Electronic Supplementary Material (ESI) for Dalton Transactions

Intramolecular Excimer Formation in Hexakis(pyrenyloxy)cyclotriphosphazene: Photophysical Properties, Crystal structure, and Theoretical Investigation

Serkan Yeşilot[a*], Bünyemin Çoşut[a], Hüsnüye Ardıç Alidağı[a], Ferda Hacıvelioğlu[a], Gül Altınbaş Özpınar[b**], Adem Kılıç[a]

Contribution from:

[a]Department of Chemistry, Gebze Institute of Technology, Gebze, Kocaeli, Turkey

[b]Department of Chemistry Technology, Biga Vocational School, Çanakkale Onsekiz Mart University, Biga 17200 Çanakkale, Turkey

[*] Author for correspondence:

Dr. Serkan Yeşilot, Department of Chemistry, Gebze Institute of Technology, P.O.Box: 141, Gebze 41400, Kocaeli, Turkey

Tel: 00 90 262 6053137

Fax: 00 90 262 6053101

e-mail : yesil@gyte.edu.tr

** Author for correspondence:

Dr. Gül Altınbaş Özpınar, Department of Chemistry Technology, Biga Vocational School, Çanakkale Onsekiz Mart University, Biga 17200 Çanakkale, Turkey

Experimental

Materials

Hexachlorocyclotriphosphazene (trimer) (Otsuka Chemical Co. Ltd) was purified by fractional crystallization from n-hexane. The deuterated solvent ($CDCl_3$) for NMR spectroscopy and the following chemicals were obtained from Aldrich: Hydroxypyrene tetrahydrofuran (THF), toluene, cesium carbonate (Cs_2CO_3), All other reagents and solvents were reagent grade quality and obtained from commercial suppliers.

Equipment

Elemental analyses were carried out using a Thermo Finnigan Flash 1112 Instrument. UV/Vis spectra were recorded with a Shimadzu 2001 UV spectrophotometer. Fluorescence excitation and emission spectra were recorded on a Varian Eclipse spectrofluoremeter using 1 cm pathlength cuvettes at room temperature. Electrochemical behaviors were investigated using a CHIModel840B electrochemical analyzer. Mass spectra were acquired in linear modes with average of 50 shots on a Bruker Daltonics Microflex mass spectrometer equipped with a nitrogen UV-Laser operating at 337 nm. Analytical thin layer chromatography (TLC) was performed on silica gel plates (Merck, Kieselgel 60, 0.25 mm thickness) with F_{254} indicator. Column chromatography was performed on silica gel (Merck, Kieselgel 60, 230-400 mesh; for 3g crude mixture, 100g silica gel was used in a column of 3 cm in diameter and 60 cm in length) . ^{1}H, ^{1} and ^{31}P NMR spectra were recorded in $CDCl_3$ solution on a Varian 500 MHz spectrometer. Thermal properties of compounds were investigated on Mettler Toledo TGA/SDTA 851 thermogravimetric analysis (TGA) and differential scanning calorimeter (DSC) DSC 821^{e} equipped with Mettler Toledo Star^{e} software at a heating rate of 10 °C min^{-1} under nitrogen flow (50 ml min^{-1}). Electrochemical behaviours were investigated using a CHI- Model 840B electrochemical analyzer.

*Synthesis of **HPCT***

Trimer, $N_3P_3Cl_6$, (0.11 g, 0.31 mmol) and 1-hydroxypyrene (0.48 g, 2.21mmol) were dissolved in dry THF (10ml) under argon atmosphere. After stirring for 15 min. at 40 °C, dry and finely powdered cessium carbonate (0.991 g, 3.06 mmol) was added portion wise over 15 min. with

efficient stirring. The reaction mixture was stirred under argon atmosphere at 40 °C for 24 h. The reaction mixture filtered off and the volatile materials were evaporated under vacuum and the product was purified by preparative TLC on silica gel using hexane: THF (1:1) as the eluent. Compound (**HPCT)** was obtained as solid; Yield: 0.40 g (83 %); (Found: C 80.05, H 3.81, N 2.75 %, $C_{96}H_{54}N_3O_6P_3$ (1438.325) requires C 80.16, H 3.78, N 2.92%). ^{1}H NMR ($CDCl_3$) δ= 7.11-7.94 (m, ArCH), ; ^{31}P NMR ($CDCl_3$) δ= 9.37. MS (MALDI) *m*/*z*(%) : 1439.13(100) $[M + H]^+$]$^+$; calculated for $C_{96}H_{54}N_3O_6P_3$.

X-ray structure determination

Slow evaporation of dichloromethane solution (50mg in 1ml) grew single crystals of **HPCT**. Unfortunately only one single crystal with a size of 0.03x0.07x0.26mm was suitable for X-ray examination. Unit cell measurements and intensity data collection was performed on a Bruker APEX II QUAZAR three-circle diffractometer using monochromatized Mo *Kα* X-radiation (λ = 0.71073 Å). The data reduction included a correction for Lorentz and polarization effects, with an applied multi-scan absorption correction (SADABS)[1]. Space groups were determined using XPREP implemented in APEX2[2]. The structure was solved using the direct methods procedure in SHELXS-97[3] and then refined by full-matrix least-squares refinements on F^2 using the SHELXL-97. All non-hydrogen atoms were refined anisotropically using all reflections with $I > 2\sigma(I)$. Aromatic C-bound H atoms were positioned geometrically and refined using a riding model and $U_{iso}(H) = 1.2U_{eq}(C)$. Crystallographic data and refinement details of the data collection for **HPCT** are given in **Table S1**. The final geometrical calculations and all the interactions (π···π, C-H···π) were found by PLATON[4]. The molecular drawings were carried out with and MERCURY[5] CSD 3.0 program.

Computational Details

All computations were done using Gaussian 09 package[6]. Geometry optimizations were done using several DFT mehods: B3LYP[7], MPW1B95[8] and B97D[9] with 6-31G(d)[10] basis set; CAM-B3LYP[11], LC-wPBE[12], and wB97XD[13] using cc-pVDZ[14] basis set. All stationary points were confirmed to be local minima by performing analytic computations of vibrational frequencies in the harmonic approximation. TD-DFT[15] computations were also carried out to calculate the

HOMO-LUMO difference of DFT optimized geometries and the first excitation energies by performing single point computations on both DFT optimized geometries and X-ray geometry. HOMO-LUMO gap and the first vertical excitation energy were also computed using TD-B97D with TZVP[16] basis set.

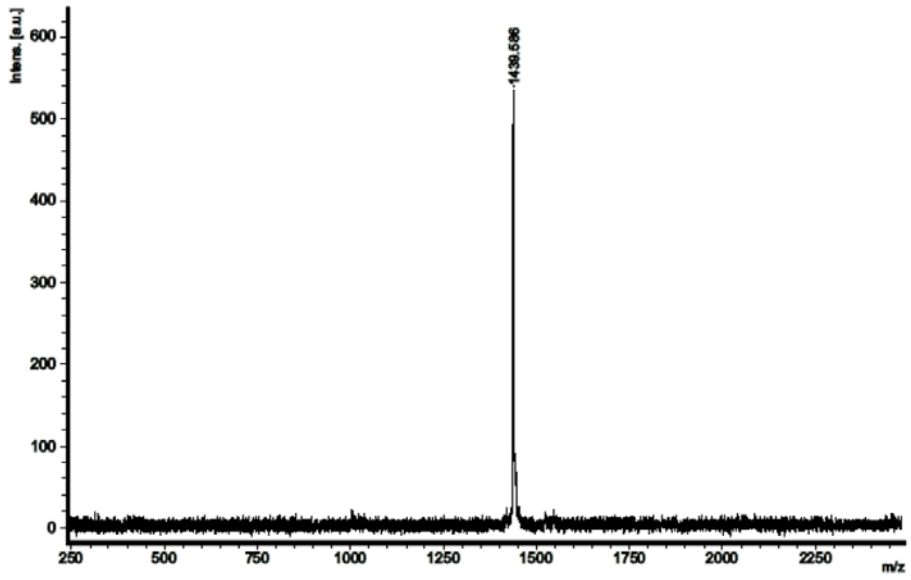

Fig. S1. Positive ion and linear mode MALDI-MS spectrum of **HPCT** was obtained in DHB (20 mg/mL THF) MALDI matrix using nitrogen laser accumulating 50 laser shots.

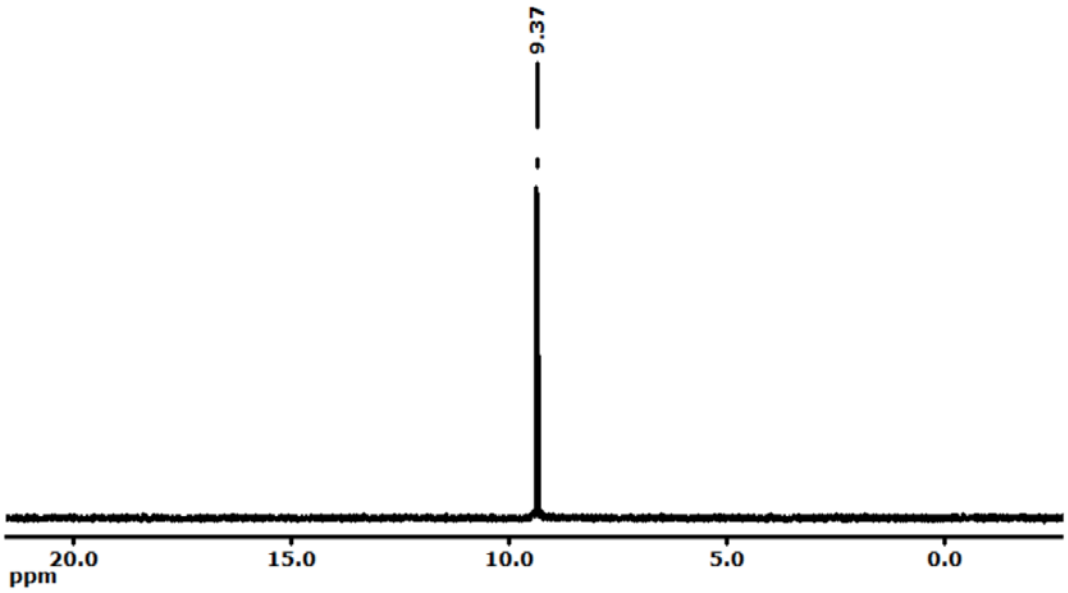

Fig. S2. Proton-decoupled ^{31}P NMR spectrum of **HPCT** in $CDCl_3$ solution.

