ solution of the compound at room temperature within 3 months. In fact, compound **3** was used for crystal growth which was apparently oxidized during crystallization to **S1**. The X-ray sample was analyzed via LDI MS and showed the characteristic molecular ion peak at m/z 450 [M-CH₃]⁺. One molecule of **S1** forms the asymmetric unit. The central N-atom has an almost ideal trigonal planar structure as all three angles around the N-core sum up to 359.8°. Overall, the molecule is slightly twisted with the N-atom having a negligible deviation from the plane defined by the adjacent C-atoms (C2-C3-C4) by 0.04 Å.

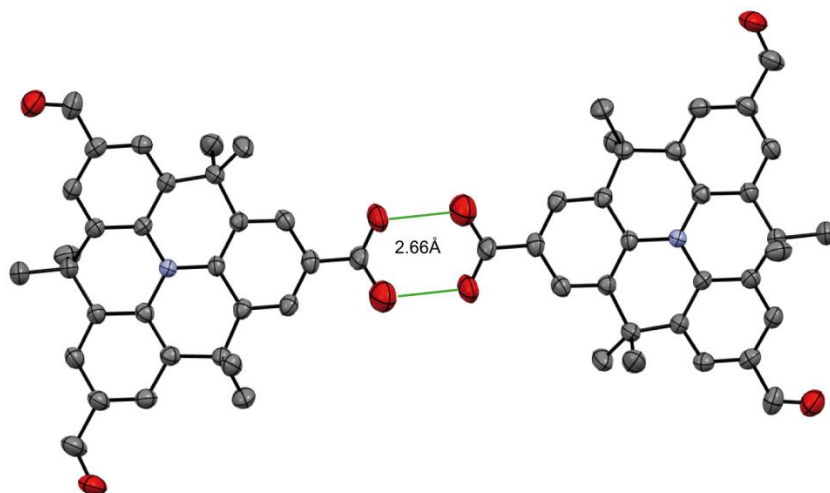
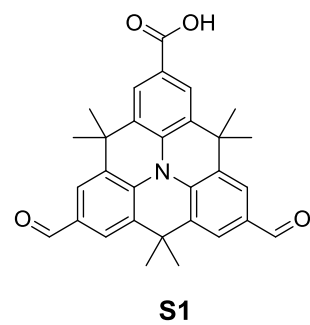
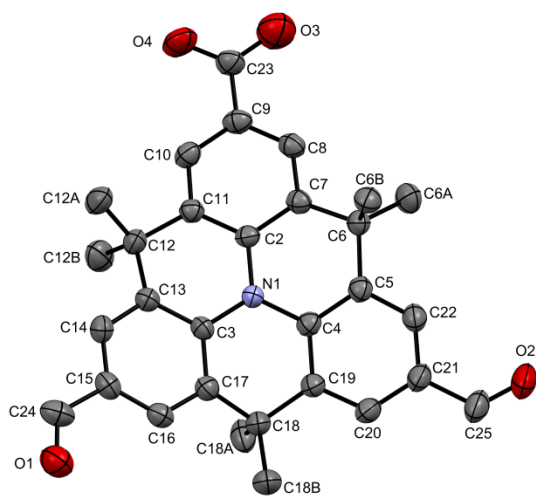


Table S3. Crystallographic data and structure refinement details for **S1**

Empirical formula	$C_{30}H_{27}NO_4$	
Formula weight	465.54	
CCDC	1537953	
Temperature/K	173.00(14)	
Wavelength	1.54184 Å	
Crystal system	triclinic	
Space group	<i>P</i> -1	
Unit cell dimensions	$a = 9.5476(15)$ Å	$\alpha = 110.256(15)^\circ$
	$b = 12.009(2)$ Å	$\beta = 98.280(13)^\circ$
	$c = 12.285(2)$ Å	$\gamma = 111.070(15)^\circ$
Volume	1173.6(4) Å ³	
Z	2	
Density calculated	1.317 mg/mm ³	
Absorption coefficient	0.699 mm ⁻¹	
F(000)	492.0	
Crystal size	0.1158 × 0.0451 × 0.0309 mm ³	
2 θ range for data collection	8.06 to 121.13°	
Index ranges	-10 ≤ h ≤ 9, -11 ≤ k ≤ 13, -12 ≤ l ≤ 13	
Reflections collected	5054	
Independent reflections	3424[R(int) = 0.0376]	
Data/restraints/parameters	3424/3/326	
Goodness-of-fit on F ²	1.083	
Final R indexes [I >= 2σ (I)]	R ₁ = 0.0725, wR ₂ = 0.2187	
Final R indexes [all data]	R ₁ = 0.0994, wR ₂ = 0.2462	
Largest diff. peak and hole	1.04 and -0.41 eÅ ⁻³	

4. (Spectro-)Electrochemistry

Electrochemistry. Electrochemical measurements were carried out in CH_2Cl_2 containing 0.1M $n\text{-Bu}_4\text{NPF}_6$ in a classical three-electrode cell by cyclic voltammetry (CV) and rotating-disk voltammetry (RDV). The working electrode was a glassy C disk (3 mm in diameter), the auxiliary electrode a Pt wire, and the reference electrode a Pt wire used as pseudo reference electrode. At the end of the studies, ferrocene is added to the solution. The cell was connected to an Autolab PGSTAT30 potentiostat (Eco Chemie, Holland) driven by a GPSE software running on a personal computer. All potentials are given vs. Fc^+/Fc used as internal reference and uncorrected from ohmic drop.

Species **1** and **2** gave rise to electrode deposits on the electrode surface. For **2**, the deposit undergoes a re-dissolution on the reverse scan (Figure S10), whereas for **1**, iterative scans gave rise to film formation which was not very adhesive at the electrode surface (Figure S11).

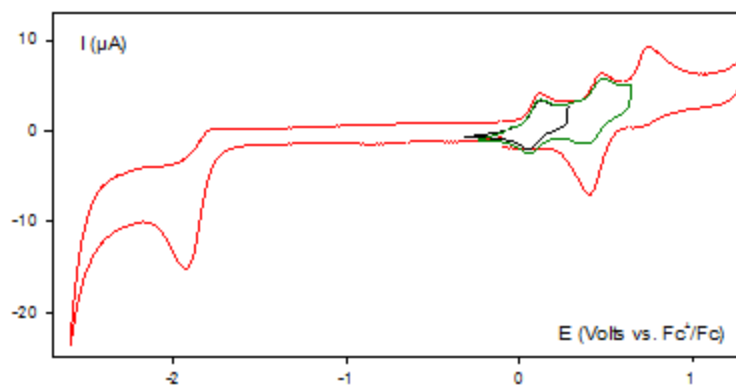


Figure S10. Cyclic voltammetry of **1** in CH_2Cl_2 + 0.1M $n\text{-Bu}_4\text{NPF}_6$ at $\nu = 0.1 \text{ V s}^{-1}$ (The two first oxidation are reversible one-electron transfers (black and green curves)).

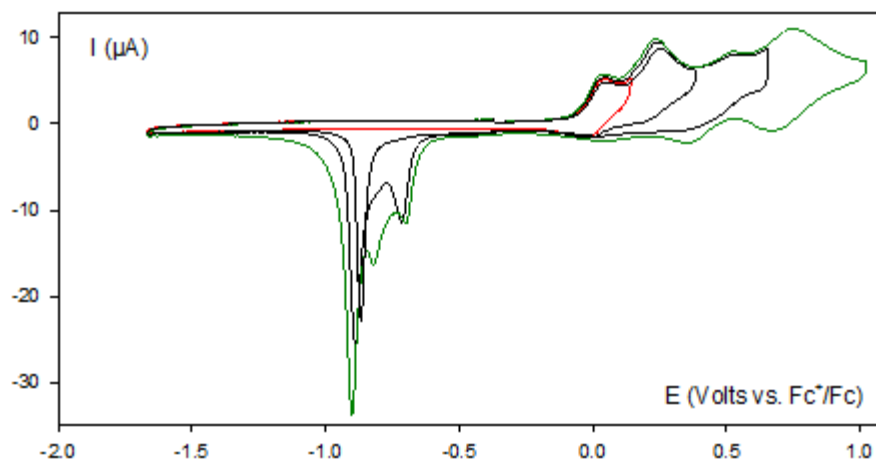


Figure S11. Cyclic voltammetry of **2** in CH_2Cl_2 + 0.1 M $n\text{-Bu}_4\text{NPF}_6$ at $v = 0.1 \text{ V s}^{-1}$.

Table S4: Electrochemical data obtained by cyclic voltammetry (CV) and rotating disk voltammetry (RDV) in CH_2Cl_2 + 0.1 M $n\text{-Bu}_4\text{NPF}_6$. All potentials are given vs. Fc^+/Fc .

Compound	CV			RDV	
	E° / V^a	$\Delta E_p / [\text{mV}]^b$	E_{pc} / V^d	$E_{1/2} / \text{V}$	Slope / $[\text{mV}]^e$
1	+0.11	60		+0.11 ($1e^-$)	60
	+0.48	85		+0.49 ($1e^-$)	60
			+0.79		
			-1.74		
2	+0.00	60		Unresolved waves	
			+0.23		
			+0.53		
			+0.74		

^a $E^\circ = (E_{pc} + E_{pa})/2$, where E_{pc} and E_{pa} correspond to the cathodic and anodic peak potentials, respectively; ^b $\Delta E_p = E_{pa} - E_{pc}$; ^c E_p = irreversible peak potential; ^d Logarithmic analysis of the wave obtained by plotting E versus $\text{Log}[I/(I_{lim} - I)]$; ^e Small amplitude signal compared to the first reduction step.

Spectroelectrochemistry. Spectroelectrochemical measurements were carried out in a homemade OTTLE cell (optical transparent thin layer electrode) connected to the potentiostat. The working electrode was a platinum grid placed in the optical pathway, the counter

electrode a platinum wire and the reference electrode (pseudo reference electrode) was a silver wire. The cell was placed in a HP 8453 diode array spectrophotometer.

Results:

First oxidation step. Time resolved UV/vis spectra could be recorded for the first oxidation of **1**. The spectral evolutions gave well resolved isosbestic points, meaning that two species are in equilibrium during that oxidation process. (Figure S12 top)

Initial spectrum: 316; 408 nm

Isosbestic points: 339; 371; 448 nm

Final spectrum: 352 (sh); 371; 557; 584 nm (sh).

Second oxidation step. The spectral evolution during the second oxidation step shows a decrease of the generated bands at 372 and 557nm with no isosbestic points. (Figure S13 bottom). The generated species did not show any absorption bands.

Reduction of the generated dication by stepwise reduction did not allow recovering of the initial spectrum (only around 50%) (Figure S13). This may be due to the film deposition observed on the platinum grid during oxidation. This deposit is not anymore dissolved under our experimental conditions.

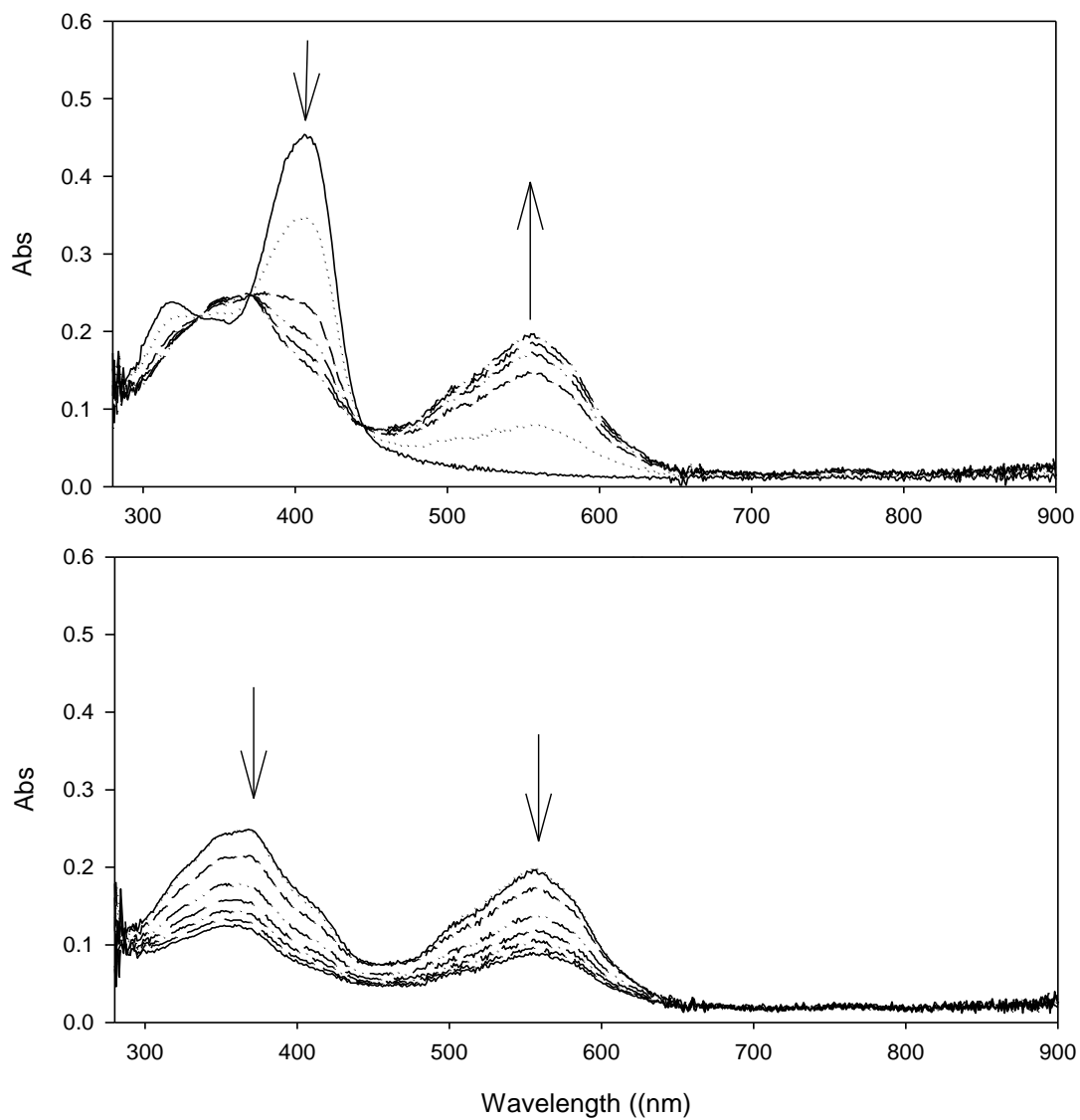


Figure S12. Time resolved UV/vis spectral evolution for the first (top) and the second (bottom) oxidation of **1** in CH_2Cl_2 containing 0.1 M $n\text{-Bu}_4\text{NPF}_6$.

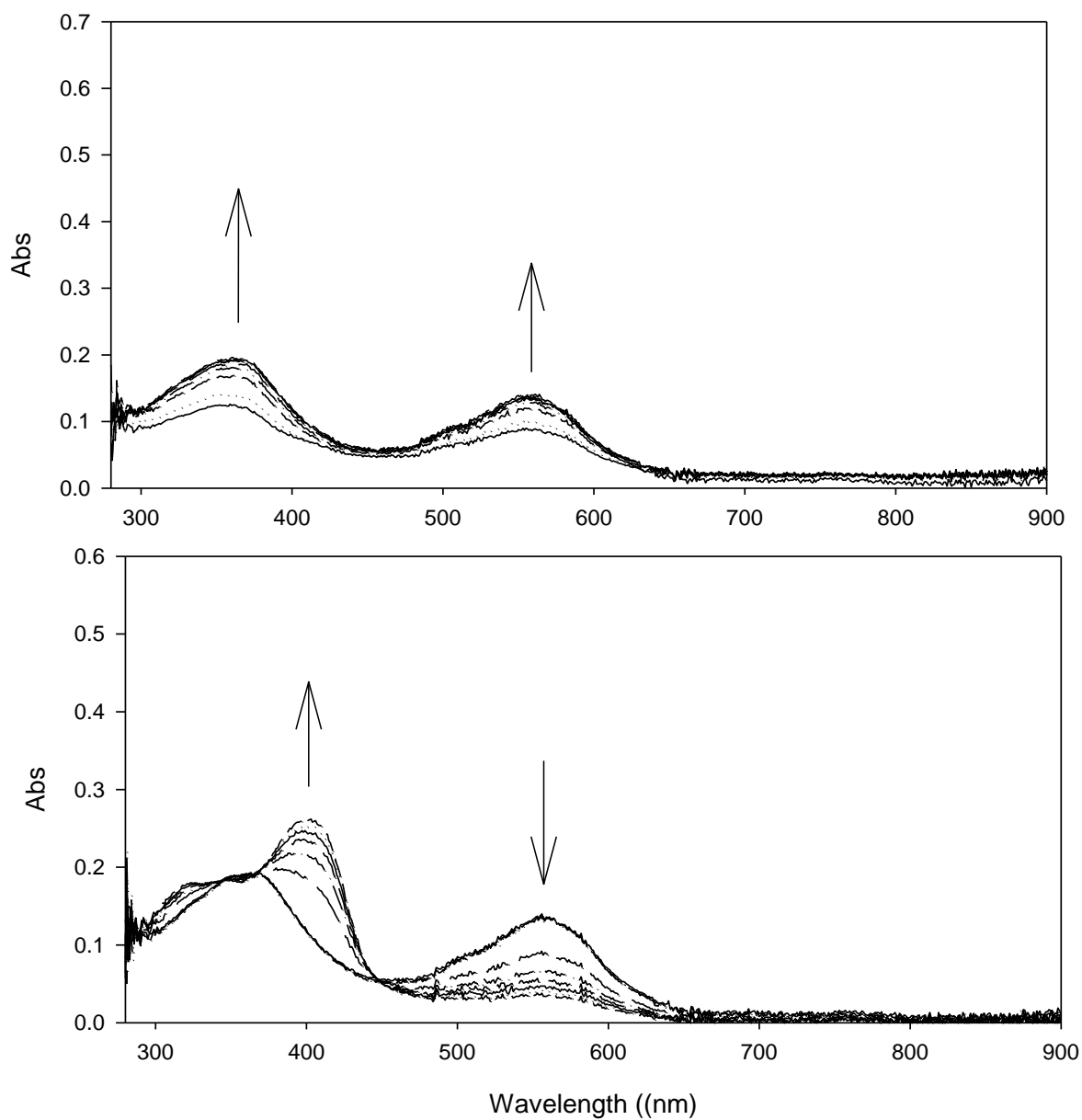


Figure S13. Time resolved UV/vis spectral evolution for the first (top) and the second (bottom) reduction of the oxidized **1** in CH_2Cl_2 containing 0.1 M $n\text{-Bu}_4\text{NPF}_6$.

5. Mass Spectrometry Experiments with **1**, **2**, and C₆₀

Positive-ion electrospray ionization (ESI) mass spectra were recorded with a hybrid quadrupole time-of-flight (QqToF) mass spectrometer (microTOF-Q II, Bruker, Bremen, Germany). The following settings were applied. Flow rate of the sample solution by syringe pump infusion 3.0 mL min⁻¹, nebulizer nitrogen pressure 400 hPa, capillary entrance voltage 3.5 kV, spray shield voltage 3 kV, nitrogen dry gas temperature 453 K, dry gas flow rate 4.0 L/min. Energy-resolved collision-induced dissociations were conducted in a collision cell (rf-only quadrupole q) following a mass selecting quadrupole (Q) and preceding the high resolution fragment ion analysis in the orthogonal reflectron TOF analyzer. Nitrogen (N₂) served as the collision gas at a pressure of 10⁻² mbar.

Compounds **1** and **2** were dissolved separately in CH₂Cl₂ and C₆₀ was dissolved in toluene. Subsequently, each DTF-substituted *N*-heterotriangulene was combined with C₆₀ and diluted with MeOH/toluene mixture (volume ratio 1:1). After thorough mixing, the resulting 10⁻⁵ M solution was introduced to the ESI-MS source by direct injection. All solvents used were of HPLC grade purity.

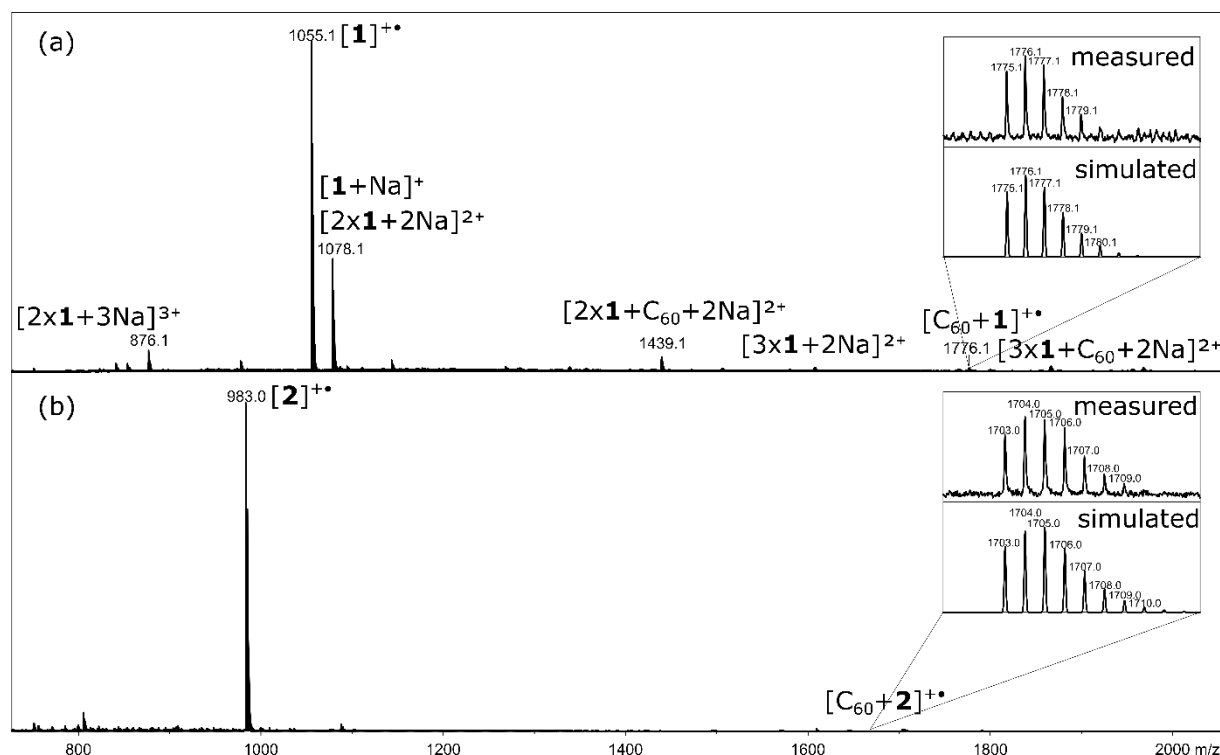


Figure S14. Positive-ion ESI mass spectrum of the noncovalent adducts formed from DTF-substituted compound **1** (a) and **2** (b) with C₆₀.

C_{60} adducts with both *N*-heterotriangulenes **1** and **2** were studied by ESI-MS. While degradation of the *N*-heterotriangulenes **2** hindered the investigation of the physicochemical behavior in solution, freshly prepared degassed solutions of *N*-heterotriangulene **2** were stable enough to obtain reliable ESI mass spectra. Figure S14 shows the positive-ion mass spectra that result from electrospraying the *N*-heterotriangulene/ C_{60} mixtures. Both spectra are dominated by the radical cation signal of the respective *N*-heterotriangulene. Both *N*-heterotriangulene radical cations form a low abundant adduct with C_{60} . In addition, **1** shows efficient Na^+ addition and, connected with this, the formation of *N*-heterotriangulene aggregates held together by up to three sodium cations. Since **2** shows no signs of sodium addition, this must be caused by the interaction of Na^+ with the dicarboxylic acid ester moieties of *N*-heterotriangulene **1**. It is interesting to note that some of the aggregates do contain a C_{60} molecule, such as the aggregate $[2x\mathbf{1}+C_{60}+2Na]^{2+}$. For its structure, it is tempting to assume a supramolecular cage-like structure of two *N*-heterotriangulene molecules on top of each other connected by sodium bridges and hosting the C_{60} inside of it. Charged C_{60} is not observed in MS^1 and does neither occur during fragmentation (CID , MS^2), indicating that the charges of the *N*-heterotriangulene fullerene clusters are always located at the *N*-heterotriangulenes.

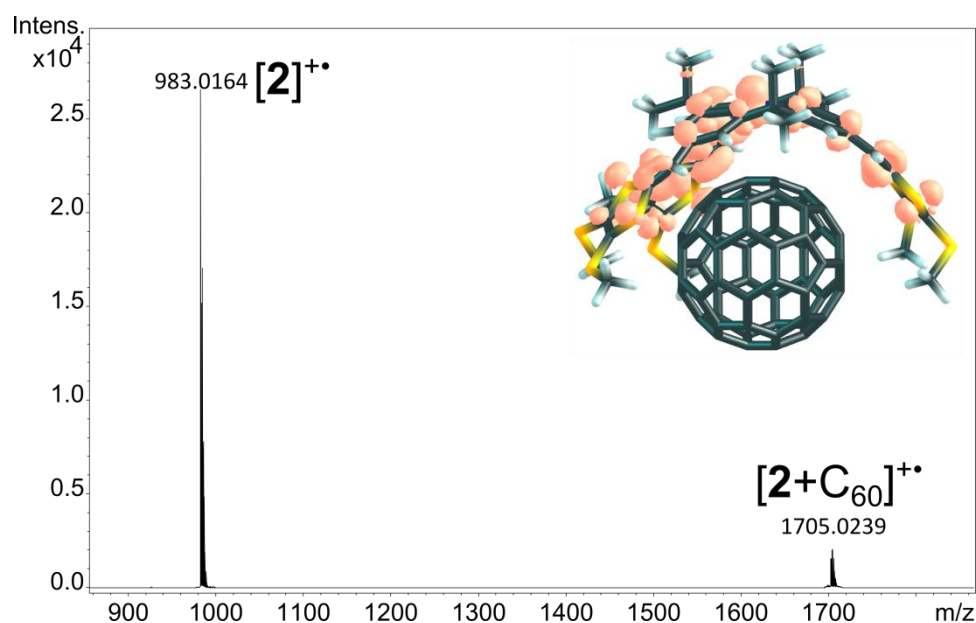


Figure S15. Positive-ion CID (MS^2) mass spectrum of the noncovalent adduct formed by DTF-substituted compound **2** and C_{60} . The $[2+C_{60}]^{+\bullet}$ adduct fragments into the radical cation $[2]^{+\bullet}$ and neutral C_{60} .

To investigate the relative interaction strength of C_{60} with **1** and **2**, the aggregates were isolated and fragmented in collisions with N_2 at different laboratory collision energies (E_{lab}) that ranged from 0 to 35 eV. The laboratory collision energy is converted to the total energy

available for dissociation, called center-of-mass collision energy (E_{com}), by the following relationship

$$E_{\text{com}} = (m_n \cdot E_{\text{lab}}) / (m_i + m_n)$$

where m_n represents the molecular mass of the neutral collision gas N_2 and m_i the molecular mass of the investigated ion.

6. Photophysical Characterization

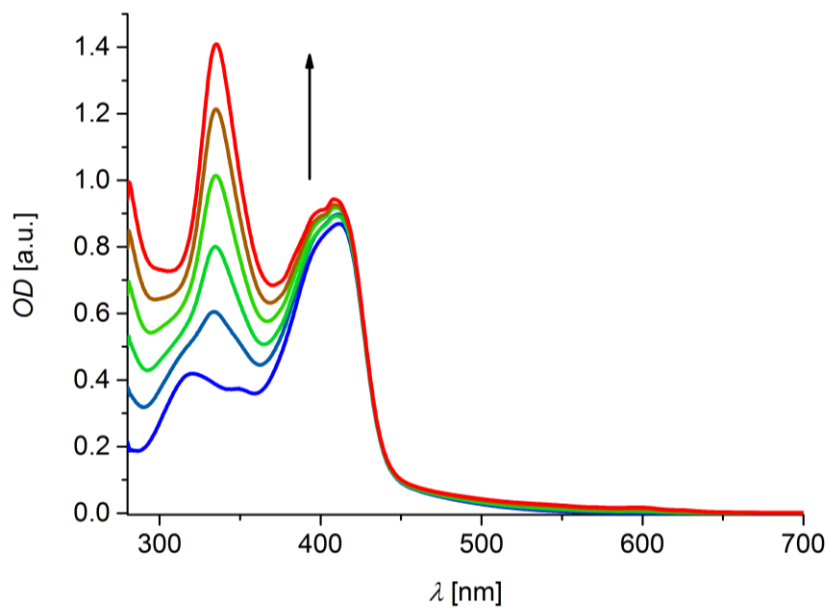


Figure S16. Absorption spectra during a titration of a solution of **1** (blue) with different amounts of C_{60} (blue→green→red) in toluene at room temperature.

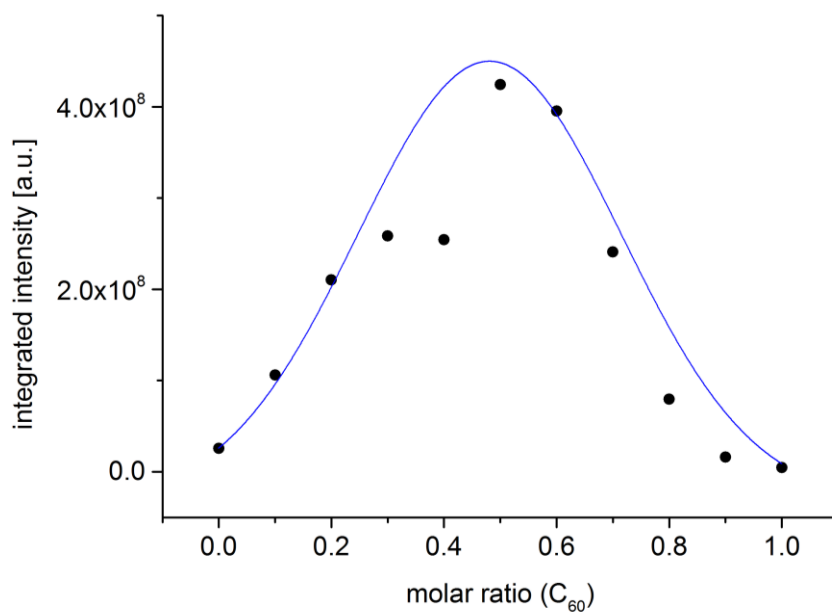


Figure S17. Job plot of **1** and C_{60} in toluene after 12 h illumination at 366 nm.

7. Theoretical Calculations

Computational Details

All density-functional theory (DFT) calculations were performed with the Gaussian 09^[3] program suite. All geometry optimizations and vibrational analyses were carried out at the B3LYP^[4-9] level of theory augmented with D3(BJ)^[10] two-body dispersion corrections. Vibrational normal modes were calculated within the harmonic approximation and imaginary frequencies below 15 cm⁻¹ were ignored. Optimizations and frontier molecular orbital (FMO), spin density and population analyses were performed with the def2-TZVP^[11] basis set. Zero-point energies (ZPEs), thermal corrections and entropies were calculated with the 6-31G(d)^[12] basis set using geometries optimized with the same basis set. All relative energies also include explicit corrections E^{ABC} for the nonadditive Axilrod–Teller–Muto three-body dispersion interaction, which were calculated with the DFTD3 program for geometries optimized with the def2-TZVP basis set.^[13] No symmetry constraints were applied during optimizations except for C₆₀-I_h. All open-shell systems were calculated using unrestricted DFT. Natural population analysis (NPA) was performed as part of the full natural bond orbital (NBO) analysis with NBO version 3.1 as implemented in Gaussian 09.^[14] Structures were visualized with Chemcraft 1.8.^[15]

Cartesian coordinates of all calculated species, archives of Gaussian 09 and outputs of DFTD3 calculations are provided separately in SI_DTF_Calculations.txt.

Structure

The average C–N bond length in **1** is 1.420 Å in the gas-phase calculations at the B3LYP^[4–9]-D3(BJ)/def2-TZVP level and is thus only slightly larger than the value of 1.417 Å obtained from X-ray crystallographic analysis. The C–N–C angles sum to 352.1° in the gas phase and 358.2° in the condensed phase. The tail groups in the condensed phase are apparently affected by intermolecular interactions, leading to the flattened X-ray geometry of **1**. On the other hand, in the gas phase, the tail groups are stabilized by intramolecular noncovalent interactions, which results in a bowl-shaped form of the computed structure (Figure S18).

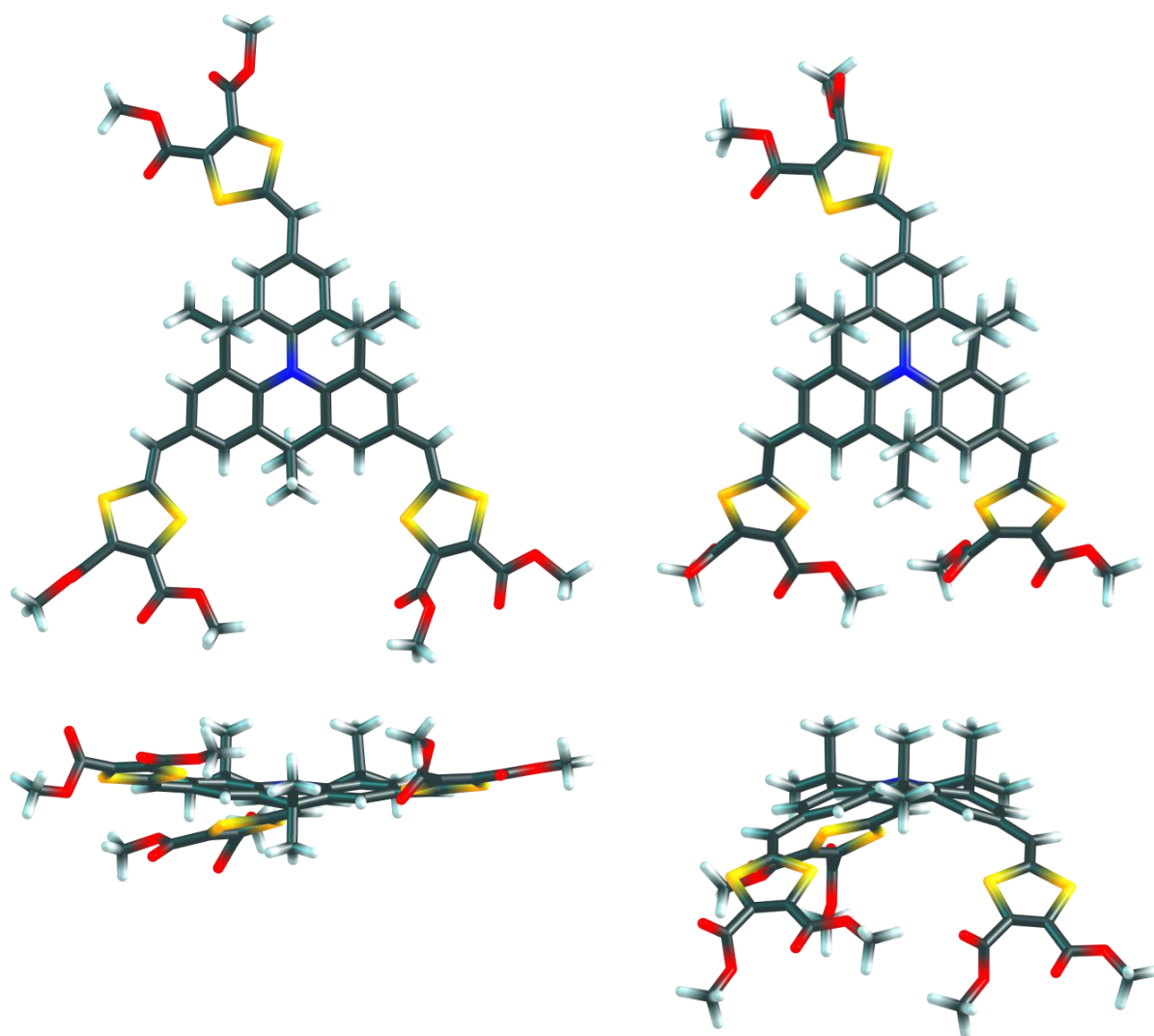


Figure S18. Top and side view on the crystallographic (left) and B3LYP-D3(BJ)/def2-TZVP (gas phase, right) structures of **1**.

Oxidation and Reduction

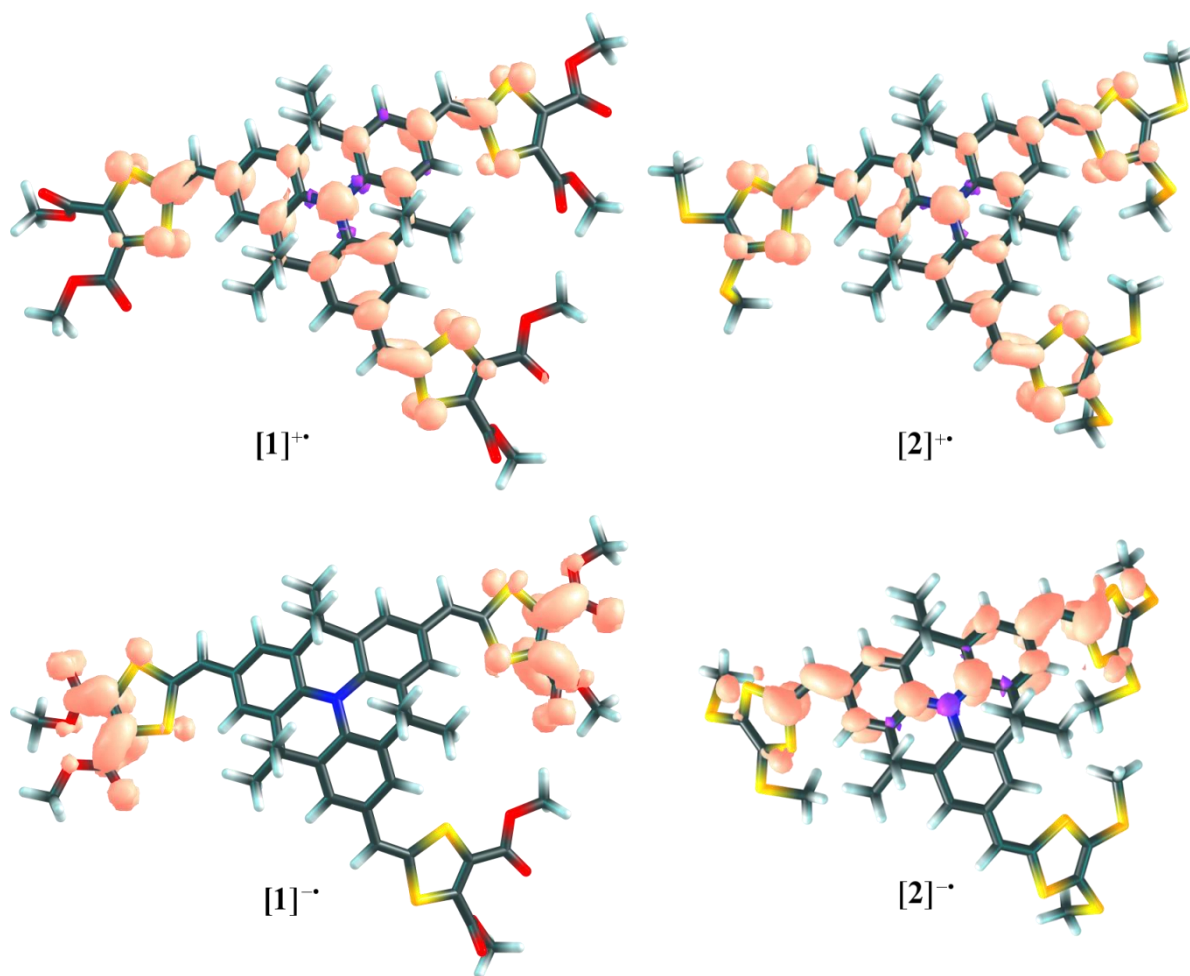


Figure S19. Spin density isosurfaces (contour value $0.0015 \text{ e Bohr}^{-3}$) for the radical cations (top) and radical anions (bottom) of **2** (left) and **1** (right) at B3LYP-D3(BJ) /def2-TZVP.

Complexation to Fullerene C₆₀

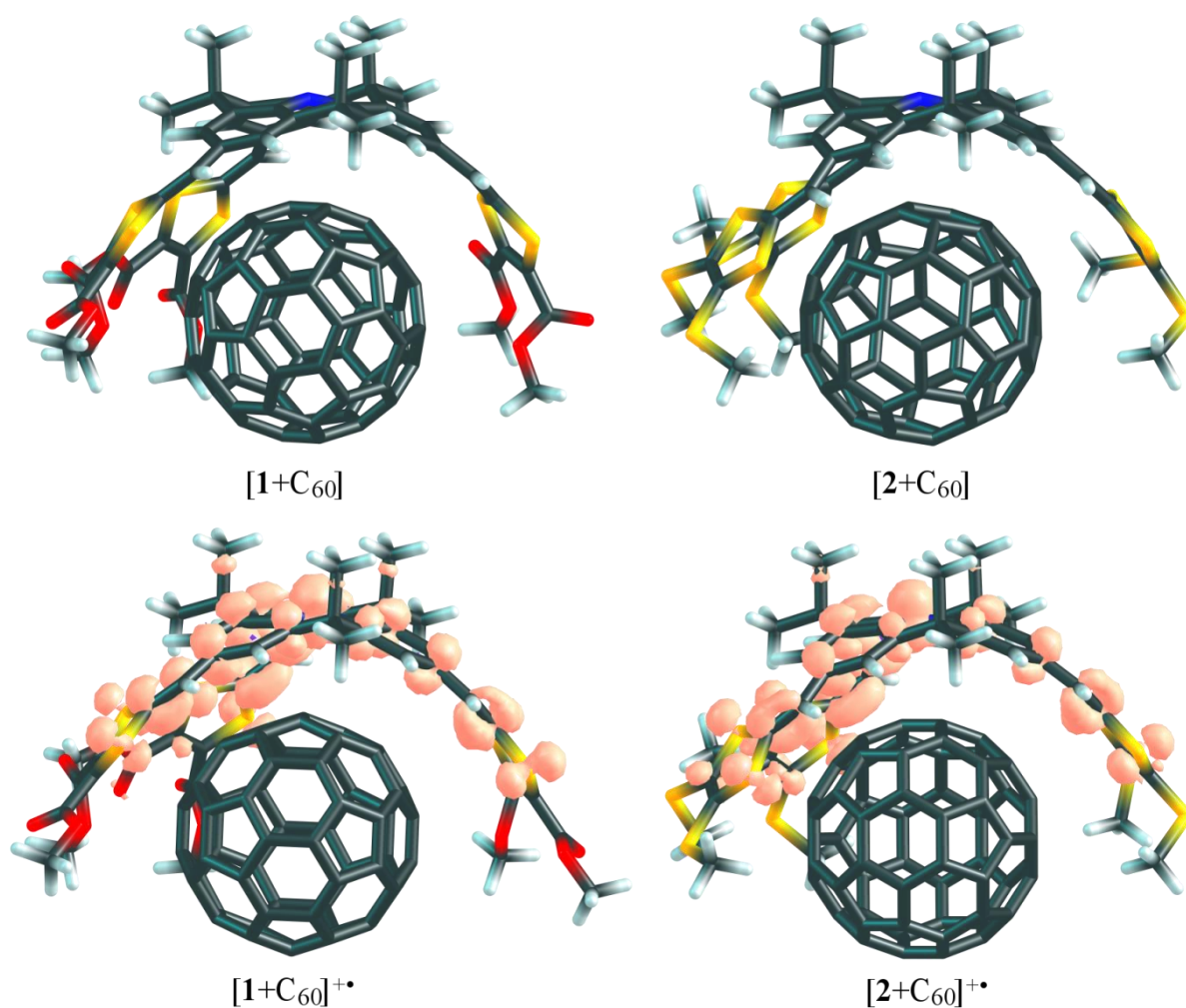


Figure S20. Complexes of **1** (left) and **2** (right) with C₆₀ calculated at B3LYP-D3(BJ)/def2-TZVP are shown at the top. The respective radical cation complexes are depicted at the bottom together with their spin density isosurfaces (contour value 0.0015 e Bohr⁻³).

Table S5. Binding energies (ΔE , $\Delta(E+ZPE)$ and $\Delta(E+ZPE+E^{ABC})$), binding internal energies (ΔU_{298}), entropy contributions ($T\Delta S_{298}$) and Helmholtz free energies (ΔA_{298}) of **1**, **2**, [**1**]⁺⁺ and [**2**]⁺⁺ to C₆₀ in kcal mol⁻¹ at the B3LYP-D3(BJ)/def2-TZVP level of theory with ZPE and thermochemical corrections calculated at B3LYP-D3(BJ)/6-31G(d).

Species	ΔE	$\Delta(E+ZPE)$	$\Delta(E+ZPE+E^{ABC})$	ΔU_{298}	$-T\Delta S_{298}$	ΔA_{298}	$K_a^\#$
[1 +C ₆₀]	-44.7	-43.1	-38.8	-37.5	16.9	-20.6	1.26×10^{15}
[2 +C ₆₀]	-45.4	-43.3	-38.8	-36.2	12.4	-23.8	2.79×10^{17}
[1 +C ₆₀] ⁺⁺	-41.7	-39.6	-35.2	-33.3	15.3	-17.9	1.32×10^{13}
[2 +C ₆₀] ⁺⁺	-40.1	-37.8	-33.1	-30.8	14.9	-16.0	5.35×10^{11}

The binding constant in the gas phase was calculated according to $K_a = e^{\frac{-\Delta A}{RT}}$ ($R = 1.987 \times 10^{-3}$ kcal mol⁻¹ K⁻¹; $T = 298.15$ K). However, we would like to emphasize that a small error in calculated ΔA leads to an exponential error in the binding energies. Comparing these values to the binding energies in solution is rather difficult as the solvent has a tremendous effect on ΔA .

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This file contains XYZ coordinates and Gaussian 09 archives of calculations at the B3LYP-D3(BJ)/def2-TZVP, B3LYP-D3(BJ)/6-31G(d), and B3LYP-D3(BJ)/6-311+G(d,p) levels of theory and DFTD3 outputs for calculations for geometries calculated at B3LYP-D3(BJ)/def2-TZVP

for

"Dithiafulvenyl-Extended N-Heterotriangulenes and Their Interaction with C60: Cooperative Fluorescence"

by

B. D. Gliemann, V. Strauss, J. F. Hitzengerger, P. O. Dral, F. Hampel, J.-P. Gisselbrecht, T. Drewello, W. Thiel, D. M. Guldi, and M. Kivala

NAMING CONVENTIONS

Each section name starts with the species number as given in the paper. Complexes of 1 and 2 with C60 are named as 1_C60 and 2_C60, respectively.

Where appropriate, species number is followed by:

'_ox1' for one-electron oxidized species
'_red1' for one-electron reduced species

Example: '1_red1' designates the radical anion of 1.

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Calculations at B3LYP-D3(BJ)/def2-TZVP

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!!!!!!

=====
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1

115

C	2.415805	-2.609908	-1.883890
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Zero-point correction= 0.867347
 (Hartree/Particle)
 Thermal correction to Energy= 0.934568
 Thermal correction to Enthalpy= 0.935512
 Thermal correction to Gibbs Free Energy= 0.758552
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 Sum of electronic and thermal Energies= -5317.775195
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	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	586.450	251.730	372.443
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	46.742
Rotational	0.889	2.981	42.583
Vibrational	584.673	245.769	283.118

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System has the following imaginary frequencies:

- 1 -9.9717 cm⁻¹
- 2 -5.5559 cm⁻¹
- 3 -3.9132 cm⁻¹

=====

1_C60

175

C	0.206495	-4.491806	-3.183387
C	1.508269	-4.079662	-2.928457

C	-2.211927	1.275240	-0.168691
C	-0.912042	1.687331	0.086140
C	-0.029260	-0.342782	-4.911406
C	-0.512980	0.811599	-4.307791
C	-0.192064	-3.616196	1.212831
C	-0.676504	-2.461225	1.813385
C	-3.589570	-2.106220	-2.799506
C	-3.622835	-2.761033	-1.574545
C	2.912752	-0.046023	-1.524707
C	2.884840	-0.697814	-0.298746
C	-0.601758	-3.781813	-4.156964
C	-0.657195	-4.888380	-2.086810
C	2.059300	-2.938694	-3.636052
C	2.005222	-4.045402	-1.565142
C	-2.706759	1.240149	-1.532174
C	-2.761426	0.133151	0.538538
C	-0.047374	2.084420	-1.010783
C	-0.102678	0.977519	1.061370
C	-0.886814	-1.505223	-5.046599
C	1.313118	-0.808301	-4.616115
C	-1.876690	0.855039	-3.813364
C	0.324482	1.554460	-3.383181
C	-1.029152	-4.355774	0.287375
C	1.170198	-3.656656	0.716725
C	-2.020613	-1.996181	1.520848
C	0.179883	-1.298118	1.944283
C	-2.743386	-2.606315	-3.866058
C	-3.560472	-0.656135	-2.847810
C	-2.809847	-3.944125	-1.361047
C	-3.627667	-1.995007	-0.341739
C	2.920894	-0.810960	-2.755484
C	2.104125	1.139922	-1.736840
C	2.856863	-2.148696	-0.250671
C	2.039982	-0.196333	0.770704
C	-0.074542	-2.689309	-4.833370
C	-0.182771	-4.855226	-0.781669
C	1.284951	-2.258552	-4.567687
C	1.177843	-4.423698	-0.514479
C	-1.883419	1.624746	-2.582487
C	-1.991700	-0.544331	1.473339
C	-0.522204	2.056797	-2.315725
C	-0.630182	-0.113987	1.736627
C	-2.191980	-1.464075	-4.573924
C	2.114043	-0.099447	-3.730287
C	-2.698613	-0.258603	-3.944648
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C	1.260842	0.934600	0.565226
C	3.028236	4.025197	1.040834
H	3.991522	3.675458	1.371346

C	0.924144	2.712879	3.715801
C	2.154547	3.524911	3.366318
C	1.719552	-3.833997	4.749258
C	-4.005434	2.572439	4.197050
H	-4.920544	3.154311	4.091889
H	-3.916208	2.314437	5.251803
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C	-0.332416	3.201916	3.325150
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H	-6.199045	-3.776809	0.752682
H	-7.627309	-4.175626	-0.249143
H	-7.832704	-3.479844	1.386519
C	-7.227283	-2.357497	-3.850560
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H	-6.323182	-2.833221	-4.217975
C	-0.151066	0.829845	4.817975
C	-1.381140	1.467374	4.611215
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H	-3.041049	5.119485	-1.317708
C	-1.829266	4.937421	0.428193
C	-0.702463	5.833749	-0.038237
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H	1.564388	5.578984	-1.550016
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H	-5.116440	4.076600	-1.691797
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C	-6.710513	0.087001	-0.121392
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C	-1.711221	4.320562	1.687375
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H	-3.656429	5.260224	4.473065
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C	-0.819672	6.210115	-1.515047
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H	-0.019043	6.891173	-1.800191
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175

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C	-1.626576	-0.124139	1.491544
C	-1.456137	1.577537	-3.018832
C	-0.395255	0.631589	1.351642
C	-2.501515	-2.692064	-3.990803
C	1.395476	-0.292986	-4.420448
C	-3.194790	-1.490165	-3.565151
C	0.702383	0.909697	-3.995217
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C	2.591906	-1.357117	0.515645
C	-1.998753	-2.554731	1.373403
C	1.896803	-0.154601	0.939870
C	-1.570857	-4.530194	-2.646902
C	-3.763727	-0.726371	-1.299405
C	-1.236542	-4.827865	-1.266912
C	-3.424932	-1.025335	0.079563
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C	0.633990	1.986591	-1.785546
C	3.162240	-2.121826	-1.752359
C	0.965932	1.681530	-0.405810
C	2.797610	4.155486	1.143262
H	3.805012	3.848614	1.365001
C	1.010982	2.510019	3.873635
C	2.147987	3.428467	3.479968
C	2.514326	-3.940331	4.340762
C	-3.865666	1.765994	4.488636

H	-4.847659	2.234534	4.448620
H	-3.725448	1.434354	5.516002
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C	-0.314787	2.887493	3.572500
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C	-6.572006	-3.932240	0.210458
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H	-6.257556	-4.539412	-0.631704
H	-7.586202	-4.184303	0.514166
C	-9.192953	-0.814316	-4.185410
H	-10.208805	-0.845868	-3.795731
H	-8.838824	-1.828926	-4.358123
H	-9.144550	-0.227120	-5.096688
C	0.181539	0.487513	4.941066
C	-1.119227	1.012391	4.840111
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C	-1.383254	2.190275	4.181339
C	-2.779433	2.767944	4.097023
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C	-4.116957	3.135719	1.978580
H	-4.918058	2.577378	2.429901
C	-4.293940	3.698760	0.704173
C	-3.321078	4.621482	0.280324
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C	-2.137007	4.796389	0.959073
C	-1.105734	5.820784	0.545941
C	0.241948	5.146928	0.677761
C	1.239795	5.314083	-0.255045
H	1.034532	5.859341	-1.163134
C	-5.335434	3.336254	-0.210092
H	-5.444700	3.976276	-1.078480
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C	1.823455	3.970939	2.104202
C	-6.845459	-0.271311	0.016735
C	-7.381744	0.142324	-1.146229
C	1.235293	1.324530	4.542013
H	2.249838	1.036137	4.751046
C	-8.250686	-0.684841	-2.027338
C	-1.881958	4.009810	2.104858
C	0.497164	4.351071	1.815652
C	-2.859345	3.974994	5.070448
H	-3.840297	4.445954	4.998816
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C	-1.158166	6.994473	1.561229
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H	-0.393411	7.731985	1.315519
H	-0.985630	6.649638	2.580115
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C	4.564417	-3.222334	3.129262
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H	7.165243	-2.615930	2.690543
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H	3.114828	5.403808	-2.040605
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O	6.799616	0.165064	-0.241652
O	6.164027	-0.487172	-2.303842
O	7.784451	1.158260	-3.924736
O	6.478384	2.499165	-5.181782
S	-6.021781	0.921850	0.979888
S	-7.116258	1.813122	-1.578864
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S	2.873736	-1.320050	4.289597
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C	-1.741997	-0.345797	2.809184
C	-3.799880	6.123204	-0.284677
C	3.925257	2.139070	1.632271
H	4.961754	1.906187	1.868061
H	3.716047	3.094567	2.109338
H	3.833147	2.259196	0.552652

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C	-2.083538	-3.741528	1.086737
C	11.156174	3.097879	-1.774869
H	10.599475	3.693083	-2.496453
H	12.173128	2.929053	-2.113897
H	11.149085	3.597332	-0.808010
C	11.943576	-0.657450	-4.129852
H	12.302661	-1.684784	-4.126755
H	12.679745	-0.014017	-3.651281
H	11.732559	-0.322411	-5.140054
C	-0.282150	2.996867	1.663221
C	1.085543	2.669138	1.716111
H	1.804334	3.453944	1.537459
C	1.525489	1.384529	1.955870
C	2.986993	1.056685	2.171005
C	3.255495	-0.310886	1.576622
C	4.483572	-0.611937	1.025402
H	5.208978	0.177422	0.956169
C	4.817121	-1.904062	0.591935
C	3.866045	-2.912911	0.828135
H	4.130084	-3.925358	0.565252
C	2.628852	-2.658012	1.376321
C	1.690118	-3.783906	1.760358
C	0.269230	-3.304766	1.555434
C	-0.740311	-4.149118	1.137184
H	-0.498565	-5.149620	0.813008
C	6.054286	-2.270420	-0.033625
H	6.174235	-3.332598	-0.217604
C	7.090087	-1.488252	-0.446636
C	-1.408155	-1.626822	2.080588
C	8.782661	0.368095	-1.126090
C	9.359607	-0.783497	-1.512289
C	-1.185310	1.993383	2.046850
H	-2.220369	2.242365	2.198414
C	10.711565	-0.943678	-2.152428
C	2.277493	-1.323241	1.682960
C	-0.054180	-1.977734	1.908468
C	3.211566	0.946008	3.705792
H	4.248960	0.679026	3.909896
H	2.568403	0.185414	4.147995
H	2.991122	1.901291	4.183294
C	9.309213	1.744921	-1.225543
C	1.873191	-4.039246	3.283153
H	2.895677	-4.360124	3.485109
H	1.185387	-4.817548	3.615496
H	1.676430	-3.137992	3.863298
C	1.988746	-5.090691	1.023157
H	2.995811	-5.436754	1.247070
H	1.888466	-4.981442	-0.057050
H	1.316522	-5.878192	1.358426
C	-1.447240	-0.559137	4.319109
H	-2.093004	-1.343100	4.716029
H	-1.636055	0.364109	4.867885
H	-0.411189	-0.851374	4.487151
C	-3.209543	0.060598	2.665281
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H	-3.860591	-0.707003	3.080060
C	-0.685307	4.305987	1.242463
H	0.094968	5.058231	1.207088

