Light-Induced Regiospecific Bromination of *meso*-Tetra(3,5-Di-*tert*-butylphenyl)Porphyrin on 2,12 β-Pyrrolic Positions

Gabriele Di Carlo,[†] Alessio Orbelli Biroli,[‡] Francesca Tessore,[†] Silvia Rizzato,[†] Alessandra Forni,[†,‡] Giulia Magnano[†] and Maddalena Pizzotti[†]*

† Department of Chemistry, University of Milan, Via C. Golgi 19, 20133 Milano, Italy

‡ Institute of Molecular Sciences and Technologies of CNR (ISTM-CNR), Via C. Golgi 19, 20133 Milano, Italy

E-mail: gabriele.dicarlo@unimi.it

Content

1. **Experimental Procedure** **p. 2**
2. **Table S1.** Details of the Data Collection and Refinement Parameters for Ni-3 **p. 4**
3. **Table S2.** Selected bond lengths [Å] and angles [°] for compound Ni-3 **p. 5**
4. **Figure S1.** Molecular structure of compound Zn-3 **p. 6**
5. **Computational Details** **p. 6**
6. **Figure S2.** Hypothetical cationic intermediates **p. 8**
7. **Table S3.** Integrated Net Charges of 2 and Zn-2 computed by QTAIM Partitioning **p. 8**
8. **Table S4.** Selected bond lengths and angles for compound Ni-3 computed **p. 9**
9. **Table S5.** M06/6-311G(d) relative energies (kcal/mol) of the hypothetical cationic intermediates **p. 10**
10. **Table S6.** Cartesian coordinates of the modelled compounds **p. 10**
11. **References** **p. 26**

EXPERIMENTAL PROCEDURES

X-ray Crystal Structure Determination

Air-stable, pink crystals of **Ni-3** were obtained by slow evaporation from a THF solution at low temperature (4°C). The single-crystal data collection was performed at 293 K on X-ray area detector diffractometer by the ω-scan method, within the limits $2<\theta<25°$. The collected intensities were corrected for Lorentz and polarization factors and empirically for absorption by using the SADABS program.[1] The structures were solved by direct methods and refined by full-matrix least-squares on F^2 (SHELX-97)[2] with the WINGX interface[3] by using anisotropic displacement parameters for all non-disordered atoms.

Four electron density peaks were located in the difference Fourier map at the 2, 3, 12, 13 positions, clearly indicating a disorder involving the bromine substituents. To identify the regioisomer, the bromine atoms were initially refined with free occupancy variables and fixed thermal isotropic parameter. The site occupancies were found very similar for the 2, 12 and 3, 13 positions. The bromine substituents were therefore refined over these two sets of positions, initially using an occupancy variable to refine freely the occupancies of the two models. In the later round of refinement the occupancies were fixed (at 0.8 and 0.2 for 2, 12 and 3, 13 respectively) allowing B-factors to converge. Then, the bromine atoms were refined with anisotropic thermal parameters. Large and highly anisotropic thermal displacement parameters were observed only for Br3, close to which a large residual electron density was located. The Br3 bromine was therefore refined isotropically on two positions with population parameters of 58% and 42%.

Three *tert*-butyl substituents of phenyl rings were found disordered and their refinement was carried out isotropically using a suitable double model for each. In all models restraints were used for equivalent distances.

The hydrogen atoms were included in the refinement at their calculated positions using a riding model. Crystallographic data and analysis parameters are given in Table S1. The diagram was drawn using ORTEPIII program.[4]

CCDC 1045781 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Details of the Data Collection and Refinement Parameters for **Ni-3**.

Formula	C76 H90 Br2 N4 Ni
Formula weight	1278.05
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	*P* -1
Unit cell dimensions	a = 14.796(4) Å b = 14.826(4) Å c = 17.185(5) Å α= 92.321(5)° β= 95.308(5)° γ = 95.191(4)°
Volume	3733.7(18) $Å^3$
Z	2
Temperature	120(2) K
Density (calculated), ρ_c	1.137 g/cm^3
Absorption coefficient, μ	1.370 mm^{-1}
F(000)	1344
Theta range for data collection	1.19 to 24.89°
Index ranges	-17<=h<=17 -17<=k<=17 -20<=l<=20
Reflections collected	36354
Independent reflections	12405 [*R*(int) = 0.0719]
Completeness to theta	95.4 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12405 / 34 / 754
Goodness-of-fit on F^2	1.070
Final R indices [I>2sigma(I)]	R1 = 0.0873, wR2 = 0.2411
R indices (all data)	R1 = 0.1360, wR2 = 0.2744
Extinction coefficient	0.036(2)
Largest diff. peak and hole	2.031 and -1.179 $e·Å^{-3}$

Table S2. Selected bond lengths [Å] and angles [°] for compound **Ni-3**.

Ni-N(4)	1.888(5)	C(11)-N(3)-C(14)	106.1(5)
Ni-N(2)	1.891(5)	C(11)-N(3)-Ni	128.3(4)
Ni-N(1)	1.908(5)	C(14)-N(3)-Ni	125.5(4)
Ni-N(3)	1.927(5)	C(9)-N(4)-C(6)	105.4(5)
Br(1)-C(2)	1.880(7)	C(9)-N(4)-Ni	127.5(5)
Br(2)-C(12)	1.904(7)	C(6)-N(4)-Ni	127.0(5)
N(1)-C(1)	1.373(8)	N(1)-C(4)-C(5)	125.7(6)
N(1)-C(4)	1.379(8)	N(1)-C(4)-C(3)	110.5(6)
N(2)-C(16)	1.371(8)	C(5)-C(4)-C(3)	123.6(6)
N(2)-C(19)	1.374(8)	C(2)-C(3)-C(4)	106.5(6)
N(3)-C(11)	1.363(8)	C(3)-C(2)-C(1)	107.8(6)
N(3)-C(14)	1.387(8)	C(3)-C(2)-Br(1)	121.2(6)
N(4)-C(9)	1.365(9)	C(1)-C(2)-Br(1)	130.7(5)
N(4)-C(6)	1.372(8)	C(20)-C(1)-N(1)	124.5(6)
C(4)-C(5)	1.391(10)	C(20)-C(1)-C(2)	125.6(6)
C(4)-C(3)	1.430(10)	N(1)-C(1)-C(2)	109.3(6)
C(3)-C(2)	1.350(10)	C(1)-C(20)-C(19)	121.4(6)
C(2)-C(1)	1.440(9)	N(2)-C(19)-C(20)	124.4(6)
C(1)-C(20)	1.371(9)	N(2)-C(19)-C(18)	111.0(6)
C(20)-C(19)	1.399(9)	C(20)-C(19)-C(18)	124.0(6)
C(19)-C(18)	1.409(9)	C(17)-C(18)-C(19)	107.1(6)
C(18)-C(17)	1.339(10)	C(18)-C(17)-C(16)	107.0(6)
C(17)-C(16)	1.431(9)	C(15)-C(16)-N(2)	125.9(6)
C(16)-C(15)	1.361(9)	C(15)-C(16)-C(17)	123.7(6)
C(15)-C(14)	1.374(9)	N(2)-C(16)-C(17)	110.0(6)
C(14)-C(13)	1.430(10)	C(16)-C(15)-C(14)	121.9(6)
C(13)-C(12)	1.339(10)	C(15)-C(14)-N(3)	125.3(6)
C(12)-C(11)	1.422(10)	C(15)-C(14)-C(13)	124.9(6)
C(11)-C(10)	1.384(9)	N(3)-C(14)-C(13)	109.3(6)
C(10)-C(9)	1.369(10)	C(12)-C(13)-C(14)	106.7(6)
C(9)-C(8)	1.418(9)	C(13)-C(12)-C(11)	108.3(6)
C(8)-C(7)	1.330(11)	C(13)-C(12)-Br(2)	120.8(6)
C(7)-C(6)	1.444(10)	C(11)-C(12)-Br(2)	130.9(5)
C(6)-C(5)	1.360(10)	N(3)-C(11)-C(10)	123.4(6)
		N(3)-C(11)-C(12)	109.4(6)
N(4)-Ni-N(2)	179.8(3)	C(10)-C(11)-C(12)	127.0(6)
N(4)-Ni-N(1)	90.5(2)	C(9)-C(10)-C(11)	121.7(7)
N(2)-Ni-N(1)	89.5(2)	C(9)-C(10)-C(27)	118.2(6)
N(4)-Ni-N(3)	89.2(2)	N(4)-C(9)-C(10)	125.5(6)
N(2)-Ni-N(3)	90.8(2)	N(4)-C(9)-C(8)	110.1(6)
N(1)-Ni-N(3)	179.7(2)	C(10)-C(9)-C(8)	123.7(7)
C(1)-N(1)-C(4)	105.9(5)	C(7)-C(8)-C(9)	108.3(7)
C(1)-N(1)-Ni	128.4(4)	C(8)-C(7)-C(6)	106.0(7)
C(4)-N(1)-Ni	125.6(4)	C(5)-C(6)-N(4)	125.9(6)
C(16)-N(2)-C(19)	104.7(5)	C(5)-C(6)-C(7)	123.8(6)
C(16)-N(2)-Ni	127.3(4)	N(4)-C(6)-C(7)	110.0(6)
C(19)-N(2)-Ni	127.9(4)	C(6)-C(5)-C(4)	120.5(6)

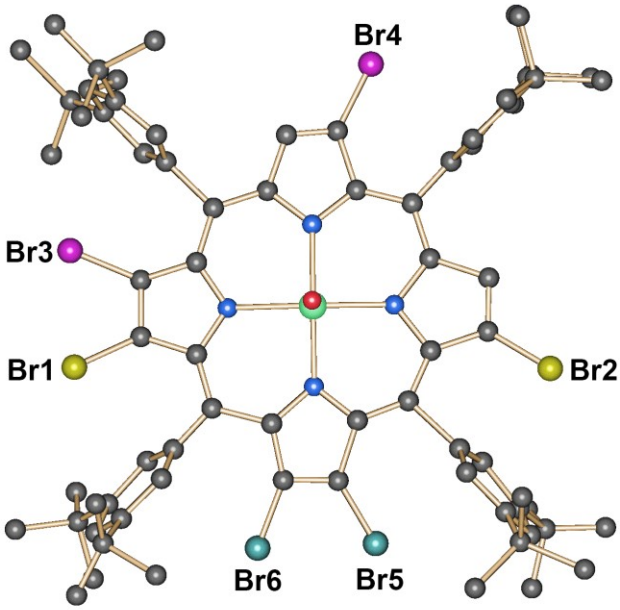


Figure S1. Molecular structure of compound **Zn-3**: [dibromo-5,10,15,20-tetra(3,5-di-tert-butylphenyl)porphyrinate Zn(H_2O)]·$n H_2O$ showing the presence in the crystal of different di-bromine regioisomers that have been refined by using a site-occupancy disorder model (isomer 2,13 (Br1, Br2), occupancy 50%; isomer 2,7 (Br3, Br4), occupancy 33%, isomer 2,3 (Br5, Br6), occupancy 17%).