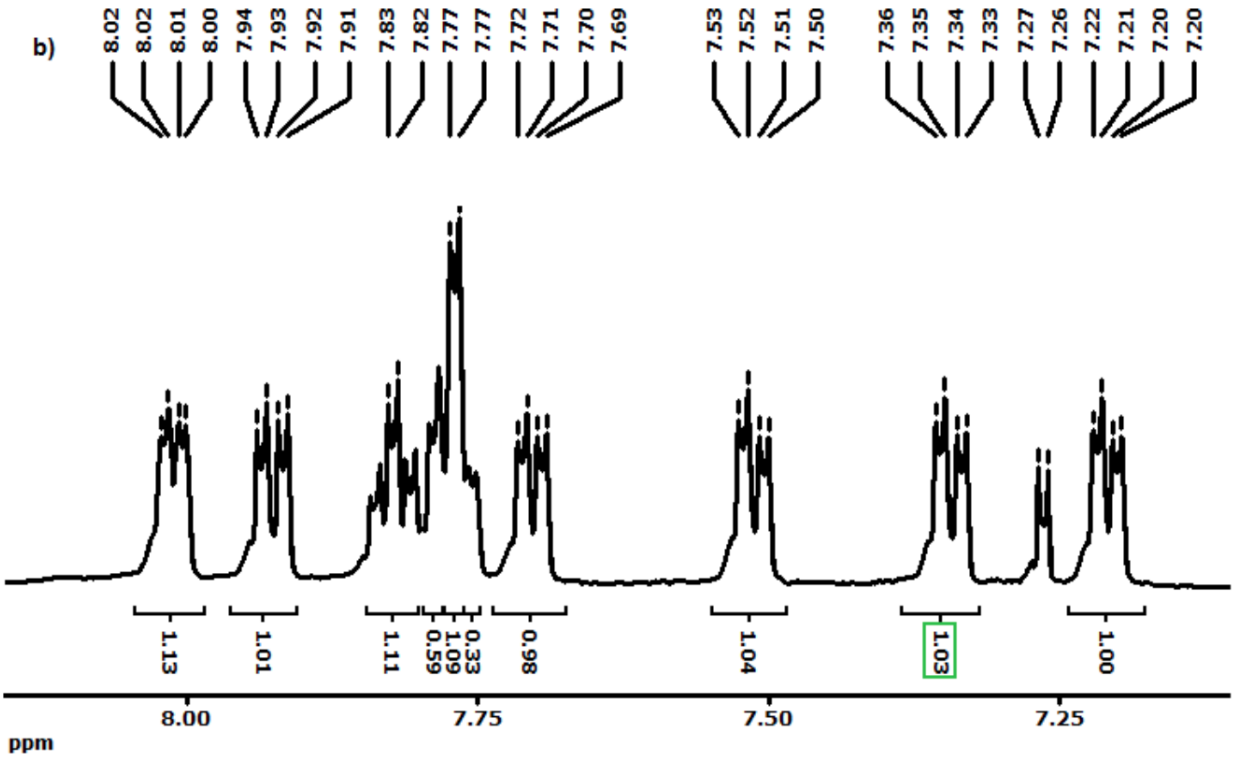

Fig. S3. ^{1}H NMR spectrum of **HPCT** in $CDCl_3$

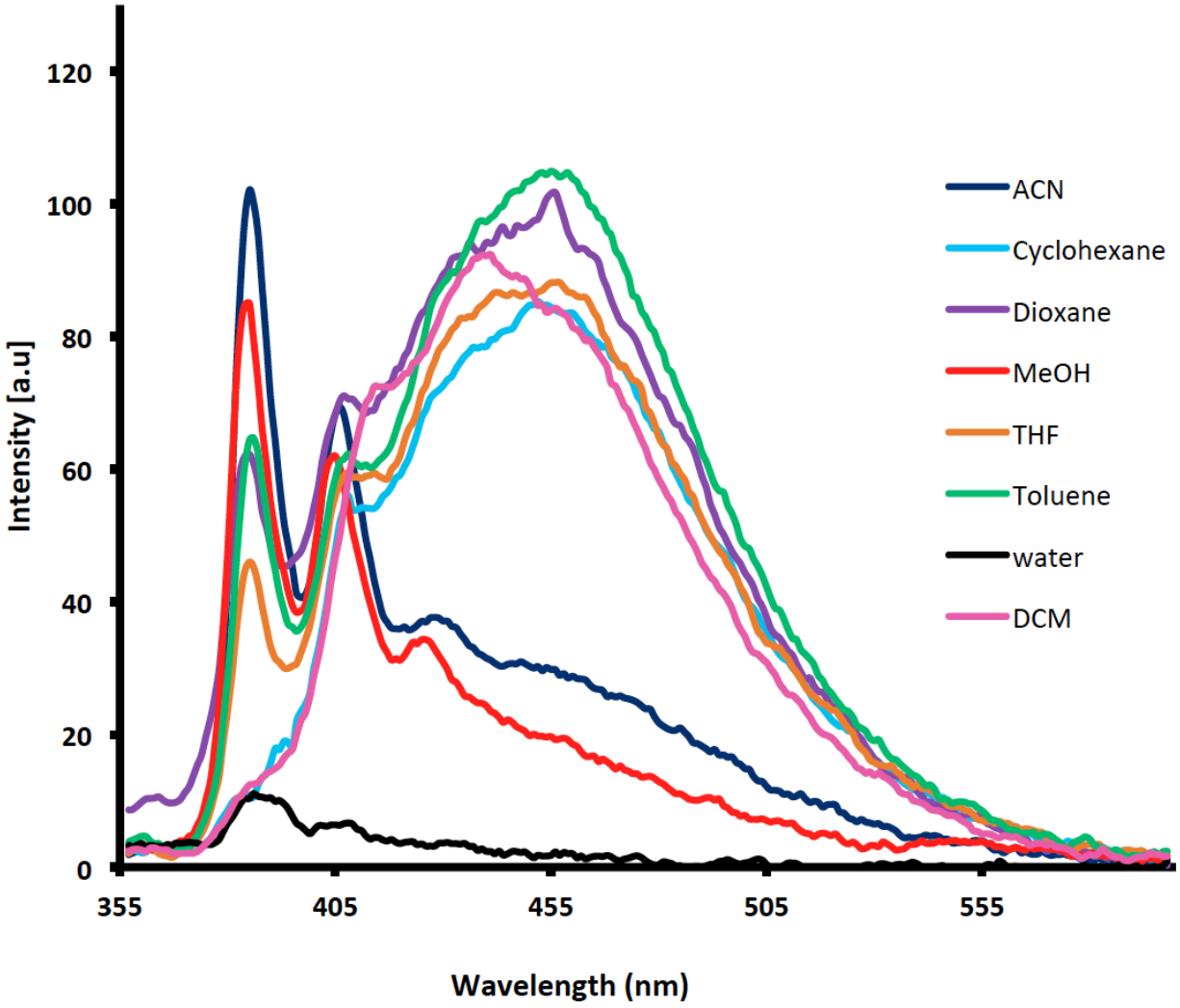

Fig. S4. Emission spectra of **HPCT** recorded in various solvents

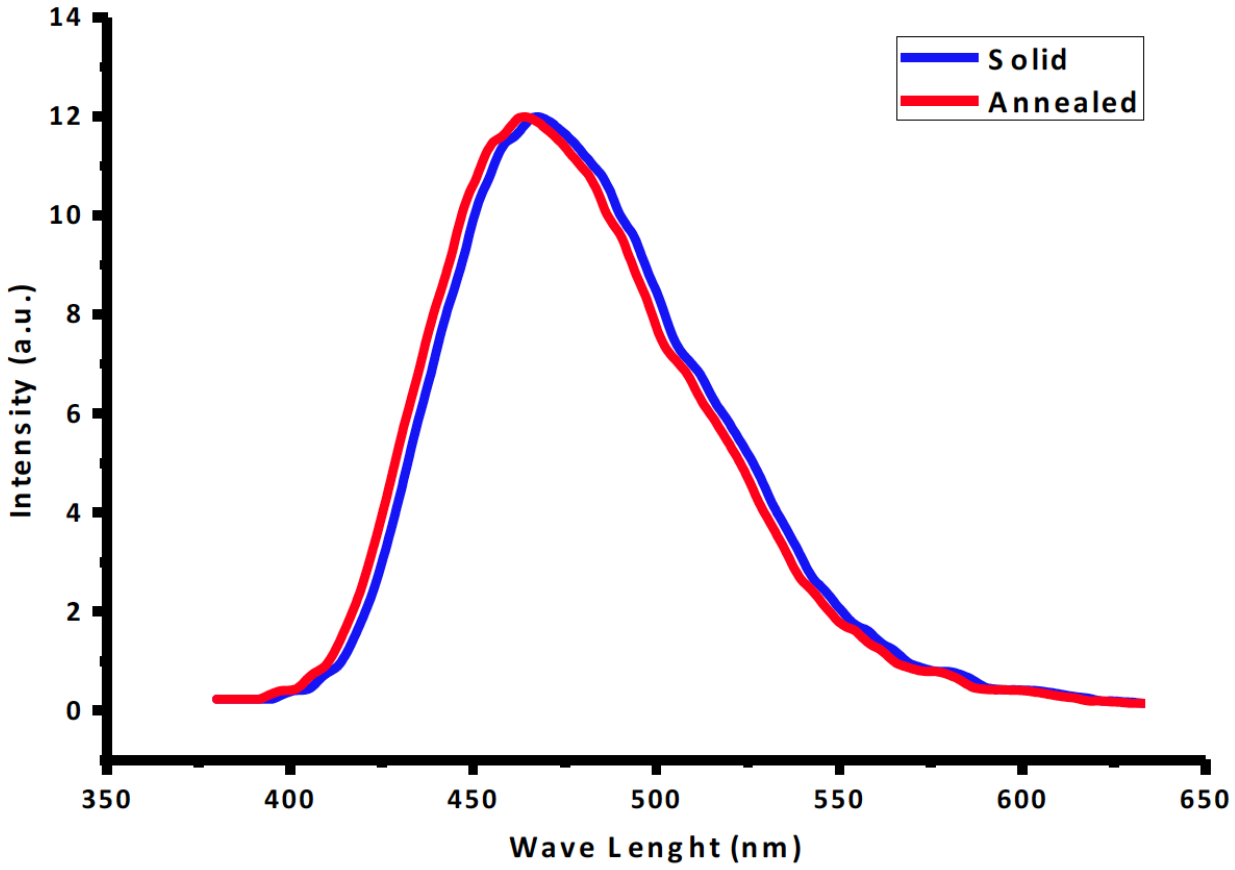

Fig. S5. Fluorescence emission spectra of **HPCT** before and after annealing at 200 °C for 24h under argon atmosphere.

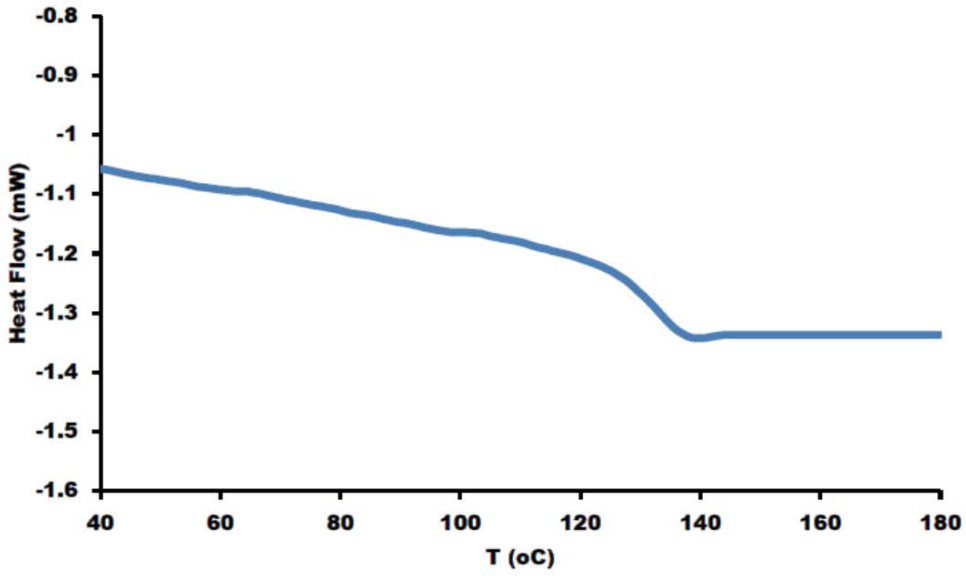

Fig.S6. DSC thermogram of **HPCT** at a heating/cooling rate of 10°Cmin^{-1} from 40 to 180°C at a heating rate of 10°C/min under N_2 atmosphere.

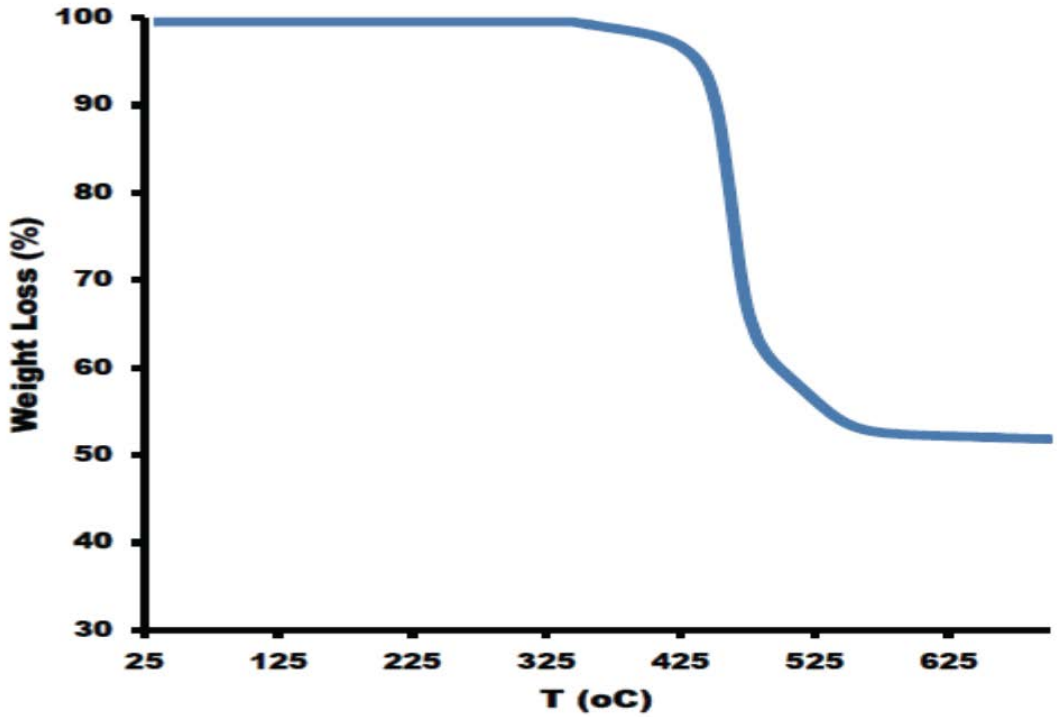

Fig. S7. TGA thermogram of **HPCT** from 25 to 700°C at a heating rate of 10°C/min under N_2 flow of 50mLmin^{-1}.