C	-1.916400	4.695551	0.802446
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H	-7.496713	2.996507	-1.746324
C	-4.506205	7.334935	-0.828477
C	-5.460328	8.296883	-2.743054
H	-5.479760	8.068545	-3.803618
H	-4.985893	9.258758	-2.559014
H	-6.465743	8.294384	-2.326332
C	-3.075181	-4.599919	0.496213
H	-2.803351	-5.643731	0.383789
C	-4.284463	-4.235094	-0.006134
C	-6.310904	-2.994145	-1.071817
C	-6.556575	-4.299580	-1.291481
C	-7.105145	-1.809496	-1.505480
C	-8.444159	-0.891160	-3.203614
H	-7.908355	0.056346	-3.225130
H	-9.310887	-0.811565	-2.550112
H	-8.742855	-1.188549	-4.203340
C	-7.797936	-4.858862	-1.900247
C	-8.703499	-6.768761	-2.946208
H	-9.102690	-6.208282	-3.789460
H	-9.475132	-6.881317	-2.186774
H	-8.329528	-7.735639	-3.266794
N	0.956265	-1.000331	2.053058
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O	11.652505	-1.404220	-1.567331
O	10.570313	1.785793	-1.658443
O	8.648761	2.708469	-0.917939
O	-6.549771	5.328866	-0.894688
O	-5.909158	3.215487	-0.418237
O	-4.802277	8.267210	-0.132654
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O	-7.226124	-0.828456	-0.810253
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O	-8.865520	-4.308281	-1.900526
O	-7.562367	-6.081308	-2.393555
S	7.211437	0.252552	-0.355229
S	8.496834	-2.245216	-1.179964
S	-2.196311	6.358594	0.318925
S	-3.320798	3.671922	0.589829
S	-4.896135	-2.593202	-0.133943
S	-5.384470	-5.433010	-0.666725

Zero-point correction=	0.867855
(Hartree/Particle)	
Thermal correction to Energy=	0.935146
Thermal correction to Enthalpy=	0.936091
Thermal correction to Gibbs Free Energy=	0.757601
Sum of electronic and zero-point Energies=	-5317.636663
Sum of electronic and thermal Energies=	-5317.569371
Sum of electronic and thermal Enthalpies=	-5317.568427
Sum of electronic and thermal Free Energies=	-5317.746917

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	586.813	251.603	375.664

Electronic	0.000	0.000	1.377
Translational	0.889	2.981	46.742
Rotational	0.889	2.981	42.683
Vibrational	585.036	245.641	284.862

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System has the following imaginary frequencies:

- 1 -9.3426 cm⁻¹
- 2 -7.8833 cm⁻¹
- 3 -5.5660 cm⁻¹

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1_red1

115

C	-2.487453	-2.385345	1.603232
H	-3.501951	-2.068347	1.771553
C	-0.737354	0.709910	2.359215
C	-1.727348	-0.319736	2.859006
C	-3.498677	6.213054	-0.294294
C	4.001487	1.993710	1.669928
H	5.033347	1.705014	1.861789
H	3.838220	2.930986	2.200656
H	3.889790	2.174094	0.600535
C	0.596115	0.317417	2.153073
C	-2.248625	-3.609669	0.972522
C	11.544134	2.601471	-0.659528
H	11.251786	3.317377	-1.428872
H	12.606444	2.379863	-0.732399
H	11.309786	3.025057	0.317558
C	12.087052	-0.241989	-3.970557
H	11.915402	-0.957344	-4.775392
H	12.927707	-0.589291	-3.368318
H	12.294657	0.744968	-4.377414
C	-0.163421	3.006639	1.795973
C	1.183089	2.624502	1.791664
H	1.930374	3.381767	1.606190
C	1.579671	1.313132	1.997596
C	3.032736	0.921297	2.172476
C	3.231273	-0.421675	1.494578
C	4.428902	-0.732536	0.868708
H	5.174832	0.037563	0.797149
C	4.698879	-2.005371	0.356277
C	3.715518	-2.980640	0.568789
H	3.924546	-3.985987	0.235282
C	2.509427	-2.712032	1.192260
C	1.540342	-3.821623	1.555925
C	0.132946	-3.277195	1.411385
C	-0.920477	-4.055765	0.958810
H	-0.721328	-5.042251	0.567056
C	5.915787	-2.392477	-0.326950
H	5.952663	-3.438734	-0.613844
C	7.005619	-1.665078	-0.663007
C	-1.459257	-1.579363	2.062094
C	8.875011	0.139069	-1.074723
C	9.340613	-1.001978	-1.681050
C	-1.093248	2.032909	2.166344
H	-2.115840	2.317102	2.345647
C	10.493379	-1.211831	-2.544991
C	2.225190	-1.395653	1.599388
C	-0.126998	-1.971128	1.860498
C	3.285623	0.724633	3.691180
H	4.316021	0.405984	3.858011
H	2.620606	-0.034051	4.103507
H	3.111561	1.660947	4.225120
C	9.525304	1.412302	-0.815565
C	1.758888	-4.163360	3.054211
H	2.775514	-4.529328	3.210203

H	1.050250	-4.931036	3.371037
H	1.612342	-3.283333	3.679973
C	1.766236	-5.100020	0.746727
H	2.767938	-5.490999	0.918594
H	1.637595	-4.930441	-0.322783
H	1.070307	-5.876379	1.061560
C	-1.418893	-0.611058	4.350129
H	-2.087791	-1.388447	4.723803
H	-1.559906	0.293492	4.945115
H	-0.391808	-0.950873	4.480862
C	-3.179256	0.151221	2.758584
H	-3.468834	0.372504	1.731394
H	-3.333830	1.044752	3.362774
H	-3.854569	-0.609500	3.147512
C	-0.534300	4.359912	1.427338
H	0.255871	5.102727	1.470302
C	-1.731563	4.778494	0.971494
C	-4.031602	4.980248	-0.242085
C	-5.348092	4.621330	-0.812418
C	-6.822877	2.803400	-1.185510
H	-7.633134	3.281013	-0.635746
H	-6.807679	1.732722	-1.006555
H	-6.933817	3.022698	-2.247079
C	-4.106019	7.398412	-0.972748
C	-4.824700	8.258111	-3.031302
H	-4.724955	7.981606	-4.076779
H	-4.381897	9.235586	-2.844734
H	-5.872761	8.268415	-2.734909
C	-3.286167	-4.428385	0.378422
H	-3.014004	-5.461626	0.187401
C	-4.522457	-4.056823	-0.026260
C	-6.624585	-2.778000	-0.935976
C	-6.876974	-4.102737	-1.219517
C	-7.322755	-1.580122	-1.354800
C	-8.871973	-0.629479	-2.843403
H	-8.250970	0.221867	-3.127126
H	-9.528186	-0.330828	-2.025269
H	-9.460044	-0.967636	-3.693012
C	-8.117356	-4.677743	-1.711514
C	-9.087393	-6.677622	-2.513562
H	-9.566889	-6.194684	-3.365879
H	-9.804180	-6.723323	-1.692311
H	-8.755411	-7.677869	-2.782901
N	0.936546	-1.054790	2.096989
O	10.918984	-0.087874	-3.167466
O	10.990030	-2.306034	-2.751885
O	10.878436	1.354787	-0.848331
O	8.919372	2.429741	-0.522215
O	-6.137755	5.411135	-1.275670
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O	-4.128014	7.239463	-2.297949
O	-7.202423	-0.497577	-0.793587
O	-8.068991	-1.743523	-2.466505
O	-9.216670	-4.164604	-1.733962
O	-7.913149	-5.971517	-2.125431
S	7.256403	0.051338	-0.381653
S	8.362884	-2.445593	-1.476345
S	-2.016430	6.480527	0.572752
S	-3.150240	3.763462	0.672858

S -5.206143 -2.438866 0.054074
S -5.619915 -5.239037 -0.736612

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2

103

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C	-2.955824	1.161783	-4.096795
H	-4.000591	0.940312	-4.321346
H	-2.339264	0.368315	-4.518395
H	-2.680934	2.101616	-4.578637
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H	-10.690535	-1.774190	4.640055
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H	-8.937513	-1.879725	4.365897
C	-6.447786	2.651071	3.421738
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H	-6.458020	3.634239	3.890512
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Zero-point correction=	0.783453
(Hartree/Particle)	
Thermal correction to Energy=	0.842682
Thermal correction to Enthalpy=	0.843626
Thermal correction to Gibbs Free Energy=	0.684473
Sum of electronic and zero-point Energies=	-6575.406654
Sum of electronic and thermal Energies=	-6575.347425
Sum of electronic and thermal Enthalpies=	-6575.346481
Sum of electronic and thermal Free Energies=	-6575.505633

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	528.791	225.425	334.965
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	46.531
Rotational	0.889	2.981	41.969
Vibrational	527.013	219.463	246.465

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System has the following imaginary frequencies:

1 -10.3117 cm⁻¹

2 -9.8107 cm⁻¹
3 -8.1660 cm⁻¹
4 -7.2536 cm⁻¹

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2_C60

163

C	-1.570124	-3.990097	2.447455
C	-0.284833	-4.500374	2.317827
C	-0.459884	0.184819	-2.991624
C	0.826305	-0.325551	-3.120602
C	-1.677065	-5.038023	-1.926804
C	-1.454866	-4.202490	-3.013763
C	0.709379	-0.112458	2.343421
C	0.932404	0.722919	1.257680
C	-3.831482	-1.373282	-0.440199
C	-3.347575	-0.390136	0.413489
C	2.602352	-3.927027	-1.086655
C	3.076985	-2.940143	-0.231705
C	-2.573338	-4.286286	1.441269
C	-1.766013	-2.620913	2.886736
C	0.054817	-5.330170	1.176749
C	0.861573	-3.664348	2.621287
C	-1.607975	-0.651753	-3.294501
C	-0.799102	1.008433	-1.846085
C	1.022097	-1.695267	-3.560316
C	1.826812	-0.031623	-2.112696
C	-2.725210	-4.724603	-0.973650
C	-0.552510	-5.587450	-1.192649
C	-2.271892	-3.017298	-3.198390
C	-0.098348	-3.880755	-3.416282
C	-0.645827	-0.433239	2.747152
C	1.527155	-1.296643	2.527408
C	-0.192351	1.265364	0.520227
C	1.982085	0.409816	0.303458
C	-3.848388	-2.758918	-0.008297
C	-3.477216	-1.347432	-1.848663
C	-2.867942	-0.745872	1.737480
C	-2.491383	0.662074	-0.100316
C	1.749373	-4.982088	-0.571649
C	2.126704	-3.572338	-2.411854
C	2.726952	-2.966002	1.177150
C	3.098392	-1.554721	-0.663013
C	-2.248649	-5.081230	0.349516
C	-0.668690	-1.819601	3.177394
C	-0.905605	-5.613859	0.214360
C	0.673954	-2.352983	3.039224
C	-1.420028	-1.962776	-3.715024
C	0.160231	1.290132	-0.885044
C	-0.076293	-2.495578	-3.849390
C	1.504387	0.763038	-1.021526
C	-3.507697	-3.589720	-1.149456
C	0.745937	-5.278564	-1.577024
C	-3.277026	-2.716801	-2.286362
C	0.978324	-4.407306	-2.714021
C	-1.722736	0.092189	2.043416
C	2.533003	-1.596078	1.616752

C	-1.489426	0.958719	0.903445
C	2.766567	-0.722888	0.479866
C	-3.390135	-3.100943	1.258557
C	-2.657455	-0.338655	-2.339864
C	-2.888668	-2.071690	2.150328
C	-2.152819	0.685125	-1.445033
C	1.411491	-5.006912	0.775551
C	2.147082	-2.245460	-2.824061
C	1.910869	-3.977929	1.669413
C	2.643691	-1.215256	-1.930175
C	2.705894	3.739645	-1.727780
H	3.724784	3.630239	-1.397463
C	1.139664	4.361090	1.432104
C	2.180741	4.906000	0.475875
C	3.588384	-0.387207	5.307227
C	-3.624178	3.925111	2.713958
H	-4.636247	4.257008	2.486081
H	-3.399622	4.266024	3.723966
H	-3.608549	2.834865	2.703023
C	-0.210607	4.410306	1.057995
C	2.328711	3.263858	-2.989066
C	0.526395	3.245528	3.507321
C	-0.814279	3.529995	3.212084
H	-1.571800	3.213778	3.913566
C	-1.193701	4.135464	2.026393
C	-2.627294	4.521647	1.720324
C	-2.890352	4.089321	0.290573
C	-4.081326	3.483578	-0.082365
H	-4.810386	3.280473	0.681436
C	-4.329164	3.090319	-1.400418
C	-3.415616	3.525412	-2.367345
H	-3.625150	3.302371	-3.402633
C	-2.227125	4.148441	-2.036497
C	-1.254522	4.646710	-3.085960
C	0.117439	4.217355	-2.611897
C	1.049508	3.619426	-3.438995
H	0.771723	3.357170	-4.448876
C	-5.353342	2.158058	-1.816104
H	-5.398333	1.989148	-2.887091
C	-6.141110	1.353289	-1.073668
C	1.793389	4.342146	-0.875372
C	-7.183560	-0.190295	0.782848
C	-7.528251	-0.769618	-0.386149
C	1.483416	3.791194	2.645795
H	2.521737	3.775411	2.924138
C	-1.900189	4.320096	-0.678603
C	0.447177	4.431740	-1.263193
C	-2.739707	6.065405	1.793486
H	-3.753107	6.378453	1.536715
H	-2.047847	6.543255	1.100681
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C	-1.305033	6.195212	-3.108224
H	-2.299541	6.531921	-3.405569
H	-0.573000	6.582933	-3.818684
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C	-1.579934	4.143108	-4.491044
H	-2.562450	4.495647	-4.802882
H	-1.568240	3.054154	-4.549129
H	-0.858329	4.534809	-5.207367
C	2.070158	6.448987	0.427313

H	2.773734	6.852586	-0.302803
H	2.299030	6.870418	1.407634
H	1.066428	6.764891	0.145773
C	3.609537	4.542220	0.879222
H	3.755932	3.463581	0.937126
H	3.853975	4.976049	1.848390
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C	0.845602	2.345367	4.594823
H	0.046918	2.146312	5.301181
C	1.965255	1.599233	4.733157
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C	4.160456	1.587454	-3.463339
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C	5.881393	-0.406934	-3.503729
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S	3.361876	1.670730	3.654997
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S	4.718948	0.335607	-4.579852
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S	6.813204	-1.781079	-4.065367
S	4.247013	-1.804443	6.094182
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S	-7.676834	-0.750219	2.363188
S	-8.441251	-2.255775	-0.541487
C	6.487365	-1.711926	-0.299343
H	6.218531	-2.466728	-1.034060
H	7.239374	-2.116037	0.377854
H	5.616034	-1.404509	0.269975
C	5.551208	-2.725199	-4.977355
H	5.230670	-2.207222	-5.878641
H	6.040479	-3.656561	-5.258704
H	4.696484	-2.941882	-4.340325
C	5.803132	0.857140	2.107299
H	5.970797	1.838844	2.544891
H	6.700744	0.554043	1.573892
H	4.973847	0.887846	1.402762
C	3.245277	-3.127401	5.339697
H	3.434163	-3.184737	4.270885
H	3.560083	-4.055126	5.816193
H	2.187516	-2.963133	5.528368
C	-7.390259	-3.192912	-1.698487
H	-7.880134	-4.158372	-1.817665
H	-7.320546	-2.703612	-2.666820
H	-6.398912	-3.339355	-1.276593
C	-6.077439	-1.028296	3.183942
H	-5.452037	-0.139821	3.143528
H	-6.311053	-1.257485	4.222783
H	-5.560694	-1.869955	2.731980

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 heck Guess=Read\BG32...C60\0,1\C,-1.5786339175,-4.0239684593,2.40988
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2_C60_ox1

163

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C	1.074583	-1.317607	2.528281
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C	-3.800883	-3.075059	-0.008762
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C	1.225742	4.213122	1.719930
C	2.340345	4.758180	0.854449
C	3.019000	-0.853796	5.521653
C	-3.627373	4.110562	2.753692
H	-4.596237	4.526055	2.480765
H	-3.432622	4.421975	3.778910
H	-3.696998	3.022770	2.726139
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C	2.647845	3.423100	-2.721509
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C	-0.883000	3.503543	3.381357

H	-1.692783	3.241499	4.045093
C	-1.157069	4.137274	2.190421
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H	-1.766398	6.623386	1.272192
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C	-1.202092	4.349859	-4.341665
H	-2.160631	4.734898	-4.685978
H	-1.211305	3.262986	-4.429415
H	-0.445835	4.747192	-5.016923
C	2.300724	6.307436	0.911389
H	3.065738	6.723418	0.254845
H	2.488551	6.647277	1.930555
H	1.332393	6.693448	0.595255
C	3.725020	4.297717	1.310094
H	3.819032	3.211615	1.292839
H	3.929088	4.649042	2.320580
H	4.496752	4.723174	0.670372
C	0.597183	2.146849	4.778426
H	-0.270038	1.957199	5.400983
C	1.654675	1.305575	4.961245
C	3.732165	-0.231805	4.553430
C	3.465797	2.579752	-3.540996
H	3.146487	2.481817	-4.573121
C	4.467373	1.742249	-3.153111
C	6.192080	0.185330	-1.940868
C	6.157916	-0.264459	-3.217096
N	-0.375677	4.608694	-0.084777
S	-5.919524	1.437627	0.601821
S	-6.985641	0.470481	-1.921801
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S	3.143165	1.330599	4.037383
S	5.172357	1.568013	-1.567110
S	5.104891	0.587319	-4.315269

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S	7.132695	-1.607745	-3.761901
S	3.503688	-2.346165	6.290676
S	5.175044	-0.901311	3.827105
S	-7.229105	-0.541884	2.325018
S	-8.558371	-1.765789	-0.703475
C	6.343368	-1.928996	-0.137888
H	6.093866	-2.563906	-0.983964
H	7.026703	-2.462017	0.522265
H	5.448400	-1.653802	0.411365
C	6.540032	-1.869724	-5.457045
H	6.748339	-1.009559	-6.090322
H	7.110321	-2.721947	-5.822505
H	5.480274	-2.116087	-5.473589
C	5.612123	0.364289	2.602220
H	5.815824	1.322859	3.075421
H	6.527431	0.009169	2.135029
H	4.844592	0.465945	1.837120
C	2.181050	-3.481692	5.759425
H	2.233862	-3.652644	4.688165
H	2.363085	-4.415654	6.288864
H	1.202705	-3.096393	6.037237
C	-7.469776	-2.989973	-1.506398
H	-8.100520	-3.849421	-1.728240
H	-7.057964	-2.597913	-2.433394
H	-6.667994	-3.287987	-0.834398
C	-6.814137	-2.309814	2.250842
H	-5.814296	-2.448253	1.852089
H	-6.843683	-2.646988	3.286079
H	-7.548153	-2.854522	1.665245

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2_ox1

103

C	-2.444257	-2.393508	1.558358
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C	-1.814937	-0.273777	2.784334
C	-4.164547	5.967667	-0.505977
C	3.745142	2.375445	1.494451
H	4.791360	2.171188	1.713904
H	3.513702	3.322824	1.977811
H	3.632353	2.495450	0.416608
C	0.454909	0.496272	2.029737
C	-2.124876	-3.605187	0.929588
C	-0.487652	3.108116	1.584703
C	0.890134	2.823139	1.611354
H	1.580790	3.627309	1.408227
C	1.373566	1.553289	1.852386
C	2.847088	1.264425	2.042877
C	3.143621	-0.092723	1.435323
C	4.371205	-0.356411	0.863190
H	5.074887	0.452009	0.787019
C	4.733071	-1.635777	0.414529
C	3.805911	-2.668425	0.642634
H	4.089367	-3.670433	0.360123
C	2.569634	-2.450857	1.209276
C	1.657369	-3.605387	1.575863
C	0.225085	-3.148771	1.397010
C	-0.774011	-3.992407	0.952234
H	-0.518265	-4.973838	0.582927
C	5.976662	-1.966032	-0.216242
H	6.113810	-3.021361	-0.427390
C	7.006049	-1.158437	-0.598898
C	-1.474060	-1.525988	2.009528
C	8.717539	0.738607	-1.188647
C	9.319308	-0.403653	-1.595354
C	-1.348895	2.084513	2.008195
H	-2.384543	2.308216	2.193898

C	2.193802	-1.130774	1.547837
C	-0.117674	-1.842055	1.800967
C	3.100400	1.153763	3.572480
H	4.148443	0.916318	3.758451
H	2.487348	0.372047	4.020408
H	2.859292	2.099444	4.059333
C	1.862033	-3.896823	3.088632
H	2.892304	-4.204376	3.271493
H	1.191610	-4.695265	3.408889
H	1.656217	-3.014107	3.693575
C	1.971660	-4.886523	0.801387
H	2.986022	-5.222201	1.007925
H	1.861165	-4.749607	-0.274723
H	1.313824	-5.693066	1.120014
C	-1.462964	-0.510264	4.277070
H	-2.073852	-1.319124	4.679497
H	-1.655210	0.396045	4.852532
H	-0.414695	-0.778786	4.402574
C	-3.296145	0.096806	2.699669
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C	-0.946596	4.391008	1.138706
H	-0.201668	5.177562	1.087439
C	-2.189630	4.717042	0.682004
C	-4.603813	4.697771	-0.350755
C	-3.104033	-4.438304	0.287853
H	-2.807724	-5.461579	0.083994
C	-4.327021	-4.059045	-0.171901
C	-6.426792	-2.814784	-1.129346
C	-6.600588	-4.104999	-1.494648
N	0.874335	-0.847183	1.954861
S	7.128892	0.572354	-0.459894
S	8.426232	-1.882426	-1.344214
S	-2.586185	6.334596	0.165521
S	-3.532944	3.597663	0.491306
S	-5.017063	-2.452073	-0.145939
S	-5.383665	-5.235953	-0.944748
S	-7.508128	-1.499196	-1.534702
S	-7.967209	-4.637962	-2.445638
S	-5.095905	7.254599	-1.240717
S	-6.170504	4.152597	-0.908351
S	9.409997	2.339892	-1.319293
S	10.900898	-0.412506	-2.338116
C	-6.743653	-0.906165	-3.082672
H	-6.759953	-1.692246	-3.833907
H	-7.350580	-0.067659	-3.422292
H	-5.724416	-0.570719	-2.902906
C	-7.588896	-6.387111	-2.748270
H	-7.561084	-6.956015	-1.820909
H	-8.416033	-6.748087	-3.357184
H	-6.660287	-6.504963	-3.302837
C	-6.084805	2.355729	-0.649111
H	-5.988938	2.103962	0.405292
H	-7.038671	1.974341	-1.008915
H	-5.279596	1.905043	-1.225910
C	-4.315978	7.338389	-2.887824
H	-4.445353	6.395651	-3.414388
H	-4.834380	8.131658	-3.424538
H	-3.261262	7.589998	-2.802219

C	11.156194	-2.169207	-2.715271
H	12.136709	-2.212144	-3.186321
H	11.173455	-2.772604	-1.809703
H	10.410226	-2.541276	-3.414816
C	8.867549	2.805089	-2.999293
H	7.781723	2.831452	-3.056489
H	9.266078	3.802840	-3.178115
H	9.275706	2.113740	-3.732821

Zero-point correction=	0.783965
(Hartree/Particle)	
Thermal correction to Energy=	0.844029
Thermal correction to Enthalpy=	0.844973
Thermal correction to Gibbs Free Energy=	0.681559
Sum of electronic and zero-point Energies=	-6575.207595
Sum of electronic and thermal Energies=	-6575.147532
Sum of electronic and thermal Enthalpies=	-6575.146587
Sum of electronic and thermal Free Energies=	-6575.310001

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	529.636	227.066	343.934
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	46.531
Rotational	0.889	2.981	42.122
Vibrational	527.858	221.104	253.904

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0572693,-0.2535016,0.0916195,0.1857577,-0.0248729,-0.0281825,-0.058009
8,-0.0600753,0.0681882,-0.001271,0.0227592,-0.0385833,-0.0265132,0.108
1677,0.0227206,-0.0160466,0.1230186,-0.0434367,-0.0503985,0.1438308,-0
.0784855,0.0168839,0.0693692,-0.0324562,-0.003464,-0.1062623,0.0294774
,0.0704199,-0.0074116,-0.0045388,-0.0600714\Polar=2813.847581,76.20807
85,1587.8951822,-48.269068,-35.0518562,628.2678113\PG=C01 [X(C45H45N1S
12)]\NImag=3\0.74687108,0.00224784,0.54677129,-0.00430141,-0.23253890

System has the following imaginary frequencies:

- 1 -11.3314 cm⁻¹
- 2 -7.3002 cm⁻¹
- 3 -5.9346 cm⁻¹

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2_red1

103

C	2.455495	-2.373230	-1.874419
H	3.503348	-2.146069	-1.989784
C	0.983576	0.830008	-2.661394
C	1.899886	-0.263594	-3.170219
C	4.067810	5.724278	0.621354
C	-3.656228	2.480123	-2.077462
H	-4.698439	2.284418	-2.323821
H	-3.390844	3.420597	-2.560220
H	-3.577988	2.605442	-0.997123
C	-0.383676	0.540974	-2.491542
C	2.091704	-3.586222	-1.245741
C	0.584299	3.137838	-1.999736
C	-0.790401	2.872899	-2.052821
H	-1.476563	3.681620	-1.847337
C	-1.288329	1.610580	-2.333323
C	-2.760889	1.347327	-2.583169
C	-3.101370	0.002301	-1.967424
C	-4.335540	-0.233893	-1.397414
H	-5.040286	0.578005	-1.342775
C	-4.722601	-1.505867	-0.927084
C	-3.812755	-2.556738	-1.170072
H	-4.118951	-3.555807	-0.895038
C	-2.570447	-2.361579	-1.732605
C	-1.666928	-3.525252	-2.106110
C	-0.230628	-3.102509	-1.857299
C	0.729580	-3.955912	-1.358413
H	0.444555	-4.940093	-1.013562
C	-5.963698	-1.791234	-0.275003
H	-6.202485	-2.847071	-0.174152
C	-6.902479	-0.946065	0.236359
C	1.521670	-1.506358	-2.392517
C	-7.877561	0.852008	1.829428
C	-8.646406	-0.240757	2.026485
C	1.438891	2.111114	-2.408638
H	2.482977	2.322964	-2.565262
C	-2.161971	-1.046889	-2.070068
C	0.145973	-1.798267	-2.257499
C	-2.957838	1.235863	-4.118524
H	-4.004243	1.020763	-4.342684
H	-2.347525	0.432937	-4.531206
H	-2.672258	2.170675	-4.606201
C	-1.827086	-3.774231	-3.629700
H	-2.858862	-4.048141	-3.860187
H	-1.161671	-4.577964	-3.951513
H	-1.577079	-2.877283	-4.195969
C	-2.032862	-4.817920	-1.376178
H	-3.049453	-5.124136	-1.620699
H	-1.954337	-4.704454	-0.294397
H	-1.374213	-5.627701	-1.688566
C	1.595793	-0.500712	-4.671030
H	2.213173	-1.317468	-5.049577
H	1.808142	0.402597	-5.247609
H	0.549890	-0.766286	-4.821125
C	3.380773	0.093142	-3.039346

H	3.663355	0.277663	-2.002717
H	3.618046	0.979123	-3.628832
H	3.998102	-0.718767	-3.421768
C	1.062686	4.416367	-1.511811
H	0.352019	5.237053	-1.523788
C	2.268279	4.678929	-0.968351
C	4.442450	4.437803	0.472716
C	3.022084	-4.417983	-0.556442
H	2.735386	-5.456188	-0.402470
C	4.237137	-4.057821	-0.043411
C	5.709732	-2.834263	1.690419
C	5.958510	-4.146645	1.891224
N	-0.829259	-0.794693	-2.464573
S	-6.804437	0.806583	0.416518
S	-8.465172	-1.531403	0.824579
S	2.748902	6.285034	-0.417731
S	3.551330	3.482755	-0.704260
S	4.853713	-2.418012	0.188667
S	5.385511	-5.230762	0.607548
S	6.238991	-1.522407	2.723361
S	6.920494	-4.794615	3.200841
S	4.852122	6.877269	1.676270
S	5.792837	3.709444	1.323562
S	-7.976494	2.333807	2.752957
S	-9.893483	-0.388748	3.244487
C	4.629583	-0.873515	3.282350
H	4.145228	-1.590340	3.942786
H	4.833120	0.048541	3.826177
H	3.988362	-0.664887	2.428981
C	5.855932	-6.147690	3.795027
H	5.703802	-6.899548	3.024596
H	6.381024	-6.591641	4.640695
H	4.895432	-5.757115	4.126242
C	5.528457	1.930661	1.050523
H	5.644049	1.659714	0.003595
H	6.304226	1.427780	1.625133
H	4.553628	1.616489	1.413767
C	3.630832	6.973900	3.027311
H	3.547052	6.010093	3.525329
H	3.999478	7.720636	3.730206
H	2.662171	7.283942	2.640580
C	-9.389640	-1.928237	4.078442
H	-10.138427	-2.115202	4.847882
H	-9.367171	-2.761422	3.380118
H	-8.412321	-1.804841	4.541630
C	-6.227690	2.602910	3.189148
H	-5.614656	2.736430	2.301485
H	-6.205932	3.512655	3.788670
H	-5.851722	1.768165	3.777574

Zero-point correction=
(Hartree/Particle)

0.779015

Thermal correction to Energy=

0.838707

Thermal correction to Enthalpy=

0.839651

Thermal correction to Gibbs Free Energy=

0.680534

Sum of electronic and zero-point Energies=

-6575.436065

Sum of electronic and thermal Energies=

-6575.376372

Sum of electronic and thermal Enthalpies=

-6575.375428

Sum of electronic and thermal Free Energies=

-6575.534545

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	526.297	227.377	334.889
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	46.531
Rotational	0.889	2.981	41.926
Vibrational	524.519	221.416	245.055

1\1\GINC-XE29TH10\Freq\UB3LYP\def2TZVP\C45H45N1S12(1-,2)\DRAL\25-Jul-2015\0\#\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk UB3LYP/def2TZVP Freq\BG32(-)\-1,2\C,2.4392181445,-2.3766607097,-1.9021250608\H,3.4888738033,-2.1554658703,-2.0125918692\C,0.9910665778,0.8445874605,-2.6591093253\C,1.9011742478,-0.2498735967,-3.1771347416\C,4.1003817249,5.6831689287,0.6820123716\C,-3.6388392631,2.5201493627,-2.0691086933\H,-4.6817446342,2.3341441981,-2.3200031076\H,-3.3658731341,3.463776966,-2.5413722518\H,-3.5624208692,2.6336504649,-0.9873348069\C,-0.3785349155,0.5631351442,-2.495573039\C,2.0656340475,-3.5936358472,-1.2870351471\C,0.6058568124,3.1480586835,-1.974327454\C,-0.7704777839,2.8930770553,-2.0334802793\H,-1.4516301529,3.7042738261,-1.8212033786\C,-1.2762826194,1.6371814191,-2.3283564863\C,-2.7499762264,1.3866075369,-2.5844766808\C,-3.1011178848,0.0375840109,-1.9836427743\C,-4.3382711653,-0.1961161796,-1.419098663\H,-5.0376125029,0.6199592427,-1.3576702202\C,-4.7351345273,-1.470256922,-0.9630203147\C,-3.8318574152,-2.5247208876,-1.2147930242\H,-4.1455193085,-3.5244918552,-0.9509519785\C,-2.5868635173,-2.3321854958,-1.7722696601\C,-1.6903574625,-3.498037858,-2.1557454662\C,-0.2518354381,-3.0877277786,-1.8990802113\C,0.701310271,-3.9528235912,-1.4068362413\H,0.408747442,-4.9385819271,-1.072976395\C,-5.9797520359,-1.7539350071,-0.3169410812\H,-6.2259621912,-2.8091127881,-0.2277046603\C,-6.9140257032,-0.9077608152,0.2009711709\C,1.512594003,-1.4980760637,-2.413375087\C,-7.8807955437,0.8802030747,1.8103998691\C,-8.6575390136,-0.2092855282,1.9941767545\C,1.4544557381,2.1198483247,-2.391884216\H,2.5003423265,2.3261896995,-2.5437778364\C,-2.1686234731,-1.0168642042,-2.0949903712\C,0.1346145066,-1.7819815806,-2.2847210412\C,-2.9438806566,1.2925182914,-4.1213807593\H,-3.9911664617,1.086916991,-4.3502900426\H,-2.338023191,0.4897961664,-4.5409657257\H,-2.6507455976,2.2303979403,-4.598573292\C,-1.848436277,-3.7300045935,-3.6822345762\H,-2.8814776987,-3.9944456619,-3.9180500214\H,-1.187708223,-4.5348585955,-4.0108313687\H,-1.5909356915,-2.8289239142,-4.2384963993\C,-2.0668770485,-4.7957245051,-1.4402453427\H,-3.0849188599,-5.0924265484,-1.690394464\H,-1.9902583752,-4.6940925186,-0.3571522061\H,-1.4129795615,-5.6066785319,-1.759497624\C,1.5991885512,-0.4692362436,-4.6810681062\H,2.2119345967,-1.2861929634,-5.0666475533\H,1.8191008043,0.4385698365,-5.2476625527\H,0.5518785717,-0.7260843114,-4.8364424422\C,3.384124297,0.0953605216,-3.0389836387\H,3.665390624,0.2671210642,-1.9998065758\H,3.6288742762,0.9858053475,-3.6186057329\H,3.9968620554,-0.7167083616,-3.428386883\C,1.0917189201,4.4181316331,-1.4719180773\H,0.3866801931,5.2437293538,-1.4770238168\C,2.2977211309,4.6667723993,-0.922849336\C,4.4666318714,4.3957875511,0.5208370894\C,2.9886290382,-4.4388759215,-0.6042340327\H,2.6944975755,-5.4766494299,-0.4618112266\C,4.2048303093,-4.0923888362,-0.0845499096\C,5.6814186849,-2.8970697082,1.6655058048\C,5.9207691015,-4.2131437797,1.8531799299\N,-0.8332563218,-0.7696676029,-2.4836356808\N,-6.8045143786,0.8422015222,0.3996735995\N,-8.4821135702,-1.4885258616,0.7792854531\N,2.7878914504,6.263726224,-0.3543197163\N,3.5719517165,3.4591786137,-0.6681945605\N,4.8319668589,-2.4593366739,0.1661352717\N,5.3435887301,-5.2798690492,0.5568706961\N,6.2170296531,-1.5997070566,2.713371508\N,6.8750837218,-4.8812954092,3.158260119\N,4.8899048491,6.8197083969,1.7508029053\N,5.809925939,3.6493892932,1.3672642145\N,-7.9719337046,2.3529251826,2.7491260475\N,-9.9086015199,-0.3614637172,3.2075668251\C,4.6106942487,-0.9457147057,3.2752451613\H,4.1198444877,-1.6660690697,3.9269868891\H,4.8191504378,-0.0307941418,3.8291

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System has the following imaginary frequencies:

- 1 -11.8753 cm⁻¹
- 2 -8.5945 cm⁻¹
- 3 -5.1159 cm⁻¹
- 4 -2.7929 cm⁻¹

=====

4

55

N	0.000000	0.035515	0.077308
C	1.217771	0.733525	-0.093466
C	1.220803	2.143371	-0.049577
C	2.372204	2.835077	-0.396508
H	2.367189	3.914049	-0.396876
C	3.543328	2.164550	-0.713245
H	4.435421	2.712961	-0.984525
C	3.564118	0.786827	-0.622377
H	4.492335	0.262025	-0.799372
C	2.423714	0.052418	-0.302189
C	2.560241	-1.445096	-0.109153
C	1.212734	-2.088844	0.169679

C	1.186277	-3.461707	0.392495
H	2.120555	-4.003155	0.437974
C	-0.000011	-4.154971	0.538080
H	-0.000014	-5.220495	0.724192
C	-1.186296	-3.461700	0.392502
H	-2.120577	-4.003143	0.437986
C	-1.212746	-2.088837	0.169689
C	-0.000004	-1.376469	0.135314
C	-2.560252	-1.445080	-0.109134
C	-2.423719	0.052435	-0.302154
C	-3.564124	0.786853	-0.622319
H	-4.492347	0.262057	-0.799303
C	-3.543329	2.164577	-0.713178
H	-4.435423	2.712994	-0.984439
C	-2.372194	2.835094	-0.396458
H	-2.367173	3.914066	-0.396821
C	-1.220791	2.143379	-0.049552
C	-1.217769	0.733534	-0.093446
C	0.000014	2.845628	0.506444
C	3.515480	-1.691809	1.081718
H	3.108644	-1.250159	1.991849
H	4.491270	-1.244554	0.893444
H	3.662051	-2.757660	1.254850
C	3.150670	-2.086815	-1.386043
H	3.271761	-3.162331	-1.260840
H	4.127604	-1.665663	-1.621438
H	2.490396	-1.915078	-2.236525
C	-3.150683	-2.086782	-1.386031
H	-2.490409	-1.915038	-2.236511
H	-4.127616	-1.665623	-1.621421
H	-3.271779	-3.162299	-1.260840
C	-3.515490	-1.691805	1.081735
H	-3.662066	-2.757657	1.254854
H	-4.491278	-1.244543	0.893468
H	-3.108651	-1.250168	1.991872
C	0.000030	2.648852	2.046459
H	-0.888432	3.109449	2.482027
H	0.888504	3.109442	2.482008
H	0.000028	1.591168	2.307757
C	0.000017	4.349452	0.228784
H	0.000006	4.566879	-0.840053
H	0.873056	4.819960	0.678545
H	-0.873009	4.819967	0.678564

Zero-point correction=	0.467857
(Hartree/Particle)	
Thermal correction to Energy=	0.490927
Thermal correction to Enthalpy=	0.491871
Thermal correction to Gibbs Free Energy=	0.417711
Sum of electronic and zero-point Energies=	-1099.984739
Sum of electronic and thermal Energies=	-1099.961668
Sum of electronic and thermal Enthalpies=	-1099.960724
Sum of electronic and thermal Free Energies=	-1100.034885

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	308.061	97.953	156.084
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.579
Rotational	0.889	2.981	35.095

Vibrational

306.284

91.991

77.411

1\1\GINC-XE30TH8\Freq\RB3LYP\def2TZVP\C27H27N1\DRAL\07-Sep-2016\0\#\#P
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99929,-0.0930705723\C,-1.2207324853,-2.1433557162,-0.0491811632\C,-2.3
72112651,-2.8350961256,-0.3961126122\H,-2.3670662264,-3.9140675105,-0.
3964806332\C,-3.5432571737,-2.1646039601,-0.7128493871\H,-4.4353334604
, -2.7130408714,-0.9841297096\C,-3.5640872672,-0.7868809608,-0.62198127
14\H,-4.4923202248,-0.262106724,-0.7989761184\C,-2.4237045952,-0.05243
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216317,0.5384755541\H,-0.0001327755,5.2205456369,0.7245874828\C,1.1862
009912,3.4617862362,0.3928978373\H,2.1204662492,4.003255969,0.43838141
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8\H,4.4923622453,-0.2618739287,-0.7989078461\C,3.5433997773,-2.1644213
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C	-2.429065	-0.039347	-0.295151
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C	-1.222732	2.086186	0.183526
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H	0.000026	5.182487	0.850258
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C	3.548750	-2.149291	-0.668703
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C	1.219902	-0.732656	-0.093517
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C	-3.554809	1.722421	1.025448
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C	-3.088896	2.083246	-1.440785
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H	-0.886933	-3.185778	2.455966
H	-0.000001	-1.661306	2.337360
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H	-0.000012	-4.550347	-0.907263
H	-0.869221	-4.845907	0.606191
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Zero-point correction=
(Hartree/Particle)

0.468659

Thermal correction to Energy= 0.491813
 Thermal correction to Enthalpy= 0.492757
 Thermal correction to Gibbs Free Energy= 0.417525
 Sum of electronic and zero-point Energies= -1099.752240
 Sum of electronic and thermal Energies= -1099.729086
 Sum of electronic and thermal Enthalpies= -1099.728142
 Sum of electronic and thermal Free Energies= -1099.803374

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	308.617	97.848	158.340
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	43.579
Rotational	0.889	2.981	35.097
Vibrational	306.840	91.886	78.286

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H	-4.407324	-2.715431	-1.069025
C	-3.535039	-0.789540	-0.734221
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C	-2.404200	-0.041308	-0.362241
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C	-1.221656	2.090095	0.221568
C	-1.193627	3.436884	0.532765
H	-2.129996	3.978940	0.586276
C	-0.000020	4.132039	0.740816
H	-0.000025	5.181899	1.002103
C	1.193593	3.436895	0.532769
H	2.129958	3.978958	0.586287
C	1.221634	2.090106	0.221571
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C	3.535042	-0.789503	-0.734237
H	4.445507	-0.266010	-0.998654
C	3.523529	-2.166099	-0.766483
H	4.407343	-2.715385	-1.069054
C	2.370805	-2.848653	-0.362286
H	2.380486	-3.926798	-0.318720
C	1.219248	-2.143551	-0.003613
C	1.206990	-0.741919	-0.081171
C	0.000016	-2.835196	0.575011
C	-3.589601	1.689757	0.962071
H	-3.235451	1.257181	1.898554
H	-4.539958	1.217331	0.707079
H	-3.772913	2.753757	1.122671
C	-3.044761	2.118791	-1.460876
H	-3.221068	3.185456	-1.313560
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H	-2.296476	1.999321	-2.245160
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H	3.975885	1.662915	-1.805711
H	3.221050	3.185499	-1.313527
C	3.589574	1.689776	0.962092

H	3.772878	2.753775	1.122705
H	4.539937	1.217357	0.707105
H	3.235416	1.257188	1.898566
C	0.000019	-2.631775	2.114641
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H	0.000015	-1.571162	2.362096
C	0.000023	-4.345109	0.319067
H	0.000020	-4.575727	-0.746941
H	-0.876711	-4.806241	0.774066
H	0.876766	-4.806231	0.774059

Zero-point correction= 0.458704
(Hartree/Particle)
Thermal correction to Energy= 0.482649
Thermal correction to Enthalpy= 0.483593
Thermal correction to Gibbs Free Energy= 0.407065
Sum of electronic and zero-point Energies= -1099.973191
Sum of electronic and thermal Energies= -1099.949246
Sum of electronic and thermal Enthalpies= -1099.948301
Sum of electronic and thermal Free Energies= -1100.024829

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	302.867	101.671	161.067
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	43.579
Rotational	0.889	2.981	35.098
Vibrational	301.089	95.710	81.012

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C	3.022852	1.744969	0.590640
C	0.725463	0.998550	-3.317688

1\1\GINC-XE34TH10\FOpt\RB3LYP\def2TZVP\C60\DRAL\27-May-2015\0\#\#P B3LYP/def2TZVP EmpiricalDispersion=GD3BJ Freq=NoRaman Name=Dral Opt=(Tight,MaxCyc=1000) SCF=NoVarAcc SCFCyc=500 Int=UltraFine\\Ih-C60\0,1\C,1.1738655856,0.3813999711,3.3177268919\C,2.2974644408,0.7464485065,2.5878091046\C,-2.2974644408,-0.7464485065,-2.5878091046\C,-1.1738655856,-0.3813999711,-3.3177268919\C,1.4197952402,-3.188481191,0.590717397\C,0.7254656539,-3.4139136438,-0.5905849611\C,-0.7254656539,3.4139136438,0.5905849611\C,-1.4197952402,3.188481191,-0.590717397\C,-2.5938225245,-1.5729180726,1.8250334997\C,-3.0229718604,-0.2521630145,1.8250157199\C,3.0229718604,0.2521630145,-1.8250157199\C,2.5938225245,1.5729180726,-1.8250334997\C,0.7254629382,-0.9985494294,3.3176877702\C,0.0000000714,1.2343012684,3.317758115\C,3.0229709911,-0.2521623048,1.8250150625\C,2.2974837862,1.9807514469,1.8250020732\C,-2.2974837862,-1.9807514469,-1.8250020732\C,-3.0229709911,0.2521623048,-1.8250150625\C,-0.0000000714,-1.2343012684,-3.317758115\C,-0.7254629382,0.9985494294,-3.3176877702\C,0.6944083061,-2.9531189681,1.8251475242\C,2.5936234349,-2.335547334,0.5906529929\C,-0.7254651357,-3.4139129355,-0.5905850978\C,1.1738983983,-2.7968958209,-1.8248731937\C,-1.1738983983,2.7968958209,1.8248731937\C,0.7254651357,3.4139129355,0.5905850978\C,-2.5936234349,2.335547334,-0.5906529929\C,-0.6944083061,2.9531189681,-1.8251475242\C,-1.4198671546,-1.9543302364,2.5878176344\C,-2.5936234106,-2.3355478667,0.5906528385\C,-2.2974639893,0.7464482809,2.5878087385\C,-3.4713035462,0.365019384,0.5906862533\C,3.4713035462,-0.365019384,-0.5906862533\C,2.2974639893,-0.7464482809,-2.5878087385\C,2.5936234106,2.3355478667,-0.5906528385\C,1.4198671546,1.9543302364,-2.5878176344\C,1.4198670411,-1.9543306059,2.5878177318\C,-0.000000458,2.4155098676,2.5876774107\C,2.5938216892,-1.5729182961,1.8250322873\C,1.1738975163,2.7968958398,1.8248725028\C,-1.1738975163,-2.7968958398,-1.8248725028\C,-2.5938216892,1.5729182

961,-1.8250322873\C,0.000000458,-2.4155098676,-2.5876774107\C,-1.41986
70411,1.9543306059,-2.5878177318\C,-0.6944085828,-2.9531186286,1.82514
76482\C,3.0228517787,-1.7449682236,-0.5906404287\C,-1.4197952441,-3.18
84806935,0.5907177702\C,2.2974841075,-1.9807516203,-1.8250023235\C,-2.
2974841075,1.9807516203,1.8250023235\C,1.4197952441,3.1884806935,-0.59
07177702\C,-3.0228517787,1.7449682236,0.5906404287\C,0.6944085828,2.95
31186286,-1.8251476482\C,-0.7254628508,-0.9985495893,3.3176878707\C,-3
.0228517965,-1.7449685499,-0.5906400574\C,-1.1738658046,0.3814000201,3
.3177268356\C,-3.4713037585,-0.365019208,-0.5906862774\C,3.4713037585,
0.365019208,0.5906862774\C,1.1738658046,-0.3814000201,-3.3177268356\C,
3.0228517965,1.7449685499,0.5906400574\C,0.7254628508,0.9985495893,-3.
3176878707\\Version=ES64L-G09RevD.01\State=1-AG\HF=-2287.1966078\RMSD=
3.599e-10\RMSF=9.540e-07\Dipole=0.,0.,0.\Quadrupole=-0.0026433,0.00019
51,0.0024482,-0.0000056,-0.000006,0.0005023\PG=CI [X(C60)]\@

=====

=====

!!
!!!!!!

DFTD3 outputs for geometries optimized at B3LYP-D3(BJ)/def2-TZVP

!!
!!!!!!

=====

=====

1

	DFTD3 V3.1 Rev 0	
	S.Grimme, University Bonn	
	June 2014	
	see dftd3 -h for options	

Please cite DFT-D3 work done with this code as:
S. Grimme, J. Antony, S. Ehrlich and H. Krieg,
J. Chem. Phys. 132 (2010), 154104
If used with BJ-damping cite also
S. Grimme, S. Ehrlich and L. Goerigk,
J. Comput. Chem. 32 (2011), 1456-1465
For DFT-D2 the reference is
S. Grimme, J. Comput. Chem., 27 (2006), 1787-1799

files read :

BG33.xyz

C6 coefficients used:

	2	C6 for element	1
Z= 1	CN= 0.912	C6(AA)= 3.03	
Z= 1	CN= 0.000	C6(AA)= 7.59	
	5	C6 for element	6
Z= 6	CN= 0.000	C6(AA)= 49.11	
Z= 6	CN= 0.987	C6(AA)= 43.25	
Z= 6	CN= 1.998	C6(AA)= 29.36	
Z= 6	CN= 2.999	C6(AA)= 25.78	
Z= 6	CN= 3.984	C6(AA)= 18.21	
	4	C6 for element	7
Z= 7	CN= 0.000	C6(AA)= 25.27	

Z=	7	CN=	0.994	C6(AA)=	22.12
Z=	7	CN=	2.014	C6(AA)=	19.68
Z=	7	CN=	2.990	C6(AA)=	15.58
			3	C6 for element	8
Z=	8	CN=	0.000	C6(AA)=	15.51
Z=	8	CN=	0.993	C6(AA)=	12.82
Z=	8	CN=	1.989	C6(AA)=	10.37
			3	C6 for element	16
Z=	16	CN=	0.000	C6(AA)=	134.01
Z=	16	CN=	0.995	C6(AA)=	131.00
Z=	16	CN=	1.990	C6(AA)=	125.81

#	XYZ [au]				R0(AA) [Ang.]	CN	C6(AA)
C8(AA)	C10(AA) [au]						
1	4.56521	-4.93201	-3.56004	c	0.566	3.251	24.7
714.3	25308.1						
2	6.52589	-4.42780	-3.77978	h	0.366	1.017	3.1
37.3	551.9						
3	1.58982	1.07938	-5.02887	c	0.566	3.310	24.2
699.4	24778.6						
4	3.42058	-0.92625	-5.92833	c	0.566	4.147	18.2
527.7	18694.4						
5	6.99044	11.37767	0.14882	c	0.566	3.264	24.6
711.5	25207.1						
6	-7.30843	3.84536	-4.07225	c	0.566	4.099	18.3
528.2	18712.3						
7	-9.26109	3.38163	-4.52557	h	0.366	1.000	3.1
37.4	553.2						
8	-6.89372	5.61585	-5.03548	h	0.366	1.000	3.1
37.4	553.2						
9	-7.16629	4.15159	-2.03978	h	0.366	0.999	3.1
37.4	553.3						
10	-0.97151	0.43966	-4.77635	c	0.566	3.351	23.7
686.5	24323.0						
11	3.94619	-7.23667	-2.43763	c	0.566	3.184	25.1
726.3	25732.1						
12	-19.28659	6.29699	5.10964	c	0.566	4.061	18.3
528.7	18731.9						
13	-17.93568	7.10782	6.43399	h	0.366	0.996	3.1
37.4	553.5						
14	-21.13461	6.10484	5.98100	h	0.366	0.997	3.1
37.4	553.5						
15	-19.39355	7.48876	3.43571	h	0.366	0.996	3.1
37.4	553.5						
16	-20.88354	-0.99864	8.93764	c	0.566	4.064	18.3
528.7	18730.2						
17	-21.79171	-2.84354	8.86517	h	0.366	0.996	3.1
37.4	553.5						
18	-22.24295	0.44946	8.39769	h	0.366	0.997	3.1
37.4	553.5						
19	-20.12816	-0.62921	10.80895	h	0.366	0.997	3.1
37.4	553.5						
20	0.63289	5.44629	-3.95517	c	0.566	3.179	25.1
727.0	25755.9						
21	-1.93531	4.82736	-4.07620	c	0.566	3.231	24.8
718.5	25455.1						
22	-3.30256	6.31229	-3.77840	h	0.366	1.007	3.1
37.3	552.7						
23	-2.76412	2.38581	-4.53071	c	0.566	3.299	24.3
702.5	24889.6						

24	-5.52239	1.76164	-4.98183	c	0.566	4.144	18.2
527.7	18695.6						
25	-6.04182	-0.77141	-3.74595	c	0.566	3.300	24.3
702.4	24885.2						
26	-8.35204	-1.28378	-2.62408	c	0.566	3.240	24.8
716.6	25389.1						
27	-9.72603	0.21201	-2.54196	h	0.366	1.022	3.1
37.2	551.5						
28	-8.97119	-3.67693	-1.69819	c	0.566	3.172	25.2
727.9	25790.0						
29	-7.21494	-5.60751	-2.12184	c	0.566	3.236	24.8
717.5	25419.8						
30	-7.71171	-7.50060	-1.54571	h	0.366	1.007	3.1
37.3	552.7						
31	-4.89242	-5.17612	-3.24294	c	0.566	3.297	24.3
703.0	24906.8						
32	-3.13723	-7.32819	-3.95012	c	0.566	4.143	18.2
527.7	18695.7						
33	-0.45605	-6.42668	-3.50855	c	0.566	3.301	24.3
702.1	24876.4						
34	1.41927	-7.99668	-2.57241	c	0.566	3.228	24.9
719.0	25472.3						
35	0.92829	-9.85611	-1.89018	h	0.366	1.007	3.1
37.3	552.7						
36	-11.31085	-4.28882	-0.41124	c	0.566	3.271	24.5
709.9	25149.9						
37	-11.67073	-6.29491	-0.18211	h	0.366	1.010	3.1
37.3	552.4						
38	-13.06089	-2.72989	0.58596	c	0.566	3.083	25.5
737.2	26117.8						
39	2.74182	-3.30897	-4.49996	c	0.566	3.311	24.2
699.3	24775.1						
40	-15.65001	0.94111	2.62425	c	0.566	3.267	24.6
710.7	25178.8						
41	-16.91020	-1.17544	3.24804	c	0.566	3.253	24.7
713.9	25293.3						
42	2.34792	3.54389	-4.58870	c	0.566	3.248	24.7
715.0	25331.5						
43	4.31516	4.00689	-4.81970	h	0.366	1.021	3.1
37.3	551.7						
44	-19.25154	-1.35398	4.83156	c	0.566	3.220	24.9
720.4	25522.3						
45	-4.21849	-2.69349	-3.91848	c	0.566	3.342	23.8
689.6	24431.8						
46	0.17976	-3.95645	-4.25710	c	0.566	3.352	23.7
686.1	24307.8						
47	-5.90163	1.44311	-7.87211	c	0.566	4.110	18.3
528.0	18707.7						
48	-7.85597	0.92157	-8.27406	h	0.366	0.999	3.1
37.4	553.3						
49	-4.67138	-0.02663	-8.62527	h	0.366	1.000	3.1
37.4	553.3						
50	-5.46690	3.21057	-8.84163	h	0.366	0.999	3.1
37.4	553.3						
51	-16.29496	3.56851	3.26990	c	0.566	3.222	24.9
720.1	25513.5						
52	-3.44735	-7.82774	-6.82341	c	0.566	4.110	18.3
528.0	18707.5						
53	-5.38075	-8.41730	-7.23240	h	0.366	0.999	3.1
37.4	553.3						