Computational Details

DFT calculations were performed on the mono-brominated free-base **2**, the Zn complex **Zn-2** and the Ni complex **Ni-3** using Gaussian 09.[5] The structures were optimized *in vacuo* and in solvent (CCl_4 and CH_2Cl_2), starting from the X-ray structure of the **Ni-3** complex with the appropriate substitutions and using the 6-311G(d) basis set, which was chosen on the basis of previous theoretical investigation on similar porphyrin derivatives.[6,7] The solvent effects have been taken into account by means of the CPCM conductor-like solvation model.[8] The **Ni-3** structure was modelled only with the aim to assess the performance of the adopted computational protocol through comparison with accurate X-ray structural information. In particular, we have evaluated the better performance between the B3LYP[9-11] and the M06[12] functionals. The former has been used in previous theoretical studies on porhpyrin

derivatives,[6,7] while the latter was properly developed to treat organometallic complexes. The better agreement with the experimental structure has been obtained with the M06 functional as far as the Ni-N distances are concerned, while the other distances and the bond angles were reproduced with similar accuracy by the two functionals (see Table S4 for a full comparison between computed and experimental bond distances and angles). The M06 functional was then chosen to investigate the free-base mono-brominated porphyrin and the **Zn-2** complex. The M06/6-311G(d) optimized wavefunctions have been submitted to topological analysis according to the Quantum Theory of Atoms in Molecules (QTAIM),[13] using AIMAll,[14] aimed at determining the atomic charges of the reactive sites in β-pyrrolic position of the mono-brominated ligand and Zn complex.

Further calculations have been performed in order to get further insight on the possible mechanism of the reaction giving the di-brominated free-base derivative starting from the mono-brominated one, though a full mechanistic study is beyond the aims of the present work. We have considered all the possible cationic intermediates approximating the transition state for this reaction, looking for the more stable one, if any, which should simulate the 'true' intermediate assuming an electrophilic aromatic substitution mechanism. Such cationic species have been freely optimized starting from the optimized mono-bromo derivative (Br in position 2, see labelling in Tables 2 and S3, M = 2H) and replacing successively each of the C(sp^2) carbon atoms in 7, 8, 12, 13, 17 and 18 position by a tetrahedral carbon atom bearing the incoming bromine ion and the outgoing proton. Both bromine additions on one side or on the other side of the porphyrinic main plane have been considered, labelled in the following with "a" and "b", respectively (see Figure S2 for exemplificative intermediates 2,12a and 2,12b). The second configuration resulted in all cases to be the more stable one. A summary of the obtained M06/6-311G(d) relative energies of the considered ionic intermediates with respect to the most stable one (2,12b) is reported in Table S5.

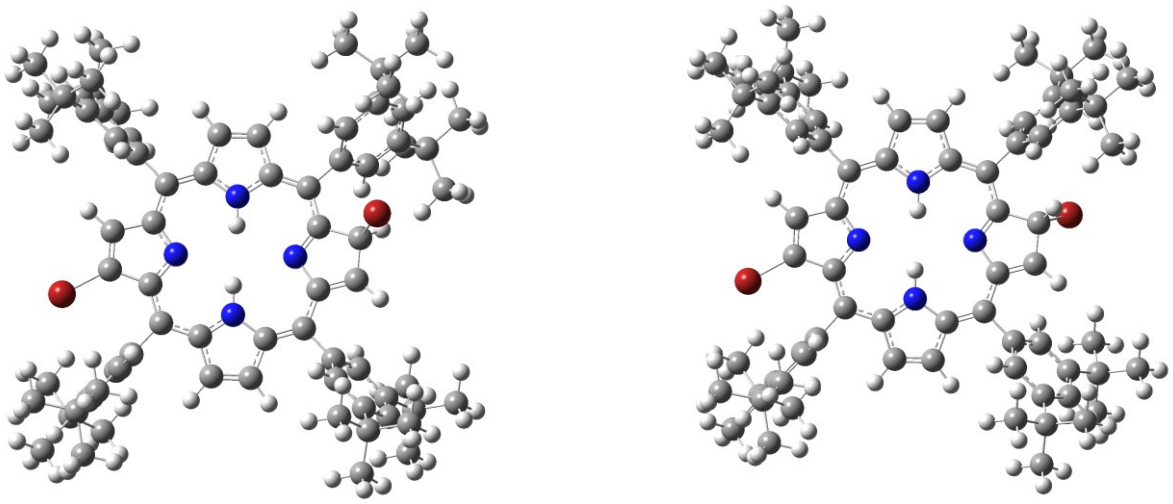
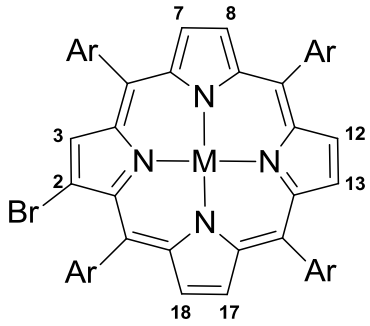


Figure S2. Hypothetical cationic intermediates leading to formation of the di-brominated free-base 2,12 regioisomer, with the second bromine atom incoming from one side (2,12a cation, left) or the other side (2,12b cation, right) of the porphyrinic main plane.

Table S3. B3LYP/6-311G(d) and M06/6-311G(d) Integrated Net Charges q (e) of the Atomic Basins of Mono-Brominated Free-Base (**2**) and its Zn Complex (**Zn-2**) *in vacuo*, Computed by QTAIM Partitioning



Atom	Free-Base (**2**)		Zn^{II}-Complex (**Zn-2**)	
	B3LYP	M06	B3LYP	M06
C3	-0.0352	-0.0421	-0.0288	-0.0345
C7	-0.0536	-0.0477	-0.0714	-0.0654
C8	-0.0551	-0.0482	-0.0713	-0.0656
C12	-0.0823	-0.0776	-0.0730	-0.0678
C13	-0.0811	-0.0769	-0.0722	-0.0659
C17	-0.0550	-0.0487	-0.0724	-0.0659
C18	-0.0525	-0.0461	-0.0691	-0.0633

Table S4. Selected bond lengths [Å] and angles [°] for compound **Ni-3**, computed at the B3LYP/6-311G(d) (1st row) and M06/6-311G(d) (2nd row) levels of theory, compared with the experimental values (3rd row)

Ni-N(2), Ni-N(4)	1.916, 1.916	N(4)-Ni-N(2)	178.7
	1.907, 1.908		179.7
	1.891(5), 1.888(5)		179.8(3)
Ni-N(1), Ni-N(3)	1.940, 1.941	N(4)-Ni-N(1)	90.7
	1.930, 1.929		90.6
	1.908(5), 1.927(5)		90.5(2)
Br(1)-C(2), Br(2)-C(12)	1.896, 1.895	N(2)-Ni-N(1)	89.3
	1.882, 1.882		89.4
	1.880(7), 1.904(7)		89.5(2)
N(1)-C(1), N(3)-C(11)	1.382, 1.383	N(4)-Ni-N(3)	89.3
	1.375, 1.374		89.4
	1.373(8), 1.363(8)		89.2(2)
N(1)-C(4), N(3)-C(14)	1.377, 1.377	N(2)-Ni-N(3)	90.7
	1.370, 1.370		90.6
	1.379(8), 1.387(8)		90.8(2)
N(2)-C(16), N(4)-C(6)	1.373, 1.374	N(1)-Ni-N(3)	178.3
	1.367, 1.367		179.2
	1.371(8), 1.372(8)		179.7(2)
N(2)-C(19), N(4)-C(9)	1.377, 1.377		
	1.369, 1.369		
	1.374(8), 1.365(9)		
C(1)-C(2), C(11)-C(12)	1.454, 1.454		
	1.446, 1.446		
	1.440(9), 1.422(10)		
C(2)-C(3), C(12)-C(13)	1.355, 1.355		
	1.351, 1.352		
	1.350(10), 1.339(10)		
C(3)-C(4), C(13)-C(14)	1.431, 1.431		
	1.424, 1.424		
	1.430(10), 1.430(10)		
C(4)-C(5), C(14)-C(15)	1.395, 1.396		
	1.389, 1.389		
	1.391(10), 1.374(9)		
C(5)-C(6), C(15)-C(16)	1.393, 1.394		
	1.387, 1.387		
	1.360(10), 1.361(9)		
C(6)-C(7), C(16)-C(17)	1.439, 1.439		
	1.433, 1.432		
	1.444(10), 1.431(9)		
C(7)-C(8), C(17)-C(18)	1.356, 1.356		
	1.351, 1.351		
	1.330(11), 1.339(10)		
C(8)-C(9), C(18)-C(19)	1.443, 1.443		
	1.436, 1.435		
	1.418(9), 1.409(9)		
C(9)-C(10), C(19)-C(20)	1.397, 1.397		
	1.390, 1.390		
	1.369(10), 1.399(9)		
C(10)-C(11), C(20)-C(1)	1.399, 1.399		
	1.393, 1.392		
	1.384(9), 1.371(9)		

Table S5. M06/6-311G(d) relative energies (kcal/mol) of the hypothetical cationic intermediates leading to formation of the di-brominated free-base 2,12 regioisomer.[a]

Cationic intermediate	"a" configuration	"b" configuration
2,7	0.930	0.789
2,8	1.872	1.241
2,12	0.519	0.0
2,13	0.061	0.024
2,17	0.978	0.620
2,18	1.474	0.545

[a]The second bromine atom enter from one side ("a" configuration) or the other side ("b" configuration) of the porphyrinic main plane. All the reported values are energy differences with respect to the value obtained for the most stable configuration 2,12b.

