SUPPORTING INFORMATION

Graphene Oxide-Arginine Composites: Efficient Dual Function Materials for Integrated CO_2 Capture and Conversion

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General Methods

^{1}H-NMR spectra were recorded on Varian 400 (400 MHz) spectrometer. Chemical shifts are reported in ppm from TMS with the solvent resonance as the internal standard (deuterochloroform: 7.24 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, dd= doublet-doublet, t = triplet, td = triple doublet, dt = double triplet, q = quartet, sext = sextet, sept = septet, p = pseudo, b = broad, m = multiplet), coupling constants (Hz). 13C-NMR spectra were recorded on a Varian 400 (100 MHz) spectrometer with complete proton decoupling. Chemical shifts are reported in ppm from TMS with the solvent as the internal standard (deuterochloroform: 77.0 ppm).

Chromatographic purification was done with 240-400 mesh silica gel. Other anhydrous solvents were supplied by Sigma Aldrich in Sureseal® bottles and used without any further purification. Commercially available chemicals were purchased from Sigma Aldrich, Stream and TCI and used without any further purification.

Anhydrous DMF was purchased from Merck and used as received. All other commercially available starting materials and (non-anhydrous) solvents were purchased from Merck, TCI chemicals, Fluorochem or Alfa Aesar and were used as such without further purification. CO_2 ≥ 99.5% purity, purchased from SIAD, was used in the Arg-GO CO_2 fixation.

Starting materials **1**, is commercially available: it was purchased from Merck and used as received.

The CO_2 adsorption/desorption capability of samples was determined *via* Thermogravimetric Analysis (TGA, STA449 F3 Jupiter Thermo-Microbalance, Netzsch-Gerätebau). The samples, weighed into a Al_2O_3 crucible, were subjected to an initial cleaning cycle at 90°C for 30 min (heating rate: 10 °C min^{-1}) in a high-purity nitrogen atmosphere (99.999%, 250 ml·min^{-1}) before the absorption of CO_2. A 100 minutes-long CO_2 isothermal adsorption cycle under a CO_2/N_2 mixture (1:2 % v/v, 185 ml min^{-1}) was set after cooling sample at 40°C (cooling rate: 1 °C min^{-1}, N_2). Finally, the temperature was increased to 90°C (heating rate: 10 °C min^{-1}) in pure N_2 for the final desorption step. In addition to the single-cycle measurements (*i.e.,* absorption/desorption), five-cycles processes were also carried out to determine the cyclability of the samples. By measuring the mass change during the TGA analysis, CO_2 uptake values were calculated and expressed as $mg_{CO2}/g_{adsorbent}$.

Synthesis and purification of the materials

Initially, 100 mg of graphene oxide (Abalonyx (S-126/36)) is uniformly dispersed in 80 mL of distilled water through sonication for 2 hours to obtain an aqueous suspension of GO (5 mg/mL). Subsequently, a variable ratio of L-arginine (100, 300, or 500 mg) and 420 mg of NaOH is dissolved in 20 mL (21 mg/mL for NaOH) of distilled water. The two dispersions are mixed together, and the solution is refluxed at 80°C for 24 hours. When the reaction is complete, the crude mixture is purified by centrifugation (9000 RPM), 15 minutes each time, with tap water until the supernatant solution reaches a neutral pH. The product is washed with a total of 2 L/g of H_2O. Finally, the purified product is lyophilized.

Table S1: Name of the different materials prepared.

GO/Arg ratio	Sample
1:1	**GO-Arg 1:1**
1:3	**GO-Arg 1:3**
1:5	**GO-Arg 1:5**

XPS-analyses

X-Ray Photoelectron spectroscopy (XPS): High-resolution XPS by using a Phoibos 100 hemispherical energy analyser (Specs GmbH, Berlin, Germany), using Mg Kα radiation (ħω = 1253.6 eV; X-Ray power = 125W) in constant analyser energy (CAE) mode, with analyser pass energies of 10 eV. Base pressure in the analysis chamber during analysis was $4.2x10^{-8}$ mbar. Spectra were fitted by using CasaXPS (www.casaxps.com) after Tougaard background subtraction and all spectra were calibrated to the C 1s binding energy (285.0 eV). XPS samples were prepared as a thin film after the material was filtered on a nylon membrane. After the deposition the membrane was dried, cut and fixated on the sample holder by conductive carbon tape.

The materials **GO-Arg 1:1**, **GO-Arg 1:3** and **GO-Arg 1:5** presents a significantly higher amount of N respect to the pristine GO. The overall oxidation (O 1s / C 1s) was lower than GO due to the presence of aliphatic chains of arginine. The presence of Ca 2p (347.5 eV) in the samples can be ascribed to the presence of Ca ions in the washing water used during purification. The parameters used for the fitting of C 1s and N 1s signal are reported in more details in our previous work.

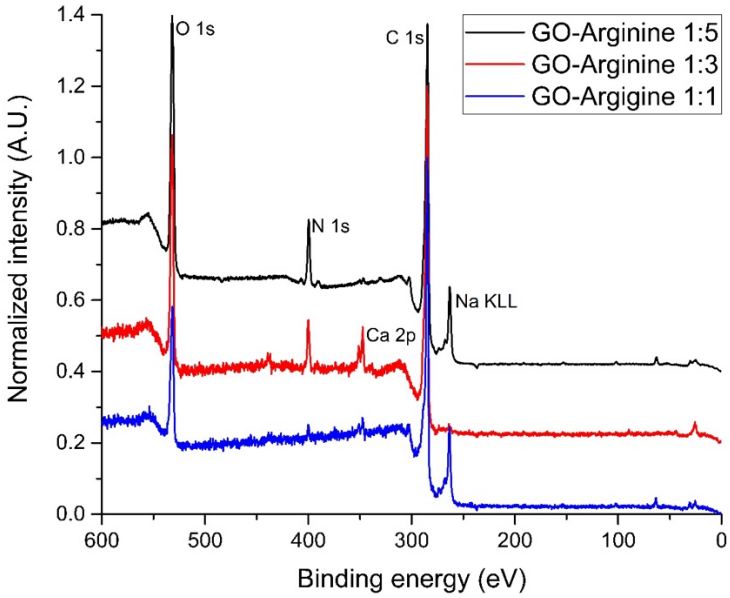


Figure S1: Survey spectra of **GO-Arg 1:1** (blue line), **GO-Arg 1:3** (red line) and **GO-Arg 1:5** (black line).

Table S2: XPS Atomic composition.

Sample	*C%*	*O%*	*N%*	*Na %*	*Ca %*	*Loading %*
GO-Arg (1:1)	84.3	14.4	1.6	< 1	< 1	5
GO-Arg (1:3)	73.7	19.6	4.5	< 1	< 1	14
GO-Arg (1:5)	73.1	21.1	5.9	< 1	1.5	18

The following X-ray photoelectron spectroscopy (XPS) measurements were performed with a Thermo Scientific ESCALAB QXi spectrometer employing a monochromatic Al Kα X-ray source (1486.6 eV) operating at 15 kV and 200 W, a concentric hemispherical analyser, and a spot size of 400 µm × 200 µm. The pressure

in the analysis chamber was better than 10^{-7} mbar. Few mg of sample powder were mounted with a double adhesive conductive carbon tape on a sample holder grounded to the instrument. Charge compensation was applied by beams of combined low energy ion (Ar^+) and electron beams. Survey scans were measured in a binding energy range of 0–1350 eV with a constant pass energy of 100 eV, at 1.0 eV/step, with a dwell time of 50 ms, accumulating 3 scans. High-resolution spectra were recorded using a constant pass energy (3 eV for C 1s and 10 eV for O1s and N1s), at 0.05 eV/step, with a dwell time of 100 ms, accumulating 5 scans for each element. The high-resolution XPS spectra were used for assessment of the elemental state as well as for quantification using the sensitivity factors provided by the manufacturer by means of the Avantage software and after background correction with the smart-background function implemented in the same software.

Peak fittings were performed in the framework of the Avantage software after background correction with the smart-background function implemented in the same software using pseudo-Voigt functions for the synthetic peaks. In the C 1s photoemission peak generated from graphene oxide, the asymmetric tail of the sp^2 carbon forms a pseudo-background that superimposes to the signal from carbon species bound to oxygen and nitrogen (laying in the range 285-290 eV). Hence, a meaningful fit must consider in a complementary way the C 1s, O 1s and N 1s peaks by comparing the atomic percentages of the C bound to O and C bound to N moieties present in the three peaks. The asymmetric tail of the sp^2 carbon have been modelled in order to have a maximum mismatch of 1% at. among the total carbon bound to oxygen and nitrogen from C 1s and the sum of oxygen bound to carbon from O 1s and the nitrogen bound to carbon from N 1s. Full details of peak fitting are given in their relative table.

Table S3: fitting parameters for C 1s of sample GO-Arg.

Ref.	Name	Peak BE (eV)	Area	FWHM (eV)	L/G Mix (%) Product	Tail Mix (%)	Tail Height (%)	Tail Exponent
I	C1s Defects	283.9	100.45	1.1	30	100	0	0
		283.50 : 283.90		K*1	K*1	fixed	fixed	fixed
J	C1s graphite	284.5	2457.22	0.97	30	45	0	0.09
		284.20 : 284.60		0.7 : 1.1	fixed	fixed	fixed	fixed
K	C1s C-C	285.1	221.22	1.1	30	100	0	0
		284.70 : 285.30		0.8 : 1.2	fixed	fixed	fixed	fixed
L	C1s C-O, C-N	286.4	433.71	1.1	30	100	0	0
		286.00 : 286.50		K*1	K*1	fixed	fixed	fixed
M	C1s C-O-C	287.1	257.58	1.1	30	100	0	0
		286.60 : 287.20		K*1	K*1	fixed	fixed	fixed
N	C1s C=O, C=N	288.3	209.81	1.1	30	100	0	0
		287.80 : 288.40		K*1	K*1	fixed	fixed	fixed
O	C1s O-C=O	289.1	95.87	1.1	30	100	0	0
		288.60 : 290.00		K*1	K*1	fixed	fixed	fixed
P	C1s satellite	291.2	24.68	1.91	30	100	0	0
		290.70 : 291.30		1.0 : 2.3	K*1	fixed	fixed	fixed

Table S4: fitting parameters for C 1s of sample for [GO-Arg]/CO_2.

Ref.	Name	Peak BE (eV)	Area	FWHM (eV)	L/G Mix (%) Product	Tail Mix (%)	Tail Height (%)	Tail Exponent
I	C1s Defects	283.8	122.59	1.1	30	100	0	0
		283.50 : 283.90		K*1	K*1	fixed	fixed	fixed
J	C1s graphite	284.5	2156.88	0.99	30	45	0	0.07
		284.20 : 284.60		0.7 : 1.1	fixed	fixed	fixed	fixed
K	C1s C-C	285.0	286.23	1.1	30	100	0	0
		284.70 : 285.20		0.8 : 1.2	fixed	fixed	fixed	fixed
L	C1s C-O, C-N	286.3	599.53	1.1	30	100	0	0
		286.00 : 286.50		K*1	K*1	fixed	fixed	fixed
M	C1s C-O-C	287.1	278.45	1.1	30	100	0	0
		286.60 : 287.20		K*1	K*1	fixed	fixed	fixed
N	C1s C=O, C=N	288.1	217.91	1.1	30	100	0	0
		287.80 : 288.40		K*1	K*1	fixed	fixed	fixed
O	C1s O-C=O, N-COO	288.9	207.89	1.1	30	100	0	0
		288.60 : 290.00		K*1	K*1	fixed	fixed	fixed
P	C1s satellite	291.0	45.41	2.12	30	100	0	0
		290.70 : 291.30		1.0 : 2.3	K*1	fixed	fixed	fixed

Table S5: fitting parameters for O 1s of sample GO-Arg.

Ref.	Name	Peak BE (eV)	Area	FWHM (eV)	L/G Mix (%) Product	Tail Mix (%)	Tail Height (%)	Tail Exponent
I	C=O	532.0	13841.98	1.2	30	100	0	0
				0.8 : 1.2	fixed	fixed	fixed	fixed
J	O=C-O Arg	530.7	4215.05	1.2	30	100	0	0
				I*1	I*1	fixed	fixed	fixed
K	C-O	532.6	10362.74	1.2	30	100	0	0
				I*1	I*1	fixed	fixed	fixed
L	adsorbed H2O	533.9	2063.98	1.2	30	100	0	0
				I*1	I*1	fixed	fixed	fixed

Table S6: fitting parameters for O 1s of sample [GO-Arg]/CO_2.

Ref.	Name	Peak BE (eV)	Area	FWHM (eV)	L/G Mix (%) Product	Tail Mix (%)	Tail Height (%)	Tail Exponent
E	C-O	531.9	8458.98	1.2	30	100	0	0
				0.8 : 1.2	fixed	fixed	fixed	fixed
F	O=C-O Arg, N-COO	530.8	4834.3	1.2	30	100	0	0
				E*1	E*1	fixed	fixed	fixed
G	C=O	532.9	5679.17	1.2	30	100	0	0
				E*1	E*1	fixed	fixed	fixed
H	adsorbed H2O	534.0	1364.86	1.2	30	100	0	0
				E*1	E*1	fixed	fixed	fixed

Table S7: fitting parameters for N 1s of sample GO-Arg.

Ref.	Name	Peak BE (eV)	Area	FWHM (eV)	L/G Mix (%) Product	Tail Mix (%)	Tail Height (%)	Tail Exponent
I	C-NH2	399.3	913.95	1.3	30	100	0	0
				0.7 : 1.3	fixed	fixed	fixed	fixed
J	N in GO	401.5	341.14	1.3	30	100	0	0
				I*1	fixed	fixed	fixed	fixed
K	guanidinium	400.2	2741.84	1.3	30	100	0	0
				I*1	fixed	fixed	fixed	fixed

Table S8: fitting parameters for N 1s of sample [GO-Arg]/CO_2.

Ref.	Name	Peak BE (eV)	Area	FWHM (eV)	L/G Mix (%) Product	Tail Mix (%)	Tail Height (%)	Tail Exponent
I	C-NH2	399.4	1015.07	1.25	30	100	0	0
				0.7 : 1.25	fixed	fixed	fixed	fixed
J	N in GO	401.5	362.03	1.25	30	100	0	0
				I*1	fixed	fixed	fixed	fixed
K	guanidinium, N-COO	400.4	3045.22	1.25	30	100	0	0
				I*1	fixed	fixed	fixed	fixed

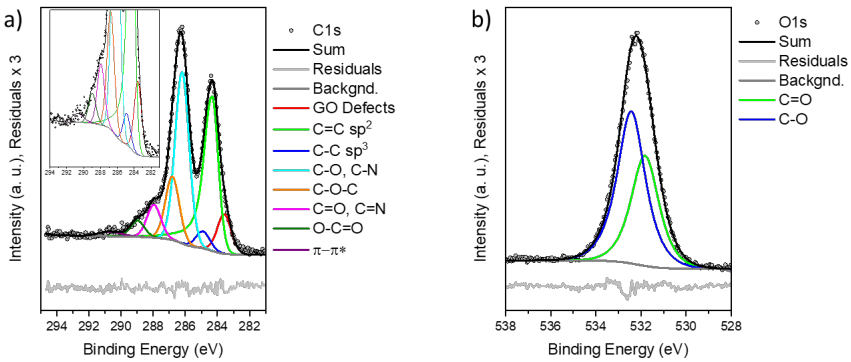


Figure S2: C 1s (a) and O1s (b) photoemission peaks and their fitting for pristine GO.

Table S9: BE and atomic percentage of the fitted C 1s, O 1s and N 1s photoemission peaks for pristine GO.

	BE (eV)	at. %
C1s		
defects	283.7	4.8
C=C	284.5	22.4
C-C	285.1	2.1
C-O, C-N	286.4	20.8
C-O-C	287.0	7.7
C=O, C=N	288.1	4.0
O-C=O	289.1	2.0
π-π*	290.9	0.9
O1s		
C-O	532.0	20.5
C=O, C-O-C	532.6	14.3
N1s		
N in GO	401.5	0.5

Table S10: fitting parameters for C 1s of pristine GO

Ref.	Name	Peak BE (eV)	Area	FWHM (eV)	L/G Mix (%) Product	Tail Mix (%)	Tail Height (%)	Tail Exponent
I	C1s Defects	283.73	389.68	1.06	30	100	0	0
		283.50 : 283.90		P*1	P*1	fixed	fixed	fixed
J	C1s graphite	284.48	1813.81	0.93	30	40	0	0.0532
		284.2 : 284.6		0.7 : 1.1	fixed	fixed	fixed	fixed
K	C1s C-C	285.05	166.09	1.06	30	100	0	0
		284.70 : 285.20			fixed	fixed	fixed	fixed
L	C1s C-O, C-N	286.35	1688.53	1.06	30	100	0	0
		286.00 : 286.50		P*1	P*1	fixed	fixed	fixed
M	C1s C-O-C	286.95	625.79	1.06	30	100	0	0
		286.60 : 287.20		P*1	P*1	fixed	fixed	fixed
N	C1s C=O, C=N	288.1	323.43	1.06	30	100	0	0
		287.80 : 288.40		P*1	P*1	fixed	fixed	fixed
O	C1s O-C=O	289.12	158.42	1.06	30	100	0	0
		288.60 : 290.00		P*1	P*1	fixed	fixed	fixed
P	C1s satellite	290.85	73.59	1.7	30	100	0	0
		290.70 : 291.30		1.7 : 2.3	P*1	fixed	fixed	fixed

Table S11: fitting parameters for O 1s of pristine GO

Ref.	Name	Peak BE (eV)	Area	FWHM (eV)	L/G Mix (%) Product	Tail Mix (%)	Tail Height (%)	Tail Exponent
C	C=O	531.97	22414.21	1.5	60	100	0	0
				01:01.5		fixed	fixed	fixed
D	C-O	532.58	30966.77	1.5	60	100	0	0
				C*1	C*1	fixed	fixed	fixed

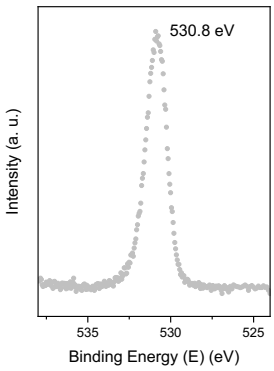
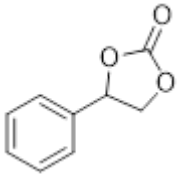


Figure S3: O1s photoemission peaks for pure arginine.

CO_2 fixation experiments

General procedure of CO_2 fixation

In a vacuum-dried and nitrogen-filled Schlenk flask, 40 mg of one of the materials is added. The nitrogen flow is switched to a CO_2 flow, by performing 3 cycles of vacuum-CO_2, and the dry material is allowed to stir in a CO_2 atmosphere for 2 hours at 100°C. Then, the Schlenk flask is simply opened and left under nitrogen at room temperature before adding the reagents for carbocatalysis: 1 mL of anhydrous DMF, 12.5 µL of compound 1 (0.01 mmol), and 37 mg of TBAI (0.01 mmol). The reaction is carried out at 100°C. After 48 hours, the reaction mixture is filtered through cotton with celite, washed with ethyl acetate, and dried. Any remaining DMF is removed using a high-vacuum pump. An NMR analysis is performed on the crude mixture, and the yield of the reaction is calculated using an internal standard (6 µL of mesitylene). Product **2** was purified by flash column chromatography (FC) on silica gel (*n*Hex/EtOAc mixtures=2:1).



2. White solid. FC eluent: nHex/EtOAc: 2:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.49 – 7.39 (m, 3H), 7.38 – 7.33 (m, 2H), 5.68 (t, *J* = 8.0 Hz, 1H), 4.80 (t, *J* = 8.4 Hz, 1H), 4.34 (dd, *J* = 8.6, 7.8 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.9, 136.9, 135.9, 129.8, 129.3, 125.9, 78.1, 71.3.

General procedure for recovery of the GO-Arg

Recycling experiments were conducted similarly to the previously mentioned reactions. After the completion of each reaction cycle, the mixture was centrifuged several times with EtOAc, to separate the product, the DMF and TBAI from the material. Then, the material was washed one final time with DI water and freeze dried, after which it was ready to be re-utilized.

General procedure for atmospheric CO_2 adsorption experiment

40 mg of **GO-Arg 1:3** was left exposed to the air overnight. The next morning the material was transferred in to a Schlenk flask. The atmosphere inside the vessel was changed with nitrogen and the reagents for carbocatalysis were added (1 mL of anhydrous DMF, 0.01 mmol of compound **1** and 0.01 mmol of TBAI). The reaction was carried out at 100°C for 48 hours. After that, the reaction mixture is filtered through cotton with celite, washed with ethyl acetate, and dried. Any remaining DMF is removed using a high-vacuum pump. An NMR analysis is performed on the crude mixture, and the yield of the reaction is calculated using an internal standard (6 µL of mesitylene). Product **2** was purified by flash column chromatography (FC) on silica gel (*n*Hex/EtOAc mixtures=2:1).

In parallel, the same amount of the same material was left under vacuum at 50 °C overnight. The next morning the material was transferred in to a Schlenk flask, treated and then used as motioned before.

