Supplementary Information

Effects of position (α or β) and linker heteroatom (O or S) of substituent on the photophysicochemical behavior of poly(oxyethylene) substituted ZnPcs and assessment of J-aggregation or protonation using TD-DFT computations

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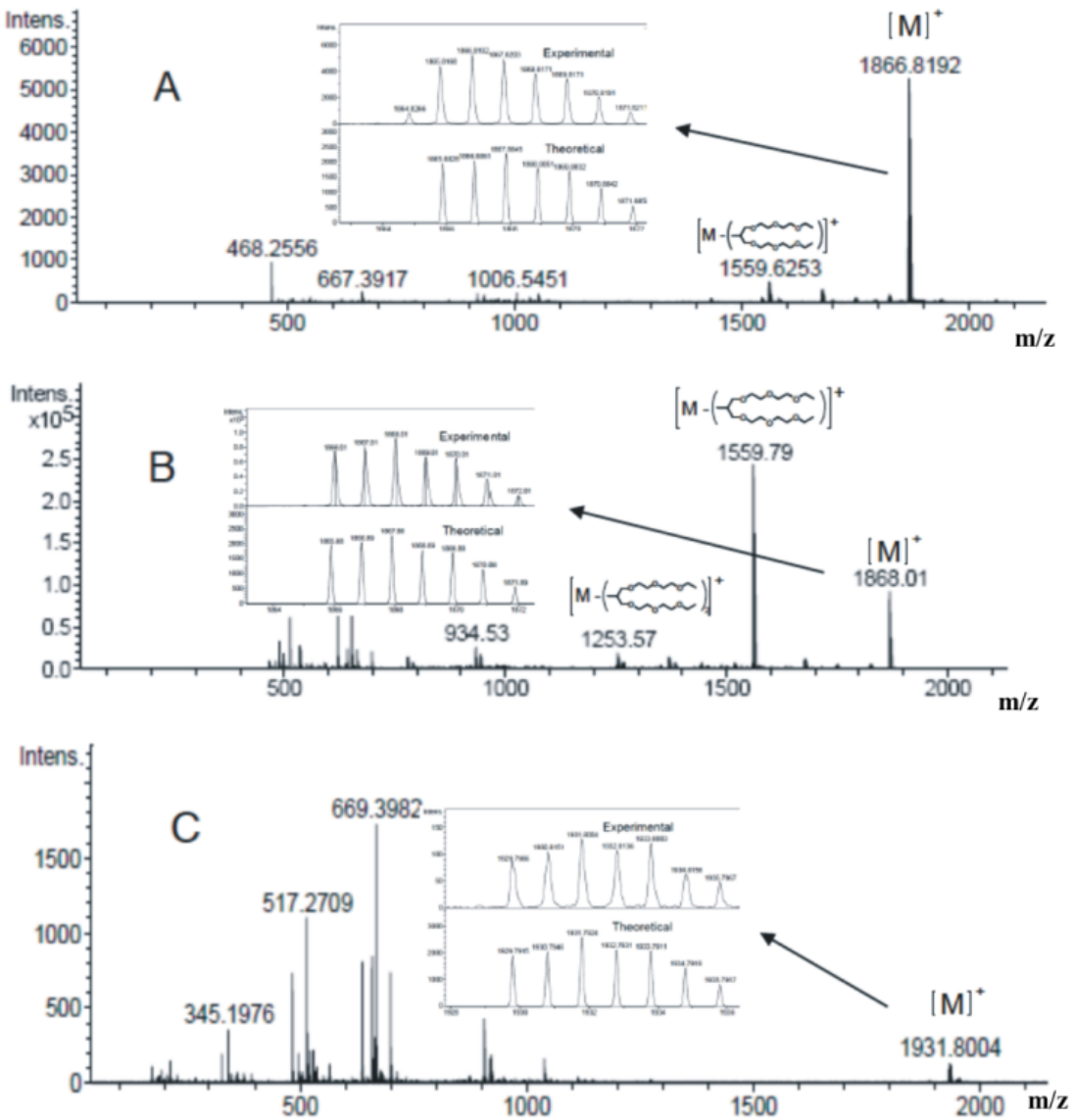

Figure S1. ESI-MS mass spectra of compounds **6a (A), 7a (B)** and **7b (C).**

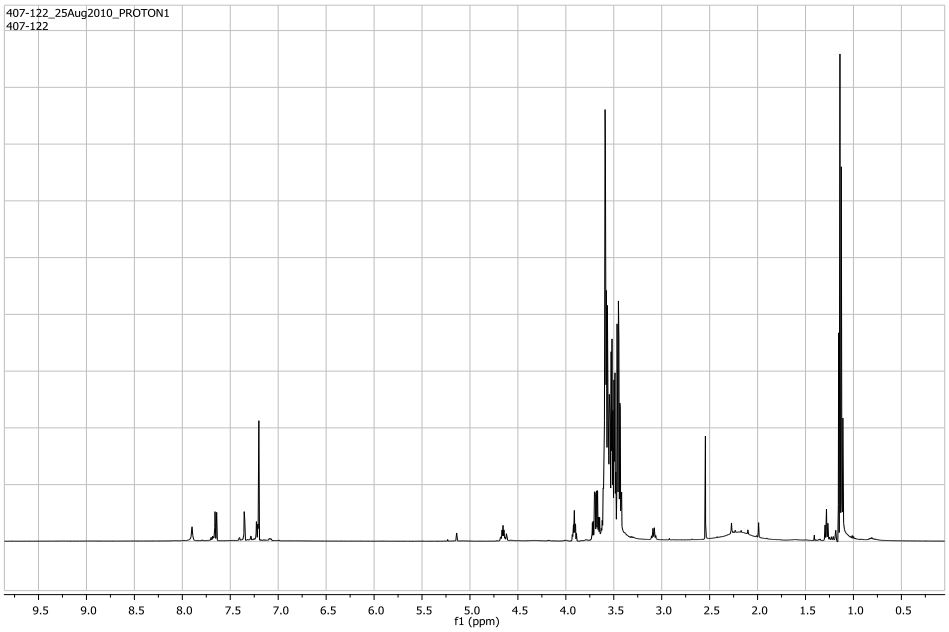

Figure S2. ^{1}H NMR (in $CDCl_3$) Spectrum of **6a.**

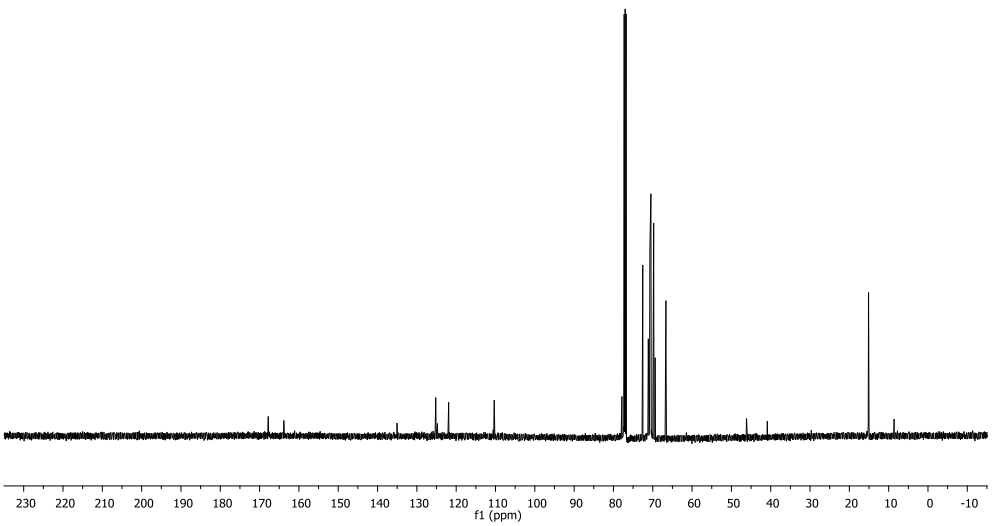

Figure S3. ^{13}C NMR (in $CDCl_3$) Spectrum of **6a.**

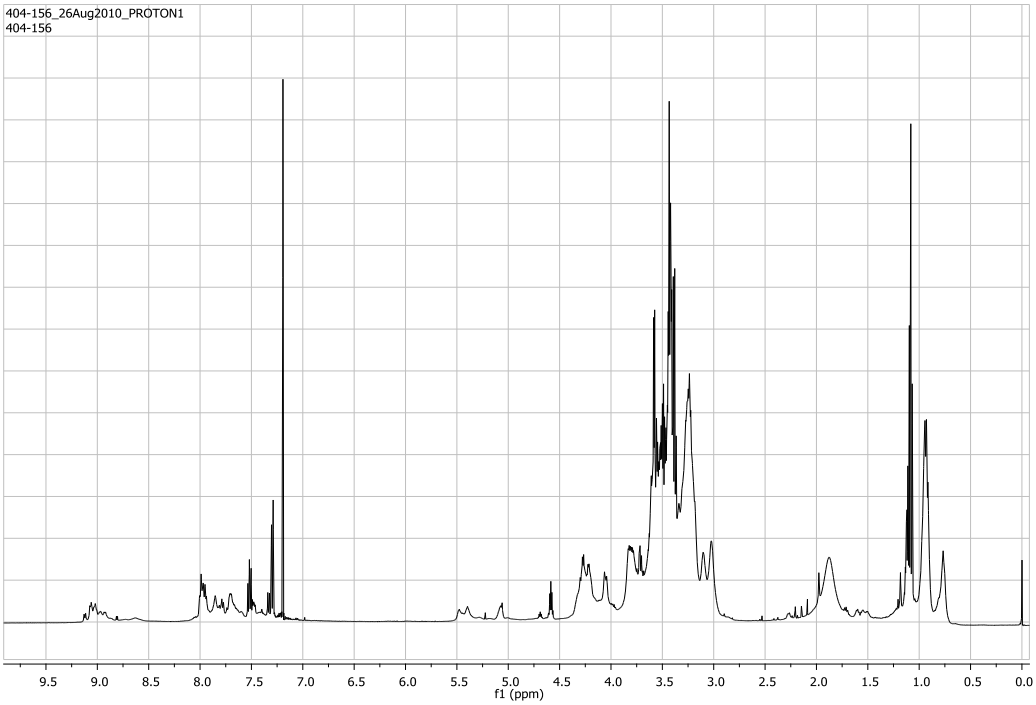

Figure S4. ^{1}H NMR (in $CDCl_3$) Spectrum of **7a.**

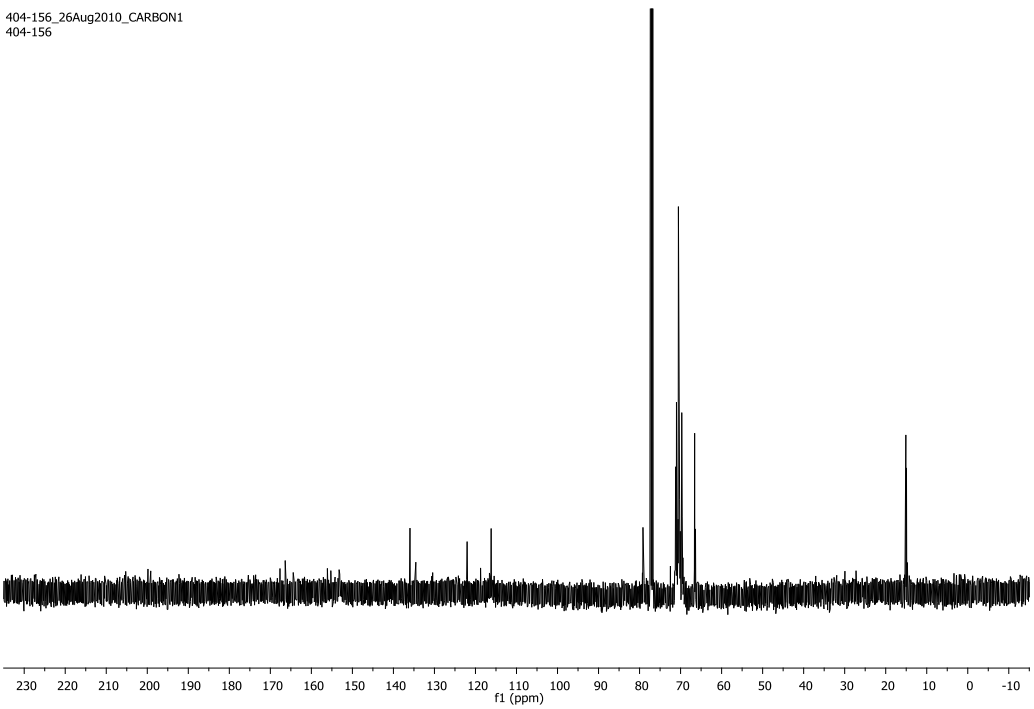

Figure S5. ^{13}C NMR (in $CDCl_3$) Spectrum of **7a.**

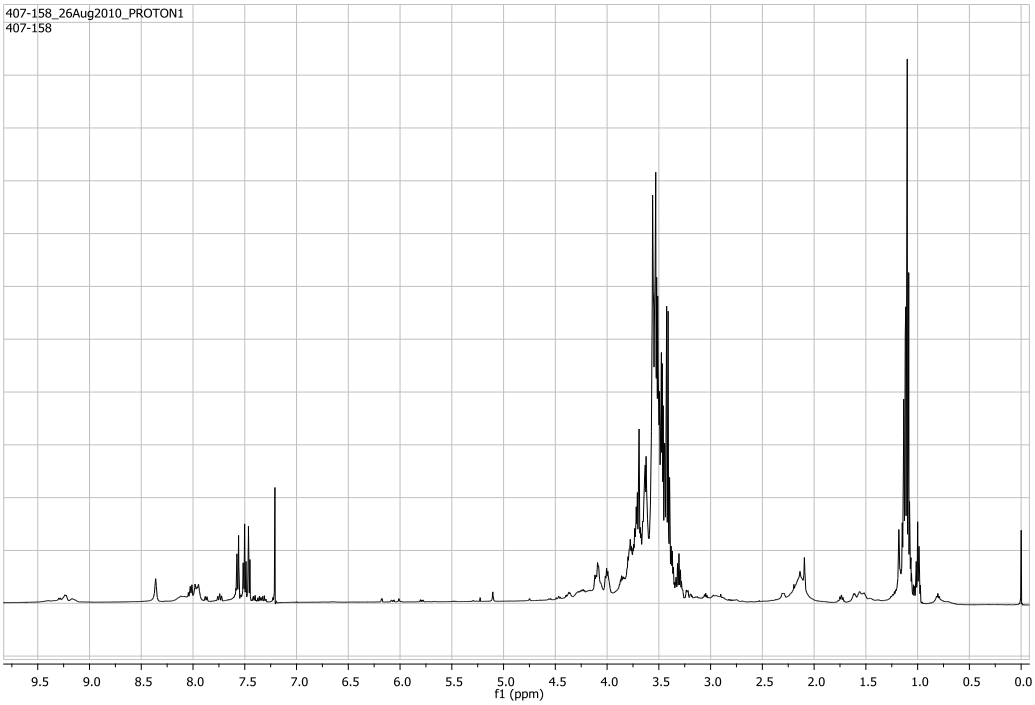

Figure S6. ^{1}H NMR (in $CDCl_3$) Spectrum of **7b.**

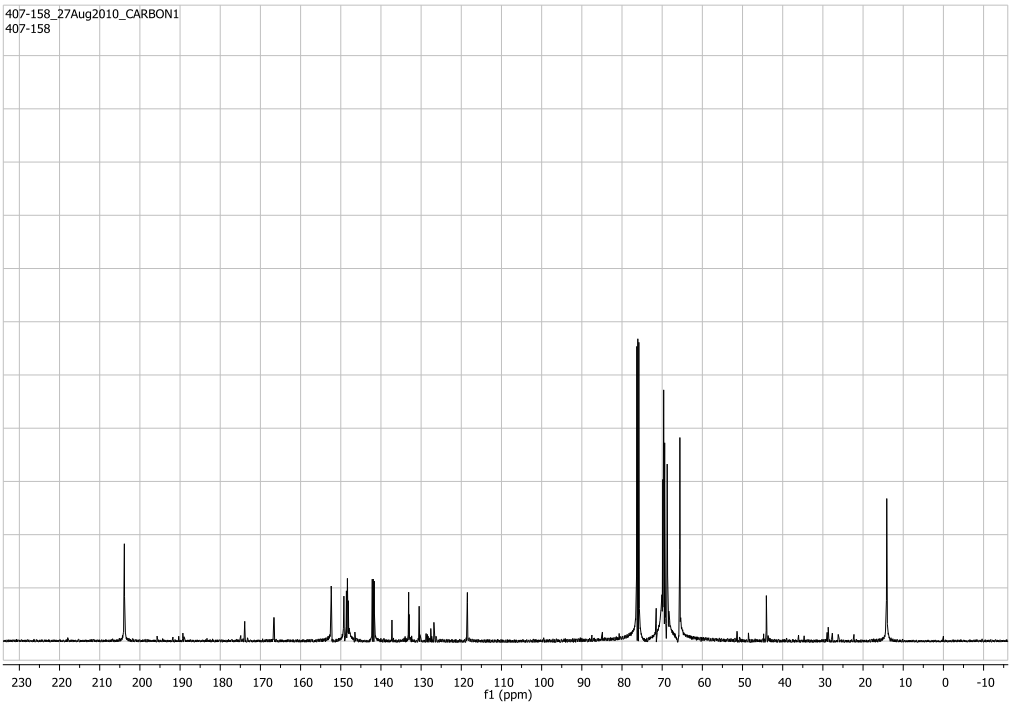

Figure S7. ^{13}C NMR (in $CDCl_3$) Spectrum of **7b.**

Photophysical and photochemical parameters

Fluorescence quantum yields (Φ_F) and lifetimes (τ_F): Fluorescence quantum yields (Φ_F) of the studied ZnPc compounds were determined in DMSO by the comparative method using equation 1.[1,2]

$$\Phi_F = \Phi_F(\text{Std})\frac{F \cdot A_{Std} \cdot n^2}{F_{Std} \cdot A \cdot n_{Std}^2} \quad (1)$$

where F and F_{Std} are the areas under the fluorescence emission curves of the ZnPcs (**6a-b** and **7a-b**) and the standard (**Std-ZnPc**), respectively. A and A_{Std} are the respective absorbances of the samples and standard at the excitation wavelengths, respectively. n^2 and n_{Std}^2 are the refractive indices of solvents used for the sample and standard, respectively. Unsubstituted ZnPc (**Std-ZnPc**) (Φ_F = 0.20 in DMSO)[3] was employed as the standard. The absorbance of the solutions at the excitation wavelength ranged between 0.04 and 0.05. The studied ZnPc compounds' (**6a-b** and **7a-b**) natural radiative lifetimes (τ_0) values were determined using PhotochemCAD program[4] which uses the Strickler-Berg equation for determination of τ_0 values. The fluorescence lifetimes (τ_F) of studied ZnPc compounds were evaluated using equation 2.

$$\Phi_F = \frac{\tau_F}{\tau_0} \quad (2)$$

Fluorescence quenching behavior of substituted ZnPcs by 1,4-benzoquinone (BQ): The fluorescence quenching studies on the substituted ZnPc compounds (**6a-b** and **7a-b**) were carried out by the addition of different concentrations of BQ to a fixed concentration of the samples, and the concentrations of BQ in the resulting mixtures were 0, 0.008, 0.016, 0.024, 0.032 and 0.040 M. The fluorescence spectra of the substituted ZnPc compounds (**6a-b** and **7a-b**) at each BQ concentration were recorded, and the changes in fluorescence intensity of ZnPc compounds (**6a-b** and **7a-b**) related to BQ concentration by the Stern–Volmer (SV) equation[5] (equation 3):

$$\frac{I_0}{I} = 1 + K_{SV}[BQ] \quad (3)$$

where I_0 and I are the fluorescence intensities of samples (**6a-b** and **7a-b**) in the absence and presence of BQ, respectively. K_{SV} is the Stern–Volmer constant; and this is the product of the bimolecular quenching constant (k_q) and the fluorescence lifetime τ_F (equation 4):

$$K_{SV} = k_q \tau_F \quad (4)$$

The ratios I_0/I were calculated and plotted against [BQ] according to equation 3, and K_{SV} determined from the slope.

Singlet oxygen quantum yields (Φ_Δ): In this study, the singlet oxygen quantum yield (Φ_Δ) determinations were carried out using the experimental set-up described in the literature.[6-8] Singlet oxygen quantum yields (Φ_Δ) of ZnPc compounds (**6a-b** and **7a-b**) were studied in DMSO using the relative method with unsubstituted ZnPc (**Std-ZnPc**) as reference. DPBF was used as chemical quencher for singlet oxygen in DMSO. The substituted ZnPcs (**6a-b** and **7a-b**) and the respective unsubstituted ZnPc (**Std-ZnPc**) solutions (C= $1x10^{-5}$ M) containing the singlet oxygen quencher were irradiated in the Q band region with the photo-irradiation set-up described in references.[6-8] Equation 5 was used for the calculations of Φ_Δ values:

$$\Phi_\Delta = \Phi_\Delta^{Std}\frac{R \cdot I_{abs}^{Std}}{R^{Std} \cdot I_{abs}} \quad (5)$$

where Φ_Δ^{Std} is the singlet oxygen quantum yield for the standard ZnPc (**Std-ZnPc**) (Φ_Δ^{Std} = 0.67 in DMSO).[9] R and R_{Std} are the DPBF photobleaching rates in the presence of the samples (**6a-b** and **7a-b**) and standard, respectively. I_{abs} and I_{abs}^{Std} are the rates of light absorption by the samples (**6a-b** and **7a-b**) and standard, respectively. To avoid chain reactions induced by DPBF in the presence of singlet oxygen, the concentration of DPBF was lowered to ~$3x10^{-5}$ M.[10] Solutions of sensitizers (C= $1x10^{-5}$ M) containing DPBF quencher were prepared in the dark and irradiated in the Q band region of samples using

the photoirradiation setup. The degradation of DPBF at 417 nm was monitored by UV-Vis spectrophotometer. The light intensity 6.54 x 10^{15} photons s^{-1} cm^{-2} was used for Φ_Δ determinations.

Photodegradation quantum yields (Φ_d): Photodegradation quantum yield (Φ_d) studies for substituted ZnPcs (**6a-b** and **7a-b**) were carried out using the experimental set-up described in the literature.[6-8] Photodegradation quantum yields of samples (**6a-b** and **7a-b**) were determined using equation 6,

$$\Phi_d = \frac{(C_0 - C_t) \cdot V \cdot N_A}{I_{abs} \cdot S \cdot t} \qquad (6)$$

where C_0 and C_t are the samples (**6a-b** and **7a-b**) concentrations before and after photoirradiation respectively, V is the reaction volume, N_A is the Avogadro's constant, S is the irradiated cell area and t is the irradiation time. I_{abs} is the overlap integral of the radiation source light intensity and the absorption of the samples (**6a-b** and **7a-b**). A light intensity of 2.18 x 10^{16} photons s^{-1} cm^{-2} was employed for Φ_d determinations.

References

1 S. Fery-Forgues and D. Lavabre, *J. Chem. Ed.,* 1999, **76**, 1260-1264.
2 D. Maree, T. Nyokong, K. Suhling and D. Phillips, *J. Porphyr. Phthalocyanines,* 2002, **6**, 373-376.
3 A. Ogunsipe, J-Y Chen and T. Nyokong, *New J. Chem.,* 2004, **28**, 822-827.
4 H. Du, R.A. Fuh, J. Li, A. Corkan and J.S. Lindsey, *Photochem. Photobiol.,* 1998, **68**, 141-142.
5 J. Rose, Advanced Physico-chemical Experiments, 1st ed., Sir Isaac Pitman & Sons Ltd., London, 1964, p. 257.
6 J.H. Brannon and D. Madge, *J. Am. Chem. Soc*., 1980, **102**, 62–65.
7 I. Seotsanyana-Mokhosi, N. Kuznetsova and T. Nyokong, *J. Photochem. Photobiol. A: Chem.,* 2001, **140**, 215-222.
8 A. Ogunsipe and T. Nyokong, *J. Photochem. Photobiol. A: Chem*. 2005, **173**, 211–220.
9 N. Kuznetsova, N. Gretsova, E. Kalmkova, E. Makarova, S. Dashkevich, V. Negrimovski, O. Kaliya and E. Luk'yanets, *Russ. J. Gen. Chem.,* 2000, **70**, 133–140.
10 W. Spiller, H. Kliesch, D. Wöhrle, S. Hackbarth, B. Roder and G. Schnurpfeil, *J. Porphyrins Phthalocyanines,* 1998, **2**, 145-158.

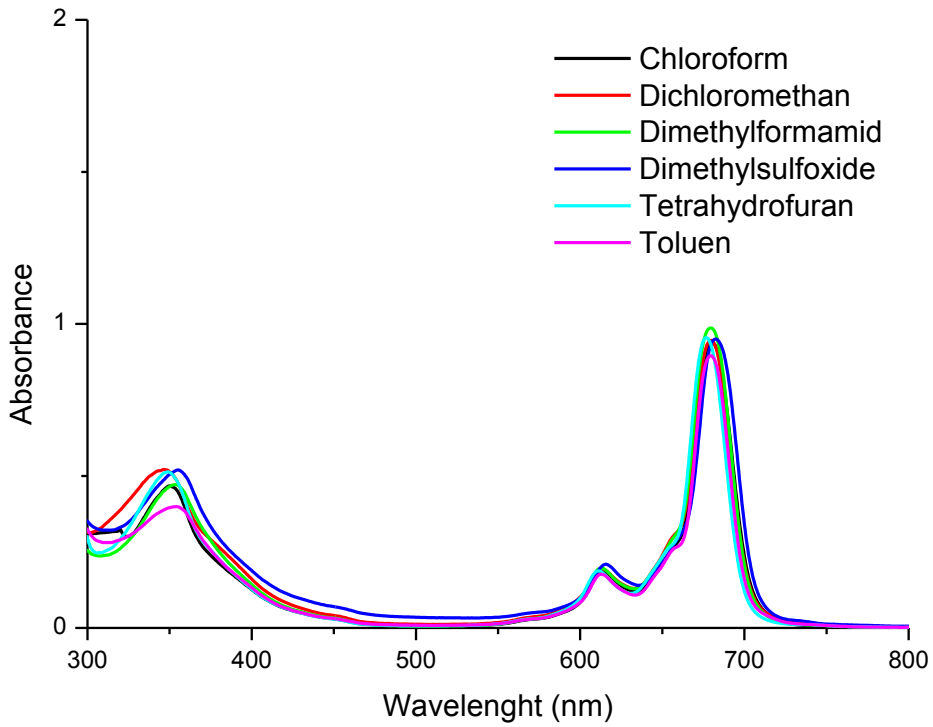

Figure S8. Absorption spectra of **6a** in different solvents. Concentration ~ 5.0x10^{-6} M.