Table S6. Cartesian coordinates of the modelled compounds

Complex **Ni-3** *in vacuo* at the B3LYP/6-311G(d) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.008092	0.002510	0.125553
2	35	0	5.979774	-0.367038	0.103777
3	35	0	-5.995302	0.386614	0.009428
4	7	0	1.829019	-0.621012	0.167664
5	7	0	0.631033	1.808185	0.093416
6	7	0	-1.845342	0.627666	0.142421
7	7	0	-0.647088	-1.803600	0.114624
8	6	0	2.233880	-1.857928	0.617149
9	6	0	3.661221	-1.915791	0.695929
10	6	0	4.124246	-0.743467	0.197720
11	6	0	2.977912	0.091461	-0.121117
12	6	0	2.992113	1.432493	-0.521130
13	6	0	1.862223	2.236213	-0.350298
14	6	0	1.883383	3.677036	-0.418444
15	6	0	0.702963	4.113833	0.085980
16	6	0	-0.085783	2.945489	0.374843
17	6	0	-1.431640	2.986481	0.734788
18	6	0	-2.253671	1.870179	0.573370
19	6	0	-3.681976	1.930793	0.632965
20	6	0	-4.140462	0.754768	0.139388
21	6	0	-2.991775	-0.087222	-0.150820
22	6	0	-3.003605	-1.435704	-0.523941
23	6	0	-1.876337	-2.237594	-0.328131
24	6	0	-1.899741	-3.679589	-0.370906
25	6	0	-0.721239	-4.109401	0.143423
26	6	0	0.067970	-2.937418	0.415891
27	6	0	1.411808	-2.973453	0.781846
28	6	0	4.222911	2.066093	-1.089524
29	6	0	4.602437	1.761223	-2.392950
30	6	0	5.725738	2.356109	-2.985119
31	6	0	6.455091	3.263914	-2.217301
32	6	0	6.102817	3.599524	-0.898481
33	6	0	4.976020	2.989994	-0.352581
34	6	0	-2.014443	4.290581	1.178338
35	6	0	-1.679193	4.798537	2.436731

36	6	0	-2.197123	6.016060	2.888927
37	6	0	-3.056121	6.712902	2.031224
38	6	0	-3.405897	6.245614	0.758620
39	6	0	-2.871052	5.020664	0.348626
40	6	0	-4.227334	-2.084308	-1.091917
41	6	0	-4.575772	-1.831996	-2.419114
42	6	0	-5.678732	-2.452796	-3.013270
43	6	0	-6.428099	-3.338508	-2.229616
44	6	0	-6.110619	-3.615926	-0.893635
45	6	0	-4.997228	-2.975909	-0.342865
46	6	0	1.998854	-4.275735	1.226399
47	6	0	1.692067	-4.778649	2.488021
48	6	0	2.214888	-6.001655	2.935303
49	6	0	3.049222	-6.703820	2.065433
50	6	0	3.374720	-6.235855	0.780816
51	6	0	2.838639	-5.013400	0.379457
52	6	0	6.101809	1.996546	-4.434495
53	6	0	6.963584	4.606227	-0.112085
54	6	0	-1.857446	6.599350	4.273826
55	6	0	-4.348921	7.077604	-0.131340
56	6	0	-6.021080	-2.151751	-4.484720
57	6	0	-6.942829	-4.579106	-0.025193
58	6	0	1.860488	-6.511176	4.344857
59	1	0	4.241468	-2.749568	1.054784
60	1	0	-4.265822	2.769420	0.973948
61	1	0	0.366757	5.131516	0.210108
62	1	0	2.709813	4.268879	-0.776994
63	1	0	-0.387262	-5.125352	0.286039
64	1	0	-2.726220	-4.276745	-0.720356
65	1	0	-3.101921	4.618419	-0.629167
66	1	0	-1.010950	4.217539	3.059224
67	1	0	-3.468215	7.658281	2.365765
68	1	0	-4.721272	-3.149537	0.691083
69	1	0	-3.962945	-1.141432	-2.988117
70	1	0	-7.282840	-3.828032	-2.672439
71	1	0	3.051084	-4.612915	-0.603213
72	1	0	1.039813	-4.196209	3.129315
73	1	0	3.465128	-7.649570	2.386721
74	1	0	4.003661	1.048731	-2.949729
75	1	0	4.669723	3.202522	0.663237
76	1	0	7.328420	3.733121	-2.651191
77	6	0	-0.897882	5.697349	5.069704
78	1	0	-1.324438	4.708333	5.256948
79	1	0	0.058871	5.563316	4.557921
80	1	0	-0.686656	6.149939	6.042294
81	6	0	-1.183549	7.979314	4.101106
82	1	0	-1.832150	8.691333	3.585510
83	1	0	-0.933463	8.407959	5.076565
84	1	0	-0.258957	7.894578	3.523470
85	6	0	-3.154891	6.763001	5.097314
86	1	0	-2.930769	7.172280	6.087247
87	1	0	-3.864474	7.439055	4.614594
88	1	0	-3.656119	5.801305	5.236521
89	6	0	-3.735978	8.475678	-0.372518
90	1	0	-4.394285	9.076972	-1.007086
91	1	0	-3.586180	9.025927	0.559293
92	1	0	-2.765879	8.399136	-0.871176
93	6	0	-5.716132	7.233616	0.572303
94	1	0	-5.625367	7.735430	1.538487
95	1	0	-6.398888	7.826172	-0.044677
96	1	0	-6.181306	6.259712	0.747688
97	6	0	-4.590744	6.422813	-1.502976
98	1	0	-3.663627	6.304812	-2.070500
99	1	0	-5.061652	5.440256	-1.414032
100	1	0	-5.259318	7.050199	-2.098491
101	6	0	-6.032540	-5.698535	0.529059
102	1	0	-5.572033	-6.268709	-0.282769
103	1	0	-5.229195	-5.303297	1.154481
104	1	0	-6.612860	-6.395426	1.141654
105	6	0	-7.564212	-3.796669	1.153867
106	1	0	-6.802434	-3.320671	1.774960
107	1	0	-8.233086	-3.010425	0.793435

108	1	0	-8.146001	-4.466948	1.794845
109	6	0	-8.085728	-5.246043	-0.811199
110	1	0	-7.714251	-5.837221	-1.652937
111	1	0	-8.637486	-5.924003	-0.154428
112	1	0	-8.801550	-4.515650	-1.197470
113	6	0	-7.263239	-2.919542	-4.970457
114	1	0	-7.464492	-2.671606	-6.016186
115	1	0	-7.125410	-4.002863	-4.914107
116	1	0	-8.157223	-2.659643	-4.396999
117	6	0	-4.829684	-2.553697	-5.383598
118	1	0	-3.920118	-2.006137	-5.126960
119	1	0	-4.610375	-3.621059	-5.291234
120	1	0	-5.055409	-2.345570	-6.434235
121	6	0	-6.298400	-0.640483	-4.649753
122	1	0	-7.135438	-0.323829	-4.021848
123	1	0	-5.433386	-0.033086	-4.374983
124	1	0	-6.548581	-0.408924	-5.689895
125	6	0	6.411310	4.871597	1.299772
126	1	0	5.400943	5.289046	1.272991
127	1	0	6.386984	3.964745	1.909600
128	1	0	7.049103	5.594259	1.816073
129	6	0	7.008888	5.954250	-0.866516
130	1	0	7.615962	6.679903	-0.316294
131	1	0	7.442243	5.853145	-1.864086
132	1	0	6.005965	6.374592	-0.982156
133	6	0	8.399516	4.052995	0.031462
134	1	0	8.870477	3.881362	-0.939158
135	1	0	9.028616	4.757599	0.584456
136	1	0	8.400728	3.103134	0.572831
137	6	0	4.930960	2.360985	-5.375324
138	1	0	4.708768	3.430776	-5.329783
139	1	0	5.180959	2.112656	-6.411592
140	1	0	4.016128	1.822257	-5.118888
141	6	0	7.353958	2.746710	-4.921912
142	1	0	8.236025	2.508738	-4.321081
143	1	0	7.577002	2.460715	-5.953354
144	1	0	7.214576	3.831256	-4.908407
145	6	0	6.383651	0.480236	-4.532020
146	1	0	7.207181	0.190890	-3.873884
147	1	0	5.513500	-0.117012	-4.251184
148	1	0	6.656182	0.206981	-5.556302
149	6	0	2.363333	-5.496432	5.396783
150	1	0	3.448454	-5.375032	5.337504
151	1	0	1.912644	-4.510738	5.262059
152	1	0	2.117080	-5.837837	6.407023
153	6	0	0.327199	-6.660118	4.470105
154	1	0	-0.192268	-5.711962	4.315012
155	1	0	-0.059138	-7.373610	3.736915
156	1	0	0.058986	-7.023598	5.466961
157	6	0	2.497570	-7.876656	4.655769
158	1	0	2.164976	-8.652602	3.960687
159	1	0	3.589904	-7.837427	4.625764
160	1	0	2.212366	-8.196863	5.661488
161	6	0	4.295873	-7.075250	-0.124372
162	6	0	4.521998	-6.421479	-1.499030
163	1	0	3.587312	-6.295865	-2.052315
164	1	0	5.001516	-5.442521	-1.416284
165	1	0	5.176574	-7.053457	-2.105171
166	6	0	3.666295	-8.467578	-0.356402
167	1	0	4.309272	-9.074896	-1.000896
168	1	0	3.525549	-9.016386	0.577640
169	1	0	2.689614	-8.381683	-0.840530
170	6	0	5.672764	-7.244489	0.557291
171	1	0	5.593389	-7.747368	1.523908
172	1	0	6.340306	-7.841792	-0.071624
173	1	0	6.149052	-6.274879	0.726597