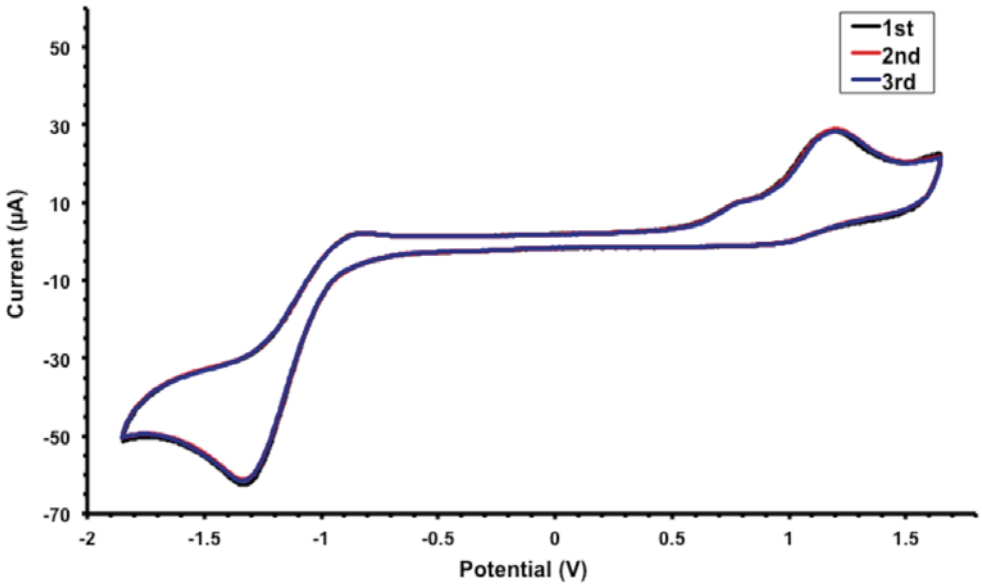

Fig. S8. CV of **HPCT** on a glassy carbon working electrode, Ag/Ag+ reference electrode and Pt counter electrode in CH_2Cl_2, with a monomer concentration of ca. 10^{-4} M, 0.1 M $TBAPF_6$ as supporting electrolyte and a scan rate of 200mVs^{-1}. The data is referenced to the Fc/Fc+ redox couple.

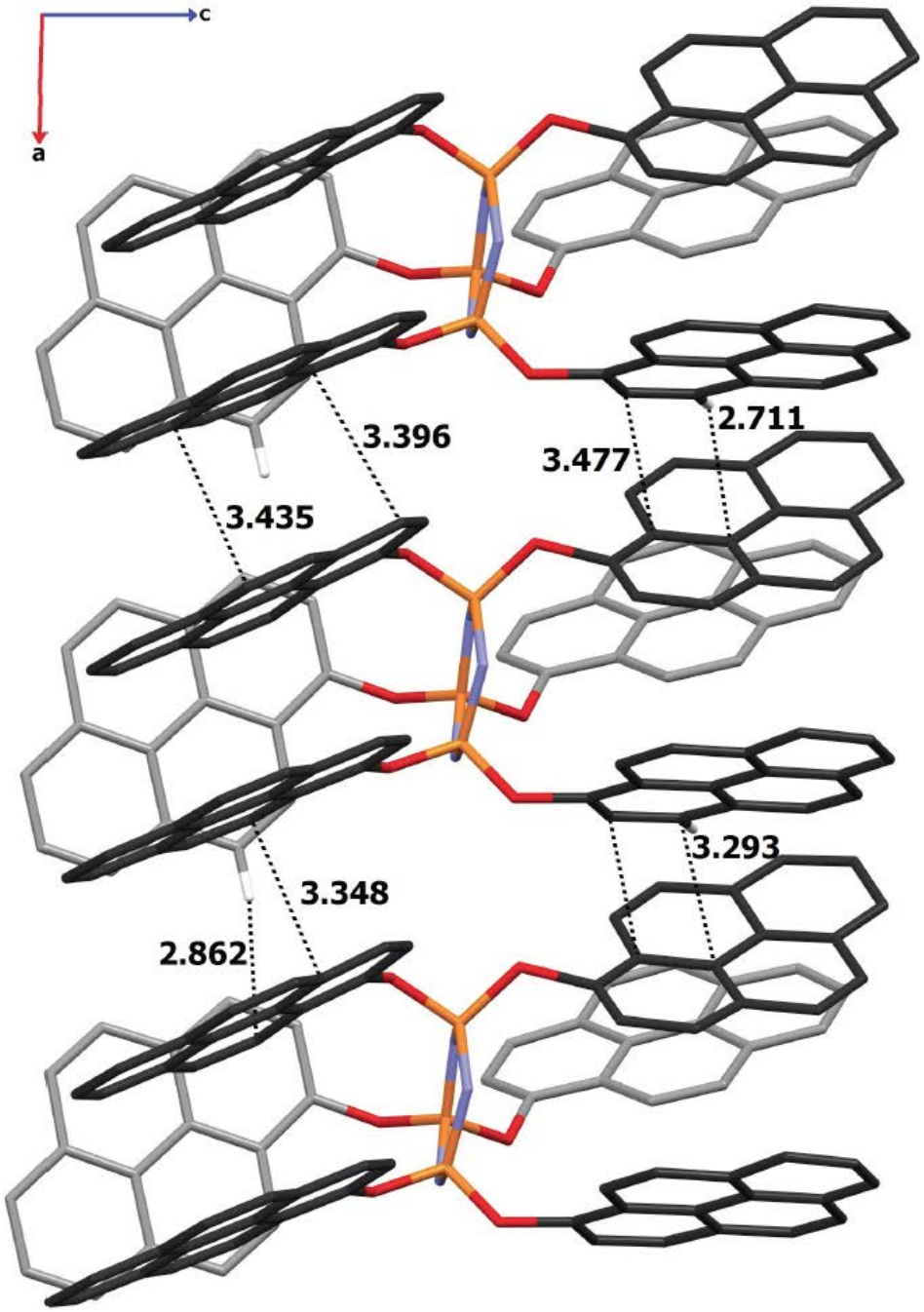

Fig. S9. Intermolecular π-stacking interactions (along *b* axis) between the **HPCT** molecules.

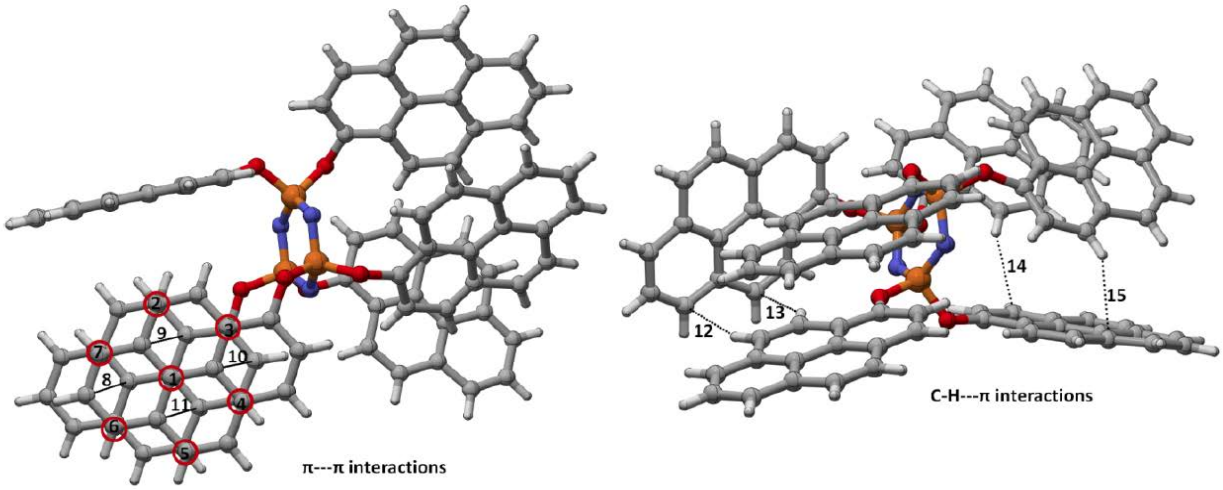

Fig. S10. Noncovalent intramolecular interactions in the **HPCT** structure. 1-11 indicate π---π interactions and 12-15 represent C-H---π interactions.

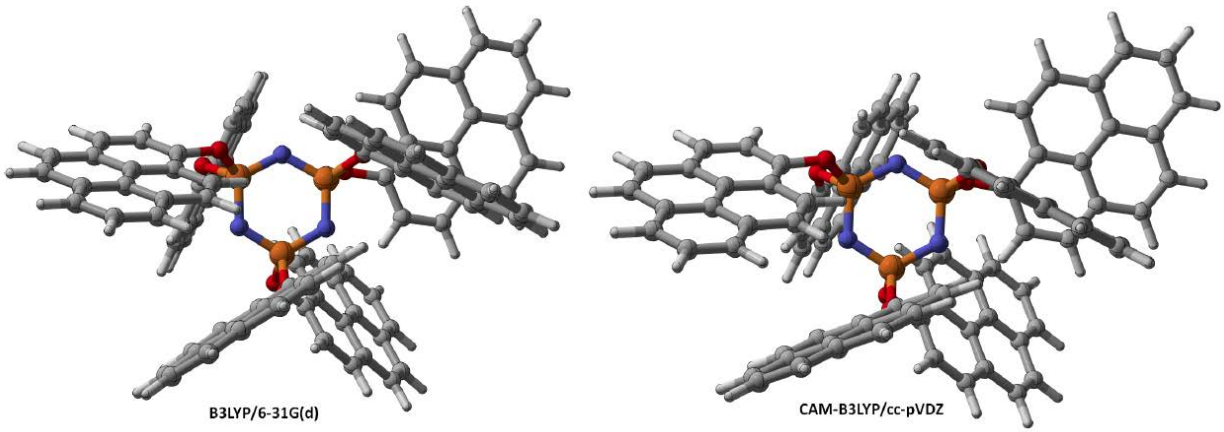

Fig. S11. Optimized geometries of **HPCT** using CAM-B3LYP/cc-pVDZ and B3LYP/6-31G(d) levels.

Table S1. Crystal data and structure refinement details for **HPCT**

Identification code	**12gyte60 (HPCT)**	
Empirical formula	$C_{97}H_{56}Cl_2N_3O_6P_3$	
Formula weight	1523.26	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	*P-1*	
Unit cell dimensions	a = 8.1849(2) Å	α = 80.0900(10)°
	b = 12.4435(3) Å	β = 89.547(2)°
	c = 35.6604(8) Å	γ = 75.642(2)°
Volume	3463.72(14) Å^3	
Z	2	
Density (calculated)	1.461 g / cm^3	
Absorption coefficient	0.230 mm^{-1}	
F(000)	1572	
Crystal	plate; colourless	
Crystal size	0.030 × 0.070 × 0.26 mm^3	
θ range for data collection	3.03 – 25.00°	
Index ranges	-9<=h<=9, -14<=k<=14, -42<=l<=38	
Reflections collected	40430	
Independent reflections	11974 [R(int) = 0.0667]	
Completeness to θ = 27.49°	97.90%	
Absorption correction	multi-scan	
Max. and min. transmission	0.9931 and 0.9425	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11974 / 377 / 1000	
Goodness-of-fit on F^2	1.02	
Final *R* indices [$I>2\sigma(I)$]	*R1 = 0.1004, wR2 = 0.2763*	
R indices (all data)	*R1 = 0.1697, wR2 = 0.3288*	
Largest diff. peak and hole	0.786 and -1.147 eÅ^{-3}	

Table S2. Comparison of inter-plane distances (Å) for π---π interactions.

π---π interactions	1	2	3	4	5	6	7	8	9	10	11
LC-wPBE/cc-pVDZ	4.333	3.978	3.835	4.270	4.770	4.782	4.413	4.173	3.769	3.588	4.039
wB97XD/cc-pVDZ	3.394	3.310	3.403	3.396	3.421	3.376	3.311	3.495	3.491	3.501	3.561
B97D/6-31G(d)	3.324	3.245	3.337	3.327	3.350	3.304	3.243	3.431	3.429	3.444	3.499
MPW1B95/6-31G(d)	3.557	3.524	3.592	3.548	3.560	3.560	3.542	3.794	3.802	3.800	3.817
Experimental	3.497(9)	3.399(9)	3.535(8)	3.607(9)	3.564(11)	3.504(10)	3.428(9)	3.527(9)	3.539(8)	3.590(9)	3.557(9)

Table S.3. Comparison of intramolecular C-H---π interaction distances (Å).

C-H---π interactions	12	13	14	15
LC-wPBE/cc-pVDZ	3.568	3.142	2.951	2.918
wB97XD/cc-pVDZ	2.643	2.849	2.719	2.682
B97D/6-31G(d)	2.620	2.815	2.763	2.640
MPW1B95/6-31G(d)	3.099	3.078	2.952	2.831
Experimental	2.814	2.875	2.762	2.737

Table S4. Calculated HOMO, LUMO, HOMO-LUMO gap (E_g) energies (eV) and the first vertical excitation energy (E_{exc}) (eV) obtained from single point TD-DFT computations for **HPCT**.