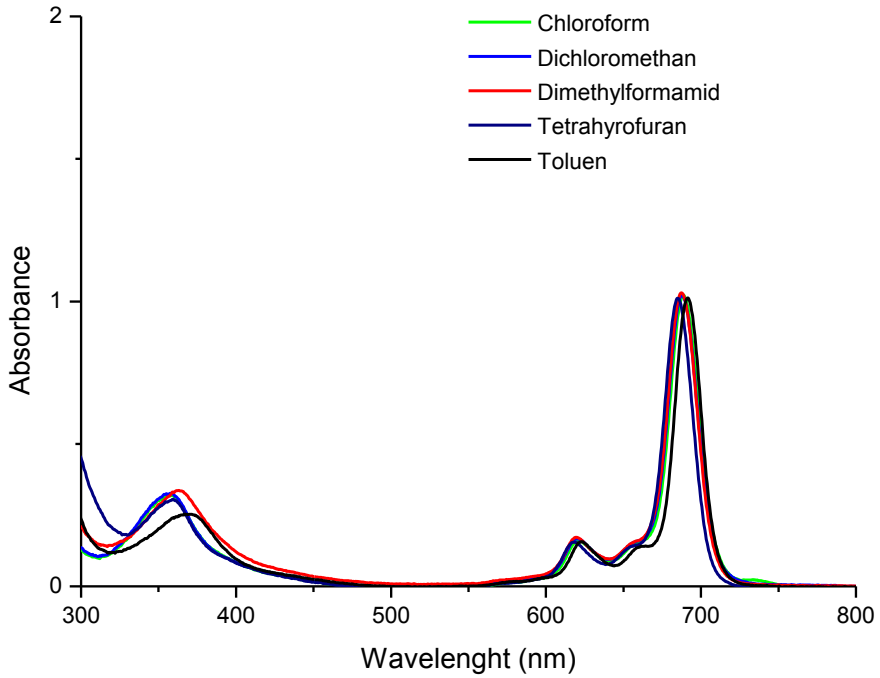

Figure S9. Absorption spectra of **6b** in different solvents. Concentration ~ 5.0×10^{-6} M.

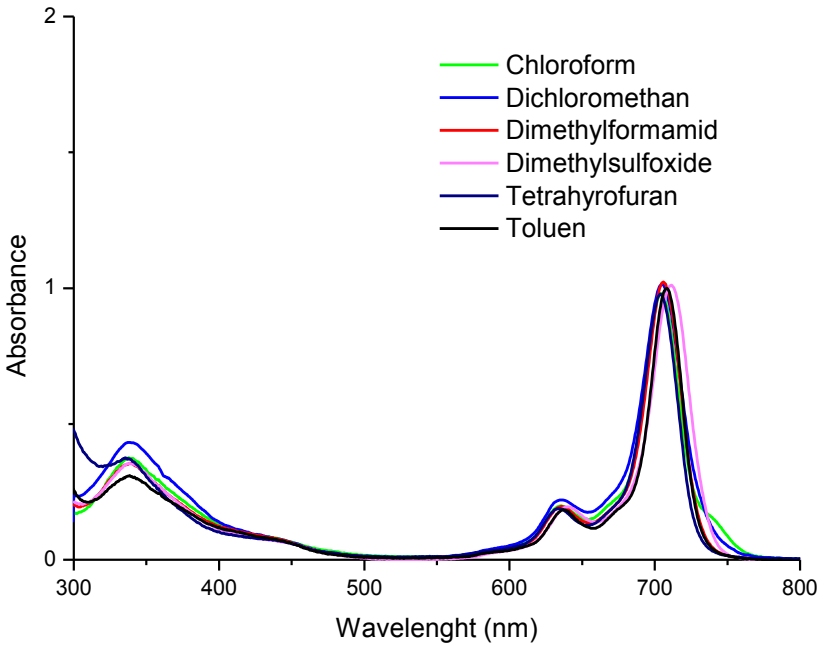

Figure S10. Absorption spectra of **7b** in different solvents. Concentration ~ 5.0×10^{-6} M.

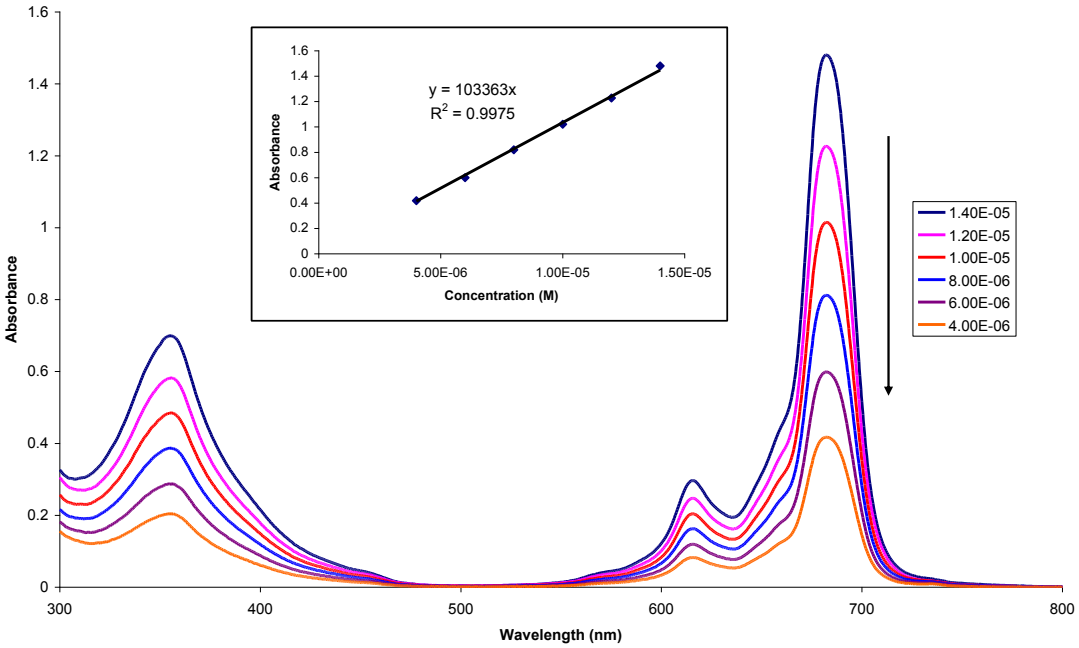

Figure S11. Absorption spectra of compound **6a** at different concentrations in DMSO.

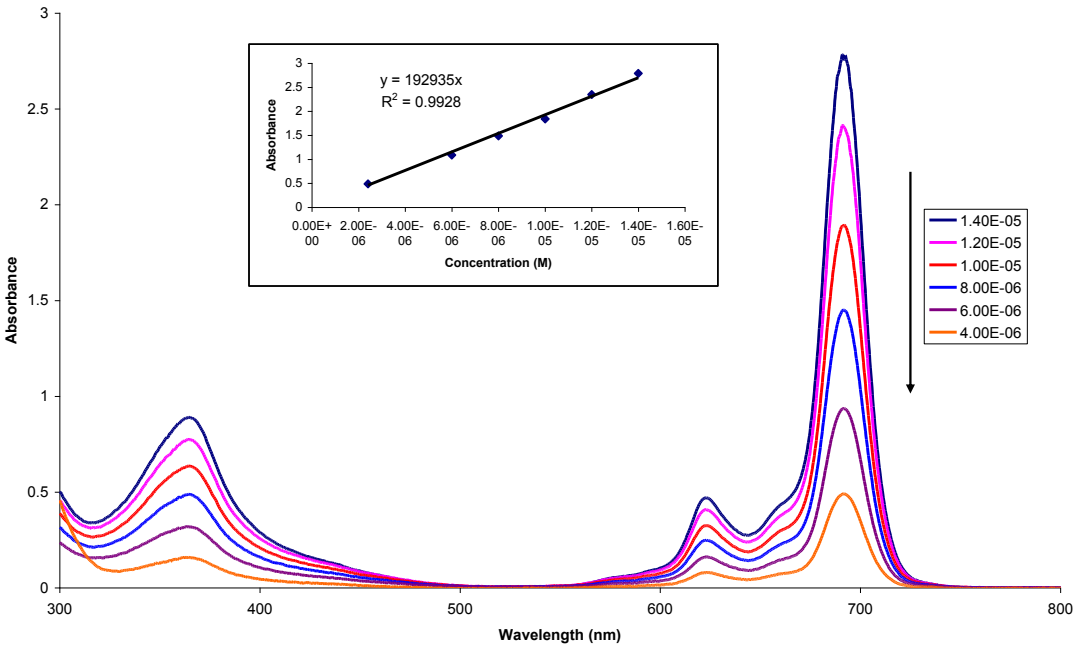

Figure S12. Absorption spectra of compound **6b** at different concentrations in DMSO.

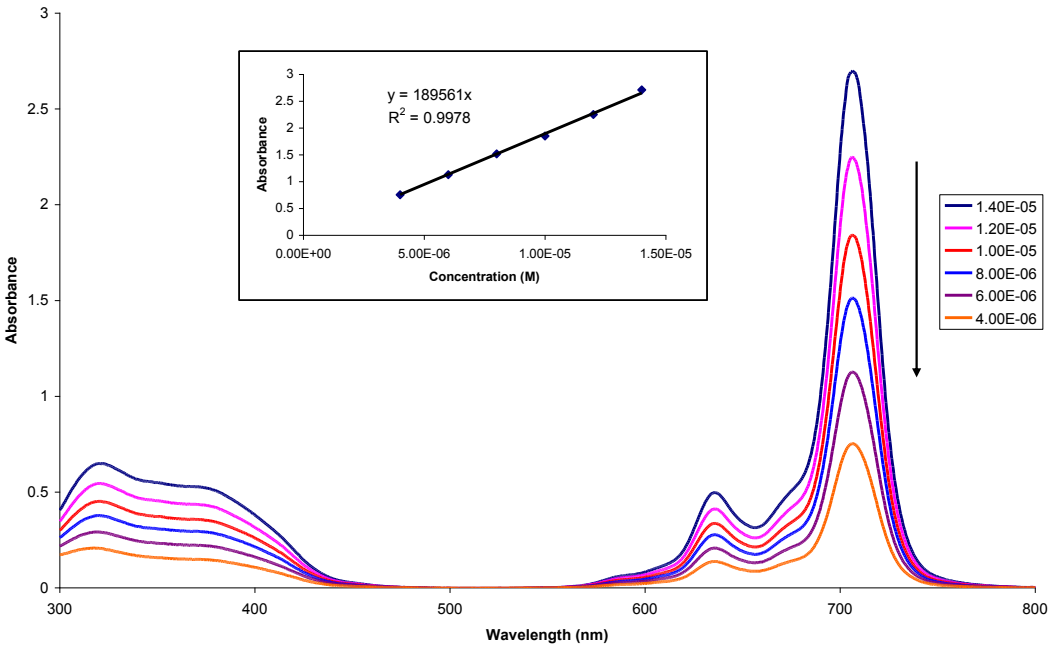

Figure S13. Absorption spectra of compound **7a** at different concentrations in DMSO.

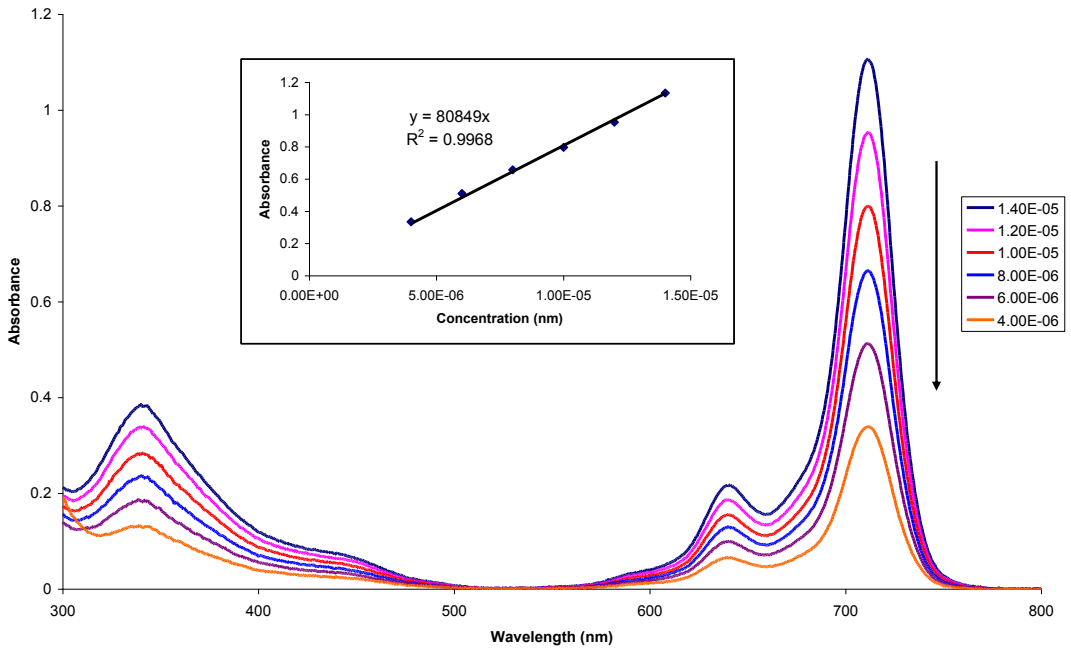

Figure S14. Absorption spectra of compound **7b** at different concentrations in DMSO.

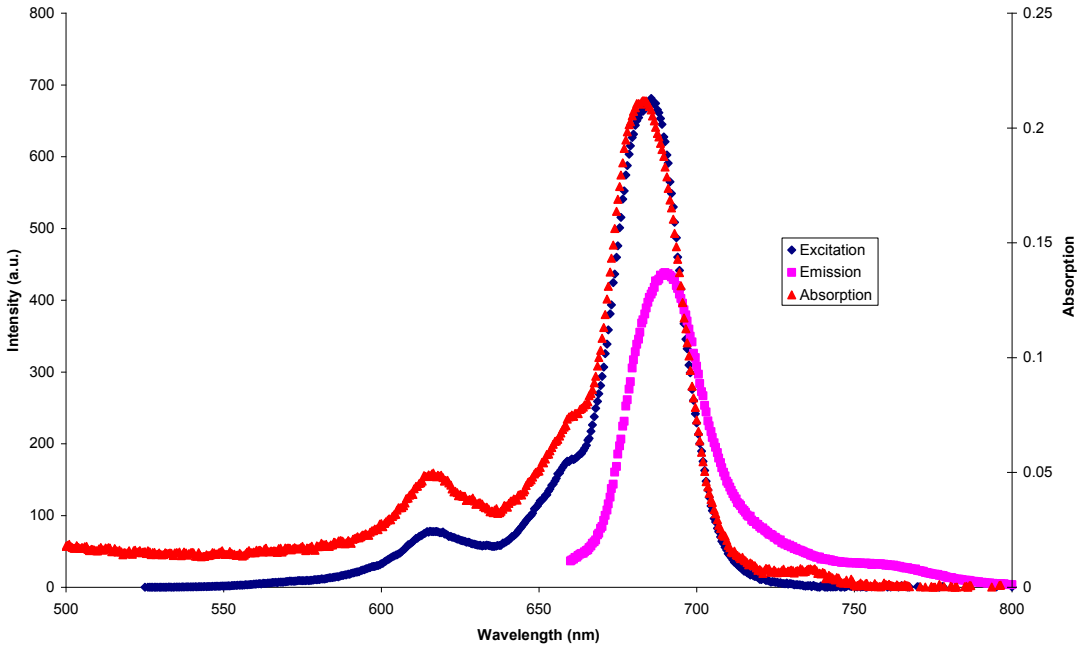

Figure S15. Absorption, fluorescence emission and excitation spectra for compound **6a** in DMSO. Excitation wavelengths = 660 nm.

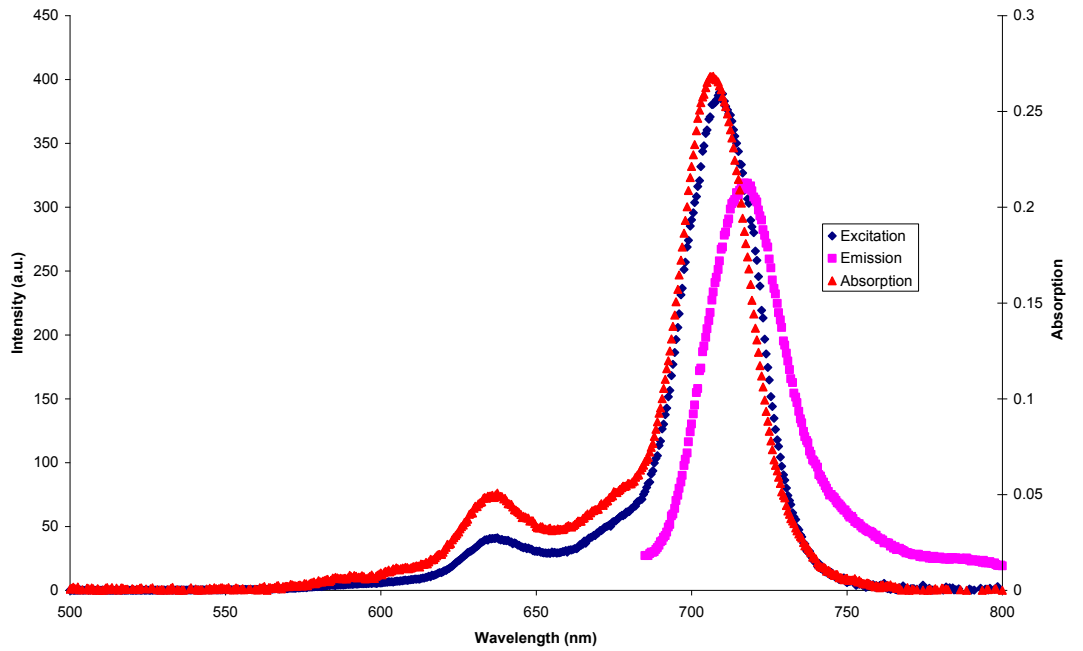

Figure S16. Absorption, fluorescence emission and excitation spectra for compound **7a** in DMSO. Excitation wavelengths = 675 nm.

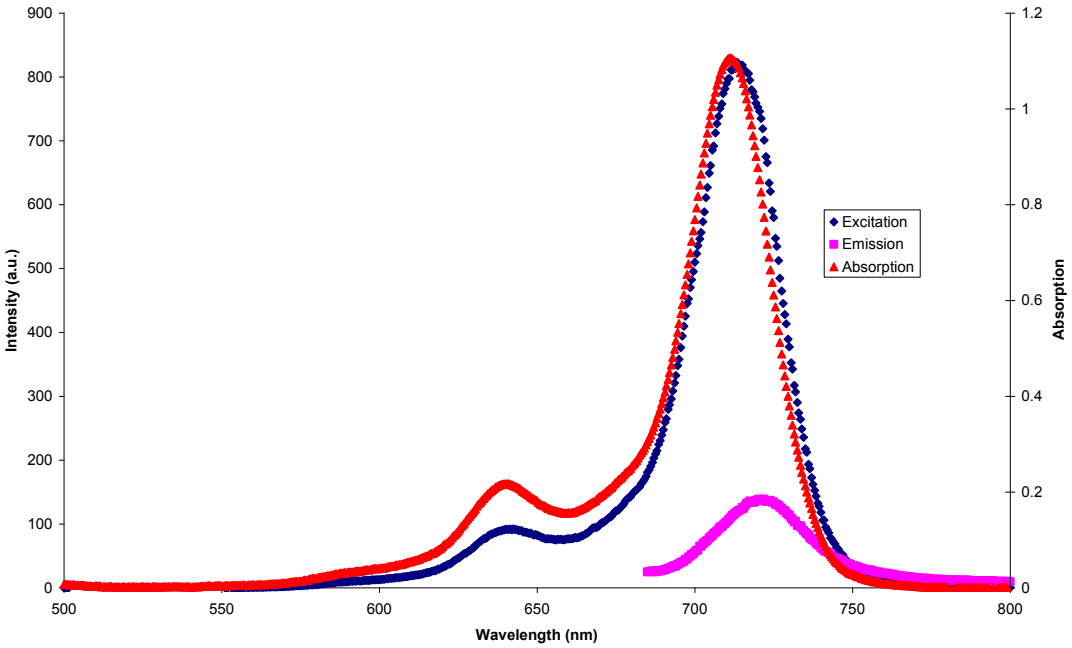

Figure S17. Absorption, fluorescence emission and excitation spectra for compound **7b** in DMSO. Excitation wavelengths = 675 nm.

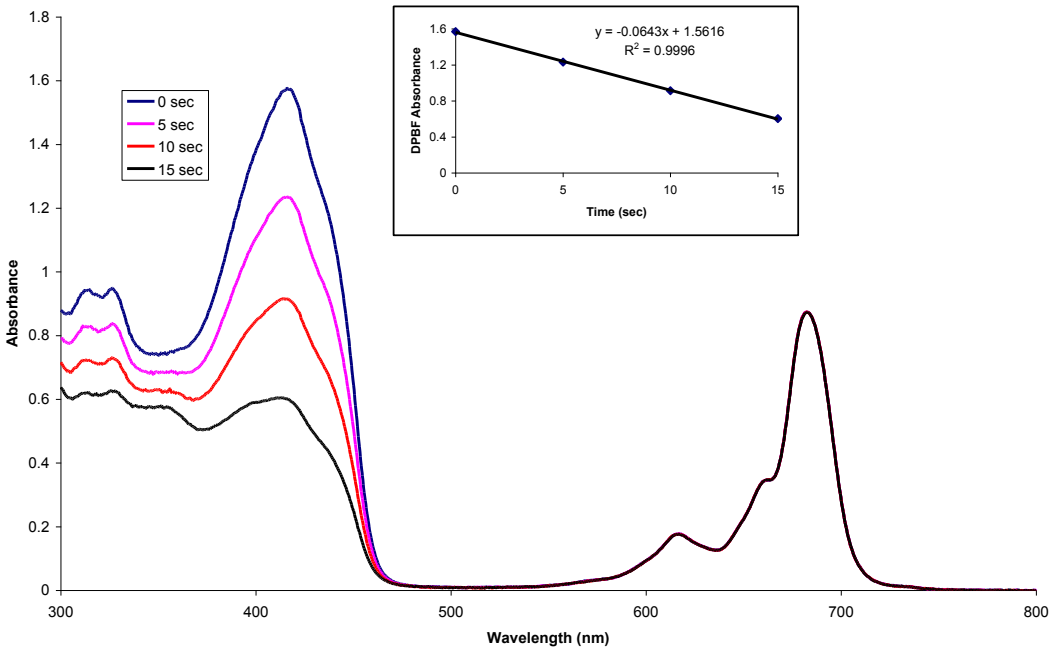

Figure S18. Absorption changes during the determination of singlet oxygen quantum yield. This determination was for compound **6a** in DMSO at a concentration of $1x10^{-5}$ M. (Inset: Plot of DPBF absorbance versus time).

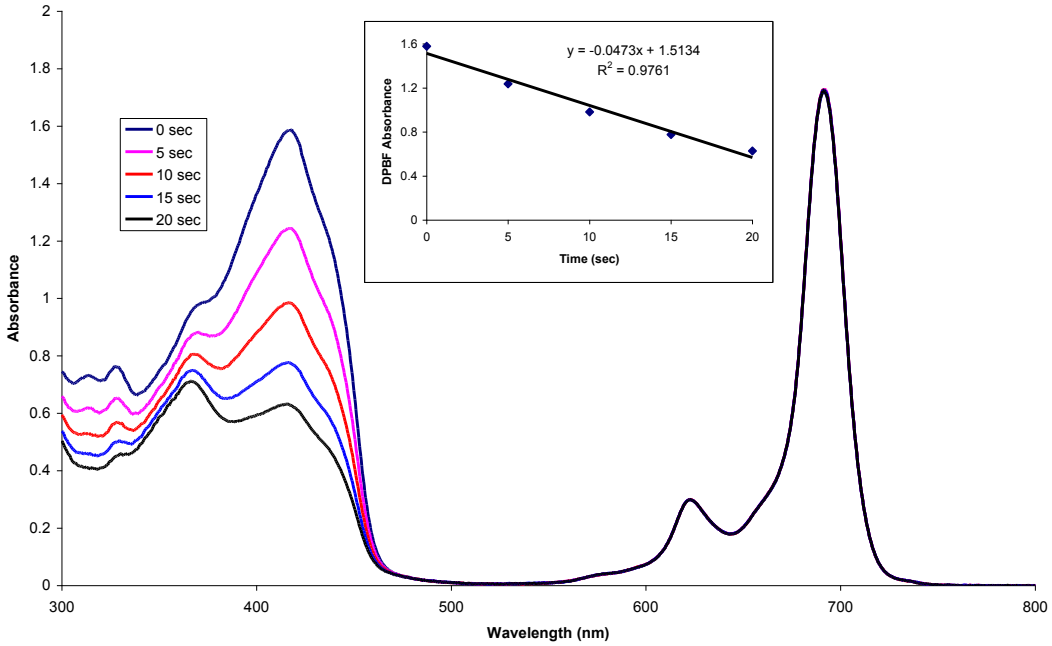

Figure S19. Absorption changes during the determination of singlet oxygen quantum yield. This determination was for compound **6b** in DMSO at a concentration of $1x10^{-5}$ M. (Inset: Plot of DPBF absorbance versus time).