Complex **Ni-3** *in vacuo* at the M06/6-311G(d) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.000494	-0.007312	-0.086920
2	35	0	-5.965997	-0.179506	0.146090
3	35	0	5.965945	0.129253	0.027185
4	7	0	-1.849135	-0.559551	-0.094077
5	7	0	-0.563339	1.814853	-0.079721
6	7	0	1.849181	0.544790	-0.106689
7	7	0	0.566709	-1.829869	-0.083328
8	6	0	-2.312783	-1.784068	-0.496036
9	6	0	-3.737042	-1.802695	-0.511124
10	6	0	-4.141733	-0.606337	-0.030237
11	6	0	-2.960029	0.192803	0.207040
12	6	0	-2.926091	1.545394	0.532929
13	6	0	-1.777496	2.300118	0.325707
14	6	0	-1.761168	3.734965	0.336319
15	6	0	-0.559944	4.114778	-0.152606
16	6	0	0.189406	2.915728	-0.380438
17	6	0	1.538055	2.905513	-0.704516
18	6	0	2.311410	1.766647	-0.519869
19	6	0	3.735133	1.777513	-0.561665
20	6	0	4.142395	0.580722	-0.083413
21	6	0	2.960621	-0.208573	0.184302
22	6	0	2.927573	-1.557307	0.529204
23	6	0	1.780732	-2.315509	0.323377
24	6	0	1.762952	-3.751121	0.334282
25	6	0	0.562952	-4.129613	-0.158342
26	6	0	-0.187002	-2.930033	-0.383420
27	6	0	-1.538616	-2.920404	-0.694738
28	6	0	-4.140784	2.243265	1.022455
29	6	0	-4.560773	2.048797	2.326017
30	6	0	-5.711285	2.670221	2.817260
31	6	0	-6.419014	3.490828	1.949532
32	6	0	-6.016452	3.720163	0.627633
33	6	0	-4.866127	3.089080	0.182876
34	6	0	2.177832	4.177989	-1.121825
35	6	0	1.908521	4.701040	-2.382853
36	6	0	2.482712	5.898008	-2.802826
37	6	0	3.325715	6.557146	-1.910516
38	6	0	3.607259	6.072953	-0.634173
39	6	0	3.020078	4.869404	-0.255358
40	6	0	4.138044	-2.237716	1.047963
41	6	0	4.585551	-1.951946	2.330730
42	6	0	5.726044	-2.558110	2.849381
43	6	0	6.400417	-3.473332	2.042276
44	6	0	5.972908	-3.791585	0.752707
45	6	0	4.834798	-3.154657	0.271837
46	6	0	-2.177082	-4.193839	-1.110481
47	6	0	-1.907297	-4.719481	-2.363635
48	6	0	-2.467469	-5.929623	-2.781987
49	6	0	-3.304880	-6.590916	-1.893864
50	6	0	-3.592343	-6.097552	-0.615366
51	6	0	-3.016497	-4.892780	-0.239741
52	6	0	-6.157023	2.394450	4.249443
53	6	0	-6.869696	4.605161	-0.275396
54	6	0	2.222985	6.501221	-4.180401
55	6	0	4.525312	6.869516	0.288770
56	6	0	6.209163	-2.178178	4.245857
57	6	0	6.722754	-4.765257	-0.151950
58	6	0	-2.146177	-6.464952	-4.174530
59	1	0	-4.360959	-2.630546	-0.820415
60	1	0	4.357502	2.598796	-0.890898
61	1	0	-0.183365	5.118372	-0.305018
62	1	0	-2.582259	4.363449	0.654786
63	1	0	0.187305	-5.133363	-0.312092
64	1	0	2.581398	-4.383210	0.653800
65	1	0	3.198664	4.447532	0.730832
66	1	0	1.240232	4.143446	-3.034752

67	1	0	3.782097	7.496009	-2.220400
68	1	0	4.481792	-3.342103	-0.741032
69	1	0	4.030447	-1.220022	2.916926
70	1	0	7.288045	-3.957771	2.435617
71	1	0	-3.196175	-4.470430	0.745981
72	1	0	-1.243814	-4.161474	-3.023203
73	1	0	-3.754761	-7.533615	-2.193511
74	1	0	-3.980527	1.378576	2.959561
75	1	0	-4.518788	3.212507	-0.839965
76	1	0	-7.324728	3.976512	2.304570
77	6	0	1.291533	5.639992	-5.025925
78	1	0	1.704541	4.640144	-5.205075
79	1	0	0.303321	5.524027	-4.565059
80	1	0	1.140241	6.109800	-6.004959
81	6	0	1.576318	7.878701	-4.018902
82	1	0	2.214832	8.575499	-3.464575
83	1	0	1.375611	8.326251	-5.000795
84	1	0	0.622679	7.804149	-3.482078
85	6	0	3.546838	6.643486	-4.934869
86	1	0	3.375399	7.063514	-5.934230
87	1	0	4.251905	7.304357	-4.418945
88	1	0	4.035238	5.669337	-5.058669
89	6	0	3.921113	8.253558	0.537071
90	1	0	4.562709	8.837145	1.209625
91	1	0	3.805723	8.829958	-0.387537
92	1	0	2.931099	8.172582	1.002147
93	6	0	5.900766	7.023083	-0.363807
94	1	0	5.850880	7.550303	-1.323033
95	1	0	6.573386	7.593064	0.289945
96	1	0	6.360456	6.044418	-0.548096
97	6	0	4.718470	6.192116	1.640608
98	1	0	3.771687	6.075066	2.181467
99	1	0	5.181026	5.202233	1.545424
100	1	0	5.379283	6.800422	2.269244
101	6	0	5.755206	-5.819102	-0.695495
102	1	0	5.284880	-6.379638	0.122181
103	1	0	4.954297	-5.382790	-1.302023
104	1	0	6.288541	-6.537040	-1.331206
105	6	0	7.335966	-3.982217	-1.315458
106	1	0	6.575334	-3.459271	-1.905806
107	1	0	8.042342	-3.227054	-0.948391
108	1	0	7.880818	-4.654828	-1.990999
109	6	0	7.845808	-5.497515	0.573938
110	1	0	7.473970	-6.070612	1.432195
111	1	0	8.327762	-6.205795	-0.110269
112	1	0	8.626331	-4.815462	0.931294
113	6	0	7.429268	-2.980704	4.682509
114	1	0	7.729069	-2.678163	5.692824
115	1	0	7.224915	-4.057985	4.711145
116	1	0	8.291557	-2.813022	4.026293
117	6	0	5.096560	-2.423981	5.266907
118	1	0	4.202395	-1.825905	5.062215
119	1	0	4.795418	-3.478565	5.274884
120	1	0	5.440115	-2.163820	6.276302
121	6	0	6.589651	-0.695457	4.251401
122	1	0	7.400496	-0.495972	3.540015
123	1	0	5.747198	-0.051556	3.975303
124	1	0	6.931463	-0.388806	5.248597
125	6	0	-6.246059	4.798094	-1.653105
126	1	0	-5.256902	5.268903	-1.594667
127	1	0	-6.139786	3.850103	-2.193775
128	1	0	-6.883898	5.449397	-2.262254
129	6	0	-7.046359	5.985711	0.359285
130	1	0	-7.658442	6.628562	-0.286228
131	1	0	-7.541221	5.937430	1.335282
132	1	0	-6.077420	6.479297	0.503658
133	6	0	-8.239840	3.949382	-0.463658
134	1	0	-8.773871	3.828624	0.485487
135	1	0	-8.871559	4.558278	-1.123379
136	1	0	-8.138786	2.954925	-0.916221
137	6	0	-5.029912	2.752419	5.220453
138	1	0	-4.758048	3.811501	5.134049

139	1	0	-5.344278	2.568906	6.255819
140	1	0	-4.123620	2.163155	5.045546
141	6	0	-7.388358	3.200407	4.646030
142	1	0	-8.262401	2.951158	4.032471
143	1	0	-7.653308	2.982110	5.687309
144	1	0	-7.214281	4.280907	4.572449
145	6	0	-6.498022	0.908347	4.384147
146	1	0	-7.315689	0.631728	3.707189
147	1	0	-5.644147	0.264892	4.144906
148	1	0	-6.813933	0.676532	5.409561
149	6	0	-2.641549	-5.468353	-5.224763
150	1	0	-3.725693	-5.322206	-5.145951
151	1	0	-2.167042	-4.486671	-5.119924
152	1	0	-2.423331	-5.835063	-6.235942
153	6	0	-0.633053	-6.646178	-4.315361
154	1	0	-0.086665	-5.704829	-4.193344
155	1	0	-0.250367	-7.351547	-3.567536
156	1	0	-0.385963	-7.042166	-5.308646
157	6	0	-2.807209	-7.810274	-4.450440
158	1	0	-2.480660	-8.581871	-3.742584
159	1	0	-3.901425	-7.749374	-4.409845
160	1	0	-2.538596	-8.155231	-5.455785
161	6	0	-4.507762	-6.896814	0.307604
162	6	0	-4.703737	-6.219456	1.659013
163	1	0	-3.757485	-6.099054	2.200084
164	1	0	-5.169558	-5.231154	1.563349
165	1	0	-5.362810	-6.829684	2.287613
166	6	0	-3.900811	-8.279379	0.557772
167	1	0	-4.540679	-8.862181	1.232631
168	1	0	-3.786312	-8.858157	-0.365258
169	1	0	-2.910428	-8.195751	1.021623
170	6	0	-5.882530	-7.054323	-0.345727
171	1	0	-5.830483	-7.581004	-1.305037
172	1	0	-6.553694	-7.626558	0.307566
173	1	0	-6.345025	-6.076842	-0.529440