Thermal analysis

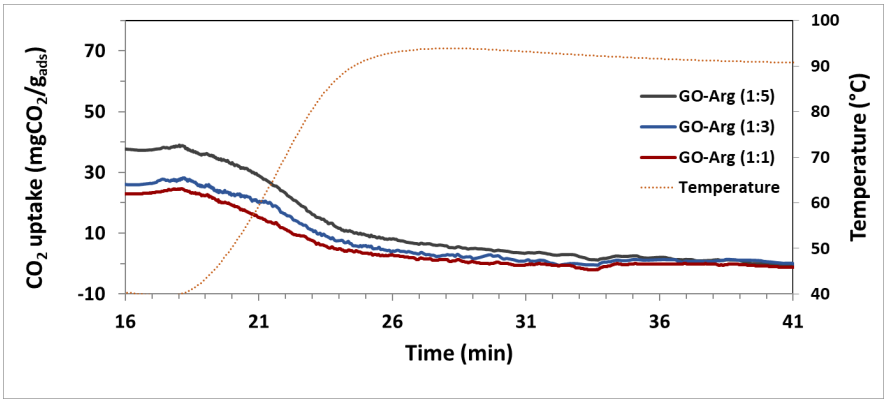
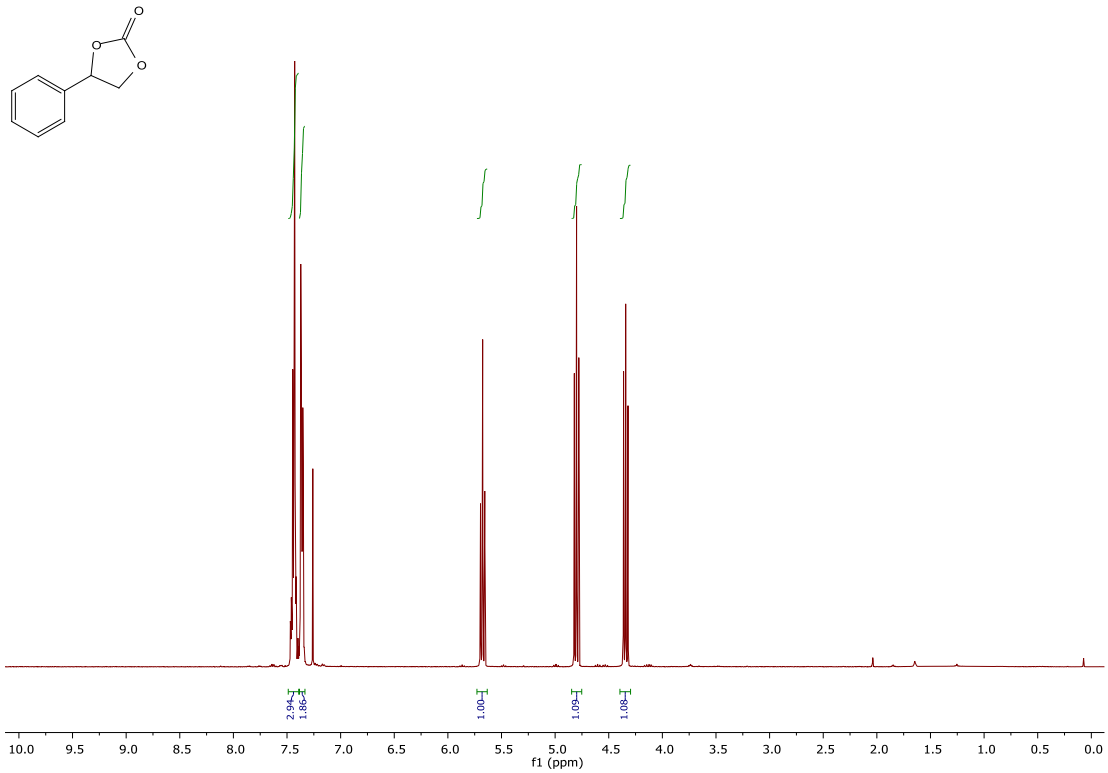


Figure S4. CO_2 desorption curves of the Arg-functionalized GO samples with different Arginine amounts after absorption test in static CO_2 for 2 hours (method b) Supporting Information).

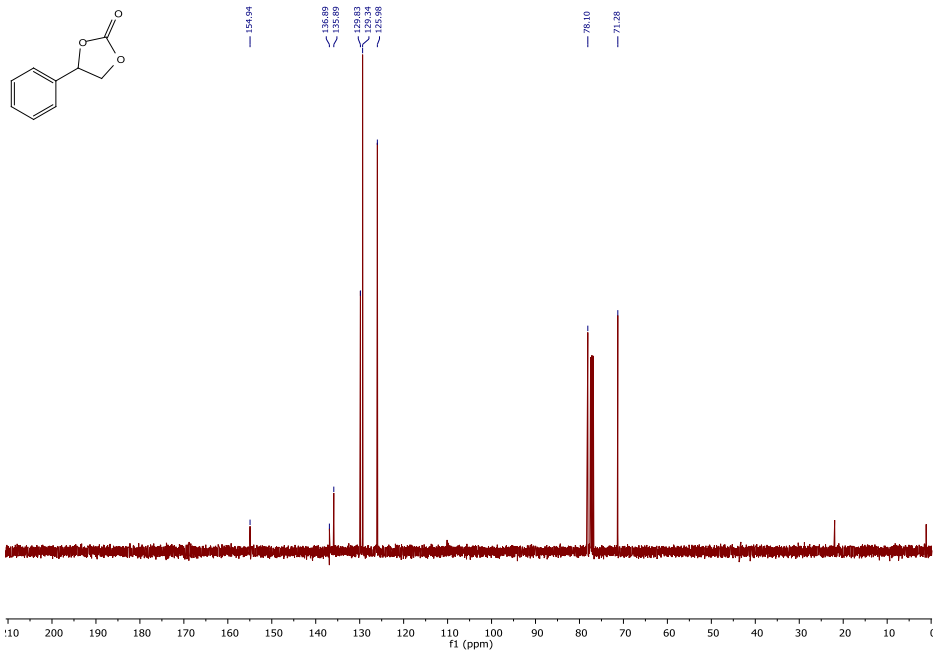
^{1}H and ^{13}C NMR spectra

Compound 2

^{1}H NMR (400 MHz, $CDCl_3$)

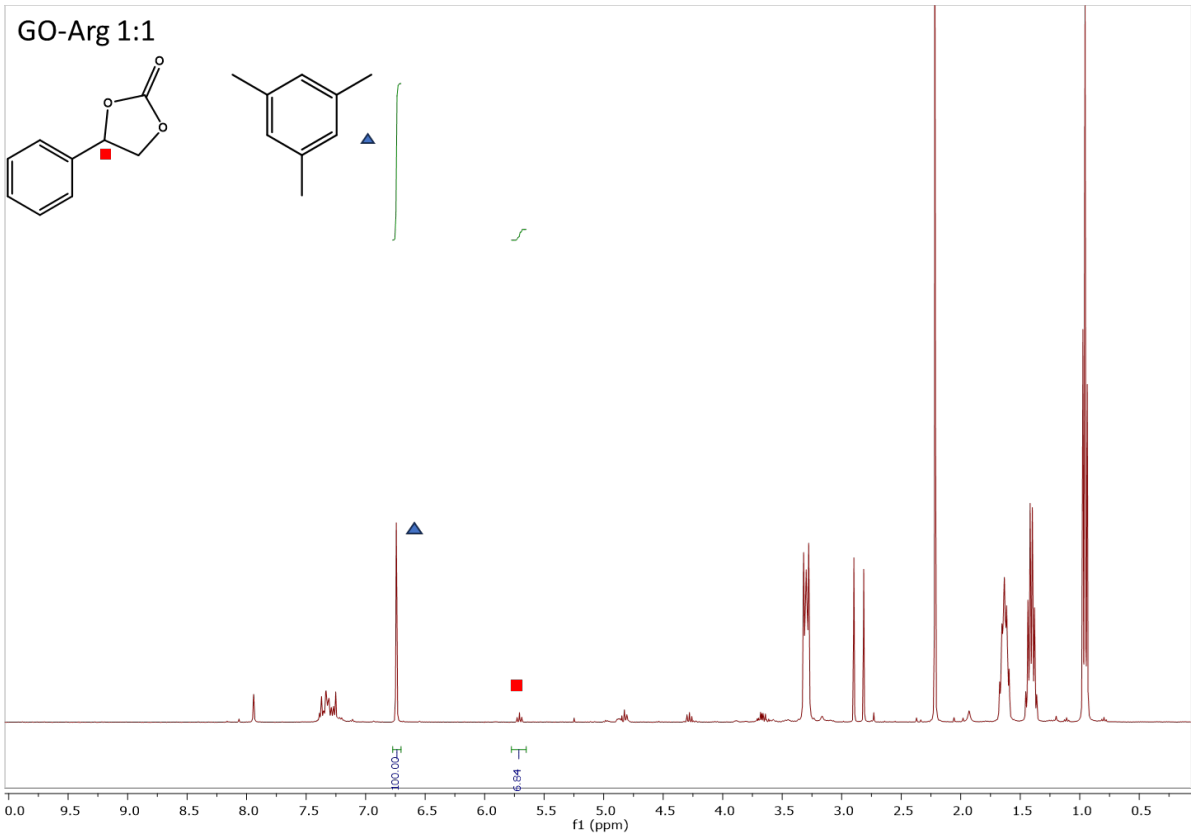


^{13}C NMR (100 MHz, $CDCl_3$)

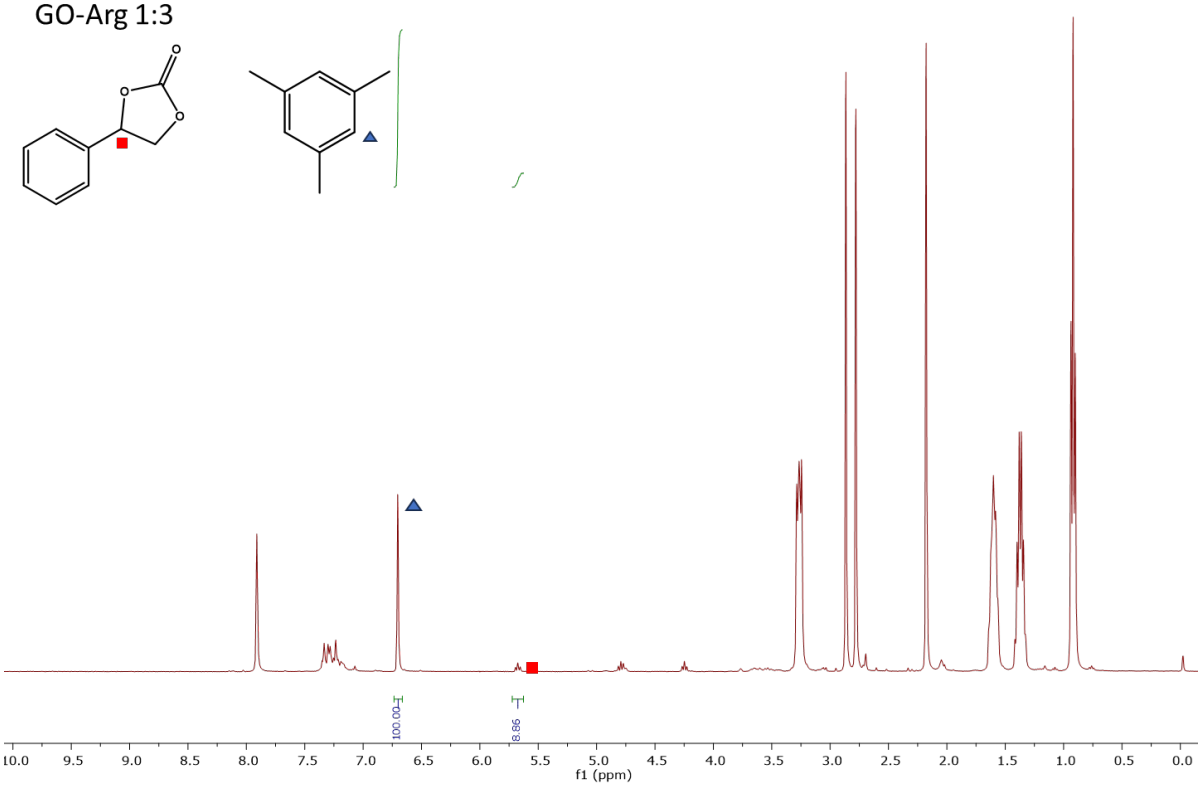

154.94
136.89
135.89
129.83
129.34
125.98
78.10
71.28
f1 (ppm)

^{1}H and ^{13}C NMR spectra

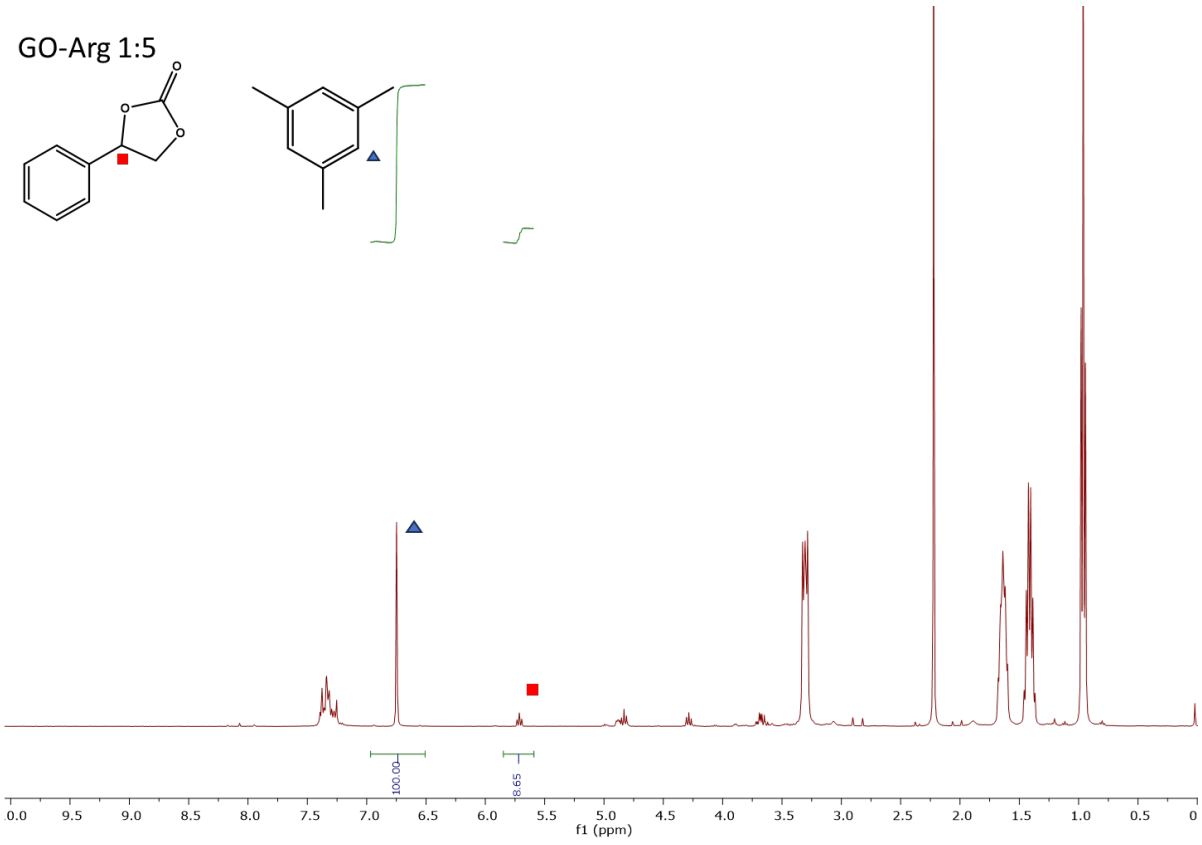
Reaction crudes of the CO_2 fixation reactions. (mesitylene was used as an internal standard)



GO-Arg 1:3



GO-Arg 1:5



Cartesian Coordinates

Rc_{syn}

ONIOM: extrapolated energy = -1602.624161

C	-4.809	-10.646	-0.192
C	-3.426	-10.810	-0.267
C	-2.581	-9.692	-0.270
C	-1.192	-9.859	-0.347
C	-0.342	-8.745	-0.355
C	1.047	-8.918	-0.443
C	1.904	-7.809	-0.466
C	3.293	-7.986	-0.575
C	4.154	-6.878	-0.623
C	5.539	-7.056	-0.748
C	6.400	-5.948	-0.817
C	7.778	-6.141	-0.946
C	8.647	-5.047	-1.031
C	10.022	-5.268	-1.155
C	-5.370	-9.363	-0.123
C	-6.752	-9.205	-0.045
C	-7.318	-7.934	0.018
C	-6.517	-6.764	-0.001
C	-3.136	-8.393	-0.199
C	-4.537	-8.224	-0.127
C	-5.105	-6.925	-0.063
C	-4.255	-5.797	-0.061
C	-0.890	-7.444	-0.278
C	-2.291	-7.267	-0.200
C	-2.845	-5.971	-0.127
C	1.365	-6.506	-0.388
C	-0.035	-6.322	-0.287
C	0.295	-3.907	-0.215
C	1.693	-4.087	-0.347
C	5.877	-4.636	-0.762
C	4.484	-4.457	-0.622
C	4.857	-1.993	-0.671
C	8.140	-3.722	-0.996
C	6.750	-3.516	-0.855
C	6.239	-2.200	-0.815
C	7.103	-1.089	-0.938
C	9.028	-2.614	-1.107
C	8.498	-1.287	-1.109
C	9.307	-0.144	-1.305
C	-7.074	-5.447	0.043
C	-8.466	-5.213	0.053
C	-8.983	-3.980	0.107
C	-8.173	-2.824	0.164
C	-4.812	-4.498	0.007
C	-6.215	-4.317	0.059
C	-6.768	-3.001	0.115
C	-5.920	-1.873	0.114
C	-2.551	-3.565	-0.045
C	-3.962	-3.376	0.018
C	-4.526	-2.069	0.080
C	-3.618	-0.899	0.093

C	-0.269	-2.534	-0.104
C	-1.657	-2.381	-0.012
C	-2.212	-1.109	0.094
C	2.022	-1.603	-0.366
C	0.626	-1.420	-0.155
C	0.116	-0.132	-0.017
C	0.943	0.976	-0.205
C	4.329	-0.693	-0.646
C	2.862	-0.512	-0.480
C	2.329	0.798	-0.423
C	3.176	1.946	-0.558
C	5.181	0.436	-0.754
C	5.475	2.894	-0.798
C	8.805	1.096	-1.272
C	6.873	2.727	-0.926
C	7.690	3.873	-0.920
C	-8.722	-1.503	0.242
C	-10.104	-1.273	0.388
C	-10.632	0.010	0.421
C	-9.814	1.150	0.312
C	-7.865	-0.371	0.189
C	-8.409	0.952	0.206
C	-7.548	2.073	0.117
C	-4.133	0.377	0.064
C	-5.614	0.573	0.078
C	-6.151	1.884	0.046
C	-5.300	3.013	-0.050
C	-3.273	1.540	-0.008
C	-3.828	2.838	-0.101
C	-2.991	3.931	-0.199
C	0.388	2.294	-0.201
C	-1.034	2.474	-0.132
C	-1.585	3.765	-0.238
C	2.641	3.211	-0.516
C	1.222	3.398	-0.370
C	0.649	4.713	-0.411
C	1.547	5.891	-0.517
C	3.525	4.408	-0.614
C	2.956	5.713	-0.602
C	7.175	5.106	-0.862
C	5.785	5.330	-0.796
C	5.195	6.711	-0.780
C	5.991	7.875	-0.871
C	-10.352	2.475	0.315
C	-11.742	2.741	0.419
C	-12.232	4.046	0.416
C	-11.365	5.123	0.306
C	-8.078	3.386	0.107
C	-9.472	3.586	0.205
C	-9.988	4.909	0.199
C	-9.126	6.006	0.087
C	-5.821	4.324	-0.079
C	-7.214	4.508	0.003
C	-3.559	5.297	-0.249
C	-4.959	5.456	-0.179

C	-5.502	6.760	-0.201
C	-4.647	7.876	-0.298
C	-2.701	6.416	-0.344
C	-3.252	7.713	-0.368
C	-2.397	8.825	-0.453
C	0.970	7.184	-0.543
C	-0.440	7.360	-0.487
C	-0.999	8.658	-0.511
C	-0.154	9.773	-0.590
C	1.805	8.313	-0.630
C	1.239	9.610	-0.650
C	2.075	10.731	-0.732
C	4.032	9.295	-0.788
C	3.460	10.575	-0.800
C	-7.745	5.819	-0.011
C	-6.890	6.929	-0.116
C	-6.465	-0.558	0.128
C	4.922	4.211	-0.735
C	6.571	0.232	-0.903
C	7.438	1.339	-1.030
C	3.622	-5.575	-0.553
C	2.226	-5.389	-0.426
C	3.950	-3.163	-0.564
C	2.566	-2.977	-0.420
C	4.643	1.755	-0.723
C	-1.315	0.058	0.404
C	-1.891	1.381	0.008
O	-1.255	0.053	1.856
C	10.416	-2.884	-1.207
C	-0.709	4.887	-0.354
C	-1.297	6.246	-0.405
C	10.897	-4.193	-1.234
C	3.208	8.151	-0.700
C	3.788	6.854	-0.692
C	5.416	9.144	-0.870
C	-1.989	-4.850	-0.123
C	-0.578	-5.022	-0.203
H	-5.442	-11.526	-0.189
H	-3.016	-11.811	-0.322
H	-0.771	-10.857	-0.405
H	1.463	-9.919	-0.504
H	3.705	-8.989	-0.634
H	5.948	-8.059	-0.799
H	8.176	-7.150	-0.985
H	10.421	-6.275	-1.185
H	-7.403	-10.072	-0.031
H	-8.391	-7.911	0.091
H	10.362	-0.217	-1.507
H	-9.184	-6.014	-0.001
H	-10.058	-3.929	0.080
H	9.498	1.902	-1.451
H	8.765	3.801	-0.952
H	-10.820	-2.069	0.504
H	-11.700	0.065	0.538
H	7.882	5.919	-0.865