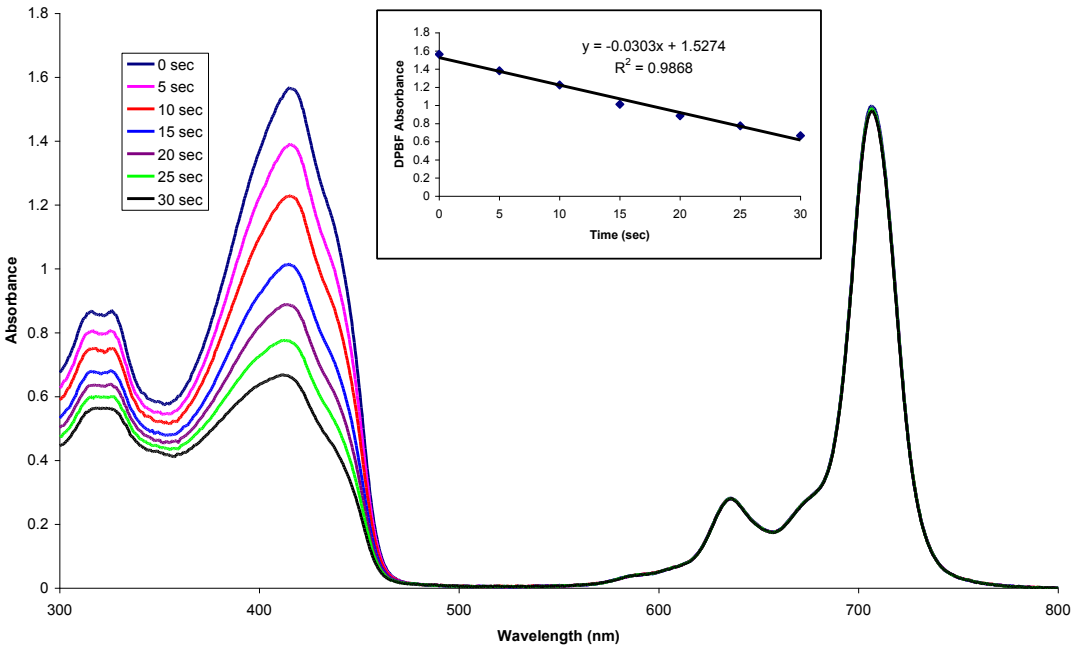

Figure S20. Absorption changes during the determination of singlet oxygen quantum yield. This determination was for compound **7a** in DMSO at a concentration of $1x10^{-5}$ M. (Inset: Plot of DPBF absorbance versus time).

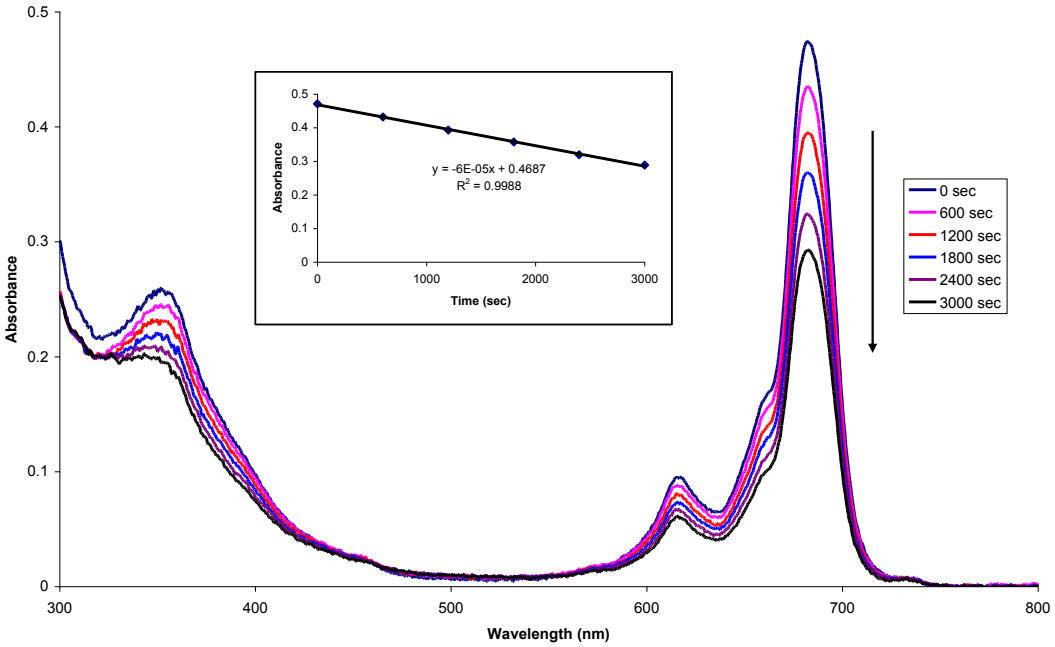

Figure S21. Absorption changes during the photodegradation studies of compound **6a** in DMSO showing the disappearance of the Q-band at 10 minutes intervals. Concentration ~ 5.0×10^{-6} M. (Inset: Plot of absorbance versus time).

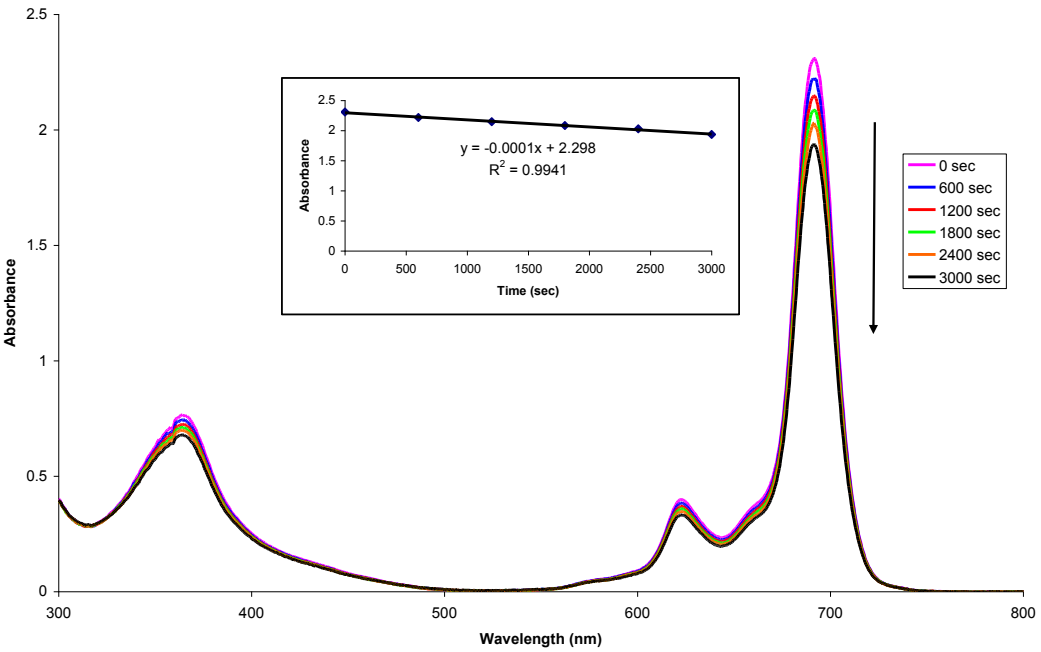

Figure S22. Absorption changes during the photodegradation studies of compound **6b** in DMSO showing the disappearance of the Q-band at 10 minutes intervals. Concentration ~ 5.0×10^{-6} M. (Inset: Plot of absorbance versus time).

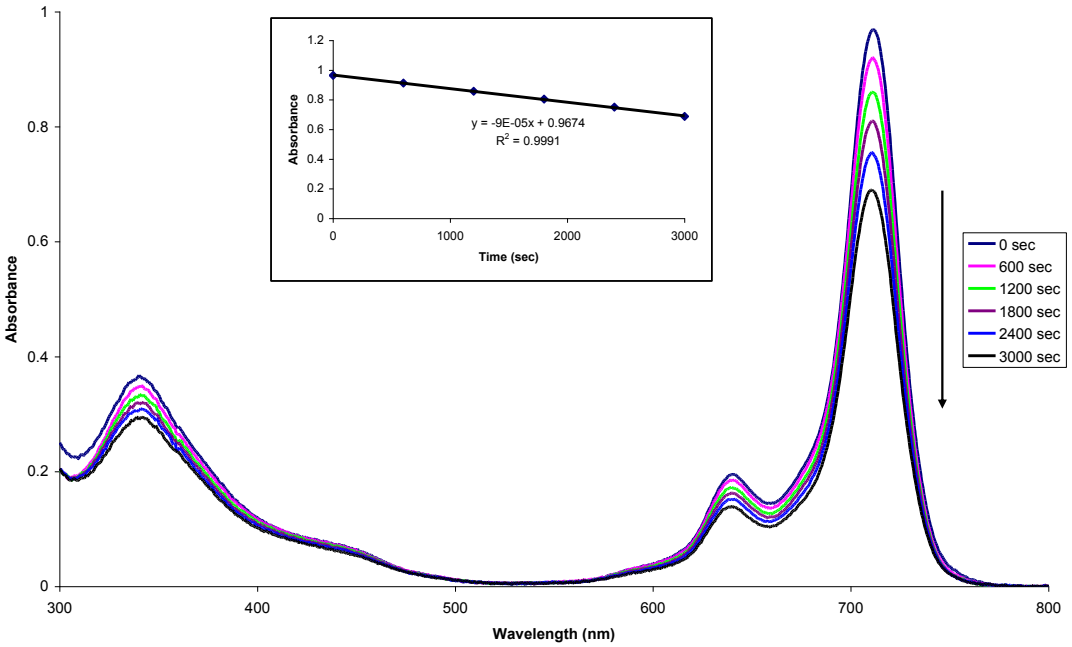

Figure S23. Absorption changes during the photodegradation studies of compound **7b** in DMSO showing the disappearance of the Q-band at 10 minutes intervals. Concentration ~ 5.0×10^{-6} M. (Inset: Plot of absorbance versus time).

Computational details:

The DFT[1] and semi-empirical calculations were carried out using Gaussian 09[2] and Spartan 10[3] packages, respectively. Considering the size of the structures **7a-b** and computational cost, we performed all computations on the model ZnPc structures (Figure 12) by replacing the poly(oxyethylene) and poly(thioethylene) bulky groups on benzene rings with methoxy and methylthio groups, respectively. Besides, symmetry isomers (C_{4h}, D_{2h}, C_{2v}, and C_s) of these model ZnPcs were also taken into consideration, since all four possible symmetry isomers can be formed during reaction. Conformational search for each symmetry (**8a-d** and **9a-d**) was done using AM1[4] method. Taking the most stable conformations as prime input, DFT optimizations were carried out using the B3LYP level of theory[5,6] using the 6-31G(d,p)[7] basis set.

To study the aggregation process, J-dimeric arrangements of **8a-d** and **9a-d** were constructed using their optimized geometries as monomers. The optimizations of model J-dimers were done with B3LYP/6-31G(d,p) level and interaction energies were calculated.

In order to calculate the proton affinities of nitrogen atoms which have different electronic environment (Figure 11) on the model monomers (**8a-d** and **9a-d**), protonated species of **8a-d** and **9a-d** were also optimized with the same level. All stationary points were confirmed to be local minima by performing analytic computations of vibrational frequencies in the harmonic approximation. Thermal corrections to the zero point energy (ZPE), enthalpy, and entropy were calculated at 298.15 K and 1 atm. Proton affinities (PA) of model monomers were calculated using the equation $PA = \Delta E_{prot} + 5RT/2$. $\Delta E_{prot} = E_{tot}(M) - E_{tot}(MH^+)$ is the difference between zero-point corrected total energies of monomer (M) and protonated monomer (MH^+). In order to compare electronic absorption spectra of the model monomers (**8a-d** and **9a-d**), J-dimers and protonated monomers in chloroform, TD-DFT computations at the B3LYP/6-31G(d,p) level combined with the polarizable continuum model (PCM)[8] were carried out on the optimized ground state geometries, by considering the first twelve singlet excited states. Absorption spectra were simulated using SpecDis Version 1.51 program package.[9]

References

1 R. G. Parr and W. Yang, Density-Functional Theory of Atoms and Molecules; Oxford University Press: New York, 1989.

2 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.

3 Spartan 10, Wavefunction Inc.: Irvine, CA.

4 M. Dewar and W. Thiel. *J. Am. Chem. Soc.* 1977, **99**, 4899-4907.

5 A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648-5652.

6 C. Lee and W. Yang, R. G. Parr, *Phys. Rev. B* 1988, **37**, 785-789.

7 R. Ditchfield, W. J. Hehre and J. A. Pople, *J. Chem. Soc.* 1971, **54**, 724-728.

8 S. Miertus, E. Scrocco and J. Tomasi, *Chem. Phys.* 1981, **55**, 117–129.

9 T. Bruhn, A. Schaumlöffel, Y. Hemberger and G. Bringmann, SpecDis version 1.53, University of Wuerzburg, Germany, 2012.

Table S1. Absolute energies (au) of the model monomers calculated with B3LYP/6-31G(d,p). ZPE: Zero point energy, H: Enthalpy, G:Gibbs energy, NIF: Number of imaginary frequency.

	ZPE	**H**	**G**	**NIF**
8a	-3903,934610	-3903,894615	-3904,006279	0
8b	-3903,929880	-3903,889566	-3904,001886	0
8c	-3903,932445	-3903,892219	-3904,004581	0
8d	-3903,932422	-3903,892236	-3904,004341	0
9a	-5195,874253	-5195,831613	-5195,950807	0
9b	-5195,85995	-5195,81742	-5195,93462	0
9c	-5195,867091	-5195,824500	-5195,942675	0
9d	-5195,867095	-5195,824531	-5195,942412	0
p-8a	-3903,950456			0
p-8b	-3903,950271			0
p-8c	-3903,952684			0
p-8d	-3903,915636			0

Table S2. Absolute energies (au) of the model J-dimers calculated with B3LYP/6-31G(d,p). ZPE: Zero point energy, H: Enthalpy, G:Gibbs energy, NIF: Number of imaginary frequency.

	ZPE	**H**	**G**	**NIF**
Dimer of 8a	-7807,882860	-7807,802297	-7808,000203	0
Dimer of 8b	-7807,885687	-7807,805321	-7808,000797	0
Dimer of 8c	-7807,882001	-7807,801463	-7807,998586	0
Dimer of 8d	-7807,886359	-7807,806075	-7808,001304	0
Dimer of 9a	-10391,762245	-10391,676780	-10391,887227	0
Dimer of 9b	-10391,736339	-10391,650852	-10391,858982	0
Dimer of 9c	-10391,745154	-10391,659701	-10391,868143	0
Dimer of 9d	-10391,739219	-10391,653676	-10391,864056	0

Table S3. Absolute zero point energies (au) of the protonated monomers calculated with B3LYP/6-31G(d,p).

Sym.	ZnPc	N type	ZPE	ZnPc	N type	ZPE	ZnPc	N type	ZPE
C_{4h}	8a	Na	-3904,342675	9a	Na	-5196,272007	*p*-8a	Na	-3904,343035
D_{2h}	8b	Na	-3904,345008	9b	Na	-5196,259478	*p*-8b	Na	-3904,344270
		Nb	-3904,320390		Nb	-5196,245827		Nb	-3904,344438
C_{2v}	8c	Na	-3904,351149	9c	Na	-5196,269759	*p*-8c	Na	-3904,341868
		Nb	-3904,336805		Nb	-5196,262001		Nb	-3904,343918
		Nc	-3904,326014		Nc	-5196,255647		Nc	-3904,346074
C_s	8d	Na	-3904,350965	9d	Na	-5196,269567	*p*-8d	Na	-3904,302674
		Nb	-3904,325870		Nb	-5196,255841		Nb	-3904,304212
		Nc	-3904,336899		Nc	-5196,262051		Nc	-3904,305914
		Nd	-3904,337194		Nd	-5196,262132		Nd	-3904,305691

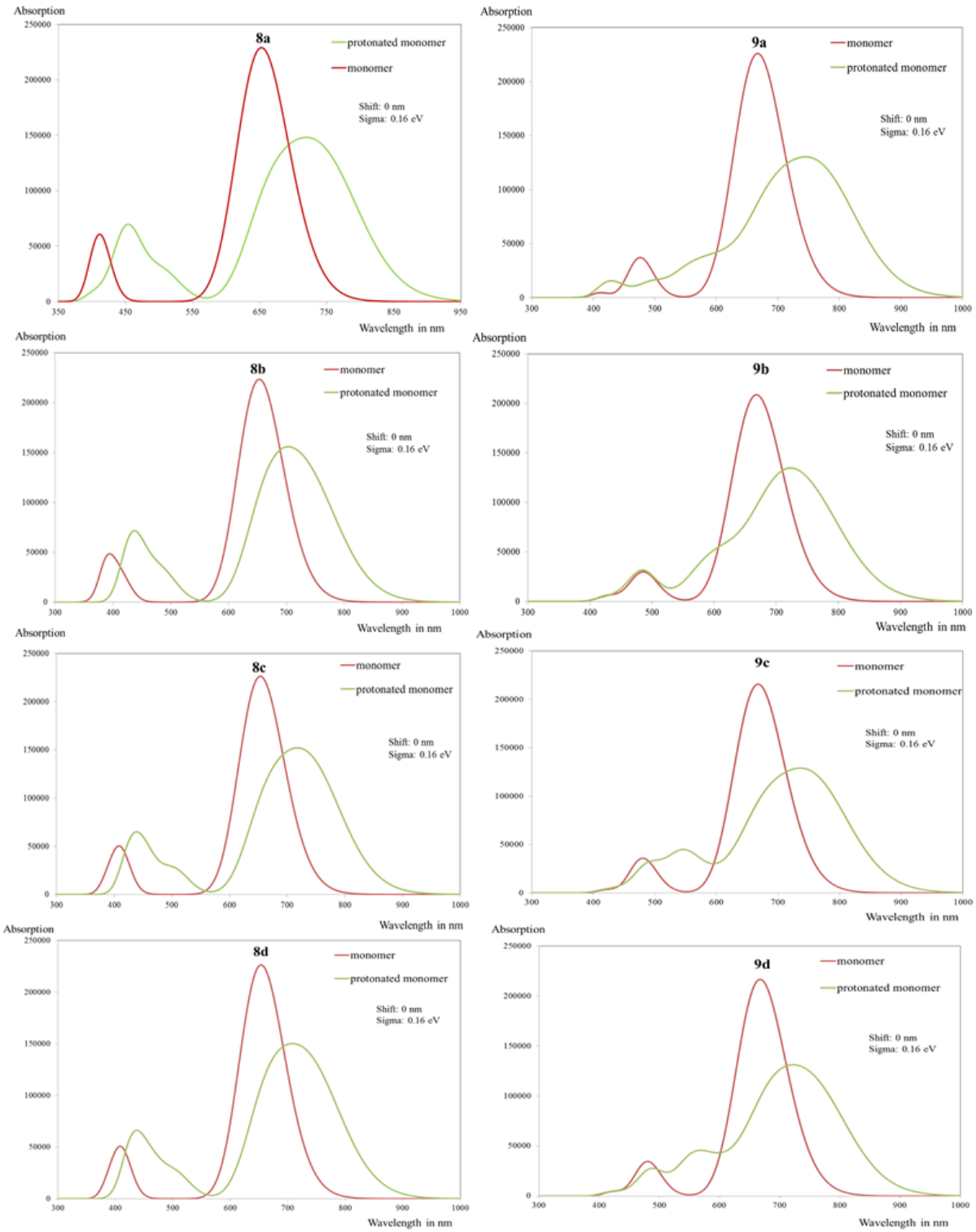

Figure S24. A comparison of the calculated absorption spectra (TD-B3LYP/6-31G(d,p)) of the model monomers and protonated monomers in chloroform.

Cartesian coordinates of optimized geometries with B3LYP/6-31G(d,p).

8a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.181298	-5.590745	0.000425
2	6	0	2.595616	-4.901224	0.000453
3	6	0	0.817276	-6.574678	0.000635
4	6	0	0.226842	-4.242395	0.000212
5	6	0	1.600261	-3.924511	0.000236
6	6	0	2.179541	-6.228333	0.000637
7	1	0	0.547103	-7.623586	0.000829
8	1	0	2.916248	-7.026608	0.000800
9	1	0	3.642635	-4.620402	0.000458
10	6	0	-0.492984	-2.971282	-0.000007
11	6	0	1.691148	-2.466877	0.000014
12	7	0	0.424752	-1.945535	-0.000134
13	7	0	-1.816898	-2.850570	-0.000062
14	6	0	-2.466812	-1.691037	-0.000195
15	6	0	-3.924486	-1.600248	-0.000109
16	6	0	-4.242413	-0.226838	-0.000191
17	6	0	-4.901179	-2.595624	0.000069
18	1	0	-4.620320	-3.642633	0.000150
19	6	0	-6.228290	-2.179581	0.000157
20	1	0	-7.026555	-2.916301	0.000299
21	6	0	-6.574681	-0.817318	0.000044
22	1	0	-7.623603	-0.547196	0.000064
23	6	0	-5.590780	0.181276	-0.000129
24	6	0	-2.971339	0.493060	-0.000346
25	7	0	-1.945543	-0.424719	-0.000285
26	7	0	-2.850568	1.816883	-0.000283
27	6	0	-1.690930	2.466781	-0.000172
28	6	0	-1.600230	3.924451	-0.000006
29	6	0	-0.817381	6.574682	0.000342
30	6	0	-0.226831	4.242429	0.000094
31	6	0	-2.595626	4.901111	0.000058
32	6	0	-2.179626	6.228244	0.000228
33	6	0	0.181245	5.590806	0.000285
34	1	0	-3.642631	4.620238	-0.000024
35	1	0	-2.916391	7.026465	0.000272
36	1	0	-0.547288	7.623611	0.000480
37	6	0	0.493148	2.971451	-0.000021
38	7	0	-0.424668	1.945541	-0.000168
39	7	0	1.816915	2.850577	0.000009
40	6	0	2.466873	1.691024	-0.000047
41	7	0	1.945582	0.424716	-0.000052
42	7	0	2.850587	-1.816900	0.000007
43	6	0	2.971396	-0.493034	-0.000060
44	6	0	3.924504	1.600256	-0.000003
45	6	0	6.574715	0.817313	0.000053
46	6	0	4.242439	0.226835	-0.000009

47	6	0	4.901213	2.595620	0.000037
48	6	0	6.228322	2.179579	0.000060
49	6	0	5.590807	-0.181269	0.000025
50	1	0	4.620387	3.642638	0.000049
51	1	0	7.026574	2.916311	0.000086
52	1	0	7.623632	0.547182	0.000070
53	30	0	-0.000094	-0.000018	-0.001062
54	8	0	1.512849	5.848728	0.000400
55	8	0	5.848703	-1.512894	0.000028
56	8	0	-1.512910	-5.848639	0.000453
57	8	0	-5.848678	1.512876	-0.000340
58	6	0	7.203440	-1.937721	0.000017
59	1	0	7.736613	-1.590792	-0.894062
60	1	0	7.173013	-3.027884	0.000012
61	1	0	7.736622	-1.590808	0.894096
62	6	0	1.937659	7.203476	0.000585
63	1	0	1.590796	7.736742	-0.893462
64	1	0	3.027822	7.173065	0.000673
65	1	0	1.590655	7.736542	0.894698
66	6	0	-7.203413	1.937704	0.001053
67	1	0	-7.737288	1.591454	-0.892876
68	1	0	-7.172989	3.027866	0.001828
69	1	0	-7.735892	1.590104	0.895279
70	6	0	-1.937742	-7.203373	-0.000163
71	1	0	-1.590288	-7.736317	-0.894170
72	1	0	-3.027905	-7.172938	-0.000797
73	1	0	-1.591364	-7.736787	0.893988

8b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.815068	2.930025	-0.012332
2	6	0	2.719464	4.869333	0.065100
3	6	0	5.080816	4.303413	0.064316
4	6	0	3.466592	2.519863	-0.024557
5	6	0	2.450306	3.504835	0.003694
6	6	0	4.056857	5.257582	0.107251
7	1	0	6.122222	4.607657	0.082254
8	1	0	4.316283	6.310698	0.162546
9	1	0	1.908419	5.588434	0.090492
10	6	0	2.774079	1.225521	-0.011347
11	6	0	1.175812	2.795657	-0.003841
12	7	0	1.415153	1.449258	-0.009692
13	7	0	3.384085	0.046256	0.025246
14	6	0	2.769598	-1.135243	0.054484
15	6	0	3.455008	-2.425254	0.111099
16	6	0	2.449624	-3.414337	0.093678
17	6	0	4.809296	-2.807888	0.189473
18	6	0	5.101155	-4.177787	0.235749

19	1	0	6.129600	-4.512364	0.293977
20	6	0	4.078254	-5.140848	0.207941
21	1	0	4.353954	-6.190747	0.245121
22	6	0	2.737799	-4.778318	0.138656
23	6	0	1.174825	-2.708458	0.035939
24	7	0	1.413167	-1.359409	0.022031
25	7	0	0.000045	-3.329264	-0.000021
26	6	0	-1.174751	-2.708490	-0.035903
27	6	0	-2.449522	-3.414402	-0.093867
28	6	0	-5.101019	-4.177916	-0.236303
29	6	0	-3.454937	-2.425350	-0.111195
30	6	0	-2.737650	-4.778385	-0.139121
31	6	0	-4.078086	-5.140947	-0.208577
32	6	0	-4.809204	-2.808018	-0.189767
33	1	0	-1.941054	-5.513282	-0.123570
34	1	0	-4.353747	-6.190849	-0.245961
35	1	0	-6.129446	-4.512518	-0.294685
36	6	0	-2.769574	-1.135324	-0.054291
37	7	0	-1.413142	-1.359448	-0.021857
38	7	0	-3.384110	0.046151	-0.024953
39	6	0	-2.774176	1.225454	0.011770
40	7	0	-1.415255	1.449215	0.010103
41	7	0	-0.000075	3.416294	-0.000026
42	6	0	-1.175944	2.795616	0.003955
43	6	0	-3.466745	2.519790	0.024684
44	6	0	-4.056889	5.257535	-0.108251
45	6	0	-2.450445	3.504763	-0.003861
46	6	0	-4.815217	2.930036	0.012354
47	6	0	-5.080866	4.303428	-0.064933
48	6	0	-2.719515	4.869243	-0.065823
49	1	0	-6.122262	4.607699	-0.082935
50	1	0	-4.316283	6.310635	-0.164007
51	30	0	-0.000013	0.044804	0.000560
52	8	0	-5.743998	-1.826248	-0.219132
53	8	0	5.897505	2.099119	-0.027870
54	6	0	-7.107271	-2.191681	-0.383453
55	1	0	-7.660898	-1.253771	-0.433202
56	1	0	-7.472455	-2.786070	0.463546
57	1	0	-7.263100	-2.753504	-1.312372
58	6	0	6.049486	1.252051	-1.175916
59	1	0	5.951323	1.836539	-2.099220
60	1	0	5.330860	0.432009	-1.156576
61	1	0	7.064909	0.854434	-1.115375
62	1	0	-1.908416	5.588274	-0.091464
63	1	0	1.941226	-5.513239	0.123042
64	8	0	-5.897847	2.099450	0.028501
65	8	0	5.744070	-1.826109	0.218926
66	6	0	7.107313	-2.191555	0.383467
67	1	0	7.262935	-2.753627	1.312268
68	1	0	7.660906	-1.253646	0.433602
69	1	0	7.472716	-2.785701	-0.463609
70	6	0	-6.049248	1.251731	1.176140
71	1	0	-7.065077	0.855012	1.116428
72	1	0	-5.949618	1.835522	2.099726