54	-2.15080	-9.31335	-7.42782	h	0.366	0.999	3.1
37.4	553.3						
55	-3.04370	-6.13217	-7.91950	h	0.366	1.000	3.1
37.4	553.2						
56	-3.73923	-9.78481	-2.55300	c	0.566	4.098	18.3
528.2	18712.7						
57	-5.64611	-10.41932	-2.99522	h	0.366	1.000	3.1
37.4	553.3						
58	-3.57515	-9.56893	-0.51002	h	0.366	0.999	3.1
37.4	553.3						
59	-2.46737	-11.28482	-3.15972	h	0.366	1.000	3.1
37.4	553.3						
60	2.95148	-1.39442	-8.78189	c	0.566	4.107	18.3
528.1	18708.7						
61	4.18635	-2.89881	-9.46415	h	0.366	0.999	3.1
37.4	553.3						
62	3.34097	0.32496	-9.85175	h	0.366	0.999	3.1
37.4	553.3						
63	1.00034	-1.94799	-9.13660	h	0.366	1.000	3.1
37.4	553.2						
64	6.18688	-0.16008	-5.58982	c	0.566	4.101	18.3
528.1	18711.4						
65	6.65393	0.20676	-3.61699	h	0.366	1.000	3.1
37.4	553.3						
66	6.60502	1.53287	-6.68281	h	0.366	1.000	3.1
37.4	553.2						
67	7.43558	-1.63659	-6.29520	h	0.366	1.000	3.1
37.4	553.2						
68	1.39083	7.97773	-3.22586	c	0.566	3.266	24.6
711.0	25189.2						
69	-0.05166	9.42739	-3.37422	h	0.366	1.009	3.1
37.3	552.5						
70	3.63806	8.70509	-2.27128	c	0.566	3.087	25.5
736.9	26106.4						
71	7.94909	9.02576	0.10759	c	0.566	3.269	24.6
710.3	25164.3						
72	10.40284	8.34009	1.24157	c	0.566	3.200	25.0
723.9	25647.2						
73	13.18286	4.94057	2.05209	c	0.566	4.057	18.3
528.8	18734.3						
74	14.72949	5.77751	0.98247	h	0.366	0.996	3.1
37.4	553.5						
75	13.14851	2.90308	1.82546	h	0.366	0.998	3.1
37.4	553.4						
76	13.38384	5.45485	4.03527	h	0.366	0.997	3.1
37.4	553.5						
77	8.19369	13.62808	1.37660	c	0.566	3.217	24.9
721.0	25544.6						
78	9.41665	15.41294	5.24105	c	0.566	4.064	18.3
528.7	18729.8						
79	9.11082	15.00236	7.22787	h	0.366	0.997	3.1
37.4	553.5						
80	8.66031	17.26208	4.74890	h	0.366	0.996	3.1
37.4	553.5						
81	11.42092	15.33927	4.78078	h	0.366	0.997	3.1
37.4	553.5						
82	5.80447	-8.82727	-1.19064	c	0.566	3.263	24.6
711.6	25211.3						
83	5.39432	-10.83449	-1.10344	h	0.366	1.008	3.1
37.3	552.6						

84	7.92708	-8.04522	-0.02707	c	0.566	3.091	25.5
736.6	26097.3						
85	11.11079	-5.46739	2.67201	c	0.566	3.271	24.5
709.8	25146.8						
86	11.72323	-7.89364	3.11256	c	0.566	3.259	24.6
712.5	25243.7						
87	12.27544	-3.19452	3.88072	c	0.566	3.222	24.9
720.1	25513.3						
88	12.97550	-1.07751	7.71089	c	0.566	4.064	18.3
528.7	18730.0						
89	12.33116	0.73973	6.99190	h	0.366	0.997	3.1
37.4	553.5						
90	15.01986	-1.21495	7.52431	h	0.366	0.997	3.1
37.4	553.5						
91	12.40475	-1.32845	9.66516	h	0.366	0.997	3.1
37.4	553.5						
92	13.79922	-8.67238	4.80409	c	0.566	3.201	25.0
723.7	25639.9						
93	15.84077	-12.17679	6.64261	c	0.566	4.059	18.3
528.7	18732.8						
94	15.70135	-11.43188	8.55601	h	0.366	0.996	3.1
37.4	553.5						
95	17.66732	-11.66153	5.84638	h	0.366	0.996	3.1
37.4	553.5						
96	15.59116	-14.21340	6.63605	h	0.366	0.997	3.1
37.4	553.5						
97	-1.72841	-2.13819	-4.74906	n	0.495	3.231	15.6
344.0	9297.2						
98	-18.74129	-0.93067	7.26566	o	0.473	2.047	10.4
209.8	5187.1						
99	-21.28658	-1.91740	3.99657	o	0.473	1.056	12.8
257.6	6368.5						
100	-18.54359	3.77800	4.42761	o	0.473	2.052	10.4
209.8	5186.6						
101	-14.95193	5.34174	2.75361	o	0.473	1.072	12.8
257.3	6361.6						
102	11.87919	9.82622	2.14720	o	0.473	1.059	12.8
257.6	6367.4						
103	10.79933	5.83806	1.09684	o	0.473	2.071	10.4
209.7	5184.8						
104	9.02674	15.38412	0.20093	o	0.473	1.056	12.8
257.6	6368.4						
105	8.10180	13.45617	3.88760	o	0.473	2.047	10.4
209.8	5187.1						
106	13.39287	-1.59825	2.70202	o	0.473	1.059	12.8
257.6	6367.2						
107	11.79162	-3.10847	6.34660	o	0.473	2.048	10.4
209.8	5187.0						
108	15.30789	-7.25426	5.75998	o	0.473	1.059	12.8
257.6	6367.4						
109	13.83228	-11.19551	5.10382	o	0.473	2.069	10.4
209.7	5185.0						
110	-12.97469	0.60374	0.67544	s	0.737	2.602	125.8
6163.7	369907.5						
111	-15.80494	-4.00262	2.01974	s	0.737	2.601	125.8
6163.7	369907.5						
112	4.21302	11.90931	-1.50479	s	0.737	2.589	125.8
6163.7	369907.7						
113	6.24448	6.72785	-1.59134	s	0.737	2.595	125.8
6163.7	369907.6						

```
114 8.83592 -4.84444 0.38061 s 0.737 2.606 125.8
6163.7 369907.4
115 10.10278 -10.18296 1.33212 s 0.737 2.575 125.8
6163.7 369908.0
```

molecular C6(AA) [au] = 186993.53

DFT-D V3(BJ)

DF b3-lyp

parameters

```
s6 : 1.0000
s8 : 1.9889
a1 : 0.3981
a2 : 4.4211
k1-k3 : 16.0000 1.3333 -4.0000
Cutoff : 94.8683 a.u.
CN-Cutoff: 40.0000 a.u.
```

Edisp /kcal,au: -202.8975 -0.32333763

```
E6 /kcal : -93.4015
E8 /kcal : -109.7462
E6(ABC) " : 0.250237
% E8 : 54.09
% E6(ABC) : -0.12
normal termination of dftd3
```

=====
1_C60

```
-----
|           DFTD3 V3.1 Rev 0           |
| S.Grimme, University Bonn           |
|           June 2014                 |
| see dftd3 -h for options           |
-----
```

Please cite DFT-D3 work done with this code as:
S. Grimme, J. Antony, S. Ehrlich and H. Krieg,
J. Chem. Phys. 132 (2010), 154104
If used with BJ-damping cite also
S. Grimme, S. Ehrlich and L. Goerigk,
J. Comput. Chem. 32 (2011), 1456-1465
For DFT-D2 the reference is
S. Grimme, J. Comput. Chem., 27 (2006), 1787-1799

files read :

BG33_C60.xyz

C6 coefficients used:

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      2 C6 for element      1
Z=  1 CN= 0.912      C6(AA)=  3.03
Z=  1 CN= 0.000      C6(AA)=  7.59
      5 C6 for element      6
Z=  6 CN= 0.000      C6(AA)= 49.11
Z=  6 CN= 0.987      C6(AA)= 43.25
Z=  6 CN= 1.998      C6(AA)= 29.36
Z=  6 CN= 2.999      C6(AA)= 25.78
Z=  6 CN= 3.984      C6(AA)= 18.21
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      4 C6 for element          7
Z=  7 CN= 0.000      C6(AA)=  25.27
Z=  7 CN= 0.994      C6(AA)=  22.12
Z=  7 CN= 2.014      C6(AA)=  19.68
Z=  7 CN= 2.990      C6(AA)=  15.58
      3 C6 for element          8
Z=  8 CN= 0.000      C6(AA)=  15.51
Z=  8 CN= 0.993      C6(AA)=  12.82
Z=  8 CN= 1.989      C6(AA)=  10.37
      3 C6 for element          16
Z= 16 CN= 0.000      C6(AA)= 134.01
Z= 16 CN= 0.995      C6(AA)= 131.00
Z= 16 CN= 1.990      C6(AA)= 125.81

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#	XYZ [au]	R0(AA) [Ang.]	CN	C6(AA)
C8(AA)	C10(AA) [au]			
1	0.39022 -8.48828 -6.01573	c 0.566	3.382	23.3
675.3	23923.8			
2	2.85022 -7.70944 -5.53398	c 0.566	3.382	23.4
675.4	23928.8			
3	-4.17994 2.40985 -0.31878	c 0.566	3.394	23.2
670.8	23766.3			
4	-1.72351 3.18859 0.16278	c 0.566	3.395	23.2
670.4	23751.2			
5	-0.05529 -0.64776 -9.28121	c 0.566	3.381	23.4
675.5	23932.2			
6	-0.96939 1.53370 -8.14054	c 0.566	3.381	23.4
675.6	23937.4			
7	-0.36295 -6.83362 2.29192	c 0.566	3.385	23.3
674.3	23889.9			
8	-1.27841 -4.65104 3.42680	c 0.566	3.386	23.3
673.6	23866.0			
9	-6.78330 -3.98018 -5.29030	c 0.566	3.384	23.3
674.5	23895.7			
10	-6.84617 -5.21760 -2.97546	c 0.566	3.382	23.3
675.1	23917.6			
11	5.50430 -0.08697 -2.88128	c 0.566	3.396	23.2
669.9	23733.1			
12	5.45156 -1.31868 -0.56455	c 0.566	3.388	23.3
672.9	23841.1			
13	-1.13716 -7.14659 -7.85552	c 0.566	3.382	23.4
675.3	23926.1			
14	-1.24192 -9.23770 -3.94350	c 0.566	3.381	23.4
675.5	23934.1			
15	3.89151 -5.55333 -6.87114	c 0.566	3.382	23.3
675.3	23924.4			
16	3.78932 -7.64470 -2.95769	c 0.566	3.381	23.4
675.6	23936.6			
17	-5.11503 2.34354 -2.89539	c 0.566	3.390	23.2
672.0	23808.9			
18	-5.21834 0.25162 1.01769	c 0.566	3.392	23.2
671.6	23794.5			
19	-0.08952 3.93898 -1.91010	c 0.566	3.389	23.2
672.4	23823.6			
20	-0.19403 1.84724 2.00570	c 0.566	3.394	23.2
670.7	23763.0			
21	-1.67584 -2.84446 -9.53669	c 0.566	3.382	23.4
675.4	23928.1			
22	2.48143 -1.52747 -8.72319	c 0.566	3.382	23.3
675.3	23923.8			

23	-3.54643	1.61579	-7.20621	c	0.566	3.381	23.4
675.5	23933.6						
24	0.61318	2.93750	-6.39328	c	0.566	3.381	23.4
675.7	23939.3						
25	-1.94482	-8.23122	0.54306	c	0.566	3.382	23.4
675.4	23928.2						
26	2.21135	-6.91008	1.35441	c	0.566	3.386	23.3
673.6	23864.7						
27	-3.81840	-3.77224	2.87399	c	0.566	3.383	23.3
675.0	23913.9						
28	0.33993	-2.45309	3.67416	c	0.566	3.397	23.1
669.4	23716.8						
29	-5.18425	-4.92522	-7.30579	c	0.566	3.382	23.3
675.2	23923.4						
30	-6.72832	-1.23992	-5.38158	c	0.566	3.386	23.3
673.6	23863.7						
31	-5.30984	-7.45332	-2.57201	c	0.566	3.382	23.3
675.3	23924.7						
32	-6.85530	-3.77002	-0.64579	c	0.566	3.387	23.3
673.3	23854.9						
33	5.51969	-1.53249	-5.20711	c	0.566	3.385	23.3
674.0	23880.4						
34	3.97622	2.15414	-3.28215	c	0.566	3.391	23.2
671.8	23802.9						
35	5.39869	-4.06045	-0.47370	c	0.566	3.384	23.3
674.4	23893.0						
36	3.85501	-0.37102	1.45642	c	0.566	3.385	23.3
674.0	23877.8						
37	-0.14086	-5.08206	-9.13374	c	0.566	3.382	23.3
675.2	23921.8						
38	-0.34539	-9.17505	-1.47714	c	0.566	3.382	23.4
675.4	23928.7						
39	2.42821	-4.26804	-8.63168	c	0.566	3.382	23.4
675.3	23926.3						
40	2.22580	-8.35958	-0.97222	c	0.566	3.382	23.3
675.3	23923.7						
41	-3.55915	3.07032	-4.88019	c	0.566	3.382	23.4
675.3	23926.7						
42	-3.76377	-1.02864	2.78421	c	0.566	3.385	23.3
674.0	23879.6						
43	-0.98682	3.88678	-4.37609	c	0.566	3.382	23.3
675.3	23924.7						
44	-1.19087	-0.21540	3.28175	c	0.566	3.392	23.2
671.3	23783.7						
45	-4.14224	-2.76670	-8.64346	c	0.566	3.382	23.3
675.2	23922.3						
46	3.99496	-0.18793	-7.04922	c	0.566	3.383	23.3
674.8	23908.3						
47	-5.09964	-0.48869	-7.45430	c	0.566	3.381	23.4
675.5	23933.9						
48	3.04164	2.09331	-5.85870	c	0.566	3.383	23.3
675.0	23915.7						
49	-4.37461	-7.38922	0.00748	c	0.566	3.381	23.4
675.7	23940.4						
50	3.76297	-4.80836	1.59888	c	0.566	3.387	23.3
673.2	23850.2						
51	-5.33328	-5.11345	1.20023	c	0.566	3.381	23.4
675.7	23939.8						
52	2.80432	-2.52856	2.78328	c	0.566	3.399	23.1
668.6	23688.4						

53	-3.71401	-7.06657	-6.92048	c	0.566	3.382	23.4
675.3	23926.1						
54	-6.73107	0.14383	-3.15416	c	0.566	3.392	23.2
671.3	23783.1						
55	-3.77892	-8.35895	-4.50361	c	0.566	3.381	23.4
675.5	23932.1						
56	-6.78762	-1.15123	-0.73790	c	0.566	3.401	23.1
667.8	23660.7						
57	5.47505	-4.15535	-5.12233	c	0.566	3.383	23.3
674.9	23911.6						
58	2.44604	3.05525	-1.35243	c	0.566	3.392	23.2
671.4	23788.8						
59	5.41228	-5.44804	-2.70369	c	0.566	3.383	23.3
675.0	23913.6						
60	2.38265	1.76614	1.06812	c	0.566	3.391	23.2
671.9	23805.7						
61	5.72254	7.60652	1.96689	c	0.566	3.247	24.7
715.1	25336.7						
62	7.54288	6.94561	2.59147	h	0.366	1.018	3.1
37.3	551.9						
63	1.74638	5.12660	7.02185	c	0.566	3.310	24.2
699.3	24776.5						
64	4.07150	6.66112	6.36142	c	0.566	4.146	18.2
527.7	18694.9						
65	3.24948	-7.24520	8.97480	c	0.566	3.273	24.5
709.2	25126.2						
66	-7.56917	4.86120	7.93127	c	0.566	4.102	18.3
528.1	18711.1						
67	-9.29848	5.96078	7.73255	h	0.366	1.000	3.1
37.4	553.2						
68	-7.40056	4.37365	9.92447	h	0.366	1.000	3.1
37.4	553.2						
69	-7.77533	3.12328	6.84430	h	0.366	1.000	3.1
37.4	553.2						
70	-0.62818	6.05074	6.28362	c	0.566	3.363	23.6
682.2	24171.1						
71	5.45557	8.54214	-0.48405	c	0.566	3.185	25.1
726.2	25729.3						
72	-13.63811	-6.60085	0.92371	c	0.566	4.063	18.3
528.7	18730.5						
73	-11.71450	-7.13713	1.42236	h	0.366	0.997	3.1
37.4	553.5						
74	-14.41352	-7.89079	-0.47081	h	0.366	0.997	3.1
37.4	553.5						
75	-14.80166	-6.57595	2.62014	h	0.366	0.997	3.1
37.4	553.5						
76	-13.65758	-4.45502	-7.27650	c	0.566	4.062	18.3
528.7	18731.1						
77	-14.71382	-3.59363	-8.81797	h	0.366	0.997	3.1
37.4	553.5						
78	-14.85650	-5.81568	-6.30341	h	0.366	0.997	3.1
37.4	553.5						
79	-11.94908	-5.35401	-7.97082	h	0.366	0.997	3.1
37.4	553.4						
80	-0.28547	1.56818	9.10465	c	0.566	3.182	25.1
726.6	25741.8						
81	-2.60998	2.77293	8.71393	c	0.566	3.243	24.8
716.0	25367.5						
82	-4.29945	1.86590	9.41033	h	0.366	1.008	3.1
37.3	552.6						

83	-2.81084	5.01037	7.38476	c	0.566	3.315	24.1
698.0	24728.7						
84	-5.28620	6.41388	7.08392	c	0.566	4.148	18.2
527.7	18694.3						
85	-5.40447	7.15144	4.32351	c	0.566	3.317	24.1
697.4	24708.7						
86	-7.57848	6.86122	2.89717	c	0.566	3.252	24.7
714.2	25303.0						
87	-9.22812	6.08449	3.79537	h	0.366	1.021	3.1
37.3	551.6						
88	-7.67488	7.55003	0.35000	c	0.566	3.187	25.1
725.8	25715.1						
89	-5.63313	8.95024	-0.58609	c	0.566	3.238	24.8
717.0	25401.6						
90	-5.74675	9.67442	-2.49011	h	0.366	1.007	3.1
37.3	552.6						
91	-3.45681	9.33037	0.80917	c	0.566	3.310	24.2
699.6	24785.5						
92	-1.32746	11.02419	-0.07226	c	0.566	4.146	18.2
527.7	18694.9						
93	1.11511	9.66455	0.54500	c	0.566	3.307	24.2
700.4	24816.3						
94	3.15409	9.68742	-1.08809	c	0.566	3.240	24.8
716.6	25387.1						
95	2.95626	10.54275	-2.92911	h	0.366	1.008	3.1
37.3	552.6						
96	-9.62897	6.74390	-1.38613	c	0.566	3.272	24.5
709.7	25142.4						
97	-9.66867	7.70366	-3.19703	h	0.366	1.010	3.1
37.3	552.5						
98	-11.16780	4.72864	-1.14238	c	0.566	3.097	25.5
736.1	26079.1						
99	3.72240	7.54233	3.65697	c	0.566	3.308	24.2
700.0	24800.5						
100	-12.68103	0.16441	-0.22940	c	0.566	3.276	24.5
708.5	25102.6						
101	-13.46032	0.65578	-2.59500	c	0.566	3.262	24.6
711.8	25217.7						
102	1.88330	2.90274	8.39939	c	0.566	3.240	24.8
716.6	25388.8						
103	3.71631	2.19610	8.91976	h	0.366	1.019	3.1
37.3	551.8						
104	-14.60877	-1.19363	-4.40899	c	0.566	3.213	25.0
721.7	25569.5						
105	-3.23374	8.16468	3.18868	c	0.566	3.363	23.6
682.4	24176.1						
106	1.33500	8.40389	2.87751	c	0.566	3.351	23.7
686.4	24317.8						
107	-5.18145	8.84519	8.71072	c	0.566	4.106	18.3
528.1	18709.3						
108	-6.90965	9.94038	8.45287	h	0.366	0.999	3.1
37.4	553.3						
109	-3.58135	10.02928	8.18532	h	0.366	1.000	3.1
37.4	553.2						
110	-4.99542	8.35377	10.70474	h	0.366	0.999	3.1
37.4	553.3						
111	-12.74943	-2.25191	1.14110	c	0.566	3.228	24.9
719.0	25473.7						
112	-1.42203	13.49257	1.50433	c	0.566	4.109	18.3
528.0	18708.0						

113	-3.20473	14.47499	1.17365	h	0.366	0.999	3.1
37.4	553.3						
114	0.13581	14.73235	0.96718	h	0.366	0.999	3.1
37.4	553.3						
115	-1.26696	13.09540	3.51855	h	0.366	1.000	3.1
37.4	553.2						
116	-1.54896	11.73542	-2.86302	c	0.566	4.100	18.3
528.1	18711.6						
117	-3.32012	12.72603	-3.20766	h	0.366	1.000	3.1
37.4	553.2						
118	-1.47135	10.07954	-4.08750	h	0.366	0.999	3.1
37.4	553.3						
119	-0.03599	13.02243	-3.40187	h	0.366	1.000	3.1
37.4	553.2						
120	4.13856	9.02027	8.09551	c	0.566	4.107	18.3
528.1	18709.0						
121	5.75577	10.20577	7.61369	h	0.366	0.999	3.1
37.4	553.3						
122	4.29848	8.44232	10.06855	h	0.366	0.999	3.1
37.4	553.3						
123	2.42654	10.14562	7.88817	h	0.366	1.000	3.1
37.4	553.2						
124	6.52540	5.18248	6.74845	c	0.566	4.102	18.3
528.1	18710.9						
125	6.60405	3.49662	5.56700	h	0.366	1.000	3.1
37.4	553.2						
126	6.71624	4.61161	8.71646	h	0.366	1.000	3.1
37.4	553.2						
127	8.15747	6.36121	6.32187	h	0.366	1.000	3.1
37.4	553.2						
128	-0.32548	-1.00080	10.04009	c	0.566	3.275	24.5
708.7	25108.3						
129	-2.15034	-1.64158	10.72104	h	0.366	1.011	3.1
37.3	552.4						
130	1.48377	-2.78666	9.89534	c	0.566	3.094	25.5
736.3	26087.1						
131	5.01594	-5.65021	8.08812	c	0.566	3.277	24.5
708.3	25093.6						
132	7.25794	-6.48523	6.66692	c	0.566	3.205	25.0
723.1	25617.8						
133	10.84199	-5.09170	4.41979	c	0.566	4.062	18.3
528.7	18730.9						
134	12.21035	-6.02406	5.64285	h	0.366	0.997	3.1
37.4	553.5						
135	11.56389	-3.30605	3.72346	h	0.366	0.998	3.1
37.4	553.4						
136	10.37361	-6.34525	2.85708	h	0.366	0.997	3.1
37.4	553.4						
137	3.24479	-10.05578	8.62739	c	0.566	3.214	24.9
721.6	25564.8						
138	2.82667	-13.28791	5.61051	c	0.566	4.063	18.3
528.7	18730.7						
139	2.27254	-13.40174	3.63794	h	0.366	0.997	3.1
37.4	553.5						
140	1.55325	-14.38713	6.79521	h	0.366	0.997	3.1
37.4	553.5						
141	4.75834	-13.94974	5.86472	h	0.366	0.997	3.1
37.4	553.5						
142	7.36417	8.32016	-2.43402	c	0.566	3.273	24.5
709.3	25128.7						

143	7.17391	9.60321	-4.02201	h	0.366	1.010	3.1
37.3	552.5						
144	9.21195	6.58218	-2.61870	c	0.566	3.093	25.5
736.4	26089.7						
145	11.55815	2.29425	-2.60575	c	0.566	3.275	24.5
708.7	25109.1						
146	12.28745	3.41316	-4.76947	c	0.566	3.260	24.6
712.4	25239.1						
147	12.14537	-0.33258	-1.78221	c	0.566	3.221	24.9
720.3	25519.6						
148	12.21951	-4.59334	-3.04154	c	0.566	4.065	18.3
528.6	18729.4						
149	11.24847	-5.27621	-1.36420	h	0.366	0.998	3.1
37.4	553.4						
150	14.25596	-4.73305	-2.78490	h	0.366	0.997	3.1
37.4	553.5						
151	11.61695	-5.64691	-4.69461	h	0.366	0.997	3.1
37.4	553.4						
152	14.05880	2.27892	-6.61672	c	0.566	3.203	25.0
723.4	25629.2						
153	15.73953	2.69868	-10.71789	c	0.566	4.060	18.3
528.7	18732.5						
154	15.31526	0.75483	-11.24355	h	0.366	0.997	3.1
37.4	553.5						
155	17.67350	2.80633	-10.02235	h	0.366	0.997	3.1
37.4	553.5						
156	15.46616	3.95910	-12.31360	h	0.366	0.997	3.1
37.4	553.5						
157	-0.83938	7.94297	4.38675	n	0.495	3.233	15.6
344.0	9297.1						
158	-12.80903	-2.55363	-5.53270	o	0.473	2.053	10.4
209.8	5186.5						
159	-16.83298	-1.33292	-4.83782	o	0.473	1.054	12.8
257.7	6369.5						
160	-13.64410	-4.16114	-0.26512	o	0.473	2.054	10.4
209.8	5186.4						
161	-12.05663	-2.46815	3.30698	o	0.473	1.075	12.7
257.3	6360.2						
162	7.83558	-8.66550	6.31767	o	0.473	1.061	12.8
257.5	6366.5						
163	8.59203	-4.49968	5.82437	o	0.473	2.073	10.4
209.7	5184.6						
164	3.59412	-11.52959	10.31836	o	0.473	1.055	12.8
257.6	6369.0						
165	2.67919	-10.65161	6.24639	o	0.473	2.052	10.4
209.8	5186.5						
166	12.97106	-0.82871	0.28405	o	0.473	1.063	12.8
257.5	6365.8						
167	11.53057	-2.01574	-3.54409	o	0.473	2.054	10.4
209.8	5186.4						
168	15.42524	0.50462	-6.20579	o	0.473	1.058	12.8
257.6	6367.9						
169	14.00486	3.55474	-8.81322	o	0.473	2.070	10.4
209.7	5184.9						
170	-11.39142	2.70401	1.49055	s	0.737	2.653	125.8
6163.7	369906.8						
171	-13.12402	3.74168	-3.67226	s	0.737	2.603	125.8
6163.7	369907.5						
172	0.79242	-5.95672	10.72149	s	0.737	2.605	125.8
6163.7	369907.4						

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173 4.59764 -2.42023 8.78549 s 0.737 2.616 125.8
6163.7 369907.3
174 9.80088 4.09669 -0.47037 s 0.737 2.626 125.8
6163.7 369907.1
175 11.29240 6.53993 -5.23054 s 0.737 2.598 125.8
6163.7 369907.6
```

molecular C6(AA) [au] = 521090.20

DFT-D V3(BJ)

DF b3-lyp

parameters

```
s6 : 1.0000
s8 : 1.9889
a1 : 0.3981
a2 : 4.4211
k1-k3 : 16.0000 1.3333 -4.0000
Cutoff : 94.8683 a.u.
CN-Cutoff: 40.0000 a.u.
```

Edisp /kcal,au: -464.1476 -0.73966625

E6 /kcal : -219.4344

E8 /kcal : -252.1836

E6(ABC) " : 7.470425

% E8 : 54.33

% E6(ABC) : -1.61

normal termination of dftd3

=====
1_C60_ox1

```
|           DFTD3 V3.1 Rev 0           |
| S.Grimme, University Bonn           |
|           June 2014                 |
| see dftd3 -h for options           |
```

Please cite DFT-D3 work done with this code as:
S. Grimme, J. Antony, S. Ehrlich and H. Krieg,
J. Chem. Phys. 132 (2010), 154104
If used with BJ-damping cite also
S. Grimme, S. Ehrlich and L. Goerigk,
J. Comput. Chem. 32 (2011), 1456-1465
For DFT-D2 the reference is
S. Grimme, J. Comput. Chem., 27 (2006), 1787-1799

files read :

BG33_C60_plm2.xyz

C6 coefficients used:

```
2 C6 for element 1
Z= 1 CN= 0.912 C6(AA)= 3.03
Z= 1 CN= 0.000 C6(AA)= 7.59
5 C6 for element 6
Z= 6 CN= 0.000 C6(AA)= 49.11
Z= 6 CN= 0.987 C6(AA)= 43.25
Z= 6 CN= 1.998 C6(AA)= 29.36
```

Z=	6	CN=	2.999	C6(AA)=	25.78	
Z=	6	CN=	3.984	C6(AA)=	18.21	
			4	C6 for element		7
Z=	7	CN=	0.000	C6(AA)=	25.27	
Z=	7	CN=	0.994	C6(AA)=	22.12	
Z=	7	CN=	2.014	C6(AA)=	19.68	
Z=	7	CN=	2.990	C6(AA)=	15.58	
			3	C6 for element		8
Z=	8	CN=	0.000	C6(AA)=	15.51	
Z=	8	CN=	0.993	C6(AA)=	12.82	
Z=	8	CN=	1.989	C6(AA)=	10.37	
			3	C6 for element		16
Z=	16	CN=	0.000	C6(AA)=	134.01	
Z=	16	CN=	0.995	C6(AA)=	131.00	
Z=	16	CN=	1.990	C6(AA)=	125.81	

#	XYZ [au]			R0(AA) [Ang.]	CN	C6(AA)	
C8(AA)	C10(AA)	[au]					
1	1.45020	-8.80602	-4.68536	c	0.566	3.382	23.3
675.1	23919.2						
2	3.67625	-7.43878	-4.93127	c	0.566	3.382	23.3
675.2	23921.9						
3	-4.81261	2.05963	-0.83460	c	0.566	3.391	23.2
671.7	23797.2						
4	-2.59139	3.43239	-1.08142	c	0.566	3.389	23.3
672.5	23826.2						
5	-1.45636	-2.43201	-9.50288	c	0.566	3.383	23.3
675.0	23913.0						
6	-2.70973	-0.25829	-8.73582	c	0.566	3.382	23.3
675.2	23921.7						
7	1.56607	-5.12001	2.97052	c	0.566	3.394	23.2
670.8	23765.9						
8	0.31312	-2.94841	3.74024	c	0.566	3.395	23.2
670.1	23740.2						
9	-6.43601	-5.84597	-3.51774	c	0.566	3.383	23.3
674.8	23906.5						
10	-5.83097	-6.38499	-1.02079	c	0.566	3.383	23.3
674.9	23909.9						
11	4.69305	1.00391	-4.74657	c	0.566	3.386	23.3
673.6	23865.0						
12	5.28540	0.45787	-2.25091	c	0.566	3.399	23.1
668.5	23685.9						
13	-0.62867	-8.36455	-6.41714	c	0.566	3.383	23.3
674.9	23910.9						
14	0.39534	-9.27458	-2.19727	c	0.566	3.383	23.3
675.1	23917.0						
15	3.92264	-5.56598	-6.92022	c	0.566	3.383	23.3
675.0	23915.7						
16	4.94688	-6.47786	-2.69912	c	0.566	3.382	23.4
675.4	23929.8						
17	-6.08678	1.09818	-3.06461	c	0.566	3.387	23.3
673.3	23853.5						
18	-5.05398	0.18420	1.15389	c	0.566	3.393	23.2
670.9	23771.0						
19	-1.53595	3.90967	-3.56962	c	0.566	3.382	23.3
675.1	23918.8						
20	-0.50988	2.98266	0.64704	c	0.566	3.397	23.2
669.6	23723.5						
21	-2.48687	-4.89879	-8.89353	c	0.566	3.383	23.3
674.9	23910.2						

22	1.27431	-2.58333	-9.30678	c	0.566	3.383	23.3
674.9	23910.4						
23	-5.05121	-0.45371	-7.32137	c	0.566	3.382	23.4
675.4	23927.6						
24	-1.28835	1.86386	-7.73754	c	0.566	3.381	23.4
675.7	23940.7						
25	0.14776	-7.24331	1.97498	c	0.566	3.384	23.3
674.7	23903.4						
26	3.91007	-4.92467	1.55691	c	0.566	3.390	23.2
672.3	23820.6						
27	-2.41847	-2.79757	3.55577	c	0.566	3.384	23.3
674.6	23900.8						
28	1.34287	-0.48036	3.12724	c	0.566	3.397	23.2
669.7	23725.6						
29	-4.97353	-6.95892	-5.55197	c	0.566	3.383	23.3
675.0	23916.3						
30	-7.09177	-3.28522	-4.25032	c	0.566	3.385	23.3
674.2	23885.0						
31	-3.73674	-8.06013	-0.44557	c	0.566	3.382	23.3
675.3	23925.5						
32	-5.85527	-4.38647	0.85693	c	0.566	3.384	23.3
674.5	23898.6						
33	4.71862	-0.99459	-6.62197	c	0.566	3.382	23.4
675.4	23927.9						
34	2.59836	2.68602	-5.32080	c	0.566	3.382	23.3
675.1	23919.4						
35	5.95386	-2.09692	-1.51407	c	0.566	3.386	23.3
673.7	23869.5						
36	3.82352	1.57214	-0.21712	c	0.566	3.395	23.2
670.3	23747.9						
37	-0.39313	-6.57368	-8.32037	c	0.566	3.383	23.3
674.9	23909.6						
38	1.61129	-8.35787	-0.05998	c	0.566	3.383	23.3
674.8	23909.3						
39	1.93125	-5.14317	-8.57639	c	0.566	3.383	23.3
675.0	23913.9						
40	3.93700	-6.92562	-0.31726	c	0.566	3.383	23.3
674.9	23911.4						
41	-5.07828	1.54801	-5.44736	c	0.566	3.382	23.4
675.4	23928.5						
42	-3.07378	-0.23459	2.81861	c	0.566	3.388	23.3
672.9	23839.8						
43	-2.75170	2.98111	-5.70477	c	0.566	3.382	23.4
675.5	23930.6						
44	-0.74692	1.19353	2.55423	c	0.566	3.396	23.2
670.0	23738.5						
45	-4.72718	-5.08726	-7.54152	c	0.566	3.383	23.3
675.0	23915.4						
46	2.63707	-0.55366	-8.35344	c	0.566	3.382	23.3
675.2	23922.8						
47	-6.03728	-2.81600	-6.73716	c	0.566	3.382	23.3
675.2	23921.8						
48	1.32731	1.71908	-7.54987	c	0.566	3.381	23.4
675.6	23937.5						
49	-2.46690	-7.09895	1.78849	c	0.566	3.381	23.4
675.5	23933.1						
50	4.89799	-2.56458	0.97443	c	0.566	3.388	23.3
673.1	23848.8						
51	-3.77710	-4.82774	2.59536	c	0.566	3.382	23.3
675.2	23922.4						

52	3.58444	-0.29215	1.77610	c	0.566	3.390	23.2
672.2	23813.9						
53	-2.96849	-8.56083	-5.00192	c	0.566	3.383	23.3
675.0	23916.3						
54	-7.11241	-1.37264	-2.45552	c	0.566	3.391	23.2
671.8	23799.8						
55	-2.33673	-9.12334	-2.39412	c	0.566	3.382	23.3
675.1	23919.9						
56	-6.47218	-1.93760	0.15035	c	0.566	3.396	23.2
669.8	23731.2						
57	5.34706	-3.44667	-5.92057	c	0.566	3.382	23.4
675.4	23929.4						
58	1.19807	3.75411	-3.37419	c	0.566	3.384	23.3
674.4	23892.9						
59	5.97577	-4.00967	-3.31148	c	0.566	3.386	23.3
673.8	23870.4						
60	1.82535	3.17763	-0.76687	c	0.566	3.394	23.2
670.8	23765.5						
61	5.28672	7.85273	2.16045	c	0.566	3.242	24.8
716.1	25372.3						
62	7.19043	7.27283	2.57948	h	0.366	1.017	3.1
37.3	551.9						
63	1.91048	4.74325	7.32011	c	0.566	3.306	24.2
700.7	24825.5						
64	4.05911	6.47886	6.57619	c	0.566	4.145	18.2
527.7	18695.1						
65	4.75139	-7.44615	8.20285	c	0.566	3.278	24.5
708.0	25084.9						
66	-7.30505	3.33724	8.48229	c	0.566	4.101	18.3
528.1	18711.2						
67	-9.16075	4.22266	8.40667	h	0.366	1.000	3.1
37.4	553.2						
68	-7.04008	2.71054	10.42373	h	0.366	1.000	3.1
37.4	553.2						
69	-7.31439	1.68640	7.24956	h	0.366	1.000	3.1
37.4	553.2						
70	-0.59486	5.45657	6.75105	c	0.566	3.354	23.7
685.4	24282.5						
71	4.74556	8.95457	-0.18809	c	0.566	3.184	25.1
726.3	25732.0						
72	-12.41929	-7.43086	0.39771	c	0.566	4.065	18.3
528.6	18729.5						
73	-11.13600	-7.66250	1.98821	h	0.366	0.997	3.1
37.4	553.5						
74	-11.82507	-8.57824	-1.19375	h	0.366	0.997	3.1
37.4	553.4						
75	-14.33584	-7.90719	0.97163	h	0.366	0.997	3.1
37.4	553.5						
76	-17.37216	-1.53883	-7.90928	c	0.566	4.058	18.3
528.8	18733.8						
77	-19.29184	-1.59846	-7.17289	h	0.366	0.997	3.1
37.4	553.5						
78	-16.70296	-3.45617	-8.23566	h	0.366	0.997	3.1
37.4	553.5						
79	-17.28069	-0.42919	-9.63134	h	0.366	0.997	3.1
37.4	553.5						
80	0.34306	0.92127	9.33726	c	0.566	3.186	25.1
726.0	25722.3						
81	-2.11503	1.91314	9.14648	c	0.566	3.243	24.8
716.0	25366.5						

82	-3.65879	0.80689	9.88745	h	0.366	1.008	3.1
37.3	552.6						
83	-2.61397	4.13902	7.90158	c	0.566	3.307	24.2
700.4	24816.3						
84	-5.25237	5.23066	7.74225	c	0.566	4.146	18.2
527.7	18694.7						
85	-5.56576	6.22015	5.08001	c	0.566	3.310	24.2
699.5	24782.8						
86	-7.77992	5.92565	3.73897	c	0.566	3.248	24.7
714.9	25328.4						
87	-9.29378	4.87054	4.59185	h	0.366	1.020	3.1
37.3	551.7						
88	-8.11437	6.98964	1.33069	c	0.566	3.186	25.1
726.0	25721.3						
89	-6.27593	8.73333	0.52974	c	0.566	3.239	24.8
716.8	25396.1						
90	-6.59694	9.74180	-1.21331	h	0.366	1.007	3.1
37.3	552.6						
91	-4.03836	9.06386	1.81239	c	0.566	3.309	24.2
699.8	24792.7						
92	-2.08953	10.99969	1.03168	c	0.566	4.147	18.2
527.7	18694.6						
93	0.45722	9.72628	1.28078	c	0.566	3.308	24.2
700.0	24800.9						
94	2.34287	10.04216	-0.48197	c	0.566	3.242	24.8
716.2	25376.0						
95	1.95498	11.07255	-2.19800	h	0.366	1.008	3.1
37.3	552.6						
96	-10.08251	6.30461	-0.39702	c	0.566	3.281	24.5
707.3	25057.3						
97	-10.28899	7.51407	-2.03803	h	0.366	1.010	3.1
37.3	552.4						
98	-11.47130	4.13862	-0.42135	c	0.566	3.095	25.5
736.2	26084.4						
99	3.44583	7.50399	3.97637	c	0.566	3.306	24.2
700.7	24826.2						
100	-12.93604	-0.51270	0.03162	c	0.566	3.278	24.5
708.1	25089.1						
101	-13.94947	0.26895	-2.16606	c	0.566	3.265	24.6
711.2	25197.2						
102	2.33437	2.50300	8.58316	c	0.566	3.246	24.7
715.5	25347.9						
103	4.25158	1.95801	8.97817	h	0.366	1.020	3.1
37.3	551.7						
104	-15.59154	-1.29416	-3.83111	c	0.566	3.201	25.0
723.7	25639.8						
105	-3.55638	7.57744	3.97760	c	0.566	3.360	23.6
683.5	24215.8						
106	0.93950	8.22233	3.43108	c	0.566	3.356	23.7
684.7	24256.7						
107	-5.40338	7.51165	9.58176	c	0.566	4.108	18.3
528.1	18708.4						
108	-7.25711	8.40163	9.44639	h	0.366	0.999	3.1
37.4	553.3						
109	-3.97232	8.92684	9.14732	h	0.366	1.000	3.1
37.4	553.3						
110	-5.11208	6.86984	11.51811	h	0.366	0.999	3.1
37.4	553.3						
111	-12.95005	-3.09459	1.17164	c	0.566	3.229	24.9
718.7	25464.2						

112	-2.18862	13.21764	2.95029	c	0.566	4.109	18.3
528.0	18708.1						
113	-4.03743	14.12507	2.87891	h	0.366	0.999	3.1
37.4	553.3						
114	-0.74344	14.61133	2.48597	h	0.366	0.999	3.1
37.4	553.3						
115	-1.86257	12.56599	4.87571	h	0.366	1.000	3.1
37.4	553.2						
116	-2.56328	12.07665	-1.60524	c	0.566	4.100	18.3
528.1	18711.7						
117	-4.39467	13.01212	-1.67673	h	0.366	1.000	3.1
37.4	553.2						
118	-2.51213	10.61596	-3.05806	h	0.366	0.999	3.1
37.4	553.3						
119	-1.15559	13.50673	-2.05995	h	0.366	1.000	3.1
37.4	553.2						
120	4.09083	8.73734	8.44989	c	0.566	4.107	18.3
528.1	18708.7						
121	5.57197	10.06868	7.92043	h	0.366	0.999	3.1
37.4	553.3						
122	4.45651	8.05815	10.36080	h	0.366	0.999	3.1
37.4	553.3						
123	2.29086	9.73740	8.45120	h	0.366	1.000	3.1
37.4	553.3						
124	6.63791	5.17525	6.68275	c	0.566	4.102	18.3
528.1	18710.9						
125	6.74061	3.56308	5.40406	h	0.366	1.000	3.1
37.4	553.2						
126	7.04125	4.52683	8.59285	h	0.366	1.000	3.1
37.4	553.2						
127	8.13586	6.49872	6.19733	h	0.366	1.000	3.1
37.4	553.2						
128	0.60696	-1.67408	10.05465	c	0.566	3.287	24.4
705.8	25004.5						
129	-1.07865	-2.55067	10.82182	h	0.366	1.011	3.1
37.3	552.4						
130	2.54253	-3.27683	9.50109	c	0.566	3.097	25.4
736.1	26077.7						
131	6.29323	-5.60619	7.37108	c	0.566	3.284	24.4
706.6	25034.9						
132	8.62550	-6.08933	5.91345	c	0.566	3.204	25.0
723.2	25622.9						
133	12.08165	-4.15112	3.86858	c	0.566	4.060	18.3
528.7	18732.6						
134	13.54035	-4.94339	5.08439	h	0.366	0.997	3.1
37.4	553.5						
135	12.56094	-2.25749	3.25619	h	0.366	0.998	3.1
37.4	553.4						
136	11.80218	-5.38692	2.24956	h	0.366	0.997	3.1
37.4	553.5						
137	5.10088	-10.22716	7.73110	c	0.566	3.212	25.0
721.8	25574.4						
138	4.90195	-13.36568	4.59272	c	0.566	4.061	18.3
528.7	18731.6						
139	4.22097	-13.47342	2.66103	h	0.366	0.997	3.1
37.4	553.5						
140	3.86492	-14.65541	5.81337	h	0.366	0.997	3.1
37.4	553.5						
141	6.91448	-13.77954	4.68656	h	0.366	0.997	3.1
37.4	553.5						

142	6.40454	8.94145	-2.33384	c	0.566	3.283	24.4
706.9	25043.6						
143	5.88617	10.21172	-3.85618	h	0.366	1.010	3.1
37.3	552.4						
144	8.33422	7.33073	-2.84475	c	0.566	3.093	25.5
736.4	26088.9						
145	11.09293	3.31737	-3.26114	c	0.566	3.278	24.5
708.0	25082.7						
146	11.34636	4.50252	-5.49768	c	0.566	3.262	24.6
711.8	25220.0						
147	12.01248	0.76189	-2.53068	c	0.566	3.226	24.9
719.4	25486.0						
148	12.61821	-3.42102	-3.90115	c	0.566	4.064	18.3
528.7	18729.9						
149	11.65927	-4.26802	-2.29169	h	0.366	0.997	3.1
37.4	553.4						
150	14.64271	-3.33328	-3.55089	h	0.366	0.997	3.1
37.4	553.5						
151	12.21908	-4.47429	-5.61426	h	0.366	0.997	3.1
37.4	553.5						
152	12.96049	3.61949	-7.63006	c	0.566	3.202	25.0
723.5	25633.5						
153	13.74972	4.13567	-11.98507	c	0.566	4.058	18.3
528.8	18733.7						
154	13.65549	2.11997	-12.38337	h	0.366	0.997	3.1
37.4	553.5						
155	15.70685	4.68030	-11.66252	h	0.366	0.997	3.1
37.4	553.5						
156	12.92790	5.22287	-13.51728	h	0.366	0.997	3.1
37.4	553.5						
157	-1.08369	7.35503	4.94547	n	0.495	3.239	15.6
344.0	9296.7						
158	-15.73226	-0.26877	-6.14228	o	0.473	2.071	10.4
209.7	5184.8						
159	-16.68769	-3.16853	-3.16804	o	0.473	1.056	12.8
257.6	6368.4						
160	-12.34216	-4.86177	-0.50201	o	0.473	2.051	10.4
209.8	5186.6						
161	-13.32752	-3.43275	3.39103	o	0.473	1.065	12.8
257.5	6364.7						
162	9.39752	-8.16912	5.39802	o	0.473	1.061	12.8
257.5	6366.5						
163	9.75035	-3.91944	5.26396	o	0.473	2.073	10.4
209.7	5184.6						
164	5.74713	-11.68728	9.33764	o	0.473	1.054	12.8
257.6	6369.4						
165	4.47346	-10.78546	5.36102	o	0.473	2.052	10.4
209.8	5186.6						
166	12.84941	0.31193	-0.45666	o	0.473	1.067	12.8
257.4	6363.9						
167	11.64832	-0.92062	-4.35363	o	0.473	2.053	10.4
209.8	5186.5						
168	14.71048	2.18879	-7.41668	o	0.473	1.056	12.8
257.6	6368.5						
169	12.24237	4.72274	-9.79215	o	0.473	2.070	10.4
209.7	5184.9						
170	-11.37952	1.74204	1.85172	s	0.737	2.679	125.8
6163.6	369906.5						
171	-13.44778	3.42630	-2.98362	s	0.737	2.628	125.8
6163.7	369907.1						

172	2.14522	-6.54154	9.94475	s	0.737	2.629	125.8
6163.7	369907.1						
173	5.43057	-2.49453	8.10616	s	0.737	2.643	125.8
6163.7	369906.9						
174	9.46065	4.91591	-0.88238	s	0.737	2.653	125.8
6163.7	369906.8						
175	9.85821	7.42910	-5.79334	s	0.737	2.627	125.8
6163.7	369907.1						

molecular C6(AA) [au] = 521057.60

DFT-D V3(BJ)

DF b3-lyp

parameters

s6 : 1.0000
s8 : 1.9889
a1 : 0.3981
a2 : 4.4211
k1-k3 : 16.0000 1.3333 -4.0000
Cutoff : 94.8683 a.u.
CN-Cutoff: 40.0000 a.u.

Edisp /kcal,au: -461.5410 -0.73551228

E6 /kcal : -217.8729
E8 /kcal : -251.0157
E6(ABC) " : 7.347630
% E8 : 54.39
% E6(ABC) : -1.59
normal termination of dftd3

=====

1_ox1

	DFTD3 V3.1 Rev 0	
	S.Grimme, University Bonn	
	June 2014	
	see dftd3 -h for options	

Please cite DFT-D3 work done with this code as:
S. Grimme, J. Antony, S. Ehrlich and H. Krieg,
J. Chem. Phys. 132 (2010), 154104
If used with BJ-damping cite also
S. Grimme, S. Ehrlich and L. Goerigk,
J. Comput. Chem. 32 (2011), 1456-1465
For DFT-D2 the reference is
S. Grimme, J. Comput. Chem., 27 (2006), 1787-1799

files read :
BG33_plm2.xyz

C6 coefficients used:

	2	C6 for element	1
Z=	1	CN= 0.912 C6(AA)=	3.03
Z=	1	CN= 0.000 C6(AA)=	7.59
	5	C6 for element	6
Z=	6	CN= 0.000 C6(AA)=	49.11

Z= 6	CN= 0.987	C6(AA)=	43.25	
Z= 6	CN= 1.998	C6(AA)=	29.36	
Z= 6	CN= 2.999	C6(AA)=	25.78	
Z= 6	CN= 3.984	C6(AA)=	18.21	
	4 C6 for element			7
Z= 7	CN= 0.000	C6(AA)=	25.27	
Z= 7	CN= 0.994	C6(AA)=	22.12	
Z= 7	CN= 2.014	C6(AA)=	19.68	
Z= 7	CN= 2.990	C6(AA)=	15.58	
	3 C6 for element			8
Z= 8	CN= 0.000	C6(AA)=	15.51	
Z= 8	CN= 0.993	C6(AA)=	12.82	
Z= 8	CN= 1.989	C6(AA)=	10.37	
	3 C6 for element			16
Z= 16	CN= 0.000	C6(AA)=	134.01	
Z= 16	CN= 0.995	C6(AA)=	131.00	
Z= 16	CN= 1.990	C6(AA)=	125.81	

#	XYZ [au]				R0(AA) [Ang.]	CN	C6(AA)
C8(AA)	C10(AA) [au]						
1	-4.51145	-4.71583	3.12272	c	0.566	3.251	24.7
714.4	25310.9						
2	-6.45751	-4.19528	3.40303	h	0.366	1.020	3.1
37.3	551.7						
3	-1.48248	1.32155	4.32100	c	0.566	3.309	24.2
699.7	24791.1						
4	-3.29190	-0.65346	5.30859	c	0.566	4.149	18.2
527.6	18694.1						
5	-7.18073	11.57118	-0.53796	c	0.566	3.269	24.6
710.3	25165.6						
6	7.41766	4.04226	3.08454	c	0.566	4.098	18.3
528.2	18712.6						
7	9.37636	3.60217	3.53012	h	0.366	1.000	3.1
37.4	553.2						
8	7.02231	5.84788	3.98607	h	0.366	1.000	3.1
37.4	553.2						
9	7.24360	4.26926	1.04436	h	0.366	0.999	3.1
37.4	553.3						
10	1.08064	0.66813	3.98909	c	0.566	3.349	23.8
687.1	24343.2						
11	-3.93732	-7.07046	2.05364	c	0.566	3.181	25.1
726.7	25746.2						
12	21.08211	5.85414	-3.35402	c	0.566	4.059	18.3
528.7	18732.9						
13	20.03010	6.97891	-4.71761	h	0.366	0.996	3.1
37.4	553.5						
14	23.00388	5.53511	-3.99469	h	0.366	0.997	3.1
37.4	553.5						
15	21.06872	6.79797	-1.52692	h	0.366	0.997	3.1
37.4	553.5						
16	22.57009	-1.24240	-7.80429	c	0.566	4.062	18.3
528.7	18731.4						
17	23.24866	-3.18378	-7.79844	h	0.366	0.997	3.1
37.4	553.5						
18	23.96124	-0.02649	-6.89992	h	0.366	0.997	3.1
37.4	553.5						
19	22.17132	-0.60927	-9.71329	h	0.366	0.997	3.1
37.4	553.5						
20	-0.53319	5.66326	3.14303	c	0.566	3.180	25.1
726.9	25755.2						

21	2.05138	5.04394	3.24298	c	0.566	3.230	24.8
718.5	25457.1						
22	3.40970	6.52701	2.90538	h	0.366	1.007	3.1
37.3	552.7						
23	2.88276	2.61638	3.69606	c	0.566	3.295	24.3
703.5	24925.6						
24	5.64460	1.99685	4.10260	c	0.566	4.143	18.2
527.7	18695.7						
25	6.15199	-0.58749	2.97938	c	0.566	3.295	24.3
703.6	24927.1						
26	8.47272	-1.15639	1.93773	c	0.566	3.238	24.8
716.9	25400.5						
27	9.84354	0.33528	1.80690	h	0.366	1.025	3.1
37.2	551.3						
28	9.10304	-3.59816	1.11859	c	0.566	3.171	25.2
728.2	25798.4						
29	7.30577	-5.50460	1.56495	c	0.566	3.238	24.8
717.0	25401.0						
30	7.80473	-7.41785	1.06817	h	0.366	1.007	3.1
37.3	552.6						
31	4.96781	-5.02291	2.60087	c	0.566	3.292	24.4
704.6	24963.0						
32	3.19386	-7.15055	3.32659	c	0.566	4.142	18.2
527.7	18696.0						
33	0.50877	-6.24510	2.93934	c	0.566	3.296	24.3
703.4	24922.5						
34	-1.39898	-7.84070	2.14897	c	0.566	3.230	24.8
718.7	25461.2						
35	-0.94215	-9.73137	1.53636	h	0.366	1.007	3.1
37.3	552.7						
36	11.44094	-4.29047	-0.06354	c	0.566	3.280	24.5
707.6	25068.0						
37	11.66761	-6.29770	-0.41121	h	0.366	1.011	3.1
37.3	552.4						
38	13.39832	-2.81239	-0.84402	c	0.566	3.085	25.5
737.0	26112.5						
39	-2.66103	-3.07425	3.93174	c	0.566	3.309	24.2
699.6	24787.4						
40	16.59682	0.69560	-2.12800	c	0.566	3.274	24.5
709.0	25118.5						
41	17.68709	-1.48059	-2.85781	c	0.566	3.258	24.6
712.8	25253.0						
42	-2.23991	3.76695	3.86799	c	0.566	3.250	24.7
714.6	25316.6						
43	-4.19589	4.23746	4.15440	h	0.366	1.023	3.1
37.2	551.5						
44	20.24192	-1.78329	-4.06750	c	0.566	3.215	24.9
721.4	25556.9						
45	4.30384	-2.50056	3.18033	c	0.566	3.337	23.9
691.2	24487.4						
46	-0.10239	-3.73738	3.60648	c	0.566	3.349	23.8
687.1	24343.8						
47	6.06898	1.78770	7.00293	c	0.566	4.111	18.3
528.0	18707.0						
48	8.02937	1.28317	7.38863	h	0.366	0.999	3.1
37.4	553.3						
49	4.85358	0.35038	7.83857	h	0.366	1.000	3.1
37.4	553.3						
50	5.65240	3.59292	7.90528	h	0.366	0.999	3.1
37.4	553.3						

51	17.59186	3.29742	-2.31594	c	0.566	3.223	24.9
719.8	25503.6						
52	3.53982	-7.63307	6.20426	c	0.566	4.112	18.3
528.0	18707.0						
53	5.47204	-8.23944	6.58590	h	0.366	0.999	3.1
37.4	553.3						
54	2.24006	-9.10385	6.83230	h	0.366	0.999	3.1
37.4	553.3						
55	3.16799	-5.92994	7.30057	h	0.366	1.000	3.1
37.4	553.3						
56	3.75818	-9.62001	1.93349	c	0.566	4.097	18.3
528.2	18713.0						
57	5.66126	-10.27398	2.35662	h	0.366	1.000	3.1
37.4	553.2						
58	3.56868	-9.41356	-0.10781	h	0.366	0.999	3.1
37.4	553.3						
59	2.48787	-11.10817	2.56705	h	0.366	1.000	3.1
37.4	553.2						
60	-2.73489	-1.05662	8.16193	c	0.566	4.108	18.3
528.0	18708.3						
61	-3.95520	-2.53809	8.91200	h	0.366	0.999	3.1
37.4	553.3						
62	-3.09170	0.68807	9.19897	h	0.366	0.999	3.1
37.4	553.3						
63	-0.77703	-1.60886	8.47949	h	0.366	1.000	3.1
37.4	553.3						
64	-6.06516	0.11451	5.03665	c	0.566	4.101	18.3
528.1	18711.2						
65	-6.59465	0.43259	3.07129	h	0.366	1.000	3.1
37.4	553.3						
66	-6.44586	1.83175	6.10380	h	0.366	1.000	3.1
37.4	553.2						
67	-7.29546	-1.33604	5.82047	h	0.366	1.000	3.1
37.4	553.2						
68	-1.29504	8.13714	2.34791	c	0.566	3.274	24.5
709.1	25121.4						
69	0.17946	9.55867	2.28107	h	0.366	1.009	3.1
37.3	552.5						
70	-3.62147	8.87330	1.51640	c	0.566	3.090	25.5
736.7	26099.6						
71	-8.18294	9.24782	-0.29629	c	0.566	3.275	24.5
708.9	25115.4						
72	-10.80205	8.57231	-1.01945	c	0.566	3.198	25.0
724.2	25656.8						
73	-13.66878	5.15705	-1.36871	c	0.566	4.054	18.3
528.8	18736.0						
74	-15.03449	5.99086	-0.07538	h	0.366	0.996	3.1
37.4	553.5						
75	-13.57880	3.12115	-1.13812	h	0.366	0.997	3.1
37.4	553.4						
76	-14.16673	5.66258	-3.30007	h	0.366	0.997	3.1
37.4	553.5						
77	-8.51549	13.86102	-1.56559	c	0.566	3.213	25.0
721.8	25571.6						
78	-10.31852	15.67884	-5.18362	c	0.566	4.062	18.3
528.7	18731.0						
79	-10.35524	15.24734	-7.18780	h	0.366	0.997	3.1
37.4	553.5						
80	-9.42197	17.49652	-4.83584	h	0.366	0.997	3.1
37.4	553.5						

81	-12.21848	15.67411	-4.39613	h	0.366	0.997	3.1
37.4	553.5						
82	-5.81125	-8.69259	0.93771	c	0.566	3.272	24.5
709.5	25136.6						
83	-5.29757	-10.66510	0.72526	h	0.366	1.009	3.1
37.3	552.5						
84	-8.09646	-8.00317	-0.01159	c	0.566	3.089	25.5
736.7	26101.3						
85	-11.92588	-5.65811	-2.02544	c	0.566	3.269	24.6
710.3	25165.1						
86	-12.39013	-8.12503	-2.44055	c	0.566	3.258	24.6
712.8	25253.9						
87	-13.42678	-3.41945	-2.84494	c	0.566	3.225	24.9
719.5	25490.3						
88	-15.95715	-1.68405	-6.05395	c	0.566	4.061	18.3
528.7	18731.5						
89	-14.94462	0.10648	-6.09461	h	0.366	0.997	3.1
37.4	553.5						
90	-17.59502	-1.53364	-4.81901	h	0.366	0.997	3.1
37.4	553.5						
91	-16.52160	-2.24603	-7.94316	h	0.366	0.997	3.1
37.4	553.5						
92	-14.73596	-9.18192	-3.59095	c	0.566	3.202	25.0
723.5	25633.8						
93	-16.44723	-12.79110	-5.56753	c	0.566	4.057	18.3
528.8	18734.0						
94	-17.20159	-11.73195	-7.16104	h	0.366	0.996	3.1
37.4	553.5						
95	-17.90540	-13.00380	-4.13240	h	0.366	0.997	3.1
37.4	553.5						
96	-15.74053	-14.61824	-6.17335	h	0.366	0.997	3.1
37.4	553.5						
97	1.80708	-1.89035	3.87972	n	0.495	3.235	15.6
344.0	9297.0						
98	20.19241	-1.07260	-6.47608	o	0.473	2.046	10.4
209.8	5187.2						
99	22.02004	-2.65359	-2.96183	o	0.473	1.056	12.8
257.6	6368.5						
100	19.97499	3.37466	-3.13400	o	0.473	2.051	10.4
209.8	5186.7						
101	16.34379	5.11826	-1.73465	o	0.473	1.075	12.7
257.3	6360.5						
102	-12.37727	10.07010	-1.69072	o	0.473	1.058	12.8
257.6	6367.9						
103	-11.16669	6.07639	-0.79035	o	0.473	2.074	10.4
209.7	5184.5						
104	-9.07499	15.62276	-0.25068	o	0.473	1.057	12.8
257.6	6368.3						
105	-8.86191	13.67303	-4.04134	o	0.473	2.046	10.4
209.8	5187.2						
106	-13.65539	-1.56555	-1.53116	o	0.473	1.067	12.8
257.4	6363.8						
107	-14.31713	-3.67075	-5.17266	o	0.473	2.049	10.4
209.8	5186.9						
108	-16.75340	-8.14147	-3.59147	o	0.473	1.055	12.8
257.6	6368.8						
109	-14.29080	-11.49201	-4.52316	o	0.473	2.069	10.4
209.7	5185.0						
110	13.62764	0.47725	-0.67129	s	0.737	2.636	125.8
6163.7	369907.0						

111	16.05669	-4.24284	-2.22981	s	0.737	2.628	125.8
6163.7	369907.1						
112	-4.15043	12.01600	0.60268	s	0.737	2.617	125.8
6163.7	369907.2						
113	-6.27540	6.93893	1.11462	s	0.737	2.633	125.8
6163.7	369907.0						
114	-9.25235	-4.90044	-0.25312	s	0.737	2.641	125.8
6163.7	369906.9						
115	-10.17517	-10.26690	-1.25993	s	0.737	2.616	125.8
6163.7	369907.3						

molecular C6(AA) [au] = 186988.06

DFT-D V3(BJ)

DF b3-lyp

parameters

s6 : 1.0000
s8 : 1.9889
a1 : 0.3981
a2 : 4.4211
k1-k3 : 16.0000 1.3333 -4.0000
Cutoff : 94.8683 a.u.
CN-Cutoff: 40.0000 a.u.

Edisp /kcal,au: -202.6191 -0.32289412

E6 /kcal : -93.2142

E8 /kcal : -109.5781

E6(ABC) " : 0.173210

% E8 : 54.08

% E6(ABC) : -0.09

normal termination of dftd3

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1_red1

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|           DFTD3 V3.1 Rev 0           |
| S.Grimme, University Bonn           |
|           June 2014                 |
| see dftd3 -h for options           |