Mono-brominated free-base **2** *in vacuo* at the M06/6-311G(d) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	5.801822	-0.164854	0.476161
2	7	0	-2.258631	0.529650	0.042982
3	7	0	-0.904322	-2.016822	0.048028
4	7	0	1.685735	-0.563178	0.058001
5	7	0	0.287125	1.961483	0.056774
6	6	0	-2.740694	1.798358	0.057745
7	6	0	-4.192822	1.806216	0.043601
8	6	0	-4.575956	0.514773	0.031109
9	6	0	-3.354775	-0.270096	0.015722
10	6	0	-3.347224	-1.673019	-0.032838
11	6	0	-2.195709	-2.460321	-0.048078
12	6	0	-2.132309	-3.874552	-0.218625
13	6	0	-0.820969	-4.241351	-0.221472
14	6	0	-0.030346	-3.066298	-0.050351
15	6	0	1.360828	-3.009784	-0.013972
16	6	0	2.136031	-1.841568	0.072082
17	6	0	3.571416	-1.888761	0.202077
18	6	0	3.982893	-0.606268	0.253115
19	6	0	2.785622	0.231430	0.151003
20	6	0	2.747844	1.633421	0.145663
21	6	0	1.582689	2.402456	0.107825
22	6	0	1.527553	3.828230	0.147933
23	6	0	0.218724	4.202139	0.135811
24	6	0	-0.578215	3.022280	0.072652
25	6	0	-1.972475	2.971016	0.064763
26	6	0	-4.648220	-2.386934	-0.102212
27	6	0	-5.466295	-2.246285	-1.211601

28	6	0	-6.707681	-2.881543	-1.288418
29	6	0	-7.088023	-3.682953	-0.219961
30	6	0	-6.284178	-3.862386	0.912224
31	6	0	-5.065936	-3.199453	0.954512
32	6	0	2.076313	-4.312450	-0.093742
33	6	0	2.055632	-5.196068	0.981094
34	6	0	2.724031	-6.416230	0.920686
35	6	0	3.411578	-6.718726	-0.253034
36	6	0	3.452849	-5.861336	-1.351299
37	6	0	2.772221	-4.651466	-1.250020
38	6	0	4.008632	2.425522	0.161725
39	6	0	4.663750	2.700175	-1.029557
40	6	0	5.835234	3.451695	-1.050955
41	6	0	6.323971	3.926776	0.165839
42	6	0	5.681735	3.680307	1.379507
43	6	0	4.512962	2.925148	1.353379
44	6	0	-2.688966	4.274229	0.067539
45	6	0	-3.404700	4.677851	1.182640
46	6	0	-4.126400	5.873596	1.191240
47	6	0	-4.084689	6.659199	0.046791
48	6	0	-3.359605	6.293841	-1.093696
49	6	0	-2.668939	5.090599	-1.065002
50	6	0	-7.587560	-2.652833	-2.513742
51	6	0	-6.771733	-4.763652	2.043758
52	6	0	2.727153	-7.412952	2.076641
53	6	0	4.233838	-6.265755	-2.598418
54	6	0	6.551829	3.686876	-2.377231
55	6	0	6.225682	4.174137	2.716264
56	6	0	-4.935553	6.247466	2.428773
57	1	0	-4.825198	2.685727	0.038861
58	1	0	4.190872	-2.773397	0.272061
59	1	0	-0.414726	-5.235752	-0.352524
60	1	0	-2.994790	-4.514454	-0.349940
61	1	0	-0.180445	5.206989	0.179993
62	1	0	2.394866	4.473453	0.192550
63	1	0	2.767819	-3.942218	-2.074565
64	1	0	1.506617	-4.901559	1.872537
65	1	0	3.940708	-7.668925	-0.313952
66	1	0	3.980854	2.690434	2.274819
67	1	0	4.247309	2.292400	-1.950231
68	1	0	7.235669	4.515376	0.167917
69	1	0	-2.104772	4.748833	-1.929503
70	1	0	-3.403428	4.027477	2.056593
71	1	0	-4.636502	7.595719	0.028276
72	1	0	-5.119788	-1.614227	-2.027945
73	1	0	-4.411442	-3.285929	1.818130
74	1	0	-8.046908	-4.192992	-0.256901
75	6	0	1.921381	-6.916929	3.272487
76	1	0	2.325208	-5.984461	3.684692
77	1	0	0.867460	-6.749124	3.019664
78	1	0	1.948953	-7.665278	4.073223
79	6	0	2.114219	-8.735773	1.612578
80	1	0	2.673770	-9.187981	0.786269
81	1	0	2.100349	-9.461238	2.436024
82	1	0	1.081087	-8.591978	1.273327
83	6	0	4.164291	-7.651525	2.545271
84	1	0	4.180906	-8.355455	3.387226
85	1	0	4.796973	-8.070686	1.755274
86	1	0	4.628338	-6.715935	2.879835
87	6	0	3.681273	-7.582035	-3.148639
88	1	0	4.229485	-7.879040	-4.051821
89	1	0	3.765716	-8.403676	-2.428903
90	1	0	2.622123	-7.482275	-3.415373
91	6	0	5.710048	-6.441577	-2.235340
92	1	0	5.862525	-7.221717	-1.481335
93	1	0	6.293350	-6.721511	-3.121963
94	1	0	6.129556	-5.509802	-1.836854
95	6	0	4.141762	-5.219354	-3.703715
96	1	0	3.108305	-5.058003	-4.033208
97	1	0	4.555563	-4.252697	-3.393250
98	1	0	4.714085	-5.552493	-4.577490
99	6	0	5.166572	5.020674	3.425815

100	1	0	4.888084	5.891777	2.819716
101	1	0	4.251246	4.456521	3.634430
102	1	0	5.550623	5.388455	4.386021
103	6	0	6.580897	2.964776	3.584357
104	1	0	5.708471	2.335776	3.793728
105	1	0	7.328098	2.332972	3.088323
106	1	0	6.995909	3.289936	4.547208
107	6	0	7.478170	5.029302	2.558400
108	1	0	7.291920	5.921530	1.948228
109	1	0	7.820136	5.371840	3.542314
110	1	0	8.305579	4.471273	2.104013
111	6	0	7.762117	4.603553	-2.235262
112	1	0	8.226263	4.757217	-3.216786
113	1	0	7.486155	5.590837	-1.844954
114	1	0	8.530085	4.178425	-1.578256
115	6	0	5.594206	4.330159	-3.382221
116	1	0	4.723792	3.700223	-3.593955
117	1	0	5.223589	5.293827	-3.011627
118	1	0	6.106205	4.511076	-4.336041
119	6	0	7.035898	2.340389	-2.920378
120	1	0	7.734046	1.864998	-2.220490
121	1	0	6.209034	1.640001	-3.082621
122	1	0	7.555055	2.474600	-3.878418
123	6	0	-5.781050	-4.833002	3.200250
124	1	0	-4.809543	-5.234973	2.888143
125	1	0	-5.612269	-3.850872	3.658049
126	1	0	-6.171297	-5.494752	3.982383
127	6	0	-6.972568	-6.184342	1.510707
128	1	0	-7.316149	-6.850548	2.312496
129	1	0	-7.716186	-6.226724	0.707543
130	1	0	-6.033896	-6.591539	1.115162
131	6	0	-8.097603	-4.231302	2.591388
132	1	0	-8.885053	-4.212308	1.830309
133	1	0	-8.452786	-4.862850	3.415795
134	1	0	-7.981870	-3.210608	2.975514
135	6	0	-6.848284	-3.107750	-3.773262
136	1	0	-6.598270	-4.174258	-3.718541
137	1	0	-7.474765	-2.953822	-4.661079
138	1	0	-5.914829	-2.557033	-3.931541
139	6	0	-8.904273	-3.417418	-2.439589
140	1	0	-9.511438	-3.113172	-1.578373
141	1	0	-9.497170	-3.220515	-3.340471
142	1	0	-8.748660	-4.501650	-2.382542
143	6	0	-7.913193	-1.160569	-2.620812
144	1	0	-8.444014	-0.811326	-1.726321
145	1	0	-7.014165	-0.544027	-2.733705
146	1	0	-8.555685	-0.967871	-3.489602
147	6	0	-5.994376	5.169628	2.674901
148	1	0	-6.673206	5.086389	1.816960
149	1	0	-5.550577	4.181826	2.842884
150	1	0	-6.597145	5.415942	3.558476
151	6	0	-4.007462	6.340237	3.641988
152	1	0	-3.498377	5.393140	3.850987
153	1	0	-3.235308	7.104116	3.489067
154	1	0	-4.576508	6.612129	4.540238
155	6	0	-5.649323	7.585986	2.278278
156	1	0	-4.945566	8.411818	2.117927
157	1	0	-6.365861	7.580717	1.448033
158	1	0	-6.212827	7.810739	3.191538
159	6	0	-3.363894	7.211312	-2.312611
160	6	0	-2.517006	6.663041	-3.455905
161	1	0	-1.464864	6.543706	-3.170495
162	1	0	-2.884677	5.694460	-3.815250
163	1	0	-2.547406	7.357291	-4.303958
164	6	0	-2.799982	8.580032	-1.924422
165	1	0	-2.783984	9.249316	-2.794239
166	1	0	-3.393602	9.069658	-1.144763
167	1	0	-1.772449	8.490257	-1.551077
168	6	0	-4.796123	7.376174	-2.826050
169	1	0	-5.458584	7.823295	-2.076980
170	1	0	-4.814368	8.025755	-3.710646
171	1	0	-5.224540	6.407722	-3.111532

172	1	0	-5.585488	0.121971	0.034674
173	1	0	0.012254	0.985756	-0.005252
174	1	0	-0.647154	-1.040373	0.155492