	E_{HOMO}	E_{LUMO}	E_g	E_{exc}
sp-TD-CAM-B3LYP/cc-pVDZ//CAM-B3LYP/cc-pVDZ	-6.56	-0.64	5.92	3.88
sp-TD-LC-wPBE/cc-pVDZ//LC-wPBE/cc-pVDZ	-7.64	0.12	7.76	4.13
sp-TD-wB97XD/cc-pVDZ//wB97XD/cc-pVDZ	-6.87	-0.28	6.59	3.72
sp-TD-B3LYP/6-31G(d) //X-ray geometry	-5.07	-1.54	3.53	3.09
sp-TD-B3LYP/6-31G+(d)//X-ray geometry	-5.36	-1.83	3.54	3.10
sp-TD-B97D/TZVP//X-ray geometry	-4.72	-2.34	2.38	2.39
MPW1B95/6-31G(d)	-5.27	-1.35	3.92	-
sp-TD-B3LYP/6-31G(d)//MPW1B95/6-31G(d)	-4.94	-1.61	3.33	2.90
sp-TD-B97D/TZVP//MPW1B95/6-31G(d)	-4.61	-2.41	2.20	2.20
B97D/6-31G(d)	-4.27	-2.29	1.98	-
sp-TD-B97D/TZVP//B97D/6-31G(d)	-4.60	-2.60	2.00	2.00
Experimental (CV)	-5.62	-3.03	2.59	
Experimental (UV)			3.45	

Table S5. Total energies (au)

	E
CAM-B3LYP/cc-pVDZ	**-5328.77530183**
LC-wPBE/cc-pVDZ	**-5327.58317127**
wB97XD/cc-pVDZ	**-5329.74978400**
B3LYP/6-31G(d)	**-5330.84750803**
B97D/6-31G(d)	**-5327.65988436**
MPW1B95/6-31G(d)	**-5329.19088080**

Cartesian Coordinates

CAM-B3LYP/cc-pVDZ

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.918370	0.384225	-0.942927
2	8	0	2.539722	0.317171	-1.026346
3	6	0	3.368153	1.366614	-0.632364
4	6	0	4.098522	2.023818	-1.629451
5	6	0	4.995105	3.051229	-1.231096
6	6	0	5.758319	3.746065	-2.219555
7	6	0	5.620499	3.408404	-3.592866
8	6	0	4.703529	2.359540	-3.957056
9	6	0	3.976714	1.697711	-3.025576
10	6	0	6.376969	4.102529	-4.544092
11	6	0	7.253494	5.109607	-4.156059
12	6	0	7.393629	5.444656	-2.813611
13	6	0	6.656521	4.776445	-1.829617
14	6	0	6.776145	5.097192	-0.430234
15	6	0	6.052035	4.439416	0.505860
16	6	0	5.132320	3.392868	0.141623
17	6	0	4.375271	2.699390	1.091291
18	6	0	3.498636	1.690404	0.711291
19	8	0	0.718905	1.843831	-1.647727
20	6	0	-0.515923	2.463679	-1.786482
21	6	0	-0.663236	3.735391	-1.218157
22	6	0	-1.898407	4.411567	-1.406180
23	6	0	-2.948751	3.799396	-2.142031
24	6	0	-2.741420	2.529065	-2.688312
25	6	0	-1.531966	1.864726	-2.522012
26	6	0	-4.190291	4.511109	-2.300343
27	6	0	-4.369660	5.741390	-1.763250
28	6	0	-3.325054	6.387840	-1.009922
29	6	0	-2.087490	5.709113	-0.837088
30	6	0	-1.042191	6.319648	-0.092192
31	6	0	0.196668	5.604437	0.072557
32	6	0	0.382179	4.373498	-0.461776

33	6	0	-1.249919	7.590161	0.457359
34	6	0	-2.461195	8.249641	0.281774
35	6	0	-3.489727	7.656640	-0.442666
36	7	0	0.388696	-0.801337	-1.884390
37	15	0	-0.647300	-1.902347	-1.345031
38	8	0	-0.105154	-3.399546	-1.726528
39	6	0	0.902635	-4.025831	-0.997039
40	6	0	2.200440	-4.046148	-1.524326
41	6	0	3.193676	-4.774446	-0.813445
42	6	0	4.530450	-4.824113	-1.317830
43	6	0	5.531691	-5.542842	-0.609198
44	6	0	5.168833	-6.211249	0.614037
45	6	0	3.902819	-6.163731	1.091565
46	6	0	2.867327	-5.444365	0.396617
47	6	0	1.555080	-5.378043	0.877159
48	6	0	0.576812	-4.675918	0.186448
49	6	0	6.834965	-5.575914	-1.118924
50	6	0	7.151464	-4.916779	-2.301874
51	6	0	6.176827	-4.211755	-2.999501
52	6	0	4.861440	-4.152306	-2.525581
53	6	0	3.827741	-3.426637	-3.217066
54	6	0	2.560010	-3.371820	-2.744632
55	8	0	-1.917171	-1.828631	-2.355137
56	6	0	-2.983600	-2.728520	-2.376017
57	6	0	-4.235461	-2.275029	-1.944273
58	6	0	-5.340506	-3.162711	-2.059510
59	6	0	-5.163116	-4.467946	-2.592297
60	6	0	-3.887878	-4.860823	-3.010924
61	6	0	-2.804886	-3.998017	-2.910622
62	6	0	-6.305479	-5.338953	-2.690119
63	6	0	-7.533306	-4.936297	-2.285830
64	6	0	-7.746290	-3.619744	-1.742208
65	6	0	-6.637291	-2.736932	-1.635655
66	6	0	-6.820323	-1.431791	-1.105332
67	6	0	-5.680177	-0.557732	-1.013552
68	6	0	-4.447961	-0.955813	-1.410021
69	6	0	-8.095765	-1.038037	-0.685305
70	6	0	-9.175569	-1.907486	-0.791089
71	6	0	-9.006020	-3.183980	-1.316025
72	7	0	-1.107039	-1.851288	0.196258
73	15	0	-0.425008	-0.799019	1.199635
74	7	0	0.378316	0.450110	0.574888
75	8	0	0.509472	-1.672863	2.214134
76	6	0	1.382176	-1.092408	3.130794
77	6	0	2.756227	-1.272894	2.925161
78	6	0	3.287535	-1.984648	1.792993
79	6	0	4.623722	-2.134083	1.631208
80	6	0	5.561612	-1.588916	2.577162
81	6	0	5.061701	-0.884659	3.705387
82	6	0	3.652451	-0.728039	3.885208
83	6	0	3.155319	-0.024923	5.015818
84	6	0	1.772416	0.111324	5.173387
85	6	0	0.889402	-0.420029	4.242097
86	6	0	4.095109	0.518536	5.962132
87	6	0	5.430316	0.371335	5.791102
88	6	0	5.965327	-0.336638	4.656247
89	6	0	7.340999	-0.501879	4.460983
90	6	0	7.823244	-1.192749	3.354363
91	6	0	6.945136	-1.732024	2.421093
92	8	0	-1.510214	-0.270520	2.293008
93	6	0	-2.552686	0.620254	2.047897
94	6	0	-2.287022	1.929838	1.669686
95	6	0	-3.337086	2.828765	1.530998
96	6	0	-4.656033	2.441804	1.787654
97	6	0	-4.916312	1.104186	2.190072
98	6	0	-3.852397	0.170365	2.312133
99	6	0	-4.144832	-1.181065	2.710015
100	6	0	-5.415590	-1.564866	2.977574
101	6	0	-6.518470	-0.644862	2.876456
102	6	0	-6.255032	0.692226	2.474324
103	6	0	-7.325087	1.621031	2.354935
104	6	0	-7.029642	2.967589	1.935370
105	6	0	-5.761271	3.356921	1.663962
106	6	0	-8.627622	1.198902	2.646388
107	6	0	-8.877140	-0.110384	3.044640
108	6	0	-7.835894	-1.024796	3.156605
109	1	0	4.603501	2.106266	-5.014562

110	1	0	3.288336	0.903820	-3.311264
111	1	0	6.270342	3.843562	-5.599465
112	1	0	7.835695	5.641539	-4.910564
113	1	0	8.083424	6.236662	-2.514784
114	1	0	7.469851	5.888694	-0.139112
115	1	0	6.153136	4.691589	1.563531
116	1	0	4.481585	2.948721	2.148599
117	1	0	2.912775	1.145631	1.449240
118	1	0	-3.541785	2.053329	-3.257987
119	1	0	-1.367298	0.881654	-2.962152
120	1	0	-4.990294	4.032127	-2.868475
121	1	0	-5.316153	6.270161	-1.893627
122	1	0	0.996261	6.080320	0.643819
123	1	0	1.325315	3.845012	-0.331816
124	1	0	-0.446407	8.059632	1.028338
125	1	0	-2.606571	9.240100	0.716499
126	1	0	-4.438971	8.179562	-0.576302
127	1	0	5.943991	-6.759566	1.153236
128	1	0	3.641931	-6.671773	2.022060
129	1	0	1.300588	-5.884668	1.809649
130	1	0	-0.445855	-4.613223	0.555121
131	1	0	7.603958	-6.128841	-0.575531
132	1	0	8.172588	-4.952724	-2.685449
133	1	0	6.431187	-3.694124	-3.926524
134	1	0	4.092110	-2.906848	-4.140147
135	1	0	1.793753	-2.801276	-3.265824
136	1	0	-3.745691	-5.859277	-3.428557
137	1	0	-1.812920	-4.295768	-3.244276
138	1	0	-6.157285	-6.339602	-3.101526
139	1	0	-8.390840	-5.607714	-2.365840
140	1	0	-5.827192	0.442870	-0.603717
141	1	0	-3.596036	-0.283641	-1.325133
142	1	0	-8.231805	-0.041469	-0.261419
143	1	0	-10.163200	-1.585604	-0.456289
144	1	0	-9.858032	-3.862204	-1.397886
145	1	0	2.592610	-2.409001	1.071247
146	1	0	5.012511	-2.680049	0.769775
147	1	0	1.383062	0.642606	6.043887
148	1	0	-0.187631	-0.320033	4.364247
149	1	0	3.702864	1.055803	6.828201
150	1	0	6.131195	0.788314	6.517381
151	1	0	8.035641	-0.080584	5.190673
152	1	0	8.899471	-1.311657	3.217321
153	1	0	7.326725	-2.273398	1.553191
154	1	0	-1.257257	2.233332	1.489952
155	1	0	-3.129395	3.855276	1.226461
156	1	0	-3.319817	-1.887748	2.782963
157	1	0	-5.628098	-2.593830	3.274362
158	1	0	-7.858028	3.672940	1.841379
159	1	0	-5.548597	4.379035	1.344370
160	1	0	-9.449345	1.912997	2.560030
161	1	0	-9.898482	-0.422853	3.269303
162	1	0	-8.038455	-2.053026	3.462262

LC-wPBE /cc-pVDZ

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.748766	0.274325	-0.950242
2	8	0	2.366307	0.236685	-1.033830
3	6	0	3.254843	1.258168	-0.748997
4	6	0	4.482042	1.189110	-1.414945
5	6	0	5.457971	2.168473	-1.126661
6	6	0	6.729102	2.115993	-1.782296
7	6	0	7.006221	1.084042	-2.708912
8	6	0	5.987979	0.096406	-2.970137
9	6	0	4.786884	0.143571	-2.358827
10	6	0	8.252466	1.049243	-3.337354

11	6	0	9.210574	2.013159	-3.059922
12	6	0	8.944852	3.026641	-2.149207
13	6	0	7.711821	3.094125	-1.499418
14	6	0	7.406229	4.130351	-0.541759
15	6	0	6.212521	4.172918	0.082471
16	6	0	5.191148	3.191250	-0.187430
17	6	0	3.953736	3.209387	0.452042
18	6	0	2.988741	2.249478	0.182920
19	8	0	0.487691	1.535036	-1.948094
20	6	0	-0.793647	1.933619	-2.300313
21	6	0	-1.213581	3.208096	-1.913660
22	6	0	-2.497180	3.639023	-2.320202
23	6	0	-3.323812	2.794859	-3.097075
24	6	0	-2.848111	1.537965	-3.468687
25	6	0	-1.589434	1.106272	-3.078557
26	6	0	-4.631930	3.264534	-3.483735
27	6	0	-5.074889	4.482735	-3.114258
28	6	0	-4.255110	5.366740	-2.320428
29	6	0	-2.964269	4.935341	-1.933215
30	6	0	-2.140608	5.782493	-1.155187
31	6	0	-0.829836	5.314551	-0.773718
32	6	0	-0.386006	4.092609	-1.132607
33	6	0	-2.618862	7.038140	-0.776495
34	6	0	-3.886538	7.455156	-1.156583
35	6	0	-4.698034	6.629043	-1.922050
36	7	0	0.261801	-1.102675	-1.601715
37	15	0	-0.658799	-2.130193	-0.789759
38	8	0	-0.006838	-3.628542	-0.884261
39	6	0	1.145344	-3.930335	-0.168405
40	6	0	2.364996	-3.968923	-0.848285
41	6	0	3.517020	-4.351101	-0.121471
42	6	0	4.785497	-4.404944	-0.783120
43	6	0	5.945164	-4.770765	-0.060067
44	6	0	5.819113	-5.085109	1.342814
45	6	0	4.623767	-5.041077	1.963875
46	6	0	3.423766	-4.673936	1.252644
47	6	0	2.178887	-4.619241	1.880187
48	6	0	1.043187	-4.251534	1.176665
49	6	0	7.173284	-4.816807	-0.721660
50	6	0	7.260354	-4.512978	-2.072769
51	6	0	6.125436	-4.155543	-2.786906
52	6	0	4.880569	-4.093005	-2.159337
53	6	0	3.681566	-3.717282	-2.868857
54	6	0	2.485737	-3.652112	-2.249839
55	8	0	-1.971410	-2.362787	-1.707989
56	6	0	-3.050309	-3.173341	-1.372799
57	6	0	-4.297332	-2.559126	-1.244228
58	6	0	-5.427193	-3.384003	-1.036184
59	6	0	-5.280664	-4.786168	-0.926199
60	6	0	-4.008056	-5.343977	-1.044231
61	6	0	-2.898270	-4.548028	-1.280158
62	6	0	-6.456799	-5.594807	-0.716281
63	6	0	-7.682818	-5.039183	-0.643688
64	6	0	-7.866552	-3.613401	-0.770530
65	6	0	-6.728808	-2.793911	-0.957247
66	6	0	-6.880677	-1.393666	-1.082855
67	6	0	-5.702059	-0.581234	-1.261107
68	6	0	-4.473928	-1.131739	-1.338751
69	6	0	-8.159861	-0.839828	-1.032151
70	6	0	-9.273297	-1.649023	-0.857705
71	6	0	-9.130193	-3.022434	-0.723774
72	7	0	-1.049407	-1.800073	0.729558
73	15	0	-0.452857	-0.493726	1.438487
74	7	0	0.201303	0.646099	0.514106
75	8	0	0.591656	-1.011141	2.577875
76	6	0	1.456362	-0.104053	3.183302
77	6	0	2.799235	-0.120655	2.800937
78	6	0	3.316926	-1.043234	1.822836
79	6	0	4.611136	-0.996734	1.448445
80	6	0	5.518518	-0.021851	2.000521
81	6	0	5.040911	0.871069	2.987083
82	6	0	3.672439	0.816156	3.401070
83	6	0	3.192842	1.717895	4.379981
84	6	0	1.849968	1.662090	4.753040
85	6	0	0.981807	0.759844	4.157152
86	6	0	4.110382	2.673405	4.952801
87	6	0	5.397484	2.731037	4.555664