73	1	0	-5.331280	0.431155	1.155506

8c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.339918	-3.967101	-0.011665
2	6	0	-5.627435	-1.412476	-0.051340
3	6	0	-5.726122	-3.855367	-0.036741
4	6	0	-3.607067	-2.780564	-0.006382
5	6	0	-4.222330	-1.512281	-0.025766
6	6	0	-6.365758	-2.604288	-0.056304
7	1	0	-6.340613	-4.751008	-0.041638
8	1	0	-7.448231	-2.573398	-0.075612
9	6	0	-2.166392	-2.542394	0.015510
10	6	0	-3.144193	-0.527123	-0.013812
11	7	0	-1.939207	-1.191452	0.010576
12	7	0	-1.266999	-3.520722	0.031780
13	6	0	0.048938	-3.324870	0.037935
14	6	0	1.019363	-4.415504	0.044745
15	6	0	2.295473	-3.815764	0.036507
16	6	0	0.843423	-5.799175	0.054249
17	1	0	-0.150565	-6.231475	0.059594
18	6	0	1.991740	-6.583613	0.056532
19	1	0	1.906908	-7.666446	0.064405
20	6	0	3.275971	-6.012525	0.048760
21	1	0	4.137291	-6.669113	0.050917
22	6	0	3.451136	-4.621900	0.038174
23	6	0	2.076005	-2.372373	0.025112
24	7	0	0.720227	-2.131967	0.029695
25	7	0	3.042435	-1.460566	0.002820
26	6	0	2.840880	-0.147458	-0.013562
27	6	0	3.932507	0.818926	-0.064363
28	6	0	5.543237	3.058004	-0.195536
29	6	0	3.338732	2.097875	-0.073626
30	6	0	5.313231	0.629799	-0.113568
31	6	0	6.105990	1.770262	-0.177477
32	6	0	4.155127	3.244399	-0.145519
33	1	0	5.731695	-0.370101	-0.105318
34	1	0	7.187472	1.677243	-0.217654
35	1	0	6.204209	3.914310	-0.249320
36	6	0	1.892825	1.884140	-0.021532
37	7	0	1.650413	0.530715	0.005847
38	7	0	0.984279	2.857931	-0.002325
39	6	0	-0.332405	2.675207	0.018328

40	7	0	-0.993220	1.468102	0.017805
41	7	0	-3.324323	0.789390	-0.028475
42	6	0	-2.343670	1.686082	-0.014295
43	6	0	-1.324545	3.757924	0.002683
44	6	0	-3.713715	5.214080	-0.194659
45	6	0	-2.589122	3.123357	-0.042424
46	6	0	-1.268537	5.166345	-0.025473
47	6	0	-2.476474	5.867626	-0.134988
48	6	0	-3.788088	3.824157	-0.136266
49	1	0	-2.420624	6.950897	-0.164828
50	1	0	-4.621126	5.805434	-0.275608
51	30	0	-0.141142	-0.332806	0.053700
52	8	0	3.545825	4.456244	-0.165114
53	8	0	4.655961	-4.000094	0.030123
54	6	0	4.349574	5.617106	-0.321578
55	1	0	5.032798	5.754558	0.526104
56	1	0	3.653688	6.455336	-0.365177
57	1	0	4.930948	5.581083	-1.250941
58	6	0	5.829279	-4.800202	0.031214
59	1	0	5.890585	-5.427511	0.929347
60	1	0	6.665738	-4.100503	0.023629
61	1	0	5.884145	-5.439340	-0.858952
62	1	0	-4.730564	3.289309	-0.173905
63	1	0	-3.839121	-4.928321	0.003179
64	8	0	-0.129536	5.917790	0.005117
65	6	0	0.709061	5.780779	1.161029
66	1	0	1.416006	6.611983	1.111298
67	1	0	1.250280	4.834143	1.143415
68	1	0	0.114858	5.874622	2.078667
69	8	0	-6.172974	-0.171666	-0.069094
70	6	0	-7.588278	-0.055669	-0.094277
71	1	0	-8.016289	-0.516684	-0.993206
72	1	0	-7.798225	1.014391	-0.104311
73	1	0	-8.047120	-0.505945	0.794848

8d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.438131	3.048129	-0.028980
2	6	0	2.199424	4.818892	-0.143993
3	6	0	4.596966	4.435541	-0.141975
4	6	0	3.125303	2.535012	-0.000102
5	6	0	2.037614	3.439877	-0.046852
6	6	0	3.502762	5.307381	-0.204036
7	1	0	5.612070	4.817780	-0.172113
8	1	0	3.681174	6.375468	-0.287704
9	1	0	1.331724	5.467991	-0.182835
10	6	0	2.529795	1.192528	0.016818
11	6	0	0.818506	2.640086	-0.017818

12	7	0	1.158786	1.315568	0.015785
13	7	0	3.222701	0.058567	-0.001922
14	6	0	2.694386	-1.164142	-0.021032
15	6	0	3.470160	-2.402888	-0.067577
16	6	0	2.537312	-3.460859	-0.058317
17	6	0	4.848597	-2.689994	-0.133376
18	6	0	5.236838	-4.035764	-0.176088
19	1	0	6.286884	-4.296415	-0.224848
20	6	0	4.284246	-5.068758	-0.157388
21	1	0	4.633514	-6.096652	-0.191600
22	6	0	2.921220	-4.801141	-0.100566
23	6	0	1.214873	-2.847932	-0.013974
24	7	0	1.356925	-1.485482	0.002699
25	7	0	0.087145	-3.552475	0.000592
26	6	0	-1.129765	-3.017942	0.019697
27	6	0	-2.353958	-3.813321	0.028866
28	6	0	-4.953374	-4.755982	0.044823
29	6	0	-3.425892	-2.897228	0.036712
30	6	0	-2.551078	-5.194208	0.028293
31	6	0	-3.866155	-5.646556	0.036735
32	6	0	-4.753706	-3.368531	0.044488
33	1	0	-1.707342	-5.874700	0.021349
34	1	0	-4.070843	-6.713282	0.037014
35	1	0	-5.957913	-5.160756	0.051192
36	6	0	-2.832589	-1.563080	0.031132
37	7	0	-1.462334	-1.689338	0.024293
38	7	0	-3.525614	-0.427950	0.024995
39	6	0	-2.982631	0.783709	0.009966
40	7	0	-1.654308	1.119444	0.005197
41	7	0	-0.395513	3.181491	-0.031956
42	6	0	-1.529671	2.489363	-0.017338
43	6	0	-3.778663	2.008597	-0.009556
44	6	0	-4.727650	4.603645	-0.052856
45	6	0	-2.865100	3.081654	-0.027362
46	6	0	-5.159657	2.200232	-0.013437
47	6	0	-5.615413	3.514407	-0.035296
48	6	0	-3.339196	4.407919	-0.049259
49	1	0	-5.833925	1.351571	0.000133
50	1	0	-6.682608	3.716908	-0.039025
51	1	0	-5.134899	5.607090	-0.069500
52	30	0	-0.151463	-0.185648	0.042487
53	8	0	-5.750742	-2.449832	0.051593
54	8	0	-2.423230	5.407341	-0.064841
55	8	0	5.583250	2.306228	0.004392
56	6	0	-2.887745	6.749322	-0.084514
57	1	0	-3.484482	6.983887	0.805848
58	1	0	-3.482781	6.958387	-0.982315
59	1	0	-1.993301	7.373124	-0.092563
60	6	0	-7.093943	-2.910948	0.057903
61	1	0	-7.312894	-3.507154	0.952594
62	1	0	-7.321769	-3.505471	-0.835679
63	1	0	-7.715549	-2.014929	0.061881
64	6	0	5.792788	1.485053	1.161867
65	1	0	5.631017	2.065904	2.078559

66	1	0	6.840227	1.178076	1.118598
67	1	0	5.148716	0.605310	1.141227
68	1	0	2.177782	-5.589884	-0.092318
69	8	0	5.712961	-1.645054	-0.154647
70	6	0	7.100084	-1.914534	-0.301978
71	1	0	7.587749	-0.940326	-0.344686
72	1	0	7.306646	-2.463294	-1.228891
73	1	0	7.495361	-2.482681	0.549545

9a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.575644	-0.333525	-0.000561
2	6	0	-4.634542	-3.051640	-0.000091
3	6	0	-6.456540	-1.426247	-0.000376
4	6	0	-4.198538	-0.635380	-0.000397
5	6	0	-3.751112	-1.974977	-0.000203
6	6	0	-5.993936	-2.751825	-0.000160
7	1	0	-7.526686	-1.260575	-0.000380
8	1	0	-6.724706	-3.555464	-0.000039
9	1	0	-4.267155	-4.071694	0.000057
10	6	0	-2.998499	0.193759	-0.000392
11	6	0	-2.291606	-1.928467	-0.000156
12	7	0	-1.890653	-0.619837	-0.000238
13	7	0	-3.014467	1.523003	-0.000341
14	6	0	-1.928564	2.291673	-0.000270
15	6	0	-1.974982	3.751133	0.000176
16	6	0	-0.635358	4.198519	0.000302
17	6	0	-3.051625	4.634617	0.000539
18	1	0	-4.071689	4.267262	0.000464
19	6	0	-2.751765	5.993983	0.000975
20	1	0	-3.555372	6.724787	0.001192
21	6	0	-1.426158	6.456548	0.001142
22	1	0	-1.260468	7.526691	0.001420
23	6	0	-0.333457	5.575647	0.000928
24	6	0	0.193671	2.998459	-0.000168
25	7	0	-0.619830	1.890669	-0.000492
26	7	0	1.523042	3.014472	-0.000298
27	6	0	2.291676	1.928693	-0.000455
28	6	0	3.751180	1.975017	-0.000632
29	6	0	6.456570	1.426108	-0.001004
30	6	0	4.198519	0.635388	-0.000687
31	6	0	4.634686	3.051623	-0.000742

32	6	0	5.994059	2.751715	-0.000931
33	6	0	5.575598	0.333441	-0.000885
34	1	0	4.267368	4.071702	-0.000687
35	1	0	6.724889	3.555300	-0.001027
36	1	0	7.526703	1.260357	-0.001157
37	6	0	2.998361	-0.193600	-0.000512
38	7	0	1.890678	0.619852	-0.000360
39	7	0	3.014482	-1.523004	-0.000369
40	6	0	1.928597	-2.291574	-0.000190
41	7	0	0.619840	-1.890599	-0.000402
42	7	0	-1.522996	-3.014461	0.000037
43	6	0	-0.193708	-2.998374	0.000027
44	6	0	1.974993	-3.751108	0.000365
45	6	0	1.426190	-6.456507	0.001508
46	6	0	0.635393	-4.198487	0.000531
47	6	0	3.051627	-4.634553	0.000761
48	6	0	2.751766	-5.993954	0.001317
49	6	0	0.333490	-5.575554	0.001149
50	1	0	4.071691	-4.267199	0.000645
51	1	0	3.555386	-6.724745	0.001624
52	1	0	1.260462	-7.526644	0.001954
53	30	0	0.000025	-0.000022	-0.001148
54	6	0	-1.213826	-7.923916	0.002636
55	1	0	-0.709090	-8.293064	-0.893284
56	1	0	-2.241420	-8.293681	0.003023
57	1	0	-0.708847	-8.291844	0.898920
58	6	0	7.923917	-1.213914	-0.001465
59	1	0	8.292222	-0.708994	-0.897627
60	1	0	8.293632	-2.241525	-0.001653
61	1	0	8.292713	-0.709140	0.894577
62	6	0	1.213834	7.923967	0.004413
63	1	0	0.710256	8.294186	-0.891715
64	1	0	2.241455	8.293642	0.006603
65	1	0	0.707713	8.290823	0.900489
66	6	0	-7.924007	1.213784	-0.002579
67	1	0	-8.291621	0.708014	-0.898544
68	1	0	-8.293750	2.241384	-0.004016
69	1	0	-8.293448	0.709830	0.893659
70	16	0	6.105330	-1.365053	-0.000992
71	16	0	1.364919	6.105325	0.001381
72	16	0	-6.105410	1.364948	-0.000982
73	16	0	-1.365041	-6.105361	0.001451

9b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.807459	2.964169	-0.315108
2	6	0	2.688644	4.876724	-0.123004
3	6	0	5.046562	4.346840	-0.298828

4	6	0	3.468677	2.535148	-0.186381
5	6	0	2.440266	3.506712	-0.126834
6	6	0	4.014990	5.289230	-0.189418
7	1	0	6.071782	4.687994	-0.399141
8	1	0	4.260309	6.347018	-0.185400
9	1	0	1.865439	5.580390	-0.065640
10	6	0	2.786804	1.232479	-0.079530
11	6	0	1.176389	2.791418	-0.047312
12	7	0	1.426826	1.448132	-0.025599
13	7	0	3.394485	0.050065	0.008400
14	6	0	2.771350	-1.124648	0.101845
15	6	0	3.451303	-2.413551	0.259611
16	6	0	2.438909	-3.396974	0.213676
17	6	0	4.796753	-2.792342	0.461855
18	6	0	5.058425	-4.168607	0.560401
19	1	0	6.073763	-4.514916	0.707476
20	6	0	4.038833	-5.128646	0.484786
21	1	0	4.304425	-6.178435	0.569153
22	6	0	2.707891	-4.758800	0.319592
23	6	0	1.172717	-2.690925	0.071264
24	7	0	1.415364	-1.345477	0.022625
25	7	0	-0.000128	-3.311628	0.000012
26	6	0	-1.172935	-2.690872	-0.071398
27	6	0	-2.439211	-3.396873	-0.213322
28	6	0	-5.058873	-4.168415	-0.559174
29	6	0	-3.451536	-2.413384	-0.259416
30	6	0	-2.708338	-4.758719	-0.318626
31	6	0	-4.039352	-5.128515	-0.483374
32	6	0	-4.797050	-2.792132	-0.461281
33	1	0	-1.905620	-5.486173	-0.277402
34	1	0	-4.305057	-6.178316	-0.567224
35	1	0	-6.074280	-4.514691	-0.705858
36	6	0	-2.771456	-1.124488	-0.102206
37	7	0	-1.415469	-1.345390	-0.023174
38	7	0	-3.394484	0.050278	-0.008730
39	6	0	-2.786689	1.232641	0.079096
40	7	0	-1.426705	1.448208	0.024989
41	7	0	0.000125	3.407564	-0.000096
42	6	0	-1.176173	2.791475	0.046996
43	6	0	-3.468449	2.535325	0.186511
44	6	0	-4.014526	5.289465	0.190698
45	6	0	-2.439982	3.506828	0.127030
46	6	0	-4.807165	2.964420	0.315730
47	6	0	-5.046148	4.347114	0.300021
48	6	0	-2.688238	4.876866	0.123785
49	1	0	-6.071319	4.688311	0.400685
50	1	0	-4.259757	6.347276	0.187133
51	30	0	0.000004	0.055064	-0.001854
52	6	0	-7.547396	-2.516949	-0.973654
53	1	0	-8.336653	-1.775116	-1.112943
54	1	0	-7.822660	-3.169477	-0.141535
55	1	0	-7.447303	-3.099429	-1.892548
56	6	0	5.849653	0.966599	-1.998217
57	1	0	5.034354	0.268525	-1.812944

58	1	0	6.754748	0.405491	-2.239643
59	1	0	5.614386	1.644975	-2.820712
60	1	0	-1.864981	5.580477	0.066489
61	1	0	1.905117	-5.486200	0.278501
62	6	0	7.547286	-2.517282	0.973286
63	1	0	7.447820	-3.099235	1.892585
64	1	0	8.336786	-1.775515	1.111535
65	1	0	7.821774	-3.170321	0.141313
66	6	0	-5.849475	0.966818	1.998693
67	1	0	-5.615540	1.645129	2.821618
68	1	0	-5.033286	0.269691	1.813722
69	1	0	-6.754058	0.404502	2.239197
70	16	0	6.241904	1.913672	-0.481545
71	16	0	6.045504	-1.542545	0.619730
72	16	0	-6.045701	-1.542275	-0.619513
73	16	0	-6.241701	1.913957	0.482045

9c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.950554	-4.561443	-0.105264
2	6	0	-5.488459	-2.132562	-0.176604
3	6	0	-5.341093	-4.582443	-0.167943
4	6	0	-3.338241	-3.311077	-0.078997
5	6	0	-4.080257	-2.110775	-0.112906
6	6	0	-6.094484	-3.398486	-0.202990
7	1	0	-5.867124	-5.532449	-0.190997
8	1	0	-7.172943	-3.482433	-0.251624
9	6	0	-1.929090	-2.931072	-0.018169
10	6	0	-3.102395	-1.029044	-0.069006
11	7	0	-1.838157	-1.564863	-0.017878
12	7	0	-0.935188	-3.813367	0.027494
13	6	0	0.350967	-3.476973	0.062822
14	6	0	1.436760	-4.453370	0.108765
15	6	0	2.641633	-3.718010	0.114768
16	6	0	1.418682	-5.845351	0.139376
17	1	0	0.481036	-6.389576	0.132820
18	6	0	2.650791	-6.492329	0.178839
19	1	0	2.691138	-7.577439	0.204721
20	6	0	3.858299	-5.776607	0.186256
21	1	0	4.783111	-6.338996	0.217712
22	6	0	3.889065	-4.373419	0.154014
23	6	0	2.257630	-2.311242	0.071382

24	7	0	0.886969	-2.217632	0.048921
25	7	0	3.125266	-1.307541	0.034172
26	6	0	2.793025	-0.019458	-0.016996
27	6	0	3.774954	1.048515	-0.141903
28	6	0	5.137720	3.417583	-0.470671
29	6	0	3.053660	2.262074	-0.197161
30	6	0	5.163576	0.993509	-0.231331
31	6	0	5.833647	2.202608	-0.386938
32	6	0	3.737377	3.482533	-0.390936
33	1	0	5.683513	0.043325	-0.186179
34	1	0	6.917414	2.217447	-0.457980
35	1	0	5.711881	4.325013	-0.610111
36	6	0	1.639896	1.900576	-0.064411
37	7	0	1.540629	0.529635	0.017026
38	7	0	0.637951	2.778261	-0.001905
39	6	0	-0.656584	2.465991	0.052067
40	7	0	-1.182001	1.192960	-0.002977
41	7	0	-3.421586	0.258937	-0.068164
42	6	0	-2.546499	1.260982	-0.020516
43	6	0	-1.767783	3.432627	0.114720
44	6	0	-4.319981	4.601085	0.032548
45	6	0	-2.949903	2.656838	0.027604
46	6	0	-1.879427	4.835205	0.229966
47	6	0	-3.167968	5.387506	0.170680
48	6	0	-4.225056	3.214640	-0.018762
49	1	0	-3.265352	6.464551	0.260699
50	1	0	-5.291409	5.085004	-0.004305
51	30	0	-0.149845	-0.512690	0.047769
52	6	0	4.117835	6.221684	-0.894520
53	1	0	4.803642	6.333836	-0.051256
54	1	0	3.583096	7.162873	-1.038980
55	1	0	4.675134	5.991228	-1.805598
56	6	0	6.680109	-4.701945	0.243245
57	1	0	6.604795	-5.299631	1.154662
58	1	0	7.624243	-4.153383	0.261190
59	1	0	6.668830	-5.350416	-0.635962
60	1	0	-5.097407	2.574651	-0.094746
61	1	0	-3.359890	-5.470168	-0.078188
62	6	0	0.253114	5.389396	1.976168
63	1	0	-0.484083	5.326919	2.779186
64	1	0	1.007532	6.135227	2.234822
65	1	0	0.741005	4.429858	1.809312
66	6	0	-8.125707	-1.165754	-0.318588
67	1	0	-8.316177	-1.741770	-1.227190
68	1	0	-8.719792	-0.250080	-0.353549
69	1	0	-8.420454	-1.740872	0.562314
70	16	0	5.387487	-3.415874	0.162368
71	16	0	2.814468	4.987739	-0.564324
72	16	0	-0.530433	5.988295	0.434244
73	16	0	-6.392468	-0.601952	-0.219308

9d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.372104	2.960220	0.208783
2	6	0	2.128604	4.716329	-0.058558
3	6	0	4.517130	4.354003	0.137001
4	6	0	3.066203	2.435985	0.096425
5	6	0	1.974524	3.333622	0.000107
6	6	0	3.424306	5.219217	-0.010433
7	1	0	5.516639	4.767317	0.224922
8	1	0	3.597853	6.290161	-0.056917
9	1	0	1.258508	5.358492	-0.141538
10	6	0	2.472980	1.087300	0.044423
11	6	0	0.761251	2.533796	-0.042245
12	7	0	1.101483	1.210754	-0.014017
13	7	0	3.155402	-0.056894	0.003645
14	6	0	2.615021	-1.274866	-0.049561
15	6	0	3.382163	-2.518859	-0.160115
16	6	0	2.437791	-3.567508	-0.098576
17	6	0	4.752559	-2.811557	-0.337807
18	6	0	5.107972	-4.168827	-0.392918
19	1	0	6.146273	-4.448934	-0.518802
20	6	0	4.154662	-5.193687	-0.301397
21	1	0	4.491788	-6.224961	-0.352374
22	6	0	2.799885	-4.910501	-0.163396
23	6	0	1.124364	-2.947018	0.005934
24	7	0	1.276091	-1.587076	0.024257
25	7	0	-0.006034	-3.647915	0.055474
26	6	0	-1.219223	-3.108189	0.081123
27	6	0	-2.450643	-3.893116	0.122859
28	6	0	-5.057004	-4.800504	0.183340
29	6	0	-3.518433	-2.969733	0.110577
30	6	0	-2.661570	-5.268834	0.164326
31	6	0	-3.983421	-5.704626	0.195066
32	6	0	-4.856853	-3.411669	0.140041
33	1	0	-1.825882	-5.959501	0.172000
34	1	0	-4.201529	-6.768140	0.228633
35	1	0	-6.061907	-5.202805	0.208402
36	6	0	-2.908438	-1.645214	0.061202
37	7	0	-1.541187	-1.777933	0.051786
38	7	0	-3.602096	-0.512332	0.020073
39	6	0	-3.056401	0.699268	-0.030124
40	7	0	-1.725611	1.018867	-0.033008
41	7	0	-0.455246	3.072118	-0.092366
42	6	0	-1.590612	2.385212	-0.088088
43	6	0	-3.839391	1.930248	-0.091725
44	6	0	-4.745096	4.534135	-0.212558
45	6	0	-2.914582	2.996304	-0.129224
46	6	0	-5.215804	2.140490	-0.113800
47	6	0	-5.650201	3.461764	-0.175203
48	6	0	-3.355896	4.333644	-0.190588
49	1	0	-5.905799	1.304682	-0.084195

50	1	0	-6.713901	3.680715	-0.194965
51	1	0	-5.147002	5.538468	-0.259193
52	30	0	-0.221247	-0.281288	0.031530
53	6	0	-3.222893	7.140020	-0.316895
54	1	0	-3.855493	7.241128	0.568091
55	1	0	-3.834141	7.157059	-1.222281
56	1	0	-2.527353	7.981361	-0.348033
57	6	0	-7.665423	-3.281690	0.180043
58	1	0	-7.709614	-3.874959	1.096424
59	1	0	-7.738478	-3.931920	-0.694882
60	1	0	-8.508313	-2.587366	0.171442
61	6	0	5.530319	1.104774	1.974866
62	1	0	4.760229	0.351644	1.812390
63	1	0	5.248436	1.797922	2.770009
64	1	0	6.466233	0.609436	2.241259
65	1	0	2.047151	-5.688984	-0.112464
66	6	0	7.484421	-2.366219	-0.828563
67	1	0	8.223891	-1.577186	-0.981121
68	1	0	7.436822	-2.981476	-1.730223
69	1	0	7.791038	-2.973614	0.026485
70	16	0	-2.165700	5.654416	-0.234533
71	16	0	5.873181	2.016400	0.424525
72	16	0	5.915616	-1.485273	-0.522622
73	16	0	-6.179591	-2.222998	0.122259

p-8a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.344849	-3.528016	-0.000019
2	6	0	-5.488148	-0.924152	-0.000029
3	6	0	-5.735806	-3.350520	-0.000013
4	6	0	-3.547459	-2.392067	-0.000032
5	6	0	-4.106404	-1.095321	-0.000035
6	6	0	-6.301756	-2.056500	-0.000018
7	1	0	-7.377850	-1.932877	-0.000013
8	1	0	-5.921757	0.070520	-0.000030
9	6	0	-2.094402	-2.215241	-0.000041
10	6	0	-2.990609	-0.158605	-0.000041
11	7	0	-1.815361	-0.870380	-0.000046
12	7	0	-1.230936	-3.224517	-0.000035
13	6	0	0.093132	-3.079721	-0.000020
14	6	0	1.030524	-4.193530	-0.000009
15	6	0	2.322253	-3.635192	0.000014

16	6	0	0.860420	-5.582381	-0.000011
17	1	0	-0.133186	-6.018054	-0.000030
18	6	0	1.992670	-6.381424	0.000011
19	1	0	1.917911	-7.463729	0.000014
20	6	0	3.290858	-5.814617	0.000035
21	6	0	3.471136	-4.428306	0.000036
22	6	0	2.146880	-2.184427	0.000000
23	7	0	0.802469	-1.902954	-0.000014
24	7	0	3.157955	-1.320855	0.000013
25	6	0	3.014052	0.002348	0.000016
26	6	0	4.127524	0.940345	-0.000005
27	6	0	5.747813	3.202208	-0.000038
28	6	0	3.568833	2.232020	-0.000002
29	6	0	5.516580	0.771784	-0.000026
30	6	0	6.315206	1.904286	-0.000042
31	6	0	4.361661	3.381447	-0.000021
32	1	0	5.953162	-0.221447	-0.000029
33	1	0	7.397578	1.830087	-0.000059
34	6	0	2.118459	2.056161	0.000018
35	7	0	1.836642	0.713556	0.000028
36	7	0	1.254398	3.068628	0.000019
37	6	0	-0.067712	2.925182	0.000009
38	7	0	-0.781244	1.749110	-0.000014
39	7	0	-3.134894	1.164404	-0.000033
40	6	0	-2.124314	2.028326	-0.000017
41	6	0	-1.005328	4.040569	0.000004
42	6	0	-3.262820	5.668390	0.000012
43	6	0	-2.301838	3.480951	-0.000009
44	6	0	-0.836274	5.422602	0.000016
45	6	0	-1.969246	6.235372	0.000020
46	6	0	-3.438627	4.277529	-0.000008
47	1	0	0.157830	5.857571	0.000027
48	1	0	-1.846616	7.311612	0.000027
49	30	0	0.012601	-0.078528	-0.000010
50	8	0	6.655310	4.219709	-0.000056
51	8	0	-4.413041	6.401890	0.000010
52	8	0	-6.470087	-4.499822	-0.000005
53	8	0	4.307825	-6.722199	0.000048
54	6	0	-4.320762	7.818189	0.000158
55	1	0	-3.805349	8.191154	0.894244
56	1	0	-5.348192	8.184690	0.000222
57	1	0	-3.805400	8.191350	-0.893879
58	6	0	6.167505	5.553383	-0.000041
59	1	0	5.566056	5.762780	-0.893566
60	1	0	7.048979	6.195886	-0.000045
61	1	0	5.566075	5.762765	0.893501
62	6	0	5.642015	-6.235175	0.000118
63	1	0	5.851662	-5.633950	0.893674
64	1	0	5.851758	-5.633953	-0.893418
65	1	0	6.283807	-7.117138	0.000152
66	6	0	-7.886479	-4.406637	0.000019
67	1	0	-8.259022	-3.890983	0.894091
68	1	0	-8.253463	-5.433875	0.000024
69	1	0	-8.259056	-3.890989	-0.894044