Mono-brominated free-base **2** in CH_2Cl_2 at the M06/6-311G(d) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	5.795156	0.126264	-0.544603
2	7	0	-2.263242	-0.513378	-0.049085
3	7	0	-0.894665	2.024225	-0.045841
4	7	0	1.687062	0.550127	-0.072489
5	7	0	0.272486	-1.965683	-0.083844
6	6	0	-2.754254	-1.780158	-0.075554
7	6	0	-4.205492	-1.777624	-0.055297
8	6	0	-4.580503	-0.483143	-0.025078
9	6	0	-3.355479	0.294396	-0.007160
10	6	0	-3.339573	1.697254	0.055263
11	6	0	-2.182449	2.477067	0.065520
12	6	0	-2.106974	3.890019	0.241720
13	6	0	-0.792895	4.247763	0.230355
14	6	0	-0.011984	3.068115	0.045355
15	6	0	1.378548	3.002369	-0.007654
16	6	0	2.144410	1.827479	-0.099708
17	6	0	3.577535	1.864089	-0.247442
18	6	0	3.980594	0.577530	-0.292176
19	6	0	2.781887	-0.252991	-0.170513
20	6	0	2.736583	-1.655744	-0.156548
21	6	0	1.566122	-2.416913	-0.124887
22	6	0	1.499712	-3.842347	-0.162488
23	6	0	0.187854	-4.206588	-0.160076
24	6	0	-0.601178	-3.021020	-0.101870
25	6	0	-1.995151	-2.959482	-0.094153
26	6	0	-4.636225	2.417886	0.141136
27	6	0	-5.445990	2.270753	1.256334
28	6	0	-6.685144	2.909830	1.346511
29	6	0	-7.069983	3.720900	0.286204
30	6	0	-6.273188	3.907189	-0.850503
31	6	0	-5.057059	3.240346	-0.907016
32	6	0	2.104688	4.299944	0.058957
33	6	0	2.066795	5.183782	-1.015720
34	6	0	2.747619	6.398179	-0.969781
35	6	0	3.464165	6.694203	0.188948
36	6	0	3.520926	5.836685	1.287281
37	6	0	2.827710	4.632251	1.200931
38	6	0	3.995023	-2.451694	-0.141265
39	6	0	4.644254	-2.675309	1.064633
40	6	0	5.814913	-3.427341	1.123336
41	6	0	6.310734	-3.950466	-0.071208
42	6	0	5.674720	-3.754861	-1.298066
43	6	0	4.503858	-3.001391	-1.309392
44	6	0	-2.722131	-4.257321	-0.104329
45	6	0	-3.438937	-4.649364	-1.223308
46	6	0	-4.168036	-5.841275	-1.238623
47	6	0	-4.131906	-6.633189	-0.097653
48	6	0	-3.405872	-6.278503	1.046288
49	6	0	-2.708089	-5.078615	1.025185
50	6	0	-7.558777	2.675072	2.575269
51	6	0	-6.764202	4.821534	-1.969915
52	6	0	2.733430	7.395636	-2.124908
53	6	0	4.330686	6.235042	2.517750
54	6	0	6.517808	-3.618925	2.464015
55	6	0	6.227800	-4.303154	-2.609845
56	6	0	-4.979087	-6.204540	-2.478132
57	1	0	-4.845081	-2.651850	-0.060160
58	1	0	4.201241	2.744642	-0.331031
59	1	0	-0.381458	5.240304	0.358689
60	1	0	-2.961410	4.538377	0.383384

61	1	0	-0.215281	-5.209809	-0.203522
62	1	0	2.359817	-4.497398	-0.200127
63	1	0	2.834929	3.924428	2.026820
64	1	0	1.495702	4.896197	-1.895515
65	1	0	4.003672	7.639004	0.237507
66	1	0	3.975084	-2.809792	-2.243001
67	1	0	4.223140	-2.232306	1.966902
68	1	0	7.222818	-4.537670	-0.045134
69	1	0	-2.142206	-4.746475	1.892404
70	1	0	-3.433309	-3.995975	-2.095084
71	1	0	-4.688866	-7.566667	-0.084797
72	1	0	-5.097322	1.631408	2.066089
73	1	0	-4.409479	3.333751	-1.775182
74	1	0	-8.026954	4.233383	0.334028
75	6	0	1.891118	6.911118	-3.300070
76	1	0	2.271944	5.973315	-3.722066
77	1	0	0.841479	6.758549	-3.020936
78	1	0	1.910602	7.660013	-4.100359
79	6	0	2.150492	8.726072	-1.643380
80	1	0	2.739949	9.170564	-0.833851
81	1	0	2.123961	9.450384	-2.467281
82	1	0	1.124780	8.595572	-1.276752
83	6	0	4.161424	7.616755	-2.629235
84	1	0	4.163881	8.325668	-3.466931
85	1	0	4.819653	8.022879	-1.853362
86	1	0	4.602498	6.676861	-2.983293
87	6	0	3.798897	7.555597	3.078687
88	1	0	4.368271	7.847141	3.970348
89	1	0	3.875562	8.376387	2.357130
90	1	0	2.744938	7.462715	3.368340
91	6	0	5.800208	6.401342	2.123529
92	1	0	5.941683	7.181381	1.367266
93	1	0	6.401813	6.677117	2.998962
94	1	0	6.205447	5.465998	1.717926
95	6	0	4.254374	5.189094	3.624701
96	1	0	3.227068	5.036277	3.977016
97	1	0	4.653326	4.219095	3.304708
98	1	0	4.849004	5.518710	4.484643
99	6	0	5.176752	-5.185669	-3.286660
100	1	0	4.903887	-6.033997	-2.646540
101	1	0	4.258620	-4.636453	-3.521526
102	1	0	5.567818	-5.588729	-4.229557
103	6	0	6.580216	-3.130710	-3.528532
104	1	0	5.704384	-2.518901	-3.772978
105	1	0	7.322490	-2.473913	-3.057403
106	1	0	7.003039	-3.496920	-4.472772
107	6	0	7.484981	-5.142425	-2.409024
108	1	0	7.300758	-6.011134	-1.765274
109	1	0	7.834969	-5.520790	-3.376681
110	1	0	8.305006	-4.560882	-1.971050
111	6	0	7.744785	-4.518218	2.360415
112	1	0	8.197883	-4.637188	3.351699
113	1	0	7.490449	-5.520069	1.993420
114	1	0	8.512912	-4.097142	1.700835
115	6	0	5.554089	-4.253524	3.469014
116	1	0	4.667567	-3.635026	3.645242
117	1	0	5.211827	-5.235427	3.119160
118	1	0	6.052016	-4.396354	4.436484
119	6	0	6.972558	-2.253131	2.984504
120	1	0	7.669699	-1.779861	2.281588
121	1	0	6.130850	-1.566747	3.129776
122	1	0	7.485659	-2.360894	3.948792
123	6	0	-5.781866	4.896533	-3.133163
124	1	0	-4.806205	5.291291	-2.824645
125	1	0	-5.621671	3.917840	-3.601574
126	1	0	-6.176338	5.567610	-3.905020
127	6	0	-6.953179	6.237856	-1.420697
128	1	0	-7.299545	6.912121	-2.214277
129	1	0	-7.691070	6.275632	-0.612012
130	1	0	-6.008656	6.636629	-1.030049
131	6	0	-8.097664	4.302097	-2.511844
132	1	0	-8.879192	4.280578	-1.744730

133	1	0	-8.454052	4.945358	-3.326383
134	1	0	-7.990449	3.285333	-2.909380
135	6	0	-6.811923	3.121939	3.833373
136	1	0	-6.563438	4.189285	3.784476
137	1	0	-7.434789	2.962014	4.722479
138	1	0	-5.878296	2.568773	3.983077
139	6	0	-8.875226	3.441117	2.511553
140	1	0	-9.486153	3.142618	1.651043
141	1	0	-9.462595	3.237852	3.414546
142	1	0	-8.719252	4.525524	2.460206
143	6	0	-7.884543	1.182257	2.676200
144	1	0	-8.418524	0.837327	1.781783
145	1	0	-6.985167	0.565367	2.785684
146	1	0	-8.524967	0.988106	3.545953
147	6	0	-6.033633	-5.120629	-2.716688
148	1	0	-6.711694	-5.040174	-1.857746
149	1	0	-5.585160	-4.134119	-2.880821
150	1	0	-6.637275	-5.361252	-3.601003
151	6	0	-4.052121	-6.292482	-3.692737
152	1	0	-3.541396	-5.345090	-3.897290
153	1	0	-3.283184	-7.061037	-3.545663
154	1	0	-4.624543	-6.557413	-4.590688
155	6	0	-5.697587	-7.541385	-2.335081
156	1	0	-4.996796	-8.370611	-2.179547
157	1	0	-6.413559	-7.538379	-1.504441
158	1	0	-6.261506	-7.756853	-3.250194
159	6	0	-3.413053	-7.205144	2.258249
160	6	0	-2.566128	-6.667233	3.406433
161	1	0	-1.513264	-6.549035	3.122923
162	1	0	-2.931936	-5.700246	3.772286
163	1	0	-2.600628	-7.368460	4.248407
164	6	0	-2.851179	-8.571496	1.858221
165	1	0	-2.837784	-9.246576	2.723365
166	1	0	-3.446077	-9.053284	1.074590
167	1	0	-1.822519	-8.480054	1.487821
168	6	0	-4.846106	-7.372648	2.768912
169	1	0	-5.508605	-7.812384	2.015517
170	1	0	-4.863442	-8.030920	3.646844
171	1	0	-5.272587	-6.406443	3.065645
172	1	0	-5.588436	-0.086534	-0.016324
173	1	0	0.004711	-0.988505	-0.017721
174	1	0	-0.647650	1.047419	-0.168664

Complex **Zn-2** *in vacuo* at the M06/6-311G(d) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	5.780150	0.012519	0.367346
2	7	0	-2.279030	0.471497	-0.003184
3	7	0	-0.816118	-1.994700	-0.001497
4	7	0	1.694309	-0.534864	0.021300
5	7	0	0.204754	1.918867	0.069561
6	6	0	-2.790862	1.736638	0.053395
7	6	0	-4.226013	1.682933	0.094924
8	6	0	-4.571017	0.374291	0.058969
9	6	0	-3.346355	-0.379111	-0.009858
10	6	0	-3.273370	-1.775812	-0.060256
11	6	0	-2.081348	-2.508310	-0.077902
12	6	0	-2.017188	-3.938371	-0.206127
13	6	0	-0.707388	-4.278987	-0.191980
14	6	0	0.039600	-3.059185	-0.056489
15	6	0	1.433297	-2.992890	-0.008881
16	6	0	2.181416	-1.809897	0.050055
17	6	0	3.605372	-1.786113	0.158037
18	6	0	3.973493	-0.483219	0.173568
19	6	0	2.767491	0.318012	0.078992
20	6	0	2.670650	1.714370	0.052545