88	6	0	5.911638	1.834564	3.547706
89	6	0	7.233144	1.896031	3.105242
90	6	0	7.693691	1.024224	2.128100
91	6	0	6.847190	0.070375	1.582941
92	8	0	-1.563942	0.167902	2.419700
93	6	0	-2.642332	0.931325	1.986873
94	6	0	-2.428623	2.221035	1.527753
95	6	0	-3.514325	3.021817	1.212011
96	6	0	-4.818735	2.555348	1.376186
97	6	0	-5.025431	1.239412	1.851130
98	6	0	-3.923985	0.400844	2.141434
99	6	0	-4.160973	-0.945836	2.597828
100	6	0	-5.417547	-1.400755	2.773963
101	6	0	-6.565390	-0.561797	2.528986
102	6	0	-6.356177	0.754814	2.056923
103	6	0	-7.463005	1.597977	1.801030
104	6	0	-7.220378	2.929860	1.299847
105	6	0	-5.966959	3.381698	1.092393
106	6	0	-8.752028	1.119308	2.041487
107	6	0	-8.950508	-0.170593	2.512826
108	6	0	-7.869256	-1.007655	2.747259
109	1	0	6.213422	-0.701970	-3.679737
110	1	0	4.025185	-0.609728	-2.556679
111	1	0	8.465696	0.252685	-4.053042
112	1	0	10.179766	1.974588	-3.560301
113	1	0	9.702589	3.782686	-1.933286
114	1	0	8.170812	4.880645	-0.330554
115	1	0	5.993869	4.956851	0.810279
116	1	0	3.745859	3.982126	1.194564
117	1	0	2.040206	2.246487	0.719226
118	1	0	-3.477185	0.883742	-4.075081
119	1	0	-1.213407	0.125207	-3.367187
120	1	0	-5.259521	2.604186	-4.085564
121	1	0	-6.067732	4.825981	-3.411413
122	1	0	-0.194940	5.979990	-0.185327
123	1	0	0.609523	3.752320	-0.850584
124	1	0	-1.982746	7.691656	-0.176202
125	1	0	-4.247128	8.439578	-0.853544
126	1	0	-5.693613	6.962959	-2.221401
127	1	0	6.720230	-5.361157	1.893841
128	1	0	4.541035	-5.279323	3.025907
129	1	0	2.101929	-4.863557	2.940958
130	1	0	0.067997	-4.196715	1.658708
131	1	0	8.068517	-5.097975	-0.163444
132	1	0	8.227280	-4.556297	-2.576834
133	1	0	6.197512	-3.920463	-3.850817
134	1	0	3.763305	-3.479404	-3.931494
135	1	0	1.590241	-3.351190	-2.790954
136	1	0	-3.888016	-6.426348	-0.969031
137	1	0	-1.908318	-4.983048	-1.405484
138	1	0	-6.330587	-6.675545	-0.624993
139	1	0	-8.566185	-5.662891	-0.492342
140	1	0	-5.823640	0.502050	-1.326749
141	1	0	-3.593785	-0.505352	-1.474047
142	1	0	-8.274265	0.241592	-1.124563
143	1	0	-10.267759	-1.201135	-0.820069
144	1	0	-10.008969	-3.655475	-0.584164
145	1	0	2.642142	-1.782759	1.394290
146	1	0	4.993479	-1.698700	0.704804
147	1	0	1.476448	2.346808	5.516815
148	1	0	-0.071738	0.719822	4.431208
149	1	0	3.733499	3.357425	5.716034
150	1	0	6.079831	3.463214	4.992583
151	1	0	7.903797	2.644340	3.532612
152	1	0	8.726737	1.091850	1.783459
153	1	0	7.210308	-0.612423	0.812384
154	1	0	-1.407872	2.586821	1.427522
155	1	0	-3.348438	4.036045	0.845603
156	1	0	-3.301368	-1.588519	2.782544
157	1	0	-5.589787	-2.424430	3.111621
158	1	0	-8.081411	3.568953	1.093100
159	1	0	-5.793002	4.390063	0.711219
160	1	0	-9.606428	1.773202	1.853969
161	1	0	-9.964175	-0.532006	2.693974
162	1	0	-8.030495	-2.025634	3.106739

wB97XD/cc-pVDZ

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.658604	0.465673	-1.134600
2	8	0	2.279497	0.430621	-1.201100
3	6	0	3.167694	1.419774	-0.816698
4	6	0	4.509797	1.145049	-1.115332
5	6	0	5.488781	2.105186	-0.750606
6	6	0	6.868371	1.844541	-1.019870
7	6	0	7.253773	0.621225	-1.630685
8	6	0	6.232734	-0.333189	-1.978077
9	6	0	4.921840	-0.084396	-1.741285
10	6	0	8.613148	0.369761	-1.855963
11	6	0	9.576363	1.306395	-1.492992
12	6	0	9.204121	2.510536	-0.900764
13	6	0	7.856246	2.798656	-0.653684
14	6	0	7.437422	4.024980	-0.020990
15	6	0	6.130814	4.265894	0.244334
16	6	0	5.109284	3.312310	-0.104225
17	6	0	3.759459	3.520319	0.189707
18	6	0	2.791527	2.583584	-0.154550
19	8	0	0.369339	1.634478	-2.238121
20	6	0	-0.951669	1.929736	-2.554814
21	6	0	-1.532207	3.079384	-2.004455
22	6	0	-2.882937	3.367918	-2.335688
23	6	0	-3.599791	2.527292	-3.228985
24	6	0	-2.957522	1.408933	-3.773165
25	6	0	-1.644755	1.103117	-3.432336
26	6	0	-4.974832	2.843359	-3.526988
27	6	0	-5.598526	3.893274	-2.938553
28	6	0	-4.901997	4.752064	-2.012553
29	6	0	-3.530528	4.494815	-1.739696
30	6	0	-2.816331	5.334015	-0.841165
31	6	0	-1.429321	5.043234	-0.576159
32	6	0	-0.816079	3.967723	-1.126695
33	6	0	-3.485209	6.399034	-0.224251
34	6	0	-4.833053	6.633985	-0.480553
35	6	0	-5.535722	5.822469	-1.367574
36	7	0	0.174247	-0.959387	-1.686537
37	15	0	-0.660003	-1.937365	-0.723838
38	8	0	-0.055152	-3.454552	-0.870248
39	6	0	1.175894	-3.743453	-0.292000
40	6	0	2.330595	-3.702452	-1.086053
41	6	0	3.562822	-4.081765	-0.484879
42	6	0	4.766361	-4.052502	-1.258938
43	6	0	6.006868	-4.405636	-0.659232
44	6	0	6.019941	-4.798599	0.728469
45	6	0	4.877603	-4.839227	1.457356
46	6	0	3.607419	-4.480208	0.879079
47	6	0	2.422011	-4.489736	1.624743
48	6	0	1.213933	-4.123044	1.045731
49	6	0	7.174351	-4.367329	-1.434176
50	6	0	7.122797	-4.009509	-2.778283
51	6	0	5.910365	-3.667516	-3.372401
52	6	0	4.723735	-3.673419	-2.628283
53	6	0	3.455282	-3.302235	-3.203889
54	6	0	2.314102	-3.311188	-2.473395
55	8	0	-2.095714	-2.150075	-1.447376
56	6	0	-3.205126	-2.744165	-0.862445
57	6	0	-4.405066	-2.024669	-0.934596
58	6	0	-5.603258	-2.688522	-0.559171
59	6	0	-5.560337	-4.008572	-0.035603
60	6	0	-4.320070	-4.643923	0.095392
61	6	0	-3.149690	-4.029656	-0.336843
62	6	0	-6.800068	-4.659609	0.305176
63	6	0	-7.993326	-4.050924	0.098283
64	6	0	-8.069235	-2.719562	-0.448905
65	6	0	-6.860173	-2.035026	-0.748441

66	6	0	-6.902133	-0.711046	-1.260429
67	6	0	-5.660648	-0.034554	-1.533349
68	6	0	-4.467723	-0.662363	-1.395087
69	6	0	-8.144695	-0.104739	-1.482344
70	6	0	-9.325408	-0.787301	-1.208443
71	6	0	-9.290270	-2.080162	-0.692362
72	7	0	-0.832198	-1.587258	0.833034
73	15	0	-0.332163	-0.155977	1.365346
74	7	0	0.096844	0.963282	0.289683
75	8	0	0.862811	-0.446692	2.433268
76	6	0	1.835177	0.507118	2.711150
77	6	0	3.155423	0.200127	2.360112
78	6	0	3.512722	-1.002365	1.652944
79	6	0	4.807297	-1.262454	1.349406
80	6	0	5.866923	-0.365045	1.724847
81	6	0	5.535085	0.839795	2.398408
82	6	0	4.171502	1.128672	2.715330
83	6	0	3.838982	2.342645	3.374401
84	6	0	2.497199	2.605559	3.676057
85	6	0	1.499633	1.691189	3.356451
86	6	0	4.897379	3.262375	3.709023
87	6	0	6.190907	2.983716	3.414959
88	6	0	6.559770	1.758133	2.752504
89	6	0	7.888570	1.446947	2.440021
90	6	0	8.208572	0.258086	1.791134
91	6	0	7.208026	-0.638631	1.430978
92	8	0	-1.435280	0.467973	2.379913
93	6	0	-2.693205	0.869238	1.929723
94	6	0	-2.834594	2.138290	1.382551
95	6	0	-4.103846	2.617176	1.080398
96	6	0	-5.239844	1.842007	1.333192
97	6	0	-5.083147	0.536936	1.873103
98	6	0	-3.787506	0.022814	2.152972
99	6	0	-3.656058	-1.316456	2.668757
100	6	0	-4.753604	-2.071480	2.916855
101	6	0	-6.084163	-1.562059	2.703696
102	6	0	-6.236207	-0.255018	2.167818
103	6	0	-7.536042	0.274847	1.945303
104	6	0	-7.661929	1.595295	1.379882
105	6	0	-6.569205	2.338012	1.079418
106	6	0	-8.652199	-0.499902	2.281250
107	6	0	-8.496867	-1.774930	2.816101
108	6	0	-7.227559	-2.307033	3.017149
109	1	0	6.535968	-1.279189	-2.429090
110	1	0	4.159611	-0.819297	-1.998183
111	1	0	8.908540	-0.574844	-2.318101
112	1	0	10.632312	1.097451	-1.675156
113	1	0	9.965294	3.241055	-0.618153
114	1	0	8.202197	4.755091	0.252770
115	1	0	5.826553	5.190785	0.738785
116	1	0	3.458988	4.427665	0.716846
117	1	0	1.754996	2.735913	0.138596
118	1	0	-3.505735	0.753303	-4.451875
119	1	0	-1.150120	0.214804	-3.823102
120	1	0	-5.513486	2.200115	-4.226243
121	1	0	-6.646376	4.108864	-3.158595
122	1	0	-0.876747	5.709688	0.089374
123	1	0	0.232124	3.758760	-0.923088
124	1	0	-2.938199	7.041267	0.468971
125	1	0	-5.341719	7.463083	0.014331
126	1	0	-6.591566	6.016359	-1.568834
127	1	0	6.976116	-5.063547	1.184358
128	1	0	4.902523	-5.133142	2.508585
129	1	0	2.452537	-4.778548	2.676777
130	1	0	0.288656	-4.112182	1.620804
131	1	0	8.127757	-4.633973	-0.973221
132	1	0	8.039635	-3.995867	-3.370563
133	1	0	5.876049	-3.382573	-4.426092
134	1	0	3.430826	-3.002708	-4.253719
135	1	0	1.368021	-3.008069	-2.917320
136	1	0	-4.275904	-5.655671	0.503608
137	1	0	-2.194958	-4.553099	-0.300069
138	1	0	-6.757759	-5.669171	0.720217
139	1	0	-8.925935	-4.562983	0.345233
140	1	0	-5.697209	1.007375	-1.853992
141	1	0	-3.538264	-0.139213	-1.615074
142	1	0	-8.173818	0.915356	-1.871136