70	1	0	4.449636	-3.965454	0.000054
71	1	0	-3.924825	-4.527220	-0.000019
72	1	0	-4.437330	3.856312	-0.000011
73	1	0	3.898169	4.359652	-0.000018

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.837505	2.785194	0.000077
2	6	0	2.835416	4.804942	0.000513
3	6	0	5.183361	4.144051	0.000451
4	6	0	3.487885	2.461307	-0.000109
5	6	0	2.486831	3.457083	0.000075
6	6	0	4.187632	5.145656	0.000680
7	6	0	2.789612	1.175162	-0.000431
8	6	0	1.205124	2.763349	-0.000316
9	7	0	1.437831	1.407292	-0.000381
10	7	0	3.412168	0.000006	-0.000465
11	6	0	2.789618	-1.175154	-0.000483
12	6	0	3.487897	-2.461298	-0.000360
13	6	0	2.486845	-3.457077	-0.000305
14	6	0	4.837517	-2.785175	-0.000207
15	1	0	5.612206	-2.027093	-0.000201
16	6	0	5.183380	-4.144033	-0.000030
17	6	0	4.187657	-5.145641	-0.000028
18	6	0	2.835439	-4.804936	-0.000133
19	6	0	1.205136	-2.763348	-0.000426
20	7	0	1.437839	-1.407289	-0.000454
21	7	0	0.028975	-3.382250	-0.000358
22	6	0	-1.148887	-2.760819	-0.000315
23	6	0	-2.429555	-3.453329	-0.000080
24	6	0	-5.125989	-4.135265	0.000334
25	6	0	-3.427184	-2.460688	-0.000022
26	6	0	-2.779519	-4.808020	0.000078
27	6	0	-4.125432	-5.137777	0.000274
28	6	0	-4.786829	-2.779224	0.000183
29	1	0	-2.014099	-5.576902	0.000037
30	1	0	-4.451950	-6.172358	0.000389
31	6	0	-2.732267	-1.175545	-0.000203
32	7	0	-1.378115	-1.406329	-0.000296
33	7	0	-3.355174	-0.000007	-0.000129
34	6	0	-2.732274	1.175534	-0.000144
35	7	0	-1.378122	1.406322	-0.000205
36	7	0	0.028962	3.382248	-0.000199
37	6	0	-1.148899	2.760814	-0.000182
38	6	0	-3.427194	2.460674	-0.000007
39	6	0	-4.125453	5.137760	0.000250
40	6	0	-2.429569	3.453318	-0.000018
41	6	0	-4.786842	2.779205	0.000135

42	6	0	-5.126005	4.135246	0.000261
43	6	0	-2.779537	4.808009	0.000119
44	1	0	-4.451969	6.172342	0.000350
45	30	0	0.027891	-0.000001	-0.001078
46	1	0	-2.014120	5.576892	0.000109
47	1	0	5.612195	2.027112	-0.000054
48	1	0	2.069831	-5.573830	-0.000128
49	1	0	2.069809	5.573836	0.000657
50	1	0	-5.528709	-1.990828	0.000188
51	1	0	-5.528718	1.990807	0.000147
52	8	0	-6.404836	-4.608491	0.000460
53	8	0	-6.404855	4.608474	0.000407
54	6	0	-7.467598	-3.667216	0.001054
55	1	0	-7.443156	-3.030845	-0.892534
56	1	0	-8.387896	-4.252745	0.001531
57	1	0	-7.442185	-3.030882	0.894636
58	6	0	-7.467625	3.667205	0.000435
59	1	0	-8.387918	4.252740	0.000577
60	1	0	-7.442790	3.030925	-0.893204
61	1	0	-7.442613	3.030781	0.893966
62	1	0	4.468052	6.191865	0.000996
63	8	0	6.522069	4.404948	0.000639
64	6	0	6.955156	5.756752	0.000477
65	1	0	8.045360	5.721129	0.000259
66	1	0	6.612028	6.292609	-0.893500
67	1	0	6.612418	6.292711	0.894547
68	1	0	4.468078	-6.191850	-0.000001
69	8	0	6.522089	-4.404922	-0.000066
70	6	0	6.955183	-5.756723	0.002024
71	1	0	6.611335	-6.291523	0.896354
72	1	0	6.613174	-6.293742	-0.891693
73	1	0	8.045386	-5.721091	0.003063

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.807716	-5.085214	0.000570
2	6	0	-4.813939	-3.055000	0.000461
3	6	0	-4.154212	-5.414201	0.000880
4	6	0	-2.457880	-3.730924	0.000154
5	6	0	-3.454812	-2.738813	0.000101
6	6	0	-5.154351	-4.411626	0.000833
7	1	0	-4.481201	-6.448634	0.001174

8	6	0	-1.175872	-3.037778	-0.000234
9	6	0	-2.759102	-1.451692	-0.000370
10	7	0	-1.404667	-1.683444	-0.000326
11	7	0	0.000655	-3.660036	-0.000108
12	6	0	1.176959	-3.037359	-0.000086
13	6	0	2.459214	-3.730052	-0.000017
14	6	0	3.455794	-2.737587	-0.000023
15	6	0	2.809532	-5.084216	0.000035
16	1	0	2.044736	-5.853699	0.000039
17	6	0	4.156149	-5.412721	0.000082
18	1	0	4.483505	-6.447036	0.000132
19	6	0	5.155928	-4.409788	0.000066
20	6	0	4.815034	-3.053285	0.000005
21	6	0	2.759625	-1.450713	-0.000023
22	7	0	1.405274	-1.682945	-0.000055
23	7	0	3.382645	-0.278305	0.000026
24	6	0	2.761302	0.901715	-0.000049
25	6	0	3.453533	2.182026	0.000266
26	6	0	4.134631	4.879106	0.000808
27	6	0	2.460462	3.179670	0.000200
28	6	0	4.808228	2.532878	0.000610
29	6	0	5.137568	3.878643	0.000860
30	6	0	2.778834	4.539467	0.000490
31	1	0	5.577591	1.767919	0.000661
32	1	0	6.171991	4.205724	0.001098
33	6	0	1.175701	2.484586	-0.000169
34	7	0	1.407574	1.129978	-0.000256
35	7	0	-0.000543	3.105815	-0.000212
36	6	0	-1.176574	2.484174	-0.000334
37	7	0	-1.407961	1.129491	-0.000467
38	7	0	-3.382533	-0.279501	-0.000372
39	6	0	-2.761614	0.900739	-0.000407
40	6	0	-2.461582	3.178804	-0.000178
41	6	0	-5.138938	3.876823	0.000101
42	6	0	-3.454298	2.180806	-0.000213
43	6	0	-2.780443	4.538485	0.000006
44	6	0	-4.136364	4.877646	0.000133
45	6	0	-4.809114	2.531176	-0.000056
46	1	0	-6.173481	4.203525	0.000212
47	30	0	0.000041	-0.274894	-0.001961
48	1	0	-5.578206	1.765942	-0.000061
49	1	0	-2.042639	-5.854420	0.000631
50	1	0	5.555525	-2.263541	-0.000018
51	1	0	-5.554713	-2.265522	0.000435
52	8	0	6.434493	-4.880569	0.000086
53	8	0	-6.432744	-4.882880	0.001184
54	6	0	-7.495522	-3.940551	0.000868
55	1	0	-7.469970	-3.304709	-0.892896
56	1	0	-8.415904	-4.525856	0.000965
57	1	0	-7.470088	-3.304238	0.894303
58	6	0	7.496904	-3.937833	0.000576
59	1	0	8.417519	-4.522774	0.000951
60	1	0	7.471555	-3.301731	-0.893015
61	1	0	7.470773	-3.301791	0.894181

62	1	0	1.990186	5.281119	0.000476
63	1	0	-1.992059	5.280418	0.000073
64	8	0	4.607559	6.157770	0.001126
65	8	0	-4.609769	6.156140	0.000304
66	6	0	3.666326	7.220605	0.000330
67	1	0	3.029677	7.196028	0.893741
68	1	0	4.251807	8.140958	0.000115
69	1	0	3.030261	7.195206	-0.893466
70	6	0	-3.668970	7.219358	0.000253
71	1	0	-4.254821	8.139477	0.000269
72	1	0	-3.032560	7.194641	0.893826
73	1	0	-3.032644	7.194622	-0.893380

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.289793	-2.207137	0.000269
2	6	0	3.565883	-4.467907	0.000404
3	6	0	5.809395	-3.510204	0.000823
4	6	0	3.910211	-2.060063	-0.000247
5	6	0	3.046246	-3.176472	-0.000191
6	6	0	4.951233	-4.631640	0.000890
7	6	0	3.051522	-0.873411	-0.000782
8	6	0	1.685096	-2.653405	-0.000733
9	7	0	1.740708	-1.279530	-0.001018
10	7	0	3.517601	0.370119	-0.000693
11	6	0	2.748484	1.458707	-0.000729
12	6	0	3.270399	2.818098	-0.000182
13	6	0	2.157391	3.678849	-0.000029
14	6	0	4.568349	3.340784	0.000319
15	1	0	5.431071	2.681967	0.000242
16	6	0	4.720470	4.718536	0.000988
17	1	0	5.704891	5.175758	0.001421
18	6	0	3.596927	5.581234	0.001198
19	6	0	2.296167	5.067660	0.000676
20	6	0	0.971692	2.823697	-0.000650
21	7	0	1.376836	1.509618	-0.000999
22	7	0	-0.271686	3.289786	-0.000541
23	6	0	-1.362002	2.523457	-0.000656
24	6	0	-2.720653	3.044670	-0.000219
25	6	0	-5.484943	3.370289	0.000524
26	6	0	-3.581668	1.930816	-0.000273
27	6	0	-3.244993	4.342380	0.000256
28	6	0	-4.622346	4.494328	0.000604
29	6	0	-4.971443	2.070502	0.000115
30	1	0	-2.586704	5.205563	0.000316
31	1	0	-5.080063	5.478560	0.000938
32	6	0	-2.726660	0.747298	-0.000672
33	7	0	-1.414631	1.150322	-0.000860

34	7	0	-3.192189	-0.500573	-0.000559
35	6	0	-2.424233	-1.584831	-0.000627
36	7	0	-1.050196	-1.640137	-0.001006
37	7	0	0.598946	-3.419081	-0.000590
38	6	0	-0.649411	-2.952781	-0.000642
39	6	0	-2.947475	-2.949372	0.000018
40	6	0	-3.295802	-5.694049	0.001351
41	6	0	-1.830377	-3.804974	0.000019
42	6	0	-4.254431	-3.440482	0.000691
43	6	0	-4.417439	-4.828998	0.001353
44	6	0	-2.003227	-5.193418	0.000705
45	1	0	-3.485463	-6.762781	0.001891
46	30	0	0.162018	-0.063836	-0.003643
47	1	0	-1.145023	-5.858141	0.000740
48	1	0	5.960649	-1.355042	0.000262
49	1	0	1.417164	5.700371	0.000761
50	1	0	2.906142	-5.330110	0.000479
51	8	0	3.899953	6.909748	0.001828
52	6	0	2.830212	7.843392	0.003015
53	1	0	3.295635	8.830557	0.004133
54	1	0	2.203059	7.737222	-0.891663
55	1	0	2.203219	7.735080	0.897541
56	1	0	-5.604323	1.191597	0.000116
57	1	0	-5.092021	-2.753884	0.000695
58	8	0	-6.814126	3.674345	0.000950
59	8	0	-5.624679	-5.462274	0.002037
60	6	0	-7.747322	2.605131	0.000251
61	1	0	-7.640442	1.977385	0.894626
62	1	0	-8.734762	3.070129	0.000194
63	1	0	-7.639947	1.978151	-0.894596
64	6	0	-6.800131	-4.666609	0.002386
65	1	0	-7.635967	-5.368450	0.003163
66	1	0	-6.856043	-4.032399	0.896802
67	1	0	-6.857090	-4.033151	-0.892499
68	1	0	5.363976	-5.633679	0.001339
69	8	0	7.170192	-3.595214	0.001301
70	6	0	7.775496	-4.878860	0.001739
71	1	0	8.852065	-4.699501	0.001949
72	1	0	7.504057	-5.453755	0.896857
73	1	0	7.504470	-5.454171	-0.893235

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	8.734807	-1.191666	-0.677405
2	6	0	7.477014	-3.709205	-0.164813
3	6	0	9.443544	-2.397548	-0.777169
4	6	0	7.374351	-1.258686	-0.320432
5	6	0	6.774091	-2.508606	-0.073210
6	6	0	8.818993	-3.630632	-0.522865
7	1	0	10.491043	-2.391678	-1.052804
8	1	0	9.410155	-4.537815	-0.610890
9	1	0	6.984001	-4.652849	0.039496
10	6	0	6.334616	-0.253431	-0.099293
11	6	0	5.381382	-2.236476	0.281363
12	7	0	5.163565	-0.888274	0.234776
13	7	0	6.537916	1.059248	-0.153595
14	6	0	5.618786	1.967011	0.164251
15	6	0	5.929057	3.392074	0.260046
16	6	0	4.753647	4.027668	0.705801
17	6	0	7.111195	4.089172	0.012049
18	1	0	7.999124	3.565232	-0.323017
19	6	0	7.088946	5.464668	0.216273
20	1	0	7.982911	6.054164	0.033286
21	6	0	5.930406	6.125705	0.660496
22	1	0	5.966322	7.198594	0.804945
23	6	0	4.746357	5.420412	0.916786
24	6	0	3.751064	2.975288	0.863488
25	7	0	4.309284	1.769775	0.504938
26	7	0	2.516543	3.178025	1.311039
27	6	0	1.621382	2.213032	1.495553
28	6	0	0.250575	2.486048	1.920315
29	6	0	-2.464076	2.428927	2.417062
30	6	0	-0.428114	1.246977	1.897845
31	6	0	-0.389480	3.683066	2.236307
32	6	0	-1.752718	3.636409	2.515219
33	6	0	-1.817539	1.241788	2.081770
34	1	0	0.168539	4.612856	2.240013
35	1	0	-2.290727	4.545770	2.763943
36	1	0	-3.540897	2.412218	2.549389
37	6	0	0.586977	0.236682	1.583700
38	7	0	1.772255	0.867359	1.314542
39	7	0	0.381164	-1.077517	1.656408
40	6	0	1.331575	-1.990435	1.456462
41	7	0	2.619618	-1.784150	1.051247
42	7	0	4.530445	-3.200424	0.617663
43	6	0	3.269311	-2.992088	0.984338
44	6	0	1.117738	-3.421963	1.669813
45	6	0	1.339309	-6.169034	1.924236
46	6	0	2.345699	-4.051425	1.384356
47	6	0	-0.008380	-4.139017	2.073589
48	6	0	0.123690	-5.518433	2.192973
49	6	0	2.469597	-5.447918	1.515269
50	1	0	-0.948223	-3.638324	2.273103
51	1	0	-0.729020	-6.117610	2.498910
52	1	0	1.390304	-7.245278	2.035569
53	30	0	3.341810	-0.009446	0.369427

54	6	0	3.821096	-7.408889	1.394128
55	1	0	3.630097	-7.722881	2.428133
56	1	0	4.857558	-7.631013	1.137019
57	1	0	3.155404	-7.965235	0.721771
58	6	0	-2.667366	-0.899731	2.799539
59	1	0	-1.669409	-1.309396	2.965138
60	1	0	-3.333006	-1.668550	2.405133
61	1	0	-3.084487	-0.484974	3.722783
62	6	0	3.577202	7.389651	1.581389
63	1	0	4.301862	7.682270	2.351742
64	1	0	2.569767	7.622412	1.928564
65	1	0	3.782300	7.954927	0.663160
66	6	0	10.643626	0.115683	-1.255486
67	1	0	11.287564	-0.291498	-0.465741
68	1	0	10.856207	1.178144	-1.380360
69	1	0	10.855060	-0.407791	-2.196656
70	6	0	-2.469197	5.447912	-1.514642
71	6	0	0.008696	4.138901	-2.073086
72	6	0	-1.338865	6.168992	-1.923550
73	6	0	-2.345391	4.051396	-1.383881
74	6	0	-1.117474	3.421876	-1.669396
75	6	0	-0.123286	5.518337	-2.192340
76	1	0	-1.389795	7.245248	-2.034800
77	1	0	0.729465	6.117488	-2.498214
78	1	0	0.948517	3.638180	-2.272635
79	6	0	-3.269080	2.992085	-0.983984
80	6	0	-1.331416	1.990342	-1.456177
81	7	0	-2.619481	1.784104	-1.051008
82	7	0	-4.530207	3.200484	-0.617322
83	6	0	-5.381232	2.236572	-0.281158
84	6	0	-6.773991	2.508766	0.073163
85	6	0	-7.374390	1.258867	0.320133
86	6	0	-7.476852	3.709406	0.164711
87	1	0	-6.983730	4.653033	-0.039410
88	6	0	-8.818916	3.630892	0.522455
89	1	0	-9.410036	4.538106	0.610436
90	6	0	-9.443610	2.397826	0.776499
91	1	0	-10.491170	2.392001	1.051903
92	6	0	-8.734936	1.191904	0.676774
93	6	0	-6.334674	0.253564	0.099123
94	7	0	-5.163495	0.888351	-0.234590
95	7	0	-6.538104	-1.059107	0.153227
96	6	0	-5.618991	-1.966903	-0.164573
97	6	0	-5.929326	-3.391948	-0.260443
98	6	0	-5.930770	-6.125570	-0.660944
99	6	0	-4.753898	-4.027594	-0.706071
100	6	0	-7.111529	-4.088987	-0.012598
101	6	0	-7.089328	-5.464481	-0.216847
102	6	0	-4.746654	-5.420333	-0.917086
103	1	0	-7.999470	-3.565007	0.322372
104	1	0	-7.983346	-6.053934	-0.033976
105	1	0	-5.966722	-7.198456	-0.805408
106	6	0	-3.751244	-2.975260	-0.863627
107	7	0	-4.309449	-1.769724	-0.505131

108	7	0	-2.516684	-3.178052	-1.311036
109	6	0	-1.621455	-2.213102	-1.495467
110	7	0	-1.772266	-0.867424	-1.314466
111	7	0	-0.381059	1.077381	-1.656194
112	6	0	-0.586939	-0.236811	-1.583580
113	6	0	-0.250651	-2.486197	-1.920168
114	6	0	2.464005	-2.429273	-2.416837
115	6	0	0.428107	-1.247159	-1.897725
116	6	0	0.389333	-3.683271	-2.236081
117	6	0	1.752584	-3.636720	-2.514934
118	6	0	1.817544	-1.242056	-2.081650
119	1	0	-0.168747	-4.613024	-2.239766
120	1	0	2.290546	-4.546130	-2.763583
121	1	0	3.540830	-2.412633	-2.549150
122	30	0	-3.341792	0.009363	-0.369278
123	6	0	2.667401	0.899408	-2.799555
124	1	0	3.083450	0.484434	-3.723194
125	1	0	3.333932	1.667704	-2.405623
126	1	0	1.669586	1.309755	-2.964321
127	6	0	-3.577442	-7.389653	-1.581335
128	1	0	-3.782633	-7.954789	-0.663041
129	1	0	-2.569974	-7.622463	-1.928377
130	1	0	-4.302025	-7.682386	-2.351717
131	6	0	-10.644010	-0.115369	1.254226
132	1	0	-10.855679	0.408058	2.195370
133	1	0	-10.856695	-1.177824	1.378974
134	1	0	-11.287702	0.291903	0.464326
135	6	0	-3.820603	7.408942	-1.393492
136	1	0	-3.155018	7.965257	-0.721002
137	1	0	-4.857106	7.631086	-1.136564
138	1	0	-3.629411	7.722955	-2.427454
139	8	0	2.607059	-0.129691	-1.788939
140	8	0	9.270503	0.034022	-0.906296
141	8	0	3.675211	-6.006319	1.236831
142	8	0	-2.606910	0.129320	1.788919
143	8	0	3.593250	5.989534	1.351018
144	8	0	-3.593516	-5.989510	-1.351176
145	8	0	-9.270777	-0.033770	0.905423
146	8	0	-3.674779	6.006360	-1.236199

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.892193	-1.473712	-1.947395
2	6	0	-0.384418	-3.851576	-2.241885
3	6	0	-2.516315	-2.691196	-2.212099
4	6	0	-0.492959	-1.417788	-1.878739
5	6	0	0.229865	-2.628121	-1.981328
6	6	0	-1.769433	-3.868374	-2.376461

7	1	0	-3.600025	-2.714285	-2.256058
8	1	0	-2.288215	-4.801169	-2.573823
9	1	0	0.209990	-4.755686	-2.313651
10	6	0	0.503894	-0.369164	-1.619804
11	6	0	1.620920	-2.303663	-1.683524
12	7	0	1.732091	-0.962309	-1.461349
13	7	0	0.240582	0.935434	-1.637163
14	6	0	1.151499	1.885865	-1.423045
15	6	0	0.917875	3.323702	-1.602136
16	6	0	2.136522	3.959171	-1.287600
17	6	0	-0.181429	4.109777	-2.002710
18	6	0	-0.004322	5.498341	-2.084835
19	1	0	-0.827903	6.132303	-2.386950
20	6	0	1.225807	6.097948	-1.774925
21	1	0	1.313513	7.177421	-1.857854
22	6	0	2.317671	5.339035	-1.369941
23	6	0	3.068969	2.904442	-0.909681
24	7	0	2.450286	1.693996	-1.018106
25	7	0	4.322744	3.162198	-0.541957
26	6	0	5.231384	2.225989	-0.289103
27	6	0	6.623476	2.537320	0.023779
28	6	0	9.332975	2.503986	0.562093
29	6	0	7.289271	1.301023	0.143643
30	6	0	7.279276	3.760086	0.165097
31	6	0	8.641983	3.721180	0.439667
32	6	0	8.672341	1.276787	0.411870
33	1	0	6.739422	4.693852	0.056218
34	1	0	9.197013	4.646960	0.561166
35	1	0	10.394591	2.526766	0.775038
36	6	0	6.283929	0.265758	-0.105268
37	7	0	5.071737	0.868919	-0.331978
38	7	0	6.551587	-1.037392	-0.156890
39	6	0	5.679445	-1.975773	-0.514882
40	7	0	4.355260	-1.790373	-0.826364
41	7	0	2.576646	-3.226407	-1.627653
42	6	0	3.824770	-2.976958	-1.245198
43	6	0	6.030983	-3.390020	-0.714847
44	6	0	5.986498	-6.082953	-1.497780
45	6	0	4.858545	-4.007411	-1.211108
46	6	0	7.202583	-4.162377	-0.580964
47	6	0	7.154193	-5.502466	-0.989879
48	6	0	4.811166	-5.341408	-1.603872
49	1	0	8.063938	-6.085198	-0.888798
50	1	0	6.000845	-7.126844	-1.797344
51	30	0	3.287782	-0.082472	-0.493222
52	8	0	9.278752	0.067289	0.511532
53	8	0	-2.709415	-0.386860	-1.646060
54	6	0	10.686973	0.027840	0.694686
55	1	0	10.956994	-1.028450	0.689927
56	1	0	10.984195	0.475162	1.651709
57	1	0	11.212696	0.538700	-0.121072
58	6	0	-2.841908	0.610806	-2.686757
59	1	0	-3.126015	0.117941	-3.621614
60	1	0	-1.909383	1.166715	-2.787395

61	1	0	-3.647893	1.269119	-2.360600
62	1	0	3.891008	-5.768484	-1.986704
63	1	0	3.277735	5.784609	-1.134810
64	8	0	8.406354	-3.720097	-0.115128
65	8	0	-1.355276	3.485273	-2.283747
66	6	0	-2.477014	4.292083	-2.627592
67	1	0	-2.734006	4.982304	-1.817026
68	1	0	-3.306470	3.602376	-2.780570
69	1	0	-2.298904	4.854879	-3.552111
70	6	0	8.433962	-3.145066	1.198449
71	1	0	9.487938	-3.119385	1.485323
72	1	0	7.890878	-3.782724	1.907508
73	1	0	8.023806	-2.134692	1.192509
74	6	0	-7.202165	-4.162597	0.580865
75	6	0	-4.810779	-5.341298	1.604236
76	6	0	-7.153684	-5.502662	0.989857
77	6	0	-6.030678	-3.390094	0.714914
78	6	0	-4.858250	-4.007329	1.211394
79	6	0	-5.986007	-6.082985	1.497986
80	1	0	-8.063339	-6.085508	0.888641
81	1	0	-6.000285	-7.126864	1.797598
82	1	0	-3.890631	-5.768245	1.987238
83	6	0	-5.679263	-1.975818	0.514932
84	6	0	-3.824594	-2.976761	1.245587
85	7	0	-4.355151	-1.790252	0.826631
86	7	0	-6.551447	-1.037540	0.156773
87	6	0	-6.283896	0.265625	0.105070
88	6	0	-7.289323	1.300790	-0.143911
89	6	0	-6.623646	2.537152	-0.024070
90	6	0	-8.672381	1.276419	-0.412187
91	6	0	-9.333128	2.503549	-0.562458
92	1	0	-10.394747	2.526226	-0.775404
93	6	0	-8.642252	3.720812	-0.440054
94	1	0	-9.197367	4.646536	-0.561586
95	6	0	-7.279555	3.759853	-0.165452
96	6	0	-5.231534	2.225957	0.288858
97	7	0	-5.071752	0.868909	0.331755
98	7	0	-4.322996	3.162260	0.541738
99	6	0	-3.069215	2.904623	0.909521
100	6	0	-2.136897	3.959451	1.287483
101	6	0	0.003717	5.498867	2.084824
102	6	0	-0.918185	3.324118	1.602040
103	6	0	-2.318227	5.339288	1.369851
104	6	0	-1.226477	6.098330	1.774900
105	6	0	0.181008	4.110328	2.002654
106	1	0	-3.278343	5.784740	1.134700
107	1	0	-1.314325	7.177789	1.857868
108	1	0	0.827210	6.132920	2.386986
109	6	0	-1.151646	1.886251	1.422935
110	7	0	-2.450404	1.694242	1.017956
111	7	0	-0.240651	0.935912	1.637128
112	6	0	-0.503898	-0.368706	1.619963
113	7	0	-1.732061	-0.961935	1.461594
114	7	0	-2.576487	-3.226064	1.628198