```

Please cite DFT-D3 work done with this code as:
S. Grimme, J. Antony, S. Ehrlich and H. Krieg,
J. Chem. Phys. 132 (2010), 154104
If used with BJ-damping cite also
S. Grimme, S. Ehrlich and L. Goerigk,
J. Comput. Chem. 32 (2011), 1456-1465
For DFT-D2 the reference is
S. Grimme, J. Comput. Chem., 27 (2006), 1787-1799

files read :

BG33_mlm2.xyz

C6 coefficients used:

	2	C6 for element	1
Z=	1	CN= 0.912	C6(AA)= 3.03
Z=	1	CN= 0.000	C6(AA)= 7.59

	5	C6 for element	6
Z=	6	CN= 0.000 C6(AA)= 49.11	
Z=	6	CN= 0.987 C6(AA)= 43.25	
Z=	6	CN= 1.998 C6(AA)= 29.36	
Z=	6	CN= 2.999 C6(AA)= 25.78	
Z=	6	CN= 3.984 C6(AA)= 18.21	
	4	C6 for element	7
Z=	7	CN= 0.000 C6(AA)= 25.27	
Z=	7	CN= 0.994 C6(AA)= 22.12	
Z=	7	CN= 2.014 C6(AA)= 19.68	
Z=	7	CN= 2.990 C6(AA)= 15.58	
	3	C6 for element	8
Z=	8	CN= 0.000 C6(AA)= 15.51	
Z=	8	CN= 0.993 C6(AA)= 12.82	
Z=	8	CN= 1.989 C6(AA)= 10.37	
	3	C6 for element	16
Z=	16	CN= 0.000 C6(AA)= 134.01	
Z=	16	CN= 0.995 C6(AA)= 131.00	
Z=	16	CN= 1.990 C6(AA)= 125.81	

#	XYZ [au]				R0(AA) [Ang.]	CN	C6(AA)
C8(AA)	C10(AA)	[au]					
1	-4.70060	-4.50765	3.02967	c	0.566	3.244	24.8
715.8	25361.1						
2	-6.61773	-3.90861	3.34775	h	0.366	1.021	3.1
37.3	551.6						
3	-1.39340	1.34154	4.45827	c	0.566	3.310	24.2
699.4	24778.2						
4	-3.26421	-0.60421	5.40274	c	0.566	4.148	18.2
527.7	18694.3						
5	-6.61154	11.74097	-0.55614	c	0.566	3.262	24.6
711.9	25221.3						
6	7.56171	3.76757	3.15571	c	0.566	4.099	18.3
528.2	18712.4						
7	9.51165	3.22201	3.51827	h	0.366	1.000	3.1
37.4	553.2						
8	7.25318	5.53876	4.15864	h	0.366	1.000	3.1
37.4	553.3						
9	7.35064	4.10844	1.13485	h	0.366	0.999	3.1
37.4	553.3						
10	1.12649	0.59983	4.06872	c	0.566	3.351	23.7
686.4	24319.3						
11	-4.24929	-6.82129	1.83780	c	0.566	3.174	25.2
727.7	25783.1						
12	21.81525	4.91607	-1.24633	c	0.566	4.065	18.3
528.6	18729.6						
13	21.26279	6.26893	-2.70018	h	0.366	0.996	3.1
37.4	553.5						
14	23.82272	4.49729	-1.38403	h	0.366	0.997	3.1
37.4	553.5						
15	21.37240	5.71653	0.60010	h	0.366	0.996	3.1
37.4	553.5						
16	22.84122	-0.45729	-7.50326	c	0.566	4.065	18.3
528.6	18729.6						
17	22.51684	-1.80912	-9.02418	h	0.366	0.996	3.1
37.4	553.5						
18	24.42982	-1.11360	-6.36520	h	0.366	0.996	3.1
37.4	553.5						
19	23.23353	1.40779	-8.27211	h	0.366	0.997	3.1
37.4	553.5						

20	-0.30882	5.68172	3.39390	c	0.566	3.180	25.1
726.8	25751.5						
21	2.23571	4.95959	3.38575	c	0.566	3.229	24.9
718.8	25465.0						
22	3.64788	6.39061	3.03526	h	0.366	1.007	3.1
37.3	552.7						
23	2.98515	2.48146	3.77491	c	0.566	3.299	24.3
702.6	24893.9						
24	5.73104	1.74100	4.10538	c	0.566	4.144	18.2
527.7	18695.5						
25	6.10622	-0.79685	2.82434	c	0.566	3.298	24.3
702.8	24900.3						
26	8.36941	-1.38429	1.64162	c	0.566	3.237	24.8
717.2	25408.6						
27	9.77901	0.07098	1.50639	h	0.366	1.025	3.1
37.2	551.3						
28	8.87959	-3.78960	0.67327	c	0.566	3.166	25.2
728.7	25818.1						
29	7.02131	-5.63259	1.07486	c	0.566	3.238	24.8
717.0	25401.4						
30	7.41632	-7.53242	0.44462	h	0.366	1.007	3.1
37.3	552.6						
31	4.74213	-5.12500	2.25304	c	0.566	3.293	24.3
704.1	24945.4						
32	2.91082	-7.22182	2.94027	c	0.566	4.143	18.2
527.7	18695.9						
33	0.25123	-6.19300	2.66713	c	0.566	3.296	24.3
703.4	24920.5						
34	-1.73945	-7.66428	1.81189	c	0.566	3.232	24.8
718.2	25445.9						
35	-1.36311	-9.52847	1.07158	h	0.366	1.007	3.1
37.3	552.7						
36	11.17922	-4.52113	-0.61785	c	0.566	3.274	24.5
709.0	25119.4						
37	11.24890	-6.49826	-1.16000	h	0.366	1.011	3.1
37.3	552.4						
38	13.23870	-3.14654	-1.25290	c	0.566	3.077	25.5
737.7	26134.7						
39	-2.75760	-2.98456	3.89679	c	0.566	3.310	24.2
699.6	24785.7						
40	16.77134	0.26280	-2.03093	c	0.566	3.243	24.8
716.1	25369.7						
41	17.65120	-1.89346	-3.17672	c	0.566	3.238	24.8
717.0	25404.1						
42	-2.06594	3.84164	4.09380	c	0.566	3.250	24.7
714.5	25312.4						
43	-3.99836	4.37869	4.43263	h	0.366	1.022	3.1
37.2	551.6						
44	19.82961	-2.29003	-4.80934	c	0.566	3.241	24.8
716.5	25383.8						
45	4.20500	-2.63740	3.02241	c	0.566	3.338	23.9
690.9	24477.5						
46	-0.23999	-3.72489	3.51583	c	0.566	3.349	23.8
687.1	24344.2						
47	6.20893	1.36936	6.97532	c	0.566	4.110	18.3
528.0	18707.5						
48	8.15610	0.76720	7.29058	h	0.366	0.999	3.1
37.4	553.3						
49	4.95223	-0.06435	7.75450	h	0.366	1.000	3.1
37.4	553.3						

50	5.88000	3.13873	7.98432	h	0.366	0.999	3.1
37.4	553.3						
51	18.00021	2.66886	-1.54119	c	0.566	3.242	24.8
716.2	25373.8						
52	3.32382	-7.86761	5.77162	c	0.566	4.110	18.3
528.0	18707.4						
53	5.24496	-8.55919	6.06640	h	0.366	0.999	3.1
37.4	553.3						
54	1.98468	-9.31831	6.37034	h	0.366	0.999	3.1
37.4	553.3						
55	3.04688	-6.20460	6.95414	h	0.366	1.000	3.1
37.4	553.3						
56	3.33770	-9.63764	1.41111	c	0.566	4.098	18.3
528.2	18712.7						
57	5.23064	-10.37648	1.73589	h	0.366	1.000	3.1
37.4	553.3						
58	3.09461	-9.31718	-0.60997	h	0.366	0.999	3.1
37.4	553.3						
59	2.02259	-11.10475	2.00606	h	0.366	1.000	3.1
37.4	553.3						
60	-2.68132	-1.15473	8.22055	c	0.566	4.107	18.3
528.1	18708.7						
61	-3.94535	-2.62378	8.92669	h	0.366	0.999	3.1
37.4	553.3						
62	-2.94779	0.55462	9.34491	h	0.366	0.999	3.1
37.4	553.3						
63	-0.74041	-1.79689	8.46760	h	0.366	1.000	3.1
37.4	553.2						
64	-6.00792	0.28577	5.21297	c	0.566	4.101	18.3
528.1	18711.3						
65	-6.55515	0.70393	3.27186	h	0.366	1.000	3.1
37.4	553.3						
66	-6.30003	1.97429	6.35472	h	0.366	1.000	3.1
37.4	553.2						
67	-7.28408	-1.15179	5.94794	h	0.366	1.000	3.1
37.4	553.2						
68	-1.00968	8.23904	2.69728	c	0.566	3.263	24.6
711.6	25211.2						
69	0.48353	9.64276	2.77847	h	0.366	1.009	3.1
37.3	552.5						
70	-3.27218	9.03004	1.83586	c	0.566	3.088	25.5
736.8	26103.6						
71	-7.61862	9.41130	-0.45747	c	0.566	3.269	24.6
710.2	25162.8						
72	-10.10643	8.73305	-1.53525	c	0.566	3.198	25.0
724.2	25659.0						
73	-12.89337	5.29766	-2.24029	c	0.566	4.053	18.3
528.8	18736.6						
74	-14.42453	6.20022	-1.20139	h	0.366	0.996	3.1
37.4	553.5						
75	-12.86465	3.27437	-1.90211	h	0.366	0.998	3.1
37.4	553.4						
76	-13.10301	5.71207	-4.24636	h	0.366	0.996	3.1
37.4	553.5						
77	-7.75925	13.98097	-1.83823	c	0.566	3.216	24.9
721.1	25548.3						
78	-9.11736	15.60557	-5.72833	c	0.566	4.065	18.3
528.6	18729.6						
79	-8.92887	15.08305	-7.70400	h	0.366	0.997	3.1
37.4	553.5						

80	-8.28058	17.45273	-5.37577	h	0.366	0.996	3.1
37.4	553.5						
81	-11.09791	15.62504	-5.16823	h	0.366	0.997	3.1
37.4	553.5						
82	-6.20996	-8.36843	0.71511	c	0.566	3.271	24.5
709.8	25146.5						
83	-5.69564	-10.32098	0.35414	h	0.366	1.009	3.1
37.3	552.5						
84	-8.54620	-7.66628	-0.04962	c	0.566	3.081	25.5
737.4	26124.8						
85	-12.51865	-5.24966	-1.76874	c	0.566	3.249	24.7
714.8	25325.1						
86	-12.99560	-7.75305	-2.30455	c	0.566	3.234	24.8
717.8	25432.2						
87	-13.83800	-2.98600	-2.56020	c	0.566	3.242	24.8
716.3	25377.6						
88	-16.76560	-1.18954	-5.37325	c	0.566	4.064	18.3
528.7	18729.9						
89	-15.59207	0.41927	-5.90941	h	0.366	0.996	3.1
37.4	553.6						
90	-18.00566	-0.62517	-3.82720	h	0.366	0.996	3.1
37.4	553.5						
91	-17.87689	-1.82857	-6.97878	h	0.366	0.997	3.1
37.4	553.5						
92	-15.33958	-8.83965	-3.23429	c	0.566	3.211	25.0
722.1	25584.0						
93	-17.17268	-12.61888	-4.74994	c	0.566	4.059	18.3
528.8	18733.2						
94	-18.07880	-11.70626	-6.36059	h	0.366	0.996	3.1
37.4	553.5						
95	-18.52721	-12.70524	-3.19800	h	0.366	0.996	3.1
37.4	553.5						
96	-16.54533	-14.50907	-5.25892	h	0.366	0.997	3.1
37.4	553.5						
97	1.76982	-1.99326	3.96273	n	0.495	3.229	15.6
344.0	9297.3						
98	20.63389	-0.16606	-5.98564	o	0.473	2.048	10.4
209.8	5187.0						
99	20.76814	-4.35777	-5.20031	o	0.473	1.073	12.8
257.3	6361.3						
100	20.55726	2.56018	-1.60311	o	0.473	2.048	10.4
209.8	5187.0						
101	16.85517	4.59154	-0.98684	o	0.473	1.075	12.7
257.3	6360.4						
102	-11.59867	10.22556	-2.41067	o	0.473	1.057	12.8
257.6	6368.1						
103	-10.49763	6.24220	-1.35546	o	0.473	2.075	10.4
209.7	5184.4						
104	-8.45101	15.84351	-0.73122	o	0.473	1.057	12.8
257.6	6368.3						
105	-7.80082	13.68060	-4.34249	o	0.473	2.048	10.4
209.8	5187.0						
106	-13.61061	-0.94028	-1.49966	o	0.473	1.076	12.7
257.3	6360.0						
107	-15.24818	-3.29478	-4.66102	o	0.473	2.049	10.4
209.8	5186.8						
108	-17.41698	-7.86996	-3.27671	o	0.473	1.054	12.8
257.6	6369.3						
109	-14.95368	-11.28453	-4.01648	o	0.473	2.079	10.4
209.7	5184.1						

110	13.71261	0.09701	-0.72122	s	0.737	2.629	125.8
6163.7	369907.1						
111	15.80356	-4.62150	-2.78989	s	0.737	2.629	125.8
6163.7	369907.1						
112	-3.81050	12.24642	1.08234	s	0.737	2.583	125.8
6163.7	369907.8						
113	-5.95309	7.11191	1.27152	s	0.737	2.605	125.8
6163.7	369907.4						
114	-9.83818	-4.60879	0.10219	s	0.737	2.629	125.8
6163.7	369907.1						
115	-10.62010	-9.90034	-1.39199	s	0.737	2.616	125.8
6163.7	369907.3						

molecular C6(AA) [au] = 187029.64

DFT-D V3(BJ)

DF b3-lyp

parameters

s6 : 1.0000
s8 : 1.9889
a1 : 0.3981
a2 : 4.4211
k1-k3 : 16.0000 1.3333 -4.0000
Cutoff : 94.8683 a.u.
CN-Cutoff: 40.0000 a.u.

Edisp /kcal,au: -202.5889 -0.32284600

E6 /kcal : -93.2103

E8 /kcal : -109.5425

E6(ABC) " : 0.163890

% E8 : 54.07

% E6(ABC) : -0.08

normal termination of dftd3

2

	DFTD3 V3.1 Rev 0	
	S.Grimme, University Bonn	
	June 2014	
	see dftd3 -h for options	

Please cite DFT-D3 work done with this code as:
S. Grimme, J. Antony, S. Ehrlich and H. Krieg,
J. Chem. Phys. 132 (2010), 154104
If used with BJ-damping cite also
S. Grimme, S. Ehrlich and L. Goerigk,
J. Comput. Chem. 32 (2011), 1456-1465
For DFT-D2 the reference is
S. Grimme, J. Comput. Chem., 27 (2006), 1787-1799

files read :

BG32.xyz

C6 coefficients used:

2 C6 for element

1

Z=	1	CN=	0.912	C6(AA)=	3.03
Z=	1	CN=	0.000	C6(AA)=	7.59
			5	C6 for element	6
Z=	6	CN=	0.000	C6(AA)=	49.11
Z=	6	CN=	0.987	C6(AA)=	43.25
Z=	6	CN=	1.998	C6(AA)=	29.36
Z=	6	CN=	2.999	C6(AA)=	25.78
Z=	6	CN=	3.984	C6(AA)=	18.21
			4	C6 for element	7
Z=	7	CN=	0.000	C6(AA)=	25.27
Z=	7	CN=	0.994	C6(AA)=	22.12
Z=	7	CN=	2.014	C6(AA)=	19.68
Z=	7	CN=	2.990	C6(AA)=	15.58
			3	C6 for element	16
Z=	16	CN=	0.000	C6(AA)=	134.01
Z=	16	CN=	0.995	C6(AA)=	131.00
Z=	16	CN=	1.990	C6(AA)=	125.81

#	XYZ [au]				R0(AA) [Ang.]	CN	C6(AA)
C8(AA)	C10(AA) [au]						
1	4.57639	-4.71474	-3.46750	c	0.566	3.250	24.7
714.6	25317.6						
2	6.55956	-4.28402	-3.63569	h	0.366	1.016	3.1
37.3	552.0						
3	1.86817	1.40815	-4.91117	c	0.566	3.311	24.2
699.1	24766.8						
4	3.61398	-0.65841	-5.83978	c	0.566	4.148	18.2
527.7	18694.3						
5	7.71373	11.02908	0.93664	c	0.566	3.267	24.6
710.6	25177.1						
6	-6.89835	4.53226	-3.86891	c	0.566	4.099	18.3
528.2	18712.3						
7	-8.86776	4.17351	-4.34389	h	0.366	1.000	3.1
37.4	553.2						
8	-6.39678	6.31397	-4.76820	h	0.366	1.000	3.1
37.4	553.2						
9	-6.75081	4.75904	-1.82608	h	0.366	0.999	3.1
37.4	553.3						
10	-0.71804	0.87303	-4.67006	c	0.566	3.352	23.7
686.2	24310.8						
11	3.84880	-6.99916	-2.36874	c	0.566	3.185	25.1
726.2	25728.5						
12	1.10830	5.77449	-3.68534	c	0.566	3.179	25.1
727.0	25757.0						
13	-1.48583	5.27329	-3.82258	c	0.566	3.230	24.8
718.5	25456.3						
14	-2.78522	6.80549	-3.46500	h	0.366	1.007	3.1
37.3	552.7						
15	-2.42269	2.88876	-4.36421	c	0.566	3.299	24.3
702.6	24893.4						
16	-5.20399	2.40087	-4.84181	c	0.566	4.143	18.2
527.7	18695.7						
17	-5.84237	-0.14450	-3.68843	c	0.566	3.298	24.3
702.7	24896.4						
18	-8.18382	-0.59150	-2.60263	c	0.566	3.241	24.8
716.5	25383.4						
19	-9.50746	0.94894	-2.50012	h	0.366	1.020	3.1
37.3	551.7						
20	-8.90833	-2.97910	-1.74334	c	0.566	3.174	25.2
727.7	25783.5						

21	-7.23277	-4.97055	-2.20532	c	0.566	3.235	24.8
717.7	25428.2						
22	-7.81273	-6.85491	-1.68023	h	0.366	1.007	3.1
37.3	552.7						
23	-4.88320	-4.60696	-3.29447	c	0.566	3.297	24.3
703.0	24906.9						
24	-3.20419	-6.81157	-4.02621	c	0.566	4.143	18.2
527.7	18695.8						
25	-0.49778	-6.02467	-3.52423	c	0.566	3.301	24.3
702.0	24871.9						
26	1.30049	-7.67130	-2.56856	c	0.566	3.227	24.9
719.1	25478.5						
27	0.72935	-9.51787	-1.91356	h	0.366	1.007	3.1
37.3	552.7						
28	-11.28157	-3.50874	-0.48012	c	0.566	3.265	24.6
711.2	25196.2						
29	-11.81229	-5.48848	-0.40486	h	0.366	1.010	3.1
37.3	552.5						
30	-12.88065	-1.88544	0.65684	c	0.566	3.083	25.5
737.2	26119.9						
31	2.83134	-3.02304	-4.43481	c	0.566	3.312	24.2
698.7	24755.6						
32	-14.84172	1.75188	3.39002	c	0.566	3.271	24.5
709.7	25144.7						
33	-16.34905	-0.26013	3.81402	c	0.566	3.256	24.7
713.2	25269.4						
34	2.73281	3.82445	-4.40729	c	0.566	3.251	24.7
714.4	25311.8						
35	4.71484	4.21108	-4.64859	h	0.366	1.022	3.1
37.2	551.6						
36	-4.10164	-2.13785	-3.90270	c	0.566	3.341	23.8
689.8	24437.7						
37	0.24389	-3.57198	-4.23016	c	0.566	3.355	23.7
685.2	24275.6						
38	-5.58570	2.19545	-7.74182	c	0.566	4.109	18.3
528.0	18707.8						
39	-7.56002	1.77693	-8.16616	h	0.366	0.999	3.1
37.4	553.3						
40	-4.42057	0.69601	-8.53853	h	0.366	1.000	3.1
37.4	553.3						
41	-5.06623	3.97148	-8.65237	h	0.366	0.999	3.1
37.4	553.3						
42	-3.49014	-7.23752	-6.91352	c	0.566	4.110	18.3
528.0	18707.6						
43	-5.43809	-7.74454	-7.36251	h	0.366	0.999	3.1
37.4	553.3						
44	-2.24154	-8.75788	-7.53239	h	0.366	0.999	3.1
37.4	553.3						
45	-3.00677	-5.53540	-7.96625	h	0.366	1.000	3.1
37.4	553.2						
46	-3.92088	-9.27224	-2.69221	c	0.566	4.098	18.3
528.2	18712.7						
47	-5.84222	-9.82597	-3.17854	h	0.366	1.000	3.1
37.4	553.3						
48	-3.78407	-9.10513	-0.64263	h	0.366	0.999	3.1
37.4	553.3						
49	-2.69348	-10.80472	-3.30980	h	0.366	1.000	3.1
37.4	553.3						
50	3.13324	-1.07329	-8.69876	c	0.566	4.107	18.3
528.1	18709.0						

51	4.30098	-2.62419	-9.39487	h	0.366	0.999	3.1
37.4	553.3						
52	3.60276	0.63858	-9.74858	h	0.366	0.999	3.1
37.4	553.3						
53	1.16034	-1.53452	-9.06441	h	0.366	1.000	3.1
37.4	553.2						
54	6.40974	-0.01735	-5.48612	c	0.566	4.101	18.3
528.1	18711.1						
55	6.88309	0.30139	-3.50623	h	0.366	1.000	3.1
37.4	553.2						
56	6.90538	1.66959	-6.55603	h	0.366	1.000	3.1
37.4	553.2						
57	7.59351	-1.54088	-6.20338	h	0.366	1.000	3.1
37.4	553.2						
58	1.98284	8.22391	-2.82273	c	0.566	3.261	24.6
712.2	25231.9						
59	0.60812	9.74442	-2.87465	h	0.366	1.009	3.1
37.3	552.5						
60	4.26357	8.80030	-1.84123	c	0.566	3.085	25.5
737.1	26113.5						
61	8.50643	8.61684	0.72347	c	0.566	3.262	24.6
711.9	25220.6						
62	5.62038	-8.64028	-1.06544	c	0.566	3.261	24.6
712.2	25233.1						
63	5.16001	-10.63729	-0.99315	h	0.366	1.008	3.1
37.3	552.6						
64	7.71876	-7.89642	0.16710	c	0.566	3.090	25.5
736.7	26099.6						
65	10.73611	-5.44870	3.21492	c	0.566	3.273	24.5
709.4	25131.8						
66	11.22362	-7.90997	3.66547	c	0.566	3.254	24.7
713.8	25288.6						
67	-1.58488	-1.66926	-4.70858	n	0.495	3.231	15.6
344.0	9297.2						
68	-12.50564	1.40378	1.02592	s	0.737	2.686	125.8
6163.6	369906.4						
69	-15.77780	-2.94623	1.93933	s	0.737	2.686	125.8
6163.6	369906.4						
70	5.07945	11.89444	-0.92014	s	0.737	2.667	125.8
6163.6	369906.6						
71	6.77316	6.65019	-1.32558	s	0.737	2.705	125.8
6163.6	369906.3						
72	8.76533	-4.75553	0.60735	s	0.737	2.694	125.8
6163.6	369906.4						
73	9.80299	-10.08750	1.58354	s	0.737	2.678	125.8
6163.6	369906.5						
74	12.03992	-2.89027	4.85671	s	0.737	2.355	125.8
6163.9	369921.0						
75	13.36013	-9.00425	5.93721	s	0.737	2.344	125.8
6163.9	369922.4						
76	9.25736	13.38669	2.66498	s	0.737	2.351	125.8
6163.9	369921.4						
77	11.25815	7.43475	2.13243	s	0.737	2.352	125.8
6163.9	369921.3						
78	-15.17964	4.72698	4.78688	s	0.737	2.353	125.8
6163.9	369921.2						
79	-18.95961	-0.23880	5.84291	s	0.737	2.348	125.8
6163.9	369921.9						
80	9.22957	-1.64262	6.41249	c	0.566	3.991	18.3
530.2	18786.2						

81	8.47930	-3.02785	7.73337	h	0.366	1.009	3.1
37.3	552.5						
82	9.83511	0.03388	7.44172	h	0.366	1.013	3.1
37.3	552.2						
83	7.79714	-1.12404	5.03281	h	0.366	1.010	3.1
37.3	552.5						
84	11.71686	-11.75008	7.20038	c	0.566	3.995	18.3
530.1	18782.5						
85	11.54579	-13.24838	5.80450	h	0.366	1.009	3.1
37.3	552.5						
86	12.88679	-12.41099	8.75974	h	0.366	1.014	3.1
37.3	552.1						
87	9.86160	-11.22270	7.91188	h	0.366	1.009	3.1
37.3	552.5						
88	10.51632	4.10095	2.53414	c	0.566	4.004	18.3
529.9	18774.5						
89	10.33749	3.12585	0.73398	h	0.366	1.010	3.1
37.3	552.4						
90	12.12271	3.30761	3.54545	h	0.366	1.015	3.1
37.3	552.0						
91	8.80886	3.85513	3.65139	h	0.366	1.010	3.1
37.3	552.5						
92	6.94108	13.98816	5.14299	c	0.566	3.989	18.3
530.3	18788.3						
93	6.69449	12.31202	6.30799	h	0.366	1.009	3.1
37.3	552.5						
94	7.70534	15.52027	6.28581	h	0.366	1.013	3.1
37.3	552.2						
95	5.14252	14.56876	4.33456	h	0.366	1.009	3.1
37.3	552.5						
96	-18.71940	-3.32695	7.34094	c	0.566	3.995	18.3
530.1	18782.5						
97	-20.20218	-3.35273	8.76843	h	0.366	1.014	3.1
37.3	552.1						
98	-19.04484	-4.85376	6.00450	h	0.366	1.009	3.1
37.3	552.5						
99	-16.88945	-3.55217	8.25035	h	0.366	1.009	3.1
37.3	552.5						
100	-12.18455	5.00980	6.46615	c	0.566	3.990	18.3
530.3	18787.2						
101	-10.59534	4.88795	5.16873	h	0.366	1.009	3.1
37.3	552.5						
102	-12.20389	6.86772	7.35200	h	0.366	1.013	3.1
37.3	552.2						
103	-12.03849	3.55609	7.91281	h	0.366	1.009	3.1
37.3	552.5						

molecular C6(AA) [au] = 184727.46

DFT-D V3(BJ)

DF b3-lyp
parameters

s6 : 1.0000
s8 : 1.9889
a1 : 0.3981
a2 : 4.4211
k1-k3 : 16.0000 1.3333 -4.0000
Cutoff : 94.8683 a.u.
CN-Cutoff: 40.0000 a.u.

Edisp /kcal,au: -203.9629 -0.32503556

E6 /kcal : -91.3417
E8 /kcal : -113.0760
E6(ABC) " : 0.454718
% E8 : 55.44
% E6(ABC) : -0.22
normal termination of dftd3

=====

2_C60

	DFTD3 V3.1 Rev 0	
	S.Grimme, University Bonn	
	June 2014	
	see dftd3 -h for options	

Please cite DFT-D3 work done with this code as:
S. Grimme, J. Antony, S. Ehrlich and H. Krieg,
J. Chem. Phys. 132 (2010), 154104
If used with BJ-damping cite also
S. Grimme, S. Ehrlich and L. Goerigk,
J. Comput. Chem. 32 (2011), 1456-1465
For DFT-D2 the reference is
S. Grimme, J. Comput. Chem., 27 (2006), 1787-1799

files read :
BG32_C60.xyz
C6 coefficients used:

	2	C6 for element	1
Z= 1	CN= 0.912	C6(AA)= 3.03	
Z= 1	CN= 0.000	C6(AA)= 7.59	
	5	C6 for element	6
Z= 6	CN= 0.000	C6(AA)= 49.11	
Z= 6	CN= 0.987	C6(AA)= 43.25	
Z= 6	CN= 1.998	C6(AA)= 29.36	
Z= 6	CN= 2.999	C6(AA)= 25.78	
Z= 6	CN= 3.984	C6(AA)= 18.21	
	4	C6 for element	7
Z= 7	CN= 0.000	C6(AA)= 25.27	
Z= 7	CN= 0.994	C6(AA)= 22.12	
Z= 7	CN= 2.014	C6(AA)= 19.68	
Z= 7	CN= 2.990	C6(AA)= 15.58	
	3	C6 for element	16
Z= 16	CN= 0.000	C6(AA)= 134.01	
Z= 16	CN= 0.995	C6(AA)= 131.00	
Z= 16	CN= 1.990	C6(AA)= 125.81	

#	XYZ [au]	R0(AA) [Ang.]	CN	C6(AA)
C8(AA)	C10(AA) [au]			
1	-2.96710 -7.54019	4.62502	c	0.566 3.382 23.3
675.2	23921.8			
2	-0.53826 -8.50447	4.38006	c	0.566 3.382 23.3
675.2	23922.1			
3	-0.86905 0.34926 -5.65335	4.38006	c	0.566 3.384 23.3
674.5	23898.3			

4	1.56149	-0.61520	-5.89708	c	0.566	3.385	23.3
674.0	23879.2						
5	-3.16919	-9.52048	-3.64113	c	0.566	3.382	23.3
675.2	23922.2						
6	-2.74930	-7.94155	-5.69519	c	0.566	3.382	23.3
675.1	23919.1						
7	1.34053	-0.21251	4.42842	c	0.566	3.399	23.1
668.5	23686.0						
8	1.76199	1.36612	2.37667	c	0.566	3.395	23.2
670.3	23749.6						
9	-7.24045	-2.59513	-0.83186	c	0.566	3.386	23.3
673.7	23869.6						
10	-6.32600	-0.73725	0.78138	c	0.566	3.392	23.2
671.3	23784.4						
11	4.91773	-7.42100	-2.05348	c	0.566	3.381	23.4
675.5	23933.6						
12	5.81466	-5.55606	-0.43786	c	0.566	3.383	23.3
674.8	23906.6						
13	-4.86290	-8.09991	2.72360	c	0.566	3.382	23.3
675.1	23917.3						
14	-3.33728	-4.95281	5.45514	c	0.566	3.382	23.4
675.4	23930.0						
15	0.10359	-10.07256	2.22373	c	0.566	3.382	23.3
675.3	23925.7						
16	1.62814	-6.92461	4.95351	c	0.566	3.383	23.3
674.8	23907.7						
17	-3.03863	-1.23163	-6.22570	c	0.566	3.383	23.3
674.9	23911.9						
18	-1.51008	1.90566	-3.48859	c	0.566	3.394	23.2
670.6	23758.3						
19	1.93148	-3.20359	-6.72802	c	0.566	3.382	23.3
675.3	23924.6						
20	3.45217	-0.05976	-3.99242	c	0.566	3.399	23.1
668.6	23689.6						
21	-5.14990	-8.92820	-1.83993	c	0.566	3.382	23.4
675.3	23926.9						
22	-1.04409	-10.55875	-2.25378	c	0.566	3.382	23.3
675.1	23919.7						
23	-4.29325	-5.70187	-6.04408	c	0.566	3.381	23.4
675.7	23939.0						
24	-0.18585	-7.33356	-6.45584	c	0.566	3.381	23.4
675.5	23932.8						
25	-1.22044	-0.81870	5.19136	c	0.566	3.386	23.3
673.9	23875.4						
26	2.88590	-2.45030	4.77611	c	0.566	3.392	23.2
671.5	23791.4						
27	-0.36349	2.39119	0.98309	c	0.566	3.399	23.1
668.5	23684.6						
28	3.74560	0.77444	0.57345	c	0.566	3.391	23.2
671.8	23801.8						
29	-7.27240	-5.21360	-0.01568	c	0.566	3.383	23.3
674.7	23904.0						
30	-6.57099	-2.54628	-3.49347	c	0.566	3.384	23.3
674.7	23903.5						
31	-5.41962	-1.40949	3.28336	c	0.566	3.387	23.3
673.2	23851.1						
32	-4.70803	1.25114	-0.18957	c	0.566	3.397	23.1
669.5	23721.0						
33	3.30584	-9.41478	-1.08026	c	0.566	3.382	23.4
675.4	23930.1						

34	4.01889	-6.75074	-4.55774	c	0.566	3.381	23.4
675.6	23936.5						
35	5.15319	-5.60493	2.22449	c	0.566	3.382	23.3
675.2	23920.4						
36	5.85511	-2.93800	-1.25291	c	0.566	3.389	23.3
672.5	23827.1						
37	-4.24933	-9.60213	0.66049	c	0.566	3.382	23.3
675.3	23924.2						
38	-1.26364	-3.43855	6.00440	c	0.566	3.383	23.3
674.8	23908.7						
39	-1.71135	-10.60866	0.40508	c	0.566	3.382	23.3
675.1	23919.9						
40	1.27359	-4.44649	5.74330	c	0.566	3.387	23.3
673.5	23860.7						
41	-2.68346	-3.70911	-7.02038	c	0.566	3.381	23.4
675.7	23940.7						
42	0.30279	2.43800	-1.67249	c	0.566	3.400	23.1
668.3	23676.1						
43	-0.14417	-4.71596	-7.27429	c	0.566	3.381	23.4
675.6	23936.8						
44	2.84288	1.44193	-1.93040	c	0.566	3.395	23.2
670.4	23752.6						
45	-6.62859	-6.78359	-2.17216	c	0.566	3.382	23.4
675.4	23930.4						
46	1.40962	-9.97504	-2.98014	c	0.566	3.382	23.3
675.3	23924.5						
47	-6.19268	-5.13401	-4.32060	c	0.566	3.381	23.4
675.6	23935.3						
48	1.84876	-8.32860	-5.12876	c	0.566	3.381	23.4
675.6	23934.2						
49	-3.25550	0.17421	3.86150	c	0.566	3.385	23.3
674.2	23887.3						
50	4.78668	-3.01615	3.05522	c	0.566	3.388	23.3
673.0	23842.6						
51	-2.81461	1.81172	1.70726	c	0.566	3.395	23.2
670.2	23744.3						
52	5.22805	-1.36606	0.90682	c	0.566	3.386	23.3
673.7	23867.1						
53	-6.40643	-5.85993	2.37833	c	0.566	3.382	23.3
675.2	23923.3						
54	-5.02186	-0.63997	-4.42170	c	0.566	3.384	23.3
674.5	23896.9						
55	-5.45879	-3.91493	4.06353	c	0.566	3.385	23.3
674.0	23878.4						
56	-4.06824	1.29470	-2.73072	c	0.566	3.397	23.1
669.5	23719.1						
57	2.66733	-9.46169	1.46558	c	0.566	3.382	23.3
675.3	23925.7						
58	4.05740	-4.24330	-5.33670	c	0.566	3.384	23.3
674.4	23892.5						
59	3.61102	-7.51720	3.15473	c	0.566	3.382	23.4
675.3	23926.9						
60	4.99585	-2.29650	-3.64750	c	0.566	3.392	23.2
671.5	23789.4						
61	5.11340	7.06690	-3.26503	c	0.566	3.238	24.8
717.0	25402.1						
62	7.03882	6.86016	-2.64082	h	0.366	1.018	3.1
37.3	551.8						
63	2.15365	8.24126	2.70628	c	0.566	3.318	24.1
697.0	24693.2						

64	4.12100	9.27100	0.89927	c	0.566	4.148	18.2
527.7	18694.2						
65	6.78106	-0.73172	10.02920	c	0.566	3.275	24.5
708.8	25113.4						
66	-6.84870	7.41738	5.12864	c	0.566	4.102	18.3
528.1	18711.1						
67	-8.76124	8.04458	4.69801	h	0.366	1.000	3.1
37.4	553.2						
68	-6.42435	8.06162	7.03728	h	0.366	1.000	3.1
37.4	553.2						
69	-6.81917	5.35712	5.10797	h	0.366	1.000	3.1
37.4	553.2						
70	-0.39799	8.33427	1.99932	c	0.566	3.364	23.6
682.0	24162.8						
71	4.40063	6.16780	-5.64852	c	0.566	3.181	25.1
726.8	25748.2						
72	0.99474	6.13316	6.62788	c	0.566	3.186	25.1
725.9	25719.4						
73	-1.53876	6.67072	6.06996	c	0.566	3.236	24.8
717.5	25420.4						
74	-2.97027	6.07316	7.39557	h	0.366	1.007	3.1
37.3	552.6						
75	-2.25577	7.81489	3.82933	c	0.566	3.308	24.2
699.9	24797.7						
76	-4.96487	8.54467	3.25094	c	0.566	4.145	18.2
527.7	18695.2						
77	-5.46197	7.72770	0.54910	c	0.566	3.308	24.2
700.0	24800.3						
78	-7.71259	6.58301	-0.15565	c	0.566	3.241	24.8
716.4	25381.8						
79	-9.09031	6.19919	1.28773	h	0.366	1.021	3.1
37.3	551.6						
80	-8.18093	5.83986	-2.64641	c	0.566	3.180	25.1
726.9	25754.7						
81	-6.45458	6.66206	-4.47363	c	0.566	3.246	24.7
715.4	25346.8						
82	-6.85054	6.24058	-6.43004	h	0.366	1.008	3.1
37.3	552.6						
83	-4.20866	7.83942	-3.84842	c	0.566	3.310	24.2
699.3	24776.1						
84	-2.37070	8.78101	-5.83162	c	0.566	4.146	18.2
527.7	18694.7						
85	0.22193	7.96965	-4.93577	c	0.566	3.313	24.2
698.5	24747.8						
86	1.98328	6.83972	-6.49876	c	0.566	3.242	24.8
716.2	25372.6						
87	1.45834	6.34413	-8.40716	h	0.366	1.007	3.1
37.3	552.6						
88	-10.11635	4.07814	-3.43194	c	0.566	3.276	24.5
708.6	25104.7						
89	-10.20137	3.75894	-5.45581	h	0.366	1.011	3.1
37.3	552.4						
90	-11.60501	2.55735	-2.02894	c	0.566	3.085	25.5
737.1	26114.7						
91	3.38901	8.20547	-1.65421	c	0.566	3.320	24.1
696.5	24675.8						
92	-13.57496	-0.35961	1.47937	c	0.566	3.267	24.6
710.8	25184.0						
93	-14.22633	-1.45437	-0.72972	c	0.566	3.264	24.6
711.3	25201.2						

94	2.80325	7.16432	4.99983	c	0.566	3.262	24.6
711.8	25219.4						
95	4.76539	7.13449	5.52582	h	0.366	1.026	3.1
37.2	551.2						
96	-3.59084	8.16380	-1.28237	c	0.566	3.355	23.7
685.2	24276.9						
97	0.84504	8.37477	-2.38709	c	0.566	3.369	23.5
680.2	24099.7						
98	-5.17730	11.46195	3.38920	c	0.566	4.107	18.3
528.1	18708.8						
99	-7.09234	12.05353	2.90397	h	0.366	0.999	3.1
37.4	553.3						
100	-3.86987	12.36496	2.07999	h	0.366	1.000	3.1
37.4	553.2						
101	-4.73809	12.11415	5.29570	h	0.366	0.999	3.1
37.4	553.3						
102	-2.46615	11.70725	-5.87369	c	0.566	4.107	18.3
528.1	18708.8						
103	-4.34550	12.34354	-6.43559	h	0.366	0.999	3.1
37.4	553.3						
104	-1.08281	12.43994	-7.21627	h	0.366	0.999	3.1
37.4	553.3						
105	-2.04549	12.49426	-4.01873	h	0.366	1.000	3.1
37.4	553.2						
106	-2.98564	7.82934	-8.48684	c	0.566	4.101	18.3
528.1	18711.5						
107	-4.84233	8.49554	-9.07613	h	0.366	1.000	3.1
37.4	553.3						
108	-2.96354	5.77151	-8.59661	h	0.366	0.999	3.1
37.4	553.3						
109	-1.62201	8.56955	-9.84050	h	0.366	1.000	3.1
37.4	553.2						
110	3.91203	12.18682	0.80750	c	0.566	4.104	18.3
528.1	18710.1						
111	5.24160	12.94951	-0.57221	h	0.366	0.999	3.1
37.4	553.3						
112	4.34454	12.98321	2.66004	h	0.366	0.999	3.1
37.4	553.3						
113	2.01526	12.78379	0.27547	h	0.366	1.000	3.1
37.4	553.2						
114	6.82104	8.58355	1.66149	c	0.566	4.103	18.3
528.1	18710.3						
115	7.09768	6.54522	1.77091	h	0.366	1.001	3.1
37.4	553.2						
116	7.28296	9.40337	3.49295	h	0.366	1.000	3.1
37.4	553.2						
117	8.16342	9.35248	0.30252	h	0.366	1.000	3.1
37.4	553.2						
118	1.59796	4.43210	8.68296	c	0.566	3.267	24.6
710.7	25178.7						
119	0.08866	4.05594	10.01778	h	0.366	1.009	3.1
37.3	552.5						
120	3.71379	3.02211	8.94437	c	0.566	3.091	25.5
736.6	26096.5						
121	7.81890	0.39595	7.99792	c	0.566	3.271	24.5
709.8	25149.2						
122	5.87435	4.46446	-7.19209	c	0.566	3.279	24.5
707.7	25074.2						
123	5.09149	4.10618	-9.05345	h	0.366	1.011	3.1
37.3	552.3						

124	7.86212	2.99985	-6.54476	c	0.566	3.086	25.5
737.0	26109.8						
125	11.44302	0.32930	-4.34824	c	0.566	3.275	24.5
708.8	25111.4						
126	11.11422	-0.76899	-6.62109	c	0.566	3.260	24.6
712.3	25235.5						
127	-1.08074	8.80354	-0.55911	n	0.495	3.232	15.6
344.0	9297.2						
128	-11.97862	2.56254	1.27570	s	0.737	2.697	125.8
6163.6	369906.3						
129	-13.51159	0.24162	-3.49217	s	0.737	2.704	125.8
6163.6	369906.3						
130	4.07389	0.72650	11.32353	s	0.737	2.657	125.8
6163.7	369906.7						
131	6.35302	3.15722	6.90694	s	0.737	2.765	125.8
6163.6	369905.9						
132	9.56423	3.00557	-3.68692	s	0.737	2.673	125.8
6163.6	369906.5						
133	8.91752	0.63421	-8.65467	s	0.737	2.702	125.8
6163.6	369906.3						
134	13.74572	-0.55342	-2.12320	s	0.737	2.359	125.8
6163.9	369920.5						
135	12.87509	-3.36575	-7.68243	s	0.737	2.362	125.8
6163.9	369920.1						
136	8.02569	-3.40990	11.51633	s	0.737	2.355	125.8
6163.9	369921.0						
137	10.48105	-0.76175	6.40289	s	0.737	2.372	125.8
6163.9	369919.0						
138	-14.50711	-1.41771	4.46578	s	0.737	2.355	125.8
6163.9	369921.0						
139	-15.95165	-4.26280	-1.02326	s	0.737	2.355	125.8
6163.9	369921.0						
140	12.25934	-3.23507	-0.56568	c	0.566	3.994	18.3
530.2	18783.4						
141	11.75132	-4.66144	-1.95409	h	0.366	1.011	3.1
37.3	552.4						
142	13.68043	-3.99873	0.71404	h	0.366	1.014	3.1
37.3	552.1						
143	10.61277	-2.65414	0.51018	h	0.366	1.011	3.1
37.3	552.3						
144	10.49026	-5.14988	-9.40584	c	0.566	4.000	18.3
530.0	18777.9						
145	9.88453	-4.17104	-11.10902	h	0.366	1.010	3.1
37.3	552.5						
146	11.41485	-6.90990	-9.93751	h	0.366	1.015	3.1
37.3	552.1						
147	8.87507	-5.55935	-8.20202	h	0.366	1.010	3.1
37.3	552.4						
148	10.96633	1.61976	3.98222	c	0.566	4.023	18.3
529.5	18758.1						
149	11.28317	3.47491	4.80915	h	0.366	1.011	3.1
37.3	552.3						
150	12.66257	1.04699	2.97422	h	0.366	1.018	3.1
37.3	551.9						
151	9.39921	1.67779	2.65084	h	0.366	1.012	3.1
37.3	552.3						
152	6.13268	-5.90993	10.09056	c	0.566	3.992	18.3
530.2	18785.8						
153	6.48963	-6.01828	8.07080	h	0.366	1.010	3.1
37.3	552.4						

154	6.72758	-7.66308	10.99101	h	0.366	1.013	3.1
37.3	552.2						
155	4.13381	-5.59951	10.44710	h	0.366	1.010	3.1
37.3	552.4						
156	-13.96556	-6.03373	-3.20967	c	0.566	3.995	18.3
530.1	18782.3						
157	-14.89129	-7.85818	-3.43489	h	0.366	1.014	3.1
37.3	552.1						
158	-13.83383	-5.10909	-5.03956	h	0.366	1.010	3.1
37.3	552.5						
159	-12.09219	-6.31047	-2.41241	h	0.366	1.010	3.1
37.3	552.4						
160	-11.48469	-1.94320	6.01678	c	0.566	3.994	18.3
530.2	18783.5						
161	-10.30286	-0.26422	5.94041	h	0.366	1.010	3.1
37.3	552.4						
162	-11.92616	-2.37630	7.97990	h	0.366	1.014	3.1
37.3	552.1						
163	-10.50819	-3.53370	5.16269	h	0.366	1.011	3.1
37.3	552.4						

molecular C6(AA) [au] = 517062.90

DFT-D V3 (BJ)

DF b3-lyp

parameters

s6 : 1.0000
s8 : 1.9889
a1 : 0.3981
a2 : 4.4211
k1-k3 : 16.0000 1.3333 -4.0000
Cutoff : 94.8683 a.u.
CN-Cutoff: 40.0000 a.u.