H	7.064	7.838	-0.953
H	-12.486	1.968	0.503
H	-13.298	4.221	0.500
H	-11.772	6.128	0.305
H	-9.532	7.012	0.081
H	-5.070	8.875	-0.313
H	-2.819	9.824	-0.470
H	-0.580	10.770	-0.607
H	1.658	11.731	-0.746
H	4.086	11.458	-0.867
H	-7.308	7.931	-0.127
H	11.163	-2.111	-1.255
H	11.962	-4.374	-1.319
H	6.060	10.013	-0.942
N	9.626	-1.122	2.397
H	10.314	-0.929	1.698
H	9.159	-1.979	2.178
C	8.651	-0.032	2.436
H	8.466	0.428	1.464
C	7.317	-0.552	2.990
C	9.182	1.095	3.331
H	6.982	-1.361	2.324
H	7.492	-1.000	3.977
C	6.220	0.508	3.074
O	8.776	2.227	3.251
H	6.517	1.310	3.758
H	6.080	0.982	2.096
C	4.887	-0.088	3.523
H	4.553	-0.831	2.790
H	5.008	-0.604	4.484
N	3.853	0.925	3.607
H	4.068	1.778	4.107
C	2.666	0.882	2.910
N	2.058	-0.167	2.483
N	2.116	2.138	2.695
H	2.475	-1.012	2.869
H	2.773	2.859	2.423
O	10.094	0.712	4.224
H	-2.159	0.195	2.187
H	1.276	2.159	2.124
H	10.071	-1.203	3.289

TS_{syn}

ONIOM: extrapolated energy = -1602.604052

C	-6.598	-9.732	-0.055
C	-5.270	-10.151	-0.126
C	-4.232	-9.209	-0.146
C	-2.900	-9.632	-0.223
C	-1.859	-8.696	-0.246
C	-0.529	-9.129	-0.337
C	0.519	-8.201	-0.375
C	1.846	-8.641	-0.486
C	2.900	-7.718	-0.543
C	4.224	-8.161	-0.663
C	5.280	-7.241	-0.731

C	6.598	-7.693	-0.846
C	7.659	-6.782	-0.917
C	8.969	-7.257	-1.030
C	-6.908	-8.366	-0.006
C	-8.236	-7.954	0.067
C	-8.555	-6.599	0.108
C	-7.548	-5.601	0.067
C	-4.533	-7.828	-0.090
C	-5.877	-7.403	-0.025
C	-6.190	-6.021	0.021
C	-5.144	-5.070	0.019
C	-2.151	-7.313	-0.180
C	-3.492	-6.878	-0.103
C	-3.792	-5.500	-0.040
C	0.237	-6.819	-0.303
C	-1.101	-6.372	-0.197
C	-0.315	-4.060	-0.110
C	1.020	-4.508	-0.259
C	5.016	-5.854	-0.683
C	3.687	-5.402	-0.553
C	4.482	-3.086	-0.590
C	7.410	-5.386	-0.877
C	6.081	-4.923	-0.761
C	5.813	-3.538	-0.724
C	6.874	-2.607	-0.812
C	8.490	-4.464	-0.953
C	8.217	-3.061	-0.914
C	9.242	-2.089	-0.965
C	-7.850	-4.206	0.078
C	-9.174	-3.720	0.031
C	-9.454	-2.414	0.055
C	-8.444	-1.430	0.136
C	-5.449	-3.692	0.079
C	-6.795	-3.257	0.107
C	-7.096	-1.864	0.141
C	-6.051	-0.916	0.159
C	-3.052	-3.181	0.036
C	-4.404	-2.745	0.098
C	-4.715	-1.364	0.162
C	-3.612	-0.382	0.167
C	-0.601	-2.609	0.035
C	-1.954	-2.185	0.093
C	-2.262	-0.854	0.203
C	1.814	-2.144	-0.195
C	0.475	-1.712	0.051
C	0.262	-0.337	0.282
C	1.238	0.611	-0.098
C	4.219	-1.702	-0.551
C	2.828	-1.237	-0.328
C	2.551	0.163	-0.321
C	3.588	1.117	-0.500
C	5.269	-0.750	-0.662
C	6.018	1.613	-0.781
C	8.978	-0.779	-0.957
C	7.355	1.186	-0.929

C	8.355	2.160	-1.117
C	-8.740	-0.032	0.171
C	-10.060	0.452	0.254
C	-10.342	1.809	0.220
C	-9.322	2.772	0.104
C	-7.685	0.917	0.130
C	-7.975	2.315	0.080
C	-6.916	3.250	-0.006
C	-3.880	0.955	0.117
C	-5.291	1.419	0.094
C	-5.577	2.803	-0.010
C	-4.529	3.745	-0.127
C	-2.813	1.937	0.044
C	-3.114	3.304	-0.128
C	-2.089	4.221	-0.253
C	0.922	1.988	-0.168
C	-0.443	2.428	-0.087
C	-0.742	3.794	-0.266
C	3.294	2.462	-0.524
C	1.944	2.914	-0.399
C	1.625	4.305	-0.500
C	2.726	5.278	-0.685
C	4.384	3.458	-0.692
C	4.072	4.837	-0.757
C	8.079	3.469	-1.124
C	6.765	3.961	-0.957
C	6.462	5.361	-0.969
C	7.463	6.361	-1.054
C	-9.605	4.170	0.024
C	-10.927	4.689	0.022
C	-11.166	6.060	-0.056
C	-10.108	6.955	-0.140
C	-7.194	4.636	-0.088
C	-8.530	5.093	-0.071
C	-8.791	6.486	-0.152
C	-7.737	7.400	-0.249
C	-4.798	5.130	-0.218
C	-6.135	5.573	-0.192
C	-2.393	5.664	-0.359
C	-3.741	6.081	-0.329
C	-4.032	7.461	-0.412
C	-2.987	8.398	-0.527
C	-1.351	6.601	-0.489
C	-1.647	7.976	-0.571
C	-0.597	8.905	-0.694
C	2.399	6.654	-0.748
C	1.044	7.095	-0.680
C	0.743	8.474	-0.749
C	1.786	9.405	-0.868
C	3.434	7.599	-0.871
C	3.124	8.979	-0.925
C	4.160	9.916	-1.032
C	5.808	8.131	-1.040
C	5.490	9.496	-1.086
C	-6.413	6.957	-0.273

C	-5.366	7.887	-0.379
C	-6.341	0.473	0.135
C	5.718	3.011	-0.803
C	6.598	-1.210	-0.795
C	7.661	-0.285	-0.899
C	2.627	-6.335	-0.481
C	1.294	-5.886	-0.349
C	3.417	-4.022	-0.492
C	2.083	-3.585	-0.328
C	4.991	0.651	-0.633
C	-1.205	0.139	0.621
C	-1.490	1.527	0.120
O	-1.320	0.147	2.065
C	9.802	-4.990	-1.072
C	0.324	4.730	-0.438
C	-0.013	6.169	-0.541
C	10.030	-6.365	-1.107
C	4.782	7.169	-0.934
C	5.106	5.786	-0.888
C	7.138	7.716	-1.091
C	-2.740	-4.553	-0.037
C	-1.386	-4.989	-0.111
H	-7.384	-10.478	-0.040
H	-5.054	-11.212	-0.166
H	-2.674	-10.692	-0.269
H	-0.311	-10.190	-0.389
H	2.059	-9.704	-0.537
H	4.433	-9.225	-0.706
H	6.799	-8.759	-0.880
H	9.173	-8.321	-1.060
H	-9.038	-8.683	0.096
H	-9.604	-6.375	0.189
H	10.284	-2.353	-1.010
H	-10.024	-4.375	-0.056
H	-10.498	-2.165	-0.021
H	9.830	-0.121	-0.988
H	9.386	1.891	-1.276
H	-10.914	-0.193	0.369
H	-11.384	2.066	0.291
H	8.919	4.121	-1.291
H	8.515	6.135	-1.078
H	-11.804	4.069	0.073
H	-12.183	6.431	-0.054
H	-10.321	8.016	-0.202
H	-7.949	8.463	-0.310
H	-3.217	9.456	-0.588
H	-0.824	9.964	-0.750
H	1.558	10.464	-0.913
H	3.941	10.977	-1.070
H	6.273	10.242	-1.165
H	-5.591	8.946	-0.440
H	10.680	-4.372	-1.148
H	11.042	-6.741	-1.198
H	7.937	8.446	-1.158
N	8.972	0.671	2.501

H	9.618	1.187	1.938
H	8.796	-0.217	2.077
C	7.717	1.416	2.611
H	7.470	2.009	1.723
C	6.564	0.440	2.900
C	7.832	2.423	3.764
H	6.511	-0.273	2.064
H	6.819	-0.143	3.795
C	5.208	1.114	3.094
O	7.111	3.385	3.851
H	5.267	1.797	3.949
H	4.948	1.735	2.225
C	4.099	0.094	3.346
H	3.916	-0.518	2.455
H	4.398	-0.584	4.156
N	2.858	0.770	3.697
H	2.922	1.526	4.368
C	1.664	0.646	3.037
N	1.242	-0.414	2.424
N	0.873	1.759	3.108
H	1.785	-1.252	2.618
H	1.305	2.665	2.982
O	8.751	2.122	4.681
H	-2.264	0.302	2.238
H	-0.055	1.640	2.722
H	9.359	0.534	3.413

Pd_{syn}

ONIOM: extrapolated energy = -1602.640164

C	-1.411	-11.276	-0.848
C	-0.046	-11.027	-0.973
C	0.440	-9.714	-0.922
C	1.809	-9.467	-1.057
C	2.299	-8.157	-1.006
C	3.669	-7.919	-1.156
C	4.168	-6.614	-1.114
C	5.539	-6.383	-1.277
C	6.046	-5.080	-1.245
C	7.420	-4.851	-1.403
C	7.932	-3.546	-1.375
C	9.305	-3.325	-1.520
C	9.823	-2.024	-1.498
C	11.200	-1.828	-1.635
C	-2.311	-10.216	-0.676
C	-3.674	-10.470	-0.560
C	-4.576	-9.423	-0.403
C	-4.144	-8.073	-0.359
C	-0.458	-8.636	-0.738
C	-1.840	-8.886	-0.621
C	-2.750	-7.812	-0.457
C	-2.257	-6.486	-0.393
C	1.410	-7.075	-0.805
C	0.028	-7.315	-0.674
C	-0.863	-6.237	-0.489
C	3.285	-5.528	-0.906

C	1.904	-5.755	-0.743
C	1.534	-3.348	-0.435
C	2.905	-3.132	-0.643
C	7.061	-2.450	-1.197
C	5.676	-2.680	-1.029
C	5.330	-0.293	-0.827
C	8.960	-0.909	-1.338
C	7.575	-1.129	-1.185
C	6.702	-0.037	-1.015
C	7.203	1.298	-1.024
C	9.487	0.413	-1.326
C	8.598	1.526	-1.180
C	9.054	2.865	-1.179
C	-5.053	-6.981	-0.226
C	-6.452	-7.166	-0.159
C	-7.304	-6.142	-0.055
C	-6.864	-4.803	0.001
C	-3.155	-5.411	-0.238
C	-4.553	-5.654	-0.167
C	-5.464	-4.568	-0.046
C	-4.974	-3.255	0.026
C	-1.241	-3.849	-0.208
C	-2.656	-4.091	-0.147
C	-3.581	-3.021	0.009
C	-3.056	-1.611	0.177
C	0.641	-2.163	-0.106
C	-0.767	-2.418	0.007
C	-1.630	-1.407	0.252
C	2.538	-0.649	-0.254
C	1.157	-0.918	0.045
C	0.379	0.194	0.722
C	0.800	1.538	0.163
C	4.481	0.770	-0.634
C	3.045	0.609	-0.282
C	2.155	1.758	-0.127
C	2.621	3.096	-0.309
C	4.942	2.204	-0.672
C	4.517	4.724	-0.630
C	8.222	3.907	-1.060
C	5.893	4.936	-0.836
C	6.327	6.268	-0.987
C	-7.773	-3.696	0.085
C	-9.170	-3.867	0.141
C	-10.038	-2.784	0.179
C	-9.572	-1.454	0.166
C	-7.271	-2.369	0.104
C	-8.166	-1.242	0.130
C	-7.659	0.089	0.108
C	-3.924	-0.572	0.199
C	-5.377	-0.879	0.136
C	-6.266	0.311	0.108
C	-5.795	1.720	0.074
C	-3.431	0.804	0.203
C	-4.322	1.900	0.077
C	-3.827	3.182	0.002

C	-0.125	2.585	0.088
C	-1.549	2.341	0.165
C	-2.438	3.419	0.005
C	1.723	4.142	-0.272
C	0.339	3.898	-0.130
C	-0.594	4.976	-0.203
C	-0.129	6.409	-0.366
C	2.201	5.577	-0.439
C	1.275	6.650	-0.464
C	5.475	7.306	-0.937
C	4.080	7.134	-0.741
C	3.159	8.229	-0.717
C	3.582	9.578	-0.815
C	-10.467	-0.338	0.179
C	-11.878	-0.487	0.244
C	-12.726	0.618	0.228
C	-12.207	1.902	0.150
C	-8.549	1.200	0.086
C	-9.943	0.983	0.120
C	-10.824	2.099	0.098
C	-10.321	3.404	0.023
C	-6.673	2.793	0.014
C	-8.054	2.539	0.029
C	-4.784	4.352	-0.091
C	-6.174	4.113	-0.067
C	-7.069	5.198	-0.134
C	-6.570	6.509	-0.233
C	-4.270	5.678	-0.200
C	-5.183	6.755	-0.269
C	-4.699	8.068	-0.372
C	-1.026	7.486	-0.415
C	-2.400	7.247	-0.355
C	-3.318	8.321	-0.414
C	-2.842	9.635	-0.517
C	-0.549	8.805	-0.535
C	-1.464	9.885	-0.575
C	-0.985	11.197	-0.680
C	1.300	10.379	-0.733
C	0.386	11.443	-0.755
C	-8.945	3.635	-0.016
C	-8.451	4.951	-0.100
C	-5.875	-2.172	0.097
C	3.595	5.812	-0.591
C	6.318	2.416	-0.879
C	6.831	3.744	-0.925
C	5.168	-3.991	-1.050
C	3.784	-4.216	-0.872
C	4.801	-1.601	-0.828
C	3.408	-1.830	-0.620
C	4.064	3.420	-0.504
C	-1.180	-0.074	0.811
C	-2.057	1.048	0.308
O	-1.446	-0.167	2.227
C	10.891	0.563	-1.465
C	-1.929	4.744	-0.141

C	-2.861	5.935	-0.242
C	11.727	-0.543	-1.616
C	0.838	9.051	-0.619
C	1.760	7.973	-0.599
C	2.668	10.628	-0.822
C	-0.357	-4.913	-0.400
C	1.023	-4.667	-0.518
H	-1.765	-12.300	-0.890
H	0.631	-11.862	-1.111
H	2.494	-10.295	-1.208
H	4.347	-8.751	-1.314
H	6.213	-7.219	-1.432
H	8.092	-5.690	-1.547
H	9.973	-4.170	-1.650
H	11.871	-2.670	-1.756
H	-4.048	-11.487	-0.593
H	-5.607	-9.718	-0.316
H	10.096	3.116	-1.280
H	-6.908	-8.140	-0.201
H	-8.346	-6.410	-0.025
H	8.676	4.884	-1.065
H	7.362	6.507	-1.167
H	-9.642	-4.833	0.156
H	-11.083	-3.038	0.205
H	5.918	8.276	-1.081
H	4.617	9.865	-0.879
H	-12.369	-1.441	0.317
H	-13.799	0.476	0.278
H	-12.889	2.745	0.136
H	-11.006	4.245	-0.002
H	-7.263	7.341	-0.286
H	-5.398	8.896	-0.422
H	-3.542	10.462	-0.556
H	-1.673	12.035	-0.706
H	0.733	12.466	-0.838
H	-9.144	5.785	-0.142
H	11.385	1.519	-1.460
H	12.796	-0.401	-1.720
H	3.036	11.645	-0.904
N	7.666	-2.867	4.045
H	8.593	-2.746	3.691
H	7.173	-3.522	3.472
C	6.967	-1.583	4.029
H	7.253	-0.929	3.198
C	5.450	-1.814	3.973
C	7.299	-0.811	5.314
H	5.227	-2.402	3.071
H	5.153	-2.430	4.832
C	4.648	-0.514	3.944
O	7.121	0.378	5.412
H	4.836	0.053	4.861
H	4.978	0.118	3.110
C	3.153	-0.780	3.800
H	2.941	-1.279	2.849
H	2.795	-1.422	4.612

N	2.415	0.485	3.835
H	2.628	1.110	4.604
C	1.561	0.954	2.913
N	0.879	0.108	2.145
N	1.315	2.276	2.912
H	0.788	-0.831	2.519
H	2.081	2.915	3.086
O	7.739	-1.564	6.319
H	-2.392	-0.367	2.326
H	0.583	2.628	2.306
H	7.710	-3.211	4.983

Rc_{anti}

ONIOM: extrapolated energy = -1602.647909

C	4.998	10.516	0.203
C	3.623	10.748	0.173
C	2.726	9.674	0.095
C	1.345	9.909	0.063
C	0.444	8.839	-0.020
C	-0.938	9.078	-0.044
C	-1.845	8.012	-0.128
C	-3.227	8.254	-0.136
C	-4.138	7.190	-0.212
C	-5.514	7.439	-0.211
C	-6.431	6.381	-0.285
C	-7.801	6.649	-0.280
C	-8.728	5.606	-0.358
C	-10.095	5.899	-0.344
C	5.498	9.207	0.163
C	6.872	8.980	0.191
C	7.376	7.682	0.161
C	6.518	6.554	0.108
C	3.220	8.349	0.047
C	4.611	8.111	0.087
C	5.116	6.786	0.051
C	4.215	5.702	-0.046
C	0.932	7.514	-0.081
C	2.323	7.268	-0.044
C	2.817	5.945	-0.098
C	-1.365	6.686	-0.201
C	0.027	6.437	-0.180
C	-0.406	4.049	-0.377
C	-1.801	4.292	-0.377
C	-5.974	5.046	-0.364
C	-4.589	4.784	-0.365
C	-5.062	2.367	-0.512
C	-8.287	4.260	-0.450
C	-6.902	3.980	-0.445
C	-6.448	2.642	-0.517
C	-7.379	1.581	-0.612
C	-9.235	3.208	-0.545
C	-8.774	1.863	-0.659
C	-9.661	0.785	-0.850
C	7.010	5.213	0.103
C	8.380	4.914	0.239

C	8.845	3.605	0.221
C	7.972	2.517	0.055
C	4.710	4.377	-0.097
C	6.102	4.126	-0.020
C	6.588	2.780	-0.052
C	5.685	1.705	-0.180
C	2.404	3.555	-0.277
C	3.809	3.301	-0.220
C	4.318	1.974	-0.284
C	3.357	0.847	-0.446
C	0.105	2.656	-0.495
C	1.461	2.429	-0.453
C	1.992	1.117	-0.568
C	-2.255	1.829	-0.555
C	-0.857	1.578	-0.605
C	-0.398	0.284	-0.745
C	-1.291	-0.791	-0.761
C	-4.624	1.014	-0.591
C	-3.154	0.782	-0.627
C	-2.679	-0.549	-0.717
C	-3.584	-1.652	-0.741
C	-5.527	-0.056	-0.663
C	-5.958	-2.461	-0.724
C	-9.205	-0.523	-0.898
C	-7.345	-2.225	-0.701
C	-8.218	-3.314	-0.558
C	8.467	1.096	0.026
C	9.837	0.781	0.073
C	10.297	-0.533	0.102
C	9.419	-1.636	0.081
C	7.543	0.034	-0.059
C	8.031	-1.374	-0.024
C	7.098	-2.426	-0.088
C	3.800	-0.488	-0.427
C	5.255	-0.806	-0.278
C	5.713	-2.148	-0.218
C	4.789	-3.218	-0.283
C	2.890	-1.577	-0.529
C	3.349	-2.925	-0.445
C	2.460	-3.964	-0.492
C	-0.801	-2.130	-0.754
C	0.607	-2.390	-0.715
C	1.068	-3.718	-0.612
C	-3.116	-2.939	-0.723
C	-1.707	-3.190	-0.713
C	-1.218	-4.528	-0.626
C	-2.205	-5.630	-0.568
C	-4.078	-4.072	-0.656
C	-3.592	-5.391	-0.589
C	-7.753	-4.620	-0.510
C	-6.380	-4.925	-0.589
C	-5.895	-6.261	-0.561
C	-6.758	-7.385	-0.561
C	9.878	-2.984	0.154
C	11.248	-3.325	0.293