143	1	0	-10.286834	-0.303817	-1.391682
144	1	0	-10.221013	-2.605883	-0.468020
145	1	0	2.723706	-1.693748	1.359089
146	1	0	5.074664	-2.162205	0.798183
147	1	0	2.233740	3.536433	4.182367
148	1	0	0.455972	1.881267	3.608301
149	1	0	4.632921	4.195175	4.212350
150	1	0	6.981726	3.690807	3.674263
151	1	0	8.676102	2.156546	2.702355
152	1	0	9.248356	0.040893	1.542575
153	1	0	7.454728	-1.559841	0.898395
154	1	0	-1.946304	2.746485	1.213460
155	1	0	-4.221730	3.619026	0.667476
156	1	0	-2.657868	-1.717017	2.836004
157	1	0	-4.643699	-3.089854	3.295340
158	1	0	-8.665554	1.984007	1.194121
159	1	0	-6.670900	3.336095	0.646222
160	1	0	-9.651272	-0.093417	2.111558
161	1	0	-9.378692	-2.367522	3.066905
162	1	0	-7.111398	-3.313542	3.423925

B3LYP/6-31G(d)

Row	Highlight		Display	Tag	Symbol	X	Y	Z
1	No	Show	1	P		0.9231180	0.5376340	-0.9308200
2	No	Show	2	O		2.5358930	0.4690850	-0.9922180
3	No	Show	3	C		3.3919830	1.5041810	-0.5992530
4	No	Show	4	C		4.1862600	2.1012140	-1.5931490
5	No	Show	5	C		5.1117580	3.1113310	-1.1880430
6	No	Show	6	C		5.9344270	3.7485010	-2.1648170
7	No	Show	7	C		5.8324520	3.3769090	-3.5400020
8	No	Show	8	C		4.8927220	2.3539720	-3.9072770
9	No	Show	9	C		4.1045620	1.7415770	-2.9810460
10	No	Show	10	C		6.6509980	4.0198670	-4.4827180
11	No	Show	11	C		7.5521560	5.0069810	-4.0882420
12	No	Show	12	C		7.6585360	5.3751150	-2.7479850
13	No	Show	13	C		6.8614400	4.7611890	-1.7686490
14	No	Show	14	C		6.9435820	5.1150060	-0.3777350

15	No	Show	15	C	6.1585540	4.5075400	0.5538430
16	No	Show	16	C	5.2152360	3.4877310	0.1861760
17	No	Show	17	C	4.3954350	2.8473120	1.1278040
18	No	Show	18	C	3.4925640	1.8590170	0.7431200
19	No	Show	19	O	0.7299720	1.9976440	-1.6124930
20	No	Show	20	C	-0.5013570	2.6309190	-1.7807620
21	No	Show	21	C	-0.6704900	3.8909180	-1.1792560
22	No	Show	22	C	-1.9032930	4.5777200	-1.4064980
23	No	Show	23	C	-2.9207960	3.9883790	-2.2183250
24	No	Show	24	C	-2.6829320	2.7325640	-2.7974470
25	No	Show	25	C	-1.4807630	2.0602780	-2.5912200
26	No	Show	26	C	-4.1506980	4.7055700	-2.4138390
27	No	Show	27	C	-4.3572120	5.9255290	-1.8449830
28	No	Show	28	C	-3.3521000	6.5478300	-1.0263440
29	No	Show	29	C	-2.1188650	5.8577410	-0.8117520
30	No	Show	30	C	-1.1039120	6.4512580	-0.0004940
31	No	Show	31	C	0.1229950	5.7316120	0.2005230
32	No	Show	32	C	0.3347210	4.5080690	-0.3588390
33	No	Show	33	C	-1.3389370	7.7119440	0.5718600
34	No	Show	34	C	-2.5434780	8.3787770	0.3564370
35	No	Show	35	C	-3.5402710	7.8060010	-0.4319290
36	No	Show	36	N	0.4043350	-0.6402750	-1.8780000
37	No	Show	37	P	-0.6056950	-1.7757300	-1.3784870
38	No	Show	38	O	-0.0529850	-3.2441590	-1.8023890
39	No	Show	39	C	0.9404830	-3.9386530	-1.1053180
40	No	Show	40	C	2.2279760	-4.0100700	-1.6664830
41	No	Show	41	C	3.1982480	-4.8209040	-0.9987390
42	No	Show	42	C	4.5168500	-4.9304680	-1.5352670
43	No	Show	43	C	5.4931680	-5.7388960	-0.8748680
44	No	Show	44	C	5.1172020	-6.4286860	0.3290680

45	No	Show	45	C	3.8599670	-6.3242560	0.8406470
46	No	Show	46	C	2.8559210	-5.5214230	0.1986070
47	No	Show	47	C	1.5529360	-5.4014130	0.7067780
48	No	Show	48	C	0.5990990	-4.6222970	0.0589680
49	No	Show	49	C	6.7831150	-5.8320750	-1.4221960
50	No	Show	50	C	7.1124610	-5.1491570	-2.5918030
51	No	Show	51	C	6.1661610	-4.3588750	-3.2417970
52	No	Show	52	C	4.8631630	-4.2342140	-2.7333730
53	No	Show	53	C	3.8608740	-3.4279130	-3.3732900
54	No	Show	54	C	2.6014040	-3.3167180	-2.8681730
55	No	Show	55	O	-1.8759450	-1.6870840	-2.3703260
56	No	Show	56	C	-2.9538880	-2.5801730	-2.4444010
57	No	Show	57	C	-4.2249220	-2.1054750	-2.0766010
58	No	Show	58	C	-5.3395850	-2.9839280	-2.2525690
59	No	Show	59	C	-5.1510330	-4.2955660	-2.7857430
60	No	Show	60	C	-3.8564700	-4.7010250	-3.1429700
61	No	Show	61	C	-2.7669260	-3.8501980	-2.9842950
62	No	Show	62	C	-6.2955000	-5.1495580	-2.9456040
63	No	Show	63	C	-7.5443050	-4.7309140	-2.6020390
64	No	Show	64	C	-7.7691200	-3.4163390	-2.0663080
65	No	Show	65	C	-6.6500390	-2.5441280	-1.8967140
66	No	Show	66	C	-6.8468520	-1.2318440	-1.3698970
67	No	Show	67	C	-5.7046730	-0.3748640	-1.2159890
68	No	Show	68	C	-4.4510680	-0.7885350	-1.5502760
69	No	Show	69	C	-8.1438980	-0.8228530	-1.0201810
70	No	Show	70	C	-9.2292890	-1.6806340	-1.1870390
71	No	Show	71	C	-9.0475890	-2.9617120	-1.7054630
72	No	Show	72	N	-1.0357210	-1.7579430	0.1666020
73	No	Show	73	P	-0.4158810	-0.6980500	1.1925360
74	No	Show	74	N	0.3484770	0.5696370	0.5700420

75	No	Show	75	O	0.5312950	-1.5377370	2.2078310
76	No	Show	76	C	1.3888490	-0.9730270	3.1573530
77	No	Show	77	C	2.7633080	-1.2460350	3.0308940
78	No	Show	78	C	3.3133650	-2.0114030	1.9469760
79	No	Show	79	C	4.6521750	-2.2474290	1.8668270
80	No	Show	80	C	5.5656380	-1.7443880	2.8545530
81	No	Show	81	C	5.0437980	-0.9822940	3.9436690
82	No	Show	82	C	3.6414430	-0.7325700	4.0358320
83	No	Show	83	C	3.1244110	0.0283070	5.1287590
84	No	Show	84	C	1.7416580	0.2539520	5.2011510
85	No	Show	85	C	0.8784570	-0.2460700	4.2304910
86	No	Show	86	C	4.0394890	0.5306630	6.1163040
87	No	Show	87	C	5.3770900	0.2935930	6.0272650
88	No	Show	88	C	5.9291210	-0.4698720	4.9415820
89	No	Show	89	C	7.3045150	-0.7285150	4.8291930
90	No	Show	90	C	7.8054150	-1.4737010	3.7628530
91	No	Show	91	C	6.9489380	-1.9772240	2.7857230
92	No	Show	92	O	-1.5285460	-0.2178860	2.2643100
93	No	Show	93	C	-2.6829430	0.5280780	2.0086980
94	No	Show	94	C	-2.5971020	1.8028560	1.4566860
95	No	Show	95	C	-3.7530620	2.5644250	1.3028460
96	No	Show	96	C	-5.0023140	2.0780070	1.7167780
97	No	Show	97	C	-5.0786140	0.7764990	2.3011210
98	No	Show	98	C	-3.9015630	-0.0197380	2.4464780
99	No	Show	99	C	-4.0078070	-1.3237960	3.0381650
100	No	Show	100	C	-5.2102360	-1.8017810	3.4622120
101	No	Show	101	C	-6.4153160	-1.0301740	3.3356890
102	No	Show	102	C	-6.3357050	0.2676750	2.7451940
103	No	Show	103	C	-7.5183400	1.0573780	2.6022330
104	No	Show	104	C	-7.4096010	2.3595350	2.0015670

105	No	Show	105	C	-6.2095620	2.8463330	1.5796460
106	No	Show	106	C	-8.7427990	0.5374640	3.0517520
107	No	Show	107	C	-8.8108270	-0.7295140	3.6290930
108	No	Show	108	C	-7.6627980	-1.5065230	3.7700990
109	No	Show	109	H	4.8204850	2.0739790	-4.9555280
110	No	Show	110	H	3.4037110	0.9678340	-3.2732840
111	No	Show	111	H	6.5736430	3.7382260	-5.5300530
112	No	Show	112	H	8.1772610	5.4942390	-4.8317460
113	No	Show	113	H	8.3642920	6.1463330	-2.4488000
114	No	Show	114	H	7.6523990	5.8849140	-0.0824450
115	No	Show	115	H	6.2329490	4.7852550	1.6025310
116	No	Show	116	H	4.4744690	3.1195110	2.1769950
117	No	Show	117	H	2.8669770	1.3594500	1.4733160
118	No	Show	118	H	-3.4483850	2.2786930	-3.4212190
119	No	Show	119	H	-1.2947570	1.0971400	-3.0531850
120	No	Show	120	H	-4.9193850	4.2490180	-3.0325530
121	No	Show	121	H	-5.2927850	6.4559160	-2.0054790
122	No	Show	122	H	0.8929360	6.1879250	0.8177410
123	No	Show	123	H	1.2675290	3.9810210	-0.1958830
124	No	Show	124	H	-0.5667170	8.1650110	1.1885990
125	No	Show	125	H	-2.7075870	9.3538000	0.8072640
126	No	Show	126	H	-4.4771690	8.3334100	-0.5942850
127	No	Show	127	H	5.8646440	-7.0410040	0.8277110
128	No	Show	128	H	3.5914490	-6.8503650	1.7533580
129	No	Show	129	H	1.2858240	-5.9291790	1.6183720
130	No	Show	130	H	-0.4086390	-4.5281570	0.4464700
131	No	Show	131	H	7.5268350	-6.4475330	-0.9218160
132	No	Show	132	H	8.1158720	-5.2334490	-3.0003800
133	No	Show	133	H	6.4313850	-3.8281980	-4.1528680
134	No	Show	134	H	4.1320500	-2.8948180	-4.2812360

135	No	Show	135	H	1.8628420	-2.6905310	-3.3545190
136	No	Show	136	H	-3.7048740	-5.6931730	-3.5602670
137	No	Show	137	H	-1.7712860	-4.1601020	-3.2759500
138	No	Show	138	H	-6.1406240	-6.1463740	-3.3515900
139	No	Show	139	H	-8.4000180	-5.3897060	-2.7294610
140	No	Show	140	H	-5.8584590	0.6225680	-0.8138150
141	No	Show	141	H	-3.6039020	-0.1253830	-1.4211300
142	No	Show	142	H	-8.2901680	0.1719440	-0.6077490
143	No	Show	143	H	-10.2259570	-1.3485880	-0.9089310
144	No	Show	144	H	-9.9000120	-3.6246200	-1.8336950
145	No	Show	145	H	2.6401750	-2.4063550	1.1954930
146	No	Show	146	H	5.0520870	-2.8298610	1.0410540
147	No	Show	147	H	1.3377750	0.8242290	6.0337330
148	No	Show	148	H	-0.1897520	-0.0797100	4.2979760
149	No	Show	149	H	3.6363760	1.1083340	6.9447610
150	No	Show	150	H	6.0560000	0.6801840	6.7836430
151	No	Show	151	H	7.9796730	-0.3391220	5.5874220
152	No	Show	152	H	8.8732570	-1.6627910	3.6926940
153	No	Show	153	H	7.3459940	-2.5563410	1.9558100
154	No	Show	154	H	-1.6295580	2.1910010	1.1619400
155	No	Show	155	H	-3.6834790	3.5574050	0.8683190
156	No	Show	156	H	-3.1087320	-1.9210150	3.1380510
157	No	Show	157	H	-5.2769730	-2.7919350	3.9064550
158	No	Show	158	H	-8.3128620	2.9558330	1.8952970
159	No	Show	159	H	-6.1411740	3.8335080	1.1289720
160	No	Show	160	H	-9.6432870	1.1378490	2.9462050
161	No	Show	161	H	-9.7675180	-1.1148900	3.9713110
162	No	Show	162	H	-7.7244920	-2.4949440	4.2186640

B97D/6-31G(d)