Edisp /kcal,au: -471.4236 -0.75126124

E6 /kcal : -220.0496

E8 /kcal : -259.1904

E6(ABC) " : 7.816427

% E8 : 54.98

% E6(ABC) : -1.66

normal termination of dftd3

=====
2_C60_ox1

	DFTD3 V3.1 Rev 0	
	S.Grimme, University Bonn	
	June 2014	
	see dftd3 -h for options	

Please cite DFT-D3 work done with this code as:
S. Grimme, J. Antony, S. Ehrlich and H. Krieg,
J. Chem. Phys. 132 (2010), 154104
If used with BJ-damping cite also
S. Grimme, S. Ehrlich and L. Goerigk,

J. Comput. Chem. 32 (2011), 1456-1465
 For DFT-D2 the reference is
 S. Grimme, J. Comput. Chem., 27 (2006), 1787-1799

files read :
 BG32_C60_plm2.xyz
 C6 coefficients used:

	2	C6 for element	1
Z=	1	CN= 0.912 C6(AA)= 3.03	
Z=	1	CN= 0.000 C6(AA)= 7.59	
	5	C6 for element	6
Z=	6	CN= 0.000 C6(AA)= 49.11	
Z=	6	CN= 0.987 C6(AA)= 43.25	
Z=	6	CN= 1.998 C6(AA)= 29.36	
Z=	6	CN= 2.999 C6(AA)= 25.78	
Z=	6	CN= 3.984 C6(AA)= 18.21	
	4	C6 for element	7
Z=	7	CN= 0.000 C6(AA)= 25.27	
Z=	7	CN= 0.994 C6(AA)= 22.12	
Z=	7	CN= 2.014 C6(AA)= 19.68	
Z=	7	CN= 2.990 C6(AA)= 15.58	
	3	C6 for element	16
Z=	16	CN= 0.000 C6(AA)= 134.01	
Z=	16	CN= 0.995 C6(AA)= 131.00	
Z=	16	CN= 1.990 C6(AA)= 125.81	

#	XYZ [au]				R0(AA) [Ang.]	CN	C6(AA)
C8(AA)	C10(AA)						
1	-2.16759	-9.52965	2.51910	c	0.566	3.383	23.3
675.0	23915.3						
2	0.18779	-10.12980	1.53089	c	0.566	3.383	23.3
675.0	23915.6						
3	-1.82293	2.01918	-3.68040	c	0.566	3.391	23.2
671.6	23795.1						
4	0.52907	1.42037	-4.66662	c	0.566	3.390	23.2
672.1	23812.2						
5	-3.73486	-7.92566	-5.68310	c	0.566	3.383	23.3
675.0	23916.3						
6	-3.66758	-5.61436	-6.92485	c	0.566	3.382	23.3
675.1	23918.1						
7	2.03067	-2.48992	4.77776	c	0.566	3.392	23.2
671.6	23794.4						
8	2.09724	-0.18051	3.53297	c	0.566	3.400	23.1
668.4	23680.6						
9	-7.28233	-3.09452	0.34775	c	0.566	3.390	23.2
672.3	23819.1						
10	-6.13240	-2.00671	2.44257	c	0.566	3.387	23.3
673.5	23861.6						
11	4.49837	-6.09659	-4.59025	c	0.566	3.382	23.3
675.3	23924.3						
12	5.65208	-5.00913	-2.49776	c	0.566	3.384	23.3
674.7	23903.2						
13	-4.35108	-9.38965	0.86639	c	0.566	3.382	23.3
675.2	23922.5						
14	-2.40243	-7.55123	4.40366	c	0.566	3.382	23.3
675.2	23921.9						
15	0.46661	-10.61568	-1.15336	c	0.566	3.383	23.3
674.9	23910.1						
16	2.41572	-8.77737	2.38162	c	0.566	3.383	23.3
674.9	23909.7						

17	-4.05179	0.67121	-4.53378	c	0.566	3.386	23.3
673.8	23870.6						
18	-2.10116	2.50685	-0.99320	c	0.566	3.396	23.2
669.9	23733.5						
19	0.76638	-0.55146	-6.55819	c	0.566	3.383	23.3
675.0	23915.7						
20	2.71094	1.27545	-3.01059	c	0.566	3.396	23.2
669.8	23728.7						
21	-5.38977	-8.27488	-3.52566	c	0.566	3.383	23.3
675.0	23913.1						
22	-1.40633	-9.28830	-5.19381	c	0.566	3.383	23.3
674.9	23910.1						
23	-5.25397	-3.54945	-6.06604	c	0.566	3.381	23.4
675.5	23933.3						
24	-1.26687	-4.56314	-7.73346	c	0.566	3.381	23.4
675.5	23932.4						
25	-0.36999	-3.53952	5.58865	c	0.566	3.383	23.3
674.7	23905.7						
26	3.61345	-4.55454	3.91097	c	0.566	3.386	23.3
673.6	23864.4						
27	-0.22885	1.18521	3.04827	c	0.566	3.391	23.2
671.9	23803.2						
28	3.75700	0.17291	1.37576	c	0.566	3.389	23.3
672.7	23834.2						
29	-7.18263	-5.81102	-0.01656	c	0.566	3.385	23.3
674.3	23888.3						
30	-7.07041	-1.90415	-2.11362	c	0.566	3.392	23.2
671.4	23787.9						
31	-4.82829	-3.58690	4.26594	c	0.566	3.382	23.3
675.2	23921.6						
32	-4.71141	0.32299	2.17104	c	0.566	3.387	23.3
673.2	23851.1						
33	3.07462	-8.42387	-4.31488	c	0.566	3.382	23.3
675.2	23920.6						
34	3.19201	-4.51627	-6.41402	c	0.566	3.383	23.3
675.1	23916.9						
35	5.43596	-6.20121	-0.03608	c	0.566	3.383	23.3
675.0	23913.3						
36	5.55116	-2.29339	-2.13487	c	0.566	3.390	23.2
672.0	23808.9						
37	-4.08411	-9.85316	-1.70234	c	0.566	3.383	23.3
674.9	23911.6						
38	-0.27105	-6.25610	5.21998	c	0.566	3.383	23.3
674.9	23910.1						
39	-1.62256	-10.48051	-2.73447	c	0.566	3.383	23.3
674.9	23911.7						
40	2.19118	-6.88264	4.18400	c	0.566	3.384	23.3
674.3	23890.9						
41	-3.83114	-1.21984	-6.34053	c	0.566	3.383	23.3
675.1	23916.7						
42	-0.01302	2.37895	0.58940	c	0.566	3.394	23.2
670.7	23762.3						
43	-1.36740	-1.84694	-7.37312	c	0.566	3.382	23.4
675.4	23927.3						
44	2.45152	1.75173	-0.44619	c	0.566	3.390	23.2
672.2	23814.9						
45	-6.90886	-6.29871	-2.70284	c	0.566	3.382	23.3
675.1	23919.4						
46	0.89046	-8.28268	-5.96689	c	0.566	3.382	23.3
675.1	23918.5						

47	-6.83885	-3.88328	-3.99947	c	0.566	3.383	23.3
674.8	23906.7						
48	0.96196	-5.86811	-7.26389	c	0.566	3.382	23.3
675.3	23925.9						
49	-2.60001	-2.23254	5.12356	c	0.566	3.381	23.4
675.5	23932.8						
50	5.20257	-4.22204	1.84909	c	0.566	3.384	23.3
674.4	23895.2						
51	-2.52742	0.18259	3.82493	c	0.566	3.385	23.3
674.1	23881.6						
52	5.27547	-1.80406	0.55052	c	0.566	3.387	23.3
673.2	23851.3						
53	-5.93365	-7.32323	1.72859	c	0.566	3.383	23.3
674.9	23910.6						
54	-5.70350	0.31823	-2.37289	c	0.566	3.396	23.2
669.7	23727.1						
55	-4.73120	-6.18717	3.91557	c	0.566	3.382	23.4
675.4	23927.6						
56	-4.49958	1.45566	-0.18740	c	0.566	3.394	23.2
670.5	23754.3						
57	2.86709	-9.56469	-1.96035	c	0.566	3.383	23.3
675.0	23915.4						
58	3.09568	-1.91672	-6.06671	c	0.566	3.385	23.3
674.1	23883.2						
59	4.07261	-8.42937	0.22502	c	0.566	3.382	23.3
675.1	23918.5						
60	4.29429	-0.78492	-3.87516	c	0.566	3.396	23.2
669.8	23729.0						
61	5.59749	7.18166	-2.65864	c	0.566	3.244	24.8
715.9	25362.8						
62	7.49504	6.93780	-1.96971	h	0.366	1.019	3.1
37.3	551.7						
63	2.31632	7.96165	3.25020	c	0.566	3.315	24.1
698.1	24734.1						
64	4.42261	8.99166	1.61467	c	0.566	4.148	18.2
527.7	18694.4						
65	5.70508	-1.61344	10.43441	c	0.566	3.279	24.5
707.7	25073.8						
66	-6.85474	7.76784	5.20372	c	0.566	4.102	18.3
528.1	18711.1						
67	-8.68563	8.55300	4.68797	h	0.366	1.000	3.1
37.4	553.2						
68	-6.48671	8.35632	7.14110	h	0.366	1.000	3.1
37.4	553.2						
69	-6.98631	5.71221	5.15166	h	0.366	1.000	3.1
37.4	553.2						
70	-0.19552	8.21509	2.40579	c	0.566	3.365	23.6
681.5	24143.8						
71	5.00370	6.46872	-5.14291	c	0.566	3.185	25.1
726.1	25725.8						
72	0.79684	5.86665	7.04794	c	0.566	3.188	25.1
725.7	25711.3						
73	-1.66863	6.62074	6.38984	c	0.566	3.237	24.8
717.2	25410.1						
74	-3.19890	6.12554	7.64412	h	0.366	1.007	3.1
37.3	552.6						
75	-2.18654	7.81831	4.13930	c	0.566	3.309	24.2
699.6	24786.6						
76	-4.79347	8.76755	3.44525	c	0.566	4.146	18.2
527.7	18694.8						

77	-5.20236	8.03004	0.71307	c	0.566	3.310	24.2
699.3	24777.4						
78	-7.46208	7.03971	-0.12137	c	0.566	3.250	24.7
714.5	25315.8						
79	-8.96003	6.77129	1.22574	h	0.366	1.021	3.1
37.2	551.6						
80	-7.84485	6.35992	-2.65664	c	0.566	3.186	25.1
726.0	25721.8						
81	-5.99918	7.15268	-4.39703	c	0.566	3.240	24.8
716.7	25392.4						
82	-6.34466	6.82998	-6.38067	h	0.366	1.008	3.1
37.3	552.6						
83	-3.72286	8.16268	-3.63701	c	0.566	3.305	24.2
700.8	24829.7						
84	-1.75383	9.08358	-5.49821	c	0.566	4.144	18.2
527.7	18695.3						
85	0.78381	8.19979	-4.51522	c	0.566	3.305	24.2
700.8	24828.3						
86	2.62834	7.21920	-6.06899	c	0.566	3.241	24.8
716.4	25382.6						
87	2.20860	6.87699	-8.03511	h	0.366	1.008	3.1
37.3	552.6						
88	-9.85368	4.76569	-3.52690	c	0.566	3.281	24.5
707.3	25059.7						
89	-10.06369	4.63002	-5.56096	h	0.366	1.010	3.1
37.3	552.4						
90	-11.26345	3.11241	-2.14527	c	0.566	3.090	25.5
736.7	26099.9						
91	3.79827	8.16191	-1.04977	c	0.566	3.314	24.1
698.2	24735.9						
92	-13.12478	0.03310	1.29150	c	0.566	3.262	24.6
711.8	25218.7						
93	-14.05326	-0.82418	-0.92471	c	0.566	3.248	24.7
715.0	25330.9						
94	2.76807	6.80628	5.53919	c	0.566	3.256	24.7
713.3	25271.6						
95	4.69062	6.63507	6.17187	h	0.366	1.024	3.1
37.2	551.4						
96	-3.21084	8.36057	-1.02583	c	0.566	3.358	23.7
684.0	24233.5						
97	1.28757	8.41439	-1.90683	c	0.566	3.360	23.6
683.2	24206.8						
98	-4.77734	11.69388	3.62490	c	0.566	4.107	18.3
528.1	18708.9						
99	-6.61164	12.44113	3.05558	h	0.366	0.999	3.1
37.4	553.3						
100	-3.33801	12.51638	2.40409	h	0.366	1.000	3.1
37.4	553.2						
101	-4.39274	12.27788	5.56357	h	0.366	0.999	3.1
37.4	553.3						
102	-1.77054	12.01611	-5.45869	c	0.566	4.108	18.3
528.0	18708.3						
103	-3.60502	12.71656	-6.08430	h	0.366	0.999	3.1
37.4	553.3						
104	-0.31252	12.74452	-6.72014	h	0.366	0.999	3.1
37.4	553.3						
105	-1.41184	12.74519	-3.56698	h	0.366	1.000	3.1
37.4	553.3						
106	-2.27162	8.22004	-8.20456	c	0.566	4.100	18.3
528.1	18711.7						

107	-4.08300	8.94766	-8.85521	h	0.366	1.000	3.1
37.4	553.2						
108	-2.28903	6.16615	-8.37038	h	0.366	0.999	3.1
37.4	553.3						
109	-0.84251	8.97089	-9.48061	h	0.366	1.000	3.1
37.4	553.2						
110	4.34774	11.91933	1.72228	c	0.566	4.105	18.3
528.1	18709.6						
111	5.79340	12.70542	0.48159	h	0.366	0.999	3.1
37.4	553.3						
112	4.70268	12.56153	3.64822	h	0.366	0.999	3.1
37.4	553.3						
113	2.51786	12.64878	1.12487	h	0.366	1.000	3.1
37.4	553.2						
114	7.03927	8.12151	2.47572	c	0.566	4.103	18.3
528.1	18710.4						
115	7.21692	6.06907	2.44311	h	0.366	1.000	3.1
37.4	553.2						
116	7.42490	8.78542	4.38526	h	0.366	1.000	3.1
37.4	553.2						
117	8.49763	8.92550	1.26682	h	0.366	1.000	3.1
37.4	553.2						
118	1.12851	4.05696	9.02992	c	0.566	3.278	24.5
708.1	25088.0						
119	-0.51030	3.69857	10.20638	h	0.366	1.010	3.1
37.3	552.5						
120	3.12688	2.46718	9.37539	c	0.566	3.093	25.5
736.4	26089.7						
121	7.05277	-0.43805	8.60473	c	0.566	3.276	24.5
708.6	25105.8						
122	6.54941	4.87502	-6.69151	c	0.566	3.287	24.4
705.9	25008.8						
123	5.94600	4.68995	-8.64195	h	0.366	1.011	3.1
37.3	552.4						
124	8.44211	3.29237	-5.95852	c	0.566	3.091	25.5
736.6	26097.5						
125	11.70133	0.35022	-3.66771	c	0.566	3.288	24.4
705.5	24995.1						
126	11.63677	-0.49976	-6.07943	c	0.566	3.267	24.6
710.8	25181.4						
127	-0.70993	8.70917	-0.16021	n	0.495	3.240	15.6
344.0	9296.7						
128	-11.18628	2.71672	1.13728	s	0.737	2.800	125.8
6163.6	369905.8						
129	-13.20095	0.88908	-3.63168	s	0.737	2.733	125.8
6163.6	369906.1						
130	3.03867	0.00487	11.56301	s	0.737	2.697	125.8
6163.6	369906.3						
131	5.93972	2.51447	7.62955	s	0.737	2.777	125.8
6163.6	369905.8						
132	9.77434	2.96311	-2.96141	s	0.737	2.695	125.8
6163.6	369906.3						
133	9.64684	1.10987	-8.15468	s	0.737	2.721	125.8
6163.6	369906.2						
134	13.70298	-0.85157	-1.32202	s	0.737	2.369	125.8
6163.9	369919.3						
135	13.47884	-3.03820	-7.10896	s	0.737	2.373	125.8
6163.9	369918.9						
136	6.62101	-4.43361	11.88765	s	0.737	2.360	125.8
6163.9	369920.4						

137	9.77941	-1.70323	7.23218	s	0.737	2.368	125.8
6163.9	369919.4						
138	-13.66103	-1.02401	4.39365	s	0.737	2.378	125.8
6163.8	369918.4						
139	-16.17298	-3.33686	-1.32937	s	0.737	2.346	125.8
6163.9	369922.1						
140	11.98723	-3.64527	-0.26057	c	0.566	3.994	18.3
530.2	18783.6						
141	11.51574	-4.84508	-1.85942	h	0.366	1.011	3.1
37.3	552.4						
142	13.27854	-4.65254	0.98694	h	0.366	1.014	3.1
37.3	552.1						
143	10.29598	-3.12523	0.77737	h	0.366	1.011	3.1
37.3	552.4						
144	12.35887	-3.53327	-10.31232	c	0.566	4.008	18.3
529.8	18770.3						
145	12.75251	-1.90779	-11.50904	h	0.366	1.010	3.1
37.3	552.4						
146	13.43656	-5.14373	-11.00294	h	0.366	1.016	3.1
37.3	552.0						
147	10.35622	-3.99882	-10.34358	h	0.366	1.010	3.1
37.3	552.4						
148	10.60537	0.68841	4.91748	c	0.566	4.020	18.3
529.5	18759.9						
149	10.99031	2.49984	5.81170	h	0.366	1.011	3.1
37.3	552.4						
150	12.33506	0.01733	4.03462	h	0.366	1.018	3.1
37.3	551.9						
151	9.15495	0.88051	3.47165	h	0.366	1.012	3.1
37.3	552.3						
152	4.12159	-6.57944	10.88373	c	0.566	3.992	18.3
530.2	18785.8						
153	4.22139	-6.90250	8.85935	h	0.366	1.011	3.1
37.3	552.4						
154	4.46558	-8.34438	11.88423	h	0.366	1.014	3.1
37.3	552.2						
155	2.27278	-5.85133	11.40872	h	0.366	1.010	3.1
37.3	552.5						
156	-14.11583	-5.65023	-2.84668	c	0.566	3.993	18.3
530.2	18785.1						
157	-15.30776	-7.27435	-3.26590	h	0.366	1.013	3.1
37.3	552.2						
158	-13.33762	-4.90934	-4.59845	h	0.366	1.010	3.1
37.3	552.5						
159	-12.60068	-6.21339	-1.57678	h	0.366	1.010	3.1
37.3	552.5						
160	-12.87685	-4.36492	4.25347	c	0.566	3.994	18.3
530.2	18783.9						
161	-10.98743	-4.62653	3.49994	h	0.366	1.012	3.1
37.3	552.3						
162	-12.93269	-5.00208	6.20979	h	0.366	1.016	3.1
37.3	552.0						
163	-14.26394	-5.39426	3.14686	h	0.366	1.012	3.1
37.3	552.2						

molecular C6(AA) [au] = 517063.92

DFT-D V3(BJ)

DF b3-lyp
parameters

s6 : 1.0000
s8 : 1.9889
a1 : 0.3981
a2 : 4.4211
k1-k3 : 16.0000 1.3333 -4.0000
Cutoff : 94.8683 a.u.
CN-Cutoff: 40.0000 a.u.

Edisp /kcal,au: -468.9859 -0.74737660

E6 /kcal : -218.6631
E8 /kcal : -257.9707
E6(ABC) " : 7.647891
% E8 : 55.01
% E6(ABC) : -1.63
normal termination of dftd3

=====

2_ox1

	DFTD3 V3.1 Rev 0	
	S.Grimme, University Bonn	
	June 2014	
	see dftd3 -h for options	

Please cite DFT-D3 work done with this code as:
S. Grimme, J. Antony, S. Ehrlich and H. Krieg,
J. Chem. Phys. 132 (2010), 154104
If used with BJ-damping cite also
S. Grimme, S. Ehrlich and L. Goerigk,
J. Comput. Chem. 32 (2011), 1456-1465
For DFT-D2 the reference is
S. Grimme, J. Comput. Chem., 27 (2006), 1787-1799

files read :
BG32_plm2.xyz
C6 coefficients used:

	2	C6 for element		1
Z= 1	CN= 0.912	C6(AA)=	3.03	
Z= 1	CN= 0.000	C6(AA)=	7.59	
	5	C6 for element		6
Z= 6	CN= 0.000	C6(AA)=	49.11	
Z= 6	CN= 0.987	C6(AA)=	43.25	
Z= 6	CN= 1.998	C6(AA)=	29.36	
Z= 6	CN= 2.999	C6(AA)=	25.78	
Z= 6	CN= 3.984	C6(AA)=	18.21	
	4	C6 for element		7
Z= 7	CN= 0.000	C6(AA)=	25.27	
Z= 7	CN= 0.994	C6(AA)=	22.12	
Z= 7	CN= 2.014	C6(AA)=	19.68	
Z= 7	CN= 2.990	C6(AA)=	15.58	
	3	C6 for element		16
Z= 16	CN= 0.000	C6(AA)=	134.01	
Z= 16	CN= 0.995	C6(AA)=	131.00	
Z= 16	CN= 1.990	C6(AA)=	125.81	

#	XYZ [au]			R0 (AA) [Ang.]	CN	C6 (AA)	
C8 (AA)	C10 (AA) [au]						
1	-4.61898	-4.52307	2.94487	c	0.566	3.250	24.7
714.5	25314.7						
2	-6.57061	-4.05366	3.27109	h	0.366	1.021	3.1
37.3	551.6						
3	-1.70846	1.51844	4.23892	c	0.566	3.312	24.2
698.9	24762.2						
4	-3.42973	-0.51736	5.26163	c	0.566	4.149	18.2
527.6	18694.0						
5	-7.86985	11.27726	-0.95616	c	0.566	3.278	24.5
708.2	25089.4						
6	7.07729	4.48894	2.82410	c	0.566	4.098	18.3
528.2	18712.6						
7	9.05436	4.10295	3.23881	h	0.366	1.000	3.1
37.4	553.2						
8	6.63993	6.27923	3.73752	h	0.366	1.000	3.1
37.4	553.2						
9	6.86415	4.71572	0.78727	h	0.366	0.999	3.1
37.4	553.3						
10	0.85965	0.93782	3.83565	c	0.566	3.353	23.7
685.9	24300.6						
11	-4.01543	-6.81282	1.75667	c	0.566	3.181	25.1
726.7	25747.0						
12	-0.92153	5.87349	2.99465	c	0.566	3.180	25.1
726.8	25751.5						
13	1.68211	5.33496	3.04502	c	0.566	3.229	24.9
718.7	25463.2						
14	2.98726	6.85462	2.66116	h	0.366	1.007	3.1
37.3	552.7						
15	2.59566	2.93529	3.50050	c	0.566	3.296	24.3
703.4	24921.1						
16	5.38022	2.38942	3.86048	c	0.566	4.143	18.2
527.7	18695.7						
17	5.94058	-0.17522	2.71237	c	0.566	3.294	24.3
703.9	24936.9						
18	8.26038	-0.67352	1.63119	c	0.566	3.237	24.8
717.2	25410.1						
19	9.59015	0.85417	1.48725	h	0.366	1.024	3.1
37.2	551.4						
20	8.94421	-3.09117	0.78335	c	0.566	3.170	25.2
728.3	25802.6						
21	7.19213	-5.04259	1.21440	c	0.566	3.238	24.8
717.0	25401.7						
22	7.72778	-6.93611	0.68053	h	0.366	1.007	3.1
37.3	552.6						
23	4.85590	-4.63145	2.28520	c	0.566	3.291	24.4
704.8	24970.6						
24	3.13197	-6.81319	2.97795	c	0.566	4.142	18.2
527.7	18696.1						
25	0.42535	-5.95031	2.63997	c	0.566	3.296	24.3
703.4	24919.6						
26	-1.46267	-7.54456	1.79946	c	0.566	3.229	24.9
718.8	25465.5						
27	-0.97938	-9.39919	1.10157	h	0.366	1.007	3.1
37.3	552.7						
28	11.29425	-3.71526	-0.40864	c	0.566	3.279	24.5
707.8	25076.9						
29	11.55343	-5.70954	-0.80765	h	0.366	1.011	3.1
37.3	552.4						

30	13.23951	-2.18913	-1.13175	c	0.566	3.081	25.5
737.3	26123.3						
31	-2.78557	-2.88370	3.79746	c	0.566	3.312	24.2
698.8	24758.4						
32	16.47376	1.39576	-2.24622	c	0.566	3.288	24.4
705.6	25000.0						
33	17.61094	-0.76279	-3.01478	c	0.566	3.263	24.6
711.7	25216.7						
34	-2.54904	3.93916	3.79494	c	0.566	3.252	24.7
714.0	25296.9						
35	-4.50613	4.36190	4.14587	h	0.366	1.023	3.1
37.2	551.5						
36	4.14568	-2.13685	2.92499	c	0.566	3.336	23.9
691.3	24493.8						
37	-0.22237	-3.48098	3.40333	c	0.566	3.353	23.7
685.9	24300.5						
38	5.85891	2.18030	6.75101	c	0.566	4.111	18.3
528.0	18707.1						
39	7.83942	1.73159	7.10244	h	0.366	0.999	3.1
37.4	553.3						
40	4.70041	0.70307	7.59747	h	0.366	1.000	3.1
37.4	553.3						
41	5.40328	3.96737	7.67103	h	0.366	0.999	3.1
37.4	553.3						
42	3.51873	-7.36393	5.83667	c	0.566	4.111	18.3
528.0	18707.1						
43	5.46566	-7.94512	6.18223	h	0.366	0.999	3.1
37.4	553.3						
44	2.25182	-8.87276	6.44187	h	0.366	0.999	3.1
37.4	553.3						
45	3.12980	-5.69584	6.97984	h	0.366	1.000	3.1
37.4	553.3						
46	3.72590	-9.23419	1.51440	c	0.566	4.097	18.3
528.2	18713.0						
47	5.64276	-9.86853	1.90470	h	0.366	1.000	3.1
37.4	553.2						
48	3.51709	-8.97546	-0.51915	h	0.366	0.999	3.1
37.4	553.3						
49	2.48277	-10.75833	2.11652	h	0.366	1.000	3.1
37.4	553.2						
50	-2.76460	-0.96426	8.08249	c	0.566	4.107	18.3
528.1	18708.8						
51	-3.91901	-2.49278	8.84297	h	0.366	0.999	3.1
37.4	553.3						
52	-3.12789	0.74842	9.16996	h	0.366	0.999	3.1
37.4	553.3						
53	-0.78366	-1.47169	8.31966	h	0.366	1.000	3.1
37.4	553.3						
54	-6.22881	0.18294	5.10163	c	0.566	4.102	18.3
528.1	18711.0						
55	-6.82930	0.52335	3.16007	h	0.366	1.000	3.1
37.4	553.2						
56	-6.61386	1.87008	6.21515	h	0.366	1.000	3.1
37.4	553.2						
57	-7.39305	-1.31785	5.89253	h	0.366	1.000	3.1
37.4	553.2						
58	-1.78881	8.29780	2.15184	c	0.566	3.270	24.5
710.0	25155.3						
59	-0.38110	9.78417	2.05496	h	0.366	1.009	3.1
37.3	552.5						

60	-4.13780	8.91392	1.28880	c	0.566	3.086	25.5
737.0	26109.8						
61	-8.69994	8.87750	-0.66283	c	0.566	3.268	24.6
710.4	25169.8						
62	-5.86577	-8.38718	0.54396	c	0.566	3.272	24.5
709.7	25142.3						
63	-5.30583	-10.32089	0.15873	h	0.366	1.009	3.1
37.3	552.5						
64	-8.17688	-7.67048	-0.32485	c	0.566	3.087	25.5
736.9	26108.2						
65	-12.14488	-5.31917	-2.13415	c	0.566	3.286	24.4
706.1	25017.0						
66	-12.47330	-7.75732	-2.82448	c	0.566	3.259	24.6
712.5	25241.9						
67	1.65225	-1.60094	3.69415	n	0.495	3.236	15.6
344.0	9296.9						
68	13.47165	1.08159	-0.86907	s	0.737	2.694	125.8
6163.6	369906.4						
69	15.92327	-3.55727	-2.54020	s	0.737	2.711	125.8
6163.6	369906.2						
70	-4.88718	11.97065	0.31279	s	0.737	2.685	125.8
6163.6	369906.4						
71	-6.67630	6.79860	0.92843	s	0.737	2.725	125.8
6163.6	369906.1						
72	-9.48087	-4.63375	-0.27578	s	0.737	2.700	125.8
6163.6	369906.3						
73	-10.17365	-9.89452	-1.78531	s	0.737	2.696	125.8
6163.6	369906.3						
74	-14.18830	-2.83307	-2.90017	s	0.737	2.365	125.8
6163.9	369919.8						
75	-15.05584	-8.76448	-4.62159	s	0.737	2.357	125.8
6163.9	369920.7						
76	-9.62986	13.70920	-2.34462	s	0.737	2.358	125.8
6163.9	369920.6						
77	-11.66056	7.84727	-1.71653	s	0.737	2.358	125.8
6163.9	369920.6						
78	17.78232	4.42175	-2.49310	s	0.737	2.363	125.8
6163.9	369920.0						
79	20.59971	-0.77952	-4.41840	s	0.737	2.362	125.8
6163.9	369920.1						
80	-12.74366	-1.71240	-5.82541	c	0.566	3.989	18.3
530.3	18788.6						
81	-12.77446	-3.19788	-7.24503	h	0.366	1.009	3.1
37.3	552.5						
82	-13.89058	-0.12786	-6.46719	h	0.366	1.013	3.1
37.3	552.2						
83	-10.81758	-1.07850	-5.48570	h	0.366	1.009	3.1
37.3	552.5						
84	-14.34093	-12.06989	-5.19348	c	0.566	4.007	18.3
529.8	18771.4						
85	-14.28838	-13.14496	-3.44102	h	0.366	1.010	3.1
37.3	552.4						
86	-15.90400	-12.75204	-6.34416	h	0.366	1.016	3.1
37.3	552.0						
87	-12.58612	-12.29260	-6.24146	h	0.366	1.010	3.1
37.3	552.5						
88	-11.49861	4.45168	-1.22664	c	0.566	4.010	18.3
529.8	18768.8						
89	-11.31745	3.97591	0.76589	h	0.366	1.010	3.1
37.3	552.4						

90	-13.30116	3.73096	-1.90657	h	0.366	1.016	3.1
37.3	552.0						
91	-9.97699	3.60001	-2.31663	h	0.366	1.010	3.1
37.3	552.5						
92	-8.15602	13.86754	-5.45720	c	0.566	3.988	18.3
530.3	18789.2						
93	-8.40050	12.08603	-6.45226	h	0.366	1.009	3.1
37.3	552.5						
94	-9.13565	15.36661	-6.47144	h	0.366	1.013	3.1
37.3	552.2						
95	-6.16289	14.34302	-5.29543	h	0.366	1.009	3.1
37.3	552.5						
96	21.08215	-4.09921	-5.13112	c	0.566	4.007	18.3
529.8	18771.0						
97	22.93505	-4.18035	-6.02127	h	0.366	1.016	3.1
37.3	552.0						
98	21.11477	-5.23946	-3.41984	h	0.366	1.010	3.1
37.3	552.4						
99	19.67247	-4.80232	-6.45307	h	0.366	1.010	3.1
37.3	552.5						
100	16.75724	5.30085	-5.66784	c	0.566	3.989	18.3
530.3	18789.1						
101	14.70532	5.35067	-5.77593	h	0.366	1.009	3.1
37.3	552.5						
102	17.51035	7.18633	-6.00577	h	0.366	1.013	3.1
37.3	552.2						
103	17.52854	3.99439	-7.05401	h	0.366	1.009	3.1
37.3	552.5						

molecular C6(AA) [au] = 184678.82

DFT-D V3(BJ)

DF b3-lyp
parameters

s6 : 1.0000
s8 : 1.9889
a1 : 0.3981
a2 : 4.4211
k1-k3 : 16.0000 1.3333 -4.0000
Cutoff : 94.8683 a.u.
CN-Cutoff: 40.0000 a.u.

Edisp /kcal,au: -204.1111 -0.32527178

E6 /kcal : -91.2225
E8 /kcal : -113.1874
E6(ABC) " : 0.298731
% E8 : 55.45
% E6(ABC) : -0.15

normal termination of dftd3

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2_red1

	DFTD3 V3.1 Rev 0	
	S.Grimme, University Bonn	
	June 2014	

| see dftd3 -h for options |

Please cite DFT-D3 work done with this code as:
S. Grimme, J. Antony, S. Ehrlich and H. Krieg,
J. Chem. Phys. 132 (2010), 154104
If used with BJ-damping cite also
S. Grimme, S. Ehrlich and L. Goerigk,
J. Comput. Chem. 32 (2011), 1456-1465
For DFT-D2 the reference is
S. Grimme, J. Comput. Chem., 27 (2006), 1787-1799

files read :
BG32_mlm2.xyz
C6 coefficients used:

	2	C6 for element	1
Z=	1	CN= 0.912 C6(AA)=	3.03
Z=	1	CN= 0.000 C6(AA)=	7.59
	5	C6 for element	6
Z=	6	CN= 0.000 C6(AA)=	49.11
Z=	6	CN= 0.987 C6(AA)=	43.25
Z=	6	CN= 1.998 C6(AA)=	29.36
Z=	6	CN= 2.999 C6(AA)=	25.78
Z=	6	CN= 3.984 C6(AA)=	18.21
	4	C6 for element	7
Z=	7	CN= 0.000 C6(AA)=	25.27
Z=	7	CN= 0.994 C6(AA)=	22.12
Z=	7	CN= 2.014 C6(AA)=	19.68
Z=	7	CN= 2.990 C6(AA)=	15.58
	3	C6 for element	16
Z=	16	CN= 0.000 C6(AA)=	134.01
Z=	16	CN= 0.995 C6(AA)=	131.00
Z=	16	CN= 1.990 C6(AA)=	125.81

#		XYZ [au]		R0 (AA) [Ang.]	CN	C6 (AA)
C8 (AA)	C10 (AA)					
1	4.64021	-4.48475 -3.54214	c	0.566	3.236	24.8
717.3	25415.1					
2	6.62037	-4.05548 -3.76015	h	0.366	1.015	3.1
37.3	552.1					
3	1.85869	1.56849 -5.02931	c	0.566	3.312	24.2
698.9	24763.2					
4	3.59026	-0.49812 -5.99085	c	0.566	4.147	18.2
527.7	18694.5					
5	7.68705	10.81732 1.17419	c	0.566	3.269	24.6
710.3	25164.6					
6	-6.90927	4.68675 -3.92583	c	0.566	4.099	18.3
528.2	18712.4					
7	-8.87876	4.31692 -4.39138	h	0.366	1.000	3.1
37.4	553.2					
8	-6.40777	6.46399 -4.83811	h	0.366	1.000	3.1
37.4	553.3					
9	-6.76142	4.92357 -1.88429	h	0.366	0.999	3.1
37.4	553.3					
10	-0.72504	1.02229 -4.70833	c	0.566	3.355	23.7
685.0	24269.9					
11	3.95275	-6.77698 -2.35411	c	0.566	3.173	25.2
727.8	25786.7					
12	1.10416	5.92965 -3.77895	c	0.566	3.181	25.1
726.7	25747.2					

13	-1.49364	5.42899	-3.87927	c	0.566	3.227	24.9
719.1	25477.5						
14	-2.79030	6.95725	-3.49096	h	0.366	1.007	3.1
37.3	552.7						
15	-2.43459	3.04355	-4.40934	c	0.566	3.298	24.3
702.8	24901.4						
16	-5.21732	2.54608	-4.88148	c	0.566	4.142	18.2
527.7	18696.0						
17	-5.86074	0.00435	-3.71789	c	0.566	3.289	24.4
705.2	24985.1						
18	-8.19298	-0.44199	-2.64073	c	0.566	3.230	24.8
718.5	25456.1						
19	-9.52476	1.09227	-2.53748	h	0.366	1.018	3.1
37.3	551.8						
20	-8.92442	-2.84568	-1.75193	c	0.566	3.165	25.2
729.0	25826.6						
21	-7.20506	-4.83153	-2.21112	c	0.566	3.230	24.8
718.7	25462.0						
22	-7.78369	-6.71950	-1.69138	h	0.366	1.007	3.1
37.3	552.7						
23	-4.85744	-4.46274	-3.27415	c	0.566	3.287	24.4
705.9	25009.6						
24	-3.15004	-6.66176	-3.97997	c	0.566	4.141	18.2
527.7	18696.5						
25	-0.43582	-5.86289	-3.50979	c	0.566	3.288	24.4
705.4	24991.7						
26	1.37871	-7.47559	-2.56703	c	0.566	3.221	24.9
720.3	25521.0						
27	0.84009	-9.33542	-1.91535	h	0.366	1.006	3.1
37.3	552.7						
28	-11.26975	-3.38494	-0.51968	c	0.566	3.246	24.7
715.3	25342.3						
29	-11.72100	-5.38018	-0.32910	h	0.366	1.010	3.1
37.3	552.5						
30	-13.04379	-1.78780	0.44665	c	0.566	3.087	25.5
736.9	26108.4						
31	2.87554	-2.84660	-4.52120	c	0.566	3.303	24.3
701.4	24849.0						
32	-14.88643	1.61006	3.45712	c	0.566	3.266	24.6
710.9	25185.2						
33	-16.33934	-0.45496	3.82950	c	0.566	3.260	24.6
712.2	25233.6						
34	2.71911	3.98943	-4.55167	c	0.566	3.254	24.7
713.7	25286.8						
35	4.69215	4.38977	-4.84764	h	0.366	1.022	3.1
37.2	551.6						
36	-4.08553	-1.97833	-3.91186	c	0.566	3.337	23.9
691.2	24489.8						
37	0.27585	-3.39823	-4.26605	c	0.566	3.352	23.7
686.1	24308.1						
38	-5.58950	2.33544	-7.78288	c	0.566	4.109	18.3
528.0	18707.8						
39	-7.56692	1.92896	-8.20648	h	0.366	0.999	3.1
37.4	553.3						
40	-4.43618	0.81813	-8.56274	h	0.366	1.000	3.1
37.4	553.3						
41	-5.04984	4.10198	-8.70446	h	0.366	0.999	3.1
37.4	553.4						
42	-3.45269	-7.13226	-6.85914	c	0.566	4.109	18.3
528.0	18708.0						

43	-5.40247	-7.64988	-7.29470	h	0.366	0.999	3.1
37.4	553.3						
44	-2.19524	-8.65110	-7.46728	h	0.366	0.999	3.1
37.4	553.3						
45	-2.98025	-5.43728	-7.92923	h	0.366	1.000	3.1
37.4	553.2						
46	-3.84155	-9.10455	-2.60060	c	0.566	4.098	18.3
528.2	18712.8						
47	-5.76263	-9.68321	-3.06268	h	0.366	1.000	3.1
37.4	553.3						
48	-3.69316	-8.89013	-0.55633	h	0.366	0.999	3.1
37.4	553.3						
49	-2.59689	-10.63481	-3.19093	h	0.366	1.000	3.1
37.4	553.3						
50	3.01561	-0.94621	-8.82697	c	0.566	4.106	18.3
528.1	18709.3						
51	4.18229	-2.48965	-9.54232	h	0.366	0.999	3.1
37.4	553.3						
52	3.41689	0.76080	-9.91654	h	0.366	0.999	3.1
37.4	553.4						
53	1.03914	-1.44807	-9.11061	h	0.366	1.000	3.1
37.4	553.2						
54	6.38873	0.17601	-5.74353	c	0.566	4.101	18.3
528.1	18711.2						
55	6.92274	0.52471	-3.78459	h	0.366	1.000	3.1
37.4	553.2						
56	6.83712	1.85027	-6.85750	h	0.366	1.000	3.1
37.4	553.3						
57	7.55532	-1.35827	-6.46620	h	0.366	1.000	3.1
37.4	553.2						
58	2.00819	8.34572	-2.85691	c	0.566	3.257	24.6
712.9	25257.8						
59	0.66522	9.89659	-2.87954	h	0.366	1.008	3.1
37.3	552.6						
60	4.28643	8.84189	-1.82992	c	0.566	3.087	25.5
736.9	26107.8						
61	8.39501	8.38623	0.89330	c	0.566	3.261	24.6
712.0	25226.2						
62	5.71091	-8.34878	-1.05152	c	0.566	3.242	24.8
716.3	25378.6						
63	5.16913	-10.31070	-0.76056	h	0.366	1.008	3.1
37.3	552.6						
64	8.00703	-7.66817	-0.08203	c	0.566	3.094	25.5
736.3	26087.1						
65	10.78983	-5.35598	3.19443	c	0.566	3.271	24.5
709.7	25143.2						
66	11.25995	-7.83602	3.57390	c	0.566	3.254	24.7
713.7	25284.2						
67	-1.56707	-1.50175	-4.65737	n	0.495	3.231	15.6
344.0	9297.2						
68	-12.85852	1.52422	0.78710	s	0.737	2.686	125.8
6163.6	369906.4						
69	-15.99686	-2.89393	1.55823	s	0.737	2.684	125.8
6163.6	369906.4						
70	5.19467	11.87699	-0.78940	s	0.737	2.648	125.8
6163.7	369906.8						
71	6.71104	6.58145	-1.33086	s	0.737	2.711	125.8
6163.6	369906.2						
72	9.17219	-4.56938	0.35653	s	0.737	2.691	125.8
6163.6	369906.4						

73	10.17714	-9.88471	1.14810	s	0.737	2.679	125.8
6163.6	369906.5						
74	11.78998	-2.87693	5.14641	s	0.737	2.339	125.8
6163.9	369923.2						
75	13.07784	-9.06051	6.04871	s	0.737	2.328	125.8
6164.0	369924.8						
76	9.16918	12.99615	3.16769	s	0.737	2.349	125.8
6163.9	369921.7						
77	10.94687	7.00983	2.50117	s	0.737	2.351	125.8
6163.9	369921.4						
78	-15.07339	4.41026	5.20233	s	0.737	2.339	125.8
6163.9	369923.1						
79	-18.69597	-0.73463	6.13119	s	0.737	2.335	125.8
6163.9	369923.7						
80	8.74864	-1.65070	6.20274	c	0.566	3.992	18.3
530.2	18785.5						
81	7.83334	-3.00531	7.45079	h	0.366	1.009	3.1
37.3	552.5						
82	9.13327	0.09173	7.23043	h	0.366	1.012	3.1
37.3	552.3						
83	7.53691	-1.25645	4.59011	h	0.366	1.011	3.1
37.3	552.4						
84	11.06611	-11.61745	7.17156	c	0.566	3.992	18.3
530.2	18785.2						
85	10.77862	-13.03825	5.71566	h	0.366	1.010	3.1
37.3	552.5						
86	12.05839	-12.45640	8.76964	h	0.366	1.013	3.1
37.3	552.2						
87	9.25102	-10.87937	7.79747	h	0.366	1.009	3.1
37.3	552.5						
88	10.44727	3.64842	1.98520	c	0.566	4.011	18.3
529.7	18768.0						
89	10.66571	3.13640	0.00679	h	0.366	1.010	3.1
37.3	552.4						
90	11.91326	2.69811	3.07106	h	0.366	1.016	3.1
37.3	552.0						
91	8.60511	3.05472	2.67163	h	0.366	1.010	3.1
37.3	552.4						
92	6.86128	13.17876	5.72079	c	0.566	3.989	18.3
530.3	18788.9						
93	6.70296	11.35743	6.66191	h	0.366	1.009	3.1
37.3	552.5						
94	7.55792	14.58989	7.04907	h	0.366	1.012	3.1
37.3	552.3						
95	5.03077	13.76465	4.98997	h	0.366	1.009	3.1
37.3	552.5						
96	-17.74385	-3.64384	7.70714	c	0.566	3.991	18.3
530.3	18786.5						
97	-19.15885	-3.99715	9.16117	h	0.366	1.013	3.1
37.3	552.2						
98	-17.70139	-5.21833	6.38750	h	0.366	1.010	3.1
37.3	552.5						
99	-15.89698	-3.41065	8.58244	h	0.366	1.009	3.1
37.3	552.5						
100	-11.76863	4.91879	6.02662	c	0.566	3.992	18.3
530.2	18785.2						
101	-10.61016	5.17110	4.34918	h	0.366	1.010	3.1
37.3	552.5						
102	-11.72751	6.63796	7.15955	h	0.366	1.013	3.1
37.3	552.2						

103 -11.05815 3.34135 7.13858 h 0.366 1.009 3.1
37.3 552.5

molecular C6(AA) [au] = 184820.34

DFT-D V3(BJ)
DF b3-lyp
parameters
s6 : 1.0000
s8 : 1.9889
a1 : 0.3981
a2 : 4.4211
k1-k3 : 16.0000 1.3333 -4.0000
Cutoff : 94.8683 a.u.
CN-Cutoff: 40.0000 a.u.

Edisp /kcal,au: -204.4570 -0.32582294

E6 /kcal : -91.7004
E8 /kcal : -113.2909
E6(ABC) " : 0.534324
% E8 : 55.41
% E6(ABC) : -0.26
normal termination of dftd3

=====

4

```
|           DFTD3 V3.1 Rev 0           |  
| S.Grimme, University Bonn           |  
|           June 2014                 |  
| see dftd3 -h for options           |
```

Please cite DFT-D3 work done with this code as:
S. Grimme, J. Antony, S. Ehrlich and H. Krieg,
J. Chem. Phys. 132 (2010), 154104
If used with BJ-damping cite also
S. Grimme, S. Ehrlich and L. Goerigk,
J. Comput. Chem. 32 (2011), 1456-1465
For DFT-D2 the reference is
S. Grimme, J. Comput. Chem., 27 (2006), 1787-1799

files read :

c4.xyz

C6 coefficients used:

2	C6 for element	1
Z= 1	CN= 0.912 C6(AA)= 3.03	
Z= 1	CN= 0.000 C6(AA)= 7.59	
5	C6 for element	6
Z= 6	CN= 0.000 C6(AA)= 49.11	
Z= 6	CN= 0.987 C6(AA)= 43.25	
Z= 6	CN= 1.998 C6(AA)= 29.36	
Z= 6	CN= 2.999 C6(AA)= 25.78	
Z= 6	CN= 3.984 C6(AA)= 18.21	
4	C6 for element	7
Z= 7	CN= 0.000 C6(AA)= 25.27	

Z= 7 CN= 0.994 C6(AA)= 22.12
 Z= 7 CN= 2.014 C6(AA)= 19.68
 Z= 7 CN= 2.990 C6(AA)= 15.58

#	XYZ [au]				R0(AA) [Ang.]	CN	C6(AA)
C8(AA)	C10(AA) [au]						
1	0.00000	0.06711	0.14609	n	0.495	3.234	15.6
344.0	9297.0						
2	2.30125	1.38616	-0.17663	c	0.566	3.327	24.0
694.3	24599.3						
3	2.30698	4.05038	-0.09369	c	0.566	3.307	24.2
700.3	24811.3						
4	4.48282	5.35752	-0.74929	c	0.566	3.184	25.1
726.3	25731.7						
5	4.47334	7.39648	-0.74999	h	0.366	1.006	3.1
37.3	552.7						
6	6.69592	4.09041	-1.34784	c	0.566	3.132	25.3
732.7	25960.5						
7	8.38173	5.12675	-1.86048	h	0.366	1.004	3.1
37.3	552.9						
8	6.73521	1.48689	-1.17612	c	0.566	3.196	25.1
724.6	25670.2						
9	8.48928	0.49516	-1.51059	h	0.366	1.006	3.1
37.3	552.8						
10	4.58016	0.09906	-0.57105	c	0.566	3.290	24.4
704.9	24975.3						
11	4.83815	-2.73084	-0.20627	c	0.566	4.138	18.2
527.7	18697.4						
12	2.29173	-3.94734	0.32065	c	0.566	3.291	24.4
704.8	24972.0						
13	2.24174	-6.54168	0.74171	c	0.566	3.198	25.0
724.1	25654.7						
14	4.00727	-7.56487	0.82765	h	0.366	1.006	3.1
37.3	552.7						
15	-0.00002	-7.85176	1.01682	c	0.566	3.130	25.3
733.0	25968.2						
16	-0.00003	-9.86530	1.36852	h	0.366	1.004	3.1
37.3	552.9						
17	-2.24177	-6.54166	0.74172	c	0.566	3.198	25.0
724.1	25654.7						
18	-4.00731	-7.56484	0.82767	h	0.366	1.006	3.1
37.3	552.7						
19	-2.29176	-3.94733	0.32067	c	0.566	3.291	24.4
704.8	24972.0						
20	-0.00001	-2.60115	0.25571	c	0.566	3.307	24.2
700.2	24807.4						
21	-4.83817	-2.73081	-0.20623	c	0.566	4.138	18.2
527.7	18697.4						
22	-4.58016	0.09909	-0.57099	c	0.566	3.290	24.4
704.9	24975.3						
23	-6.73522	1.48694	-1.17601	c	0.566	3.196	25.1
724.5	25670.2						
24	-8.48930	0.49522	-1.51046	h	0.366	1.006	3.1
37.3	552.8						
25	-6.69592	4.09046	-1.34771	c	0.566	3.132	25.3
732.7	25960.5						
26	-8.38173	5.12682	-1.86032	h	0.366	1.004	3.1
37.3	552.9						
27	-4.48280	5.35755	-0.74920	c	0.566	3.184	25.1
726.3	25731.7						

28	-4.47331	7.39651	-0.74988	h	0.366	1.006	3.1
37.3	552.7						
29	-2.30696	4.05040	-0.09364	c	0.566	3.307	24.2
700.3	24811.3						
30	-2.30125	1.38618	-0.17659	c	0.566	3.327	24.0
694.3	24599.3						
31	0.00003	5.37746	0.95704	c	0.566	4.145	18.2
527.7	18695.2						
32	6.64329	-3.19706	2.04415	c	0.566	4.099	18.3
528.2	18712.2						
33	5.87449	-2.36246	3.76405	h	0.366	0.999	3.1
37.4	553.3						
34	8.48727	-2.35187	1.68836	h	0.366	0.999	3.1
37.4	553.3						
35	6.92027	-5.21122	2.37132	h	0.366	0.999	3.1
37.4	553.3						
36	5.95390	-3.94351	-2.61924	c	0.566	4.099	18.3
528.2	18712.3						
37	6.18273	-5.97594	-2.38264	h	0.366	0.999	3.1
37.4	553.3						
38	7.80004	-3.14765	-3.06407	h	0.366	0.999	3.1
37.4	553.3						
39	4.70617	-3.61897	-4.22642	h	0.366	0.999	3.1
37.4	553.3						
40	-5.95393	-3.94345	-2.61922	c	0.566	4.099	18.3
528.2	18712.3						
41	-4.70619	-3.61890	-4.22639	h	0.366	0.999	3.1
37.4	553.3						
42	-7.80006	-3.14757	-3.06404	h	0.366	0.999	3.1
37.4	553.3						
43	-6.18277	-5.97588	-2.38264	h	0.366	0.999	3.1
37.4	553.3						
44	-6.64331	-3.19705	2.04418	c	0.566	4.099	18.3
528.2	18712.2						
45	-6.92030	-5.21122	2.37133	h	0.366	0.999	3.1
37.4	553.3						
46	-8.48728	-2.35185	1.68841	h	0.366	0.999	3.1
37.4	553.3						
47	-5.87450	-2.36247	3.76409	h	0.366	0.999	3.1
37.4	553.3						
48	0.00006	5.00560	3.86725	c	0.566	4.111	18.3
528.0	18707.3						
49	-1.67889	5.87601	4.69035	h	0.366	0.999	3.1
37.4	553.3						
50	1.67903	5.87599	4.69031	h	0.366	0.999	3.1
37.4	553.3						
51	0.00005	3.00687	4.36103	h	0.366	1.000	3.1
37.4	553.2						
52	0.00003	8.21927	0.43234	c	0.566	4.099	18.3
528.2	18712.4						
53	0.00001	8.63015	-1.58747	h	0.366	0.999	3.1
37.4	553.3						
54	1.64984	9.10840	1.28226	h	0.366	1.000	3.1
37.4	553.3						
55	-1.64975	9.10842	1.28230	h	0.366	1.000	3.1
37.4	553.3						

molecular C6(AA) [au] = 32067.98

DFT-D V3 (BJ)

DF b3-lyp
parameters
s6 : 1.0000
s8 : 1.9889
a1 : 0.3981
a2 : 4.4211
k1-k3 : 16.0000 1.3333 -4.0000
Cutoff : 94.8683 a.u.
CN-Cutoff: 40.0000 a.u.

Edisp /kcal,au: -92.2211 -0.14696370

E6 /kcal : -43.7702
E8 /kcal : -48.8090
E6(ABC) " : 0.358051
% E8 : 52.93
% E6(ABC) : -0.39
normal termination of dftd3

=====

4_ox1

| DFTD3 V3.1 Rev 0 |
| S.Grimme, University Bonn |
| June 2014 |
| see dftd3 -h for options |

Please cite DFT-D3 work done with this code as:
S. Grimme, J. Antony, S. Ehrlich and H. Krieg,
J. Chem. Phys. 132 (2010), 154104
If used with BJ-damping cite also
S. Grimme, S. Ehrlich and L. Goerigk,
J. Comput. Chem. 32 (2011), 1456-1465
For DFT-D2 the reference is
S. Grimme, J. Comput. Chem., 27 (2006), 1787-1799

files read :

c4_plm2.xyz

C6 coefficients used:

	2	C6 for element		1
Z=	1	CN= 0.912	C6(AA)=	3.03
Z=	1	CN= 0.000	C6(AA)=	7.59
	5	C6 for element		6
Z=	6	CN= 0.000	C6(AA)=	49.11
Z=	6	CN= 0.987	C6(AA)=	43.25
Z=	6	CN= 1.998	C6(AA)=	29.36
Z=	6	CN= 2.999	C6(AA)=	25.78
Z=	6	CN= 3.984	C6(AA)=	18.21
	4	C6 for element		7
Z=	7	CN= 0.000	C6(AA)=	25.27
Z=	7	CN= 0.994	C6(AA)=	22.12
Z=	7	CN= 2.014	C6(AA)=	19.68
Z=	7	CN= 2.990	C6(AA)=	15.58

#	XYZ [au]	R0(AA) [Ang.]	CN	C6(AA)
C8(AA)	C10(AA) [au]			

1	0.00000	-0.05287	0.03257	n	0.495	3.232	15.6
344.0	9297.2						
2	-2.30529	-1.38449	-0.17672	c	0.566	3.325	24.0
695.1	24626.1						
3	-2.30570	-4.06045	-0.06722	c	0.566	3.303	24.3
701.6	24855.9						
4	-4.49833	-5.34787	-0.65800	c	0.566	3.185	25.1
726.2	25729.3						
5	-4.51578	-7.38430	-0.63314	h	0.366	1.007	3.1
37.3	552.7						
6	-6.70621	-4.06150	-1.26366	c	0.566	3.136	25.3
732.3	25946.3						
7	-8.39652	-5.09837	-1.75750	h	0.366	1.004	3.1
37.3	552.9						
8	-6.74690	-1.45598	-1.14202	c	0.566	3.194	25.1
724.9	25681.0						
9	-8.49822	-0.46987	-1.49172	h	0.366	1.006	3.1
37.3	552.7						
10	-4.59027	-0.07436	-0.55775	c	0.566	3.294	24.3
704.0	24941.8						
11	-4.83008	2.74469	-0.24269	c	0.566	4.142	18.2
527.7	18696.0						
12	-2.31063	3.94232	0.34681	c	0.566	3.293	24.3
704.2	24950.4						
13	-2.25468	6.50987	0.86583	c	0.566	3.196	25.1
724.5	25669.9						
14	-4.00949	7.54253	0.98716	h	0.366	1.006	3.1
37.3	552.7						
15	0.00005	7.79389	1.18568	c	0.566	3.134	25.3
732.5	25952.2						
16	0.00005	9.79348	1.60675	h	0.366	1.004	3.1
37.3	552.9						
17	2.25475	6.50985	0.86583	c	0.566	3.196	25.1
724.5	25669.9						
18	4.00958	7.54248	0.98718	h	0.366	1.006	3.1
37.3	552.7						
19	2.31067	3.94229	0.34682	c	0.566	3.293	24.3
704.2	24950.4						
20	0.00002	2.60721	0.22587	c	0.566	3.311	24.2
699.2	24773.3						
21	4.83011	2.74464	-0.24268	c	0.566	4.142	18.2
527.7	18696.0						
22	4.59027	-0.07440	-0.55775	c	0.566	3.294	24.3
704.0	24941.8						
23	6.74688	-1.45606	-1.14203	c	0.566	3.194	25.1
724.9	25681.0						
24	8.49821	-0.46996	-1.49174	h	0.366	1.006	3.1
37.3	552.7						
25	6.70616	-4.06157	-1.26367	c	0.566	3.136	25.3
732.3	25946.3						
26	8.39646	-5.09847	-1.75751	h	0.366	1.004	3.1
37.3	552.9						
27	4.49827	-5.34792	-0.65800	c	0.566	3.185	25.1
726.2	25729.3						
28	4.51570	-7.38435	-0.63314	h	0.366	1.007	3.1
37.3	552.7						
29	2.30565	-4.06048	-0.06722	c	0.566	3.303	24.3
701.6	24855.9						
30	2.30528	-1.38452	-0.17672	c	0.566	3.325	24.0
695.1	24626.1						

31	-0.00003	-5.41445	0.92012	c	0.566	4.144	18.2
527.7	18695.5						
32	-6.71761	3.25490	1.93782	c	0.566	4.100	18.3
528.1	18711.6						
33	-6.02402	2.45470	3.70435	h	0.366	0.999	3.1
37.4	553.3						
34	-8.54811	2.41621	1.52186	h	0.366	0.999	3.1
37.4	553.3						
35	-7.00264	5.27320	2.20603	h	0.366	0.999	3.1
37.4	553.3						
36	-5.83717	3.93676	-2.72269	c	0.566	4.100	18.3
528.1	18711.8						
37	-6.04885	5.97161	-2.50846	h	0.366	0.999	3.1
37.4	553.3						
38	-7.67498	3.15471	-3.21393	h	0.366	0.999	3.1
37.4	553.3						
39	-4.54086	3.57995	-4.28316	h	0.366	0.999	3.1
37.4	553.3						
40	5.83720	3.93670	-2.72269	c	0.566	4.100	18.3
528.1	18711.8						
41	4.54089	3.57987	-4.28317	h	0.366	0.999	3.1
37.4	553.3						
42	7.67502	3.15465	-3.21392	h	0.366	0.999	3.1
37.4	553.3						
43	6.04887	5.97155	-2.50848	h	0.366	0.999	3.1
37.4	553.3						
44	6.71765	3.25485	1.93781	c	0.566	4.100	18.3
528.1	18711.6						
45	7.00270	5.27314	2.20601	h	0.366	0.999	3.1
37.4	553.3						
46	8.54814	2.41613	1.52187	h	0.366	0.999	3.1
37.4	553.3						
47	6.02405	2.45467	3.70435	h	0.366	0.999	3.1
37.4	553.3						
48	-0.00003	-5.11980	3.85212	c	0.566	4.111	18.3
528.0	18707.2						
49	1.67598	-6.02029	4.64110	h	0.366	0.999	3.1
37.4	553.3						
50	-1.67606	-6.02025	4.64110	h	0.366	0.999	3.1
37.4	553.3						
51	-0.00000	-3.13941	4.41697	h	0.366	0.999	3.1
37.4	553.3						
52	-0.00004	-8.24244	0.31456	c	0.566	4.098	18.3
528.2	18712.6						
53	-0.00002	-8.59891	-1.71448	h	0.366	0.999	3.1
37.4	553.3						
54	-1.64259	-9.15744	1.14553	h	0.366	1.000	3.1
37.4	553.2						
55	1.64248	-9.15746	1.14557	h	0.366	1.000	3.1
37.4	553.2						

molecular C6(AA) [au] = 32067.70

DFT-D V3(BJ)

DF b3-lyp
parameters

s6 : 1.0000
s8 : 1.9889
a1 : 0.3981
a2 : 4.4211

k1-k3 : 16.0000 1.3333 -4.0000
Cutoff : 94.8683 a.u.
CN-Cutoff: 40.0000 a.u.