C	11.657	-4.656	0.364
C	10.724	-5.684	0.305
C	7.550	-3.761	-0.024
C	8.930	-4.042	0.101
C	9.363	-5.391	0.176
C	8.433	-6.434	0.128
C	5.244	-4.551	-0.204
C	6.621	-4.823	-0.075
C	2.959	-5.349	-0.367
C	4.327	-5.616	-0.243
C	4.775	-6.952	-0.147
C	3.850	-8.009	-0.161
C	2.017	-6.423	-0.364
C	2.474	-7.753	-0.260
C	1.549	-8.810	-0.250
C	-1.707	-6.964	-0.481
C	-0.309	-7.232	-0.424
C	0.167	-8.559	-0.327
C	-0.743	-9.621	-0.302
C	-2.606	-8.048	-0.442
C	-2.120	-9.377	-0.360
C	-3.020	-10.449	-0.333
C	-4.886	-8.907	-0.454
C	-4.393	-10.216	-0.383
C	7.068	-6.162	0.006
C	6.144	-7.215	-0.030
C	6.168	0.282	-0.177
C	-5.460	-3.849	-0.665
C	-6.915	0.233	-0.670
C	-7.843	-0.823	-0.751
C	-3.668	5.860	-0.290
C	-2.278	5.612	-0.289
C	-4.125	3.454	-0.444
C	-2.726	3.228	-0.459
C	-5.041	-1.397	-0.731
C	1.055	0.033	-0.980
C	1.520	-1.340	-0.666
O	1.098	0.017	-2.468
C	-10.612	3.547	-0.504
C	0.129	-4.788	-0.575
C	0.618	-6.182	-0.455
C	-11.028	4.873	-0.410
C	-3.995	-7.810	-0.482
C	-4.494	-6.485	-0.544
C	-6.259	-8.681	-0.503
C	1.909	4.870	-0.210
C	0.511	5.116	-0.258
H	5.673	11.362	0.260
H	3.260	11.769	0.207
H	0.970	10.926	0.104
H	-1.309	10.096	0.006
H	-3.594	9.273	-0.080
H	-5.874	8.461	-0.151
H	-8.148	7.675	-0.214
H	-10.443	6.923	-0.273

H 7.565 9.812 0.235
H 8.450 7.603 0.164
H -10.720 0.915 -0.988
H 9.131 5.670 0.389
H 9.906 3.480 0.357
H -9.945 -1.287 -1.074
H -9.282 -3.181 -0.446
H 10.599 1.542 0.082
H 11.366 -0.646 0.137
H -8.511 -5.373 -0.377
H -7.830 -7.304 -0.623
H 12.032 -2.592 0.359
H 12.709 -4.892 0.470
H 11.068 -6.710 0.364
H 8.773 -7.463 0.189
H 4.201 -9.032 -0.084
H 1.905 -9.832 -0.174
H -0.378 -10.640 -0.234
H -2.662 -11.471 -0.273
H -5.071 -11.061 -0.362
H 6.491 -8.241 0.039
H -11.399 2.813 -0.523
H -12.085 5.108 -0.384
H -6.953 -9.514 -0.498
H 1.943 0.384 -2.775
N -6.907 -0.316 2.961
H -6.816 0.460 2.336
H -7.009 0.020 3.897
C -5.720 -1.151 2.873
H -5.728 -1.684 1.921
C -4.389 -0.390 2.993
C -5.812 -2.185 3.977
H -4.356 0.328 2.159
H -4.394 0.194 3.922
C -3.153 -1.284 2.926
O -6.107 -1.928 5.117
H -3.116 -1.962 3.787
H -3.211 -1.901 2.017
C -1.873 -0.469 2.833
H -1.902 0.129 1.906
H -1.764 0.255 3.651
N -0.716 -1.355 2.845
H -0.925 -2.347 2.845
C 0.512 -1.013 2.364
N 0.882 0.153 1.928
N 1.416 -2.065 2.349
H 0.105 0.816 1.980
H 1.333 -2.732 3.107
H 2.370 -1.750 2.220
O -5.474 -3.420 3.563
H -7.712 -0.854 2.710

TS_{anti}

ONIOM: extrapolated energy = -1602.633383

C 5.908 10.064 0.632

C	4.562	10.419	0.550
C	3.580	9.434	0.385
C	2.230	9.793	0.298
C	1.245	8.811	0.132
C	-0.105	9.177	0.048
C	-1.097	8.202	-0.106
C	-2.446	8.573	-0.181
C	-3.446	7.600	-0.311
C	-4.792	7.977	-0.375
C	-5.799	7.007	-0.477
C	-7.139	7.397	-0.533
C	-8.154	6.439	-0.613
C	-9.488	6.854	-0.666
C	6.292	8.717	0.554
C	7.637	8.367	0.627
C	8.025	7.031	0.558
C	7.072	5.989	0.424
C	3.957	8.072	0.304
C	5.317	7.709	0.393
C	5.703	6.346	0.320
C	4.716	5.351	0.141
C	1.615	7.449	0.050
C	2.974	7.078	0.134
C	3.350	5.719	0.047
C	-0.736	6.838	-0.184
C	0.623	6.461	-0.115
C	-0.013	4.121	-0.380
C	-1.380	4.495	-0.413
C	-5.463	5.635	-0.518
C	-4.108	5.249	-0.479
C	-4.785	2.896	-0.613
C	-7.836	5.056	-0.638
C	-6.482	4.655	-0.595
C	-6.146	3.284	-0.627
C	-7.168	2.303	-0.675
C	-8.873	4.087	-0.704
C	-8.533	2.700	-0.716
C	-9.513	1.690	-0.778
C	7.441	4.610	0.380
C	8.769	4.188	0.571
C	9.123	2.852	0.495
C	8.175	1.849	0.213
C	5.090	3.989	0.053
C	6.449	3.613	0.169
C	6.816	2.234	0.087
C	5.821	1.246	-0.110
C	2.742	3.379	-0.243
C	4.100	3.003	-0.145
C	4.467	1.642	-0.235
C	3.430	0.609	-0.457
C	0.373	2.695	-0.538
C	1.706	2.347	-0.476
C	2.096	0.998	-0.618
C	-2.038	2.091	-0.645
C	-0.672	1.710	-0.705

C	-0.332	0.377	-0.878
C	-1.324	-0.612	-0.916
C	-4.454	1.523	-0.669
C	-3.025	1.131	-0.720
C	-2.681	-0.240	-0.829
C	-3.694	-1.253	-0.779
C	-5.463	0.534	-0.690
C	-6.115	-1.828	-0.657
C	-9.175	0.345	-0.763
C	-7.476	-1.459	-0.616
C	-8.430	-2.488	-0.473
C	8.543	0.475	0.095
C	9.889	0.061	0.089
C	10.239	-1.279	0.044
C	9.266	-2.293	-0.005
C	7.540	-0.518	-0.046
C	7.900	-1.902	-0.080
C	6.892	-2.889	-0.183
C	3.765	-0.736	-0.494
C	5.193	-1.131	-0.315
C	5.538	-2.506	-0.303
C	4.536	-3.504	-0.399
C	2.765	-1.755	-0.645
C	3.115	-3.123	-0.535
C	2.136	-4.089	-0.578
C	-0.960	-1.993	-0.903
C	0.424	-2.369	-0.863
C	0.774	-3.724	-0.707
C	-3.338	-2.580	-0.748
C	-1.953	-2.965	-0.790
C	-1.576	-4.346	-0.670
C	-2.634	-5.384	-0.569
C	-4.369	-3.645	-0.625
C	-3.997	-5.008	-0.558
C	-8.075	-3.834	-0.423
C	-6.736	-4.267	-0.507
C	-6.371	-5.648	-0.479
C	-7.330	-6.692	-0.458
C	9.615	-3.679	0.005
C	10.956	-4.134	0.105
C	11.260	-5.495	0.118
C	10.248	-6.442	0.043
C	7.235	-4.263	-0.167
C	8.587	-4.655	-0.070
C	8.913	-6.037	-0.046
C	7.903	-7.003	-0.103
C	4.870	-4.875	-0.342
C	6.222	-5.253	-0.235
C	2.500	-5.519	-0.466
C	3.859	-5.875	-0.373
C	4.208	-7.241	-0.294
C	3.203	-8.225	-0.282
C	1.491	-6.503	-0.432
C	1.846	-7.864	-0.338
C	0.838	-8.843	-0.298

C	-2.252	-6.741	-0.471
C	-0.881	-7.114	-0.433
C	-0.520	-8.478	-0.341
C	-1.520	-9.459	-0.296
C	-3.246	-7.736	-0.409
C	-2.875	-9.099	-0.330
C	-3.870	-10.086	-0.286
C	-5.597	-8.382	-0.380
C	-5.219	-9.730	-0.315
C	6.562	-6.624	-0.189
C	5.558	-7.605	-0.217
C	6.182	-0.133	-0.157
C	-5.730	-3.277	-0.600
C	-6.822	0.919	-0.681
C	-7.835	-0.078	-0.683
C	-3.097	6.233	-0.373
C	-1.737	5.854	-0.323
C	-3.762	3.885	-0.543
C	-2.395	3.521	-0.532
C	-5.120	-0.838	-0.719
C	1.096	0.017	-1.181
C	1.431	-1.402	-0.845
O	1.283	0.094	-2.588
C	-10.213	4.553	-0.751
C	-0.254	-4.710	-0.628
C	0.130	-6.133	-0.484
C	-10.507	5.914	-0.735
C	-4.612	-7.372	-0.426
C	-4.994	-6.006	-0.485
C	-6.946	-8.030	-0.407
C	2.359	4.731	-0.137
C	0.991	5.101	-0.212
H	6.651	10.843	0.756
H	4.288	11.466	0.613
H	1.945	10.838	0.361
H	-0.384	10.224	0.109
H	-2.719	9.622	-0.129
H	-5.058	9.028	-0.338
H	-7.393	8.452	-0.510
H	-9.744	7.907	-0.652
H	8.398	9.132	0.734
H	9.087	6.857	0.594
H	-10.566	1.900	-0.844
H	9.569	4.866	0.814
H	10.158	2.637	0.703
H	-9.999	-0.344	-0.845
H	-9.482	-2.286	-0.360
H	10.714	0.753	0.090
H	11.296	-1.481	0.041
H	-8.895	-4.520	-0.290
H	-8.390	-6.514	-0.498
H	11.801	-3.472	0.184
H	12.291	-5.817	0.192
H	10.510	-7.493	0.059
H	8.164	-8.057	-0.075

H	3.476	-9.273	-0.217
H	1.111	-9.890	-0.229
H	-1.243	-10.506	-0.232
H	-3.604	-11.135	-0.231
H	-5.969	-10.512	-0.284
H	5.828	-8.654	-0.168
H	-11.064	3.897	-0.800
H	-11.538	6.244	-0.774
H	-7.713	-8.796	-0.390
H	0.969	0.960	-2.893
N	-7.334	-0.770	2.938
H	-7.218	-0.118	2.188
H	-7.430	-0.273	3.800
C	-6.172	-1.640	3.008
H	-6.200	-2.346	2.171
C	-4.815	-0.910	3.004
C	-6.285	-2.439	4.293
H	-4.769	-0.316	2.079
H	-4.802	-0.199	3.839
C	-3.602	-1.840	3.073
O	-6.608	-1.963	5.352
H	-3.471	-2.236	4.086
H	-3.765	-2.703	2.409
C	-2.336	-1.116	2.630
H	-2.526	-0.752	1.610
H	-2.143	-0.253	3.278
N	-1.191	-2.008	2.678
H	-1.398	-2.976	2.452
C	0.065	-1.597	2.290
N	0.437	-0.401	1.976
N	0.968	-2.646	2.226
H	-0.354	0.243	1.981
H	0.901	-3.331	2.968
H	1.918	-2.343	2.051
O	-5.935	-3.729	4.139
H	-8.153	-1.320	2.777

Pd_{anti}

ONIOM: extrapolated energy = -1602.703145

C	-1.093	-11.312	-0.491
C	0.270	-11.040	-0.589
C	0.727	-9.716	-0.597
C	2.095	-9.447	-0.691
C	2.559	-8.127	-0.696
C	3.933	-7.871	-0.773
C	4.410	-6.557	-0.770
C	5.789	-6.311	-0.819
C	6.277	-4.998	-0.800
C	7.656	-4.757	-0.823
C	8.150	-3.446	-0.796
C	9.528	-3.219	-0.804
C	10.034	-1.916	-0.775
C	11.419	-1.711	-0.768
C	-2.019	-10.265	-0.398
C	-3.380	-10.543	-0.302

C	-4.308	-9.510	-0.212
C	-3.905	-8.151	-0.211
C	-0.199	-8.649	-0.508
C	-1.578	-8.924	-0.407
C	-2.515	-7.864	-0.315
C	-2.055	-6.526	-0.334
C	1.640	-7.053	-0.618
C	0.257	-7.315	-0.521
C	-0.666	-6.249	-0.436
C	3.500	-5.477	-0.709
C	2.109	-5.723	-0.634
C	1.694	-3.315	-0.604
C	3.080	-3.075	-0.667
C	7.256	-2.352	-0.758
C	5.864	-2.591	-0.739
C	5.461	-0.194	-0.697
C	9.151	-0.805	-0.753
C	7.754	-1.024	-0.743
C	6.851	0.065	-0.717
C	7.327	1.405	-0.722
C	9.674	0.511	-0.736
C	8.719	1.669	-0.744
C	9.169	3.009	-0.790
C	-4.837	-7.074	-0.121
C	-6.229	-7.283	0.018
C	-7.098	-6.267	0.074
C	-6.680	-4.925	-0.005
C	-2.981	-5.465	-0.260
C	-4.367	-5.736	-0.163
C	-5.295	-4.662	-0.105
C	-4.832	-3.335	-0.147
C	-1.138	-3.855	-0.378
C	-2.524	-4.130	-0.291
C	-3.456	-3.069	-0.246
C	-2.987	-1.663	-0.323
C	0.746	-2.180	-0.539
C	-0.669	-2.452	-0.433
C	-1.575	-1.433	-0.447
C	2.628	-0.609	-0.572
C	1.230	-0.907	-0.491
C	0.288	0.209	-0.129
C	0.794	1.587	-0.450
C	4.516	0.934	-0.673
C	3.071	0.679	-0.573
C	2.157	1.822	-0.542
C	2.633	3.167	-0.606
C	5.039	2.292	-0.694
C	4.578	4.745	-0.691
C	8.332	4.055	-0.789
C	5.962	5.023	-0.721
C	6.377	6.372	-0.711
C	-7.658	-3.779	0.033
C	-9.051	-3.976	0.072
C	-9.952	-2.912	0.132
C	-9.528	-1.567	0.153

C	-7.174	-2.458	0.015
C	-8.138	-1.315	0.084
C	-7.649	0.004	0.082
C	-3.863	-0.623	-0.250
C	-5.318	-0.885	-0.108
C	-6.268	0.232	-0.012
C	-5.753	1.601	-0.018
C	-3.395	0.766	-0.265
C	-4.299	1.851	-0.130
C	-3.842	3.151	-0.141
C	-0.134	2.636	-0.482
C	-1.554	2.363	-0.373
C	-2.459	3.437	-0.257
C	1.736	4.225	-0.569
C	0.335	3.970	-0.508
C	-0.618	5.033	-0.412
C	-0.149	6.432	-0.427
C	2.236	5.633	-0.594
C	1.312	6.706	-0.517
C	5.508	7.395	-0.675
C	4.112	7.201	-0.642
C	3.134	8.340	-0.572
C	3.539	9.692	-0.561
C	-10.439	-0.469	0.238
C	-11.845	-0.641	0.315
C	-12.702	0.455	0.407
C	-12.195	1.748	0.428
C	-8.539	1.095	0.172
C	-9.930	0.861	0.255
C	-10.816	1.964	0.351
C	-10.319	3.273	0.368
C	-6.660	2.677	0.080
C	-8.046	2.426	0.179
C	-4.819	4.257	-0.043
C	-6.188	4.007	0.073
C	-7.088	5.094	0.180
C	-6.610	6.425	0.177
C	-4.333	5.645	-0.058
C	-5.236	6.706	0.058
C	-4.747	8.027	0.053
C	-1.058	7.496	-0.310
C	-2.437	7.234	-0.193
C	-3.365	8.295	-0.069
C	-2.892	9.617	-0.062
C	-0.589	8.823	-0.296
C	-1.517	9.887	-0.172
C	-1.054	11.210	-0.153
C	1.240	10.439	-0.371
C	0.311	11.483	-0.254
C	-8.944	3.514	0.280
C	-8.461	4.834	0.287
C	-5.794	-2.206	-0.078
C	3.617	5.882	-0.649
C	6.420	2.497	-0.718
C	6.940	3.884	-0.743

C	5.374	-3.914	-0.752
C	3.983	-4.155	-0.713
C	4.963	-1.512	-0.703
C	3.567	-1.756	-0.671
C	4.097	3.423	-0.679
C	-1.081	-0.042	-0.770
C	-2.043	1.048	-0.401
O	-0.950	0.066	-2.187
C	11.079	0.680	-0.709
C	-1.953	4.778	-0.284
C	-2.891	5.911	-0.189
C	11.934	-0.421	-0.728
C	0.799	9.097	-0.393
C	1.750	8.045	-0.499
C	2.605	10.722	-0.462
C	-0.200	-4.910	-0.458
C	1.196	-4.644	-0.567
H	-1.423	-12.345	-0.487
H	0.969	-11.865	-0.660
H	2.802	-10.267	-0.756
H	4.633	-8.698	-0.828
H	6.484	-7.143	-0.863
H	8.347	-5.593	-0.859
H	10.212	-4.062	-0.830
H	12.104	-2.551	-0.787
H	-3.732	-11.569	-0.299
H	-5.337	-9.819	-0.155
H	10.218	3.247	-0.835
H	-6.661	-8.266	0.093
H	-8.135	-6.533	0.191
H	8.779	5.034	-0.830
H	7.422	6.635	-0.724
H	-9.489	-4.959	0.048
H	-10.991	-3.190	0.159
H	5.936	8.384	-0.663
H	4.574	9.984	-0.626
H	-12.319	-1.607	0.307
H	-13.772	0.298	0.465
H	-12.884	2.582	0.501
H	-11.006	4.109	0.445
H	-7.313	7.246	0.266
H	-5.446	8.851	0.148
H	-3.595	10.437	0.036
H	-1.750	12.035	-0.058
H	0.641	12.515	-0.234
H	-9.157	5.662	0.369
H	11.547	1.648	-0.668
H	13.007	-0.271	-0.713
H	2.955	11.748	-0.450
N	6.875	-2.658	3.757
H	7.796	-2.448	3.428
H	6.476	-3.381	3.192
C	6.042	-1.459	3.674
H	6.305	-0.801	2.839
C	4.563	-1.863	3.557

C 6.224 -0.623 4.949
H 4.452 -2.482 2.658
H 4.310 -2.504 4.412
C 3.607 -0.673 3.487
O 5.909 0.540 5.002
H 3.690 -0.092 4.412
H 3.887 0.002 2.667
C 2.154 -1.111 3.305
H 1.994 -1.612 2.343
H 1.860 -1.802 4.100
N 1.262 0.053 3.393
H 1.353 0.578 4.258
C 0.717 0.732 2.375
N 0.130 0.060 1.374
N 0.628 2.062 2.462
H -0.050 -0.913 1.617
H 1.325 2.590 2.971
O 6.698 -1.295 5.994
H -0.477 -0.717 -2.519
H 0.062 2.570 1.790
H 6.923 -2.966 4.707

Rc

ONIOM: extrapolated energy = -9066.460724

C -6.462 -9.347 -0.859
C -5.149 -9.815 -0.855
C -4.077 -8.913 -0.856
C -2.760 -9.387 -0.854
C -1.684 -8.491 -0.858
C -0.368 -8.974 -0.850
C 0.716 -8.088 -0.851
C 2.029 -8.578 -0.829
C 3.120 -7.696 -0.819
C 4.428 -8.190 -0.783
C 5.521 -7.313 -0.765
C 6.819 -7.824 -0.719
C 7.920 -6.963 -0.695
C 9.212 -7.497 -0.640
C -6.723 -7.970 -0.861
C -8.037 -7.508 -0.873
C -8.306 -6.142 -0.871
C -7.262 -5.183 -0.845
C -4.328 -7.521 -0.861
C -5.657 -7.045 -0.859
C -5.920 -5.653 -0.858
C -4.841 -4.740 -0.872
C -1.926 -7.097 -0.870
C -3.252 -6.610 -0.868
C -3.503 -5.220 -0.876
C 0.484 -6.695 -0.870
C -0.841 -6.197 -0.881
C 0.030 -3.923 -0.911
C 1.355 -4.419 -0.887
C 5.314 -5.914 -0.789
C 3.999 -5.409 -0.828