21	6	0	1.469697	2.435361	0.047611
22	6	0	1.405204	3.872659	0.024711
23	6	0	0.094707	4.210476	0.046570
24	6	0	-0.651470	2.984183	0.072040
25	6	0	-2.047241	2.917802	0.078807
26	6	0	-4.554797	-2.526959	-0.101682
27	6	0	-5.388495	-2.423343	-1.203188
28	6	0	-6.619428	-3.081447	-1.252677
29	6	0	-6.974152	-3.866054	-0.163396
30	6	0	-6.154565	-4.006514	0.963543
31	6	0	-4.947388	-3.322607	0.977084
32	6	0	2.183993	-4.277039	-0.026074
33	6	0	2.157517	-5.118127	1.082320
34	6	0	2.860116	-6.320035	1.090015
35	6	0	3.590115	-6.649517	-0.050531
36	6	0	3.639081	-5.835632	-1.181078
37	6	0	2.921355	-4.643290	-1.147940
38	6	0	3.911020	2.535655	-0.009477
39	6	0	4.534999	2.742366	-1.231259
40	6	0	5.693280	3.507946	-1.330232
41	6	0	6.206189	4.063204	-0.158199
42	6	0	5.596618	3.886113	1.084126
43	6	0	4.435568	3.120167	1.134148
44	6	0	-2.796100	4.204177	0.114984
45	6	0	-2.974629	4.872706	1.313918
46	6	0	-3.669503	6.084219	1.373962
47	6	0	-4.175558	6.594984	0.185752
48	6	0	-4.012253	5.948975	-1.045658
49	6	0	-3.317720	4.747045	-1.059344
50	6	0	-7.516343	-2.890387	-2.471862
51	6	0	-6.616174	-4.886602	2.122059
52	6	0	2.856366	-7.268865	2.285155
53	6	0	4.463433	-6.267929	-2.390483
54	6	0	6.372581	3.668305	-2.686991
55	6	0	6.169545	4.465168	2.374127
56	6	0	-3.844615	6.781556	2.719625
57	1	0	-4.881897	2.542585	0.156621
58	1	0	4.258956	-2.645031	0.233900
59	1	0	-0.277221	-5.268202	-0.285184
60	1	0	-2.870822	-4.595157	-0.314922
61	1	0	-0.336603	5.203894	0.035995
62	1	0	2.258998	4.537324	-0.006684
63	1	0	2.918676	-3.968561	-2.000968
64	1	0	1.575422	-4.805329	1.945948
65	1	0	4.147173	-7.585557	-0.056792
66	1	0	3.926643	2.942896	2.081489
67	1	0	4.103821	2.270540	-2.113938
68	1	0	7.110774	4.659705	-0.214761
69	1	0	-3.158409	4.200290	-1.986086
70	1	0	-2.558168	4.427629	2.217067
71	1	0	-4.722029	7.534523	0.206410
72	1	0	-5.063413	-1.801226	-2.035923
73	1	0	-4.280623	-3.379239	1.833939
74	1	0	-7.924670	-4.393070	-0.178401
75	6	0	2.000019	-6.750491	3.435412
76	1	0	2.362277	-5.789142	3.818860
77	1	0	0.949309	-6.628120	3.146002
78	1	0	2.027706	-7.463878	4.267548
79	6	0	2.297286	-8.627360	1.856759
80	1	0	2.897894	-9.095492	1.069050
81	1	0	2.275482	-9.319170	2.708614
82	1	0	1.272888	-8.528873	1.477113
83	6	0	4.284683	-7.445087	2.805461
84	1	0	4.297227	-8.119149	3.671650
85	1	0	4.954507	-7.869605	2.049673
86	1	0	4.708895	-6.484323	3.121359
87	6	0	3.938945	-7.604851	-2.918008
88	1	0	4.516257	-7.923565	-3.795395
89	1	0	4.008586	-8.403400	-2.171145
90	1	0	2.887341	-7.523001	-3.218442
91	6	0	5.929598	-6.419634	-1.978838
92	1	0	6.067752	-7.179464	-1.201734

93	1	0	6.541376	-6.715597	-2.840694
94	1	0	6.328640	-5.474153	-1.591783
95	6	0	4.397431	-5.254828	-3.528180
96	1	0	3.374900	-5.119433	-3.900574
97	1	0	4.784589	-4.273323	-3.229629
98	1	0	5.007199	-5.603278	-4.370054
99	6	0	5.127556	5.361249	3.046428
100	1	0	4.844652	6.194979	2.391928
101	1	0	4.212439	4.817114	3.303026
102	1	0	5.528697	5.784914	3.976248
103	6	0	6.541174	3.315355	3.313491
104	1	0	5.674062	2.701796	3.581840
105	1	0	7.279609	2.651875	2.846453
106	1	0	6.974495	3.702717	4.244739
107	6	0	7.421551	5.301982	2.135333
108	1	0	7.226061	6.158573	1.478743
109	1	0	7.789079	5.699711	3.088707
110	1	0	8.234688	4.712541	1.694968
111	6	0	7.566271	4.615648	-2.639641
112	1	0	8.001559	4.712214	-3.641402
113	1	0	7.280731	5.621604	-2.308270
114	1	0	8.360338	4.249927	-1.977840
115	6	0	5.375531	4.222239	-3.706574
116	1	0	4.515052	3.560908	-3.850528
117	1	0	4.992646	5.200343	-3.390642
118	1	0	5.857726	4.348741	-4.684423
119	6	0	6.872012	2.297730	-3.151432
120	1	0	7.608961	1.891521	-2.447626
121	1	0	6.058738	1.567352	-3.228721
122	1	0	7.350605	2.373880	-4.136599
123	6	0	-5.608060	-4.918681	3.265175
124	1	0	-4.636195	-5.315131	2.947354
125	1	0	-5.445120	-3.924760	3.699034
126	1	0	-5.978859	-5.567682	4.067199
127	6	0	-6.810386	-6.321513	1.625874
128	1	0	-7.132976	-6.971872	2.449131
129	1	0	-7.567059	-6.391072	0.836842
130	1	0	-5.874143	-6.727851	1.223915
131	6	0	-7.939464	-4.354535	2.676343
132	1	0	-8.737622	-4.360942	1.926206
133	1	0	-8.276555	-4.969934	3.520390
134	1	0	-7.828419	-3.323985	3.034765
135	6	0	-6.784256	-3.357844	-3.730955
136	1	0	-6.518091	-4.419391	-3.659347
137	1	0	-7.422606	-3.229592	-4.614438
138	1	0	-5.860596	-2.796898	-3.909698
139	6	0	-8.820379	-3.673117	-2.368765
140	1	0	-9.423252	-3.361399	-1.507203
141	1	0	-9.425637	-3.502879	-3.266814
142	1	0	-8.647723	-4.753573	-2.292375
143	6	0	-7.866503	-1.405482	-2.603819
144	1	0	-8.392772	-1.047371	-1.710122
145	1	0	-6.978423	-0.777578	-2.738352
146	1	0	-8.521428	-1.239298	-3.468812
147	6	0	-4.644818	5.875319	3.658004
148	1	0	-5.638537	5.663321	3.244923
149	1	0	-4.147316	4.914937	3.831551
150	1	0	-4.781635	6.357637	4.634487
151	6	0	-2.470307	7.063788	3.331548
152	1	0	-1.895265	6.148129	3.505033
153	1	0	-1.873698	7.710541	2.676580
154	1	0	-2.577895	7.571393	4.298644
155	6	0	-4.584957	8.108748	2.600711
156	1	0	-4.052549	8.821151	1.958921
157	1	0	-5.599765	7.983035	2.204104
158	1	0	-4.678996	8.569884	3.590859
159	6	0	-4.596741	6.576860	-2.307760
160	6	0	-4.291720	5.757749	-3.556944
161	1	0	-3.213574	5.665202	-3.734543
162	1	0	-4.716720	4.748388	-3.503408
163	1	0	-4.726412	6.247384	-4.436330
164	6	0	-4.008002	7.974738	-2.508736

165	1	0	-4.406718	8.429299	-3.424726
166	1	0	-4.242717	8.650205	-1.679038
167	1	0	-2.916209	7.930475	-2.602871
168	6	0	-6.117535	6.677122	-2.168207
169	1	0	-6.416727	7.295300	-1.314663
170	1	0	-6.558167	7.123332	-3.069169
171	1	0	-6.564788	5.684870	-2.031571
172	30	0	-0.299166	-0.036478	0.021997
173	1	0	-5.568049	-0.047476	0.091592