Edisp /kcal,au: -92.1965 -0.14692441

E6 /kcal : -43.7525
E8 /kcal : -48.7991
E6(ABC) " : 0.355126
% E8 : 52.93
% E6(ABC) : -0.39
normal termination of dftd3

=====

4_red1

	DFTD3 V3.1 Rev 0	
	S.Grimme, University Bonn	
	June 2014	
	see dftd3 -h for options	

Please cite DFT-D3 work done with this code as:
S. Grimme, J. Antony, S. Ehrlich and H. Krieg,
J. Chem. Phys. 132 (2010), 154104
If used with BJ-damping cite also
S. Grimme, S. Ehrlich and L. Goerigk,
J. Comput. Chem. 32 (2011), 1456-1465
For DFT-D2 the reference is
S. Grimme, J. Comput. Chem., 27 (2006), 1787-1799

files read :

c4_mlm2.xyz

C6 coefficients used:

	2	C6 for element	1
Z= 1	CN= 0.912	C6(AA)= 3.03	
Z= 1	CN= 0.000	C6(AA)= 7.59	
	5	C6 for element	6
Z= 6	CN= 0.000	C6(AA)= 49.11	
Z= 6	CN= 0.987	C6(AA)= 43.25	
Z= 6	CN= 1.998	C6(AA)= 29.36	
Z= 6	CN= 2.999	C6(AA)= 25.78	
Z= 6	CN= 3.984	C6(AA)= 18.21	
	4	C6 for element	7
Z= 7	CN= 0.000	C6(AA)= 25.27	
Z= 7	CN= 0.994	C6(AA)= 22.12	
Z= 7	CN= 2.014	C6(AA)= 19.68	
Z= 7	CN= 2.990	C6(AA)= 15.58	

#	XYZ [au]	R0(AA) [Ang.]	CN	C6(AA)	
C8(AA)	C10(AA) [au]				
1	0.00000 -0.08124 0.19919	n	0.495	3.235	15.6
344.0	9297.0				
2	-2.28087 -1.40205 -0.15338	c	0.566	3.330	24.0
693.5	24570.6				
3	-2.30400 -4.05075 -0.00681	c	0.566	3.298	24.3
702.8	24899.5				

4	-4.48012	-5.38322	-0.68459	c	0.566	3.174	25.2
727.8	25783.7						
5	-4.49840	-7.42062	-0.60227	h	0.366	1.006	3.1
37.3	552.8						
6	-6.65847	-4.09340	-1.44841	c	0.566	3.125	25.4
733.5	25986.7						
7	-8.32863	-5.13142	-2.02016	h	0.366	1.003	3.1
37.3	553.0						
8	-6.68025	-1.49201	-1.38748	c	0.566	3.182	25.1
726.6	25741.1						
9	-8.40079	-0.50277	-1.88715	h	0.366	1.005	3.1
37.3	552.8						
10	-4.54328	-0.07806	-0.68454	c	0.566	3.283	24.4
706.9	25045.9						
11	-4.81247	2.74250	-0.29576	c	0.566	4.132	18.2
527.8	18699.3						
12	-2.30860	3.94971	0.41870	c	0.566	3.279	24.5
707.9	25079.0						
13	-2.25563	6.49477	1.00678	c	0.566	3.186	25.1
726.0	25722.4						
14	-4.02511	7.51911	1.10790	h	0.366	1.006	3.1
37.3	552.8						
15	-0.00004	7.80842	1.39994	c	0.566	3.121	25.4
733.8	25999.5						
16	-0.00005	9.79237	1.89370	h	0.366	1.003	3.1
37.3	553.0						
17	2.25556	6.49479	1.00679	c	0.566	3.186	25.1
726.0	25722.4						
18	4.02504	7.51914	1.10792	h	0.366	1.006	3.1
37.3	552.8						
19	2.30855	3.94973	0.41871	c	0.566	3.279	24.5
707.9	25079.0						
20	-0.00001	2.57434	0.28169	c	0.566	3.308	24.2
700.1	24805.4						
21	4.81244	2.74254	-0.29574	c	0.566	4.132	18.2
527.8	18699.3						
22	4.54328	-0.07801	-0.68455	c	0.566	3.283	24.4
706.9	25045.9						
23	6.68026	-1.49194	-1.38751	c	0.566	3.182	25.1
726.6	25741.1						
24	8.40079	-0.50269	-1.88718	h	0.366	1.005	3.1
37.3	552.8						
25	6.65850	-4.09333	-1.44844	c	0.566	3.125	25.4
733.5	25986.7						
26	8.32867	-5.13133	-2.02022	h	0.366	1.003	3.1
37.3	553.0						
27	4.48017	-5.38317	-0.68462	c	0.566	3.174	25.2
727.8	25783.7						
28	4.49847	-7.42057	-0.60229	h	0.366	1.006	3.1
37.3	552.8						
29	2.30404	-4.05072	-0.00683	c	0.566	3.298	24.3
702.8	24899.5						
30	2.28088	-1.40202	-0.15339	c	0.566	3.330	24.0
693.5	24570.6						
31	0.00003	-5.35774	1.08661	c	0.566	4.144	18.2
527.7	18695.6						
32	-6.78336	3.19318	1.81805	c	0.566	4.098	18.3
528.2	18712.6						
33	-6.11412	2.37573	3.58775	h	0.366	0.999	3.1
37.4	553.3						

34	-8.57928	2.30042	1.33619	h	0.366	0.999	3.1
37.4	553.3						
35	-7.12977	5.20385	2.12154	h	0.366	0.999	3.1
37.4	553.4						
36	-5.75376	4.00393	-2.76066	c	0.566	4.099	18.3
528.2	18712.4						
37	-6.08694	6.01964	-2.48227	h	0.366	0.999	3.1
37.4	553.3						
38	-7.51333	3.14235	-3.41234	h	0.366	0.999	3.1
37.4	553.3						
39	-4.33971	3.77817	-4.24274	h	0.366	0.999	3.1
37.4	553.3						
40	5.75375	4.00401	-2.76062	c	0.566	4.099	18.3
528.2	18712.4						
41	4.33971	3.77825	-4.24272	h	0.366	0.999	3.1
37.4	553.3						
42	7.51333	3.14245	-3.41230	h	0.366	0.999	3.1
37.4	553.3						
43	6.08690	6.01972	-2.48221	h	0.366	0.999	3.1
37.4	553.3						
44	6.78331	3.19321	1.81809	c	0.566	4.098	18.3
528.2	18712.6						
45	7.12971	5.20388	2.12160	h	0.366	0.999	3.1
37.4	553.4						
46	8.57924	2.30047	1.33623	h	0.366	0.999	3.1
37.4	553.3						
47	6.11405	2.37574	3.58777	h	0.366	0.999	3.1
37.4	553.3						
48	0.00004	-4.97333	3.99609	c	0.566	4.105	18.3
528.1	18709.7						
49	1.68155	-5.83700	4.82731	h	0.366	0.998	3.1
37.4	553.4						
50	-1.68147	-5.83701	4.82732	h	0.366	0.998	3.1
37.4	553.4						
51	0.00003	-2.96907	4.46371	h	0.366	1.000	3.1
37.4	553.2						
52	0.00004	-8.21107	0.60295	c	0.566	4.099	18.3
528.2	18712.1						
53	0.00004	-8.64687	-1.41151	h	0.366	0.999	3.1
37.4	553.3						
54	-1.65674	-9.08248	1.46277	h	0.366	0.999	3.1
37.4	553.3						
55	1.65685	-9.08246	1.46276	h	0.366	0.999	3.1
37.4	553.3						

molecular C6(AA) [au] = 32101.26

DFT-D V3(BJ)

DF b3-lyp

parameters

s6 : 1.0000
s8 : 1.9889
a1 : 0.3981
a2 : 4.4211
k1-k3 : 16.0000 1.3333 -4.0000
Cutoff : 94.8683 a.u.
CN-Cutoff: 40.0000 a.u.

Edisp /kcal,au: -91.9989 -0.14660956

```

E6      /kcal :   -43.6681
E8      /kcal :   -48.6966
E6(ABC) "   :    0.365814
% E8           :   52.93
% E6(ABC)     :   -0.40
normal termination of dftd3

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C60