C	4.882	-3.117	-0.837
C	7.730	-5.557	-0.724
C	6.419	-5.027	-0.771
C	6.203	-3.624	-0.797
C	7.297	-2.725	-0.786
C	8.853	-4.697	-0.704
C	8.624	-3.218	-0.748
C	9.688	-2.297	-0.766
C	-7.512	-3.778	-0.821
C	-8.816	-3.244	-0.717
C	-9.044	-1.928	-0.725
C	-7.999	-0.993	-0.846
C	-5.096	-3.351	-0.893
C	-6.424	-2.868	-0.876
C	-6.672	-1.465	-0.888
C	-5.597	-0.547	-0.917
C	-2.688	-2.925	-0.898
C	-4.020	-2.442	-0.916
C	-4.277	-1.050	-0.945
C	-3.142	-0.099	-0.989
C	-0.199	-2.463	-0.894
C	-1.560	-1.966	-0.909
C	-1.807	-0.636	-1.011
C	2.225	-2.073	-0.847
C	0.860	-1.618	-0.791
C	0.593	-0.171	-0.507
C	1.758	0.732	-0.833
C	4.665	-1.716	-0.867
C	3.269	-1.204	-0.880
C	3.049	0.238	-0.897
C	4.143	1.140	-0.906
C	5.754	-0.810	-0.857
C	6.602	1.506	-0.830
C	9.477	-0.978	-0.795
C	7.929	1.043	-0.792
C	8.972	1.989	-0.699
C	-8.250	0.482	-0.881
C	-9.548	1.010	-0.964
C	-9.773	2.377	-0.930
C	-8.711	3.295	-0.817
C	-7.154	1.373	-0.854
C	-7.382	2.782	-0.811
C	-6.284	3.672	-0.762
C	-3.358	1.241	-0.955
C	-4.745	1.771	-0.879
C	-4.964	3.169	-0.796
C	-3.870	4.070	-0.747
C	-2.241	2.178	-0.932
C	-2.477	3.564	-0.802
C	-1.414	4.445	-0.753
C	1.504	2.104	-0.889
C	0.148	2.595	-0.898
C	-0.085	3.973	-0.796
C	3.909	2.511	-0.864
C	2.581	3.007	-0.862

C	2.310	4.410	-0.774
C	3.447	5.357	-0.690
C	5.034	3.481	-0.787
C	4.779	4.874	-0.704
C	8.746	3.310	-0.654
C	7.448	3.858	-0.698
C	7.192	5.335	-0.637
C	8.234	6.286	-0.585
C	-8.933	4.702	-0.728
C	-10.232	5.275	-0.683
C	-10.412	6.654	-0.600
C	-9.317	7.505	-0.551
C	-6.502	5.068	-0.687
C	-7.819	5.580	-0.666
C	-8.020	6.982	-0.580
C	-6.927	7.852	-0.519
C	-4.084	5.464	-0.656
C	-5.403	5.960	-0.628
C	-1.661	5.899	-0.632
C	-2.989	6.370	-0.596
C	-3.223	7.760	-0.504
C	-2.140	8.656	-0.444
C	-0.574	6.800	-0.570
C	-0.817	8.185	-0.475
C	0.264	9.081	-0.419
C	3.177	6.741	-0.590
C	1.841	7.222	-0.552
C	1.589	8.609	-0.456
C	2.664	9.508	-0.400
C	4.247	7.654	-0.525
C	3.987	9.042	-0.433
C	5.057	9.946	-0.374
C	6.643	8.110	-0.486
C	6.374	9.484	-0.401
C	-5.622	7.354	-0.542
C	-4.537	8.240	-0.479
C	-5.834	0.863	-0.884
C	6.350	2.981	-0.780
C	7.072	-1.320	-0.817
C	8.177	-0.436	-0.805
C	2.899	-6.302	-0.840
C	1.579	-5.804	-0.870
C	3.781	-4.016	-0.847
C	2.458	-3.532	-0.869
C	5.528	0.595	-0.875
C	-0.645	0.280	-1.301
C	-0.936	1.721	-1.008
O	-0.377	0.236	-2.704
C	10.145	-5.270	-0.637
C	1.024	4.873	-0.729
C	0.756	6.325	-0.610
C	10.315	-6.653	-0.608
C	5.579	7.184	-0.549
C	5.851	5.794	-0.630
C	7.962	7.651	-0.510

C	-2.419	-4.312	-0.888
C	-1.078	-4.804	-0.897
H	-7.276	-10.063	-0.861
H	-4.972	-10.884	-0.852
H	-2.572	-10.455	-0.848
H	-0.188	-10.044	-0.838
H	2.204	-9.649	-0.812
H	4.596	-9.262	-0.765
H	6.974	-8.898	-0.699
H	9.369	-8.569	-0.617
H	-8.865	-8.207	-0.890
H	-9.348	-5.876	-0.910
H	10.717	-2.618	-0.763
H	-9.686	-3.867	-0.604
H	-10.071	-1.620	-0.614
H	10.355	-0.356	-0.814
H	10.003	1.687	-0.640
H	-10.418	0.385	-1.076
H	-10.803	2.679	-1.007
H	9.616	3.939	-0.569
H	9.274	6.005	-0.605
H	-11.134	4.690	-0.697
H	-11.413	7.066	-0.568
H	-9.484	8.573	-0.485
H	-7.093	8.922	-0.452
H	-2.327	9.722	-0.374
H	0.075	10.146	-0.348
H	2.471	10.573	-0.329
H	4.876	11.012	-0.305
H	7.185	10.202	-0.353
H	-4.716	9.308	-0.412
H	11.042	-4.676	-0.603
H	11.312	-7.073	-0.560
H	8.788	8.351	-0.469
N	-6.954	-1.162	2.636
H	-7.610	-1.775	2.197
H	-6.888	-0.313	2.112
C	-4.536	-0.741	2.712
C	-5.550	-2.655	3.963
H	-4.649	-0.116	1.816
H	-4.693	-0.082	3.577
C	-3.129	-1.328	2.741
O	-4.761	-3.557	4.098
H	-2.980	-1.885	3.673
H	-3.007	-2.055	1.927
C	-2.057	-0.251	2.609
H	-2.091	0.209	1.619
H	-2.196	0.561	3.332
N	-0.746	-0.848	2.809
H	-0.594	-1.295	3.705
C	0.294	-0.893	1.948
N	0.267	0.009	0.924
N	1.331	-1.688	2.130
H	-0.123	0.924	1.183
H	1.131	-2.417	2.811

O	-6.381	-2.274	4.936
H	-0.285	-0.697	-2.961
C	6.021	1.684	2.731
C	5.487	0.402	2.863
C	6.328	-0.714	2.825
C	7.698	-0.548	2.651
C	8.234	0.736	2.536
C	7.397	1.850	2.578
H	5.365	2.550	2.751
H	5.905	-1.712	2.913
H	8.348	-1.417	2.601
H	9.303	0.866	2.400
H	7.812	2.847	2.475
C	4.022	0.209	3.038
C	3.026	1.009	2.318
O	3.381	-0.341	1.827
H	3.677	-0.318	3.926
H	3.329	1.769	1.604
H	2.007	1.084	2.695
C	-0.981	-4.170	5.398
O	-1.394	-5.069	6.001
O	-0.544	-3.267	4.802
I	-0.044	2.938	2.738
C	-5.640	-1.808	2.686
H	-5.454	-2.491	1.848
H	2.653	-0.951	1.966
H	-7.260	-0.957	3.566

TS1

ONIOM: extrapolated energy = -9066.424544

C	-2.863	-10.678	-1.202
C	-1.470	-10.657	-1.252
C	-0.781	-9.437	-1.230
C	0.618	-9.418	-1.271
C	1.313	-8.203	-1.235
C	2.714	-8.196	-1.265
C	3.420	-6.988	-1.217
C	4.823	-6.987	-1.250
C	5.536	-5.781	-1.204
C	6.935	-5.781	-1.252
C	7.650	-4.575	-1.226
C	9.045	-4.586	-1.290
C	9.767	-3.388	-1.281
C	11.163	-3.423	-1.347
C	-3.588	-9.481	-1.129
C	-4.979	-9.508	-1.074
C	-5.707	-8.325	-0.993
C	-5.064	-7.062	-0.959
C	-1.502	-8.222	-1.162
C	-2.912	-8.242	-1.111
C	-3.644	-7.032	-1.033
C	-2.950	-5.801	-1.013
C	0.600	-6.984	-1.163
C	-0.812	-6.993	-1.136
C	-1.531	-5.780	-1.067

C	2.716	-5.767	-1.133
C	1.301	-5.761	-1.107
C	1.327	-3.327	-0.923
C	2.735	-3.336	-0.956
C	6.961	-3.344	-1.139
C	5.554	-3.337	-1.069
C	5.577	-0.888	-0.955
C	9.090	-2.143	-1.208
C	7.680	-2.125	-1.130
C	6.988	-0.896	-1.046
C	7.706	0.321	-1.057
C	9.827	-0.928	-1.213
C	9.125	0.315	-1.155
C	9.791	1.560	-1.202
C	-5.786	-5.835	-0.863
C	-7.193	-5.788	-0.750
C	-7.862	-4.632	-0.697
C	-7.207	-3.386	-0.757
C	-3.670	-4.591	-0.924
C	-5.081	-4.603	-0.866
C	-5.797	-3.376	-0.809
C	-5.102	-2.152	-0.806
C	-1.571	-3.351	-0.897
C	-2.979	-3.365	-0.884
C	-3.695	-2.150	-0.833
C	-2.978	-0.854	-0.889
C	0.600	-2.049	-0.765
C	-0.847	-2.060	-0.806
C	-1.543	-0.893	-0.868
C	2.734	-0.845	-0.706
C	1.302	-0.897	-0.568
C	0.527	0.351	-0.213
C	1.320	1.618	-0.432
C	4.888	0.345	-0.863
C	3.410	0.333	-0.701
C	2.702	1.602	-0.574
C	3.412	2.831	-0.650
C	5.596	1.574	-0.874
C	5.591	4.037	-0.766
C	9.133	2.720	-1.122
C	6.993	4.069	-0.859
C	7.643	5.322	-0.814
C	-7.963	-2.086	-0.747
C	-9.367	-2.047	-0.773
C	-10.060	-0.847	-0.730
C	-9.387	0.389	-0.665
C	-7.257	-0.859	-0.731
C	-7.965	0.376	-0.682
C	-7.244	1.593	-0.644
C	-3.649	0.330	-0.836
C	-5.137	0.366	-0.772
C	-5.828	1.582	-0.688
C	-5.111	2.789	-0.631
C	-2.922	1.593	-0.761
C	-3.630	2.808	-0.648

C	-2.947	4.002	-0.548
C	0.608	2.818	-0.501
C	-0.832	2.809	-0.565
C	-1.534	4.021	-0.501
C	2.721	4.034	-0.572
C	1.305	4.040	-0.515
C	0.563	5.264	-0.465
C	1.292	6.555	-0.426
C	3.446	5.334	-0.563
C	2.715	6.558	-0.478
C	6.975	6.480	-0.706
C	5.569	6.538	-0.624
C	4.815	7.833	-0.515
C	5.461	9.088	-0.479
C	-10.087	1.630	-0.588
C	-11.504	1.716	-0.561
C	-12.152	2.945	-0.469
C	-11.421	4.123	-0.401
C	-7.935	2.820	-0.557
C	-9.347	2.841	-0.525
C	-10.024	4.084	-0.429
C	-9.300	5.278	-0.361
C	-5.803	4.025	-0.528
C	-7.213	4.036	-0.495
C	-3.696	5.278	-0.462
C	-5.098	5.258	-0.450
C	-5.798	6.480	-0.346
C	-5.093	7.697	-0.266
C	-2.978	6.502	-0.374
C	-3.688	7.716	-0.283
C	-2.985	8.932	-0.210
C	0.561	7.758	-0.347
C	-0.856	7.743	-0.317
C	-1.577	8.954	-0.234
C	-0.882	10.171	-0.178
C	1.248	8.984	-0.306
C	0.522	10.195	-0.219
C	1.212	11.414	-0.178
C	3.336	10.244	-0.323
C	2.607	11.439	-0.231
C	-7.905	5.266	-0.392
C	-7.196	6.473	-0.318
C	-5.847	-0.857	-0.769
C	4.847	5.329	-0.646
C	7.008	1.557	-0.972
C	7.734	2.772	-0.984
C	4.840	-4.556	-1.111
C	3.429	-4.552	-1.072
C	4.861	-2.115	-0.962
C	3.453	-2.129	-0.874
C	4.899	2.810	-0.777
C	-0.755	0.382	-1.066
C	-1.542	1.618	-0.753
O	-0.419	0.490	-2.447
C	11.243	-1.011	-1.271

C	-0.804	5.250	-0.436
C	-1.555	6.523	-0.376
C	11.892	-2.242	-1.338
C	2.661	9.005	-0.359
C	3.399	7.795	-0.450
C	4.731	10.272	-0.382
C	-0.833	-4.550	-1.002
C	0.594	-4.539	-1.015
H	-3.375	-11.634	-1.217
H	-0.931	-11.595	-1.304
H	1.167	-10.353	-1.323
H	3.256	-9.134	-1.323
H	5.360	-7.927	-1.316
H	7.470	-6.723	-1.321
H	9.573	-5.532	-1.352
H	11.693	-4.367	-1.403
H	-5.512	-10.452	-1.094
H	-6.776	-8.441	-0.968
H	10.859	1.639	-1.313
H	-7.797	-6.677	-0.692
H	-8.931	-4.710	-0.598
H	9.732	3.613	-1.175
H	8.716	5.401	-0.860
H	-9.970	-2.936	-0.835
H	-11.132	-0.931	-0.750
H	7.574	7.375	-0.684
H	6.532	9.187	-0.523
H	-12.148	0.855	-0.607
H	-13.234	2.985	-0.447
H	-11.949	5.067	-0.329
H	-9.828	6.224	-0.284
H	-5.640	8.630	-0.190
H	-3.534	9.865	-0.142
H	-1.433	11.103	-0.110
H	0.671	12.351	-0.109
H	3.117	12.394	-0.202
H	-7.735	7.411	-0.235
H	11.885	-0.148	-1.255
H	12.973	-2.279	-1.383
H	5.263	11.217	-0.356
N	-2.974	-6.076	2.398
H	-2.859	-6.850	1.776
H	-3.721	-5.496	2.074
C	-2.047	-3.830	2.775
C	-0.819	-5.889	3.518
H	-2.701	-3.425	1.990
H	-2.620	-3.788	3.711
C	-0.792	-2.972	2.870
O	0.375	-5.695	3.547
H	-0.119	-3.352	3.641
H	-0.239	-3.026	1.919
C	-1.101	-1.513	3.169
H	-1.707	-1.024	2.411
H	-1.644	-1.375	4.108
N	0.150	-0.756	3.271

H	0.750	-0.988	4.054
C	0.778	-0.204	2.220
N	0.047	0.236	1.188
N	2.122	-0.065	2.180
H	-0.920	0.514	1.389
H	2.538	-0.771	2.795
O	-1.448	-6.607	4.447
H	0.004	-0.342	-2.718
C	5.393	-0.264	2.840
C	4.865	0.425	3.943
C	4.652	-0.260	5.150
C	4.934	-1.617	5.242
C	5.449	-2.295	4.136
C	5.689	-1.619	2.940
H	5.582	0.262	1.913
H	4.244	0.276	6.004
H	4.749	-2.149	6.170
H	5.668	-3.356	4.209
H	6.100	-2.148	2.087
C	4.512	1.833	3.856
C	4.110	2.495	2.593
O	2.828	2.159	3.131
H	4.483	2.439	4.756
H	4.316	1.944	1.676
H	4.241	3.570	2.482
C	2.539	-3.764	2.926
O	2.269	-3.058	3.817
O	2.882	-4.412	2.027
I	-3.434	1.044	2.594
H	2.490	1.111	2.695
C	-1.736	-5.297	2.442
H	-1.165	-5.330	1.510
H	-3.188	-6.414	3.315

Int1

ONIOM: extrapolated energy = -9066.451523

C	5.709	9.954	-0.571
C	4.364	10.323	-0.557
C	3.362	9.345	-0.572
C	2.013	9.719	-0.566
C	1.006	8.746	-0.584
C	-0.342	9.130	-0.588
C	-1.358	8.165	-0.608
C	-2.705	8.556	-0.623
C	-3.727	7.594	-0.645
C	-5.071	7.987	-0.668
C	-6.093	7.028	-0.695
C	-7.431	7.432	-0.719
C	-8.459	6.484	-0.747
C	-9.790	6.911	-0.771
C	6.072	8.600	-0.603
C	7.416	8.236	-0.629
C	7.786	6.895	-0.668
C	6.817	5.860	-0.676
C	3.716	7.975	-0.598

C	5.077	7.600	-0.616
C	5.443	6.231	-0.654
C	4.433	5.242	-0.670
C	1.352	7.374	-0.601
C	2.711	6.988	-0.610
C	3.064	5.621	-0.637
C	-1.021	6.794	-0.616
C	0.337	6.395	-0.612
C	-0.361	4.062	-0.619
C	-1.718	4.458	-0.614
C	-5.777	5.651	-0.695
C	-4.427	5.248	-0.665
C	-5.135	2.899	-0.670
C	-8.158	5.096	-0.751
C	-6.808	4.682	-0.721
C	-6.488	3.306	-0.714
C	-7.518	2.339	-0.751
C	-9.206	4.137	-0.786
C	-8.880	2.746	-0.797
C	-9.869	1.739	-0.865
C	7.170	4.477	-0.719
C	8.512	4.032	-0.693
C	8.832	2.735	-0.754
C	7.853	1.728	-0.862
C	4.788	3.878	-0.732
C	6.149	3.494	-0.773
C	6.496	2.116	-0.849
C	5.487	1.137	-0.877
C	2.421	3.271	-0.665
C	3.782	2.892	-0.744
C	4.138	1.527	-0.828
C	3.083	0.485	-0.852
C	-0.024	2.622	-0.587
C	1.369	2.228	-0.644
C	1.711	0.921	-0.783
C	-2.409	2.054	-0.528
C	-1.015	1.700	-0.454
C	-0.635	0.272	-0.190
C	-1.739	-0.709	-0.524
C	-4.816	1.520	-0.664
C	-3.389	1.111	-0.585
C	-3.064	-0.310	-0.599
C	-4.089	-1.286	-0.711
C	-5.838	0.540	-0.715
C	-6.516	-1.830	-0.764
C	-9.559	0.439	-0.865
C	-7.873	-1.465	-0.765
C	-8.847	-2.486	-0.722
C	8.211	0.268	-0.945
C	9.544	-0.161	-1.051
C	9.873	-1.510	-1.069
C	8.883	-2.511	-0.989
C	7.191	-0.713	-0.930
C	7.523	-2.100	-0.942
C	6.491	-3.070	-0.907

C	3.398	-0.840	-0.885
C	4.818	-1.285	-0.899
C	5.137	-2.663	-0.883
C	4.112	-3.640	-0.842
C	2.350	-1.855	-0.841
C	2.687	-3.229	-0.811
C	1.690	-4.185	-0.782
C	-1.388	-2.055	-0.664
C	-0.002	-2.447	-0.728
C	0.330	-3.809	-0.749
C	-3.758	-2.635	-0.747
C	-2.398	-3.032	-0.729
C	-2.028	-4.416	-0.747
C	-3.094	-5.446	-0.750
C	-4.812	-3.685	-0.769
C	-4.457	-5.060	-0.757
C	-8.527	-3.788	-0.711
C	-7.192	-4.240	-0.735
C	-6.829	-5.697	-0.715
C	-7.800	-6.722	-0.675
C	9.208	-3.902	-0.969
C	10.544	-4.379	-0.981
C	10.824	-5.744	-0.964
C	9.794	-6.674	-0.931
C	6.810	-4.447	-0.897
C	8.160	-4.861	-0.926
C	8.463	-6.247	-0.910
C	7.436	-7.196	-0.870
C	4.427	-5.017	-0.829
C	5.778	-5.418	-0.857
C	2.041	-5.623	-0.772
C	3.400	-6.000	-0.794
C	3.734	-7.373	-0.782
C	2.718	-8.345	-0.750
C	1.022	-6.602	-0.744
C	1.365	-7.969	-0.733
C	0.350	-8.941	-0.707
C	-2.724	-6.811	-0.724
C	-1.357	-7.196	-0.719
C	-1.005	-8.564	-0.701
C	-2.012	-9.539	-0.678
C	-3.724	-7.800	-0.702
C	-3.365	-9.168	-0.676
C	-4.366	-10.148	-0.647
C	-6.081	-8.429	-0.665
C	-5.713	-9.782	-0.640
C	6.098	-6.794	-0.844
C	5.079	-7.758	-0.806
C	5.841	-0.314	-0.908
C	-6.160	-3.283	-0.763
C	-7.191	0.955	-0.750
C	-8.227	-0.007	-0.789
C	-3.400	6.221	-0.645
C	-2.046	5.823	-0.627
C	-4.104	3.876	-0.644