115	6	0	-1.620826	-2.303253	1.683992
116	6	0	0.493002	-1.417240	1.879079
117	6	0	1.769594	-3.867658	2.377302
118	6	0	-0.229764	-2.627586	1.981893
119	6	0	1.892235	-1.473083	1.947735
120	6	0	2.516420	-2.690479	2.212699
121	6	0	0.384579	-3.850959	2.242697
122	1	0	3.600132	-2.713508	2.256665
123	1	0	2.288418	-4.800388	2.574860
124	30	0	-3.287736	-0.082355	0.493206
125	8	0	1.354950	3.485990	2.283654
126	8	0	-8.405896	-3.720508	0.114764
127	6	0	2.476600	4.292951	2.627417
128	1	0	3.306180	3.603362	2.780262
129	1	0	2.298511	4.855671	3.551987
130	1	0	2.733388	4.983258	1.816860
131	6	0	-8.433336	-3.145351	-1.198758
132	1	0	-7.889523	-3.782553	-1.907668
133	1	0	-8.023819	-2.134719	-1.192533
134	1	0	-9.487207	-3.120351	-1.486088
135	1	0	-0.209782	-4.755086	2.314627
136	1	0	-6.739791	4.693672	-0.056584
137	8	0	2.709372	-0.386253	1.646108
138	8	0	-9.278679	0.066862	-0.511812
139	6	0	-10.686850	0.027284	-0.695318
140	1	0	-11.212820	0.538048	0.120343
141	1	0	-10.956763	-1.029034	-0.690682
142	1	0	-10.983884	0.474629	-1.652387
143	6	0	2.841995	0.611595	2.686605
144	1	0	3.647876	1.269907	2.360192
145	1	0	3.126296	0.118916	3.621502
146	1	0	1.909453	1.167466	2.787314

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.941618	-3.650042	2.402298
2	6	0	2.164150	-1.103503	2.204704
3	6	0	2.292109	-3.484063	2.697068
4	6	0	0.208753	-2.518430	2.049598
5	6	0	0.781875	-1.227967	2.009484
6	6	0	2.902458	-2.224974	2.575384
7	1	0	2.899299	-4.340111	2.973576
8	1	0	3.973030	-2.117098	2.715120
9	6	0	-1.172031	-2.367853	1.597242
10	6	0	-0.311066	-0.311688	1.666269
11	7	0	-1.434972	-1.043039	1.390940
12	7	0	-1.982816	-3.403170	1.408729
13	6	0	-3.223461	-3.294233	0.942009

14	6	0	-4.108371	-4.444965	0.778049
15	6	0	-5.337391	-3.938132	0.311026
16	6	0	-3.901055	-5.804993	1.014473
17	1	0	-2.948557	-6.163224	1.388728
18	6	0	-4.965815	-6.662483	0.758428
19	1	0	-4.853368	-7.730015	0.925138
20	6	0	-6.201034	-6.184376	0.287322
21	1	0	-6.998160	-6.894290	0.103589
22	6	0	-6.409903	-4.816922	0.059984
23	6	0	-5.176323	-2.487746	0.222000
24	7	0	-3.889535	-2.157975	0.575563
25	7	0	-6.158595	-1.644710	-0.081348
26	6	0	-6.052960	-0.321706	-0.008542
27	6	0	-7.199112	0.563247	-0.198714
28	6	0	-8.974409	2.671272	-0.348810
29	6	0	-6.735181	1.872769	0.035018
30	6	0	-8.528124	0.278108	-0.508375
31	6	0	-9.405159	1.354737	-0.584115
32	6	0	-7.638074	2.952068	-0.031149
33	1	0	-8.846633	-0.744819	-0.673724
34	1	0	-10.450948	1.186909	-0.825375
35	1	0	-9.696966	3.475457	-0.414702
36	6	0	-5.308642	1.752841	0.348690
37	7	0	-4.953075	0.428379	0.301542
38	7	0	-4.520205	2.782710	0.652093
39	6	0	-3.239913	2.685542	0.997765
40	7	0	-2.494869	1.535467	1.084993
41	7	0	-0.216501	1.015203	1.727031
42	6	0	-1.235115	1.846394	1.506486
43	6	0	-2.404847	3.829796	1.387422
44	6	0	-0.318744	5.434849	2.349739
45	6	0	-1.140560	3.288915	1.720145
46	6	0	-2.613317	5.216112	1.524505
47	6	0	-1.558124	5.993887	2.017998
48	6	0	-0.089583	4.069457	2.193869
49	1	0	-1.733498	7.059159	2.127645
50	1	0	0.472841	6.079934	2.719455
51	30	0	-3.063995	-0.303193	0.419809
52	8	0	-7.159924	4.197910	0.217672
53	8	0	-7.572013	-4.283780	-0.392696
54	6	0	-8.078818	5.279920	0.257285
55	1	0	-8.545140	5.453410	-0.721043
56	1	0	-7.493932	6.155965	0.539004
57	1	0	-8.863441	5.113783	1.005466
58	6	0	-8.663825	-5.156544	-0.641871
59	1	0	-8.425236	-5.891712	-1.420949
60	1	0	-9.480165	-4.520553	-0.986070
61	1	0	-8.975633	-5.685055	0.267680
62	1	0	0.868568	3.623111	2.432571
63	1	0	0.467397	-4.624905	2.422753
64	8	0	-3.779067	5.874881	1.251809
65	6	0	-4.240416	5.833472	-0.104575
66	1	0	-5.020964	6.594644	-0.174602
67	1	0	-4.656028	4.854695	-0.347228

68	1	0	-3.427248	6.095364	-0.793849
69	8	0	2.861856	0.059571	1.881352
70	6	0	2.845116	1.115524	2.865083
71	1	0	1.817425	1.441526	3.034310
72	1	0	3.436738	1.928511	2.442416
73	1	0	3.306930	0.762806	3.792858
74	6	0	7.058447	4.512658	-0.055640
75	6	0	4.606124	5.647394	-0.993952
76	6	0	6.937847	5.877391	-0.295042
77	6	0	5.930357	3.725240	-0.285697
78	6	0	4.713612	4.264514	-0.747724
79	6	0	5.736168	6.442248	-0.755989
80	1	0	7.787158	6.533372	-0.126730
81	1	0	5.695939	7.510896	-0.928104
82	6	0	5.718463	2.285412	-0.152619
83	6	0	3.787163	3.141354	-0.876789
84	7	0	4.426922	1.987080	-0.486439
85	7	0	6.692431	1.443890	0.186038
86	6	0	6.560533	0.120661	0.166606
87	6	0	7.676269	-0.790088	0.420272
88	6	0	7.175510	-2.092802	0.229646
89	6	0	9.005012	-0.542297	0.762773
90	1	0	9.363121	0.472029	0.897008
91	6	0	9.835678	-1.647230	0.919838
92	1	0	10.878400	-1.506094	1.189608
93	6	0	9.362529	-2.957583	0.736804
94	1	0	10.050703	-3.783264	0.870787
95	6	0	8.027364	-3.203205	0.385840
96	6	0	5.765777	-1.943254	-0.131679
97	7	0	5.445489	-0.607511	-0.138200
98	7	0	4.959760	-2.954735	-0.433254
99	6	0	3.688863	-2.819273	-0.801509
100	6	0	2.856318	-3.967241	-1.142525
101	6	0	0.852253	-5.730376	-1.817922
102	6	0	1.578497	-3.461150	-1.455576
103	6	0	3.164136	-5.325934	-1.166665
104	6	0	2.139279	-6.199740	-1.510167
105	6	0	0.549495	-4.361177	-1.798031
106	1	0	4.163888	-5.665195	-0.920614
107	1	0	2.323131	-7.269901	-1.541891
108	1	0	0.085266	-6.450753	-2.072720
109	6	0	1.673492	-2.003266	-1.314133
110	7	0	2.950186	-1.677732	-0.921444
111	7	0	0.674950	-1.149308	-1.542172
112	6	0	0.804760	0.177416	-1.512279
113	7	0	1.948204	0.892353	-1.265388
114	7	0	2.542872	3.246245	-1.328125
115	6	0	1.713105	2.219597	-1.483402
116	6	0	-0.272100	1.117264	-1.852183
117	6	0	-1.733203	3.413194	-2.537219
118	6	0	0.329580	2.394767	-1.910977
119	6	0	-1.658850	1.030476	-2.036049
120	6	0	-2.371994	2.169642	-2.403081
121	6	0	-0.375561	3.544618	-2.260447

122	1	0	-3.445360	2.083395	-2.537017
123	1	0	-2.321167	4.281784	-2.817414
124	30	0	3.570969	0.153902	-0.300099
125	8	0	-0.680147	-3.859492	-2.087442
126	8	0	7.500834	-4.438305	0.189841
127	6	0	-1.730724	-4.779803	-2.358898
128	1	0	-1.516967	-5.383979	-3.249289
129	1	0	-2.619335	-4.175801	-2.540993
130	1	0	-1.918825	-5.437398	-1.503149
131	6	0	8.354213	-5.564853	0.323364
132	1	0	9.184891	-5.530678	-0.392689
133	1	0	7.732585	-6.435576	0.111313
134	1	0	8.759257	-5.649281	1.339820
135	1	0	0.131587	4.502585	-2.292433
136	1	0	7.983034	4.067759	0.294051
137	8	0	-2.390179	-0.115562	-1.730809
138	6	0	-2.387057	-1.157277	-2.734865
139	1	0	-3.141380	-1.876536	-2.414124
140	1	0	-1.404076	-1.627397	-2.776509
141	1	0	-2.675196	-0.728570	-3.699759
142	8	0	3.416194	6.120365	-1.441831
143	6	0	3.295379	7.511836	-1.695262
144	1	0	3.456071	8.104923	-0.786017
145	1	0	2.273819	7.662571	-2.046139
146	1	0	3.997120	7.845065	-2.470230

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-8.431081	1.099775	0.697742
2	6	0	-7.033878	3.586958	0.604967
3	6	0	-9.049830	2.307032	1.045871
4	6	0	-7.073078	1.136701	0.325456
5	6	0	-6.409822	2.384982	0.282129
6	6	0	-8.367345	3.529859	1.004724
7	1	0	-10.091967	2.264363	1.345607
8	1	0	-8.894156	4.439745	1.277650
9	1	0	-6.483557	4.519761	0.548593
10	6	0	-6.062284	0.132678	-0.039106
11	6	0	-5.034720	2.115514	-0.128500
12	7	0	-4.868171	0.768148	-0.276753
13	7	0	-6.303636	-1.170931	-0.141778
14	6	0	-5.413210	-2.078492	-0.543272
15	6	0	-5.716714	-3.500166	-0.730402
16	6	0	-4.537925	-4.094317	-1.223834
17	6	0	-6.856641	-4.297856	-0.507690
18	6	0	-6.770911	-5.664602	-0.807831

19	1	0	-7.627040	-6.309425	-0.651631
20	6	0	-5.585665	-6.225438	-1.312250
21	1	0	-5.567255	-7.289222	-1.531262
22	6	0	-4.449614	-5.452658	-1.526444
23	6	0	-3.541761	-3.029864	-1.303713
24	7	0	-4.102292	-1.855393	-0.884427
25	7	0	-2.294778	-3.244306	-1.713441
26	6	0	-1.367596	-2.294930	-1.786639
27	6	0	0.026345	-2.568364	-2.128491
28	6	0	2.772122	-2.516149	-2.433123
29	6	0	0.709157	-1.334845	-2.028704
30	6	0	0.683914	-3.761342	-2.424628
31	6	0	2.064609	-3.718483	-2.596968
32	6	0	2.107233	-1.329914	-2.131857
33	1	0	0.127419	-4.689520	-2.493678
34	1	0	2.614037	-4.627185	-2.821850
35	1	0	3.854607	-2.498616	-2.503162
36	6	0	-0.313194	-0.329103	-1.726211
37	7	0	-1.515333	-0.959128	-1.541337
38	7	0	-0.096929	0.984551	-1.732498
39	6	0	-1.030454	1.891799	-1.452666
40	7	0	-2.297444	1.676845	-0.991158
41	7	0	-4.154020	3.086287	-0.353373
42	6	0	-2.914890	2.885366	-0.794934
43	6	0	-0.811109	3.330400	-1.604611
44	6	0	-1.010699	6.089278	-1.698276
45	6	0	-1.998203	3.957646	-1.178220
46	6	0	0.281598	4.054496	-2.079885
47	6	0	0.159566	5.439436	-2.122876
48	6	0	-2.103775	5.360655	-1.211400
49	1	0	1.188694	3.553993	-2.397004
50	1	0	0.986333	6.043473	-2.484596
51	1	0	-1.052134	7.170608	-1.743425
52	30	0	-3.071354	-0.138142	-0.513384
53	8	0	2.879440	-0.212186	-1.817277
54	8	0	-3.256326	5.920763	-0.754804
55	8	0	-9.190078	-0.033278	0.789357
56	6	0	-3.404158	7.330091	-0.851331
57	1	0	-3.330209	7.673313	-1.890563
58	1	0	-2.658762	7.859904	-0.244648
59	1	0	-4.401570	7.551539	-0.469523
60	6	0	2.958767	0.810541	-2.834516
61	1	0	1.968870	1.239293	-2.999686
62	1	0	3.363679	0.379385	-3.755381
63	1	0	3.643795	1.566553	-2.449131
64	6	0	-9.448446	-0.719726	-0.443320
65	1	0	-9.841666	-0.023070	-1.194599
66	1	0	-10.215386	-1.462465	-0.213477
67	1	0	-8.550868	-1.220618	-0.808513
68	1	0	-3.526624	-5.875163	-1.906769
69	8	0	-7.965311	-3.696956	-0.005723
70	6	0	-9.088556	-4.506047	0.310875
71	1	0	-9.826270	-3.832047	0.747230
72	1	0	-8.831657	-5.282416	1.042016

73	1	0	-9.513124	-4.980089	-0.583204
74	6	0	-1.604433	-1.567147	1.849018
75	6	0	-0.007379	-3.898526	2.022840
76	6	0	-2.178904	-2.814294	2.085401
77	6	0	-0.210210	-1.458292	1.748733
78	6	0	0.556162	-2.645049	1.791763
79	6	0	-1.387069	-3.969269	2.189446
80	1	0	-3.259742	-2.877627	2.155031
81	1	0	-1.868884	-4.925908	2.365742
82	1	0	0.624331	-4.779700	2.047305
83	6	0	0.743441	-0.367505	1.503355
84	6	0	1.928369	-2.264000	1.477180
85	7	0	1.987311	-0.911143	1.301773
86	7	0	0.436662	0.927499	1.565964
87	6	0	1.308499	1.915386	1.361303
88	6	0	1.030979	3.338434	1.590570
89	6	0	2.220328	4.025034	1.271043
90	6	0	-0.087664	4.074238	2.032830
91	6	0	0.044320	5.465197	2.151412
92	1	0	-0.794852	6.060631	2.487768
93	6	0	1.247787	6.115508	1.837235
94	1	0	1.300388	7.194797	1.948821
95	6	0	2.355753	5.407130	1.388460
96	6	0	3.179941	3.016416	0.838382
97	7	0	2.603862	1.782036	0.918398
98	7	0	4.415746	3.328631	0.451290
99	6	0	5.348122	2.432387	0.146536
100	6	0	6.717726	2.799950	-0.210074
101	6	0	9.399163	2.867104	-0.877937
102	6	0	7.421101	1.591154	-0.380004
103	6	0	7.324726	4.046322	-0.360855
104	6	0	8.673881	4.057391	-0.699615
105	6	0	8.788287	1.615245	-0.717498
106	1	0	6.759177	4.959696	-0.215677
107	1	0	9.190820	5.003578	-0.831901
108	1	0	10.447499	2.930733	-1.142553
109	6	0	6.465760	0.516747	-0.110193
110	7	0	5.238365	1.070256	0.165141
111	7	0	6.782990	-0.773030	-0.071128
112	6	0	5.939715	-1.734286	0.296141
113	7	0	4.615782	-1.628402	0.613739
114	7	0	2.907343	-3.157520	1.372768
115	6	0	4.144587	-2.863451	0.990852
116	6	0	6.364566	-3.124057	0.460322
117	6	0	6.575869	-5.831322	0.966763
118	6	0	5.233364	-3.836329	0.902954
119	6	0	7.604618	-3.730828	0.265336
120	6	0	7.688203	-5.095212	0.523837
121	6	0	5.331698	-5.216117	1.166723
122	1	0	8.455453	-3.149474	-0.071289
123	1	0	8.631442	-5.616069	0.385476
124	1	0	6.695198	-6.891357	1.154980
125	30	0	3.494712	0.048927	0.342258
126	8	0	9.423941	0.426768	-0.871592

127	8	0	4.217219	-5.861102	1.595311
128	8	0	-2.465818	-0.499979	1.604937
129	6	0	4.308397	-7.248300	1.881535
130	1	0	5.032042	-7.450552	2.681239
131	1	0	4.584585	-7.828985	0.992153
132	1	0	3.313822	-7.549765	2.212476
133	6	0	10.805026	0.437288	-1.199685
134	1	0	11.401491	0.935458	-0.425059
135	1	0	10.989179	0.925843	-2.164966
136	1	0	11.102977	-0.609840	-1.264857
137	6	0	-2.604407	0.458187	2.681926
138	1	0	-2.832127	-0.076795	3.608851
139	1	0	-3.450545	1.088872	2.407230
140	1	0	-1.693908	1.051888	2.767896
141	1	0	3.292270	5.892340	1.138320
142	8	0	-1.234717	3.402821	2.314920
143	6	0	-2.381429	4.159783	2.693619
144	1	0	-3.177233	3.433704	2.856167
145	1	0	-2.689293	4.846088	1.897699
146	1	0	-2.204834	4.716215	3.622339

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.619535	1.644716	0.364801
2	6	0	7.131504	4.054779	-0.132778
3	6	0	9.221042	2.912099	0.405059
4	6	0	7.240621	1.610590	0.073430
5	6	0	6.523170	2.802154	-0.167859
6	6	0	8.491869	4.087094	0.160598
7	1	0	10.276910	3.004793	0.626898
8	1	0	9.013761	5.038863	0.202666
9	1	0	6.559738	4.954884	-0.329285
10	6	0	6.276871	0.523579	-0.072983
11	6	0	5.143692	2.408338	-0.445945
12	7	0	5.041213	1.047398	-0.363145
13	7	0	6.597933	-0.762653	0.026084
14	6	0	5.753214	-1.764790	-0.209281
15	6	0	6.165723	-3.165878	-0.220740
16	6	0	5.025171	-3.916469	-0.577510
17	6	0	7.399807	-3.762666	0.026048
18	1	0	8.263671	-3.162804	0.289948
19	6	0	7.463558	-5.148598	-0.086276
20	1	0	8.401678	-5.663899	0.099250
21	6	0	6.338805	-5.911576	-0.439489
22	1	0	6.454854	-6.985862	-0.511322
23	6	0	5.093271	-5.319167	-0.698834
24	6	0	3.949512	-2.948692	-0.770304

25	7	0	4.425095	-1.684898	-0.522665
26	7	0	2.724448	-3.282612	-1.164994
27	6	0	1.751410	-2.408719	-1.404482
28	6	0	0.422020	-2.800251	-1.868364
29	6	0	-2.223123	-2.906974	-2.664215
30	6	0	-0.328959	-1.610497	-1.978299
31	6	0	-0.120730	-4.046052	-2.174272
32	6	0	-1.449728	-4.077966	-2.585181
33	6	0	-1.683263	-1.653544	-2.353534
34	1	0	0.477059	-4.946284	-2.087043
35	1	0	-1.918674	-5.025446	-2.832129
36	1	0	-3.261737	-2.999081	-2.955775
37	6	0	0.584790	-0.523431	-1.634570
38	7	0	1.799278	-1.048017	-1.282770
39	7	0	0.257741	0.762364	-1.726401
40	6	0	1.109269	1.764451	-1.521071
41	7	0	2.413209	1.682159	-1.122036
42	7	0	4.187732	3.282320	-0.750788
43	6	0	2.941752	2.947267	-1.070083
44	6	0	0.758371	3.166793	-1.735380
45	6	0	0.713295	5.915074	-1.975026
46	6	0	1.919567	3.916552	-1.453094
47	6	0	-0.431281	3.765732	-2.139757
48	6	0	-0.433300	5.153812	-2.249658
49	6	0	1.919486	5.319964	-1.572735
50	1	0	-1.311239	3.169134	-2.352064
51	1	0	-1.340012	5.670415	-2.549632
52	1	0	0.646888	6.990820	-2.079485
53	30	0	3.305257	0.000421	-0.435004
54	6	0	2.889358	7.959813	-1.530867
55	1	0	2.592512	8.111722	-2.571281
56	1	0	3.777151	8.562877	-1.328477
57	1	0	2.087936	8.279603	-0.860549
58	6	0	-4.253655	-0.672811	-3.022510
59	1	0	-4.132630	-1.044485	-4.041733
60	1	0	-4.870462	0.227757	-3.041921
61	1	0	-4.742647	-1.419315	-2.395795
62	6	0	4.253156	-7.954320	-1.203498
63	1	0	5.040790	-8.085431	-1.949250
64	1	0	3.390792	-8.557313	-1.495956
65	1	0	4.601983	-8.292917	-0.224902
66	6	0	11.194047	0.703592	0.994149
67	1	0	11.626155	1.217445	0.132210
68	1	0	11.771019	-0.203576	1.186130
69	1	0	11.243023	1.343964	1.878059
70	6	0	-1.919469	-5.319955	1.572745
71	6	0	0.431289	-3.765715	2.139779
72	6	0	-0.713279	-5.915061	1.975044
73	6	0	-1.919555	-3.916544	1.453103
74	6	0	-0.758363	-3.166782	1.735395
75	6	0	0.433312	-5.153795	2.249681
76	1	0	-0.646869	-6.990807	2.079505
77	1	0	1.340024	-5.670394	2.549662
78	1	0	1.311243	-3.169113	2.352090

79	6	0	-2.941741	-2.947263	1.070086
80	6	0	-1.109266	-1.764441	1.521082
81	7	0	-2.413203	-1.682154	1.122037
82	7	0	-4.187718	-3.282322	0.750785
83	6	0	-5.143679	-2.408345	0.445934
84	6	0	-6.523153	-2.802166	0.167836
85	6	0	-7.240607	-1.610605	-0.073458
86	6	0	-7.131481	-4.054794	0.132749
87	1	0	-6.559713	-4.954896	0.329261
88	6	0	-8.491844	-4.087114	-0.160637
89	1	0	-9.013731	-5.038886	-0.202709
90	6	0	-9.221020	-2.912122	-0.405103
91	1	0	-10.276886	-3.004821	-0.626950
92	6	0	-8.619519	-1.644737	-0.364840
93	6	0	-6.276864	-0.523590	0.072965
94	7	0	-5.041204	-1.047405	0.363133
95	7	0	-6.597931	0.762640	-0.026100
96	6	0	-5.753218	1.764782	0.209275
97	6	0	-6.165734	3.165867	0.220738
98	6	0	-6.338831	5.911563	0.439494
99	6	0	-5.025188	3.916463	0.577515
100	6	0	-7.399820	3.762650	-0.026055
101	6	0	-7.463578	5.148581	0.086273
102	6	0	-5.093294	5.319160	0.698843
103	1	0	-8.263680	3.162785	-0.289961
104	1	0	-8.401699	5.663879	-0.099256
105	1	0	-6.454884	6.985848	0.511329
106	6	0	-3.949525	2.948690	0.770313
107	7	0	-4.425101	1.684895	0.522666
108	7	0	-2.724464	3.282614	1.165007
109	6	0	-1.751421	2.408726	1.404494
110	7	0	-1.799283	1.048023	1.282779
111	7	0	-0.257740	-0.762351	1.726413
112	6	0	-0.584793	0.523443	1.634581
113	6	0	-0.422034	2.800263	1.868381
114	6	0	2.223106	2.906995	2.664241
115	6	0	0.328951	1.610512	1.978312
116	6	0	0.120708	4.046065	2.174296
117	6	0	1.449705	4.077984	2.585210
118	6	0	1.683254	1.653564	2.353551
119	1	0	-0.477085	4.946295	2.087069
120	1	0	1.918645	5.025465	2.832166
121	1	0	3.261717	2.999107	2.955807
122	30	0	-3.305255	-0.000417	0.435001
123	6	0	4.253647	0.672830	3.022537
124	1	0	4.742636	1.419352	2.395841
125	1	0	4.870462	-0.227734	3.041928
126	1	0	4.132618	1.044481	4.041767
127	6	0	-4.253195	7.954315	1.203525
128	1	0	-4.602020	8.292916	0.224929
129	1	0	-3.390835	8.557310	1.495991
130	1	0	-5.040833	8.085416	1.949274
131	6	0	-11.194028	-0.703624	-0.994212
132	1	0	-11.242992	-1.343995	-1.878123

133	1	0	-11.771002	0.203542	-1.186199
134	1	0	-11.626144	-1.217478	-0.132277
135	6	0	-2.889331	-7.959809	1.530872
136	1	0	-2.087904	-8.279594	0.860559
137	1	0	-3.777120	-8.562876	1.328476
138	1	0	-2.592492	-8.111717	2.571288
139	16	0	-9.495524	-0.123941	-0.661318
140	16	0	-3.638313	6.236155	1.158203
141	16	0	-2.645141	-0.139569	-2.341482
142	16	0	3.402659	6.237180	-1.213397
143	16	0	2.645138	0.139592	2.341495
144	16	0	9.495536	0.123916	0.661274
145	16	0	3.638283	-6.236157	-1.158185
146	16	0	-3.402637	-6.237177	1.213399

Dimer of 9b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.440683	3.907337	-2.337160
2	6	0	-1.902659	5.314840	-1.502725
3	6	0	0.364436	5.308286	-2.356688
4	6	0	-0.677380	3.201567	-1.845733
5	6	0	-1.830687	3.925735	-1.466394
6	6	0	-0.776315	6.005613	-1.937425
7	1	0	1.220122	5.860029	-2.731892
8	1	0	-0.781034	7.090728	-1.978732
9	1	0	-2.811338	5.821723	-1.196969
10	6	0	-1.013697	1.783234	-1.611599
11	6	0	-2.834629	2.950504	-1.063937
12	7	0	-2.310764	1.696057	-1.164724
13	7	0	-0.180169	0.761576	-1.801301
14	6	0	-0.525915	-0.522058	-1.696140
15	6	0	0.392089	-1.639254	-1.947985
16	6	0	-0.398359	-2.807753	-1.902709
17	6	0	1.776758	-1.741735	-2.183060
18	6	0	2.303426	-3.018323	-2.411725
19	1	0	3.363326	-3.146528	-2.591172
20	6	0	1.490556	-4.163556	-2.397119
21	1	0	1.949937	-5.130358	-2.579110
22	6	0	0.128617	-4.076191	-2.133150
23	6	0	-1.753010	-2.381398	-1.575672
24	7	0	-1.775514	-1.022351	-1.438609
25	7	0	-2.771017	-3.228642	-1.475964
26	6	0	-4.015328	-2.864197	-1.184139
27	6	0	-5.134465	-3.796589	-1.221490
28	6	0	-7.587419	-5.046202	-1.230321
29	6	0	-6.293017	-3.051252	-0.915203
30	6	0	-5.172107	-5.155878	-1.521739
31	6	0	-6.419514	-5.771197	-1.510049