Row	Highlight	Display	Tag	Symbol	X	Y	Z
1	No	Show	1	P	0.6796590	0.4589090	-1.2027120
2	No	Show	2	O	2.3038480	0.4443140	-1.1950220
3	No	Show	3	C	3.1796680	1.4535420	-0.7783280
4	No	Show	4	C	4.5421840	1.1992950	-1.0562390
5	No	Show	5	C	5.5024370	2.1870820	-0.6543890
6	No	Show	6	C	6.8923270	1.9634180	-0.9003080
7	No	Show	7	C	7.3240390	0.7472750	-1.5275720
8	No	Show	8	C	6.3346990	-0.2223580	-1.9098530
9	No	Show	9	C	4.9982650	-0.0082680	-1.6904720
10	No	Show	10	C	8.7040990	0.5334740	-1.7335940
11	No	Show	11	C	9.6433400	1.4951380	-1.3383780
12	No	Show	12	C	9.2294090	2.6894470	-0.7323200
13	No	Show	13	C	7.8606450	2.9454260	-0.4999960
14	No	Show	14	C	7.4028970	4.1510910	0.1386160
15	No	Show	15	C	6.0699200	4.3608660	0.3840370
16	No	Show	16	C	5.0795670	3.3911570	0.0029670
17	No	Show	17	C	3.7088170	3.5663410	0.2727850
18	No	Show	18	C	2.7630780	2.6091480	-0.1061810
19	No	Show	19	O	0.4167850	1.6398070	-2.3050370
20	No	Show	20	C	-0.9216050	1.9011620	-2.6474870
21	No	Show	21	C	-1.5716060	3.0045680	-2.0535300
22	No	Show	22	C	-2.9377380	3.2484300	-2.4238680

23	No	Show	23	C	-3.5868570	2.4190310	-3.4004550
24	No	Show	24	C	-2.8699650	1.3459650	-3.9708200
25	No	Show	25	C	-1.5498970	1.0804180	-3.5914770
26	No	Show	26	C	-4.9586690	2.6922700	-3.7403850
27	No	Show	27	C	-5.6600720	3.6947340	-3.1184950
28	No	Show	28	C	-5.0431930	4.5268720	-2.1180410
29	No	Show	29	C	-3.6599770	4.3097700	-1.7951210
30	No	Show	30	C	-3.0127830	5.1440300	-0.8208250
31	No	Show	31	C	-1.6271300	4.9016410	-0.5156610
32	No	Show	32	C	-0.9341250	3.8732940	-1.1017180
33	No	Show	33	C	-3.7606730	6.1551070	-0.1791480
34	No	Show	34	C	-5.1166010	6.3435310	-0.4807960
35	No	Show	35	C	-5.7522110	5.5432880	-1.4406210
36	No	Show	36	N	0.2450250	-0.9744930	-1.7887050
37	No	Show	37	P	-0.6178050	-1.9871100	-0.8783580
38	No	Show	38	O	0.0282170	-3.4920400	-0.9973760
39	No	Show	39	C	1.2554730	-3.7411980	-0.3608470
40	No	Show	40	C	2.4475040	-3.6753290	-1.1170920
41	No	Show	41	C	3.6715380	-4.0401470	-0.4573270
42	No	Show	42	C	4.9053290	-3.9916090	-1.1794370
43	No	Show	43	C	6.1373230	-4.3344120	-0.5227010
44	No	Show	44	C	6.0975290	-4.7289050	0.8615300
45	No	Show	45	C	4.9127780	-4.7812010	1.5518490

46	No	Show	46	C	3.6648610	-4.4404360	0.9224960
47	No	Show	47	C	2.4395480	-4.4634920	1.6225320
48	No	Show	48	C	1.2429200	-4.1179800	0.9873230
49	No	Show	49	C	7.3441680	-4.2699590	-1.2543030
50	No	Show	50	C	7.3446830	-3.8952770	-2.6047020
51	No	Show	51	C	6.1466590	-3.5633790	-3.2534770
52	No	Show	52	C	4.9175990	-3.5940280	-2.5595370
53	No	Show	53	C	3.6721540	-3.2336190	-3.1844040
54	No	Show	54	C	2.4855470	-3.2685300	-2.4967600
55	No	Show	55	O	-2.0059190	-2.2428580	-1.6791120
56	No	Show	56	C	-3.1538340	-2.7890470	-1.0799370
57	No	Show	57	C	-4.3067420	-1.9763630	-1.0549540
58	No	Show	58	C	-5.5405510	-2.5925030	-0.6538930
59	No	Show	59	C	-5.5639140	-3.9594490	-0.2150500
60	No	Show	60	C	-4.3558550	-4.6898510	-0.1940010
61	No	Show	61	C	-3.1609030	-4.1187180	-0.6449260
62	No	Show	62	C	-6.8247380	-4.5460840	0.1538170
63	No	Show	63	C	-7.9945210	-3.8344990	0.0611720
64	No	Show	64	C	-8.0049890	-2.4713140	-0.3968130
65	No	Show	65	C	-6.7564290	-1.8465010	-0.7294160
66	No	Show	66	C	-6.7333240	-0.4790850	-1.1620160
67	No	Show	67	C	-5.4669440	0.1306850	-1.4609440
68	No	Show	68	C	-4.2993180	-0.5872560	-1.4256470

69	No	Show	69	C	-7.9511820	0.2224770	-1.2832000
70	No	Show	70	C	-9.1683900	-0.4019230	-0.9835580
71	No	Show	71	C	-9.1968140	-1.7288530	-0.5352560
72	No	Show	72	N	-0.8857680	-1.6371420	0.6727010
73	No	Show	73	P	-0.3905100	-0.2182770	1.2558660
74	No	Show	74	N	0.0319980	0.9305160	0.1995790
75	No	Show	75	O	0.8135660	-0.5327770	2.3152680
76	No	Show	76	C	1.7759090	0.4452290	2.6263610
77	No	Show	77	C	3.1182550	0.1589600	2.2962800
78	No	Show	78	C	3.5189640	-1.0249070	1.5855110
79	No	Show	79	C	4.8405750	-1.2535600	1.3016910
80	No	Show	80	C	5.8688050	-0.3373000	1.7067170
81	No	Show	81	C	5.4912810	0.8629580	2.3945260
82	No	Show	82	C	4.1161680	1.1165470	2.6875510
83	No	Show	83	C	3.7409920	2.3282110	3.3602210
84	No	Show	84	C	2.3765190	2.5592210	3.6376540
85	No	Show	85	C	1.4001290	1.6220180	3.2835940
86	No	Show	86	C	4.7702240	3.2642290	3.7276760
87	No	Show	87	C	6.0909700	3.0154050	3.4516100
88	No	Show	88	C	6.4985330	1.8092830	2.7824060
89	No	Show	89	C	7.8487420	1.5288260	2.4853250
90	No	Show	90	C	8.2096430	0.3479390	1.8245990
91	No	Show	91	C	7.2318370	-0.5740150	1.4325130

92	No	Show	92	O	-1.4920440	0.3720660	2.2880830
93	No	Show	93	C	-2.7811410	0.7696790	1.8733280
94	No	Show	94	C	-2.9521100	2.0660900	1.3779030
95	No	Show	95	C	-4.2443470	2.5580240	1.1669420
96	No	Show	96	C	-5.3751860	1.7707450	1.4697220
97	No	Show	97	C	-5.1859050	0.4274040	1.9413480
98	No	Show	98	C	-3.8628140	-0.1025480	2.1217980
99	No	Show	99	C	-3.7013060	-1.4636270	2.5582130
100	No	Show	100	C	-4.7962000	-2.2429030	2.8322590
101	No	Show	101	C	-6.1343720	-1.7272930	2.7271800
102	No	Show	102	C	-6.3184530	-0.3792990	2.2680460
103	No	Show	103	C	-7.6420370	0.1645080	2.1564690
104	No	Show	104	C	-7.7994400	1.5118790	1.6769960
105	No	Show	105	C	-6.7140090	2.2801720	1.3403200
106	No	Show	106	C	-8.7429370	-0.6388860	2.5204380
107	No	Show	107	C	-8.5549990	-1.9496130	2.9762290
108	No	Show	108	C	-7.2681070	-2.4936280	3.0691670
109	No	Show	109	H	6.6683240	-1.1531600	-2.3697380
110	No	Show	110	H	4.2663930	-0.7614510	-1.9754610
111	No	Show	111	H	9.0291780	-0.3983130	-2.2026630
112	No	Show	112	H	10.7075390	1.3143830	-1.5056750
113	No	Show	113	H	9.9663380	3.4360490	-0.4262950
114	No	Show	114	H	8.1466560	4.8935430	0.4381100

115	No	Show	115	H	5.7334580	5.2701430	0.8867850
116	No	Show	116	H	3.3812300	4.4584450	0.8091760
117	No	Show	117	H	1.7202760	2.7338350	0.1713060
118	No	Show	118	H	-3.3655010	0.7008500	-4.6983430
119	No	Show	119	H	-1.0010540	0.2314040	-3.9947580
120	No	Show	120	H	-5.4406520	2.0589090	-4.4880990
121	No	Show	121	H	-6.7068250	3.8782510	-3.3717910
122	No	Show	122	H	-1.1352160	5.5530640	0.2103450
123	No	Show	123	H	0.1102530	3.6942310	-0.8585960
124	No	Show	124	H	-3.2697430	6.7842660	0.5666610
125	No	Show	125	H	-5.6815120	7.1240060	0.0326710
126	No	Show	126	H	-6.8064500	5.7023060	-1.6789650
127	No	Show	127	H	7.0382670	-4.9813210	1.3558430
128	No	Show	128	H	4.8972930	-5.0726960	2.6041500
129	No	Show	129	H	2.4337480	-4.7473580	2.6764640
130	No	Show	130	H	0.2936120	-4.1181360	1.5202710
131	No	Show	131	H	8.2801740	-4.5281210	-0.7536670
132	No	Show	132	H	8.2864400	-3.8599890	-3.1561990
133	No	Show	133	H	6.1527250	-3.2646710	-4.3040390
134	No	Show	134	H	3.6903110	-2.9180790	-4.2299140
135	No	Show	135	H	1.5556310	-2.9696820	-2.9744400
136	No	Show	136	H	-4.3673070	-5.7294040	0.1409330
137	No	Show	137	H	-2.2385140	-4.6964650	-0.6878170

138	No	Show	138	H	-6.8319160	-5.5832990	0.4977420
139	No	Show	139	H	-8.9465010	-4.2954770	0.3343610
140	No	Show	140	H	-5.4508540	1.1867390	-1.7224270
141	No	Show	141	H	-3.3525540	-0.1122330	-1.6734380
142	No	Show	142	H	-7.9265380	1.2641870	-1.6084860
143	No	Show	143	H	-10.1026800	0.1546380	-1.0846860
144	No	Show	144	H	-10.1475270	-2.2052340	-0.2851950
145	No	Show	145	H	2.7561490	-1.7326810	1.2690150
146	No	Show	146	H	5.1369670	-2.1400290	0.7481140
147	No	Show	147	H	2.0847050	3.4787920	4.1499460
148	No	Show	148	H	0.3478680	1.7870450	3.5126740
149	No	Show	149	H	4.4733840	4.1844350	4.2371330
150	No	Show	150	H	6.8615310	3.7366190	3.7330740
151	No	Show	151	H	8.6128650	2.2567620	2.7658630
152	No	Show	152	H	9.2566180	0.1632600	1.5814900
153	No	Show	153	H	7.5085720	-1.4792600	0.8891580
154	No	Show	154	H	-2.0754790	2.6794900	1.1779090
155	No	Show	155	H	-4.3844400	3.5728880	0.7971350
156	No	Show	156	H	-2.6945630	-1.8676230	2.6393450
157	No	Show	157	H	-4.6654030	-3.2812700	3.1441250
158	No	Show	158	H	-8.8122350	1.9094710	1.5800800
159	No	Show	159	H	-6.8420840	3.2997960	0.9689750
160	No	Show	160	H	-9.7494950	-0.2239210	2.4354760

161	No	Show	161	H	-9.4205910	-2.5580170	3.2464380
162	No	Show	162	H	-7.1272700	-3.5218830	3.4079190

MPW1B95/6-31G(d)

Row	Highlight		Display Tag		Symbol X	Y	Z
1	No	Show	1	P	0.5410210	0.7021820	-1.2305670
2	No	Show	2	O	2.1213420	0.7763180	-1.4387380
3	No	Show	3	C	3.0321560	1.7063960	-0.9839930
4	No	Show	4	C	4.3687200	1.3825300	-1.2356400
5	No	Show	5	C	5.3670190	2.3073270	-0.8487160
6	No	Show	6	C	6.7312480	2.0146640	-1.1075500
7	No	Show	7	C	7.0894880	0.7985160	-1.7424470
8	No	Show	8	C	6.0547830	-0.1193410	-2.1015000
9	No	Show	9	C	4.7515080	0.1588270	-1.8665500
10	No	Show	10	C	8.4382710	0.5283430	-1.9787310
11	No	Show	11	C	9.4170000	1.4366200	-1.6090820
12	No	Show	12	C	9.0733740	2.6313810	-0.9953250
13	No	Show	13	C	7.7379460	2.9407770	-0.7347430
14	No	Show	14	C	7.3481960	4.1587320	-0.0931350
15	No	Show	15	C	6.0479470	4.4330560	0.1612810
16	No	Show	16	C	5.0118590	3.5176370	-0.2018000
17	No	Show	17	C	3.6648560	3.7684010	0.0517700
18	No	Show	18	C	2.6766920	2.8744230	-0.3296030