C	-2.749	3.491	-0.598
C	-5.510	-0.844	-0.738
C	0.605	-0.068	-1.039
C	1.014	-1.492	-0.814
O	0.275	-0.014	-2.435
C	-10.542	4.617	-0.804
C	-0.711	-4.788	-0.739
C	-0.339	-6.222	-0.733
C	-10.820	5.982	-0.798
C	-5.087	-7.426	-0.700
C	-5.459	-6.057	-0.729
C	-7.428	-8.065	-0.653
C	2.050	4.634	-0.635
C	0.678	5.024	-0.622
H	6.467	10.729	-0.561
H	4.108	11.376	-0.535
H	1.746	10.771	-0.550
H	-0.602	10.184	-0.579
H	-2.960	9.610	-0.619
H	-5.322	9.043	-0.667
H	-7.673	8.490	-0.717
H	-10.033	7.968	-0.767
H	8.191	8.995	-0.625
H	8.845	6.708	-0.703
H	-10.919	1.965	-0.928
H	9.342	4.712	-0.605
H	9.882	2.501	-0.700
H	-10.385	-0.249	-0.937
H	-9.899	-2.259	-0.685
H	10.367	0.529	-1.137
H	10.922	-1.731	-1.155
H	-9.352	-4.480	-0.681
H	-8.857	-6.517	-0.658
H	11.402	-3.729	-0.993
H	11.853	-6.083	-0.974
H	10.040	-7.730	-0.919
H	7.680	-8.253	-0.859
H	2.982	-9.398	-0.742
H	0.616	-9.993	-0.696
H	-1.743	-10.590	-0.662
H	-4.107	-11.200	-0.627
H	-6.469	-10.558	-0.615
H	5.336	-8.812	-0.797
H	-11.400	3.969	-0.820
H	-11.849	6.322	-0.812
H	-8.202	-8.824	-0.624
N	7.229	0.512	2.640
H	7.954	1.008	2.161
H	7.021	-0.333	2.147
C	4.779	0.455	2.734
C	6.093	2.178	3.989
H	4.795	-0.159	1.824
H	4.856	-0.240	3.581
C	3.461	1.220	2.801
O	5.449	3.190	4.164

H 3.381 1.742 3.761
H 3.420 1.992 2.021
C 2.273 0.274 2.643
H 2.232 -0.121 1.624
H 2.382 -0.588 3.312
N 1.031 0.973 2.931
H 1.013 1.481 3.808
C -0.128 1.032 2.218
N -0.298 0.070 1.239
N -1.075 1.891 2.482
H 0.209 -0.797 1.420
H -0.717 2.642 3.074
O 6.897 1.683 4.928
H 0.102 0.914 -2.674
C -5.408 -2.421 2.677
C -3.982 -2.386 2.583
C -3.248 -3.609 2.514
C -3.916 -4.819 2.546
C -5.313 -4.827 2.628
C -6.059 -3.634 2.689
H -5.979 -1.501 2.735
H -2.163 -3.544 2.452
H -3.367 -5.754 2.499
H -5.838 -5.777 2.645
H -7.140 -3.677 2.749
C -3.256 -1.201 2.547
C -3.771 0.191 2.684
O -3.162 0.725 3.839
H -2.165 -1.276 2.487
H -4.857 0.253 2.765
H -3.442 0.747 1.796
C -3.950 4.635 2.963
O -3.096 3.946 3.347
O -4.805 5.316 2.565
I 0.518 -3.033 2.876
H -2.378 1.239 3.496
C 6.029 1.346 2.706
H 5.942 2.063 1.884
H 7.533 0.291 3.567

Int2

ONIOM: extrapolated energy = -9066.508583

C -8.591 -7.612 -0.568
C -7.407 -8.344 -0.652
C -6.172 -7.686 -0.721
C -4.986 -8.424 -0.804
C -3.749 -7.773 -0.876
C -2.565 -8.521 -0.949
C -1.321 -7.881 -1.012
C -0.138 -8.635 -1.062
C 1.112 -8.000 -1.104
C 2.291 -8.755 -1.135
C 3.543 -8.123 -1.161
C 4.713 -8.886 -1.185
C 5.967 -8.265 -1.203

C	7.124	-9.050	-1.226
C	-8.557	-6.211	-0.547
C	-9.742	-5.484	-0.467
C	-9.719	-4.093	-0.440
C	-8.499	-3.373	-0.486
C	-6.126	-6.272	-0.707
C	-7.323	-5.529	-0.615
C	-7.289	-4.112	-0.592
C	-6.045	-3.445	-0.675
C	-3.695	-6.360	-0.871
C	-4.887	-5.606	-0.784
C	-4.842	-4.194	-0.771
C	-1.258	-6.471	-1.016
C	-2.449	-5.706	-0.948
C	-1.124	-3.664	-1.002
C	0.066	-4.426	-1.061
C	3.626	-6.712	-1.157
C	2.444	-5.946	-1.131
C	3.784	-3.891	-1.131
C	6.068	-6.850	-1.197
C	4.889	-6.072	-1.172
C	4.969	-4.662	-1.159
C	6.229	-4.024	-1.170
C	7.344	-6.224	-1.213
C	7.423	-4.797	-1.205
C	8.656	-4.109	-1.238
C	-8.447	-1.947	-0.441
C	-9.603	-1.153	-0.264
C	-9.550	0.182	-0.254
C	-8.340	0.880	-0.426
C	-6.004	-2.033	-0.661
C	-7.197	-1.283	-0.552
C	-7.145	0.141	-0.540
C	-5.906	0.815	-0.626
C	-3.567	-2.120	-0.816
C	-4.765	-1.368	-0.740
C	-4.724	0.048	-0.734
C	-3.419	0.741	-0.837
C	-1.041	-2.191	-0.933
C	-2.265	-1.418	-0.874
C	-2.231	-0.064	-0.939
C	1.410	-2.314	-1.016
C	0.176	-1.589	-0.854
C	0.220	-0.125	-0.509
C	1.546	0.518	-0.828
C	3.866	-2.478	-1.109
C	2.612	-1.686	-1.042
C	2.702	-0.236	-0.962
C	3.958	0.419	-1.033
C	5.123	-1.825	-1.117
C	6.442	0.258	-1.077
C	8.725	-2.774	-1.212
C	7.642	-0.474	-1.088
C	8.863	0.230	-1.015
C	-8.280	2.376	-0.451

C	-9.441	3.164	-0.467
C	-9.373	4.548	-0.430
C	-8.138	5.223	-0.381
C	-7.021	3.019	-0.488
C	-6.947	4.444	-0.444
C	-5.686	5.085	-0.462
C	-3.348	2.096	-0.781
C	-4.587	2.905	-0.636
C	-4.504	4.317	-0.556
C	-3.244	4.969	-0.568
C	-2.060	2.777	-0.802
C	-1.993	4.181	-0.668
C	-0.766	4.817	-0.660
C	1.589	1.912	-0.883
C	0.368	2.680	-0.840
C	0.433	4.077	-0.739
C	4.022	1.807	-0.989
C	2.831	2.570	-0.929
C	2.865	3.999	-0.841
C	4.178	4.687	-0.816
C	5.329	2.518	-0.974
C	5.376	3.934	-0.881
C	8.922	1.569	-0.959
C	7.770	2.379	-0.967
C	7.832	3.877	-0.893
C	9.053	4.587	-0.869
C	-8.055	6.646	-0.290
C	-9.200	7.476	-0.169
C	-9.084	8.862	-0.090
C	-7.834	9.465	-0.120
C	-5.603	6.495	-0.393
C	-6.780	7.271	-0.303
C	-6.680	8.684	-0.222
C	-5.427	9.306	-0.237
C	-3.157	6.377	-0.488
C	-4.340	7.138	-0.403
C	-0.697	6.292	-0.566
C	-1.894	7.032	-0.488
C	-1.827	8.441	-0.408
C	-0.579	9.089	-0.403
C	0.557	6.945	-0.561
C	0.613	8.351	-0.477
C	1.860	8.998	-0.468
C	4.209	6.097	-0.714
C	3.006	6.849	-0.634
C	3.054	8.258	-0.542
C	4.296	8.910	-0.524
C	5.448	6.764	-0.687
C	5.489	8.175	-0.592
C	6.726	8.833	-0.564
C	7.886	6.705	-0.720
C	7.915	8.104	-0.627
C	-4.258	8.547	-0.325
C	-3.010	9.186	-0.330
C	-5.840	2.244	-0.582

C	6.509	1.753	-1.017
C	6.305	-2.603	-1.145
C	7.571	-1.972	-1.147
C	1.184	-6.591	-1.106
C	-0.003	-5.828	-1.070
C	2.520	-4.539	-1.119
C	1.328	-3.789	-1.080
C	5.198	-0.405	-1.091
C	-0.910	0.596	-1.256
C	-0.882	2.057	-0.919
O	-0.702	0.546	-2.667
C	8.491	-7.058	-1.232
C	1.709	4.723	-0.738
C	1.756	6.200	-0.641
C	8.375	-8.447	-1.239
C	6.650	6.023	-0.752
C	6.619	4.608	-0.844
C	9.076	5.978	-0.782
C	-3.594	-3.533	-0.846
C	-2.390	-4.294	-0.939
H	-9.534	-8.142	-0.517
H	-7.458	-9.426	-0.664
H	-5.026	-9.508	-0.811
H	-2.613	-9.605	-0.947
H	-0.191	-9.719	-1.057
H	2.235	-9.839	-1.133
H	4.648	-9.969	-1.187
H	7.062	-10.132	-1.231
H	-10.698	-5.995	-0.428
H	-10.682	-3.616	-0.400
H	9.601	-4.621	-1.290
H	-10.578	-1.581	-0.110
H	-10.483	0.696	-0.088
H	9.713	-2.347	-1.251
H	9.808	-0.284	-0.987
H	-10.427	2.735	-0.524
H	-10.320	5.059	-0.454
H	9.908	1.999	-0.895
H	10.009	4.093	-0.920
H	-10.204	7.091	-0.116
H	-9.973	9.473	0.002
H	-7.771	10.545	-0.055
H	-5.362	10.388	-0.174
H	-0.536	10.171	-0.340
H	1.902	10.080	-0.400
H	4.334	9.992	-0.452
H	6.775	9.913	-0.491
H	8.859	8.635	-0.602
H	-2.958	10.268	-0.268
H	9.497	-6.678	-1.236
H	9.266	-9.063	-1.254
H	10.033	6.488	-0.763
N	-5.685	-2.981	2.773
H	-6.025	-3.760	2.246
H	-5.960	-2.130	2.325

C	-3.647	-1.628	3.030
C	-3.829	-3.911	4.051
H	-4.021	-1.002	2.207
H	-4.042	-1.202	3.964
C	-2.123	-1.609	3.024
O	-2.736	-4.407	4.176
H	-1.745	-2.315	3.770
H	-1.767	-1.946	2.038
C	-1.519	-0.238	3.318
H	-1.914	0.517	2.631
H	-1.766	0.088	4.333
N	-0.050	-0.266	3.211
H	0.351	-0.865	3.932
C	0.472	-0.665	1.952
N	-0.112	0.044	0.921
N	1.381	-1.536	1.767
H	-0.351	1.000	1.171
H	1.648	-1.998	2.635
O	-4.780	-4.036	4.978
H	-0.782	-0.382	-2.948
C	4.415	-1.068	2.591
C	3.928	-0.162	3.540
C	3.285	-0.662	4.677
C	3.132	-2.039	4.862
C	3.634	-2.930	3.915
C	4.277	-2.438	2.777
H	4.917	-0.689	1.706
H	2.904	0.032	5.423
H	2.632	-2.414	5.750
H	3.517	-4.000	4.059
H	4.658	-3.125	2.026
C	3.999	1.329	3.331
C	2.920	1.859	2.368
O	1.706	2.065	3.054
H	3.887	1.853	4.282
H	2.817	1.159	1.527
H	3.214	2.834	1.973
C	-0.273	-4.317	2.876
O	0.278	-3.820	3.774
O	-0.792	-4.820	1.967
I	5.962	1.958	2.629
H	1.226	1.231	3.214
C	-4.223	-3.043	2.847
H	-3.755	-3.503	1.969
H	-6.067	-3.011	3.697

TS2

ONIOM: extrapolated energy = -9066.495929

C	-11.390	-1.836	-0.490
C	-10.807	-3.102	-0.530
C	-9.415	-3.237	-0.600
C	-8.833	-4.510	-0.630
C	-7.441	-4.652	-0.688
C	-6.867	-5.931	-0.705
C	-5.476	-6.087	-0.748

C -4.906 -7.369 -0.759
C -3.513 -7.531 -0.794
C -2.946 -8.812 -0.809
C -1.553 -8.976 -0.848
C -1.000 -10.259 -0.866
C 0.388 -10.433 -0.910
C 0.920 -11.726 -0.925
C -10.589 -0.686 -0.521
C -11.176 0.575 -0.471
C -10.389 1.723 -0.498
C -8.975 1.650 -0.583
C -8.596 -2.083 -0.636
C -9.184 -0.801 -0.597
C -8.374 0.362 -0.626
C -6.968 0.229 -0.690
C -6.616 -3.504 -0.722
C -7.195 -2.215 -0.701
C -6.378 -1.063 -0.727
C -4.644 -4.946 -0.775
C -5.215 -3.649 -0.767
C -2.983 -2.681 -0.820
C -2.410 -3.974 -0.818
C -0.706 -7.846 -0.868
C -1.268 -6.554 -0.846
C 0.984 -5.581 -0.897
C 1.253 -9.308 -0.938
C 0.700 -8.009 -0.912
C 1.544 -6.877 -0.932
C 2.947 -7.041 -0.990
C 2.662 -9.490 -0.990
C 3.514 -8.344 -1.032
C 4.919 -8.451 -1.130
C -8.147 2.813 -0.617
C -8.678 4.122 -0.619
C -7.897 5.206 -0.619
C -6.492 5.111 -0.614
C -6.153 1.383 -0.704
C -6.734 2.671 -0.662
C -5.903 3.829 -0.665
C -4.496 3.701 -0.727
C -4.169 -0.041 -0.785
C -4.753 1.250 -0.763
C -3.936 2.406 -0.796
C -2.465 2.260 -0.903
C -2.100 -1.497 -0.803
C -2.695 -0.178 -0.828
C -1.919 0.930 -0.953
C -0.126 -2.953 -0.794
C -0.752 -1.659 -0.707
C 0.094 -0.442 -0.433
C 1.554 -0.656 -0.766
C 1.832 -4.447 -0.915
C 1.225 -3.093 -0.854
C 2.099 -1.926 -0.868
C 3.505 -2.080 -0.989

C	3.238	-4.596	-0.981
C	5.487	-3.586	-1.050
C	5.713	-7.376	-1.151
C	6.083	-4.860	-1.062
C	7.491	-4.945	-1.038
C	-5.607	6.321	-0.572
C	-6.125	7.624	-0.447
C	-5.333	8.700	-0.414
C	-3.926	8.597	-0.494
C	-4.206	6.153	-0.631
C	-3.358	7.297	-0.589
C	-1.954	7.137	-0.628
C	-1.656	3.351	-0.888
C	-2.242	4.712	-0.777
C	-1.393	5.845	-0.719
C	0.017	5.695	-0.738
C	-0.205	3.208	-0.916
C	0.626	4.347	-0.825
C	1.999	4.204	-0.836
C	2.356	0.478	-0.911
C	1.764	1.791	-0.926
C	2.591	2.923	-0.899
C	4.325	-0.958	-1.020
C	3.754	0.338	-1.000
C	4.574	1.513	-0.987
C	6.047	1.361	-0.959
C	5.807	-1.087	-1.030
C	6.630	0.070	-0.987
C	8.281	-3.861	-1.021
C	7.766	-2.550	-1.024
C	8.646	-1.334	-0.988
C	10.056	-1.416	-0.973
C	-3.075	9.744	-0.463
C	-3.574	11.071	-0.412
C	-2.713	12.166	-0.364
C	-1.338	11.981	-0.370
C	-1.109	8.269	-0.568
C	-1.666	9.565	-0.488
C	-0.803	10.691	-0.434
C	0.585	10.520	-0.446
C	0.866	6.822	-0.669
C	0.299	8.110	-0.587
C	2.872	5.396	-0.760
C	2.281	6.674	-0.679
C	3.114	7.812	-0.603
C	4.513	7.664	-0.601
C	4.277	5.248	-0.759
C	5.100	6.389	-0.676
C	6.497	6.240	-0.665
C	6.852	2.522	-0.880
C	6.265	3.814	-0.819
C	7.084	4.963	-0.733
C	8.478	4.821	-0.713
C	8.253	2.393	-0.850
C	9.067	3.548	-0.771

C	10.462	3.413	-0.746
C	10.253	0.997	-0.869
C	11.050	2.148	-0.797
C	1.144	9.242	-0.520
C	2.538	9.086	-0.527
C	-3.652	4.854	-0.718
C	6.369	-2.377	-1.041
C	3.794	-5.897	-1.013
C	5.196	-6.070	-1.073
C	-2.674	-6.396	-0.814
C	-3.243	-5.104	-0.805
C	-0.428	-5.423	-0.855
C	-1.006	-4.140	-0.825
C	4.084	-3.452	-1.018
C	-0.451	0.736	-1.252
C	0.378	1.956	-0.984
O	-0.302	0.491	-2.648
C	3.158	-10.819	-0.993
C	4.010	2.758	-0.920
C	4.865	3.965	-0.835
C	2.295	-11.914	-0.963
C	8.846	1.111	-0.896
C	8.038	-0.054	-0.959
C	10.844	-0.267	-0.914
C	-4.972	-1.204	-0.771
C	-4.386	-2.505	-0.792
H	-12.469	-1.756	-0.433
H	-11.446	-3.977	-0.503
H	-9.464	-5.391	-0.603
H	-7.505	-6.808	-0.681
H	-5.548	-8.243	-0.740
H	-3.591	-9.684	-0.793
H	-1.652	-11.126	-0.848
H	0.271	-12.594	-0.903
H	-12.253	0.678	-0.406
H	-10.929	2.652	-0.438
H	5.421	-9.401	-1.203
H	-9.737	4.315	-0.630
H	-8.403	6.156	-0.631
H	6.770	-7.564	-1.240
H	7.996	-5.896	-1.018
H	-7.182	7.811	-0.361
H	-5.836	9.645	-0.306
H	9.342	-4.046	-0.997
H	10.580	-2.356	-1.005
H	-4.624	11.307	-0.418
H	-3.119	13.170	-0.324
H	-0.690	12.849	-0.330
H	1.235	11.388	-0.399
H	5.147	8.542	-0.539
H	7.130	7.119	-0.599
H	9.108	5.702	-0.648
H	11.099	4.287	-0.685
H	12.130	2.070	-0.775
H	3.177	9.961	-0.471

H 4.208 -11.056 -1.009
H 2.699 -12.919 -0.967
H 11.923 -0.370 -0.899
N -7.309 -0.691 2.741
H -8.012 -1.239 2.287
H -7.175 0.163 2.238
C -4.874 -0.459 2.856
C -6.046 -2.349 4.010
H -4.961 0.231 2.004
H -4.990 0.152 3.761
C -3.493 -1.112 2.839
O -5.350 -3.326 4.097
H -3.376 -1.778 3.701
H -3.375 -1.744 1.949
C -2.392 -0.049 2.855
H -2.427 0.530 1.926
H -2.572 0.659 3.673
N -1.061 -0.613 3.032
H -0.994 -1.283 3.795
C -0.196 -0.964 2.025
N -0.047 -0.029 0.997
N 0.497 -2.039 2.139
H -0.639 0.787 1.120
H 1.263 -2.116 1.476
O -6.849 -1.940 4.998
H -0.900 -0.235 -2.894
C 3.921 -1.005 2.455
C 3.591 -0.126 3.494
C 3.001 -0.641 4.649
C 2.770 -2.011 4.782
C 3.131 -2.881 3.757
C 3.703 -2.371 2.590
H 4.388 -0.617 1.553
H 2.723 0.036 5.453
H 2.310 -2.395 5.687
H 2.958 -3.948 3.855
H 3.980 -3.047 1.785
C 3.826 1.352 3.373
C 3.036 2.021 2.248
O 1.652 1.901 2.471
H 3.618 1.849 4.322
H 3.330 1.571 1.297
H 3.279 3.088 2.207
C -0.085 -3.897 3.018
O -0.891 -3.531 3.796
O 0.613 -4.609 2.397
I 5.932 1.797 2.973
H 1.335 1.096 2.026
C -6.051 -1.441 2.773
H -5.907 -2.103 1.912
H -7.598 -0.485 3.676