32	6	0	-7.561194	-3.672710	-0.939888
33	1	0	-4.261640	-5.695496	-1.756759
34	1	0	-6.504915	-6.831270	-1.731224
35	1	0	-8.532103	-5.574864	-1.252346
36	6	0	-5.834480	-1.680580	-0.664490
37	7	0	-4.473872	-1.620980	-0.844486
38	7	0	-6.642673	-0.678157	-0.308574
39	6	0	-6.267087	0.595813	-0.208822
40	7	0	-5.009446	1.088389	-0.474393
41	7	0	-4.061128	3.305713	-0.696259
42	6	0	-5.041208	2.450698	-0.427077
43	6	0	-7.167654	1.722754	0.108213
44	6	0	-8.241122	4.303757	0.381183
45	6	0	-6.384437	2.887405	-0.072771
46	6	0	-8.517103	1.862576	0.497721
47	6	0	-9.024490	3.166214	0.615615
48	6	0	-6.896453	4.175659	0.048893
49	1	0	-10.058683	3.285063	0.922145
50	1	0	-8.687695	5.287682	0.489068
51	30	0	-3.288431	0.016347	-0.580163
52	6	0	-10.360713	-3.922319	-0.870840
53	1	0	-11.282141	-3.354102	-0.726678
54	1	0	-10.321761	-4.722019	-0.127071
55	1	0	-10.363900	-4.345045	-1.878316
56	6	0	1.374950	2.199988	-4.353732
57	1	0	0.807982	2.829818	-5.042100
58	1	0	0.779681	1.353471	-4.012250
59	1	0	2.271213	1.832486	-4.858305
60	1	0	-6.255125	5.034667	-0.114731
61	1	0	-0.509844	-4.951792	-2.097989
62	6	0	4.416889	-0.867157	-2.678880
63	1	0	4.846335	-1.591598	-1.985868
64	1	0	5.055761	0.017220	-2.708144
65	1	0	4.347350	-1.289785	-3.682958
66	6	0	-8.806159	-0.388240	2.166054
67	1	0	-9.526496	-1.124484	2.528920
68	1	0	-8.532304	0.280877	2.984713
69	1	0	-7.935586	-0.906166	1.764824
70	6	0	8.517045	1.861521	-0.499937
71	6	0	6.897162	4.175152	-0.051062
72	6	0	9.024780	3.165001	-0.618108
73	6	0	7.167658	1.722157	-0.109977
74	6	0	6.384809	2.887072	0.070955
75	6	0	8.241803	4.302798	-0.383643
76	1	0	10.058915	3.283525	-0.924968
77	1	0	8.688646	5.286574	-0.491770
78	1	0	6.256116	5.034375	0.112538
79	6	0	6.266931	0.595568	0.207802
80	6	0	5.041575	2.450814	0.425796
81	7	0	5.009473	1.088538	0.473557
82	7	0	6.642285	-0.678424	0.308141
83	6	0	5.833991	-1.680509	0.664723
84	6	0	6.292333	-3.051144	0.915976
85	6	0	5.133701	-3.796155	1.222751

86	6	0	7.560416	-3.672776	0.940742
87	6	0	7.586477	-5.046139	1.231818
88	1	0	8.531084	-5.574933	1.253964
89	6	0	6.418497	-5.770821	1.512033
90	1	0	6.503760	-6.830805	1.733688
91	6	0	5.171180	-5.155312	1.523597
92	6	0	4.014715	-2.863581	1.185119
93	7	0	4.473416	-1.620600	0.844889
94	7	0	2.770358	-3.227684	1.477194
95	6	0	1.752529	-2.380186	1.576632
96	6	0	0.397832	-2.806149	1.903977
97	6	0	-2.303957	-3.016131	2.413139
98	6	0	-0.392413	-1.637492	1.948853
99	6	0	-0.129324	-4.074419	2.134924
100	6	0	-1.491263	-4.161490	2.398987
101	6	0	-1.777104	-1.739715	2.183966
102	1	0	0.509015	-4.950120	2.100057
103	1	0	-1.950778	-5.128151	2.581378
104	1	0	-3.363875	-3.144081	2.592680
105	6	0	0.525829	-0.520549	1.696613
106	7	0	1.775280	-1.021208	1.439036
107	7	0	0.180458	0.763197	1.801592
108	6	0	1.014220	1.784605	1.611580
109	7	0	2.311117	1.697017	1.164241
110	7	0	4.061809	3.306141	0.695131
111	6	0	2.835335	2.951290	1.063255
112	6	0	0.678449	3.203057	1.845852
113	6	0	0.778530	6.007107	1.937639
114	6	0	1.831858	3.926834	1.466085
115	6	0	-0.439145	3.909265	2.337769
116	6	0	-0.362307	5.310184	2.357340
117	6	0	1.904415	5.315910	1.502447
118	1	0	-1.217611	5.862248	2.732946
119	1	0	0.783682	7.092217	1.979031
120	30	0	3.288269	0.016925	0.580002
121	6	0	-4.417110	-0.864585	2.679511
122	1	0	-5.055935	0.019848	2.708065
123	1	0	-4.347578	-1.286428	3.683919
124	1	0	-4.846610	-1.589543	1.987068
125	6	0	8.804318	-0.390227	-2.167464
126	1	0	8.529401	0.278605	-2.986001
127	1	0	7.934307	-0.908217	-1.765110
128	1	0	9.524454	-1.126368	-2.530937
129	1	0	2.813191	5.822410	1.196346
130	1	0	4.260666	-5.694699	1.758967
131	6	0	10.359835	-3.922918	0.871106
132	1	0	10.363267	-4.345156	1.878787
133	1	0	11.281337	-3.354967	0.726368
134	1	0	10.320477	-4.722971	0.127739
135	6	0	-1.373648	2.201749	4.354226
136	1	0	-2.269965	1.834511	4.858895
137	1	0	-0.806128	2.830947	5.042720
138	1	0	-0.778948	1.355071	4.012163
139	16	0	9.018788	-2.705082	0.649096

140	16	0	9.664609	0.537559	-0.845681
141	16	0	1.966284	3.183469	-2.927110
142	16	0	2.784126	-0.263729	-2.128795
143	16	0	-2.784338	-0.261656	2.128904
144	16	0	-1.964893	3.186209	2.928246
145	16	0	-9.665173	0.538907	0.843016
146	16	0	-9.019465	-2.704643	-0.649006

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.444804	4.443466	-2.314272
2	6	0	2.051794	2.093072	-2.449585
3	6	0	1.783927	4.520448	-2.677559
4	6	0	-0.078719	3.185186	-2.024838
5	6	0	0.690871	2.001278	-2.092380
6	6	0	2.571477	3.360632	-2.741268
7	1	0	2.235807	5.480345	-2.906400
8	1	0	3.618504	3.440172	-3.013961
9	6	0	-1.410917	2.801832	-1.577635
10	6	0	-0.227114	0.915709	-1.713554
11	7	0	-1.452167	1.447762	-1.402678
12	7	0	-2.384493	3.688677	-1.395259
13	6	0	-3.613361	3.363421	-1.011986
14	6	0	-4.688836	4.342544	-0.869458
15	6	0	-5.844459	3.618239	-0.509761
16	6	0	-4.705163	5.724928	-1.039430
17	1	0	-3.806264	6.260679	-1.323214
18	6	0	-5.918849	6.373324	-0.828968
19	1	0	-5.983517	7.451410	-0.945349
20	6	0	-7.077952	5.667791	-0.467366
21	1	0	-7.991171	6.230492	-0.318257
22	6	0	-7.074891	4.274081	-0.301826
23	6	0	-5.438070	2.216980	-0.454460
24	7	0	-4.099014	2.115668	-0.731739
25	7	0	-6.285754	1.218355	-0.231825
26	6	0	-5.957117	-0.069136	-0.299225
27	6	0	-6.953727	-1.130843	-0.246338
28	6	0	-8.373032	-3.483098	-0.360047
29	6	0	-6.263729	-2.343691	-0.455002
30	6	0	-8.334276	-1.065028	-0.079611
31	6	0	-9.031793	-2.267951	-0.125649
32	6	0	-6.982719	-3.555670	-0.547626
33	1	0	-8.828572	-0.112137	0.071716
34	1	0	-10.109872	-2.276783	0.007158
35	1	0	-8.970049	-4.385071	-0.405549
36	6	0	-4.845405	-1.983820	-0.579917
37	7	0	-4.719821	-0.617632	-0.487079

38	7	0	-3.863570	-2.868299	-0.750574
39	6	0	-2.586158	-2.559412	-0.975421
40	7	0	-2.072871	-1.291031	-1.107473
41	7	0	0.090787	-0.375999	-1.719721
42	6	0	-0.755106	-1.370213	-1.449955
43	6	0	-1.509831	-3.541157	-1.206019
44	6	0	0.932820	-4.736337	-1.900127
45	6	0	-0.365928	-2.773057	-1.531014
46	6	0	-1.406818	-4.948348	-1.179063
47	6	0	-0.175475	-5.513952	-1.545077
48	6	0	0.853709	-3.347662	-1.878929
49	1	0	-0.083322	-6.594757	-1.519610
50	1	0	1.867176	-5.225359	-2.158116
51	30	0	-2.980124	0.423610	-0.534231
52	6	0	-7.479035	-6.281795	-1.026301
53	1	0	-7.987132	-6.411130	-0.067493
54	1	0	-6.989222	-7.221006	-1.292310
55	1	0	-8.203048	-6.031530	-1.805467
56	6	0	-9.790469	4.616374	0.343239
57	1	0	-9.536699	5.331617	1.129219
58	1	0	-10.693849	4.077969	0.637654
59	1	0	-9.985978	5.140931	-0.594995
60	1	0	1.709416	-2.726586	-2.114383
61	1	0	-0.184755	5.323617	-2.242145
62	6	0	-3.127021	-5.573536	0.961221
63	1	0	-3.814353	-6.331798	1.342207
64	1	0	-3.628539	-4.606806	0.948397
65	1	0	-2.231343	-5.546573	1.583450
66	6	0	2.618779	-0.408781	-3.704647
67	1	0	1.617891	-0.748347	-3.444686
68	1	0	3.317093	-1.248887	-3.715306
69	1	0	2.634543	0.084409	-4.678029
70	6	0	8.715286	-1.545020	-1.044525
71	6	0	7.258536	-3.966773	-0.521343
72	6	0	9.299397	-2.797042	-1.219223
73	6	0	7.392065	-1.519653	-0.612849
74	6	0	6.665425	-2.700123	-0.352059
75	6	0	8.590658	-3.981478	-0.964740
76	1	0	10.328410	-2.871174	-1.559095
77	1	0	9.101346	-4.923961	-1.117966
78	6	0	6.492858	-0.403651	-0.319277
79	6	0	5.342953	-2.267477	0.093443
80	7	0	5.280789	-0.897643	0.073372
81	7	0	6.871364	0.869014	-0.388502
82	6	0	6.085444	1.888034	-0.049309
83	6	0	6.548038	3.275449	-0.033356
84	6	0	5.459118	4.055734	0.407357
85	6	0	7.781468	3.837012	-0.351756
86	1	0	8.605113	3.216158	-0.685932
87	6	0	7.899848	5.218192	-0.220060
88	1	0	8.840839	5.705847	-0.458074
89	6	0	6.826684	6.009817	0.217944
90	1	0	6.982588	7.078242	0.300517
91	6	0	5.580238	5.452651	0.545674

92	6	0	4.362737	3.118997	0.641985
93	7	0	4.781668	1.843956	0.354573
94	7	0	3.161391	3.488400	1.067911
95	6	0	2.162806	2.642713	1.313497
96	6	0	0.840607	3.085161	1.737453
97	6	0	-1.819483	3.328574	2.422569
98	6	0	0.050806	1.922585	1.878178
99	6	0	0.337484	4.363731	1.967931
100	6	0	-1.001060	4.466522	2.328395
101	6	0	-1.318144	2.043020	2.188220
102	1	0	0.975793	5.233387	1.858806
103	1	0	-1.441021	5.440769	2.518526
104	1	0	-2.865491	3.469899	2.664000
105	6	0	0.948269	0.793053	1.610431
106	7	0	2.173973	1.280106	1.231224
107	7	0	0.628660	-0.481755	1.829581
108	6	0	1.450037	-1.513642	1.640126
109	7	0	2.680492	-1.465111	1.026731
110	7	0	4.399405	-3.100546	0.512548
111	6	0	3.215756	-2.718774	0.991960
112	6	0	1.181209	-2.897911	2.067650
113	6	0	1.380531	-5.664355	2.501581
114	6	0	2.295375	-3.650415	1.626416
115	6	0	0.160204	-3.548336	2.792337
116	6	0	0.286844	-4.932476	2.985865
117	6	0	2.413362	-5.023361	1.826539
118	1	0	-0.485532	-5.440967	3.553919
119	1	0	1.425557	-6.733920	2.683585
120	30	0	3.590493	0.188070	0.293650
121	6	0	-3.948457	1.198692	2.806855
122	1	0	-3.830164	1.608500	3.811677
123	1	0	-4.597461	0.322312	2.853226
124	1	0	-4.399420	1.936945	2.142709
125	6	0	4.861591	8.102768	1.153220
126	1	0	5.696653	8.191697	1.852091
127	1	0	4.038884	8.726179	1.509939
128	1	0	5.161269	8.451998	0.162204
129	1	0	3.289001	-5.553539	1.467998
130	1	0	9.255991	-0.624493	-1.233668
131	6	0	-0.606861	-1.581016	4.657547
132	1	0	-1.458338	-1.176413	5.209383
133	1	0	-0.098001	-0.774397	4.130870
134	1	0	0.066051	-2.084068	5.354751
135	6	0	7.498810	-6.768833	-0.566179
136	1	0	7.802663	-6.754866	-1.615567
137	1	0	6.956594	-7.696373	-0.370430
138	1	0	8.377848	-6.733894	0.081627
139	16	0	-8.511798	3.327884	0.152652
140	16	0	-6.126581	-5.060186	-0.933069
141	16	0	-2.698649	-6.099962	-0.738778
142	16	0	-1.308782	-2.780233	3.465590
143	16	0	-2.349570	0.578801	2.179774
144	16	0	3.238503	0.748333	-2.430399
145	16	0	6.313834	-5.435564	-0.178637

146	16	0	4.187746	6.406822	1.109636

Dimer of 9d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.444804	4.443466	-2.314272
2	6	0	2.051794	2.093072	-2.449585
3	6	0	1.783927	4.520448	-2.677559
4	6	0	-0.078719	3.185186	-2.024838
5	6	0	0.690871	2.001278	-2.092380
6	6	0	2.571477	3.360632	-2.741268
7	1	0	2.235807	5.480345	-2.906400
8	1	0	3.618504	3.440172	-3.013961
9	6	0	-1.410917	2.801832	-1.577635
10	6	0	-0.227114	0.915709	-1.713554
11	7	0	-1.452167	1.447762	-1.402678
12	7	0	-2.384493	3.688677	-1.395259
13	6	0	-3.613361	3.363421	-1.011986
14	6	0	-4.688836	4.342544	-0.869458
15	6	0	-5.844459	3.618239	-0.509761
16	6	0	-4.705163	5.724928	-1.039430
17	1	0	-3.806264	6.260679	-1.323214
18	6	0	-5.918849	6.373324	-0.828968
19	1	0	-5.983517	7.451410	-0.945349
20	6	0	-7.077952	5.667791	-0.467366
21	1	0	-7.991171	6.230492	-0.318257
22	6	0	-7.074891	4.274081	-0.301826
23	6	0	-5.438070	2.216980	-0.454460
24	7	0	-4.099014	2.115668	-0.731739
25	7	0	-6.285754	1.218355	-0.231825
26	6	0	-5.957117	-0.069136	-0.299225
27	6	0	-6.953727	-1.130843	-0.246338
28	6	0	-8.373032	-3.483098	-0.360047
29	6	0	-6.263729	-2.343691	-0.455002
30	6	0	-8.334276	-1.065028	-0.079611
31	6	0	-9.031793	-2.267951	-0.125649
32	6	0	-6.982719	-3.555670	-0.547626
33	1	0	-8.828572	-0.112137	0.071716
34	1	0	-10.109872	-2.276783	0.007158
35	1	0	-8.970049	-4.385071	-0.405549
36	6	0	-4.845405	-1.983820	-0.579917
37	7	0	-4.719821	-0.617632	-0.487079
38	7	0	-3.863570	-2.868299	-0.750574
39	6	0	-2.586158	-2.559412	-0.975421
40	7	0	-2.072871	-1.291031	-1.107473
41	7	0	0.090787	-0.375999	-1.719721
42	6	0	-0.755106	-1.370213	-1.449955
43	6	0	-1.509831	-3.541157	-1.206019
44	6	0	0.932820	-4.736337	-1.900127

45	6	0	-0.365928	-2.773057	-1.531014
46	6	0	-1.406818	-4.948348	-1.179063
47	6	0	-0.175475	-5.513952	-1.545077
48	6	0	0.853709	-3.347662	-1.878929
49	1	0	-0.083322	-6.594757	-1.519610
50	1	0	1.867176	-5.225359	-2.158116
51	30	0	-2.980124	0.423610	-0.534231
52	6	0	-7.479035	-6.281795	-1.026301
53	1	0	-7.987132	-6.411130	-0.067493
54	1	0	-6.989222	-7.221006	-1.292310
55	1	0	-8.203048	-6.031530	-1.805467
56	6	0	-9.790469	4.616374	0.343239
57	1	0	-9.536699	5.331617	1.129219
58	1	0	-10.693849	4.077969	0.637654
59	1	0	-9.985978	5.140931	-0.594995
60	1	0	1.709416	-2.726586	-2.114383
61	1	0	-0.184755	5.323617	-2.242145
62	6	0	-3.127021	-5.573536	0.961221
63	1	0	-3.814353	-6.331798	1.342207
64	1	0	-3.628539	-4.606806	0.948397
65	1	0	-2.231343	-5.546573	1.583450
66	6	0	2.618779	-0.408781	-3.704647
67	1	0	1.617891	-0.748347	-3.444686
68	1	0	3.317093	-1.248887	-3.715306
69	1	0	2.634543	0.084409	-4.678029
70	6	0	8.715286	-1.545020	-1.044525
71	6	0	7.258536	-3.966773	-0.521343
72	6	0	9.299397	-2.797042	-1.219223
73	6	0	7.392065	-1.519653	-0.612849
74	6	0	6.665425	-2.700123	-0.352059
75	6	0	8.590658	-3.981478	-0.964740
76	1	0	10.328410	-2.871174	-1.559095
77	1	0	9.101346	-4.923961	-1.117966
78	6	0	6.492858	-0.403651	-0.319277
79	6	0	5.342953	-2.267477	0.093443
80	7	0	5.280789	-0.897643	0.073372
81	7	0	6.871364	0.869014	-0.388502
82	6	0	6.085444	1.888034	-0.049309
83	6	0	6.548038	3.275449	-0.033356
84	6	0	5.459118	4.055734	0.407357
85	6	0	7.781468	3.837012	-0.351756
86	1	0	8.605113	3.216158	-0.685932
87	6	0	7.899848	5.218192	-0.220060
88	1	0	8.840839	5.705847	-0.458074
89	6	0	6.826684	6.009817	0.217944
90	1	0	6.982588	7.078242	0.300517
91	6	0	5.580238	5.452651	0.545674
92	6	0	4.362737	3.118997	0.641985
93	7	0	4.781668	1.843956	0.354573
94	7	0	3.161391	3.488400	1.067911
95	6	0	2.162806	2.642713	1.313497
96	6	0	0.840607	3.085161	1.737453
97	6	0	-1.819483	3.328574	2.422569
98	6	0	0.050806	1.922585	1.878178

99	6	0	0.337484	4.363731	1.967931
100	6	0	-1.001060	4.466522	2.328395
101	6	0	-1.318144	2.043020	2.188220
102	1	0	0.975793	5.233387	1.858806
103	1	0	-1.441021	5.440769	2.518526
104	1	0	-2.865491	3.469899	2.664000
105	6	0	0.948269	0.793053	1.610431
106	7	0	2.173973	1.280106	1.231224
107	7	0	0.628660	-0.481755	1.829581
108	6	0	1.450037	-1.513642	1.640126
109	7	0	2.680492	-1.465111	1.026731
110	7	0	4.399405	-3.100546	0.512548
111	6	0	3.215756	-2.718774	0.991960
112	6	0	1.181209	-2.897911	2.067650
113	6	0	1.380531	-5.664355	2.501581
114	6	0	2.295375	-3.650415	1.626416
115	6	0	0.160204	-3.548336	2.792337
116	6	0	0.286844	-4.932476	2.985865
117	6	0	2.413362	-5.023361	1.826539
118	1	0	-0.485532	-5.440967	3.553919
119	1	0	1.425557	-6.733920	2.683585
120	30	0	3.590493	0.188070	0.293650
121	6	0	-3.948457	1.198692	2.806855
122	1	0	-3.830164	1.608500	3.811677
123	1	0	-4.597461	0.322312	2.853226
124	1	0	-4.399420	1.936945	2.142709
125	6	0	4.861591	8.102768	1.153220
126	1	0	5.696653	8.191697	1.852091
127	1	0	4.038884	8.726179	1.509939
128	1	0	5.161269	8.451998	0.162204
129	1	0	3.289001	-5.553539	1.467998
130	1	0	9.255991	-0.624493	-1.233668
131	6	0	-0.606861	-1.581016	4.657547
132	1	0	-1.458338	-1.176413	5.209383
133	1	0	-0.098001	-0.774397	4.130870
134	1	0	0.066051	-2.084068	5.354751
135	6	0	7.498810	-6.768833	-0.566179
136	1	0	7.802663	-6.754866	-1.615567
137	1	0	6.956594	-7.696373	-0.370430
138	1	0	8.377848	-6.733894	0.081627
139	16	0	-8.511798	3.327884	0.152652
140	16	0	-6.126581	-5.060186	-0.933069
141	16	0	-2.698649	-6.099962	-0.738778
142	16	0	-1.308782	-2.780233	3.465590
143	16	0	-2.349570	0.578801	2.179774
144	16	0	3.238503	0.748333	-2.430399
145	16	0	6.313834	-5.435564	-0.178637
146	16	0	4.187746	6.406822	1.109636

Na-Protonated 8a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.638313	-5.323699	0.000139
2	6	0	1.218388	-5.446373	0.000110
3	6	0	-0.974676	-6.551882	0.000259
4	6	0	-0.855916	-4.159077	-0.000002
5	6	0	0.554384	-4.220226	-0.000017
6	6	0	0.433176	-6.598116	0.000242
7	1	0	-1.531385	-7.480844	0.000369
8	1	0	0.913010	-7.571624	0.000338
9	1	0	2.301146	-5.490742	0.000103
10	6	0	-1.183465	-2.761291	-0.000133
11	6	0	1.027726	-2.839409	-0.000159
12	7	0	-0.070080	-1.996891	-0.000215
13	7	0	-2.445567	-2.256835	-0.000092
14	6	0	-2.853586	-0.960930	-0.000098
15	6	0	-4.230769	-0.516878	0.000051
16	6	0	-4.155344	0.896864	0.000060
17	6	0	-5.449336	-1.199843	0.000185
18	1	0	-5.510288	-2.283737	0.000182
19	6	0	-6.607326	-0.427106	0.000320
20	1	0	-7.576939	-0.914625	0.000420
21	6	0	-6.561888	0.974301	0.000328
22	1	0	-7.494387	1.524228	0.000431
23	6	0	-5.339049	1.665163	0.000204
24	6	0	-2.744415	1.248970	-0.000073
25	7	0	-1.997582	0.079916	-0.000163
26	7	0	-2.269706	2.488146	-0.000032
27	6	0	-0.984650	2.815738	-0.000056
28	6	0	-0.514578	4.199653	0.000127
29	6	0	0.940702	6.546323	0.000452
30	6	0	0.894328	4.143079	0.000110
31	6	0	-1.217006	5.399316	0.000309
32	6	0	-0.459625	6.571753	0.000467
33	6	0	1.650175	5.331168	0.000278
34	1	0	-2.300562	5.410440	0.000324
35	1	0	-0.959389	7.535507	0.000605
36	1	0	1.478538	7.486095	0.000578
37	6	0	1.253269	2.728987	-0.000078
38	7	0	0.099293	1.976181	-0.000166
39	7	0	2.499535	2.267554	-0.000080
40	6	0	2.831897	0.980607	-0.000130
41	7	0	2.004050	-0.107249	-0.000208
42	7	0	2.309585	-2.502853	-0.000157
43	6	0	2.768939	-1.256704	-0.000174
44	6	0	4.221450	0.521983	-0.000024
45	6	0	6.581938	-0.910721	0.000161
46	6	0	4.178335	-0.887653	-0.000058
47	6	0	5.413655	1.235882	0.000107
48	6	0	6.593784	0.489925	0.000194
49	6	0	5.374064	-1.631550	0.000039
50	1	0	5.413196	2.319500	0.000137
51	1	0	7.552575	0.999086	0.000291

52	1	0	7.527002	-1.439255	0.000232
53	30	0	0.022749	0.005047	-0.001011
54	8	0	2.993380	5.228633	0.000255
55	8	0	5.283344	-2.976521	0.000002
56	8	0	-2.990107	-5.136213	0.000149
57	8	0	-5.216104	3.004063	0.000201
58	6	0	6.486110	-3.745081	0.000089
59	1	0	7.085762	-3.547541	-0.895486
60	1	0	6.168413	-4.787456	0.000036
61	1	0	7.085605	-3.547584	0.895780
62	6	0	3.773976	6.423835	0.000414
63	1	0	3.582375	7.025246	-0.895247
64	1	0	4.812906	6.095322	0.000360
65	1	0	3.582391	7.024999	0.896245
66	6	0	-6.399036	3.805296	0.000399
67	1	0	-7.002409	3.623077	-0.895675
68	1	0	-6.052254	4.838021	0.000417
69	1	0	-7.002183	3.622969	0.896604
70	6	0	-3.837340	-6.292658	0.000216
71	1	0	-3.669633	-6.897909	-0.896186
72	1	0	-4.859538	-5.915629	0.000144
73	1	0	-3.669702	-6.897754	0.896735
74	1	0	-3.167367	-2.974554	-0.000015