19	No	Show	19	O	0.0897820	1.8681270	-2.2427400
20	No	Show	20	C	-1.2544140	2.1199690	-2.4729490
21	No	Show	21	C	-1.7766950	3.3399620	-2.0397420
22	No	Show	22	C	-3.1394950	3.6167220	-2.3155420
23	No	Show	23	C	-3.9368050	2.6730960	-3.0101700
24	No	Show	24	C	-3.3520400	1.4797600	-3.4341910
25	No	Show	25	C	-2.0200290	1.2023070	-3.1738920
26	No	Show	26	C	-5.3132000	2.9783590	-3.2516900
27	No	Show	27	C	-5.8597860	4.1403510	-2.8256020
28	No	Show	28	C	-5.0811710	5.1109480	-2.1197850
29	No	Show	29	C	-3.7109670	4.8386940	-1.8738330
30	No	Show	30	C	-2.9201690	5.7805810	-1.1673020
31	No	Show	31	C	-1.5448110	5.4731410	-0.9218390
32	No	Show	32	C	-0.9955410	4.3082960	-1.3386070
33	No	Show	33	C	-3.5078810	6.9669540	-0.7248300
34	No	Show	34	C	-4.8477190	7.2254950	-0.9676030
35	No	Show	35	C	-5.6274220	6.3095460	-1.6567830
36	No	Show	36	N	0.1070740	-0.7256030	-1.7662250
37	No	Show	37	P	-0.6667060	-1.7673380	-0.8537950
38	No	Show	38	O	0.0220870	-3.2172580	-0.9925910
39	No	Show	39	C	1.1514620	-3.5940300	-0.2908330
40	No	Show	40	C	2.3544950	-3.7081430	-0.9906520
41	No	Show	41	C	3.4781180	-4.2168970	-0.2923360

42	No	Show	42	C	4.7202140	-4.3501210	-0.9662490
43	No	Show	43	C	5.8551380	-4.8393330	-0.2703410
44	No	Show	44	C	5.7155290	-5.1997580	1.1073020
45	No	Show	45	C	4.5294080	-5.0794760	1.7474600
46	No	Show	46	C	3.3693260	-4.5849950	1.0738230
47	No	Show	47	C	2.1402210	-4.4388280	1.7183180
48	No	Show	48	C	1.0353240	-3.9498580	1.0431430
49	No	Show	49	C	7.0706530	-4.9492710	-0.9479060
50	No	Show	50	C	7.1710800	-4.5935080	-2.2840100
51	No	Show	51	C	6.0647360	-4.1187650	-2.9718800
52	No	Show	52	C	4.8311470	-3.9840930	-2.3321180
53	No	Show	53	C	3.6722100	-3.4831570	-3.0051080
54	No	Show	54	C	2.4859140	-3.3456520	-2.3673230
55	No	Show	55	O	-2.0464070	-2.0686750	-1.6039790
56	No	Show	56	C	-3.0001360	-3.0033500	-1.2245180
57	No	Show	57	C	-4.3008890	-2.5400150	-1.0135310
58	No	Show	58	C	-5.3088250	-3.5008280	-0.7424600
59	No	Show	59	C	-4.9866980	-4.8792360	-0.6577280
60	No	Show	60	C	-3.6693140	-5.2764180	-0.8766650
61	No	Show	61	C	-2.6861400	-4.3519910	-1.1789150
62	No	Show	62	C	-6.0275310	-5.8193060	-0.3823980
63	No	Show	63	C	-7.3111150	-5.4193110	-0.2358280
64	No	Show	64	C	-7.6733360	-4.0406760	-0.3498270

65	No	Show	65	C	-6.6558630	-3.0825970	-0.5899750
66	No	Show	66	C	-6.9915760	-1.7098870	-0.7053860
67	No	Show	67	C	-5.9415450	-0.7635150	-0.9265430
68	No	Show	68	C	-4.6542450	-1.1560050	-1.0759740
69	No	Show	69	C	-8.3301250	-1.3293830	-0.6103430
70	No	Show	70	C	-9.3213790	-2.2732000	-0.3907680
71	No	Show	71	C	-8.9978520	-3.6130880	-0.2511520
72	No	Show	72	N	-0.8806310	-1.4067780	0.6803480
73	No	Show	73	P	-0.3062900	-0.0488420	1.2754590
74	No	Show	74	N	0.0859650	1.0976720	0.2414160
75	No	Show	75	O	0.9297880	-0.4220880	2.2298640
76	No	Show	76	C	1.9162010	0.5007090	2.5521630
77	No	Show	77	C	3.2354200	0.1576350	2.2508090
78	No	Show	78	C	3.5896850	-1.0529360	1.5784750
79	No	Show	79	C	4.8869000	-1.3408090	1.3198750
80	No	Show	80	C	5.9427190	-0.4556770	1.6966220
81	No	Show	81	C	5.6124270	0.7596570	2.3446080
82	No	Show	82	C	4.2558080	1.0717300	2.6192510
83	No	Show	83	C	3.9300890	2.2907600	3.2662320
84	No	Show	84	C	2.5912150	2.5769170	3.5314000
85	No	Show	85	C	1.5896730	1.6862690	3.1865480
86	No	Show	86	C	4.9860470	3.1870380	3.6205430
87	No	Show	87	C	6.2792030	2.8870790	3.3595620

88	No	Show	88	C	6.6400340	1.6646430	2.7109890
89	No	Show	89	C	7.9664220	1.3322490	2.4330930
90	No	Show	90	C	8.2825770	0.1386260	1.8028580
91	No	Show	91	C	7.2826130	-0.7484230	1.4379150
92	No	Show	92	O	-1.3158560	0.5386610	2.3695390
93	No	Show	93	C	-2.5388400	1.0979500	2.0170860
94	No	Show	94	C	-2.5661730	2.3823070	1.5034280
95	No	Show	95	C	-3.7822620	2.9842720	1.2343380
96	No	Show	96	C	-4.9822820	2.3189940	1.4883990
97	No	Show	97	C	-4.9431610	1.0111650	2.0335880
98	No	Show	98	C	-3.7011870	0.3743820	2.2866160
99	No	Show	99	C	-3.6867500	-0.9558690	2.8079860
100	No	Show	100	C	-4.8451800	-1.6022150	3.0771440
101	No	Show	101	C	-6.1159570	-0.9823670	2.8631430
102	No	Show	102	C	-6.1520550	0.3307920	2.3318440
103	No	Show	103	C	-7.3988400	0.9637720	2.0951320
104	No	Show	104	C	-7.4066210	2.2751610	1.5234980
105	No	Show	105	C	-6.2536450	2.9208880	1.2296980
106	No	Show	106	C	-8.5749040	0.2873950	2.4219560
107	No	Show	107	C	-8.5320670	-0.9951560	2.9446730
108	No	Show	108	C	-7.3181560	-1.6295740	3.1527520
109	No	Show	109	H	6.3355350	-1.0590150	-2.5639600
110	No	Show	110	H	3.9778080	-0.5475380	-2.1328590

111	No	Show	111	H	8.7112590	-0.4049740	-2.4581410
112	No	Show	112	H	10.4593250	1.2132500	-1.8035290
113	No	Show	113	H	9.8434810	3.3397060	-0.7109750
114	No	Show	114	H	8.1239370	4.8623810	0.1875730
115	No	Show	115	H	5.7660280	5.3556730	0.6559260
116	No	Show	116	H	3.3845060	4.6794260	0.5674810
117	No	Show	117	H	1.6406320	3.0724700	-0.0950720
118	No	Show	118	H	-3.9531010	0.7547580	-3.9701010
119	No	Show	119	H	-1.5664480	0.2765130	-3.4998270
120	No	Show	120	H	-5.9132620	2.2498700	-3.7849650
121	No	Show	121	H	-6.9052180	4.3577440	-3.0124350
122	No	Show	122	H	-0.9423710	6.2031640	-0.3933250
123	No	Show	123	H	0.0502560	4.0970130	-1.1659280
124	No	Show	124	H	-2.9026040	7.6857250	-0.1844660
125	No	Show	125	H	-5.2891260	8.1500220	-0.6160130
126	No	Show	126	H	-6.6745480	6.5181680	-1.8447820
127	No	Show	127	H	6.5881730	-5.5713970	1.6319510
128	No	Show	128	H	4.4379950	-5.3513790	2.7925680
129	No	Show	129	H	2.0533790	-4.7118900	2.7630990
130	No	Show	130	H	0.0788430	-3.8338390	1.5335030
131	No	Show	131	H	7.9382810	-5.3232190	-0.4164110
132	No	Show	132	H	8.1209230	-4.6901040	-2.7957350
133	No	Show	133	H	6.1482110	-3.8463450	-4.0179810

134	No	Show	134	H	3.7652100	-3.2043240	-4.0485690
135	No	Show	135	H	1.6208610	-2.9471380	-2.8799610
136	No	Show	136	H	-3.4180230	-6.3298290	-0.8351630
137	No	Show	137	H	-1.6778760	-4.6703550	-1.3929990
138	No	Show	138	H	-5.7639340	-6.8682050	-0.3070680
139	No	Show	139	H	-8.0949680	-6.1422560	-0.0399530
140	No	Show	140	H	-6.1968390	0.2907920	-0.9570720
141	No	Show	141	H	-3.8723210	-0.4267040	-1.2413770
142	No	Show	142	H	-8.5850980	-0.2808290	-0.7084770
143	No	Show	143	H	-10.3561630	-1.9597820	-0.3221180
144	No	Show	144	H	-9.7760560	-4.3471580	-0.0745520
145	No	Show	145	H	2.8040400	-1.7359190	1.2814890
146	No	Show	146	H	5.1508370	-2.2538750	0.8025220
147	No	Show	147	H	2.3352610	3.5053910	4.0286240
148	No	Show	148	H	0.5527130	1.8969940	3.4122740
149	No	Show	149	H	4.7248320	4.1168480	4.1136320
150	No	Show	150	H	7.0704100	3.5757500	3.6333660
151	No	Show	151	H	8.7514030	2.0279180	2.7071600
152	No	Show	152	H	9.3164170	-0.0935040	1.5776150
153	No	Show	153	H	7.5278420	-1.6753630	0.9313270
154	No	Show	154	H	-1.6335550	2.8959880	1.3151320
155	No	Show	155	H	-3.8055850	3.9929400	0.8417590
156	No	Show	156	H	-2.7303910	-1.4349330	2.9680070

157	**No**	**Show**	**157**	**H**	**-4.8278050**	**-2.6139910**	**3.4655920**
158	**No**	**Show**	**158**	**H**	**-8.3645690**	**2.7465760**	**1.3334780**
159	**No**	**Show**	**159**	**H**	**-6.2693890**	**3.9142460**	**0.7954450**
160	**No**	**Show**	**160**	**H**	**-9.5280740**	**0.7758800**	**2.2521570**
161	**No**	**Show**	**161**	**H**	**-9.4547160**	**-1.5112620**	**3.1801590**
162	**No**	**Show**	**162**	**H**	**-7.2911560**	**-2.6386550**	**3.5476340**

References

[1] Bruker, SADABS, Bruker AXS Inc., Madison, Wisconsin, USA, 2005.

[2] Bruker (2008). *APEX2* (Version 2012.2-0). Bruker AXS Inc., Madison, Wisconsin, USA.

[3] Sheldrick GM. Acta Cryst 2008; A64: 112–122.

[4] Spek A L. J Appl Crystallogr 2003;36: 7-13.

[5] Macrae CF, Edgington PR, McCabe P, Pidcock E, Shields GP, Taylor R, Towler VDS. J Appl Cryst 2006;39: 453-457.

[6] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

[7] A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648-5652.

[8] Y. Zhao and D. G. Truhlar *J. Phys. Chem. A*, **2004**, ***108*** (33), 6908.

[9] S. Grimme, *J. Comp. Chem.*, 2006, **27**, 1787.

[10] R. Ditchfield, W. J. Hehre, J. A. Pople, *J. Chem. Phys.*, 1971, **54**, 724.

[11] T. Yanai, D. Tew, N. Handy, *Chem. Phys. Lett.*, 2004, **393**, 51.

[12] O. A. Vydrov, G. E. Scuseria, *J. Chem. Phys.*, 2006, **125**, 234109.

[13] J.-D. Chai, M. Head-Gordon, *Phys. Chem. Chem. Phys.*, 2008, **10**, 6615.

[14] T. H. Dunning Jr., *J. Chem. Phys.*, 1989, **90**, 1007.

[15] *(a)* F. Furche and R. Ahlrichs, *J. Chem. Phys.*, 2002, **117**, 7433. *(b)* G. Scalmani, M. J. Frisch, B. Mennucci, J. Tomasi, R. Cammi, and V. Barone, *J. Chem. Phys.*, 2006, **124**, 094107: 1-15. *(c)* C. Van Caillie and R. D. Amos, *Chem. Phys. Lett.*, 2000, **317**, 159. *(d)* C. Van Caillie and R. D. Amos, *Chem. Phys. Lett.*, 1999, **308**, 249.

[16] A. Schaefer, C. Huber, and R. Ahlrichs, *J. Chem. Phys.*, 1994, **100**, 5829-35.