```

|           DFTD3 V3.1 Rev 0           |
| S.Grimme, University Bonn           |
|           June 2014                 |
| see dftd3 -h for options           |

```

Please cite DFT-D3 work done with this code as:
S. Grimme, J. Antony, S. Ehrlich and H. Krieg,
J. Chem. Phys. 132 (2010), 154104
If used with BJ-damping cite also
S. Grimme, S. Ehrlich and L. Goerigk,
J. Comput. Chem. 32 (2011), 1456-1465
For DFT-D2 the reference is
S. Grimme, J. Comput. Chem., 27 (2006), 1787-1799

files read :

C60.xyz

C6 coefficients used:

	5	C6 for element	6
Z= 6 CN= 0.000	C6(AA)=	49.11	
Z= 6 CN= 0.987	C6(AA)=	43.25	
Z= 6 CN= 1.998	C6(AA)=	29.36	
Z= 6 CN= 2.999	C6(AA)=	25.78	
Z= 6 CN= 3.984	C6(AA)=	18.21	

#	XYZ [au]	R0(AA) [Ang.]	CN	C6(AA)
C8(AA)	C10(AA) [au]			
1	2.21829 0.72074 6.26959	c 0.566	3.382	23.3
675.1	23919.0			
2	4.34158 1.41058 4.89025	c 0.566	3.382	23.3
675.2	23920.2			
3	-4.34158 -1.41058 -4.89025	c 0.566	3.382	23.3
675.2	23920.2			
4	-2.21829 -0.72074 -6.26959	c 0.566	3.382	23.3
675.1	23919.0			
5	2.68302 -6.02536 1.11629	c 0.566	3.382	23.3
675.1	23919.3			
6	1.37093 -6.45136 -1.11604	c 0.566	3.382	23.3
675.1	23918.4			
7	-1.37093 6.45136 1.11604	c 0.566	3.382	23.3
675.1	23918.4			
8	-2.68302 6.02536 -1.11629	c 0.566	3.382	23.3
675.1	23919.3			
9	-4.90161 -2.97238 3.44881	c 0.566	3.382	23.3
675.2	23921.3			
10	-5.71259 -0.47652 3.44878	c 0.566	3.382	23.3
675.2	23920.8			

11	5.71259	0.47652	-3.44878	c	0.566	3.382	23.3
675.2	23920.8						
12	4.90161	2.97238	-3.44881	c	0.566	3.382	23.3
675.2	23921.3						
13	1.37093	-1.88698	6.26952	c	0.566	3.382	23.3
675.1	23919.3						
14	0.00000	2.33249	6.26965	c	0.566	3.382	23.3
675.1	23919.6						
15	5.71259	-0.47652	3.44878	c	0.566	3.382	23.3
675.2	23920.8						
16	4.34162	3.74308	3.44875	c	0.566	3.382	23.3
675.2	23920.5						
17	-4.34162	-3.74308	-3.44875	c	0.566	3.382	23.3
675.2	23920.5						
18	-5.71259	0.47652	-3.44878	c	0.566	3.382	23.3
675.2	23920.8						
19	0.00000	-2.33249	-6.26965	c	0.566	3.382	23.3
675.1	23919.6						
20	-1.37093	1.88698	-6.26952	c	0.566	3.382	23.3
675.1	23919.3						
21	1.31224	-5.58059	3.44903	c	0.566	3.382	23.3
675.2	23922.3						
22	4.90124	-4.41354	1.11617	c	0.566	3.382	23.3
675.1	23919.3						
23	-1.37093	-6.45136	-1.11604	c	0.566	3.382	23.3
675.1	23918.4						
24	2.21835	-5.28537	-3.44851	c	0.566	3.382	23.3
675.1	23919.2						
25	-2.21835	5.28537	3.44851	c	0.566	3.382	23.3
675.1	23919.2						
26	1.37093	6.45136	1.11604	c	0.566	3.382	23.3
675.1	23918.4						
27	-4.90124	4.41354	-1.11617	c	0.566	3.382	23.3
675.1	23919.3						
28	-1.31224	5.58059	-3.44903	c	0.566	3.382	23.3
675.2	23922.3						
29	-2.68316	-3.69315	4.89027	c	0.566	3.382	23.3
675.1	23919.6						
30	-4.90124	-4.41355	1.11617	c	0.566	3.382	23.3
675.1	23919.3						
31	-4.34158	1.41058	4.89025	c	0.566	3.382	23.3
675.2	23920.2						
32	-6.55981	0.68979	1.11623	c	0.566	3.382	23.3
675.2	23920.3						
33	6.55981	-0.68979	-1.11623	c	0.566	3.382	23.3
675.2	23920.3						
34	4.34158	-1.41058	-4.89025	c	0.566	3.382	23.3
675.2	23920.2						
35	4.90124	4.41355	-1.11617	c	0.566	3.382	23.3
675.1	23919.3						
36	2.68316	3.69315	-4.89027	c	0.566	3.382	23.3
675.1	23919.6						
37	2.68316	-3.69315	4.89027	c	0.566	3.382	23.3
675.1	23919.6						
38	0.00000	4.56465	4.89000	c	0.566	3.382	23.3
675.1	23918.6						
39	4.90161	-2.97238	3.44881	c	0.566	3.382	23.3
675.2	23921.3						
40	2.21835	5.28537	3.44851	c	0.566	3.382	23.3
675.1	23919.2						

41	-2.21835	-5.28537	-3.44851	c	0.566	3.382	23.3
675.1	23919.2						
42	-4.90161	2.97238	-3.44881	c	0.566	3.382	23.3
675.2	23921.3						
43	0.00000	-4.56465	-4.89000	c	0.566	3.382	23.3
675.1	23918.6						
44	-2.68316	3.69315	-4.89027	c	0.566	3.382	23.3
675.1	23919.6						
45	-1.31224	-5.58059	3.44903	c	0.566	3.382	23.3
675.2	23922.3						
46	5.71236	-3.29751	-1.11615	c	0.566	3.382	23.3
675.2	23920.1						
47	-2.68302	-6.02536	1.11630	c	0.566	3.382	23.3
675.1	23919.3						
48	4.34162	-3.74308	-3.44875	c	0.566	3.382	23.3
675.2	23920.5						
49	-4.34162	3.74308	3.44875	c	0.566	3.382	23.3
675.2	23920.5						
50	2.68302	6.02536	-1.11630	c	0.566	3.382	23.3
675.1	23919.3						
51	-5.71236	3.29751	1.11615	c	0.566	3.382	23.3
675.2	23920.1						
52	1.31224	5.58059	-3.44903	c	0.566	3.382	23.3
675.2	23922.3						
53	-1.37093	-1.88699	6.26952	c	0.566	3.382	23.3
675.1	23919.3						
54	-5.71236	-3.29751	-1.11615	c	0.566	3.382	23.3
675.2	23920.1						
55	-2.21829	0.72074	6.26959	c	0.566	3.382	23.3
675.1	23919.0						
56	-6.55981	-0.68979	-1.11623	c	0.566	3.382	23.3
675.2	23920.3						
57	6.55981	0.68979	1.11623	c	0.566	3.382	23.3
675.2	23920.3						
58	2.21829	-0.72074	-6.26959	c	0.566	3.382	23.3
675.1	23919.0						
59	5.71236	3.29751	1.11615	c	0.566	3.382	23.3
675.2	23920.1						
60	1.37093	1.88699	-6.26952	c	0.566	3.382	23.3
675.1	23919.3						

molecular C6(AA) [au] = 84038.28

DFT-D V3(BJ)

DF b3-lyp
parameters

s6 : 1.0000
s8 : 1.9889
a1 : 0.3981
a2 : 4.4211
k1-k3 : 16.0000 1.3333 -4.0000
Cutoff : 94.8683 a.u.
CN-Cutoff: 40.0000 a.u.

Edisp /kcal,au: -195.2922 -0.31121792

E6 /kcal : -88.3458
E8 /kcal : -109.8515
E6(ABC) " : 2.905090
% E8 : 56.25

% E6(ABC) : -1.49
normal termination of dftd3

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Calculations at B3LYP-D3(BJ)/6-31G(d)

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C	2.440851	-2.629035	-1.890593
H	3.479581	-2.352785	-2.007807
C	0.818417	0.518807	-2.761537
C	1.812905	-0.540071	-3.202024
C	3.491243	6.093159	-0.010120
C	-3.940899	1.915625	-2.377345
H	-4.968815	1.643383	-2.630591
H	-3.727214	2.843893	-2.913780
H	-3.889556	2.112484	-1.301834
C	-0.538555	0.159745	-2.641338
C	2.122520	-3.842309	-1.266510
C	-9.893593	3.390005	2.777966
H	-9.282054	3.643436	3.647689
H	-10.952291	3.389845	3.036147
H	-9.689985	4.104131	1.976622
C	-10.824501	-0.207392	4.882025
H	-11.141181	-1.232572	5.087372
H	-11.667602	0.353786	4.470625
H	-10.445878	0.270363	5.785111
C	0.258235	2.841859	-2.259159
C	-1.098252	2.488436	-2.335507
H	-1.840376	3.266898	-2.204759
C	-1.511651	1.177901	-2.550526
C	-2.964055	0.812423	-2.806642
C	-3.225501	-0.513445	-2.110540
C	-4.453787	-0.790603	-1.519146
H	-5.207602	-0.017370	-1.517684
C	-4.760913	-2.050680	-0.987766
C	-3.813483	-3.068182	-1.178678
H	-4.061727	-4.067769	-0.842572
C	-2.578911	-2.835160	-1.772258
C	-1.626281	-3.969103	-2.114463
C	-0.214865	-3.463205	-1.871942
C	0.787809	-4.268306	-1.341339
H	0.536930	-5.248413	-0.953337
C	-6.004386	-2.367927	-0.301059
H	-6.235178	-3.429440	-0.226165
C	-6.883361	-1.527913	0.288691
C	1.464739	-1.792174	-2.418407
C	-8.090389	0.435362	1.545188
C	-8.813945	-0.666224	1.843830

C	1.193336	1.841497	-2.557198
H	2.233431	2.108504	-2.675834
C	-9.978432	-0.774635	2.772338
C	-2.240238	-1.520900	-2.163710
C	0.108438	-2.157026	-2.299512
C	-3.131858	0.589117	-4.336390
H	-4.160095	0.285182	-4.561592
H	-2.456438	-0.192286	-4.696974
H	-2.907449	1.513849	-4.879290
C	-8.337135	1.836920	1.956946
C	-1.767308	-4.263751	-3.635196
H	-2.786502	-4.596409	-3.860693
H	-1.062530	-5.047364	-3.934521
H	-1.559274	-3.370103	-4.230610
C	-1.934686	-5.263873	-1.352251
H	-2.939422	-5.621514	-1.592430
H	-1.862528	-5.127558	-0.268418
H	-1.243270	-6.056380	-1.651090
C	1.584612	-0.828478	-4.711645
H	2.256961	-1.625065	-5.048945
H	1.781585	0.074032	-5.300525
H	0.555063	-1.144540	-4.903163
C	3.272237	-0.104465	-3.015019
H	3.503868	0.118400	-1.968558
H	3.487002	0.784636	-3.613836
H	3.953869	-0.885076	-3.363767
C	0.630969	4.205080	-1.908780
H	-0.133995	4.964651	-2.060765
C	1.793484	4.619233	-1.356887
C	4.003233	4.844666	0.043500
C	5.285261	4.505581	0.704947
C	6.704530	2.718360	1.304538
H	7.539965	3.123257	0.727774
H	6.681730	1.631502	1.247182
H	6.793145	3.056306	2.340773
C	4.064558	7.309965	0.648611
C	4.808092	8.211941	2.677295
H	4.714475	7.963917	3.734113
H	4.348701	9.179043	2.460635
H	5.858495	8.227266	2.376547
C	3.113807	-4.660028	-0.578677
H	2.909300	-5.727583	-0.516224
C	4.227775	-4.218742	0.044205
C	5.893274	-2.805300	1.476854
C	6.230871	-4.087579	1.735329
C	6.485010	-1.583420	2.102834
C	7.005953	-0.515061	4.121927
H	6.589009	0.444612	3.806989
H	8.078661	-0.537231	3.916489
H	6.812261	-0.691420	5.179212
C	7.347772	-4.480505	2.624620
C	8.422549	-6.313172	3.638193
H	8.387550	-5.873532	4.637979
H	9.381759	-6.071727	3.173569
H	8.274167	-7.391513	3.684552
N	-0.917926	-1.215871	-2.600476
O	-9.724762	-0.196961	3.955696
O	-10.993254	-1.377538	2.497949
O	-9.609017	2.051406	2.338953
O	-7.488589	2.703938	1.889853

O	6.091151	5.312704	1.121891
O	5.455645	3.170167	0.747700
O	4.371209	8.310774	0.040051
O	4.124091	7.158625	1.976531
O	6.956241	-0.673490	1.452439
O	6.356272	-1.597001	3.431391
O	8.182365	-3.724475	3.077438
O	7.339653	-5.812694	2.837004
S	-6.720475	0.241506	0.443226
S	-8.373724	-2.161757	1.038391
S	2.078667	6.346997	-1.014086
S	3.157918	3.579162	-0.863804
S	4.690414	-2.501929	0.234562
S	5.387695	-5.337129	0.809118

Zero-point correction=	0.873992
(Hartree/Particle)	
Thermal correction to Energy=	0.941088
Thermal correction to Enthalpy=	0.942032
Thermal correction to Gibbs Free Energy=	0.765610
Sum of electronic and zero-point Energies=	-5316.529395
Sum of electronic and thermal Energies=	-5316.462298
Sum of electronic and thermal Enthalpies=	-5316.461354
Sum of electronic and thermal Free Energies=	-5316.637776

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	590.542	251.284	371.312
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	46.742
Rotational	0.889	2.981	42.573
Vibrational	588.764	245.322	281.997

1\1\GINC-XE30TH52\Freq\RB3LYP\6-31G(d)\C51H45N1O12S6\DRAL\08-Jun-2015\0\#\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d) Freq\BG33\0,1\C,3.0472999505,3.8590297067,0.8430956503\H,4.022827721,3.6324971472,1.2505775843\C,0.9052499722,2.4173238232,3.4185276319\C,2.0559953983,3.3657675188,3.1348074429\C,2.6492596849,-3.7381018953,5.6223556825\C,-4.0140300983,1.6787485829,3.4891463244\H,-4.9856833608,2.1600247642,3.3508558002\H,-3.9681079821,1.3736002595,4.5378987256\H,-3.9787311461,0.7827092263,2.8614681215\C,-0.3700056614,2.7349682287,2.9110116198\C,2.9475281579,4.3159346872,-0.4775604211\C,-10.0438950159,-2.3173369385,0.0456562977\H,-9.4693219511,-3.1705993125,-0.3237143815\H,-11.0831319981,-2.3823781355,-0.2756745286\H,-9.976322248,-2.2848911408,1.1355943683\C,-10.322768694,-1.1411615775,-4.0499214337\H,-10.4594009103,-0.5250054649,-4.9416222485\H,-11.2547910253,-1.1590233664,-3.478952491\H,-10.0148857502,-2.1510569671,-4.3191591003\C,-0.0286411484,0.4842242657,4.5820268647\C,-1.3076072084,0.9351088423,4.2190657487\H,-2.1676365495,0.3738983305,4.5643753705\C,-1.4985985715,2.0572385197,3.4197015405\C,-2.8730491638,2.652647205,3.1647102666\C,-2.89665875,3.132701619,1.7225493129\C,-4.0510500784,3.0492978232,0.9507504218\H,-4.9238583046,2.5833599616,1.3834597376\C,-4.1334493927,3.602839038,-0.3342739244\C,-3.0319160202,4.3528149717,-0.7742080382\H,-3.10323281,4.8520923402,-1.7330625086\C,-1.8639541463,4.4682794132,-0.0303410958\C,-0.7402419611,5.4057256025,-0.4413179177\C,0.5700081976,4.7249481711,-0.085463484\C,1.7022352876,4.8147230126,-0.8886350508\H,1.6259074231,5.2642607663,-1.871581701\C,-5.2945068389,3.4828711398,-1.2037506193\H,-5.3425341432,4.2064998545,-2.0159926813\C,-6.2921874176,2.572412192,-1.1622129866\C,1.9359672222,3.7419531368,1.6695040035\C,-7.7908080214,0.4374332105,-0.8686963524\C,-8.3141116798,1.0867342634,-1.932071746\C,1.05

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System has the following imaginary frequencies:

- 1 -8.8789 cm⁻¹
- 2 -4.4555 cm⁻¹
- 3 -3.0103 cm⁻¹

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1_C60

175

C	0.403238	-4.515659	-3.078978
C	1.691098	-4.081512	-2.763968
C	-2.239839	1.300386	-0.300008
C	-0.953311	1.733778	0.015051
C	0.213899	-0.390511	-4.905473
C	-0.315309	0.774768	-4.348346
C	-0.234811	-3.555680	1.286490
C	-0.764598	-2.390410	1.841320
C	-3.443145	-2.158753	-2.939924
C	-3.534696	-2.793474	-1.700251
C	2.980924	0.007998	-1.367278
C	2.896181	-0.622414	-0.125437
C	-0.362682	-3.832260	-4.110046
C	-0.514514	-4.901803	-2.017878
C	2.267507	-2.944969	-3.466797
C	2.116827	-4.014436	-1.373978
C	-2.663823	1.233090	-1.690672
C	-2.814077	0.162107	0.401745
C	-0.034335	2.119855	-1.046785
C	-0.186175	1.050962	1.047580
C	-0.625114	-1.568547	-5.061943
C	1.547539	-0.835845	-4.531214
C	-1.706974	0.811899	-3.924881
C	0.466949	1.547591	-3.394459
C	-1.016346	-4.325595	0.331786
C	1.155890	-3.589834	0.860956

C	-2.099846	-1.945281	1.468455
C	0.073974	-1.211380	1.993833
C	-2.535298	-2.670783	-3.953536
C	-3.429783	-0.705300	-3.016918
C	-2.719094	-3.965202	-1.420424
C	-3.612217	-2.001408	-0.482266
C	3.061421	-0.782399	-2.583853
C	2.169558	1.183482	-1.645217
C	2.880719	-2.076025	-0.049946
C	1.989494	-0.108216	0.892091
C	0.189565	-2.742033	-4.782759
C	-0.107573	-4.837465	-0.684803
C	1.532503	-2.289200	-4.455237
C	1.236297	-4.383323	-0.355488
C	-1.787088	1.608439	-2.708987
C	-2.084770	-0.490426	1.394831
C	-0.442198	2.063177	-2.380022
C	-0.739234	-0.037947	1.720054
C	-1.959025	-1.533174	-4.656519
C	2.296726	-0.097364	-3.615405
C	-2.512311	-0.318494	-4.077083
C	1.745916	1.119440	-3.035304
C	-2.295755	-3.898793	-0.028400
C	1.959860	-2.460821	1.010238
C	-2.850455	-2.685284	0.553260
C	1.406705	-1.245329	1.587963
C	-1.754143	-3.795898	-3.686124
C	-3.500983	0.053426	-1.849282
C	-1.848060	-4.456820	-2.393659
C	-3.587929	-0.610145	-0.557422
C	3.050622	-2.175640	-2.512288
C	1.298485	1.671591	-0.672937
C	2.957559	-2.836520	-1.218533
C	1.205630	1.013801	0.622002
C	3.013367	4.082486	1.032682
H	3.970726	3.758786	1.413696
C	0.805377	2.824687	3.665480
C	2.051597	3.630469	3.340806
C	1.407337	-3.755840	4.836937
C	-4.149599	2.767647	4.041243
H	-5.057427	3.361477	3.901397
H	-4.082178	2.541332	5.109247
H	-4.262138	1.828309	3.490666
C	-0.440051	3.317391	3.227032
C	2.914183	4.525078	-0.292225
C	-6.971767	-3.543038	0.562848
H	-5.919761	-3.769883	0.753107
H	-7.410409	-4.277017	-0.112471
H	-7.513207	-3.514864	1.511102
C	-6.903418	-2.709383	-3.713420
H	-7.319829	-2.298658	-4.636064
H	-7.643016	-3.360651	-3.240610
H	-5.977887	-3.249275	-3.908227
C	-0.325609	0.971578	4.782314
C	-1.546384	1.621206	4.529775
H	-2.459122	1.159601	4.886596
C	-1.620465	2.795313	3.795467
C	-2.916433	3.557007	3.586645
C	-2.940752	3.890475	2.107216
C	-4.078478	3.716161	1.328846

H	-4.976965	3.354094	1.804534
C	-4.086695	4.006055	-0.042792
C	-2.982094	4.712284	-0.549363
H	-3.008069	5.038737	-1.581989
C	-1.845297	4.945679	0.213700
C	-0.700495	5.820701	-0.260991
C	0.586189	5.123794	0.146421
C	1.700312	5.108758	-0.681479
H	1.625110	5.515006	-1.682466
C	-5.106209	3.534197	-0.964024
H	-5.121499	4.005861	-1.944654
C	-5.914888	2.462801	-0.796459
C	1.917230	4.066201	1.889946
C	-6.615457	0.022305	-0.234227
C	-7.022601	0.218892	-1.505730
C	0.845181	1.658731	4.424850
H	1.805637	1.278382	4.736707
C	-7.522763	-0.813618	-2.469900
C	-1.767710	4.389839	1.509920
C	0.664174	4.507755	1.415924
C	-2.853356	4.876024	4.402592
H	-3.758379	5.468411	4.228954
H	-1.988048	5.480166	4.115339
H	-2.776715	4.654013	5.472542
C	-6.581806	-1.229659	0.546584
C	-0.781364	7.170127	0.506007
H	-1.722810	7.680091	0.274207
H	0.053981	7.817322	0.217039
H	-0.734300	7.012290	1.587414
C	-0.769476	6.118410	-1.763718
H	-1.705554	6.628513	-2.006883
H	-0.702741	5.203632	-2.361578
H	0.039527	6.791064	-2.060928
C	2.055037	4.901038	4.234237
H	2.923892	5.525115	3.997839
H	2.099484	4.618282	5.291644
H	1.151442	5.497318	4.076445
C	3.343667	2.846514	3.608580
H	3.403251	1.939667	2.998453
H	3.405453	2.562469	4.662514
H	4.221812	3.464770	3.404296
C	-0.387573	-0.379002	5.312822
H	-1.376550	-0.687410	5.647359
C	0.550588	-1.351957	5.304445
C	2.390481	-2.944374	4.392119
C	3.587223	-3.430114	3.674275
C	5.500390	-2.761046	2.478180
H	6.221371	-3.218238	3.161088
H	5.889203	-1.838963	2.052556
H	5.251247	-3.477438	1.691714
C	1.324926	-5.236254	4.620887
C	1.261604	-6.905041	2.965399
H	1.093135	-6.932945	1.889032
H	0.486366	-7.460582	3.497952
H	2.245034	-7.311643	3.213242
C	3.956067	4.363243	-1.292307
H	3.872394	5.001540	-2.170128
C	4.937075	3.435660	-1.324695
C	6.127810	1.130368	-1.203605
C	6.531770	1.657050	-2.381222

C	6.384711	-0.250927	-0.707400
C	6.460561	-2.521861	-1.315649
H	5.888214	-2.871905	-0.455773
H	7.531094	-2.581596	-1.107580
H	6.203537	-3.099924	-2.201968
C	7.459417	0.986638	-3.327245
C	8.371750	1.097968	-5.493709
H	8.121375	0.061058	-5.730597
H	9.395323	1.142037	-5.113475
H	8.255020	1.734043	-6.370461
N	-0.516047	4.296126	2.190002
O	-6.536184	-1.650638	-2.813386
O	-8.645556	-0.829121	-2.919669
O	-7.086596	-2.282512	-0.119272
O	-6.141115	-1.283866	1.679027
O	3.894721	-4.598242	3.546338
O	4.306192	-2.397829	3.193722
O	1.291098	-6.045625	5.519254
O	1.216778	-5.512705	3.316080
O	6.751647	-0.486423	0.426148
O	6.100911	-1.167193	-1.635303
O	8.162078	0.033643	-3.067151
O	7.453647	1.619575	-4.518584
S	-6.019944	1.436420	0.650243
S	-6.947009	1.863505	-2.123960
S	0.117244	-3.022030	5.770499
S	2.238715	-1.218503	4.773315
S	5.232195	2.174438	-0.104409
S	6.054624	3.325621	-2.710321

Zero-point correction=	1.253403
(Hartree/Particle)	
Thermal correction to Energy=	1.343024
Thermal correction to Enthalpy=	1.343968
Thermal correction to Gibbs Free Energy=	1.130087
Sum of electronic and zero-point Energies=	-7602.728926
Sum of electronic and thermal Energies=	-7602.639306
Sum of electronic and thermal Enthalpies=	-7602.638362
Sum of electronic and thermal Free Energies=	-7602.852242

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	842.760	372.116	450.149
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	48.292
Rotational	0.889	2.981	43.047
Vibrational	840.983	366.154	358.810

1\1\GINC-XE33TH6\Freq\RB3LYP\6-31G(d)\C111H45N1O12S6\DRAL\25-May-2015\0\#\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d) Freq\BG33...C60\0,1\C,0.324723272,-4.649689635,-2.8740446037\C,1.6199910627,-4.2122525592,-2.5961468805\C,-2.2359637929,1.3100658065,-0.332564595\C,-0.9420323326,1.7467619865,-0.054566783\C,0.1429608782,-0.611634963,-4.8864709493\C,-0.3697352196,0.5824501529,-4.3769310964\C,-0.2475854301,-3.4843140092,1.450344442\C,-0.7608914513,-2.2903390009,1.957598048\C,-3.5011101297,-2.2568635378,-2.7941017868\C,-3.5810242085,-2.8330103625,-1.5253589809\C,2.9599406274,-0.0736435757,-1.4066362143\C,2.8868960176,-0.6454426079,-0.136014483\C,-0.4495730745,-4.0081510968,-3.9255498725\C,-0.5817526287,-4.9788642461,-1.784431663\C,2.1957500616,-3.1141466081,-3.3581252562\C,2.064731895,-4.0847636027,-1.2163753311

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System has the following imaginary frequencies:

- 1 -6.5362 cm⁻¹
- 2 -1.7634 cm⁻¹

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1_C60_ox1

175

C	0.714963	-4.671547	-2.438288
C	1.925023	-3.983009	-2.521429
C	-2.484329	1.182187	-0.431288
C	-1.276525	1.874270	-0.515266
C	-0.630070	-1.208977	-5.002220
C	-1.270734	-0.036876	-4.601791
C	0.707523	-2.763551	1.650220
C	0.067142	-1.592477	2.053572
C	-3.436042	-2.967885	-1.936037
C	-3.166214	-3.279524	-0.602812
C	2.608275	0.477644	-2.351690
C	2.869235	0.161610	-1.018972
C	-0.349120	-4.389979	-3.389442
C	0.104330	-4.916533	-1.140025
C	2.122969	-2.982085	-3.559578

C	2.576456	-3.509546	-1.309594
C	-3.137797	0.708049	-1.642040
C	-2.678999	0.179439	0.606550
C	-0.665001	2.124633	-1.813539
C	-0.211061	1.587216	0.433493
C	-1.230052	-2.502509	-4.713147
C	0.811252	-1.338635	-4.852287
C	-2.539952	-0.107563	-3.893364
C	-0.497550	1.057312	-4.034035
C	-0.063357	-3.858933	1.084438
C	1.976738	-2.692495	0.940101
C	-1.375008	-1.463132	1.909703
C	0.666418	-0.298137	1.760219
C	-2.644443	-3.571290	-2.996651
C	-3.726956	-1.593912	-2.318958
C	-2.095956	-4.208138	-0.272517
C	-3.177309	-2.230824	0.406220
C	2.619289	-0.571505	-3.358494
C	1.537571	1.410594	-2.680576
C	3.167012	-1.209205	-0.633239
C	2.078743	0.766601	0.041667
C	-0.159545	-3.431237	-4.384371
C	0.728386	-4.463870	0.022473
C	1.101996	-2.712218	-4.470807
C	1.990617	-3.743607	-0.064764
C	-2.552252	0.943423	-2.887212
C	-1.664826	-0.087775	1.523772
C	-1.289365	1.663925	-2.974105
C	-0.401606	0.629511	1.431246
C	-2.446506	-2.571083	-4.035068
C	1.553896	-0.290319	-4.309357
C	-3.115211	-1.348411	-3.615826
C	0.885329	0.933415	-3.890812
C	-1.445439	-3.734497	0.940989
C	2.552844	-1.453319	0.663305
C	-2.114074	-2.511675	1.360916
C	1.883438	-0.230032	1.081698
C	-1.617435	-4.460958	-2.680431
C	-3.735567	-0.588123	-1.353282
C	-1.337753	-4.786199	-1.290460
C	-3.449266	-0.915047	0.035716
C	2.898157	-1.889524	-2.991664
C	0.778555	1.991692	-1.663793
C	3.175680	-2.215196	-1.600529
C	1.054924	1.658094	-0.274554
C	2.852605	4.150385	1.198224
H	3.860136	3.841060	1.432370
C	1.011082	2.505404	3.916112
C	2.165737	3.412547	3.530857
C	2.339362	-4.010039	4.377392
C	-3.896823	1.805884	4.475471
H	-4.878681	2.282964	4.422616
H	-3.773108	1.473041	5.508959
H	-3.897672	0.929388	3.819812
C	-0.313017	2.898478	3.601189
C	2.583225	4.741437	-0.050152
C	-6.495956	-3.907520	0.022043
H	-5.821119	-4.035253	0.870695
H	-6.169895	-4.506171	-0.826343
H	-7.515758	-4.165620	0.314635

C	-8.946753	-0.770114	-4.432236
H	-9.976561	-0.840804	-4.075290
H	-8.555969	-1.773562	-4.614365
H	-8.886098	-0.159584	-5.331801
C	0.144332	0.494972	4.998503
C	-1.154290	1.031871	4.874276
H	-1.984826	0.454440	5.259084
C	-1.400686	2.211667	4.199658
C	-2.794365	2.802122	4.095019
C	-2.938264	3.323087	2.678917
C	-4.108199	3.177791	1.952403
H	-4.924794	2.629910	2.396669
C	-4.261439	3.739898	0.668754
C	-3.272170	4.656654	0.254997
H	-3.423425	5.188797	-0.675580
C	-2.091162	4.824539	0.951924
C	-1.046264	5.844656	0.551790
C	0.297374	5.159312	0.701398
C	1.312069	5.323465	-0.221928
H	1.118936	5.870762	-1.135578
C	-5.290034	3.384409	-0.271549
H	-5.369835	4.028023	-1.144851
C	-6.034022	2.240267	-0.308325
C	1.860366	3.963629	2.149487
C	-6.786792	-0.244792	-0.119476
C	-7.277203	0.169642	-1.309015
C	1.215623	1.319032	4.601993
H	2.226897	1.021487	4.831250
C	-8.087219	-0.667314	-2.240584
C	-1.857991	4.035806	2.106991
C	0.535991	4.359220	1.846208
C	-2.875707	4.016417	5.065360
H	-3.854962	4.498217	4.980210
H	-2.105974	4.760530	4.840559
H	-2.736040	3.679006	6.097283
C	-6.772887	-1.620008	0.464619
C	-1.104170	7.021211	1.569019
H	-2.082486	7.509910	1.519857
H	-0.328719	7.756975	1.333203
H	-0.945922	6.673139	2.593812
C	-1.275712	6.414637	-0.852728
H	-2.245185	6.916634	-0.905962
H	-1.241427	5.634394	-1.620020
H	-0.521460	7.170121	-1.086940
C	2.187908	4.609194	4.526466
H	2.985207	5.308014	4.253910
H	2.368029	4.245857	5.543266
H	1.237804	5.151564	4.518526
C	3.524866	2.701253	3.596760
H	3.569278	1.844894	2.916359
H	3.728692	2.353494	4.612344
H	4.333072	3.392394	3.346001
C	0.258738	-0.880689	5.402572
H	-0.644691	-1.318015	5.821726
C	1.263784	-1.759693	5.118412
C	3.180079	-3.057280	3.921756
C	4.364231	-3.347299	3.080868
C	6.106013	-2.371500	1.828422
H	6.936167	-2.787780	2.404035
H	6.342869	-1.380365	1.450318

H	5.860303	-3.050998	1.009405
C	2.424217	-5.477412	4.053523
C	2.293082	-7.021444	2.283898
H	1.929911	-7.001613	1.257284
H	1.709108	-7.712363	2.895020
H	3.349909	-7.294756	2.318820
C	3.473820	4.740110	-1.183415
H	3.211787	5.431007	-1.981880
C	4.483718	3.872696	-1.464853
C	5.856700	1.684419	-1.729756
C	6.004023	2.321423	-2.912892
C	6.297013	0.303958	-1.378475
C	6.529237	-1.896634	-2.174325
H	6.099234	-2.358169	-1.284062
H	7.617213	-1.856959	-2.092252
H	6.226083	-2.436927	-3.069389
C	6.823095	1.821099	-4.054630
C	7.312579	2.172769	-6.332717
H	7.149666	1.127269	-6.603204
H	8.373259	2.334047	-6.128145
H	6.960996	2.837730	-7.119993
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O	-8.656442	-1.689200	-1.935367
O	-6.454687	-2.543228	-0.442834
O	-6.952204	-1.818754	1.647209
O	4.741498	-4.464211	2.796564
O	4.953404	-2.208474	2.681584
O	2.650740	-6.331293	4.875375
O	2.135856	-5.670141	2.762867
O	6.794089	0.032452	-0.304329
O	6.005749	-0.565285	-2.344969
O	7.663604	0.954503	-3.976266
O	6.526757	2.509074	-5.170770
S	-6.042006	0.966738	0.909759
S	-7.029551	1.862018	-1.722310
S	1.012306	-3.494090	5.384063
S	2.808399	-1.387696	4.355350
S	5.058890	2.561162	-0.431457
S	5.290175	3.924039	-3.043811

Zero-point correction=	1.253565
(Hartree/Particle)	
Thermal correction to Energy=	1.344220
Thermal correction to Enthalpy=	1.345164
Thermal correction to Gibbs Free Energy=	1.125464
Sum of electronic and zero-point Energies=	-7602.525150
Sum of electronic and thermal Energies=	-7602.434496
Sum of electronic and thermal Enthalpies=	-7602.433552
Sum of electronic and thermal Free Energies=	-7602.653251

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	843.510	374.083	462.397
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	48.292
Rotational	0.889	2.981	43.097
Vibrational	841.733	368.121	369.630

n-2015\0\#\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk UB3LYP/6-31G
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System has the following imaginary frequencies:

1 -3.2724 cm⁻¹

=====

1_ox1

115

C	2.413402	-2.531451	-1.692526
H	3.445856	-2.253731	-1.843309
C	0.779590	0.648394	-2.390456
C	1.754720	-0.397425	-2.890838
C	3.673541	6.150948	0.237599

C	-3.974166	2.052037	-1.842717
H	-5.007151	1.800095	-2.093633
H	-3.765776	3.001319	-2.341781
H	-3.904633	2.200518	-0.760701
C	-0.581045	0.290749	-2.228886
C	2.113289	-3.771052	-1.098584
C	-10.940930	3.195279	1.758662
H	-10.498269	3.655345	2.644961
H	-12.018320	3.086269	1.873382
H	-10.701370	3.796332	0.878988
C	-11.847352	-0.283706	4.207877
H	-12.005397	-1.307454	4.553279
H	-12.689037	0.022841	3.582571
H	-11.718429	0.396321	5.048510
C	0.238913	2.957321	-1.807705
C	-1.128958	2.614022	-1.876859
H	-1.861045	3.395475	-1.716549
C	-1.553045	1.315552	-2.102592
C	-3.010352	0.964089	-2.337361
C	-3.271491	-0.393230	-1.707927
C	-4.504851	-0.697146	-1.156982
H	-5.251401	0.079969	-1.125928
C	-4.824565	-1.986079	-0.688596
C	-3.862847	-2.995621	-0.904588
H	-4.118045	-4.007731	-0.617783
C	-2.619557	-2.738866	-1.453366
C	-1.664578	-3.863570	-1.814655
C	-0.247183	-3.366191	-1.600305
C	0.770373	-4.194964	-1.152586
H	0.533449	-5.192168	-0.803542
C	-6.062207	-2.348656	-0.048450
H	-6.204243	-3.417294	0.099468
C	-7.064193	-1.553746	0.430079
C	1.426279	-1.673971	-2.143333
C	-8.657982	0.347857	1.272809
C	-9.268706	-0.802594	1.633475
C	1.163363	1.956611	-2.166140
H	2.199264	2.221219	-2.312152
C	-10.554304	-0.984616	2.382645
C	-2.279495	-1.402150	-1.785920
C	0.069717	-2.038993	-1.979044
C	-3.204444	0.808900	-3.876006
H	-4.237988	0.521288	-4.093853
H	-2.540792	0.042021	-4.286490
H	-2.985914	1.756883	-4.377923
C	-9.119155	1.753540	1.418769
C	-1.829290	-4.138265	-3.340064
H	-2.850540	-4.471536	-3.550810
H	-1.128323	-4.916709	-3.658033
H	-1.633447	-3.238231	-3.930384
C	-1.959438	-5.168604	-1.062891
H	-2.964421	-5.528860	-1.294420
H	-1.871581	-5.045571	0.021077
H	-1.273785	-5.956639	-1.383161
C	1.473480	-0.636734	-4.403321
H	2.132568	-1.422763	-4.785476
H	1.657001	0.283479	-4.967098
H	0.437742	-0.943773	-4.575306
C	3.221505	0.027704	-2.739335
H	3.490999	0.213982	-1.694886

H	3.419780	0.933798	-3.317259
H	3.887278	-0.741105	-3.139132
C	0.621066	4.284022	-1.402593
H	-0.165539	5.035363	-1.421237
C	1.833397	4.690269	-0.917340
C	4.212643	4.914138	0.161943
C	5.598722	4.560606	0.572718
C	7.071827	2.741648	0.900811
H	7.790489	3.122918	0.171598
H	7.008217	1.655590	0.858010
H	7.358218	3.083468	1.898475
C	4.321940	7.382004	0.804949
C	5.458584	8.272014	2.651224
H	5.626548	7.977069	3.685788
H	4.893066	9.204206	2.594774
H	6.406522	8.379792	2.119693
C	3.110559	-4.609593	-0.475583
H	2.851910	-5.659572	-0.355644
C	4.304360	-4.215028	0.050207
C	6.292353	-2.913415	1.154274
C	6.559339	-4.216102	1.400650
C	7.047847	-1.701302	1.586212
C	8.377181	-0.731991	3.260534
H	7.796269	0.192274	3.305801
H	9.222064	-0.605708	2.580309
H	8.719966	-1.023628	4.251738
C	7.802111	-4.745168	2.039872
C	8.736742	-6.651373	3.063403
H	9.091471	-6.096710	3.934680
H	9.536881	-6.715779	2.322748
H	8.387538	-7.642362	3.348887
N	-0.953252	-1.071172	-2.151068
O	-10.618162	-0.195165	3.456419
O	-11.378485	-1.811075	2.060135
O	-10.439851	1.852533	1.593847
O	-8.352951	2.691595	1.320195
O	6.470329	5.361372	0.826327
O	5.748068	3.223983	0.582895
O	4.413751	8.410600	0.174692
O	4.702087	7.190178	2.066495
O	7.114834	-0.706609	0.888855
O	7.545202	-1.820786	2.813083
O	8.857677	-4.158696	2.092316
O	7.586608	-5.991640	2.494378
S	-7.105336	0.211272	0.445307
S	-8.494876	-2.299858	1.158805
S	2.094656	6.382479	-0.476058
S	3.233274	3.658233	-0.598083
S	4.885333	-2.544699	0.166389
S	5.417075	-5.394881	0.763961

Zero-point correction=
(Hartree/Particle)

0.874299

Thermal correction to Energy=

0.941519

Thermal correction to Enthalpy=

0.942463

Thermal correction to Gibbs Free Energy=

0.764487

Sum of electronic and zero-point Energies=

-5316.330190

Sum of electronic and thermal Energies=

-5316.262971

Sum of electronic and thermal Enthalpies=

-5316.262026

Sum of electronic and thermal Free Energies=

-5316.440003

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	590.812	251.265	374.583
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	46.742
Rotational	0.889	2.981	42.674
Vibrational	589.035	245.303	283.790

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72293,-0.2665743,0.1772405,-0.0599582,0.1680722,0.0062366,0.287301,-0.07968,0.0057462,0.0158825,-0.0330517,0.0269383,0.0543467,0.0490751,0.0362664,-0.0218928,0.0108605,-0.0482213,-0.0124239,0.0483398,0.0601473,-0.0056125,-0.0158052,-0.0266925,0.0688021,-0.0536305,0.0125485,-0.0189551,-0.0047538,0.0384466,-0.0534525,-0.0730416,-0.0284751,-0.0714651,0.8103394,0.9485559,0.3410036,0.8536597,2.3391071,-0.1344795,1.0085082,1.3199164,1.6338353,0.5324455,0.4181867,0.1969172,0.4120438,0.8545653,0.2971577,0.3175903,0.4613201,0.4978113,0.0395351,-0.0562974,-0.0291093,-0.0136485,0.0232533,0.045866,-0.0667804,-0.0489842,-0.0798545,-0.0158915,0.0440088,-0.0303447,-0.0243427,-0.096611,-0.0665595,-0.0336455,0.012614,0.0495188,-0.0610098,-0.0693963,-0.0019425,-0.0301006,-0.0043875,-0.0643263,0.05715,-0.0220089,-0.0008226,-2.9175408,2.0707545,-0.59181,0.0768359,-0.0565859,-0.0852719,-1.5017546,0.9920597,-0.4628961,-0.090743,0.0485774,-0.0516246,0.079005,-0.0793732,0.04223,0.1185159,-0.0722171,0.1257259,3.2379174,-2.0945015,0.8192081,1.04643,-0.5613718,0.2516852,1.1682212,-0.7493402,0.2449913,-0.2667602,-0.0111541,0.0051378,-0.234189,-0.4605843,-0.1740597,-0.2155516,0.05904,-0.0175567,-0.5939076,0.7461915,-0.1910033,0.1294507,0.3228263,0.2191413,-0.5956471,0.5341041,-0.2286018,1.2208179,0.1122268,0.5046135,0.9952147,0.7042952,0.0276069,1.3331741,-0.0937136,1.5937814,0.7004288,0.0818365,0.2508484,0.4889868,0.3352353,0.2945027,0.336973,0.0749825,0.447212,-0.0653229,0.0666644,-0.0312446,-0.0470213,-0.0440521,-0.0828677,-0.0067286,0.0037567,0.0563183,-0.0492084,-0.0224772,-0.0013156,-0.080699,0.0379658,-0.0691335,0.077079,-0.001271,-0.0126457,0.0229502,-0.0121095,-0.0513453,-0.0010015,0.0456873,0.0433764,-0.0932115,0.014059,-0.0554914,2.3383662,-0.8056406,0.503892,-1.0588227,1.9912379,-0.7953308,1.1065122,-1.0547674,0.8319111,0.8662615,-0.561201,0.2800886,-0.516828,0.7186643,-0.241081,0.3853505,-0.3631778,0.4524237,-0.0496876,0.1073634,-0.0700789,0.0005866,-0.0184878,-0.0716773,-0.0717718,0.0095365,-0.040112,-0.0871864,0.1192593,-0.0094731,0.0179321,0.0277096,0.0362437,0.043541,0.0239004,-0.0442328,0.0216948,-0.043567,0.0004443,0.0405372,-0.0854918,0.0703955,-0.0284447,0.0497438,0.0598854,3.3655349,-0.0760951,-0.1832529,0.465418,2.4202965,-0.4370123,-0.4567265,-0.628601,-0.1997448,-1.4555204,-0.0923939,0.5321289,0.4540254,-0.4562406,-0.4908426,1.5781691,-0.1937901,-1.3281769,-1.4646445,-0.3993948,0.1265816,-0.2557153,-0.6158319,-0.2125247,0.6605416,-0.017783,-0.6892407,-2.3518921,0.6746627,0.3139732,1.1927051,-0.8612215,-0.1893973,0.262686,-0.0862154,-0.2773328,-1.0006418,0.075076,0.0925832,0.6060078,-0.8368015,-0.1217811,0.1284347,0.023533,-0.3306475,-1.3520049,-0.8782043,-0.1639271,-0.224322,-0.7782263,-0.0435072,-0.3221402,-0.2621829,-0.3412959,-1.2163742,-0.1924689,-0.1694619,0.7449398,-0.6442069,0.1445429,-0.3003225,-0.0682753,-0.2864837,-0.5057567,-0.4227936,-0.0570711,-0.4187909,-1.4368874,0.2288927,-0.2749674,-0.3015882,-0.714751,-0.6846032,-0.6818546,-0.3768926,-0.5102536,-1.1367782,-0.1971749,-0.8961665,-1.1510178,-1.2549968,-0.6841865,-0.0156917,-0.1180469,-0.4021735,-0.5916728,0.1761144,-0.3657073,0.1280473,-0.7161014,-0.9900161,-0.0911931,-0.5032222,-0.6092878,-0.3740661,-0.2559171,-1.2155836,-0.0251301,-1.2066457,-1.5247429,0.3270846,-0.2574036,0.0702103,-0.6482658,0.143552,-0.4178216,0.3037265,-0.4482709,-1.110344,0.5181806,-0.306518,1.0051838,-1.6382112,0.6715965,-0.7463733,0.8104913,-0.6618631,0.5682444,-0.0929623,-0.0337368,1.6492921,0.020066,-0.3550233,-0.5597289,0.0214115,0.1350334,-1.3278792,0.0839278,0.3235361,-1.1020742,-0.2507015,0.2672813,0.576336,-0.0835589,-0.0464081,-0.0747633,0.2069208,-0.0564965,-0.9302591,-1.3425972,-0.1293959,-0.1017004,0.0955254,0.0517725,-0.4488668,-0.7594849,-0.0755431,0.8822353,1.048564,0.0488415,0.2404,0.2864419,0.032691,-0.1963775,0.1882321,-0.1117738,-1.2017007,0.5866659,-0.3407534,0.3898208,-0.1844538,0.0948544,-0.6575939,0.1582824,-0.202313,1.0763799,-0.778844,0.2978728,-0.1876675,-0.0232469,0.0197864\Polar=2152.848801,73.4246142,1375.679476,-20.5781354,-55.0020442,525.6852077\PG=C01 [X(C51H45N1O12S6)]\NImag=3\0.75375

System has the following imaginary frequencies:

- 1 -9.0262 cm⁻¹
- 2 -5.8845 cm⁻¹
- 3 -4.7510 cm⁻¹

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1_red1

115

C	2.515289	-2.437425	-1.649762
H	3.534954	-2.121546	-1.812105
C	0.750144	0.635978	-2.499955
C	1.758591	-0.397297	-2.967034
C	3.362496	6.219932	0.219954
C	-4.033394	1.891832	-1.957049
H	-5.060591	1.588372	-2.173827
H	-3.862018	2.822323	-2.505726
H	-3.955950	2.097342	-0.884952
C	-0.589710	0.234889	-2.317292
C	2.271269	-3.649629	-0.987188
C	-11.177917	2.880826	1.209786
H	-10.772038	3.506817	2.010717
H	-12.253298	2.746684	1.340307
H	-10.966448	3.363800	0.250852
C	-11.844150	-0.289302	4.213241
H	-11.670266	-1.083418	4.945752
H	-12.728708	-0.548490	3.622759
H	-11.990255	0.668328	4.716086
C	0.139350	2.943529	-1.984491
C	-1.208324	2.549430	-2.005656
H	-1.968754	3.304765	-1.845524
C	-1.589999	1.226167	-2.200205
C	-3.037566	0.814064	-2.407137
C	-3.239917	-0.515807	-1.697054
C	-4.449993	-0.824814	-1.083810
H	-5.219394	-0.069251	-1.063813
C	-4.714335	-2.089996	-0.537390
C	-3.720067	-3.067098	-0.715776
H	-3.926022	-4.069247	-0.358996
C	-2.501072	-2.801692	-1.328530
C	-1.513512	-3.911593	-1.655190
C	-0.110904	-3.350774	-1.488066
C	0.943306	-4.110500	-0.990560
H	0.742780	-5.090122	-0.572567
C	-5.944106	-2.467906	0.139591
H	-6.030381	-3.532895	0.350734
C	-6.983938	-1.706002	0.561085
C	1.486534	-1.646240	-2.147393
C	-8.708871	0.185375	1.234039
C	-9.239541	-0.979698	1.743055
C	1.090692	1.970894	-2.321418
H	2.115920	2.267882	-2.488560
C	-10.368185	-1.201053	2.638852
C	-2.220668	-1.487589	-1.761351
C	0.149365	-2.049013	-1.964639
C	-3.244198	0.574981	-3.929853
H	-4.269500	0.238770	-4.120322
H	-2.556960	-0.189900	-4.303684

H	-3.063384	1.501624	-4.486687
C	-9.268223	1.525756	1.132197
C	-1.696480	-4.276649	-3.156111
H	-2.710182	-4.654668	-3.331378
H	-0.972183	-5.045250	-3.449182
H	-1.542827	-3.400527	-3.792928
C	-1.746801	-5.183610	-0.829522
H	-2.744736	-5.588479	-1.017778
H	-1.643053	-4.996369	0.243977
H	-1.034832	-5.961682	-1.118029
C	1.473306	-0.719956	-4.459760
H	2.154985	-1.502526	-4.811332
H	1.615943	0.176811	-5.073661
H	0.446694	-1.071496	-4.598671
C	3.209524	0.088788	-2.852602
H	3.481554	0.331683	-1.820789
H	3.367721	0.975759	-3.472952
H	3.900003	-0.675696	-3.218711
C	0.490468	4.313052	-1.636309
H	-0.298356	5.055681	-1.746871
C	1.664512	4.746921	-1.126193
C	3.897159	4.979790	0.231747
C	5.198168	4.637449	0.860587
C	6.639984	2.829804	1.366052
H	7.461424	3.303539	0.822285
H	6.638737	1.751355	1.212432
H	6.724517	3.080207	2.427432
C	3.917226	7.421690	0.913178
C	4.715452	8.243189	2.955302
H	4.659650	7.948961	4.003202
H	4.239721	9.214037	2.796691
H	5.756037	8.284541	2.623432
C	3.307606	-4.444692	-0.347502
H	3.048647	-5.484951	-0.155281
C	4.521753	-4.037917	0.100486
C	6.572651	-2.689191	1.074262
C	6.850052	-4.007714	1.383654
C	7.228542	-1.462087	1.483816
C	8.719709	-0.419391	2.963519
H	8.050287	0.392013	3.269755
H	9.335247	-0.070786	2.128867
H	9.351383	-0.723292	3.799561
C	8.088498	-4.545588	1.928249
C	9.085381	-6.517352	2.755210
H	9.505237	-6.022706	3.636637
H	9.846327	-6.525788	1.968077
H	8.780098	-7.536354	3.000287
N	-0.921349	-1.145057	-2.245918
O	-10.705393	-0.110042	3.373357
O	-10.918551	-2.288731	2.776048
O	-10.620807	1.568594	1.255805
O	-8.595157	2.520701	0.881832
O	6.004043	5.444779	1.281227
O	5.378295	3.307533	0.856639
O	4.177436	8.461750	0.347800
O	4.022650	7.214397	2.232832
O	7.066215	-0.387674	0.901344
O	7.981201	-1.582718	2.601702
O	9.173792	-3.994618	2.015781
O	7.902925	-5.855068	2.316253

S	-7.114937	0.060537	0.457020
S	-8.394189	-2.479246	1.323750
S	1.935670	6.475996	-0.769791
S	3.067477	3.725506	-0.701567
S	5.167772	-2.387386	0.028244
S	5.627430	-5.194921	0.876878

Zero-point correction=	0.870740
(Hartree/Particle)	
Thermal correction to Energy=	0.937939
Thermal correction to Enthalpy=	0.938883
Thermal correction to Gibbs Free Energy=	0.763046
Sum of electronic and zero-point Energies=	-5316.586690
Sum of electronic and thermal Energies=	-5316.519491
Sum of electronic and thermal Enthalpies=	-5316.518547
Sum of electronic and thermal Free Energies=	-5316.694384

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	588.565	252.180	370.080
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	46.742
Rotational	0.889	2.981	42.670
Vibrational	586.788	246.219	279.291

1\1\GINC-XE29TH16\Freq\UB3LYP\6-31G(d)\C51H45N1O12S6(1-,2)\DRAL\27-Jun-2015\0\#\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk UB3LYP/6-31G(d) Freq\BG33(-)\-1,2\C,2.4486964015,-2.536521882,-1.5997441402\H,3.4784678478,-2.2551102855,-1.7616982105\C,0.7853966465,0.5818820142,-2.4904540785\C,1.7619748736,-0.4881304098,-2.9422882129\C,3.565152666,6.1097518135,0.1775884686\C,-3.9574908259,1.9954377192,-1.9795479138\H,-4.993093446,1.7224537376,-2.1968542437\H,-3.754643843,2.9138262413,-2.5377985042\H,-3.8772132646,2.2103087974,-0.9094964165\C,-0.567185978,0.2257341249,-2.3084545946\C,2.1638671111,-3.7328801054,-0.9247719694\C,-11.0776691393,3.2467238152,1.1491119937\H,-10.6547839344,3.868354754,1.9446225872\H,-12.1572232196,3.148366131,1.2770306319\H,-10.8476131949,3.7120028954,0.1857181066\C,-11.8549744182,0.1330871969,4.1847973555\H,-11.7090215664,-0.6579530747,4.9266730705\H,-12.7453165803,-0.1043563504,3.5938631275\H,-11.9721896676,1.1004289876,4.6764948359\C,0.2467414254,2.9133175929,-2.0027832517\C,-1.1127357098,2.562134024,-2.0247041876\H,-1.849234866,3.3430439758,-1.8757924297\C,-1.535748423,1.2496135976,-2.20609385\C,-2.9950030255,0.881548584,-2.4139490257\C,-3.2421002125,-0.4332077815,-1.6900159913\C,-4.4635146178,-0.6966623695,-1.0779884375\H,-5.2084917657,0.083200997,-1.0692382704\C,-4.7699464605,-1.9466157356,-0.5186553381\C,-3.8067393092,-2.9568179963,-0.6824897294\H,-4.0457746241,-3.9478614997,-0.3154631265\C,-2.5778036248,-2.7372186841,-1.2935125036\C,-1.6250280884,-3.8815836108,-1.6041715347\C,-0.205829728,-3.363898683,-1.4379324535\C,0.8219005174,-4.1512274895,-0.9280903633\H,0.588800221,-5.1192470815,-0.5000832393\C,-6.0134609662,-2.2775960478,0.1577899779\H,-6.1343815539,-3.3368780396,0.3803349386\C,-7.0299064022,-1.4783077844,0.5669160158\C,1.4474120945,-1.7185635788,-2.1099616761\C,-8.6959414586,0.4744336408,1.2124358238\C,-9.265243266,-0.6674019852,1.7322550493\C,1.1677301605,1.9071794885,-2.3253594604\H,2.2024762886,2.1694797007,-2.4918829009\C,-10.4034418071,-0.8426996007,2.62615763\C,-2.2541478426,-1.4376188327,-1.7397337665\C,0.0974577675,-2.0764786498,-1.9278416975\C,-3.2039252902,0.6322174183,-3.9347080201\H,-4.2387680456,0.3267338095,-4.1253392886\H,-2.5401517549,-0.1582841553,-4.2974767778\H,-2.9917401741,1.5463683078,-4.5010371637\C,-9.2119080398,1.8307329003,1.0937022258\C,-1.8143909097,-4.2573276508,-3.1016587044\H,-2.8390258337,-4.6047945778,-3.2765840172\H,-1.1139732773,-5.0

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-1.9015993748,-5.1362457871,-0.7654168831\H,-2.9112866065,-5.511194552
1,-0.9529744641\H,-1.7956187038,-4.9404544502,0.3063368045\H,-1.213820
5556,-5.9397667838,-1.0426283731\C,1.4716716251,-0.8181512979,-4.43243
53954\H,2.1292492238,-1.6259051144,-4.7727724005\H,1.6449426891,0.0667
217097,-5.0556430376\H,0.4348534507,-1.1383383473,-4.5713480547\C,3.22
72715232,-0.0472625442,-2.8277297486\H,3.5033645574,0.1983253272,-1.79
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373845317,-3.1827691419\C,0.6401603922,4.2747557483,-1.6683972618\H,-0
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8921434,3.0711695618,0.8275594285\H,6.6937863191,1.5504218681,1.231679
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,6.7207330712,-4.210191076,1.4671962099\C,7.1798714273,-1.6769535123,1
.5407140056\C,8.698443901,-0.665861767,3.0144657152\H,8.0541927884,0.1
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061666,3.7523001378\H,9.6331522257,-6.8157573549,2.090692512\H,8.53169
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8062\O,-10.7082028993,0.2666150239,3.3473055231\O,-10.9886838158,-1.91
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System has the following imaginary frequencies:

1	-9.8155 cm ⁻¹
2	-4.0166 cm ⁻¹
3	-3.4547 cm ⁻¹

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2

103

C	2.406447	-2.522208	-1.912535
H	3.463087	-2.307972	-1.997984
C	1.001931	0.731962	-2.714836
C	1.920090	-0.375758	-3.197265
C	4.105279	5.780368	0.484350
C	-3.643564	2.434627	-2.210308
H	-4.688667	2.251952	-2.472950
H	-3.363257	3.374123	-2.693963
H	-3.576967	2.565108	-1.125403
C	-0.375231	0.461781	-2.594879
C	2.003104	-3.725548	-1.319434
C	0.612853	3.055006	-2.070183
C	-0.766522	2.802509	-2.150559
H	-1.450717	3.621123	-1.961148
C	-1.273341	1.539595	-2.440027
C	-2.748558	1.290291	-2.705215
C	-3.101423	-0.049872	-2.079584
C	-4.347307	-0.272757	-1.501665
H	-5.051018	0.545934	-1.462724
C	-4.739052	-1.533008	-1.030496
C	-3.862681	-2.602123	-1.270412
H	-4.177664	-3.597195	-0.979717
C	-2.613407	-2.424434	-1.852496
C	-1.731903	-3.602350	-2.235810
C	-0.294804	-3.196726	-1.958670
C	0.648734	-4.074349	-1.434012
H	0.333561	-5.047335	-1.075726
C	-6.001619	-1.790058	-0.353288
H	-6.336882	-2.826053	-0.360650
C	-6.787749	-0.915337	0.312205
C	1.491357	-1.619630	-2.441450
C	-7.646605	0.986812	1.925831
C	-8.512784	-0.036940	2.110308

C	1.469689	2.013305	-2.450683
H	2.522706	2.214856	-2.582026
C	-2.187627	-1.118891	-2.184933
C	0.114221	-1.901271	-2.342171
C	-2.936279	1.163643	-4.243642
H	-3.984183	0.946181	-4.478012
H	-2.319340	0.356909	-4.650227
H	-2.647969	2.098162	-4.737411
C	-1.874713	-3.824811	-3.768394
H	-2.910008	-4.084258	-4.015656
H	-1.216468	-4.637566	-4.094708
H	-1.605978	-2.922044	-4.324373
C	-2.128652	-4.905258	-1.530851
H	-3.150059	-5.190946	-1.796027
H	-2.062754	-4.817478	-0.441572
H	-1.481664	-5.725233	-1.854352
C	1.665660	-0.606823	-4.712025
H	2.278651	-1.439308	-5.074653
H	1.923203	0.295097	-5.278058
H	0.615663	-0.844335	-4.905548
C	3.406584	-0.046920	-3.008104
H	3.656200	0.130788	-1.956910
H	3.680632	0.840922	-3.584340
H	4.029912	-0.865054	-3.379274
C	1.089199	4.351553	-1.612153
H	0.380289	5.175334	-1.675313
C	2.287430	4.631354	-1.049533
C	4.490987	4.486461	0.401793
C	2.933169	-4.597865	-0.613596
H	2.704020	-5.662189	-0.600785
C	4.018850	-4.195432	0.081768
C	5.523696	-2.883965	1.794315
C	5.803152	-4.188552	2.022665
N	-0.847682	-0.885122	-2.613055
S	-6.460907	0.810058	0.605533
S	-8.355865	-1.412927	0.995049
S	2.748127	6.275778	-0.558690
S	3.577164	3.444619	-0.708367
S	4.527993	-2.508630	0.363310
S	5.134056	-5.350788	0.851194
S	6.127317	-1.516679	2.731995
S	6.876288	-4.793425	3.283505
S	4.909060	7.023393	1.441940
S	5.904256	3.820006	1.225541
S	-7.665240	2.520382	2.794842
S	-9.852685	-0.044020	3.256880
C	4.554320	-0.890551	3.444154
H	4.120229	-1.633785	4.115979
H	4.808309	0.009094	4.010643
H	3.842925	-0.636624	2.655755
C	5.806344	-6.051893	4.082919
H	5.542421	-6.852381	3.389493
H	6.396319	-6.465887	4.904679
H	4.901952	-5.588432	4.482541
C	5.442650	2.057285	1.421759
H	5.378430	1.538702	0.462926
H	6.251947	1.605874	2.000263
H	4.502815	1.954463	1.967628
C	3.672341	7.246988	2.780644
H	3.589163	6.334991	3.375284

H	4.036066	8.063795	3.409562
H	2.699725	7.515167	2.362519
C	-9.512811	-1.594538	4.178298
H	-10.303132	-1.675618	4.929014
H	-9.548186	-2.465676	3.521576
H	-8.542607	-1.539205	4.676372
C	-6.007640	2.482920	3.584009
H	-5.216389	2.406124	2.835859
H	-5.906586	3.428236	4.123401
H	-5.939861	1.651643	4.288835

Zero-point correction=	0.789698
(Hartree/Particle)	
Thermal correction to Energy=	0.848897
Thermal correction to Enthalpy=	0.849841
Thermal correction to Gibbs Free Energy=	0.691194
Sum of electronic and zero-point Energies=	-6574.380623
Sum of electronic and thermal Energies=	-6574.321424
Sum of electronic and thermal Enthalpies=	-6574.320480
Sum of electronic and thermal Free Energies=	-6574.479127

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	532.691	224.875	333.901
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	46.531
Rotational	0.889	2.981	41.935
Vibrational	530.913	218.913	245.435

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1\1\GINC-XE30TH52\Freq\RB3LYP\6-31G(d)\C45H45N1S12\DRAL\08-Jun-2015\0\
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107,0.0353302,0.0301487,0.2689251,-0.1801914,0.1049523,0.0966084,-0.2534504,-0.1721381,-0.2415123,0.2035997,-0.0203025,0.1830535,-0.0382287,-0.0681706,0.1186173,-0.2789526,-0.0618182,-0.1633683,0.2394987,-0.0898587,-0.1461349,-0.1201601,0.2163148,-2.4220448,-0.1536394,0.0989626,-0.157487,-0.3227208,-0.0257364,-0.1575659,-0.0780518,-1.8087447,-0.056339,-0.0201386,-0.1071145,-0.1003555,-0.0785426,-0.0582248,0.5584883,0.47109,-0.3031515,-0.8058495,-0.5021748,0.0354992,0.0285263,-0.1189141,0.2073763,-0.1693683,0.0068257,-0.1745066,-0.2953066,0.1434291,-0.029621,0.1307884,-0.0499683,-0.0853932,-0.4965088,0.409878,-0.6443875,-0.4602902,0.2974641,-0.2083998,-0.0865944,-0.0402478,0.0887228,0.3777271,-0.1389752,0.0664606,-0.1840894,0.1609615,0.0658109,0.0369367,-0.0659001,-0.0921775,-0.4280281,0.3537354,-0.1204849,-0.5606729,0.4270655,0.1970739,0.0369407,-0.1223937,0.2129009,0.313252,-0.1625596,-0.3386981,0.0651541,0.0453948,0.1130497,0.0946062,-0.1141643,-0.1182688,0.0015604,0.0436946,-0.0628657,0.035648,0.0707395,0.1017491,0.0333118,-0.1231939,0.0248754,0.1452627,-0.0354092,-0.1087867,0.0203988,0.0421261,0.2360971,0.1116931,-0.044222,-0.059827,0.0381644,0.0201113,0.0023181,-0.1335792,0.0296862,0.287582,0.0421049,-0.0927598,-0.0596733,0.1391066,-0.0541915,0.0198403,0.0199268,-0.0397242,-0.1335165,-0.1436639,-0.1186995,-0.0512114,-0.0305193,0.0732347,-0.0127946,-0.0623998,-0.0849575,-0.0914149,-0.0219302,-0.1173604,0.0568815,-0.1563418,0.008144,0.004067,0.0695334,0.103037,-0.110156,0.1013893,0.0567646,0.0619493,-0.1247238,0.006327,0.0302149,-0.0282394,-0.1009833,0.0262914,-0.0651759,0.0182522,-0.0226042,-0.0098515,-0.0744705,-0.0230166,0.0415353,-0.0206325,0.0284072,-0.0057111,0.0224519,0.1370177,-0.021172,0.1025363,-0.0240418,-0.0736377,0.0123406,0.0795298,0.0100428,-0.0051495,-0.0347252,0.0443754,-0.0274896,0.0923258,-0.0581117,0.0860701,0.104326,0.1239247,0.05153,-0.0112262,0.051694,0.0624245,0.1905561,0.0614932,-0.0332219,-0.1221356,-0.0178952,-0.0022196,0.0677249,-0.0827329,0.0381245,-0.0008673,0.0464499,0.0433947,0.0047645,0.0879568,-0.0163017,-0.1090881,0.0479312,-0.0861252,-0.005878,-0.0353021,-0.11585,-0.0641948,-0.0648289,0.043366,-0.0002338,0.0095085,-0.0197118,-0.0279798,-0.0823147,0.0511416,-0.0528273,0.052937,0.0308514,-0.0225839,0.0408719,-0.0043011,0.225977,0.1090169,-0.0014754,-0.0682544,0.0234656,-0.0382011,0.0605879,-0.0295004,0.0381527,-0.059024,0.0204407,0.0441684,0.0701897,0.0650357,0.0473101,-0.0521042,0.0664384,-0.0355377,0.0590178,-0.012422,-0.0629811,-0.111544,-0.0640238,0.0469862,0.001627,-0.030493,-0.0157107,-0.0605273,0.0227619,0.1202731,-0.1468795,0.1066111,0.1446611,0.0534441,-0.0844916,0.0088345,-0.0430082,0.0210333,-0.0955379,0.0233108,-0.0589197,-0.0267292,-0.0345327,-0.0030923,-0.0889763,-0.0145414,0.0632614,-0.0149742,0.0037331,0.0239179,-0.0571703,0.1588771,-0.0368491,0.0845273,-0.0022498,-0.0828166,-0.0305182,0.0429373,-0.0086271,0.0156627,-0.0502414,0.0273458,-0.043747,0.1096308,-0.0933596,-0.0572076,0.0159683,-0.1127084,0.0657238,0.0481574,0.0633435,0.0966553,0.1940535,0.0060618,-0.0755149,-0.0153787,-0.1288838,-0.0127578,-0.0612577,-0.0589622,-0.0615051,0.0281279,0.1302674,0.0438059,0.0667768,0.0389477,-0.0014085,0.0480893,0.0387294,0.0221775,-0.0678771,-0.0039984,0.1087421,0.0491256,0.064281,0.0291367,-0.0354063,-0.0211659,-0.0671084,-0.0420321,0.1509305,-0.0969401,0.0621833,-0.0645875,0.0803514,0.0797945,0.1002707,0.0388957,-0.0347491,-0.0936692,-0.0177538,0.0049303,-0.0214635,-0.0036023,-0.019834,0.0081514,-0.0350737,0.0939734,0.0446243,0.0499554,-0.0488372,0.0226334,0.0024764,0.1035205,-0.0016254,0.082377,-0.0171685,-0.0313,0.0813369,-0.0138858,0.0580375,0.0079843,-0.043356,0.0194932,-0.1015332,-0.0047093\Polar=1006.4050344,-31.324509,605.7249011,9.5121224,-60.9371063,857.6520477\PG=C01 [X(C45H45N1S12)]\NImag=4\0.74088129,-0.03649792,0.2078014

System has the following imaginary frequencies:

- 1 -10.4213 cm⁻¹
- 2 -8.5648 cm⁻¹
- 3 -5.6990 cm⁻¹

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2_C60

163

C	-1.419535	-4.037053	2.437069
C	-0.132377	-4.533730	2.231664
C	-0.609899	0.286337	-2.968907
C	0.678732	-0.210040	-3.173126
C	-1.731993	-4.989518	-1.963929
C	-1.570144	-4.123207	-3.045215
C	0.826422	-0.124835	2.312224
C	0.990291	0.741801	1.232363
C	-3.850791	-1.368611	-0.285057
C	-3.330491	-0.396622	0.570645
C	2.587187	-3.852986	-1.306511
C	3.098627	-2.877109	-0.449164
C	-2.470848	-4.320678	1.471770
C	-1.606055	-2.676551	2.918691
C	0.159082	-5.336173	1.053631
C	1.023203	-3.691344	2.498835
C	-1.767724	-0.557114	-3.235299
C	-0.900551	1.081401	-1.785467
C	0.863620	-1.571859	-3.653364
C	1.728243	0.070655	-2.205418
C	-2.737125	-4.706992	-0.951084
C	-0.565088	-5.546544	-1.296602
C	-2.407922	-2.939129	-3.162826
C	-0.234143	-3.778349	-3.506930
C	-0.508248	-0.468034	2.775919
C	1.665341	-1.307004	2.430163
C	-0.176838	1.290622	0.561210
C	1.998328	0.460830	0.219097
C	-3.832544	-2.767757	0.115954
C	-3.565475	-1.307326	-1.712317
C	-2.783033	-0.778401	1.865747
C	-2.507537	0.678272	0.039257
C	1.767752	-4.931323	-0.773789
C	2.041266	-3.471398	-2.600966
C	2.817289	-2.938642	0.978396
C	3.088774	-1.477750	-0.849841
C	-2.191898	-5.090201	0.342321
C	-0.498340	-1.867742	3.174847
C	-0.849206	-5.608472	0.128837
C	0.844144	-2.386080	2.958315
C	-1.588894	-1.861806	-3.696804
C	0.107209	1.351328	-0.861947
C	-0.245103	-2.379641	-3.908877
C	1.451690	0.840340	-1.076460
C	-3.540300	-3.571470	-1.062889
C	0.715839	-5.215351	-1.738431
C	-3.374455	-2.668299	-2.192256
C	0.884560	-4.312932	-2.867350
C	-1.627522	0.065489	2.135252
C	2.633513	-1.577064	1.460663
C	-1.456918	0.961931	1.002035
C	2.805074	-0.672878	0.331439

C	-3.307951	-3.136131	1.356561
C	-2.774697	-0.275535	-2.221015
C	-2.771308	-2.119962	2.249542
C	-2.233096	0.733564	-1.325479
C	1.495387	-4.989902	0.593236
C	2.029749	-2.129557	-2.983347
C	2.030658	-3.973797	1.487686
C	2.564831	-1.112784	-2.090287
C	2.685530	3.786207	-1.719528
H	3.714909	3.693282	-1.404939
C	1.142047	4.362169	1.471368
C	2.168786	4.932073	0.507899
C	3.685735	-0.466505	5.233257
C	-3.617879	3.873779	2.808906
H	-4.637906	4.209938	2.603723
H	-3.376803	4.198166	3.825068
H	-3.601189	2.779541	2.777521
C	-0.217979	4.403874	1.112629
C	2.296695	3.311352	-2.983029
C	0.559629	3.198225	3.539728
C	-0.791710	3.476281	3.264526
H	-1.541722	3.135433	3.968213
C	-1.191638	4.104261	2.090443
C	-2.633750	4.489839	1.807013
C	-2.913503	4.073564	0.371724
C	-4.113614	3.470450	0.004183
H	-4.837968	3.261529	0.775898
C	-4.376555	3.089071	-1.319436
C	-3.469729	3.532405	-2.295326
H	-3.688779	3.315366	-3.333769
C	-2.273238	4.156965	-1.971453
C	-1.311552	4.665977	-3.030886
C	0.070999	4.241627	-2.572352
C	1.003241	3.653817	-3.416245
H	0.713323	3.390868	-4.426466
C	-5.413199	2.164459	-1.740234
H	-5.470682	2.018258	-2.817592
C	-6.203279	1.347285	-1.006353
C	1.772478	4.373482	-0.847605
C	-7.235821	-0.247641	0.836891
C	-7.604132	-0.795777	-0.344810
C	1.505396	3.776424	2.678196
H	2.548620	3.777879	2.952537
C	-1.932375	4.320960	-0.611034
C	0.416361	4.453772	-1.222125
C	-2.749470	6.035865	1.900787
H	-3.770440	6.351691	1.659896
H	-2.065130	6.525462	1.201940
H	-2.503831	6.372088	2.914085
C	-1.370215	6.217883	-3.044188
H	-2.373038	6.553610	-3.330064
H	-0.644814	6.616255	-3.761992
H	-1.138919	6.630897	-2.058314
C	-1.648979	4.163184	-4.438747
H	-2.639832	4.512139	-4.742721
H	-1.631211	3.070006	-4.497837
H	-0.934013	4.561622	-5.164277
C	2.036744	6.477336	0.474761
H	2.728789	6.899850	-0.261917
H	2.271093	6.895740	1.459769

H	1.021658	6.782835	0.205976
C	3.610289	4.579219	0.893626
H	3.767357	3.496852	0.938719
H	3.862674	5.007368	1.868012
H	4.311785	5.002452	0.168871
C	0.898701	2.274513	4.608615
H	0.104592	2.053379	5.319048
C	2.028767	1.531483	4.720741
C	4.223955	0.168495	4.168648
C	3.075413	2.420651	-3.823440
H	2.650693	2.248933	-4.811229
C	4.131443	1.634444	-3.504819
C	6.048779	0.198673	-2.357139
C	5.868517	-0.370978	-3.570067
N	-0.598017	4.671384	-0.238593
S	-6.384238	1.313052	0.760102
S	-7.242992	0.141920	-1.804892
S	2.236207	0.274093	5.956804
S	3.426913	1.648334	3.626378
S	5.044857	1.616009	-1.978241
S	4.701893	0.396110	-4.651735
S	7.278255	-0.264880	-1.168755
S	6.722455	-1.796187	-4.177757
S	4.367914	-1.911616	5.978497
S	5.650173	-0.406047	3.297324
S	-7.665459	-0.865748	2.430187
S	-8.499162	-2.303583	-0.558233
C	6.495822	-1.704448	-0.349258
H	6.274561	-2.482674	-1.080855
H	7.233999	-2.080242	0.364750
H	5.592156	-1.414299	0.185679
C	5.353877	-3.020737	-4.108315
H	4.500255	-2.690955	-4.702656
H	5.753325	-3.947798	-4.527460
H	5.038537	-3.192505	-3.077299
C	5.845364	0.881607	2.014078
H	5.987381	1.869703	2.456955
H	6.745506	0.615227	1.458452
H	4.999803	0.888992	1.321571
C	3.485758	-3.228995	5.052859
H	3.731007	-3.178798	3.990630
H	3.834092	-4.180498	5.463657
H	2.407688	-3.143834	5.193223
C	-7.214104	-3.317832	-1.390083
H	-7.701148	-4.252347	-1.679973
H	-6.833458	-2.814895	-2.281294
H	-6.393191	-3.529259	-0.703288
C	-6.011077	-1.227760	3.130250
H	-5.361400	-0.352262	3.086867
H	-6.175279	-1.504712	4.174785
H	-5.547694	-2.060612	2.600933

Zero-point correction=	1.169919
(Hartree/Particle)	
Thermal correction to Energy=	1.253811
Thermal correction to Enthalpy=	1.254755
Thermal correction to Gibbs Free Energy=	1.051438
Sum of electronic and zero-point Energies=	-8860.578305
Sum of electronic and thermal Energies=	-8860.494413
Sum of electronic and thermal Enthalpies=	-8860.493469

Sum of electronic and thermal Free Energies= -8860.696786

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	786.778	351.370	427.916
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	48.169
Rotational	0.889	2.981	42.775
Vibrational	785.001	345.408	336.972

1\1\GINC-XE33TH13\Freq\RB3LYP\6-31G(d)\C105H45N1S12\DRAL\26-May-2015\0
\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G(d) Freq
\BG32...C60\0,1\C,-1.4521001923,-4.057918595,2.3765966801\C,-0.16314
56184,-4.5529675379,2.1786647649\C,-0.5922584168,0.3132147844,-2.98303
52031\C,0.698158297,-0.1815454728,-3.179765468\C,-1.7240335215,-4.9711
749362,-2.0353886257\C,-1.5521422739,-4.0953144314,-3.1073919716\C,0.7
952533481,-0.1451247247,2.3072540598\C,0.9691510812,0.7310470963,1.236
6976943\C,-3.857911781,-1.3649761179,-0.3440069919\C,-3.345442336,-0.4
007185743,0.5250641376\C,2.5889980402,-3.8412605288,-1.3280870304\C,3.
0925926535,-2.8731290744,-0.4574180601\C,-2.4944886872,-4.3327743891,1
.3991592235\C,-1.64293629,-2.7017197484,2.8685532607\C,0.1390980885,-5
.3449569489,0.9962823243\C,0.9899949928,-3.7131849342,2.4639593197\C,-
1.7476502731,-0.5276393325,-3.2675819694\C,-0.8937449287,1.0977777824,
-1.7953046369\C,0.8873499556,-1.5390726976,-3.6703648876\C,1.738722761
3,0.0903601055,-2.1999620911\C,-2.7384402542,-4.6974931603,-1.02938607
36\C,-0.5633818319,-5.5343077399,-1.3623062101\C,-2.388696027,-2.91009
63259,-3.2221940734\C,-0.2119087557,-3.7465918333,-3.5536817934\C,-0.5
436666094,-0.492206957,2.7555513063\C,1.632945534,-1.3284375357,2.4224
114165\C,-0.1916902166,1.2860097834,0.5597141605\C,1.9864670793,0.4589
23685,0.2303133056\C,-3.8434865428,-2.7676344715,0.0447012293\C,-3.559
4381386,-1.291055121,-1.7679742847\C,-2.8099872124,-0.7940871549,1.821
7151824\C,-2.5175283638,0.6787162726,0.0108649303\C,1.7645901452,-4.92
41521685,-0.8125519029\C,2.0550734573,-3.4480896377,-2.6240783218\C,2.
7980942759,-2.9473016226,0.9668831168\C,3.0865577669,-1.470262671,-0.8
457129444\C,-2.2051996622,-5.0922753874,0.2655350089\C,-0.5375606501,-
1.895406824,3.1420944234\C,-0.8606408323,-5.6088557462,0.0598447002\C,
0.8068186379,-2.4120269847,2.9333542289\C,-1.5646842925,-1.8282079745,
-3.7389975663\C,0.1054773804,1.3593146514,-0.8601662651\C,-0.219039680
6,-2.3443650059,-3.9432635151\C,1.4518353992,0.8500261419,-1.066804371
7\C,-3.540450987,-3.5608867865,-1.1384942109\C,0.721595373,-5.19941704
38,-1.7893411979\C,-3.3641170703,-2.6477404494,-2.2582098993\C,0.90080
03505,-4.2870272962,-2.9085891328\C,-1.6569375541,0.0471792984,2.10935
6827\C,2.6099957782,-1.5900324259,1.4595196829\C,-1.4758104131,0.95362
92111,0.9857753129\C,2.7920441714,-0.6758746551,0.3400088529\C,-3.3303
908929,-3.1471090142,1.2867697103\C,-2.7639111612,-0.2549172718,-2.260
1645813\C,-2.8019191777,-2.1390080848,2.1936604127\C,-2.2305063536,0.7
460904904,-1.3507366217\C,1.4796229224,-4.9948339126,0.5513283793\C,2.
0472005965,-2.1029017565,-2.9946052851\C,2.0067091908,-3.9868091525,1.
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.801284453,-1.6722532221\H,3.7182364925,3.7053931102,-1.3490219937\C,1
.1190103893,4.3491223315,1.5092667781\C,2.1546423165,4.9273937835,0.56
0411577\C,3.6274716243,-0.5132282502,5.2513808968\C,-3.6530924141,3.84
96669913,2.7984531028\H,-4.671154197,4.1878088127,2.5868676582\H,-3.42
13709399,4.1649685092,3.8196388767\H,-3.6362091608,2.755748252,2.75749
76251\C,-0.2376448017,4.3942440264,1.1383841171\C,2.3146053678,3.33774
47473,-2.9434580042\C,0.5174381648,3.1669382683,3.5617385138\C,-0.8312
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1781\C,-1.2203077527,4.0861159235,2.104474802\C,-2.6597108294,4.474442
0256,1.8111950648\C,-2.926249103,4.0709878057,0.3697433061\C,-4.122971
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163

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C	-6.923416	-0.096161	0.806584
C	-7.420039	-0.588652	-0.353889
C	1.476858	3.687242	2.831494
H	2.503279	3.621077	3.155650
C	-1.768469	4.411049	-0.610980
C	0.612262	4.467458	-1.121586
C	-2.574427	6.214947	1.838415
H	-3.558056	6.597683	1.547882
H	-1.826818	6.646503	1.166643
H	-2.352884	6.547303	2.857671
C	-1.077416	6.308722	-3.015229
H	-2.063515	6.658842	-3.336943
H	-0.321408	6.695620	-3.706083
H	-0.875624	6.718741	-2.021412
C	-1.334220	4.258406	-4.426869
H	-2.308955	4.619883	-4.764405
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H	-0.594749	4.654754	-5.127503
C	2.238552	6.381619	0.749823
H	2.988191	6.802487	0.072130
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H	1.254874	6.748145	0.442847
C	3.706141	4.393111	1.155464
H	3.813902	3.303570	1.151222
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C	0.649311	2.244085	4.722888
H	-0.212793	2.057761	5.359515
C	1.720903	1.416040	4.915630
C	3.822916	-0.119010	4.522383
C	3.369929	2.554331	-3.671021
H	3.006818	2.415346	-4.687447
C	4.382158	1.720303	-3.291090
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S	-8.495009	-1.978543	-0.525986
C	6.353298	-1.891636	-0.161792
H	6.114948	-2.557700	-0.992099

H	7.060975	-2.389667	0.506402
H	5.453671	-1.627366	0.392807
C	5.598550	-2.673214	-4.791676
H	5.316953	-2.130372	-5.696239
H	6.052155	-3.625026	-5.078426
H	4.721104	-2.861811	-4.169807
C	5.669415	0.453553	2.513583
H	5.863862	1.433813	2.955080
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H	4.883216	0.518298	1.757222
C	2.367834	-3.401818	5.658280
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H	-6.899643	-2.794754	-2.199014
H	-6.527344	-3.433250	-0.570909
C	-6.638202	-2.371269	2.452047
H	-5.599852	-2.433866	2.129772