Int3
ONIOM: extrapolated energy = -9066.502246
C 11.616 0.195 -0.393

C	11.233	1.535	-0.423
C	9.878	1.882	-0.501
C	9.497	3.228	-0.520
C	8.143	3.582	-0.581
C	7.770	4.933	-0.588
C	6.419	5.299	-0.629
C	6.051	6.653	-0.630
C	4.698	7.025	-0.659
C	4.333	8.378	-0.668
C	2.981	8.752	-0.698
C	2.629	10.104	-0.717
C	1.284	10.488	-0.753
C	0.955	11.846	-0.775
C	10.650	-0.819	-0.444
C	11.037	-2.156	-0.402
C	10.085	-3.170	-0.449
C	8.700	-2.881	-0.547
C	8.893	0.866	-0.555
C	9.279	-0.491	-0.529
C	8.302	-1.517	-0.579
C	6.934	-1.170	-0.651
C	7.153	2.573	-0.630
C	7.529	1.211	-0.625
C	6.546	0.197	-0.672
C	5.423	4.298	-0.665
C	5.790	2.930	-0.674
C	3.437	2.313	-0.739
C	3.067	3.678	-0.710
C	1.971	7.764	-0.711
C	2.330	6.402	-0.699
C	-0.044	5.783	-0.728
C	0.257	9.508	-0.767
C	0.606	8.140	-0.742
C	-0.402	7.150	-0.751
C	-1.764	7.525	-0.792
C	-1.108	9.902	-0.809
C	-2.126	8.900	-0.833
C	-3.500	9.219	-0.911
C	7.704	-3.904	-0.600
C	8.031	-5.278	-0.615
C	7.093	-6.230	-0.628
C	5.720	-5.921	-0.624
C	5.952	-2.186	-0.685
C	6.331	-3.547	-0.653
C	5.333	-4.565	-0.671
C	3.963	-4.224	-0.746
C	4.208	-0.476	-0.760
C	4.589	-1.841	-0.753
C	3.606	-2.859	-0.806
C	2.175	-2.490	-0.922
C	2.385	1.277	-0.749
C	2.771	-0.116	-0.806
C	1.837	-1.092	-0.950
C	0.653	3.017	-0.686
C	1.076	1.642	-0.648

C	0.054	0.564	-0.405
C	-1.356	0.999	-0.709
C	-1.056	4.792	-0.743
C	-0.661	3.361	-0.721
C	-1.703	2.341	-0.755
C	-3.071	2.708	-0.836
C	-2.424	5.153	-0.786
C	-4.800	4.497	-0.859
C	-4.448	8.277	-0.922
C	-5.196	5.845	-0.846
C	-6.575	6.143	-0.811
C	4.661	-6.982	-0.588
C	4.974	-8.347	-0.442
C	4.028	-9.290	-0.420
C	2.656	-8.977	-0.533
C	3.303	-6.604	-0.669
C	2.292	-7.606	-0.642
C	0.929	-7.237	-0.707
C	1.210	-3.446	-0.932
C	1.583	-4.881	-0.835
C	0.571	-5.874	-0.799
C	-0.800	-5.513	-0.837
C	-0.202	-3.086	-0.965
C	-1.197	-4.087	-0.909
C	-2.533	-3.737	-0.926
C	-2.321	0.002	-0.860
C	-1.934	-1.385	-0.932
C	-2.923	-2.380	-0.951
C	-4.050	1.722	-0.888
C	-3.682	0.355	-0.914
C	-4.670	-0.683	-0.952
C	-6.103	-0.310	-0.926
C	-5.495	2.075	-0.910
C	-6.483	1.055	-0.915
C	-7.520	5.191	-0.822
C	-7.210	3.817	-0.868
C	-8.263	2.747	-0.871
C	-9.645	3.041	-0.851
C	1.641	-9.982	-0.520
C	1.933	-11.369	-0.454
C	0.916	-12.322	-0.424
C	-0.415	-11.932	-0.464
C	-0.078	-8.228	-0.666
C	0.275	-9.593	-0.578
C	-0.748	-10.576	-0.544
C	-2.094	-10.198	-0.587
C	-1.810	-6.499	-0.791
C	-1.446	-7.858	-0.711
C	-3.576	-4.785	-0.879
C	-3.187	-6.138	-0.815
C	-4.183	-7.139	-0.764
C	-5.543	-6.780	-0.772
C	-4.943	-4.425	-0.876
C	-5.930	-5.431	-0.822
C	-7.289	-5.071	-0.810

C	-7.075	-1.337	-0.896
C	-6.691	-2.705	-0.888
C	-7.675	-3.719	-0.839
C	-9.031	-3.367	-0.811
C	-8.440	-0.999	-0.862
C	-9.420	-2.019	-0.823
C	-10.778	-1.675	-0.793
C	-10.205	0.684	-0.831
C	-11.167	-0.335	-0.799
C	-2.452	-8.850	-0.666
C	-3.806	-8.486	-0.696
C	2.953	-5.236	-0.758
C	-5.854	3.435	-0.888
C	-2.775	6.524	-0.804
C	-4.136	6.907	-0.850
C	3.696	6.032	-0.680
C	4.062	4.668	-0.687
C	1.327	5.413	-0.706
C	1.704	4.056	-0.702
C	-3.434	4.151	-0.827
C	0.415	-0.672	-1.238
C	-0.589	-1.757	-0.996
O	0.301	-0.375	-2.627
C	-1.395	11.292	-0.822
C	-4.303	-2.002	-0.957
C	-5.330	-3.066	-0.914
C	-0.375	12.242	-0.807
C	-8.831	0.359	-0.862
C	-7.857	1.390	-0.886
C	-10.597	2.024	-0.831
C	5.178	0.550	-0.719
C	4.798	1.926	-0.718
H	12.669	-0.049	-0.327
H	11.997	2.302	-0.380
H	10.255	4.003	-0.479
H	8.534	5.703	-0.554
H	6.818	7.419	-0.608
H	5.104	9.141	-0.654
H	3.406	10.861	-0.707
H	1.729	12.605	-0.765
H	12.085	-2.422	-0.328
H	10.476	-4.170	-0.392
H	-3.852	10.234	-0.978
H	9.048	-5.630	-0.628
H	7.447	-7.247	-0.654
H	-5.465	8.624	-1.000
H	-6.929	7.159	-0.762
H	5.989	-8.689	-0.327
H	4.381	-10.299	-0.294
H	-8.541	5.533	-0.788
H	-10.020	4.050	-0.850
H	2.935	-11.760	-0.434
H	1.165	-13.374	-0.371
H	-1.187	-12.692	-0.438
H	-2.868	-10.958	-0.556

H	-6.303	-7.553	-0.730
H	-8.047	-5.846	-0.768
H	-9.787	-4.145	-0.776
H	-11.541	-2.445	-0.765
H	-12.224	-0.095	-0.776
H	-4.571	-9.254	-0.657
H	-2.396	11.686	-0.837
H	-0.621	13.296	-0.820
H	-11.648	2.288	-0.812
N	7.434	-0.736	2.804
H	8.261	-0.374	2.373
H	7.080	-1.496	2.259
C	5.023	-0.309	2.907
C	6.638	1.120	4.177
H	4.937	-0.948	2.017
H	4.946	-0.975	3.777
C	3.879	0.706	2.912
O	6.193	2.228	4.332
H	3.896	1.297	3.833
H	3.998	1.418	2.086
C	2.536	-0.006	2.767
H	2.513	-0.533	1.808
H	2.414	-0.755	3.561
N	1.437	0.943	2.837
H	1.485	1.748	3.492
C	0.402	1.061	2.019
N	0.132	0.114	1.041
N	-0.430	2.084	2.144
H	0.717	-0.709	1.144
H	-1.271	2.081	1.576
O	7.315	0.468	5.126
H	1.000	0.259	-2.862
C	-5.927	0.804	2.496
C	-4.668	0.350	2.894
C	-3.652	1.303	3.089
C	-3.881	2.659	2.856
C	-5.149	3.095	2.471
C	-6.170	2.165	2.307
H	-6.739	0.101	2.350
H	-2.679	0.978	3.442
H	-3.072	3.373	2.991
H	-5.338	4.153	2.312
H	-7.168	2.490	2.024
C	-4.328	-1.101	3.182
C	-3.191	-1.669	2.321
O	-1.948	-1.103	2.688
H	-4.070	-1.224	4.237
H	-3.427	-1.461	1.278
H	-3.134	-2.754	2.455
C	-0.160	3.405	2.857
O	0.827	3.371	3.606
O	-0.987	4.252	2.544
I	-5.987	-2.482	2.902
H	-1.530	-0.700	1.909
C	6.423	0.320	2.885

H 6.475 1.045 2.064
H 7.652 -1.060 3.725

TS3

ONIOM: extrapolated energy = -9066.492145

C -2.153 -10.913 -0.943
C -0.772 -10.758 -1.055
C -0.205 -9.477 -1.097
C 1.182 -9.324 -1.210
C 1.755 -8.047 -1.247
C 3.146 -7.904 -1.351
C 3.731 -6.631 -1.369
C 5.125 -6.494 -1.449
C 5.719 -5.223 -1.435
C 7.112 -5.090 -1.493
C 7.709 -3.821 -1.458
C 9.100 -3.702 -1.509
C 9.707 -2.442 -1.463
C 11.101 -2.346 -1.517
C -2.989 -9.790 -0.871
C -4.369 -9.951 -0.768
C -5.208 -8.841 -0.701
C -4.692 -7.521 -0.729
C -1.039 -8.336 -1.023
C -2.438 -8.492 -0.911
C -3.283 -7.356 -0.841
C -2.714 -6.063 -0.887
C 0.928 -6.902 -1.171
C -0.473 -7.046 -1.061
C -1.306 -5.908 -0.987
C 2.913 -5.482 -1.294
C 1.506 -5.616 -1.200
C 1.293 -3.191 -1.127
C 2.698 -3.056 -1.204
C 6.908 -2.661 -1.365
C 5.506 -2.786 -1.313
C 5.299 -0.348 -1.144
C 8.916 -1.267 -1.362
C 7.510 -1.381 -1.315
C 6.706 -0.224 -1.209
C 7.308 1.052 -1.152
C 9.538 0.009 -1.307
C 8.724 1.178 -1.192
C 9.276 2.475 -1.101
C -5.531 -6.366 -0.662
C -6.933 -6.451 -0.497
C -7.712 -5.364 -0.464
C -7.186 -4.064 -0.603
C -3.550 -4.926 -0.841
C -4.953 -5.073 -0.744
C -5.786 -3.921 -0.714
C -5.216 -2.636 -0.772
C -1.578 -3.487 -0.942
C -2.983 -3.637 -0.885
C -3.821 -2.498 -0.862

C	-3.230	-1.138	-0.898
C	0.452	-1.985	-0.978
C	-0.988	-2.129	-0.946
C	-1.793	-1.036	-0.976
C	2.461	-0.579	-0.947
C	1.037	-0.771	-0.812
C	0.168	0.393	-0.413
C	0.826	1.732	-0.637
C	4.497	0.812	-1.010
C	3.025	0.659	-0.885
C	2.202	1.855	-0.743
C	2.792	3.144	-0.764
C	5.086	2.099	-0.977
C	4.847	4.548	-0.829
C	8.511	3.566	-1.005
C	6.241	4.712	-0.903
C	6.767	6.021	-0.907
C	-8.063	-2.840	-0.593
C	-9.464	-2.935	-0.602
C	-10.267	-1.805	-0.525
C	-9.713	-0.511	-0.439
C	-7.479	-1.552	-0.590
C	-8.297	-0.388	-0.496
C	-7.695	0.893	-0.457
C	-4.009	-0.026	-0.792
C	-5.489	-0.141	-0.675
C	-6.289	1.018	-0.540
C	-5.695	2.302	-0.483
C	-3.409	1.304	-0.728
C	-4.221	2.449	-0.550
C	-3.644	3.702	-0.472
C	0.004	2.860	-0.645
C	-1.432	2.716	-0.646
C	-2.240	3.855	-0.514
C	1.989	4.274	-0.676
C	0.580	4.141	-0.623
C	-0.272	5.289	-0.527
C	0.340	6.638	-0.486
C	2.583	5.639	-0.651
C	1.748	6.783	-0.555
C	5.991	7.112	-0.815
C	4.588	7.035	-0.710
C	3.717	8.252	-0.598
C	4.242	9.563	-0.557
C	-10.524	0.658	-0.313
C	-11.938	0.605	-0.220
C	-12.699	1.767	-0.103
C	-12.084	3.011	-0.068
C	-8.496	2.051	-0.338
C	-9.902	1.935	-0.266
C	-10.692	3.108	-0.145
C	-10.085	4.368	-0.099
C	-6.491	3.462	-0.354
C	-7.894	3.334	-0.287
C	-4.497	4.906	-0.351

C	-5.897	4.753	-0.295
C	-6.710	5.903	-0.178
C	-6.123	7.180	-0.127
C	-3.908	6.190	-0.295
C	-4.728	7.332	-0.188
C	-4.142	8.608	-0.147
C	-0.505	7.768	-0.384
C	-1.916	7.620	-0.315
C	-2.745	8.760	-0.214
C	-2.168	10.037	-0.183
C	0.061	9.056	-0.354
C	-0.775	10.193	-0.254
C	-0.205	11.473	-0.226
C	2.019	10.511	-0.394
C	1.181	11.631	-0.295
C	-8.696	4.491	-0.167
C	-8.102	5.761	-0.116
C	-6.080	-1.420	-0.684
C	3.982	5.765	-0.724
C	6.495	2.216	-1.046
C	7.106	3.490	-0.991
C	4.910	-4.069	-1.352
C	3.505	-4.202	-1.293
C	4.701	-1.635	-1.202
C	3.302	-1.779	-1.138
C	4.273	3.261	-0.860
C	-1.152	0.313	-1.200
C	-2.035	1.464	-0.808
O	-0.921	0.495	-2.592
C	10.955	0.060	-1.373
C	-1.631	5.148	-0.457
C	-2.503	6.340	-0.350
C	11.716	-1.102	-1.475
C	1.464	9.213	-0.425
C	2.312	8.080	-0.527
C	3.404	10.672	-0.459
C	-0.730	-4.616	-1.013
C	0.685	-4.469	-1.119
H	-2.568	-11.914	-0.913
H	-0.145	-11.641	-1.110
H	1.817	-10.202	-1.267
H	3.775	-8.785	-1.406
H	5.750	-7.378	-1.507
H	7.733	-5.977	-1.558
H	9.714	-4.593	-1.581
H	11.716	-3.235	-1.594
H	-4.806	-10.943	-0.743
H	-6.260	-9.060	-0.643
H	10.338	2.651	-1.097
H	-7.441	-7.392	-0.373
H	-8.764	-5.535	-0.308
H	9.029	4.507	-0.929
H	7.825	6.202	-0.995
H	-9.976	-3.879	-0.685
H	-11.327	-1.987	-0.544

H	6.501	8.061	-0.832
H	5.300	9.762	-0.596
H	-12.495	-0.316	-0.224
H	-13.778	1.700	-0.035
H	-12.698	3.899	0.024
H	-10.700	5.258	-0.007
H	-6.754	8.058	-0.041
H	-4.774	9.486	-0.067
H	-2.803	10.913	-0.106
H	-0.831	12.354	-0.150
H	1.598	12.631	-0.270
H	-8.727	6.644	-0.025
H	11.513	0.980	-1.356
H	12.796	-1.037	-1.522
H	3.844	11.662	-0.432
N	-6.183	-2.117	2.710
H	-6.672	-2.839	2.221
H	-6.290	-1.252	2.221
C	-3.937	-1.174	2.964
C	-4.549	-3.364	4.014
H	-4.233	-0.477	2.165
H	-4.227	-0.704	3.915
C	-2.422	-1.376	2.905
O	-3.610	-4.108	4.122
H	-2.106	-2.217	3.530
H	-2.115	-1.620	1.880
C	-1.715	-0.101	3.377
H	-2.098	0.783	2.848
H	-1.944	0.078	4.432
N	-0.261	-0.134	3.280
H	0.183	-0.753	3.955
C	0.413	-0.143	2.099
N	-0.256	0.280	1.005
N	1.641	-0.612	2.095
H	-1.171	0.672	1.188
H	2.210	-0.436	1.276
O	-5.474	-3.219	4.970
H	-0.445	-0.284	-2.926
C	4.350	0.484	4.504
C	4.874	0.049	3.282
C	5.397	1.007	2.404
C	5.384	2.360	2.720
C	4.848	2.785	3.937
C	4.340	1.843	4.826
H	3.926	-0.233	5.199
H	5.861	0.669	1.483
H	5.803	3.082	2.025
H	4.836	3.841	4.191
H	3.926	2.161	5.779
C	4.831	-1.399	2.867
C	4.119	-2.354	3.829
O	2.758	-2.045	3.976
H	4.385	-1.499	1.874
H	4.610	-2.322	4.811
H	4.219	-3.371	3.436

C 1.728 -2.678 2.584
O 0.626 -2.770 3.047
O 2.494 -3.013 1.724
I 6.849 -2.171 2.542
H 2.344 -0.825 3.242
C -4.760 -2.459 2.792
H -4.385 -3.019 1.929
H -6.558 -2.027 3.633

Int4

ONIOM: extrapolated energy = -9066.493794

C -2.918 -10.900 -0.862
C -1.530 -10.833 -0.969
C -0.882 -9.592 -0.999
C 0.512 -9.529 -1.105
C 1.166 -8.292 -1.132
C 2.563 -8.239 -1.236
C 3.229 -7.008 -1.260
C 4.628 -6.962 -1.353
C 5.302 -5.732 -1.365
C 6.699 -5.690 -1.440
C 7.377 -4.462 -1.434
C 8.772 -4.433 -1.487
C 9.459 -3.214 -1.465
C 10.856 -3.210 -1.515
C -3.680 -9.726 -0.787
C -5.066 -9.798 -0.677
C -5.832 -8.638 -0.610
C -5.235 -7.353 -0.660
C -1.641 -8.399 -0.921
C -3.047 -8.465 -0.818
C -3.818 -7.277 -0.750
C -3.167 -6.023 -0.775
C 0.415 -7.095 -1.052
C -0.993 -7.149 -0.947
C -1.751 -5.959 -0.868
C 2.487 -5.809 -1.181
C 1.075 -5.851 -1.077
C 1.018 -3.419 -1.013
C 2.430 -3.375 -1.104
C 6.652 -3.251 -1.365
C 5.246 -3.286 -1.299
C 5.197 -0.836 -1.205
C 8.746 -1.990 -1.392
C 7.335 -2.012 -1.348
C 6.608 -0.804 -1.272
C 7.292 0.432 -1.232
C 9.449 -0.755 -1.359
C 8.713 0.466 -1.269
C 9.347 1.727 -1.200
C -6.000 -6.148 -0.618
C -7.413 -6.150 -0.582
C -8.122 -5.019 -0.523
C -7.503 -3.757 -0.492
C -3.928 -4.833 -0.713

C	-5.338	-4.891	-0.636
C	-6.097	-3.688	-0.582
C	-5.452	-2.429	-0.632
C	-1.867	-3.525	-0.809
C	-3.280	-3.583	-0.742
C	-4.045	-2.391	-0.717
C	-3.363	-1.078	-0.790
C	0.258	-2.157	-0.905
C	-1.187	-2.210	-0.829
C	-1.925	-1.069	-0.862
C	2.355	-0.884	-0.910
C	0.925	-0.978	-0.782
C	0.145	0.246	-0.410
C	0.871	1.533	-0.702
C	4.472	0.374	-1.074
C	2.996	0.317	-0.909
C	2.251	1.565	-0.810
C	2.923	2.812	-0.857
C	5.143	1.621	-1.061
C	5.062	4.081	-0.941
C	8.654	2.866	-1.122
C	6.462	4.155	-1.029
C	7.070	5.429	-1.058
C	-8.287	-2.487	-0.391
C	-9.679	-2.477	-0.184
C	-10.402	-1.291	-0.117
C	-9.781	-0.037	-0.242
C	-7.607	-1.257	-0.471
C	-8.380	0.015	-0.387
C	-7.700	1.249	-0.412
C	-4.073	0.081	-0.746
C	-5.557	0.047	-0.634
C	-6.287	1.268	-0.525
C	-5.609	2.518	-0.505
C	-3.392	1.370	-0.725
C	-4.127	2.568	-0.579
C	-3.468	3.783	-0.531
C	0.119	2.706	-0.723
C	-1.324	2.654	-0.693
C	-2.057	3.846	-0.586
C	2.192	3.992	-0.786
C	0.778	3.950	-0.727
C	0.001	5.149	-0.639
C	0.698	6.457	-0.608
C	2.872	5.315	-0.771
C	2.113	6.511	-0.678
C	6.366	6.567	-0.967
C	4.963	6.580	-0.840
C	4.173	7.850	-0.717
C	4.783	9.123	-0.659
C	-10.551	1.242	-0.187
C	-11.963	1.281	-0.133
C	-12.642	2.495	-0.056
C	-11.938	3.693	-0.039
C	-8.422	2.466	-0.303