Complex **Zn-2** in CCl_4 at the M06/6-311G(d) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	5.781894	0.014429	-0.383202
2	7	0	-2.279627	-0.481686	-0.001737
3	7	0	-0.826294	1.995590	-0.007014
4	7	0	1.694635	0.543745	-0.025789
5	7	0	0.214266	-1.921134	-0.071993
6	6	0	-2.784606	-1.749331	-0.056387
7	6	0	-4.220777	-1.702019	-0.098554
8	6	0	-4.571672	-0.394498	-0.064846
9	6	0	-3.349776	0.364758	0.003402
10	6	0	-3.282566	1.762700	0.052369
11	6	0	-2.093775	2.502140	0.069734
12	6	0	-2.036182	3.933116	0.200047
13	6	0	-0.727503	4.279601	0.187992
14	6	0	0.025253	3.062628	0.051122
15	6	0	1.420126	3.001253	0.005699
16	6	0	2.174451	1.821172	-0.054506
17	6	0	3.598943	1.804074	-0.165177
18	6	0	3.972311	0.502266	-0.182932
19	6	0	2.770162	-0.305071	-0.086030
20	6	0	2.679071	-1.702784	-0.058376
21	6	0	1.481512	-2.430661	-0.050620
22	6	0	1.423329	-3.869042	-0.024960
23	6	0	0.113880	-4.212696	-0.044436
24	6	0	-0.637897	-2.988955	-0.071789
25	6	0	-2.034819	-2.927595	-0.078742
26	6	0	-4.567673	2.507928	0.093896
27	6	0	-5.401340	2.399500	1.195242
28	6	0	-6.635161	3.052764	1.244745
29	6	0	-6.992613	3.836948	0.155677
30	6	0	-6.173113	3.981828	-0.971096
31	6	0	-4.962835	3.302939	-0.984673
32	6	0	2.165635	4.288538	0.028595
33	6	0	2.135955	5.135068	-1.075846
34	6	0	2.832673	6.340721	-1.076523
35	6	0	3.560297	6.667762	0.066592
36	6	0	3.612206	5.848195	1.193239
37	6	0	2.900350	4.652307	1.153271
38	6	0	3.923503	-2.518290	0.003051
39	6	0	4.549247	-2.721248	1.224854
40	6	0	5.709804	-3.483932	1.323816
41	6	0	6.223202	-4.039329	0.151744
42	6	0	5.612102	-3.865346	-1.090534
43	6	0	4.448744	-3.102434	-1.140649
44	6	0	-2.777796	-4.217789	-0.110856
45	6	0	-2.955331	-4.889877	-1.308150
46	6	0	-3.643293	-6.105939	-1.363341
47	6	0	-4.143155	-6.616914	-0.172273
48	6	0	-3.980577	-5.966917	1.057447
49	6	0	-3.293135	-4.760594	1.066470
50	6	0	-7.532178	2.857251	2.463224
51	6	0	-6.637518	4.861637	-2.128787
52	6	0	2.824050	7.296503	-2.266186
53	6	0	4.433655	6.278116	2.405505
54	6	0	6.391095	-3.640955	2.680048

55	6	0	6.185732	-4.444925	-2.380039
56	6	0	-3.818325	-6.807747	-2.706755
57	1	0	-4.874019	-2.563886	-0.158342
58	1	0	4.248715	2.666046	-0.240785
59	1	0	-0.302929	5.271212	0.282298
60	1	0	-2.892071	4.587203	0.307803
61	1	0	-0.312063	-5.208511	-0.032057
62	1	0	2.279148	-4.531267	0.006062
63	1	0	2.900345	3.973929	2.003464
64	1	0	1.556285	4.824613	-1.942000
65	1	0	4.112670	7.606422	0.078311
66	1	0	3.938782	-2.928594	-2.088112
67	1	0	4.117750	-2.250017	2.107736
68	1	0	7.129260	-4.633607	0.208219
69	1	0	-3.134915	-4.211422	1.992037
70	1	0	-2.544053	-4.445050	-2.213840
71	1	0	-4.683856	-7.559846	-0.189191
72	1	0	-5.074780	1.778202	2.028020
73	1	0	-4.296380	3.363838	-1.841497
74	1	0	-7.945178	4.360144	0.170955
75	6	0	1.970890	6.780267	-3.419791
76	1	0	2.338188	5.822912	-3.808520
77	1	0	0.920622	6.651164	-3.131556
78	1	0	1.995902	7.498968	-4.247358
79	6	0	2.257483	8.649363	-1.829608
80	1	0	2.855705	9.116001	-1.039171
81	1	0	2.232672	9.345310	-2.677910
82	1	0	1.233188	8.542898	-1.451643
83	6	0	4.251599	7.484061	-2.784824
84	1	0	4.259476	8.163913	-3.646444
85	1	0	4.918616	7.907811	-2.026112
86	1	0	4.680893	6.527765	-3.107696
87	6	0	3.905550	7.612126	2.937033
88	1	0	4.481736	7.928200	3.816045
89	1	0	3.974632	8.413488	2.193127
90	1	0	2.853966	7.526544	3.236822
91	6	0	5.899935	6.434988	1.995925
92	1	0	6.036586	7.197578	1.221232
93	1	0	6.509125	6.730178	2.859823
94	1	0	6.301989	5.491272	1.607384
95	6	0	4.368486	5.260833	3.539546
96	1	0	3.345572	5.121033	3.909372
97	1	0	4.759408	4.281591	3.238354
98	1	0	4.975665	5.608931	4.383382
99	6	0	5.144914	-5.342821	-3.051881
100	1	0	4.863596	-6.176857	-2.396991
101	1	0	4.229275	-4.799887	-3.309351
102	1	0	5.547583	-5.766120	-3.981132
103	6	0	6.555228	-3.295114	-3.320364
104	1	0	5.686515	-2.683960	-3.589419
105	1	0	7.293367	-2.630593	-2.854038
106	1	0	6.989000	-3.683122	-4.251057
107	6	0	7.439027	-5.279653	-2.140550
108	1	0	7.244692	-6.135764	-1.482993
109	1	0	7.806249	-5.677522	-3.093934
110	1	0	8.251418	-4.688676	-1.700859
111	6	0	7.585830	-4.587065	2.633120
112	1	0	8.021889	-4.680437	3.634818
113	1	0	7.300854	-5.594037	2.304355
114	1	0	8.378605	-4.221980	1.969431
115	6	0	5.396089	-4.193082	3.702682
116	1	0	4.535736	-3.531616	3.847199
117	1	0	5.013794	-5.172493	3.389856
118	1	0	5.880950	-4.316972	4.679464
119	6	0	6.889484	-2.268588	3.140580
120	1	0	7.625132	-1.863451	2.434538
121	1	0	6.074648	-1.539792	3.218297
122	1	0	7.369902	-2.342455	4.124934
123	6	0	-5.629390	4.898705	-3.271753
124	1	0	-4.659188	5.298892	-2.953412
125	1	0	-5.462546	3.905825	-3.706609
126	1	0	-6.003376	5.547169	-4.072665

127	6	0	-6.836821	6.295203	-1.630433
128	1	0	-7.161895	6.944765	-2.453264
129	1	0	-7.593868	6.360675	-0.841395
130	1	0	-5.901642	6.704504	-1.228765
131	6	0	-7.959120	4.325831	-2.683739
132	1	0	-8.757296	4.328388	-1.933567
133	1	0	-8.297647	4.942112	-3.526483
134	1	0	-7.844205	3.296557	-3.044901
135	6	0	-6.801789	3.324113	3.723635
136	1	0	-6.538659	4.386662	3.654323
137	1	0	-7.441152	3.192548	4.605810
138	1	0	-5.877242	2.764458	3.902295
139	6	0	-8.838117	3.636933	2.360741
140	1	0	-9.440055	3.324700	1.498724
141	1	0	-9.442380	3.463610	3.258833
142	1	0	-8.667981	4.717866	2.285530
143	6	0	-7.878230	1.371086	2.592407
144	1	0	-8.402748	1.012931	1.697638
145	1	0	-6.988369	0.745739	2.727718
146	1	0	-8.533753	1.202694	3.456442
147	6	0	-4.628863	-5.909398	-3.643888
148	1	0	-5.622714	-5.704257	-3.227464
149	1	0	-4.138439	-4.946108	-3.821823
150	1	0	-4.765643	-6.395591	-4.618384
151	6	0	-2.444393	-7.080720	-3.323827
152	1	0	-1.877769	-6.160805	-3.503018
153	1	0	-1.840050	-7.721389	-2.669862
154	1	0	-2.553195	-7.591886	-4.288835
155	6	0	-4.548188	-8.140208	-2.581669
156	1	0	-4.007761	-8.846930	-1.940307
157	1	0	-5.562264	-8.021192	-2.181186
158	1	0	-4.642258	-8.603642	-3.570707
159	6	0	-4.558154	-6.595167	2.322574
160	6	0	-4.254035	-5.771818	3.569211
161	1	0	-3.175858	-5.672858	3.743417
162	1	0	-4.685026	-4.765011	3.514917
163	1	0	-4.683632	-6.262767	4.450310
164	6	0	-3.961698	-7.989725	2.524504
165	1	0	-4.356621	-8.443918	3.442237
166	1	0	-4.195079	-8.667793	1.696503
167	1	0	-2.869927	-7.939504	2.616982
168	6	0	-6.078827	-6.703874	2.187063
169	1	0	-6.376604	-7.325355	1.335401
170	1	0	-6.513712	-7.151109	3.090235
171	1	0	-6.531795	-5.714065	2.050850
172	30	0	-0.299232	0.036124	-0.027016
173	1	0	-5.571049	0.021936	-0.097049

References:

(1) Bruker; Bruker-AXS Inc.: Madison, Wisconsin, USA, 2005.

(2) Sheldrick, G. *Acta Crystallogr., Sect. A* **2008**, *64*, 112.

(3) Farrugia, L. *J. Appl. Crystallogr.* **1999**, *32*, 837.

(4) Farrugia, L. *J. Appl. Crystallogr.* **1997**, *30*, 565.

(5) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Gaussian, Inc.: Wallingford, CT, USA, 2013.

(6) Orbelli Biroli, A.; Tessore, F.; Pizzotti, M.; Biaggi, C.; Ugo, R.; Caramori, S.; Aliprandi, A.; Bignozzi, C. A.; De Angelis, F.; Giorgi, G.; Licandro, E.; Longhi, E. *J. Phys. Chem. C* **2011**, *115*, 23170.

(7) Di Carlo, G.; Orbelli Biroli, A.; Pizzotti, M.; Tessore, F.; Trifiletti, V.; Ruffo, R.; Abbotto, A.; Amat, A.; De Angelis, F.; Mussini, P. R. *Chem. Eur. J.* **2013**, *19*, 10723.

(8) Barone, V.; Cossi, M. *J. Phys. Chem. A* **1998**, *102*, 1995.

(9) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.

(10) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648.

(11) Vosko, S. H.; Wilk, L.; Nusair, M. *Can. J. Phys.* **1980**, *58*, 1200.

(12) Zhao, Y.; Truhlar, D. *Theor. Chem. Acc.* **2008**, *120*, 215.

(13) *Atoms in Molecules. A Quantum Theory*; Bader, R. F. W., Ed. Clarendon: Oxford 1990.

(14) Todd, K. A.; TK Gristmill Software: Overland Park KS, USA, 2012.