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Zero-point correction=	1.170212
(Hartree/Particle)	
Thermal correction to Energy=	1.253118
Thermal correction to Enthalpy=	1.254063
Thermal correction to Gibbs Free Energy=	1.054646
Sum of electronic and zero-point Energies=	-8860.379118
Sum of electronic and thermal Energies=	-8860.296212
Sum of electronic and thermal Enthalpies=	-8860.295267
Sum of electronic and thermal Free Energies=	-8860.494684

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	786.344	349.121	419.707
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	48.169
Rotational	0.889	2.981	42.772
Vibrational	784.566	343.160	327.390

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System has the following imaginary frequencies:

1 -2.2942 cm⁻¹

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2_ox1

103

C	2.455049	-2.414418	-1.627271
H	3.493055	-2.172138	-1.801012
C	0.908041	0.774825	-2.377078
C	1.823863	-0.311827	-2.901983
C	4.152539	5.914093	0.462591
C	-3.766351	2.356017	-1.683080
H	-4.814120	2.147234	-1.911585
H	-3.529714	3.299218	-2.181378
H	-3.665680	2.494181	-0.601974
C	-0.457246	0.469323	-2.166670
C	2.130458	-3.616704	-0.972375
C	0.482296	3.092317	-1.738439
C	-0.900058	2.807788	-1.771999
H	-1.594526	3.614806	-1.573897
C	-1.382964	1.529796	-2.004523
C	-2.858032	1.233609	-2.204650
C	-3.155761	-0.115785	-1.571499
C	-4.389300	-0.374617	-0.997624
H	-5.107532	0.428351	-0.953065
C	-4.748086	-1.650925	-0.523188
C	-3.820223	-2.691366	-0.739504
H	-4.103078	-3.692362	-0.439351
C	-2.576739	-2.479742	-1.307441
C	-1.658007	-3.639389	-1.657025
C	-0.224646	-3.176516	-1.470058
C	0.777453	-4.012155	-0.999422
H	0.520180	-4.988544	-0.607790
C	-5.995835	-1.971054	0.118566
H	-6.167060	-3.033865	0.279141
C	-6.982871	-1.142829	0.573560
C	1.482652	-1.553191	-2.102467
C	-8.585167	0.804657	1.352647
C	-9.243775	-0.334228	1.686982
C	1.350576	2.064746	-2.154868
H	2.387963	2.294429	-2.345462
C	-2.201869	-1.159389	-1.665972
C	0.120998	-1.872516	-1.897510
C	-3.095945	1.092688	-3.737889
H	-4.145241	0.847410	-3.931227
H	-2.473888	0.301055	-4.166026
H	-2.851478	2.032676	-4.243100
C	-1.849857	-3.944278	-3.172729
H	-2.882088	-4.255600	-3.363116
H	-1.173193	-4.747275	-3.482535
H	-1.639235	-3.062818	-3.785502
C	-1.976933	-4.918359	-0.871370

H	-2.992247	-5.260606	-1.084872
H	-1.876166	-4.771229	0.208540
H	-1.311803	-5.729174	-1.178267
C	1.472119	-0.575720	-4.394057
H	2.086103	-1.393996	-4.783800
H	1.663868	0.323698	-4.988065
H	0.420036	-0.848812	-4.515785
C	3.309077	0.063890	-2.821069
H	3.625987	0.263153	-1.792101
H	3.513924	0.949954	-3.427518
H	3.929792	-0.739133	-3.226512
C	0.944760	4.381128	-1.293775
H	0.210274	5.183753	-1.284026
C	2.178028	4.686926	-0.787998
C	4.563680	4.626122	0.348635
C	3.112721	-4.436631	-0.304908
H	2.834073	-5.471754	-0.117915
C	4.313738	-4.027450	0.195006
C	6.349989	-2.721253	1.248918
C	6.556967	-4.014235	1.601440
N	-0.876232	-0.878635	-2.072957
S	-7.008374	0.613957	0.567050
S	-8.439001	-1.853674	1.296839
S	2.595126	6.317326	-0.276904
S	3.486762	3.520959	-0.511479
S	4.952557	-2.381318	0.212016
S	5.395148	-5.193709	0.983053
S	7.373420	-1.364555	1.721069
S	7.925670	-4.523349	2.590425
S	5.083506	7.201113	1.228291
S	6.107700	4.047508	0.979048
S	-9.183842	2.439551	1.626528
S	-10.826496	-0.315115	2.463963
C	6.543125	-0.868995	3.284651
H	6.587924	-1.685087	4.008022
H	7.095623	-0.009156	3.672743
H	5.505908	-0.583277	3.095963
C	7.514992	-6.266230	2.962273
H	7.505462	-6.880011	2.058482
H	8.321667	-6.613386	3.612204
H	6.565891	-6.349888	3.495847
C	5.970837	2.236227	0.751636
H	5.898938	1.963050	-0.303843
H	6.901660	1.824784	1.148010
H	5.130692	1.820055	1.312461
C	4.334179	7.183594	2.906389
H	4.506155	6.219097	3.387668
H	4.836697	7.970743	3.474101
H	3.265443	7.401085	2.852966
C	-11.127654	-2.089828	2.783866
H	-12.098184	-2.125499	3.284212
H	-11.190749	-2.660640	1.854433
H	-10.370806	-2.513780	3.447672
C	-8.609947	2.708349	3.352646
H	-7.521005	2.651650	3.408585
H	-8.938071	3.712929	3.631442
H	-9.067830	1.977258	4.021406

Zero-point correction=
(Hartree/Particle)

0.790192

Thermal correction to Energy= 0.850191
 Thermal correction to Enthalpy= 0.851135
 Thermal correction to Gibbs Free Energy= 0.687933
 Sum of electronic and zero-point Energies= -6574.184993
 Sum of electronic and thermal Energies= -6574.124994
 Sum of electronic and thermal Enthalpies= -6574.124050
 Sum of electronic and thermal Free Energies= -6574.287252

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	533.503	226.528	343.488
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	46.531
Rotational	0.889	2.981	42.106
Vibrational	531.725	220.566	253.475

1\1\GINC-XE34TH8\Freq\UB3LYP\6-31G(d)\C45H45N1S12(1+,2)\DRAL\10-Jun-20
 15\0\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk UB3LYP/6-31G(d)
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System has the following imaginary frequencies:

- 1 -10.6311 cm⁻¹
- 2 -7.0633 cm⁻¹
- 3 -5.6387 cm⁻¹

=====

2_red1

103

C	2.455820	-2.367918	-1.935140
H	3.510108	-2.153710	-2.053533
C	1.005674	0.857208	-2.717327
C	1.913923	-0.245108	-3.233685
C	4.117596	5.706618	0.657288

C	-3.639496	2.547208	-2.142523
H	-4.685048	2.361879	-2.401327
H	-3.360062	3.490667	-2.621211
H	-3.571780	2.668711	-1.056781
C	-0.369141	0.578443	-2.549105
C	2.079236	-3.582973	-1.308626
C	0.620988	3.171524	-2.038016
C	-0.760546	2.918055	-2.092037
H	-1.442965	3.732272	-1.875952
C	-1.270237	1.656911	-2.383053
C	-2.747036	1.403870	-2.643295
C	-3.101186	0.058763	-2.026757
C	-4.341461	-0.170478	-1.456499
H	-5.046665	0.646269	-1.404755
C	-4.739017	-1.444831	-0.985551
C	-3.835376	-2.506831	-1.234590
H	-4.149908	-3.507585	-0.959659
C	-2.586566	-2.319469	-1.798523
C	-1.689067	-3.490738	-2.177982
C	-0.246630	-3.078804	-1.923113
C	0.710819	-3.944087	-1.423856
H	0.416566	-4.929308	-1.077612
C	-5.986112	-1.724374	-0.334375
H	-6.237827	-2.782390	-0.247577
C	-6.918307	-0.874344	0.193245
C	1.526442	-1.488388	-2.454095
C	-7.821425	0.883515	1.891567
C	-8.606214	-0.205980	2.069418
C	1.471525	2.139221	-2.459050
H	2.518396	2.350191	-2.625176
C	-2.167696	-1.002899	-2.134636
C	0.143508	-1.773442	-2.322762
C	-2.933100	1.290744	-4.183035
H	-3.982802	1.080294	-4.416781
H	-2.322768	0.479088	-4.589817
H	-2.636488	2.225073	-4.674643
C	-1.847292	-3.729024	-3.706550
H	-2.884076	-3.995432	-3.943534
H	-1.184184	-4.537828	-4.035120
H	-1.589278	-2.826434	-4.268353
C	-2.066730	-4.789108	-1.454358
H	-3.088900	-5.088297	-1.703106
H	-1.989084	-4.682788	-0.367629
H	-1.411557	-5.605456	-1.771801
C	1.601161	-0.478075	-4.736688
H	2.210817	-1.303474	-5.121252
H	1.819360	0.426550	-5.317028
H	0.548119	-0.735117	-4.882655
C	3.402600	0.099960	-3.105456
H	3.689900	0.279635	-2.064441
H	3.648627	0.988559	-3.695161
H	4.014764	-0.718923	-3.493329
C	1.113236	4.448152	-1.544242
H	0.415538	5.284272	-1.571910
C	2.317645	4.689037	-0.978246
C	4.468190	4.407473	0.520093
C	3.005458	-4.431253	-0.622659
H	2.713525	-5.474591	-0.488273
C	4.218134	-4.082332	-0.088775
C	5.645218	-2.883343	1.721360

C	5.886166	-4.203007	1.909888
N	-0.827714	-0.758641	-2.530907
S	-6.795124	0.885409	0.419051
S	-8.495688	-1.457306	0.790313
S	2.823162	6.301697	-0.419954
S	3.579087	3.455584	-0.684054
S	4.839327	-2.434276	0.179949
S	5.362318	-5.277511	0.570706
S	6.115592	-1.578865	2.814536
S	6.778254	-4.895272	3.264243
S	4.889228	6.853360	1.750349
S	5.792615	3.643812	1.410575
S	-7.827191	2.327824	2.902682
S	-9.802478	-0.409014	3.349031
C	4.457640	-0.959474	3.303828
H	3.944733	-1.698444	3.923391
H	4.615501	-0.042916	3.878961
H	3.858075	-0.741948	2.417617
C	5.584938	-6.160075	3.849310
H	5.346095	-6.868607	3.054290
H	6.071114	-6.684854	4.676571
H	4.668588	-5.684481	4.206444
C	5.435074	1.859474	1.194327
H	5.539689	1.544706	0.153987
H	6.182299	1.329918	1.789812
H	4.438826	1.608462	1.561364
C	3.642189	6.890810	3.098178
H	3.578985	5.912391	3.578918
H	3.977012	7.637243	3.823899
H	2.665877	7.178251	2.701487
C	-9.218472	-1.972781	4.111018
H	-9.946651	-2.234287	4.883906
H	-9.169377	-2.770187	3.367223
H	-8.235725	-1.831376	4.566653
C	-6.048503	2.448287	3.339869
H	-5.429973	2.526652	2.444289
H	-5.940046	3.354327	3.942473
H	-5.740396	1.579625	3.925941

Zero-point correction=	0.785526
(Hartree/Particle)	
Thermal correction to Energy=	0.846041
Thermal correction to Enthalpy=	0.846985
Thermal correction to Gibbs Free Energy=	0.683458
Sum of electronic and zero-point Energies=	-6574.400376
Sum of electronic and thermal Energies=	-6574.339861
Sum of electronic and thermal Enthalpies=	-6574.338917
Sum of electronic and thermal Free Energies=	-6574.502444

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	530.899	228.758	344.171
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	46.531
Rotational	0.889	2.981	41.926
Vibrational	529.121	222.796	254.337

1\1\GINC-XE29TH7\Freq\UB3LYP\6-31G(d)\C45H45N1S12(1-,2)\DRAL\27-Jun-20
 15\0\#\#P Geom=AllCheck Guess=TCheck SCRF=Check GenChk UB3LYP/6-31G(d)
 Freq\BG32(-)\-1,2\C,2.4470182793,-2.4300324862,-1.8556793048\H,3.50

20117549,-2.2221368434,-1.9789398873\C,1.0064990098,0.775287154,-2.731
471199\C,1.9122953962,-0.343791254,-3.2150407492\C,4.1279986239,5.7108
650283,0.5066118949\C,-3.6346646571,2.4935362841,-2.2105840174\H,-4.68
04396706,2.3036934032,-2.4651816121\H,-3.3521498572,3.4221585492,-2.71
57437261\H,-3.5677813412,2.6458694423,-1.1286853091\C,-0.3692500322,0.
5051498091,-2.5569232647\C,2.0664556474,-3.6256481631,-1.1950968353\C,
0.6273889434,3.1091171571,-2.1190842854\C,-0.7547712485,2.857926336,-2
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,1.5903484804,-2.4228254984\C,-2.7447858623,1.3339418029,-2.6774189045
\C,-3.1032573785,0.0079818739,-2.0230613777\C,-4.3447622696,-0.2015115
632,-1.447903991\H,-5.0477946324,0.6182766252,-1.4203559524\C,-4.74629
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3641237339,-1.7262968058\C,-1.7006492294,-3.5481805023,-2.0710641325\C
, -0.2573697198,-3.1330067833,-1.8264257547\C,0.6971846721,-3.986225933
6,-1.301521537\H,0.3998789257,-4.9603427236,-0.9275738631\C,-5.9948399
617,-1.7182356109,-0.2836785956\H,-6.2495288228,-2.7726547584,-0.16693
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System has the following imaginary frequencies:

1	-11.2101 cm ⁻¹
2	-6.2481 cm ⁻¹
3	-2.9674 cm ⁻¹

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4

55

N	0.000000	0.036077	0.078462
C	1.222348	0.736449	-0.093239
C	1.224488	2.151217	-0.052566
C	2.381731	2.844957	-0.399278
H	2.375127	3.927821	-0.402881
C	3.558311	2.171715	-0.712743
H	4.454893	2.721627	-0.982066
C	3.578563	0.788359	-0.619514
H	4.509873	0.259585	-0.793072
C	2.432522	0.051655	-0.301331
C	2.569187	-1.449964	-0.107554
C	1.217318	-2.095317	0.169028
C	1.190785	-3.474541	0.388275
H	2.129654	-4.016262	0.432063
C	-0.000017	-4.171693	0.531166
H	-0.000020	-5.241766	0.714176
C	-1.190813	-3.474531	0.388281
H	-2.129686	-4.016245	0.432072
C	-1.217336	-2.095307	0.169037
C	-0.000006	-1.380672	0.135417
C	-2.569201	-1.449942	-0.107538
C	-2.432528	0.051679	-0.301290
C	-3.578570	0.788396	-0.619443
H	-4.509887	0.259629	-0.792990

C	-3.558310	2.171752	-0.712659
H	-4.454892	2.721674	-0.981958
C	-2.381717	2.844981	-0.399215
H	-2.375103	3.927846	-0.402811
C	-1.224471	2.151229	-0.052534
C	-1.222345	0.736461	-0.093214
C	0.000019	2.855039	0.504828
C	3.523098	-1.696271	1.089772
H	3.110615	-1.253978	2.001881
H	4.503167	-1.245758	0.905852
H	3.673157	-2.765916	1.265361
C	3.162212	-2.092377	-1.387999
H	3.281991	-3.172827	-1.265641
H	4.144805	-1.672737	-1.623618
H	2.501275	-1.917139	-2.242396
C	-3.162223	-2.092329	-1.387998
H	-2.501281	-1.917080	-2.242388
H	-4.144813	-1.672680	-1.623614
H	-3.282007	-3.172781	-1.265659
C	-3.523118	-1.696267	1.089779
H	-3.673185	-2.765914	1.265347
H	-4.503184	-1.245745	0.905864
H	-3.110637	-1.253994	2.001899
C	0.000038	2.656963	2.048020
H	-0.891834	3.118324	2.486624
H	0.891928	3.118315	2.486600
H	0.000036	1.595017	2.309103
C	0.000023	4.363740	0.226643
H	0.000010	4.582229	-0.846275
H	0.875962	4.836964	0.678242
H	-0.875897	4.836974	0.678266

Zero-point correction=	0.471163
(Hartree/Particle)	
Thermal correction to Energy=	0.494142
Thermal correction to Enthalpy=	0.495086
Thermal correction to Gibbs Free Energy=	0.421536
Sum of electronic and zero-point Energies=	-1099.598753
Sum of electronic and thermal Energies=	-1099.575774
Sum of electronic and thermal Enthalpies=	-1099.574830
Sum of electronic and thermal Free Energies=	-1099.648380

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	310.079	97.616	154.799
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	43.579
Rotational	0.889	2.981	35.115
Vibrational	308.301	91.654	76.106

1\1\GINC-XE30TH25\Freq\RB3LYP\6-31G(d)\C27H27N1\DRAL\07-Sep-2016\0\#\#P
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 816359307,-2.8450148164,-0.399296454\H,-2.3749988028,-3.927879514,-0.4
 028995955\C,-3.5582368619,-2.171809314,-0.7127618136\H,-4.4548015346,-
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\C,1.2172792168,2.0953591149,0.169018217\C,-0.0000285455,1.38068679,0.
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.0515892778,-0.3013080845\C,3.5786015198,-0.7882710832,-0.619461724\H,
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4_ox1

55

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C	-3.563610	-2.157085	-0.670789
H	-4.462029	-2.707063	-0.930927
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C	0.000038	4.144588	0.606922
H	0.000046	5.208142	0.821379
C	1.197934	3.460239	0.443380
H	2.130624	4.007632	0.504252
C	1.227562	2.093681	0.177879
C	0.000013	1.384874	0.115806
C	2.566921	1.456975	-0.123483
C	2.438263	-0.038677	-0.295163
C	3.584903	-0.772256	-0.603439
H	4.515091	-0.247404	-0.784688
C	3.563573	-2.157147	-0.670787
H	4.461984	-2.707141	-0.930921
C	2.389456	-2.840769	-0.354071
H	2.397530	-3.922076	-0.344845
C	1.223465	-2.156953	-0.040895
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C	3.116474	2.091801	-1.431896
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H	4.096372	1.678600	-1.683578
H	3.228365	3.172676	-1.316143
C	3.554600	1.720923	1.047562
H	3.708875	2.792184	1.196119
H	4.528677	1.272791	0.838483
H	3.172772	1.294492	1.979685
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H	0.890268	-3.192815	2.459654
H	-0.890328	-3.192788	2.459654
H	-0.000006	-1.663067	2.336972
C	-0.000038	-4.377007	0.165514
H	-0.000037	-4.568602	-0.911835
H	-0.872015	-4.862730	0.608493
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Zero-point correction=	0.471757
(Hartree/Particle)	
Thermal correction to Energy=	0.494862
Thermal correction to Enthalpy=	0.495806
Thermal correction to Gibbs Free Energy=	0.421001
Sum of electronic and zero-point Energies=	-1099.375683
Sum of electronic and thermal Energies=	-1099.352579
Sum of electronic and thermal Enthalpies=	-1099.351635
Sum of electronic and thermal Free Energies=	-1099.426439

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	310.530	97.639	157.439
Electronic	0.000	0.000	1.377

Translational	0.889	2.981	43.579
Rotational	0.889	2.981	35.118
Vibrational	308.753	91.677	77.364

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Zero-point correction= 0.462613
(Hartree/Particle)
Thermal correction to Energy= 0.486297
Thermal correction to Enthalpy= 0.487241
Thermal correction to Gibbs Free Energy= 0.411762
Sum of electronic and zero-point Energies= -1099.570331
Sum of electronic and thermal Energies= -1099.546647
Sum of electronic and thermal Enthalpies= -1099.545703
Sum of electronic and thermal Free Energies= -1099.621182

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	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	305.156	100.874	158.858
Electronic	0.000	0.000	1.377
Translational	0.889	2.981	43.579
Rotational	0.889	2.981	35.116
Vibrational	303.378	94.913	78.786

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C60

60

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C	-1.177070	-0.382453	-3.329085
C	1.424869	-3.198809	0.593244
C	0.727469	-3.425408	-0.593244
C	-0.727469	3.425408	0.593244
C	-1.424869	3.198809	-0.593244
C	-2.601939	-1.578711	1.830889
C	-3.032956	-0.252177	1.830889
C	3.032956	0.252177	-1.830889
C	2.601939	1.578711	-1.830889
C	0.727469	-1.001275	3.329085
C	0.000000	1.237644	3.329085
C	3.032956	-0.252177	1.830889
C	2.305487	1.986743	1.830889
C	-2.305487	-1.986743	-1.830889
C	-3.032956	0.252177	-1.830889
C	0.000000	-1.237644	-3.329085
C	-0.727469	1.001275	-3.329085
C	0.697400	-2.962440	1.830889
C	2.601939	-2.343618	0.593244
C	-0.727469	-3.425408	-0.593244
C	1.177070	-2.806586	-1.830889
C	-1.177070	2.806586	1.830889
C	0.727469	3.425408	0.593244
C	-2.601939	2.343618	-0.593244
C	-0.697400	2.962440	-1.830889
C	-1.424869	-1.961164	2.595795
C	-2.601939	-2.343618	0.593244
C	-2.305487	0.749098	2.595795
C	-3.482557	0.366645	0.593244
C	3.482557	-0.366645	-0.593244
C	2.305487	-0.749098	-2.595795
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C	1.424869	1.961164	-2.595795
C	1.424869	-1.961164	2.595795
C	0.000000	2.424133	2.595795
C	2.601939	-1.578711	1.830889
C	1.177070	2.806586	1.830889
C	-1.177070	-2.806586	-1.830889
C	-2.601939	1.578711	-1.830889

C	0.000000	-2.424133	-2.595795
C	-1.424869	1.961164	-2.595795
C	-0.697400	-2.962440	1.830889
C	3.032956	-1.750374	-0.593244
C	-1.424869	-3.198809	0.593244
C	2.305487	-1.986743	-1.830889
C	-2.305487	1.986743	1.830889
C	1.424869	3.198809	-0.593244
C	-3.032956	1.750374	0.593244
C	0.697400	2.962440	-1.830889
C	-0.727469	-1.001275	3.329085
C	-3.032956	-1.750374	-0.593244
C	-1.177070	0.382453	3.329085
C	-3.482557	-0.366645	-0.593244
C	3.482557	0.366645	0.593244
C	1.177070	-0.382453	-3.329085
C	3.032956	1.750374	0.593244
C	0.727469	1.001275	-3.329085

Zero-point correction=	0.376875
(Hartree/Particle)	
Thermal correction to Energy=	0.397393
Thermal correction to Enthalpy=	0.398337
Thermal correction to Gibbs Free Energy=	0.333912
Sum of electronic and zero-point Energies=	-2286.113493
Sum of electronic and thermal Energies=	-2286.092975
Sum of electronic and thermal Enthalpies=	-2286.092030
Sum of electronic and thermal Free Energies=	-2286.156456

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	249.368	113.829	135.594
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	45.602
Rotational	0.889	2.981	37.556
Vibrational	247.590	107.868	52.436

1\1\GINC-XE29TH21\Freq\RB3LYP\6-31G(d)\C60\DRAL\29-May-2015\0\#\#P Geom
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Single-point calculations at B3LYP-D3(BJ)/6-311+G(d,p)
on B3LYP-D3(BJ)/def2-TZVP geometries

!!!!!!
!!!!!!

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1

115

C	2.415805	-2.609908	-1.883890
H	3.453350	-2.343091	-2.000172
C	0.841296	0.571185	-2.661166

C	1.810094	-0.490153	-3.137140
C	3.699184	6.020803	0.078750
C	-3.867455	2.034878	-2.154942
H	-4.900760	1.789484	-2.394831
H	-3.647999	2.971780	-2.664659
H	-3.792238	2.196926	-1.079407
C	-0.514099	0.232659	-2.527534
C	2.088236	-3.829481	-1.289936
C	-10.206025	3.332222	2.703907
H	-9.491156	3.761297	3.404722
H	-11.183955	3.230545	3.165008
H	-10.262624	3.962881	1.818100
C	-11.051095	-0.528459	4.729594
H	-11.531676	-1.504735	4.691244
H	-11.770461	0.237842	4.443869
H	-10.651364	-0.332966	5.719852
C	0.334913	2.882052	-2.092984
C	-1.024124	2.554528	-2.157032
H	-1.747642	3.340318	-1.999444
C	-1.462709	1.262515	-2.397547
C	-2.922323	0.932221	-2.636269
C	-3.197192	-0.408215	-1.982269
C	-4.419712	-0.679347	-1.388602
H	-5.146794	0.112189	-1.345150
C	-4.747352	-1.945747	-0.898644
C	-3.817981	-2.967369	-1.122827
H	-4.080864	-3.969148	-0.817953
C	-2.588960	-2.739086	-1.716089
C	-1.660150	-3.877910	-2.090313
C	-0.241330	-3.400852	-1.856647
C	0.751046	-4.231660	-1.361263
H	0.491231	-5.215631	-1.000238
C	-5.985444	-2.269547	-0.217620
H	-6.175887	-3.331123	-0.096366
C	-6.911524	-1.444597	0.310079
C	1.450907	-1.751033	-2.381275
C	-8.281630	0.498012	1.388692
C	-8.948491	-0.622014	1.718789
C	1.242468	1.875345	-2.428237
H	2.283482	2.120354	-2.550478
C	-10.187475	-0.716498	2.556750
C	-2.232331	-1.425333	-2.073568
C	0.095124	-2.093661	-2.252761
C	-3.123006	0.763662	-4.165743
H	-4.157202	0.487672	-4.378446
H	-2.471987	-0.014090	-4.564296
H	-2.892961	1.698961	-4.678789
C	-8.622922	1.888373	1.730359
C	-1.824257	-4.142263	-3.610791
H	-2.847370	-4.454244	-3.827219
H	-1.138154	-4.928412	-3.930633
H	-1.610658	-3.245007	-4.190818
C	-1.978717	-5.177901	-1.350987
H	-2.987794	-5.513668	-1.585002
H	-1.891886	-5.063658	-0.269890
H	-1.305677	-5.971671	-1.672051
C	1.561858	-0.737895	-4.647178
H	2.215319	-1.533983	-5.008211
H	1.767967	0.171963	-5.213321
H	0.529356	-1.030830	-4.834879

C	3.273958	-0.084710	-2.958004
H	3.521108	0.109414	-1.914029
H	3.495225	0.811158	-3.536391
H	3.934742	-0.866048	-3.331278
C	0.735997	4.221631	-1.707051
H	-0.027335	4.988761	-1.785561
C	1.925177	4.606535	-1.201908
C	4.206477	4.776227	0.056932
C	5.504944	4.413385	0.657009
C	6.976069	2.614437	1.085922
H	7.794509	3.057329	0.519903
H	6.957894	1.536242	0.965994
H	7.082422	2.886584	2.135372
C	4.335913	7.211671	0.728463
C	4.983076	8.156177	2.773445
H	4.821239	7.938907	3.824823
H	4.582839	9.134702	2.513012
H	6.043689	8.117194	2.529882
C	3.071596	-4.671188	-0.630059
H	2.854553	-5.733365	-0.583917
C	4.194830	-4.257348	-0.014325
C	5.879579	-2.893220	1.413967
C	6.203669	-4.177134	1.647095
C	6.495885	-1.690466	2.053590
C	6.866341	-0.570192	4.080426
H	6.525371	0.391450	3.699956
H	7.948168	-0.642924	3.981694
H	6.564312	-0.702987	5.114582
C	7.302234	-4.589228	2.542216
C	8.382575	-6.443683	3.515119
H	8.308796	-6.049489	4.527647
H	9.349143	-6.171016	3.093772
H	8.250487	-7.521410	3.511649
N	-0.914634	-1.131482	-2.513097
O	-9.917467	-0.492491	3.844824
O	-11.264372	-1.014647	2.114893
O	-9.812847	1.999233	2.342991
O	-7.912219	2.826725	1.457147
O	6.286195	5.199814	1.136252
O	5.714759	3.089367	0.580423
O	4.776747	8.140927	0.106329
O	4.287286	7.120697	2.057232
O	7.087204	-0.845760	1.429847
O	6.239857	-1.644929	3.358475
O	8.100589	-3.838789	3.048048
O	7.319730	-5.924409	2.700823
S	-6.865912	0.319483	0.357429
S	-8.363615	-2.118095	1.068803
S	2.229433	6.302138	-0.796300
S	3.304435	3.560223	-0.842099
S	4.675766	-2.563566	0.201408
S	5.346162	-5.388589	0.704929

1\1\GINC-XE30TH10\SP\RB3LYP\6-311+G(d,p)\C51H45N1O12S6\DRAL\13-May-2016\0\#P B3LYP/6-311+G(d,p) EmpiricalDispersion=GD3BJ Name=DrAl Pop=(Full,NBO) GFINPUT GFPRINT Density=Current SCF=(Tight,NoVarAcc) SCFCyc=500 Int=UltraFine\BG33\0,1\C,0,2.415805,-2.609908,-1.88389\H,0,3.45335,-2.343091,-2.000172\C,0,0.841296,0.571185,-2.661166\C,0,1.810094,-0.490153,-3.13714\C,0,3.699184,6.020803,0.07875\C,0,-3.867455,2.034878,-2

.154942\H,0,-4.90076,1.789484,-2.394831\H,0,-3.647999,2.97178,-2.66465
9\H,0,-3.792238,2.196926,-1.079407\C,0,-0.514099,0.232659,-2.527534\C,
0,2.088236,-3.829481,-1.289936\C,0,-10.206025,3.332222,2.703907\H,0,-9
.491156,3.761297,3.404722\H,0,-11.183955,3.230545,3.165008\H,0,-10.262
624,3.962881,1.8181\C,0,-11.051095,-0.528459,4.729594\H,0,-11.531676,-
1.504735,4.691244\H,0,-11.770461,0.237842,4.443869\H,0,-10.651364,-0.3
32966,5.719852\C,0,0.334913,2.882052,-2.092984\C,0,-1.024124,2.554528,
-2.157032\H,0,-1.747642,3.340318,-1.999444\C,0,-1.462709,1.262515,-2.3
97547\C,0,-2.922323,0.932221,-2.636269\C,0,-3.197192,-0.408215,-1.9822
69\C,0,-4.419712,-0.679347,-1.388602\H,0,-5.146794,0.112189,-1.34515\C
,0,-4.747352,-1.945747,-0.898644\C,0,-3.817981,-2.967369,-1.122827\H,0
, -4.080864,-3.969148,-0.817953\C,0,-2.58896,-2.739086,-1.716089\C,0,-1
.66015,-3.87791,-2.090313\C,0,-0.24133,-3.400852,-1.856647\C,0,0.75104
6,-4.23166,-1.361263\H,0,0.491231,-5.215631,-1.000238\C,0,-5.985444,-2
.269547,-0.21762\H,0,-6.175887,-3.331123,-0.096366\C,0,-6.911524,-1.44
4597,0.310079\C,0,1.450907,-1.751033,-2.381275\C,0,-8.28163,0.498012,1
.388692\C,0,-8.948491,-0.622014,1.718789\C,0,1.242468,1.875345,-2.4282
37\H,0,2.283482,2.120354,-2.550478\C,0,-10.187475,-0.716498,2.55675\C,
0,-2.232331,-1.425333,-2.073568\C,0,0.095124,-2.093661,-2.252761\C,0,-
3.123006,0.763662,-4.165743\H,0,-4.157202,0.487672,-4.378446\H,0,-2.47
1987,-0.01409,-4.564296\H,0,-2.892961,1.698961,-4.678789\C,0,-8.622922
,1.888373,1.730359\C,0,-1.824257,-4.142263,-3.610791\H,0,-2.84737,-4.4
54244,-3.827219\H,0,-1.138154,-4.928412,-3.930633\H,0,-1.610658,-3.245
007,-4.190818\C,0,-1.978717,-5.177901,-1.350987\H,0,-2.987794,-5.51366
8,-1.585002\H,0,-1.891886,-5.063658,-0.26989\H,0,-1.305677,-5.971671,-
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,4.221631,-1.707051\H,0,-0.027335,4.988761,-1.785561\C,0,1.925177,4.60
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,0,6.957894,1.536242,0.965994\H,0,7.082422,2.886584,2.135372\C,0,4.335
913,7.211671,0.728463\C,0,4.983076,8.156177,2.773445\H,0,4.821239,7.93
8907,3.824823\H,0,4.582839,9.134702,2.513012\H,0,6.043689,8.117194,2.5
29882\C,0,3.071596,-4.671188,-0.630059\H,0,2.854553,-5.733365,-0.58391
7\C,0,4.19483,-4.257348,-0.014325\C,0,5.879579,-2.89322,1.413967\C,0,6
.203669,-4.177134,1.647095\C,0,6.495885,-1.690466,2.05359\C,0,6.866341
, -0.570192,4.080426\H,0,6.525371,0.39145,3.699956\H,0,7.948168,-0.6429
24,3.981694\H,0,6.564312,-0.702987,5.114582\C,0,7.302234,-4.589228,2.5
42216\C,0,8.382575,-6.443683,3.515119\H,0,8.308796,-6.049489,4.527647\
H,0,9.349143,-6.171016,3.093772\H,0,8.250487,-7.52141,3.511649\N,0,-0.
914634,-1.131482,-2.513097\O,0,-9.917467,-0.492491,3.844824\O,0,-11.26
4372,-1.014647,2.114893\O,0,-9.812847,1.999233,2.342991\O,0,-7.912219,
2.826725,1.457147\O,0,6.286195,5.199814,1.136252\O,0,5.714759,3.089367
,0.580423\O,0,4.776747,8.140927,0.106329\O,0,4.287286,7.120697,2.05723
2\O,0,7.087204,-0.84576,1.429847\O,0,6.239857,-1.644929,3.358475\O,0,8
.100589,-3.838789,3.048048\O,0,7.31973,-5.924409,2.700823\S,0,-6.86591
2,0.319483,0.357429\S,0,-8.363615,-2.118095,1.068803\S,0,2.229433,6.30
2138,-0.7963\S,0,3.304435,3.560223,-0.842099\S,0,4.675766,-2.563566,0.
201408\S,0,5.346162,-5.388589,0.704929\\Version=ES64L-G09RevD.01\State
=1-A\HF=-5318.3371325\RMSD=5.777e-09\Dipole=-1.1182139,-1.7535249,2.00
80798\Quadrupole=-0.8372853,-8.9620251,9.7993104,-32.1274785,-4.926654
5,8.3665342\PG=C01 [X(C51H45N1O12S6)]\@

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1_ox1

C	-2.387357	-2.495508	1.652472
H	-3.417169	-2.220046	1.800805
C	-0.784493	0.699333	2.286576
C	-1.741997	-0.345797	2.809184
C	-3.799880	6.123204	-0.284677
C	3.925257	2.139070	1.632271
H	4.961754	1.906187	1.868061
H	3.716047	3.094567	2.109338
H	3.833147	2.259196	0.552652
C	0.571852	0.353557	2.110937
C	-2.083538	-3.741528	1.086737
C	11.156174	3.097879	-1.774869
H	10.599475	3.693083	-2.496453
H	12.173128	2.929053	-2.113897
H	11.149085	3.597332	-0.808010
C	11.943576	-0.657450	-4.129852
H	12.302661	-1.684784	-4.126755
H	12.679745	-0.014017	-3.651281
H	11.732559	-0.322411	-5.140054
C	-0.282150	2.996867	1.663221
C	1.085543	2.669138	1.716111
H	1.804334	3.453944	1.537459
C	1.525489	1.384529	1.955870
C	2.986993	1.056685	2.171005
C	3.255495	-0.310886	1.576622
C	4.483572	-0.611937	1.025402
H	5.208978	0.177422	0.956169
C	4.817121	-1.904062	0.591935
C	3.866045	-2.912911	0.828135
H	4.130084	-3.925358	0.565252
C	2.628852	-2.658012	1.376321
C	1.690118	-3.783906	1.760358
C	0.269230	-3.304766	1.555434
C	-0.740311	-4.149118	1.137184
H	-0.498565	-5.149620	0.813008
C	6.054286	-2.270420	-0.033625
H	6.174235	-3.332598	-0.217604
C	7.090087	-1.488252	-0.446636
C	-1.408155	-1.626822	2.080588
C	8.782661	0.368095	-1.126090
C	9.359607	-0.783497	-1.512289
C	-1.185310	1.993383	2.046850
H	-2.220369	2.242365	2.198414
C	10.711565	-0.943678	-2.152428
C	2.277493	-1.323241	1.682960
C	-0.054180	-1.977734	1.908468
C	3.211566	0.946008	3.705792
H	4.248960	0.679026	3.909896
H	2.568403	0.185414	4.147995
H	2.991122	1.901291	4.183294
C	9.309213	1.744921	-1.225543
C	1.873191	-4.039246	3.283153
H	2.895677	-4.360124	3.485109
H	1.185387	-4.817548	3.615496
H	1.676430	-3.137992	3.863298
C	1.988746	-5.090691	1.023157
H	2.995811	-5.436754	1.247070
H	1.888466	-4.981442	-0.057050
H	1.316522	-5.878192	1.358426

C	-1.447240	-0.559137	4.319109
H	-2.093004	-1.343100	4.716029
H	-1.636055	0.364109	4.867885
H	-0.411189	-0.851374	4.487151
C	-3.209543	0.060598	2.665281
H	-3.489741	0.228918	1.625259
H	-3.411001	0.969320	3.229992
H	-3.860591	-0.707003	3.080060
C	-0.685307	4.305987	1.242463
H	0.094968	5.058231	1.207088
C	-1.916400	4.695551	0.802446
C	-4.330225	4.893738	-0.156788
C	-5.716197	4.536274	-0.539469
C	-7.233208	2.728995	-0.724288
H	-7.955911	3.170225	-0.039891
H	-7.185591	1.651641	-0.602265
H	-7.496713	2.996507	-1.746324
C	-4.506205	7.334935	-0.828477
C	-5.460328	8.296883	-2.743054
H	-5.479760	8.068545	-3.803618
H	-4.985893	9.258758	-2.559014
H	-6.465743	8.294384	-2.326332
C	-3.075181	-4.599919	0.496213
H	-2.803351	-5.643731	0.383789
C	-4.284463	-4.235094	-0.006134
C	-6.310904	-2.994145	-1.071817
C	-6.556575	-4.299580	-1.291481
C	-7.105145	-1.809496	-1.505480
C	-8.444159	-0.891160	-3.203614
H	-7.908355	0.056346	-3.225130
H	-9.310887	-0.811565	-2.550112
H	-8.742855	-1.188549	-4.203340
C	-7.797936	-4.858862	-1.900247
C	-8.703499	-6.768761	-2.946208
H	-9.102690	-6.208282	-3.789460
H	-9.475132	-6.881317	-2.186774
H	-8.329528	-7.735639	-3.266794
N	0.956265	-1.000331	2.053058
O	10.685365	-0.567595	-3.426996
O	11.652505	-1.404220	-1.567331
O	10.570313	1.785793	-1.658443
O	8.648761	2.708469	-0.917939
O	-6.549771	5.328866	-0.894688
O	-5.909158	3.215487	-0.418237
O	-4.802277	8.267210	-0.132654
O	-4.689520	7.235459	-2.138585
O	-7.226124	-0.828456	-0.810253
O	-7.576302	-1.942477	-2.737254
O	-8.865520	-4.308281	-1.900526
O	-7.562367	-6.081308	-2.393555
S	7.211437	0.252552	-0.355229
S	8.496834	-2.245216	-1.179964
S	-2.196311	6.358594	0.318925
S	-3.320798	3.671922	0.589829
S	-4.896135	-2.593202	-0.133943
S	-5.384470	-5.433010	-0.666725

op=(Full,NBO) GFINPUT GFPRINT Density=Current SCF=(Tight,NoVarAcc) SCF
Cyc=500 Int=UltraFine\\BG33(.+)\1,2\C,0,-2.387357,-2.495508,1.652472\
H,0,-3.417169,-2.220046,1.800805\C,0,-0.784493,0.699333,2.286576\C,0,-
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67,2.109338\H,0,3.833147,2.259196,0.552652\C,0,0.571852,0.353557,2.110
937\C,0,-2.083538,-3.741528,1.086737\C,0,11.156174,3.097879,-1.774869\
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2661,-1.684784,-4.126755\H,0,12.679745,-0.014017,-3.651281\H,0,11.7325
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115

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C	11.544134	2.601471	-0.659528
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H	11.915402	-0.957344	-4.775392
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C	1.183089	2.624502	1.791664
H	1.930374	3.381767	1.606190
C	1.579671	1.313132	1.997596
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C	3.231273	-0.421675	1.494578
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H	5.174832	0.037563	0.797149
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C	2.509427	-2.712032	1.192260
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C	0.132946	-3.277195	1.411385
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C	-1.459257	-1.579363	2.062094
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C	-0.126998	-1.971128	1.860498
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H	4.316021	0.405984	3.858011
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H	3.111561	1.660947	4.225120
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H	1.050250	-4.931036	3.371037

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H	-5.872761	8.268415	-2.734909
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H	-3.014004	-5.461626	0.187401
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H	-9.460044	-0.967636	-3.693012
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C	-9.087393	-6.677622	-2.513562
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H	-9.804180	-6.723323	-1.692311
H	-8.755411	-7.677869	-2.782901
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O	10.990030	-2.306034	-2.751885
O	10.878436	1.354787	-0.848331
O	8.919372	2.429741	-0.522215
O	-6.137755	5.411135	-1.275670
O	-5.555107	3.303228	-0.717276
O	-4.472081	8.384025	-0.386943
O	-4.128014	7.239463	-2.297949
O	-7.202423	-0.497577	-0.793587
O	-8.068991	-1.743523	-2.466505
O	-9.216670	-4.164604	-1.733962
O	-7.913149	-5.971517	-2.125431
S	7.256403	0.051338	-0.381653
S	8.362884	-2.445593	-1.476345
S	-2.016430	6.480527	0.572752
S	-3.150240	3.763462	0.672858
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S -5.619915 -5.239037 -0.736612

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103

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H	-4.692618	2.208524	-2.298687
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C	2.036699	-3.703795	-1.253481
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C	-0.786265	2.790505	-2.022823
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C	-1.282033	1.528667	-2.309441
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C	-4.330693	-0.313009	-1.377253
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C	-3.827416	-2.630302	-1.167005
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C	-0.263416	-3.188116	-1.864941
C	0.688191	-4.059480	-1.359225
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C	-5.969949	-1.856744	-0.254070
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C	-6.816147	-0.997731	0.347584
C	1.498281	-1.599722	-2.346801
C	-7.853900	0.927057	1.793921
C	-8.651545	-0.137656	2.018292
C	1.446139	2.023814	-2.332238
H	2.494987	2.228406	-2.459926
C	-2.170497	-1.131302	-2.065221
C	0.129061	-1.890210	-2.238504
C	-2.955824	1.161783	-4.096795
H	-4.000591	0.940312	-4.321346
H	-2.339264	0.368315	-4.518395
H	-2.680934	2.101616	-4.578637
C	-1.846905	-3.829932	-3.658477
H	-2.877714	-4.098235	-3.896071
H	-1.186174	-4.634472	-3.985968
H	-1.591112	-2.929207	-4.215556
C	-2.074838	-4.906656	-1.424658
H	-3.091571	-5.199682	-1.682009
H	-2.002445	-4.818226	-0.340063
H	-1.425329	-5.717613	-1.751471

C	1.658041	-0.567963	-4.603184
H	2.275981	-1.388663	-4.971553
H	1.906501	0.337920	-5.158725
H	0.614027	-0.812031	-4.796680
C	3.391891	-0.009183	-2.903130
H	3.642376	0.159491	-1.855415
H	3.654169	0.883510	-3.469303
H	4.018315	-0.815399	-3.282689
C	1.049275	4.351906	-1.493724
H	0.321804	5.156524	-1.521202
C	2.256186	4.656918	-0.974338
C	4.501408	4.559838	0.382846
C	2.974175	-4.572239	-0.563808
H	2.730562	-5.629012	-0.525550
C	4.084591	-4.178607	0.088424
C	5.681303	-2.883330	1.701261
C	5.939284	-4.185778	1.939682
N	-0.838685	-0.883336	-2.491674
S	-6.617698	0.742848	0.542891
S	-8.349253	-1.559076	1.026249
S	2.687928	6.294269	-0.486919
S	3.584201	3.519128	-0.701465
S	4.638414	-2.516519	0.321397
S	5.187517	-5.338075	0.837971
S	6.371251	-1.529463	2.570061
S	7.069879	-4.764844	3.141839
S	4.898783	7.083931	1.410249
S	5.957557	3.934298	1.128431
S	-8.032721	2.501412	2.533110
S	-10.032993	-0.126369	3.091936
C	4.884079	-0.869237	3.393342
H	4.487051	-1.602269	4.092324
H	5.204516	0.017929	3.937991
H	4.126067	-0.594814	2.663247
C	6.200295	-6.217877	3.810280
H	6.109769	-7.010743	3.071612
H	6.819397	-6.567614	4.635453
H	5.218532	-5.938796	4.186785
C	5.564996	2.170129	1.341009
H	5.470365	1.654131	0.388405
H	6.415061	1.750313	1.876172
H	4.661451	2.040047	1.932230
C	3.673061	7.402216	2.721554
H	3.542570	6.515243	3.338045
H	4.077490	8.212973	3.326307
H	2.721306	7.709459	2.293748
C	-9.905880	-1.760546	3.884659
H	-10.690535	-1.774190	4.640055
H	-10.078094	-2.568497	3.177446
H	-8.937513	-1.879725	4.365897
C	-6.447786	2.651071	3.421738
H	-5.606813	2.586592	2.735176
H	-6.458020	3.634239	3.890512
H	-6.370494	1.881801	4.187280

1\1\GINC-XE30TH52\SP\RB3LYP\6-311+G(d,p)\C45H45N1S12\DRAL\13-May-2016\0\#\#P B3LYP/6-311+G(d,p) EmpiricalDispersion=GD3BJ Name=Dral Pop=(Full,NBO) GFINPUT GFPRINT Density=Current SCF=(Tight,NoVarAcc) SCFCyc=500 Int=UltraFine\BG32\0,1\C,0,2.421721,-2.494935,-1.83492\H,0,3.471172,

-2.267008,-1.923924\C,0,0.988595,0.745159,-2.598877\C,0,1.912437,-0.348418,-3.090281\C,0,4.081932,5.836339,0.495646\C,0,-3.650448,2.398369,-2.04734\H,0,-4.692618,2.208524,-2.298687\H,0,-3.385033,3.341209,-2.523222\H,0,-3.572377,2.518374,-0.966318\C,0,-0.379973,0.461989,-2.471291\C,0,2.036699,-3.703795,-1.253481\C,0,0.586486,3.055727,-1.950199\C,0,-0.786265,2.790505,-2.022823\H,0,-1.473876,3.601312,-1.833599\C,0,-1.282033,1.528667,-2.309441\C,0,-2.753834,1.270487,-2.562177\C,0,-3.091649,-0.076467,-1.951831\C,0,-4.330693,-0.313009,-1.377253\H,0,-5.03113,0.502156,-1.323008\C,0,-4.714088,-1.576473,-0.922537\C,0,-3.827416,-2.630302,-1.167005\H,0,-4.13432,-3.627463,-0.889141\C,0,-2.584078,-2.4379,-1.74336\C,0,-1.695582,-3.60453,-2.130578\C,0,-0.263416,-3.188116,-1.864941\C,0,0.688191,-4.05948,-1.359225\H,0,0.385953,-5.036643,-1.012613\C,0,-5.969949,-1.856744,-0.25407\H,0,-6.250794,-2.904381,-0.214244\C,0,-6.816147,-0.997731,0.347584\C,0,1.498281,-1.599722,-2.346801\C,0,-7.8539,0.927057,1.793921\C,0,-8.651545,-0.137656,2.018292\C,0,1.446139,2.023814,-2.332238\H,0,2.494987,2.228406,-2.459926\C,0,-2.170497,-1.131302,-2.065221\C,0,0.129061,-1.89021,-2.238504\C,0,-2.955824,1.161783,-4.096795\H,0,-4.000591,0.940312,-4.321346\H,0,-2.339264,0.368315,-4.518395\H,0,-2.680934,2.101616,-4.578637\C,0,-1.846905,-3.829932,-3.658477\H,0,-2.877714,-4.098235,-3.896071\H,0,-1.186174,-4.634472,-3.985968\H,0,-1.591112,-2.929207,-4.215556\C,0,-2.074838,-4.906656,-1.424658\H,0,-3.091571,-5.199682,-1.682009\H,0,-2.002445,-4.818226,-0.340063\H,0,-1.425329,-5.717613,-1.751471\C,0,1.658041,-0.567963,-4.603184\H,0,2.275981,-1.388663,-4.971553\H,0,1.906501,0.33792,-5.158725\H,0,0.614027,-0.812031,-4.79668\C,0,3.391891,-0.009183,-2.90313\H,0,3.642376,0.159491,-1.855415\H,0,3.654169,0.88351,-3.469303\H,0,4.018315,-0.815399,-3.282689\C,0,1.049275,4.351906,-1.493724\H,0,0.321804,5.156524,-1.521202\C,0,2.256186,4.656918,-0.974338\C,0,4.501408,4.559838,0.382846\C,0,2.974175,-4.572239,-0.563808\H,0,2.730562,-5.629012,-0.52555\C,0,4.084591,-4.178607,0.088424\C,0,5.681303,-2.88333,1.701261\C,0,5.939284,-4.185778,1.939682\N,0,-0.838685,-0.883336,-2.491674\S,0,-6.617698,0.742848,0.542891\S,0,-8.349253,-1.559076,1.026249\S,0,2.687928,6.294269,-0.486919\S,0,3.584201,3.519128,-0.701465\S,0,4.638414,-2.516519,0.321397\S,0,5.187517,-5.338075,0.837971\S,0,6.371251,-1.529463,2.570061\S,0,7.069879,-4.764844,3.141839\S,0,4.898783,7.083931,1.410249\S,0,5.957557,3.934298,1.128431\S,0,-8.032721,2.501412,2.53311\S,0,-10.032993,-0.126369,3.091936\C,0,4.884079,-0.869237,3.393342\H,0,4.487051,-1.602269,4.092324\H,0,5.204516,0.017929,3.937991\H,0,4.126067,-0.594814,2.663247\C,0,6.200295,-6.217877,3.81028\H,0,6.109769,-7.010743,3.071612\H,0,6.819397,-6.567614,4.635453\H,0,5.218532,-5.938796,4.186785\C,0,5.564996,2.170129,1.341009\H,0,5.470365,1.654131,0.388405\H,0,6.415061,1.750313,1.876172\H,0,4.661451,2.040047,1.93223\C,0,3.673061,7.402216,2.721554\H,0,3.54257,6.515243,3.338045\H,0,4.07749,8.212973,3.326307\H,0,2.721306,7.709459,2.293748\C,0,-9.90588,-1.760546,3.884659\H,0,-10.690535,-1.77419,4.640055\H,0,-10.078094,-2.568497,3.177446\H,0,-8.937513,-1.879725,4.365897\C,0,-6.447786,2.651071,3.421738\H,0,-5.606813,2.586592,2.735176\H,0,-6.45802,3.634239,3.890512\H,0,-6.370494,1.881801,4.18728\Version=ES64L-G09RevD.01\State=1-A\HF=-6575.9208919\RMSD=2.963e-09\Dipole=-0.8738425,-1.5286253,1.6500543\Quadrupole=-30.3946343,12.3238083,18.0708259,-0.2515487,-0.601234,-0.1907242\PG=C01 [X(C45H45N1S12)]\@

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2_ox1

103

C	-2.444257	-2.393508	1.558358
H	-3.477018	-2.145106	1.730987
C	-0.904077	0.803526	2.243140

C	-1.814937	-0.273777	2.784334
C	-4.164547	5.967667	-0.505977
C	3.745142	2.375445	1.494451
H	4.791360	2.171188	1.713904
H	3.513702	3.322824	1.977811
H	3.632353	2.495450	0.416608
C	0.454909	0.496272	2.029737
C	-2.124876	-3.605187	0.929588
C	-0.487652	3.108116	1.584703
C	0.890134	2.823139	1.611354
H	1.580790	3.627309	1.408227
C	1.373566	1.553289	1.852386
C	2.847088	1.264425	2.042877
C	3.143621	-0.092723	1.435323
C	4.371205	-0.356411	0.863190
H	5.074887	0.452009	0.787019
C	4.733071	-1.635777	0.414529
C	3.805911	-2.668425	0.642634
H	4.089367	-3.670433	0.360123
C	2.569634	-2.450857	1.209276
C	1.657369	-3.605387	1.575863
C	0.225085	-3.148771	1.397010
C	-0.774011	-3.992407	0.952234
H	-0.518265	-4.973838	0.582927
C	5.976662	-1.966032	-0.216242
H	6.113810	-3.021361	-0.427390
C	7.006049	-1.158437	-0.598898
C	-1.474060	-1.525988	2.009528
C	8.717539	0.738607	-1.188647
C	9.319308	-0.403653	-1.595354
C	-1.348895	2.084513	2.008195
H	-2.384543	2.308216	2.193898
C	2.193802	-1.130774	1.547837
C	-0.117674	-1.842055	1.800967
C	3.100400	1.153763	3.572480
H	4.148443	0.916318	3.758451
H	2.487348	0.372047	4.020408
H	2.859292	2.099444	4.059333
C	1.862033	-3.896823	3.088632
H	2.892304	-4.204376	3.271493
H	1.191610	-4.695265	3.408889
H	1.656217	-3.014107	3.693575
C	1.971660	-4.886523	0.801387
H	2.986022	-5.222201	1.007925
H	1.861165	-4.749607	-0.274723
H	1.313824	-5.693066	1.120014
C	-1.462964	-0.510264	4.277070
H	-2.073852	-1.319124	4.679497
H	-1.655210	0.396045	4.852532
H	-0.414695	-0.778786	4.402574
C	-3.296145	0.096806	2.699669
H	-3.613911	0.276947	1.672238
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C	-0.946596	4.391008	1.138706
H	-0.201668	5.177562	1.087439
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C	-4.603813	4.697771	-0.350755
C	-3.104033	-4.438304	0.287853
H	-2.807724	-5.461579	0.083994

C	-4.327021	-4.059045	-0.171901
C	-6.426792	-2.814784	-1.129346
C	-6.600588	-4.104999	-1.494648
N	0.874335	-0.847183	1.954861
S	7.128892	0.572354	-0.459894
S	8.426232	-1.882426	-1.344214
S	-2.586185	6.334596	0.165521
S	-3.532944	3.597663	0.491306
S	-5.017063	-2.452073	-0.145939
S	-5.383665	-5.235953	-0.944748
S	-7.508128	-1.499196	-1.534702
S	-7.967209	-4.637962	-2.445638
S	-5.095905	7.254599	-1.240717
S	-6.170504	4.152597	-0.908351
S	9.409997	2.339892	-1.319293
S	10.900898	-0.412506	-2.338116
C	-6.743653	-0.906165	-3.082672
H	-6.759953	-1.692246	-3.833907
H	-7.350580	-0.067659	-3.422292
H	-5.724416	-0.570719	-2.902906
C	-7.588896	-6.387111	-2.748270
H	-7.561084	-6.956015	-1.820909
H	-8.416033	-6.748087	-3.357184
H	-6.660287	-6.504963	-3.302837
C	-6.084805	2.355729	-0.649111
H	-5.988938	2.103962	0.405292
H	-7.038671	1.974341	-1.008915
H	-5.279596	1.905043	-1.225910
C	-4.315978	7.338389	-2.887824
H	-4.445353	6.395651	-3.414388
H	-4.834380	8.131658	-3.424538
H	-3.261262	7.589998	-2.802219
C	11.156194	-2.169207	-2.715271
H	12.136709	-2.212144	-3.186321
H	11.173455	-2.772604	-1.809703
H	10.410226	-2.541276	-3.414816
C	8.867549	2.805089	-2.999293
H	7.781723	2.831452	-3.056489
H	9.266078	3.802840	-3.178115
H	9.275706	2.113740	-3.732821

1\1\GINC-XE30TH64\SP\UB3LYP\6-311+G(d,p)\C45H45N1S12(1+,2)\DRAL\13-May-2016\0\#\#P B3LYP/6-311+G(d,p) EmpiricalDispersion=GD3BJ Name=Dral Pop=(Full,NBO) GFINPUT GFPRINT Density=Current SCF=(Tight,NoVarAcc) SCFCy c=500 Int=UltraFine\BG32(+)\1,2\C,0,-2.444257,-2.393508,1.558358\H,0,-3.477018,-2.145106,1.730987\C,0,-0.904077,0.803526,2.24314\C,0,-1.814937,-0.273777,2.784334\C,0,-4.164547,5.967667,-0.505977\C,0,3.745142,2.375445,1.494451\H,0,4.79136,2.171188,1.713904\H,0,3.513702,3.322824,1.977811\H,0,3.632353,2.49545,0.416608\C,0,0.454909,0.496272,2.029737\C,0,-2.124876,-3.605187,0.929588\C,0,-0.487652,3.108116,1.584703\C,0,0.890134,2.823139,1.611354\H,0,1.58079,3.627309,1.408227\C,0,1.373566,1.553289,1.852386\C,0,2.847088,1.264425,2.042877\C,0,3.143621,-0.092723,1.435323\C,0,4.371205,-0.356411,0.86319\H,0,5.074887,0.452009,0.787019\C,0,4.733071,-1.635777,0.414529\C,0,3.805911,-2.668425,0.642634\H,0,4.089367,-3.670433,0.360123\C,0,2.569634,-2.450857,1.209276\C,0,1.657369,-3.605387,1.575863\C,0,0.225085,-3.148771,1.39701\C,0,-0.774011,-3.992407,0.952234\H,0,-0.518265,-4.973838,0.582927\C,0,5.976662,-1.966032,-0.216242\H,0,6.11381,-3.021361,-0.42739\C,0,7.006049,-1.158437,-0.598898\C,0,-1.47406,-1.525988,2.009528\C,0,8.717539,0.738607,-1.188647

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2532\H,0,-0.414695,-0.778786,4.402574\C,0,-3.296145,0.096806,2.699669\
H,0,-3.613911,0.276947,1.672238\H,0,-3.499905,0.989605,3.288914\H,0,-3
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7771,-0.350755\C,0,-3.104033,-4.438304,0.287853\H,0,-2.807724,-5.46157
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4861\S,0,7.128892,0.572354,-0.459894\S,0,8.426232,-1.882426,-1.344214\
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,-2.212144,-3.186321\H,0,11.173455,-2.772604,-1.809703\H,0,10.410226,-
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8607\Quadrupole=54.8875509,-5.2510116,-49.6365393,3.2355208,-2.5559467
,-0.0468684\PG=C01 [X(C45H45N1S12)]\@

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2_red1

103

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H	3.503348	-2.146069	-1.989784
C	0.983576	0.830008	-2.661394
C	1.899886	-0.263594	-3.170219
C	4.067810	5.724278	0.621354
C	-3.656228	2.480123	-2.077462
H	-4.698439	2.284418	-2.323821
H	-3.390844	3.420597	-2.560220
H	-3.577988	2.605442	-0.997123
C	-0.383676	0.540974	-2.491542
C	2.091704	-3.586222	-1.245741
C	0.584299	3.137838	-1.999736
C	-0.790401	2.872899	-2.052821
H	-1.476563	3.681620	-1.847337
C	-1.288329	1.610580	-2.333323
C	-2.760889	1.347327	-2.583169

C	-3.101370	0.002301	-1.967424
C	-4.335540	-0.233893	-1.397414
H	-5.040286	0.578005	-1.342775
C	-4.722601	-1.505867	-0.927084
C	-3.812755	-2.556738	-1.170072
H	-4.118951	-3.555807	-0.895038
C	-2.570447	-2.361579	-1.732605
C	-1.666928	-3.525252	-2.106110
C	-0.230628	-3.102509	-1.857299
C	0.729580	-3.955912	-1.358413
H	0.444555	-4.940093	-1.013562
C	-5.963698	-1.791234	-0.275003
H	-6.202485	-2.847071	-0.174152
C	-6.902479	-0.946065	0.236359
C	1.521670	-1.506358	-2.392517
C	-7.877561	0.852008	1.829428
C	-8.646406	-0.240757	2.026485
C	1.438891	2.111114	-2.408638
H	2.482977	2.322964	-2.565262
C	-2.161971	-1.046889	-2.070068
C	0.145973	-1.798267	-2.257499
C	-2.957838	1.235863	-4.118524
H	-4.004243	1.020763	-4.342684
H	-2.347525	0.432937	-4.531206
H	-2.672258	2.170675	-4.606201
C	-1.827086	-3.774231	-3.629700
H	-2.858862	-4.048141	-3.860187
H	-1.161671	-4.577964	-3.951513
H	-1.577079	-2.877283	-4.195969
C	-2.032862	-4.817920	-1.376178
H	-3.049453	-5.124136	-1.620699
H	-1.954337	-4.704454	-0.294397
H	-1.374213	-5.627701	-1.688566
C	1.595793	-0.500712	-4.671030
H	2.213173	-1.317468	-5.049577
H	1.808142	0.402597	-5.247609
H	0.549890	-0.766286	-4.821125
C	3.380773	0.093142	-3.039346
H	3.663355	0.277663	-2.002717
H	3.618046	0.979123	-3.628832
H	3.998102	-0.718767	-3.421768
C	1.062686	4.416367	-1.511811
H	0.352019	5.237053	-1.523788
C	2.268279	4.678929	-0.968351
C	4.442450	4.437803	0.472716
C	3.022084	-4.417983	-0.556442
H	2.735386	-5.456188	-0.402470
C	4.237137	-4.057821	-0.043411
C	5.709732	-2.834263	1.690419
C	5.958510	-4.146645	1.891224
N	-0.829259	-0.794693	-2.464573
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S	-8.465172	-1.531403	0.824579
S	2.748902	6.285034	-0.417731
S	3.551330	3.482755	-0.704260
S	4.853713	-2.418012	0.188667
S	5.385511	-5.230762	0.607548
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S	4.852122	6.877269	1.676270

S	5.792837	3.709444	1.323562
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S	-9.893483	-0.388748	3.244487
C	4.629583	-0.873515	3.282350
H	4.145228	-1.590340	3.942786
H	4.833120	0.048541	3.826177
H	3.988362	-0.664887	2.428981
C	5.855932	-6.147690	3.795027
H	5.703802	-6.899548	3.024596
H	6.381024	-6.591641	4.640695
H	4.895432	-5.757115	4.126242
C	5.528457	1.930661	1.050523
H	5.644049	1.659714	0.003595
H	6.304226	1.427780	1.625133
H	4.553628	1.616489	1.413767
C	3.630832	6.973900	3.027311
H	3.547052	6.010093	3.525329
H	3.999478	7.720636	3.730206
H	2.662171	7.283942	2.640580
C	-9.389640	-1.928237	4.078442
H	-10.138427	-2.115202	4.847882
H	-9.367171	-2.761422	3.380118
H	-8.412321	-1.804841	4.541630
C	-6.227690	2.602910	3.189148
H	-5.614656	2.736430	2.301485
H	-6.205932	3.512655	3.788670
H	-5.851722	1.768165	3.777574

1\1\GINC-XE30TH52\SP\UB3LYP\6-311+G(d,p)\C45H45N1S12(1-,2)\DRAL\13-May-2016\0\#\#P B3LYP/6-311+G(d,p) EmpiricalDispersion=GD3BJ Name=DrAl Pop=(Full,NBO) GFINPUT GFPRINT Density=Current SCF=(Tight,NoVarAcc) SCFCy c=500 Int=UltraFine\BG32(-)\-1,2\C,0,2.455495,-2.37323,-1.874419\H,0,3.503348,-2.146069,-1.989784\C,0,0.983576,0.830008,-2.661394\C,0,1.899886,-0.263594,-3.170219\C,0,4.06781,5.724278,0.621354\C,0,-3.656228,2.480123,-2.077462\H,0,-4.698439,2.284418,-2.323821\H,0,-3.390844,3.420597,-2.56022\H,0,-3.577988,2.605442,-0.997123\C,0,-0.383676,0.540974,-2.491542\C,0,2.091704,-3.586222,-1.245741\C,0,0.584299,3.137838,-1.999736\C,0,-0.790401,2.872899,-2.052821\H,0,-1.476563,3.68162,-1.847337\C,0,-1.288329,1.61058,-2.333323\C,0,-2.760889,1.347327,-2.583169\C,0,-3.10137,0.002301,-1.967424\C,0,-4.33554,-0.233893,-1.397414\H,0,-5.040286,0.578005,-1.342775\C,0,-4.722601,-1.505867,-0.927084\C,0,-3.812755,-2.556738,-1.170072\H,0,-4.118951,-3.555807,-0.895038\C,0,-2.570447,-2.361579,-1.732605\C,0,-1.666928,-3.525252,-2.10611\C,0,-0.230628,-3.102509,-1.857299\C,0,0.72958,-3.955912,-1.358413\H,0,0.444555,-4.940093,-1.013562\C,0,-5.963698,-1.791234,-0.275003\H,0,-6.202485,-2.847071,-0.174152\C,0,-6.902479,-0.946065,0.236359\C,0,1.52167,-1.506358,-2.392517\C,0,-7.877561,0.852008,1.829428\C,0,-8.646406,-0.240757,2.026485\C,0,1.438891,2.111114,-2.408638\H,0,2.482977,2.322964,-2.565262\C,0,-2.161971,-1.046889,-2.070068\C,0,0.145973,-1.798267,-2.257499\C,0,-2.957838,1.235863,-4.118524\H,0,-4.004243,1.020763,-4.342684\H,0,-2.347525,0.432937,-4.531206\H,0,-2.672258,2.170675,-4.606201\C,0,-1.827086,-3.774231,-3.6297\H,0,-2.858862,-4.048141,-3.860187\H,0,-1.161671,-4.577964,-3.951513\H,0,-1.577079,-2.877283,-4.195969\C,0,-2.032862,-4.81792,-1.376178\H,0,-3.049453,-5.124136,-1.620699\H,0,-1.954337,-4.704454,-0.294397\H,0,-1.374213,-5.627701,-1.688566\C,0,1.595793,-0.500712,-4.67103\H,0,2.213173,-1.317468,-5.049577\H,0,1.808142,0.402597,-5.247609\H,0,0.54989,-0.766286,-4.821125\C,0,3.380773,0.093142,-3.039346\H,0,3.663355,0.277663,-2.002717\H,0,3.618046,0.979123,-3.628832\H,0,3.998102,-0.718767,-3.421768\C,0,1.062686,4.416367,-1.511811\H,0,0.352019,5.2370

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C	1.220802	2.143371	-0.049577
C	2.372203	2.835078	-0.396508
H	2.367187	3.914050	-0.396876
C	3.543327	2.164551	-0.713245
H	4.435420	2.712963	-0.984525
C	3.564118	0.786828	-0.622377
H	4.492335	0.262027	-0.799372
C	2.423714	0.052419	-0.302189
C	2.560242	-1.445095	-0.109153
C	1.212735	-2.088844	0.169679
C	1.186278	-3.461707	0.392495
H	2.120557	-4.003154	0.437974
C	-0.000009	-4.154971	0.538080
H	-0.000012	-5.220495	0.724192
C	-1.186295	-3.461700	0.392502
H	-2.120575	-4.003144	0.437986
C	-1.212745	-2.088837	0.169689
C	-0.000003	-1.376469	0.135314
C	-2.560251	-1.445081	-0.109134
C	-2.423719	0.052434	-0.302154
C	-3.564124	0.786852	-0.622319
H	-4.492347	0.262055	-0.799303
C	-3.543330	2.164576	-0.713178
H	-4.435424	2.712992	-0.984439
C	-2.372195	2.835093	-0.396458
H	-2.367175	3.914065	-0.396821
C	-1.220792	2.143379	-0.049552

C	-1.217769	0.733534	-0.093446
C	0.000013	2.845628	0.506444
C	3.515481	-1.691808	1.081718
H	3.108644	-1.250158	1.991849
H	4.491270	-1.244552	0.893444
H	3.662052	-2.757659	1.254850
C	3.150671	-2.086814	-1.386043
H	3.271762	-3.162330	-1.260840
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H	-4.127615	-1.665625	-1.621421
H	-3.271778	-3.162300	-1.260840
C	-3.515489	-1.691806	1.081735
H	-3.662065	-2.757658	1.254854
H	-4.491278	-1.244545	0.893468
H	-3.108651	-1.250169	1.991872
C	0.000029	2.648852	2.046459
H	-0.888433	3.109449	2.482027
H	0.888503	3.109442	2.482008
H	0.000027	1.591168	2.307757
C	0.000015	4.349452	0.228784
H	0.000004	4.566879	-0.840053
H	0.873054	4.819960	0.678545
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0.262025,-0.799372\C,0,2.423714,0.052418,-0.302189\C,0,2.560241,-1.445
096,-0.109153\C,0,1.212734,-2.088844,0.169679\C,0,1.186277,-3.461707,0
.392495\H,0,2.120555,-4.003155,0.437974\C,0,-0.000011,-4.154971,0.5380
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2331,-1.26084\H,0,4.127604,-1.665663,-1.621438\H,0,2.490396,-1.915078,
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.236511\H,0,-4.127616,-1.665623,-1.621421\H,0,-3.271779,-3.162299,-1.2
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2,0.228784\H,0,0.000006,4.566879,-0.840053\H,0,0.873056,4.81996,0.6785
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783\PG=C01 [X(C27H27N1)]\@

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4_ox1

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C	1.220118	2.148702	-0.035571
C	2.380408	2.829973	-0.348198
H	2.389641	3.907605	-0.335044
C	3.548770	2.149260	-0.668700
H	4.443244	2.697952	-0.930031
C	3.570303	0.770479	-0.604331
H	4.497064	0.248650	-0.789386
C	2.429065	0.039351	-0.295151
C	2.555973	-1.452425	-0.128425
C	1.222736	-2.086184	0.183526
C	1.193130	-3.444874	0.458175
H	2.121740	-3.991331	0.522382
C	-0.000016	-4.124352	0.627437
H	-0.000016	-5.182487	0.850258
C	-1.193156	-3.444866	0.458179
H	-2.121774	-3.991311	0.522394
C	-1.222749	-2.086173	0.183528
C	-0.000007	-1.379675	0.119525
C	-2.555982	-1.452408	-0.128423
C	-2.429066	0.039368	-0.295149
C	-3.570297	0.770505	-0.604334
H	-4.497062	0.248683	-0.789397
C	-3.548754	2.149284	-0.668703
H	-4.443223	2.697987	-0.930033
C	-2.380387	2.829992	-0.348198
H	-2.389614	3.907624	-0.335045
C	-1.220104	2.148713	-0.035571
C	-1.219903	0.732654	-0.093517
C	0.000010	2.865203	0.486904
C	3.554812	-1.722414	1.025448
H	3.187775	-1.298964	1.960256
H	4.523470	-1.278598	0.805336
H	3.705641	-2.790449	1.167379
C	3.088900	-2.083240	-1.440785
H	3.200920	-3.160034	-1.327422
H	4.061429	-1.669392	-1.700738
H	2.402922	-1.894425	-2.266552
C	-3.088907	-2.083219	-1.440785
H	-2.402935	-1.894392	-2.266554
H	-4.061442	-1.669379	-1.700733
H	-3.200919	-3.160015	-1.327429
C	-3.554824	-1.722398	1.025447
H	-3.705664	-2.790431	1.167369
H	-4.523479	-1.278571	0.805338
H	-3.187786	-1.298959	1.960258
C	0.000009	2.709280	2.038452
H	-0.886897	3.185800	2.455967
H	0.886927	3.185780	2.455966
H	-0.000002	1.661306	2.337360
C	0.000014	4.361711	0.166460
H	0.000004	4.550347	-0.907263

H	0.869212	4.845909	0.606191
H	-0.869171	4.845916	0.606209

1\1\GINC-XE30TH50\SP\UB3LYP\6-311+G(d,p)\C27H27N1(1+,2)\DRAL\08-Sep-2016\0\#\#P B3LYP/6-311+G(d,p) EmpiricalDispersion=GD3BJ Name=DrAl Pop=(Full,NBO) GFINPUT GFPRINT Density=Current SCF=(Tight,NoVarAcc) SCFCyc=500 Int=UltraFine\4(.+)\1,2\N,0,0.000001,-0.027975,0.017236\C,0,-1.219909,-0.732643,-0.093518\C,0,-1.220122,-2.1487,-0.035571\C,0,-2.380413,-2.829969,-0.348198\H,0,-2.389648,-3.907601,-0.335044\C,0,-3.548774,-2.149253,-0.6687\H,0,-4.443249,-2.697944,-0.930031\C,0,-3.570304,-0.770472,-0.604331\H,0,-4.497065,-0.248642,-0.789386\C,0,-2.429065,-0.039347,-0.295151\C,0,-2.55597,1.45243,-0.128425\C,0,-1.222732,2.086186,0.183526\C,0,-1.193124,3.444876,0.458175\H,0,-2.121733,3.991335,0.522382\C,0,0.000024,4.124352,0.627437\H,0,0.000026,5.182487,0.850258\C,0,1.193162,3.444864,0.458179\H,0,2.121781,3.991307,0.522394\C,0,1.222753,2.086171,0.183528\C,0,0.000009,1.379675,0.119525\C,0,2.555985,1.452403,-0.128423\C,0,2.429066,-0.039373,-0.295149\C,0,3.570296,-0.770512,-0.604334\H,0,4.497061,-0.248691,-0.789397\C,0,3.54875,-2.149291,-0.668703\H,0,4.443218,-2.697995,-0.930033\C,0,2.380382,-2.829996,-0.348198\H,0,2.389607,-3.907628,-0.335045\C,0,1.2201,-2.148715,-0.035571\C,0,1.219902,-0.732656,-0.093517\C,0,-0.000015,-2.865203,0.486904\C,0,-3.554809,1.722421,1.025448\H,0,-3.187773,1.29897,1.960256\H,0,-4.523468,1.278606,0.805336\H,0,-3.705636,2.790456,1.167379\C,0,-3.088896,2.083246,-1.440785\H,0,-3.200914,3.16004,-1.327422\H,0,-4.061426,1.669399,-1.700738\H,0,-2.402919,1.894429,-2.266552\C,0,3.088911,2.083213,-1.440785\H,0,2.402938,1.894388,-2.266554\H,0,4.061445,1.669371,-1.700733\H,0,3.200925,3.160009,-1.327429\C,0,3.554827,1.722391,1.025447\H,0,3.705669,2.790424,1.167369\H,0,4.523481,1.278563,0.805338\H,0,3.187788,1.298953,1.960258\C,0,-0.000014,-2.70928,2.038452\H,0,0.886891,-3.185802,2.455967\H,0,-0.886933,-3.185778,2.455966\H,0,-0.000001,-1.661306,2.33736\C,0,-0.000022,-4.361711,0.16646\H,0,-0.000012,-4.550347,-0.907263\H,0,-0.869221,-4.845907,0.606191\H,0,0.869162,-4.845918,0.606209\Version=ES64L-G09RevD.01\State=2-A\HF=-1100.1004381\S2=0.76777\S2-1=0.\S2A=0.750306\RMSD=7.297e-09\Dipole=0.0000071,0.0452196,0.0112434\Quadrupole=12.035803,12.0164509,-24.0522539,0.0000061,-0.0000018,0.7998574\PG=C01 [X(C27H27N1)]\@

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4_red1

55

N	0.000000	0.042993	0.105409
C	1.206985	0.741931	-0.081166
C	1.219226	2.143564	-0.003606
C	2.370780	2.848678	-0.362272
H	2.380449	3.926823	-0.318707
C	3.523512	2.166136	-0.766463
H	4.407324	2.715431	-1.069025
C	3.535039	0.789540	-0.734221
H	4.445509	0.266057	-0.998638
C	2.404200	0.041308	-0.362241
C	2.546648	-1.451266	-0.156508
C	1.221656	-2.090095	0.221568
C	1.193627	-3.436884	0.532765
H	2.129996	-3.978940	0.586276
C	0.000020	-4.132039	0.740816
H	0.000025	-5.181899	1.002103

C	-1.193593	-3.436895	0.532769
H	-2.129958	-3.978958	0.586287
C	-1.221634	-2.090106	0.221571
C	0.000007	-1.362284	0.149066
C	-2.546634	-1.451290	-0.156501
C	-2.404198	0.041283	-0.362249
C	-3.535042	0.789503	-0.734237
H	-4.445507	0.266010	-0.998654
C	-3.523529	2.166099	-0.766483
H	-4.407343	2.715385	-1.069054
C	-2.370805	2.848653	-0.362286
H	-2.380486	3.926798	-0.318720
C	-1.219248	2.143551	-0.003613
C	-1.206990	0.741919	-0.081171
C	-0.000016	2.835196	0.575011
C	3.589601	-1.689757	0.962071
H	3.235451	-1.257181	1.898554
H	4.539958	-1.217331	0.707079
H	3.772913	-2.753757	1.122671
C	3.044761	-2.118791	-1.460876
H	3.221068	-3.185456	-1.313560
H	3.975884	-1.662858	-1.805735
H	2.296476	-1.999321	-2.245160
C	-3.044754	-2.118833	-1.460855
H	-2.296478	-1.999366	-2.245149
H	-3.975885	-1.662915	-1.805711
H	-3.221050	-3.185499	-1.313527
C	-3.589574	-1.689776	0.962092
H	-3.772878	-2.753775	1.122705
H	-4.539937	-1.217357	0.707105
H	-3.235416	-1.257188	1.898566
C	-0.000019	2.631775	2.114641
H	-0.889840	3.088806	2.554503
H	0.889794	3.088814	2.554508
H	-0.000015	1.571162	2.362096
C	-0.000023	4.345109	0.319067
H	-0.000020	4.575727	-0.746941
H	0.876711	4.806241	0.774066
H	-0.876766	4.806231	0.774059

1\1\GINC-XE30TH41\SP\UB3LYP\6-311+G(d,p)\C27H27N1(1-,2)\DRAL\08-Sep-2016\0\#\#P B3LYP/6-311+G(d,p) EmpiricalDispersion=GD3BJ Name=Dral Pop=(Full,NBO) GFINPUT GFPRINT Density=Current SCF=(Tight,NoVarAcc) SCFCyc=500 Int=UltraFine\4(-)\-1,2\N,0,0.,-0.042993,0.105409\C,0,-1.206985,-0.741931,-0.081166\C,0,-1.219226,-2.143564,-0.003606\C,0,-2.37078,-2.848678,-0.362272\H,0,-2.380449,-3.926823,-0.318707\C,0,-3.523512,-2.166136,-0.766463\H,0,-4.407324,-2.715431,-1.069025\C,0,-3.535039,-0.78954,-0.734221\H,0,-4.445509,-0.266057,-0.998638\C,0,-2.4042,-0.041308,-0.362241\C,0,-2.546648,1.451266,-0.156508\C,0,-1.221656,2.090095,0.221568\C,0,-1.193627,3.436884,0.532765\H,0,-2.129996,3.97894,0.586276\C,0,-0.00002,4.132039,0.740816\H,0,-0.000025,5.181899,1.002103\C,0,1.193593,3.436895,0.532769\H,0,2.129958,3.978958,0.586287\C,0,1.221634,2.090106,0.221571\C,0,-0.000007,1.362284,0.149066\C,0,2.546634,1.45129,-0.156501\C,0,2.404198,-0.041283,-0.362249\C,0,3.535042,-0.789503,-0.734237\H,0,4.445507,-0.26601,-0.998654\C,0,3.523529,-2.166099,-0.766483\H,0,4.407343,-2.715385,-1.069054\C,0,2.370805,-2.848653,-0.362286\H,0,2.380486,-3.926798,-0.31872\C,0,1.219248,-2.143551,-0.003613\C,0,1.20699,-0.741919,-0.081171\C,0,0.000016,-2.835196,0.575011\C,0,-3.589601,1.689757,0.962071\H,0,-3.235451,1.257181,1.898554\H,0,-4.539958,1.217331,0.

707079\H,0,-3.772913,2.753757,1.122671\C,0,-3.044761,2.118791,-1.46087
6\H,0,-3.221068,3.185456,-1.31356\H,0,-3.975884,1.662858,-1.805735\H,0
, -2.296476,1.999321,-2.24516\C,0,3.044754,2.118833,-1.460855\H,0,2.296
478,1.999366,-2.245149\H,0,3.975885,1.662915,-1.805711\H,0,3.22105,3.1
85499,-1.313527\C,0,3.589574,1.689776,0.962092\H,0,3.772878,2.753775,1
.122705\H,0,4.539937,1.217357,0.707105\H,0,3.235416,1.257188,1.898566\
C,0,0.000019,-2.631775,2.114641\H,0,0.88984,-3.088806,2.554503\H,0,-0.
889794,-3.088814,2.554508\H,0,0.000015,-1.571162,2.362096\C,0,0.000023
, -4.345109,0.319067\H,0,0.00002,-4.575727,-0.746941\H,0,-0.876711,-4.8
06241,0.774066\H,0,0.876766,-4.806231,0.774059\\Version=ES64L-G09RevD.
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572e-09\Dipole=-0.0000128,-0.1572138,0.2209569\Quadrupole=-3.8577177,-
5.2337444,9.091462,0.0000339,0.0000691,-3.3736572\PG=C01 [X(C27H27N1)]
\\@