C	-9.836	2.462	-0.200
C	-10.540	3.689	-0.115
C	-9.845	4.900	-0.110
C	-6.325	3.732	-0.388
C	-7.732	3.703	-0.298
C	-4.237	5.042	-0.426
C	-5.644	4.983	-0.357
C	-6.377	6.186	-0.252
C	-5.708	7.422	-0.221
C	-3.565	6.285	-0.390
C	-4.308	7.479	-0.289
C	-3.641	8.715	-0.256
C	-0.070	7.639	-0.500
C	-1.486	7.583	-0.426
C	-2.239	8.775	-0.323
C	-1.581	10.012	-0.288
C	0.579	8.888	-0.463
C	-0.181	10.077	-0.355
C	0.471	11.317	-0.315
C	2.627	10.213	-0.489
C	1.863	11.384	-0.380
C	-8.451	4.918	-0.194
C	-7.772	6.143	-0.176
C	-6.206	-1.215	-0.592
C	4.276	5.351	-0.844
C	6.556	1.646	-1.141
C	7.247	2.880	-1.106
C	4.569	-4.528	-1.291
C	3.161	-4.570	-1.198
C	4.518	-2.083	-1.209
C	3.115	-2.139	-1.089
C	4.408	2.833	-0.952
C	-1.205	0.222	-1.148
C	-2.009	1.438	-0.801
O	-0.993	0.331	-2.555
C	10.866	-0.797	-1.419
C	-1.364	5.097	-0.557
C	-2.156	6.343	-0.456
C	11.551	-2.008	-1.495
C	1.988	8.954	-0.533
C	2.760	7.769	-0.644
C	4.020	10.284	-0.550
C	-1.093	-4.707	-0.886
C	0.329	-4.653	-0.994
H	-3.397	-11.871	-0.838
H	-0.962	-11.754	-1.027
H	1.089	-10.446	-1.164
H	3.133	-9.160	-1.296
H	5.194	-7.885	-1.410
H	7.262	-6.616	-1.493
H	9.327	-5.364	-1.542
H	11.413	-4.138	-1.573
H	-5.565	-10.760	-0.640
H	-6.892	-8.792	-0.511
H	10.418	1.834	-1.198

H	-7.991	-7.057	-0.612
H	-9.194	-5.126	-0.518
H	9.231	3.773	-1.060
H	8.136	5.541	-1.165
H	-10.244	-3.383	-0.052
H	-11.461	-1.387	0.056
H	6.933	7.483	-1.005
H	5.852	9.252	-0.689
H	-12.567	0.389	-0.162
H	-13.724	2.506	-0.012
H	-12.488	4.625	0.024
H	-10.392	5.834	-0.038
H	-6.279	8.341	-0.143
H	-4.215	9.632	-0.178
H	-2.158	10.927	-0.208
H	-0.097	12.236	-0.231
H	2.345	12.354	-0.344
H	-8.333	7.069	-0.097
H	11.483	0.084	-1.416
H	12.633	-2.014	-1.539
H	4.523	11.243	-0.510
N	-7.455	-0.563	3.007
H	-8.206	-1.084	2.602
H	-7.297	0.266	2.471
C	-5.004	-0.471	2.974
C	-6.200	-2.221	4.294
H	-5.076	0.155	2.075
H	-5.040	0.211	3.834
C	-3.674	-1.225	2.951
O	-5.501	-3.195	4.406
H	-3.503	-1.712	3.918
H	-3.699	-2.022	2.198
C	-2.533	-0.268	2.623
H	-2.646	0.077	1.591
H	-2.570	0.612	3.281
N	-1.242	-0.932	2.750
H	-1.107	-1.531	3.557
C	-0.174	-0.772	1.947
N	-0.141	0.274	1.073
N	0.847	-1.585	2.038
H	-0.788	1.022	1.301
H	0.922	-2.432	2.614
O	-6.957	-1.752	5.289
H	-0.560	-0.483	-2.863
C	7.308	-1.768	2.555
C	6.481	-1.282	3.574
C	6.537	-1.876	4.833
C	7.397	-2.949	5.072
C	8.212	-3.427	4.052
C	8.165	-2.831	2.788
H	7.270	-1.311	1.570
H	5.891	-1.510	5.628
H	7.423	-3.410	6.055
H	8.879	-4.265	4.234
H	8.790	-3.206	1.983

C	5.493	-0.187	3.310
C	4.487	-0.508	2.202
O	3.473	-1.366	2.655
H	4.967	0.100	4.222
H	5.030	-0.977	1.381
H	4.000	0.414	1.865
C	3.611	-2.812	2.397
O	2.595	-3.410	2.792
O	4.637	-3.157	1.827
I	6.521	1.656	2.694
H	1.789	-1.280	1.780
C	-6.240	-1.381	3.010
H	-6.187	-2.091	2.176
H	-7.691	-0.313	3.946

TS4

ONIOM: extrapolated energy = -9066.465816

C	8.325	8.180	0.040
C	7.137	8.908	0.025
C	5.908	8.252	-0.116
C	4.718	8.987	-0.125
C	3.485	8.338	-0.256
C	2.300	9.084	-0.255
C	1.061	8.446	-0.367
C	-0.123	9.198	-0.349
C	-1.369	8.564	-0.438
C	-2.551	9.315	-0.406
C	-3.800	8.682	-0.479
C	-4.973	9.439	-0.439
C	-6.224	8.816	-0.501
C	-7.384	9.595	-0.452
C	8.301	6.784	-0.089
C	9.490	6.061	-0.066
C	9.476	4.675	-0.196
C	8.263	3.959	-0.363
C	5.870	6.844	-0.244
C	7.071	6.105	-0.234
C	7.047	4.694	-0.366
C	5.806	4.029	-0.499
C	3.438	6.929	-0.381
C	4.634	6.179	-0.377
C	4.596	4.772	-0.500
C	1.003	7.039	-0.489
C	2.193	6.276	-0.501
C	0.866	4.238	-0.718
C	-0.313	4.996	-0.685
C	-3.876	7.275	-0.587
C	-2.689	6.514	-0.623
C	-4.009	4.471	-0.776
C	-6.319	7.404	-0.609
C	-5.136	6.633	-0.650
C	-5.208	5.227	-0.746
C	-6.474	4.584	-0.805
C	-7.594	6.776	-0.669
C	-7.669	5.353	-0.775

C	-8.903	4.664	-0.858
C	8.224	2.541	-0.510
C	9.396	1.755	-0.569
C	9.351	0.424	-0.655
C	8.131	-0.277	-0.689
C	5.774	2.622	-0.627
C	6.973	1.877	-0.621
C	6.929	0.458	-0.721
C	5.693	-0.214	-0.860
C	3.337	2.701	-0.740
C	4.539	1.957	-0.766
C	4.506	0.550	-0.919
C	3.202	-0.136	-1.084
C	0.808	2.765	-0.802
C	2.037	2.004	-0.869
C	2.004	0.665	-1.092
C	-1.633	2.877	-0.784
C	-0.397	2.145	-0.751
C	-0.436	0.651	-0.597
C	-1.777	0.039	-0.945
C	-4.068	3.074	-0.860
C	-2.838	2.253	-0.850
C	-2.941	0.795	-0.944
C	-4.199	0.132	-1.041
C	-5.384	2.401	-0.923
C	-6.691	0.275	-1.026
C	-8.971	3.330	-0.934
C	-7.887	1.017	-0.985
C	-9.108	0.306	-0.967
C	8.072	-1.771	-0.712
C	9.225	-2.557	-0.562
C	9.165	-3.939	-0.611
C	7.945	-4.615	-0.798
C	6.820	-2.414	-0.843
C	6.753	-3.838	-0.877
C	5.497	-4.483	-0.971
C	3.139	-1.491	-1.137
C	4.387	-2.297	-1.037
C	4.309	-3.717	-1.037
C	3.052	-4.381	-1.092
C	1.852	-2.177	-1.209
C	1.798	-3.588	-1.164
C	0.578	-4.234	-1.189
C	-1.812	-1.346	-1.127
C	-0.583	-2.105	-1.206
C	-0.640	-3.509	-1.209
C	-4.253	-1.251	-1.104
C	-3.054	-2.007	-1.157
C	-3.086	-3.439	-1.187
C	-4.401	-4.132	-1.140
C	-5.563	-1.970	-1.099
C	-5.603	-3.385	-1.103
C	-9.164	-1.037	-0.988
C	-8.008	-1.845	-1.028
C	-8.062	-3.345	-1.029

C	-9.277	-4.064	-0.989
C	7.878	-6.038	-0.878
C	9.034	-6.862	-0.897
C	8.930	-8.250	-0.949
C	7.685	-8.861	-0.992
C	5.427	-5.896	-0.991
C	6.610	-6.669	-0.955
C	6.523	-8.085	-1.000
C	5.276	-8.714	-1.053
C	2.985	-5.790	-1.090
C	4.172	-6.547	-1.052
C	0.546	-5.709	-1.155
C	1.735	-6.452	-1.126
C	1.672	-7.868	-1.132
C	0.428	-8.534	-1.153
C	-0.730	-6.415	-1.163
C	-0.776	-7.814	-1.157
C	-2.025	-8.462	-1.151
C	-4.438	-5.536	-1.126
C	-3.182	-6.311	-1.143
C	-3.225	-7.720	-1.137
C	-4.472	-8.367	-1.113
C	-5.659	-6.219	-1.090
C	-5.676	-7.634	-1.085
C	-6.909	-8.303	-1.052
C	-8.093	-6.180	-1.021
C	-8.106	-7.583	-1.019
C	4.102	-7.959	-1.073
C	2.859	-8.606	-1.115
C	5.636	-1.639	-0.924
C	-6.751	-1.214	-1.055
C	-6.556	3.167	-0.889
C	-7.817	2.525	-0.936
C	-1.435	7.159	-0.551
C	-0.248	6.398	-0.582
C	-2.752	5.111	-0.717
C	-1.558	4.353	-0.740
C	-5.453	0.924	-1.009
C	0.679	0.027	-1.450
C	0.663	-1.465	-1.264
O	0.423	0.231	-2.836
C	-8.744	7.605	-0.610
C	-1.921	-4.159	-1.197
C	-1.959	-5.637	-1.165
C	-8.633	8.990	-0.505
C	-6.865	-5.487	-1.059
C	-6.844	-4.068	-1.065
C	-9.289	-5.460	-0.986
C	3.350	4.110	-0.620
C	2.137	4.867	-0.617
H	9.264	8.708	0.154
H	7.180	9.987	0.126
H	4.752	10.067	-0.027
H	2.343	10.164	-0.157
H	-0.074	10.278	-0.255

H	-2.499	10.395	-0.318
H	-4.912	10.520	-0.354
H	-7.325	10.674	-0.369
H	10.440	6.568	0.058
H	10.439	4.199	-0.144
H	-9.849	5.177	-0.866
H	10.382	2.187	-0.560
H	10.300	-0.082	-0.711
H	-9.958	2.903	-0.997
H	-10.054	0.819	-0.928
H	10.198	-2.131	-0.385
H	10.101	-4.450	-0.467
H	-10.149	-1.473	-0.972
H	-10.235	-3.574	-0.959
H	10.036	-6.470	-0.894
H	9.826	-8.858	-0.961
H	7.631	-9.943	-1.031
H	5.220	-9.797	-1.079
H	0.399	-9.618	-1.156
H	-2.065	-9.546	-1.150
H	-4.508	-9.451	-1.110
H	-6.947	-9.386	-1.050
H	-9.044	-8.124	-0.993
H	2.817	-9.690	-1.128
H	-9.748	7.222	-0.635
H	-9.526	9.601	-0.461
H	-10.241	-5.978	-0.956
N	6.345	-0.921	2.808
H	7.158	-0.516	2.390
H	6.053	-1.712	2.270
C	3.915	-0.651	2.924
C	5.454	0.963	4.076
H	3.845	-1.322	2.055
H	3.915	-1.287	3.820
C	2.698	0.273	2.923
O	4.999	2.075	4.150
H	2.749	0.996	3.744
H	2.677	0.851	1.989
C	1.411	-0.542	3.052
H	1.343	-1.290	2.255
H	1.391	-1.109	3.986
N	0.222	0.296	3.062
H	-0.182	0.564	3.965
C	-0.375	0.806	1.984
N	-0.074	0.268	0.788
N	-1.226	1.826	2.130
H	0.250	-0.694	0.859
H	-1.506	1.989	3.108
O	6.131	0.388	5.075
H	0.543	1.175	-3.036
C	-5.032	-3.999	2.940
C	-4.233	-3.012	3.550
C	-4.345	-2.864	4.942
C	-5.245	-3.645	5.666
C	-6.047	-4.596	5.038

C -5.932 -4.777 3.663
H -4.942 -4.169 1.868
H -3.716 -2.152 5.454
H -5.313 -3.504 6.741
H -6.746 -5.195 5.614
H -6.534 -5.523 3.148
C -3.382 -2.211 2.605
C -3.661 -0.742 2.267
O -3.460 0.307 3.181
H -3.662 -2.615 1.617
H -4.727 -0.704 1.988
H -3.084 -0.532 1.356
C -2.514 0.019 4.170
O -2.013 1.026 4.712
O -2.282 -1.190 4.298
I -0.912 -3.088 2.346
H -1.999 1.881 1.476
C 5.267 0.072 2.843
H 5.265 0.753 1.989
H 6.560 -1.213 3.740

Pc

ONIOM: extrapolated energy = -9066.546187

C 8.179 8.277 -0.352
C 6.977 8.983 -0.345
C 5.755 8.300 -0.395
C 4.550 9.012 -0.383
C 3.326 8.335 -0.432
C 2.124 9.057 -0.414
C 0.893 8.391 -0.458
C -0.307 9.118 -0.427
C -1.544 8.456 -0.462
C -2.740 9.184 -0.423
C -3.978 8.524 -0.455
C -5.165 9.260 -0.411
C -6.405 8.611 -0.441
C -7.580 9.367 -0.388
C 8.178 6.877 -0.411
C 9.381 6.176 -0.413
C 9.390 4.786 -0.474
C 8.186 4.040 -0.545
C 5.742 6.886 -0.456
C 6.957 6.170 -0.465
C 6.956 4.753 -0.530
C 5.725 4.061 -0.582
C 3.303 6.922 -0.498
C 4.515 6.195 -0.509
C 4.502 4.783 -0.571
C 0.861 6.981 -0.530
C 2.070 6.243 -0.553
C 0.791 4.175 -0.685
C -0.417 4.909 -0.643
C -4.029 7.114 -0.528
C -2.830 6.375 -0.565
C -4.123 4.293 -0.663

C	-6.473	7.196	-0.522
C	-5.277	6.446	-0.562
C	-5.324	5.037	-0.632
C	-6.571	4.372	-0.674
C	-7.735	6.542	-0.560
C	-7.781	5.118	-0.657
C	-8.999	4.406	-0.756
C	8.169	2.614	-0.622
C	9.352	1.844	-0.680
C	9.328	0.509	-0.716
C	8.120	-0.214	-0.694
C	5.715	2.649	-0.649
C	6.927	1.925	-0.661
C	6.906	0.501	-0.711
C	5.679	-0.197	-0.785
C	3.272	2.685	-0.697
C	4.489	1.960	-0.717
C	4.479	0.547	-0.811
C	3.188	-0.168	-0.943
C	0.744	2.699	-0.754
C	1.986	1.957	-0.785
C	1.981	0.612	-0.967
C	-1.710	2.767	-0.702
C	-0.456	2.061	-0.703
C	-0.467	0.573	-0.516
C	-1.780	-0.072	-0.884
C	-4.174	2.879	-0.735
C	-2.902	2.111	-0.747
C	-2.958	0.660	-0.869
C	-4.201	-0.010	-0.976
C	-5.415	2.201	-0.787
C	-6.686	0.093	-0.880
C	-9.036	3.071	-0.814
C	-7.899	0.796	-0.791
C	-9.099	0.062	-0.680
C	8.086	-1.710	-0.668
C	9.253	-2.473	-0.514
C	9.215	-3.858	-0.518
C	8.003	-4.560	-0.665
C	6.843	-2.378	-0.757
C	6.799	-3.805	-0.754
C	5.553	-4.472	-0.823
C	3.146	-1.525	-0.999
C	4.405	-2.311	-0.913
C	4.354	-3.727	-0.900
C	3.110	-4.406	-0.950
C	1.874	-2.234	-1.081
C	1.840	-3.644	-1.036
C	0.630	-4.309	-1.071
C	-1.789	-1.453	-1.084
C	-0.551	-2.192	-1.132
C	-0.585	-3.593	-1.121
C	-4.232	-1.398	-1.058
C	-3.022	-2.134	-1.115
C	-3.023	-3.567	-1.103

C	-4.319	-4.284	-1.031
C	-5.522	-2.139	-1.002
C	-5.535	-3.558	-0.990
C	-9.128	-1.279	-0.700
C	-7.961	-2.059	-0.834
C	-7.989	-3.558	-0.857
C	-9.192	-4.295	-0.808
C	7.955	-5.986	-0.696
C	9.122	-6.794	-0.689
C	9.038	-8.185	-0.691
C	7.801	-8.814	-0.708
C	5.501	-5.885	-0.804
C	6.695	-6.638	-0.746
C	6.627	-8.056	-0.740
C	5.389	-8.704	-0.768
C	3.054	-5.817	-0.913
C	4.253	-6.555	-0.845
C	0.594	-5.786	-1.002
C	1.807	-6.501	-0.938
C	1.772	-7.913	-0.888
C	0.539	-8.588	-0.886
C	-0.645	-6.466	-0.987
C	-0.669	-7.874	-0.926
C	-1.900	-8.549	-0.897
C	-4.315	-5.697	-0.979
C	-3.095	-6.422	-0.977
C	-3.110	-7.835	-0.916
C	-4.335	-8.515	-0.866
C	-5.538	-6.392	-0.914
C	-5.544	-7.806	-0.862
C	-6.765	-8.493	-0.798
C	-7.975	-6.389	-0.820
C	-7.970	-7.790	-0.779
C	4.204	-7.968	-0.817
C	2.970	-8.633	-0.835
C	5.645	-1.626	-0.828
C	-6.718	-1.402	-0.916
C	-6.614	2.952	-0.742
C	-7.864	2.294	-0.776
C	-1.585	7.047	-0.534
C	-0.380	6.312	-0.571
C	-2.874	4.968	-0.630
C	-1.665	4.245	-0.663
C	-5.458	0.783	-0.890
C	0.676	-0.048	-1.338
C	0.681	-1.535	-1.156
O	0.445	0.153	-2.731
C	-8.901	7.347	-0.490
C	-1.847	-4.266	-1.092
C	-1.860	-5.746	-1.021
C	-8.817	8.736	-0.407
C	-6.757	-5.679	-0.890
C	-6.760	-4.261	-0.918
C	-9.182	-5.689	-0.789
C	3.267	4.097	-0.629

C	2.043	4.831	-0.626
H	9.112	8.827	-0.311
H	7.003	10.066	-0.298
H	4.566	10.096	-0.334
H	2.147	10.140	-0.361
H	-0.279	10.201	-0.372
H	-2.708	10.266	-0.366
H	-5.124	10.342	-0.351
H	-7.542	10.448	-0.323
H	10.325	6.706	-0.364
H	10.365	4.330	-0.455
H	-9.953	4.901	-0.802
H	10.331	2.290	-0.710
H	10.283	0.015	-0.780
H	-10.010	2.620	-0.908
H	-10.048	0.556	-0.553
H	10.221	-2.025	-0.366
H	10.162	-4.350	-0.377
H	-10.098	-1.736	-0.597
H	-10.159	-3.822	-0.786
H	10.118	-6.389	-0.701
H	9.942	-8.780	-0.683
H	7.762	-9.898	-0.706
H	5.348	-9.788	-0.755
H	0.520	-9.672	-0.842
H	-1.917	-9.633	-0.849
H	-4.346	-9.599	-0.821
H	-6.787	-9.576	-0.760
H	-8.900	-8.343	-0.727
H	2.942	-9.717	-0.805
H	-9.897	6.940	-0.481
H	-9.722	9.329	-0.355
H	-10.125	-6.221	-0.744
N	6.918	-0.581	2.736
H	7.717	-0.168	2.300
H	6.628	-1.381	2.211
C	4.482	-0.344	2.827
C	5.980	1.257	4.039
H	4.410	-0.959	1.918
H	4.487	-1.038	3.678
C	3.264	0.574	2.902
O	5.474	2.346	4.146
H	3.269	1.133	3.844
H	3.301	1.318	2.095
C	1.984	-0.246	2.771
H	1.932	-0.719	1.788
H	1.933	-1.059	3.501
N	0.802	0.600	2.949
H	0.644	0.972	3.879
C	-0.043	0.992	1.992
N	-0.170	0.230	0.902
N	-0.734	2.138	2.159
H	-0.041	-0.780	1.104
H	-0.654	2.595	3.059
O	6.680	0.685	5.021

H	0.551	1.100	-2.924
C	-4.896	-3.818	2.726
C	-5.012	-2.495	3.158
C	-6.274	-1.911	3.279
C	-7.415	-2.650	2.973
C	-7.300	-3.973	2.545
C	-6.039	-4.557	2.425
H	-3.907	-4.261	2.621
H	-6.360	-0.881	3.617
H	-8.396	-2.193	3.068
H	-8.190	-4.547	2.304
H	-5.945	-5.587	2.095
C	-3.748	-1.706	3.323
C	-3.429	-0.900	2.071
O	-2.775	0.259	2.597
H	-2.905	-2.351	3.585
H	-4.339	-0.577	1.561
H	-2.749	-1.424	1.400
C	-3.079	0.379	3.906
O	-2.727	1.308	4.581
O	-3.823	-0.659	4.321
I	-0.343	-2.934	2.402
H	-1.680	2.131	1.791
C	5.827	0.395	2.780
H	5.821	1.091	1.934
H	7.153	-0.860	3.667