Na-Protonated 8b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.855170	2.720986	-0.057257
2	6	0	2.864264	4.771819	-0.106058
3	6	0	5.213193	4.071270	-0.098712
4	6	0	3.486654	2.407036	-0.038619
5	6	0	2.508298	3.425201	-0.063693
6	6	0	4.225094	5.072132	-0.122216
7	1	0	6.255584	4.364069	-0.113354
8	1	0	4.544400	6.108870	-0.154396
9	1	0	2.107782	5.547340	-0.125412
10	6	0	2.756209	1.167269	0.000664
11	6	0	1.213983	2.754658	-0.037172
12	7	0	1.420401	1.389083	0.001132
13	7	0	3.307855	-0.074146	0.026490
14	6	0	2.686195	-1.283853	0.042463
15	6	0	3.344655	-2.563101	0.051271
16	6	0	2.309660	-3.524624	0.044137
17	6	0	4.693206	-2.954881	0.062185
18	6	0	4.974326	-4.323421	0.064942
19	1	0	5.998395	-4.675249	0.073418
20	6	0	3.930812	-5.267255	0.056406
21	1	0	4.191055	-6.320874	0.058461
22	6	0	2.589640	-4.890377	0.045739

23	6	0	1.056738	-2.781217	0.032953
24	7	0	1.340467	-1.428888	0.035983
25	7	0	-0.138979	-3.354956	0.008662
26	6	0	-1.293629	-2.701175	-0.008380
27	6	0	-2.590957	-3.366462	-0.073682
28	6	0	-5.263248	-4.038791	-0.235157
29	6	0	-3.562536	-2.343598	-0.084643
30	6	0	-2.919594	-4.716258	-0.134330
31	6	0	-4.276352	-5.031958	-0.212328
32	6	0	-4.929001	-2.674005	-0.174422
33	1	0	-2.151387	-5.480355	-0.124107
34	1	0	-4.585723	-6.071345	-0.260491
35	1	0	-6.301611	-4.338332	-0.301354
36	6	0	-2.835201	-1.078653	-0.014195
37	7	0	-1.484994	-1.343655	0.020075
38	7	0	-3.412084	0.120958	0.016034
39	6	0	-2.772969	1.285483	0.041712
40	7	0	-1.407980	1.470747	0.028841
41	7	0	0.054516	3.396524	-0.053365
42	6	0	-1.138171	2.812006	-0.023042
43	6	0	-3.433698	2.595437	0.024451
44	6	0	-3.953526	5.336123	-0.247858
45	6	0	-2.392499	3.553389	-0.054103
46	6	0	-4.771793	3.036345	0.005777
47	6	0	-4.998331	4.415699	-0.151721
48	6	0	-2.622132	4.916743	-0.183853
49	1	0	-6.031101	4.746185	-0.179161
50	1	0	-4.185352	6.390700	-0.358133
51	30	0	-0.054604	0.022899	0.087741
52	8	0	-5.825333	-1.668014	-0.200056
53	8	0	5.717219	1.667990	-0.032754
54	6	0	-7.209164	-1.979062	-0.369378
55	1	0	-7.720887	-1.018255	-0.412367
56	1	0	-7.593453	-2.562318	0.474956
57	1	0	-7.380990	-2.524461	-1.303608
58	6	0	7.121211	1.944967	-0.060161
59	1	0	7.423295	2.526535	0.816780
60	1	0	7.397645	2.478448	-0.975279
61	1	0	7.617761	0.975868	-0.041685
62	1	0	-1.795441	5.614912	-0.246894
63	1	0	1.790720	-5.622374	0.039065
64	8	0	-5.876357	2.255964	0.093942
65	8	0	5.613540	-1.951765	0.070586
66	6	0	6.999177	-2.308854	0.094416
67	1	0	7.239381	-2.886719	0.992661
68	1	0	7.550324	-1.369649	0.109870
69	1	0	7.272846	-2.878213	-0.799733
70	6	0	-6.014289	1.401349	1.243110
71	1	0	-7.072025	1.134973	1.280374
72	1	0	-5.752511	1.946986	2.156608
73	1	0	-5.404723	0.504243	1.138760
74	1	0	4.328799	-0.103190	0.026612

Na-Protonated 8c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.739356	-5.221217	0.000772
2	6	0	4.818155	-3.246285	0.000436
3	6	0	4.087800	-5.581555	0.001090
4	6	0	2.453149	-3.860841	0.000251
5	6	0	3.460094	-2.872930	0.000081
6	6	0	5.108504	-4.622355	0.000927
7	1	0	4.364010	-6.631376	0.001475
8	1	0	6.137749	-4.958754	0.001198
9	6	0	1.175217	-3.149317	-0.000170
10	6	0	2.776771	-1.586595	-0.000394
11	7	0	1.413367	-1.802479	-0.000548
12	7	0	-0.001217	-3.768632	0.000005
13	6	0	-1.177237	-3.148531	-0.000020
14	6	0	-2.455616	-3.859250	0.000285
15	6	0	-3.461943	-2.870717	0.000258
16	6	0	-2.742635	-5.219450	0.000584
17	1	0	-1.950612	-5.958902	0.000611
18	6	0	-4.091301	-5.578969	0.000842
19	1	0	-4.368160	-6.628619	0.001064
20	6	0	-5.111412	-4.619142	0.000823
21	1	0	-6.140865	-4.954909	0.001031
22	6	0	-4.820231	-3.243246	0.000546
23	6	0	-2.777796	-1.584815	-0.000047
24	7	0	-1.414541	-1.801521	-0.000123
25	7	0	-3.383504	-0.403160	-0.000032
26	6	0	-2.768693	0.770393	-0.000183
27	6	0	-3.475913	2.045300	0.000134
28	6	0	-4.203757	4.729019	0.000629
29	6	0	-2.487187	3.053687	0.000016
30	6	0	-4.833593	2.359890	0.000525
31	6	0	-5.174974	3.710762	0.000757
32	6	0	-2.842900	4.412019	0.000265
33	1	0	-5.582692	1.576907	0.000632
34	1	0	-6.221225	3.999453	0.001045
35	1	0	-4.528303	5.762133	0.000824
36	6	0	-1.225885	2.359769	-0.000368
37	7	0	-1.408488	1.019401	-0.000455
38	7	0	0.000915	2.947006	-0.000366
39	6	0	1.227369	2.359036	-0.000418
40	7	0	1.409133	1.018565	-0.000682
41	7	0	3.383206	-0.405306	-0.000387
42	6	0	2.769171	0.768670	-0.000432
43	6	0	2.489112	3.052142	0.000051
44	6	0	5.177316	3.707525	0.001012
45	6	0	3.477205	2.043123	0.000046
46	6	0	2.845692	4.410245	0.000548
47	6	0	4.206741	4.726399	0.001025
48	6	0	4.835087	2.356874	0.000540

49	1	0	4.531945	5.759307	0.001418
50	1	0	6.223750	3.995551	0.001394
51	30	0	-0.000064	-0.414715	-0.003040
52	8	0	-1.815582	5.305762	0.000114
53	8	0	-5.745950	-2.263360	0.000517
54	6	0	-2.135307	6.700317	0.000201
55	1	0	-2.702095	6.972940	-0.895956
56	1	0	-1.181501	7.226201	-0.000083
57	1	0	-2.701579	6.972952	0.896682
58	6	0	-7.126755	-2.624770	0.000813
59	1	0	-7.388861	-3.199333	-0.894669
60	1	0	-7.676577	-1.683938	0.000739
61	1	0	-7.388558	-3.199016	0.896587
62	1	0	5.583702	1.573427	0.000554
63	1	0	1.946892	-5.960198	0.000909
64	8	0	1.818936	5.304642	0.000515
65	6	0	2.139558	6.698986	0.000982
66	1	0	1.186093	7.225486	0.000830
67	1	0	2.706543	6.971488	-0.895088
68	1	0	2.705992	6.971016	0.897544
69	8	0	5.744464	-2.266950	0.000277
70	6	0	7.125051	-2.629196	0.000525
71	1	0	7.386580	-3.203442	0.896380
72	1	0	7.675441	-1.688698	0.000231
73	1	0	7.386731	-3.204089	-0.894870
74	1	0	0.001212	3.968119	-0.000151

Na-Protonated 8d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.571286	2.709748	0.001712
2	6	0	-2.490811	4.670682	0.001415
3	6	0	-4.868655	4.075207	0.003105
4	6	0	-3.218317	2.334500	0.000006
5	6	0	-2.196029	3.308700	-0.000114
6	6	0	-3.836702	5.031601	0.002943
7	1	0	-5.896991	4.414561	0.004344
8	1	0	-4.110244	6.081914	0.004075
9	1	0	-1.697009	5.408315	0.001394
10	6	0	-2.542052	1.063378	-0.001575
11	6	0	-0.930878	2.583517	-0.001752
12	7	0	-1.198849	1.227366	-0.002482
13	7	0	-3.145192	-0.154790	-0.001256
14	6	0	-2.575063	-1.390114	-0.001354
15	6	0	-3.287297	-2.640495	0.000568
16	6	0	-2.294185	-3.645305	0.000856
17	6	0	-4.651372	-2.974538	0.002115
18	6	0	-4.990715	-4.329665	0.003908
19	1	0	-6.028936	-4.637386	0.005083

20	6	0	-3.988288	-5.317274	0.004222
21	1	0	-4.293299	-6.358831	0.005647
22	6	0	-2.632317	-4.997841	0.002766
23	6	0	-1.010112	-2.956572	-0.000953
24	7	0	-1.236924	-1.593207	-0.002177
25	7	0	0.160210	-3.581593	-0.000542
26	6	0	1.342374	-2.977575	-0.000964
27	6	0	2.614103	-3.696832	0.000813
28	6	0	5.265718	-4.471667	0.003987
29	6	0	3.625987	-2.714036	0.000595
30	6	0	2.893888	-5.059063	0.002668
31	6	0	4.240395	-5.425696	0.004185
32	6	0	4.982167	-3.093645	0.002258
33	1	0	2.098458	-5.794908	0.002875
34	1	0	4.511512	-6.476876	0.005562
35	1	0	6.293328	-4.812942	0.005207
36	6	0	2.950195	-1.421496	-0.001268
37	7	0	1.588611	-1.629218	-0.002062
38	7	0	3.571375	-0.245969	-0.001139
39	6	0	2.961924	0.933862	-0.001509
40	7	0	1.618491	1.194133	-0.002794
41	7	0	0.250735	3.183187	-0.001571
42	6	0	1.423543	2.559797	-0.001776
43	6	0	3.691739	2.202019	0.000496
44	6	0	4.496320	4.843386	0.004073
45	6	0	2.720091	3.224144	0.000267
46	6	0	5.056436	2.464524	0.002550
47	6	0	5.438778	3.807105	0.004263
48	6	0	3.115413	4.575785	0.002156
49	1	0	5.778441	1.656490	0.002769
50	1	0	6.492867	4.066771	0.005795
51	1	0	4.849397	5.867032	0.005446
52	30	0	0.215757	-0.201435	-0.012894
53	8	0	5.913326	-2.120167	0.001993
54	8	0	2.151423	5.518184	0.001914
55	8	0	-5.479998	1.695819	0.001799
56	6	0	2.536417	6.892530	0.003793
57	1	0	3.116381	7.145517	-0.890844
58	1	0	3.114228	7.143667	0.900340
59	1	0	1.605192	7.458470	0.003253
60	6	0	7.292424	-2.488517	0.003668
61	1	0	7.552167	-3.065121	-0.891181
62	1	0	7.550516	-3.063136	0.900268
63	1	0	7.846471	-1.550260	0.003133
64	6	0	-6.869655	2.036370	0.003672
65	1	0	-7.132672	2.606186	0.900768
66	1	0	-7.409864	1.090641	0.003507
67	1	0	-7.134726	2.607682	-0.891865
68	1	0	-1.865114	-5.763040	0.003058
69	8	0	-5.528125	-1.932614	0.001623
70	6	0	-6.927774	-2.229610	0.002932
71	1	0	-7.438002	-1.267373	0.002014
72	1	0	-7.208977	-2.790438	0.900173
73	1	0	-7.210149	-2.792736	-0.892498

74	1	0	-4.166303	-0.141747	-0.000333

Na-Protonated 9a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.576878	-0.394618	-0.078785
2	6	0	-4.634533	-3.118973	-0.137009
3	6	0	-6.455311	-1.493266	-0.108364
4	6	0	-4.197849	-0.697706	-0.078891
5	6	0	-3.749222	-2.042225	-0.106642
6	6	0	-5.994728	-2.815476	-0.137339
7	1	0	-7.524991	-1.328641	-0.110673
8	1	0	-6.723334	-3.619456	-0.162056
9	1	0	-4.297046	-4.150398	-0.163949
10	6	0	-3.008072	0.136757	-0.056916
11	6	0	-2.303037	-1.956813	-0.097565
12	7	0	-1.886483	-0.673621	-0.068581
13	7	0	-3.030591	1.463669	-0.025357
14	6	0	-1.957603	2.245528	-0.005175
15	6	0	-2.023022	3.704907	0.043238
16	6	0	-0.688631	4.167008	0.056784
17	6	0	-3.109376	4.569061	0.074871
18	1	0	-4.125909	4.193277	0.064084
19	6	0	-2.822570	5.935596	0.120630
20	1	0	-3.634755	6.655452	0.146191
21	6	0	-1.507235	6.411462	0.134793
22	1	0	-1.353687	7.482397	0.170943
23	6	0	-0.396265	5.544376	0.103720
24	6	0	0.152989	2.977129	0.016052
25	7	0	-0.645241	1.855817	-0.019802
26	7	0	1.479935	3.010003	0.019905
27	6	0	2.266784	1.935550	-0.005316
28	6	0	3.726799	2.012666	0.006618
29	6	0	6.439960	1.522996	0.014122
30	6	0	4.202170	0.682637	-0.022290
31	6	0	4.580951	3.107069	0.039951
32	6	0	5.950563	2.833993	0.042662
33	6	0	5.583941	0.405189	-0.018712
34	1	0	4.194018	4.119213	0.062408
35	1	0	6.662836	3.652835	0.067417
36	1	0	7.513043	1.380099	0.017852
37	6	0	3.020227	-0.166447	-0.050075
38	7	0	1.888695	0.624199	-0.038819
39	7	0	3.053650	-1.491497	-0.074446
40	6	0	1.988823	-2.285251	-0.091401
41	7	0	0.660737	-1.911194	-0.094644
42	7	0	-1.454001	-3.012735	-0.109510
43	6	0	-0.094666	-3.031574	-0.103992

44	6	0	2.062084	-3.738332	-0.100281
45	6	0	1.562999	-6.467080	-0.114231
46	6	0	0.729168	-4.221427	-0.105952
47	6	0	3.148232	-4.612633	-0.090476
48	6	0	2.881951	-5.980021	-0.096434
49	6	0	0.466175	-5.602198	-0.107121
50	1	0	4.162050	-4.227953	-0.082403
51	1	0	3.703093	-6.689457	-0.098602
52	1	0	1.391084	-7.538380	-0.142220
53	30	0	0.012967	-0.006889	-0.118164
54	6	0	-1.384083	-6.972039	1.516668
55	1	0	-0.667979	-7.784667	1.642498
56	1	0	-2.396739	-7.376803	1.570223
57	1	0	-1.245508	-6.220012	2.294263
58	6	0	7.969295	-1.090647	-0.041429
59	1	0	8.331491	-0.561044	-0.924928
60	1	0	8.352491	-2.112704	-0.064419
61	1	0	8.322651	-0.604667	0.870279
62	6	0	1.118740	7.914757	0.179551
63	1	0	0.611970	8.306185	-0.704883
64	1	0	2.144632	8.288172	0.188778
65	1	0	0.616932	8.248275	1.090194
66	6	0	-7.930304	1.143506	-0.061785
67	1	0	-8.290979	0.663137	-0.973622
68	1	0	-8.292498	2.173251	-0.042610
69	1	0	-8.305581	0.624482	0.822576
70	16	0	6.152817	-1.271142	-0.054989
71	16	0	1.284430	6.097596	0.120160
72	16	0	-6.110700	1.290571	-0.044319
73	16	0	-1.217019	-6.232404	-0.158205
74	1	0	-1.866463	-3.953123	-0.116881

Na-Protonated 9b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.762658	2.977157	0.238395
2	6	0	-2.651400	4.895820	0.227396
3	6	0	-5.018351	4.348250	0.327350
4	6	0	-3.422547	2.565492	0.120121
5	6	0	-2.386506	3.531404	0.122565
6	6	0	-3.980923	5.295179	0.327035
7	1	0	-6.048336	4.683889	0.393172
8	1	0	-4.226953	6.349445	0.400850
9	1	0	-1.837267	5.611910	0.228413
10	6	0	-2.737923	1.286167	0.002384
11	6	0	-1.130406	2.812748	0.025703
12	7	0	-1.394535	1.460903	-0.040588
13	7	0	-3.335715	0.062168	-0.070456
14	6	0	-2.771193	-1.176829	-0.126160

15	6	0	-3.454894	-2.460868	-0.221171
16	6	0	-2.411679	-3.420579	-0.179682
17	6	0	-4.793708	-2.899483	-0.359302
18	6	0	-5.012492	-4.283031	-0.432906
19	1	0	-6.023499	-4.658450	-0.530814
20	6	0	-3.963036	-5.208935	-0.381571
21	1	0	-4.194889	-6.267318	-0.443175
22	6	0	-2.642074	-4.789736	-0.255346
23	6	0	-1.159221	-2.695386	-0.080741
24	7	0	-1.423064	-1.346230	-0.060009
25	7	0	0.017786	-3.303603	-0.005245
26	6	0	1.190406	-2.689759	0.052434
27	6	0	2.452712	-3.394738	0.234594
28	6	0	5.060899	-4.155992	0.655531
29	6	0	3.464137	-2.409917	0.273815
30	6	0	2.713693	-4.749938	0.384730
31	6	0	4.045786	-5.114420	0.588086
32	6	0	4.806456	-2.776498	0.511454
33	1	0	1.914561	-5.481113	0.349091
34	1	0	4.308024	-6.161035	0.707241
35	1	0	6.072796	-4.498109	0.830827
36	6	0	2.787376	-1.127088	0.072676
37	7	0	1.430701	-1.344628	-0.030362
38	7	0	3.414999	0.043923	-0.022060
39	6	0	2.814259	1.229655	-0.109723
40	7	0	1.456702	1.449610	-0.052052
41	7	0	0.051091	3.415246	0.007397
42	6	0	1.222598	2.798748	-0.048975
43	6	0	3.509860	2.526188	-0.196551
44	6	0	4.089067	5.266551	-0.095638
45	6	0	2.492190	3.506417	-0.107801
46	6	0	4.853830	2.935972	-0.310042
47	6	0	5.107595	4.318548	-0.233092
48	6	0	2.753089	4.870276	-0.055054
49	1	0	6.136666	4.652303	-0.315298
50	1	0	4.347348	6.319723	-0.050817
51	30	0	0.036541	0.055088	-0.120772
52	6	0	7.554514	-2.495793	1.045069
53	1	0	8.338875	-1.745885	1.165269
54	1	0	7.835677	-3.170253	0.233533
55	1	0	7.448816	-3.045277	1.982749
56	6	0	-6.602334	1.814384	2.008052
57	1	0	-5.767050	1.538823	2.653178
58	1	0	-7.398741	1.074101	2.106790
59	1	0	-6.987342	2.796848	2.284034
60	1	0	1.941645	5.585118	0.021998
61	1	0	-1.814085	-5.488096	-0.221887
62	6	0	-7.537463	-2.665560	-1.058286
63	1	0	-7.290481	-3.162907	-1.997532
64	1	0	-8.314067	-1.920458	-1.239697
65	1	0	-7.899286	-3.382249	-0.319445
66	6	0	5.846693	0.941003	-2.037937
67	1	0	5.557193	1.618713	-2.842956
68	1	0	5.065736	0.210938	-1.831098

69	1	0	6.762198	0.418341	-2.321991
70	16	0	-6.104783	1.792726	0.238205
71	16	0	-6.109702	-1.718395	-0.430736
72	16	0	6.053458	-1.535047	0.650100
73	16	0	6.276898	1.889176	-0.532488
74	1	0	-4.361557	0.118827	-0.071419

Na-Protonated 9c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.772536	-4.728698	-0.073338
2	6	0	-5.415188	-2.361436	-0.133628
3	6	0	-5.166443	-4.806008	-0.113212
4	6	0	-3.217801	-3.455911	-0.064640
5	6	0	-4.008489	-2.286643	-0.093129
6	6	0	-5.965967	-3.657855	-0.142716
7	1	0	-5.652040	-5.776827	-0.122091
8	1	0	-7.040325	-3.787003	-0.173433
9	6	0	-1.822942	-3.017027	-0.028256
10	6	0	-3.073392	-1.170731	-0.071136
11	7	0	-1.782042	-1.651276	-0.033765
12	7	0	-0.795511	-3.860783	0.008717
13	6	0	0.475759	-3.476544	0.033333
14	6	0	1.595065	-4.417240	0.091985
15	6	0	2.774779	-3.642236	0.102693
16	6	0	1.616838	-5.804489	0.134510
17	1	0	0.699026	-6.380773	0.125400
18	6	0	2.873809	-6.411497	0.189604
19	1	0	2.947979	-7.493943	0.224240
20	6	0	4.053647	-5.659481	0.202266
21	1	0	4.995368	-6.191650	0.246820
22	6	0	4.044314	-4.251233	0.159767
23	6	0	2.341478	-2.252978	0.048745
24	7	0	0.965644	-2.199502	0.010478
25	7	0	3.166217	-1.217628	0.032437
26	6	0	2.803108	0.060120	-0.002801
27	6	0	3.764371	1.143722	-0.068291
28	6	0	5.128771	3.526597	-0.269559
29	6	0	3.032487	2.358314	-0.100071
30	6	0	5.153055	1.099920	-0.138944
31	6	0	5.827878	2.313011	-0.243796
32	6	0	3.729865	3.582607	-0.201613
33	1	0	5.672014	0.148511	-0.119466
34	1	0	6.911510	2.329745	-0.300373

35	1	0	5.693357	4.449316	-0.336513
36	6	0	1.634769	1.945283	-0.047938
37	7	0	1.533586	0.590085	0.006628
38	7	0	0.533433	2.749379	-0.043299
39	6	0	-0.789573	2.415486	-0.026901
40	7	0	-1.226812	1.132179	-0.065000
41	7	0	-3.434421	0.102947	-0.075007
42	6	0	-2.605229	1.140412	-0.056138
43	6	0	-1.913627	3.341624	0.022403
44	6	0	-4.491831	4.421432	0.109794
45	6	0	-3.064087	2.514707	-0.008522
46	6	0	-2.063236	4.737866	0.111416
47	6	0	-3.362165	5.254450	0.141307
48	6	0	-4.354824	3.038281	0.036442
49	1	0	-3.493695	6.330910	0.184204
50	1	0	-5.480026	4.868896	0.137665
51	30	0	-0.129139	-0.549554	-0.049980
52	6	0	3.882037	6.218170	-1.231671
53	1	0	4.775268	6.543149	-0.696532
54	1	0	3.260534	7.090119	-1.443672
55	1	0	4.147719	5.726234	-2.168249
56	6	0	6.846979	-4.492517	0.270611
57	1	0	6.788610	-5.084207	1.186377
58	1	0	7.768153	-3.906857	0.290197
59	1	0	6.863379	-5.141646	-0.607216
60	1	0	-5.212610	2.375223	0.014363
61	1	0	-3.147187	-5.613586	-0.050591
62	6	0	-0.693628	6.425878	1.884423
63	1	0	-1.605196	6.995646	2.069173
64	1	0	0.170978	7.082211	2.001647
65	1	0	-0.617031	5.593884	2.585626
66	6	0	-8.096541	-1.506835	-0.229386
67	1	0	-8.283990	-2.092281	-1.131808
68	1	0	-8.721653	-0.612155	-0.256394
69	1	0	-8.348503	-2.083297	0.663053
70	16	0	5.508012	-3.255734	0.177085
71	16	0	2.843724	5.118886	-0.202210
72	16	0	-0.646480	5.829329	0.146507
73	16	0	-6.383293	-0.879673	-0.171831
74	1	0	0.701425	3.763123	-0.065857

Na-Protonated 9d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.364730	2.930168	0.052257
2	6	0	2.137555	4.712280	-0.035404
3	6	0	4.534346	4.317858	0.054959
4	6	0	3.051938	2.428727	-0.017476
5	6	0	1.959244	3.330230	-0.054693

6	6	0	3.440829	5.197852	0.017060
7	1	0	5.542322	4.719207	0.081821
8	1	0	3.622242	6.267700	0.023762
9	1	0	1.277641	5.372460	-0.061679
10	6	0	2.442242	1.105443	-0.042539
11	6	0	0.746818	2.536242	-0.081841
12	7	0	1.089795	1.201166	-0.074276
13	7	0	3.102941	-0.088686	-0.043220
14	6	0	2.607615	-1.359370	-0.033406
15	6	0	3.364731	-2.605901	-0.057789
16	6	0	2.376927	-3.622972	-0.022481
17	6	0	4.728404	-2.970436	-0.132945
18	6	0	5.031069	-4.338633	-0.171698
19	1	0	6.067329	-4.651990	-0.218573
20	6	0	4.035431	-5.323425	-0.141823
21	1	0	4.328408	-6.367835	-0.174714
22	6	0	2.689557	-4.977733	-0.063401
23	6	0	1.082654	-2.970166	0.018271
24	7	0	1.270585	-1.607024	0.010320
25	7	0	-0.060074	-3.647723	0.049951
26	6	0	-1.267254	-3.102997	0.056142
27	6	0	-2.505526	-3.878186	0.101618
28	6	0	-5.116558	-4.758946	0.173615
29	6	0	-3.563516	-2.943757	0.088841
30	6	0	-2.724679	-5.248454	0.150105
31	6	0	-4.055615	-5.670626	0.185757
32	6	0	-4.907473	-3.365912	0.125079
33	1	0	-1.898659	-5.950068	0.159646
34	1	0	-4.283231	-6.731363	0.224013
35	1	0	-6.124909	-5.151333	0.202855
36	6	0	-2.939925	-1.626771	0.035896
37	7	0	-1.571213	-1.768481	0.018701
38	7	0	-3.624149	-0.489470	0.010230
39	6	0	-3.070916	0.719536	-0.028952
40	7	0	-1.741087	1.029376	-0.042924
41	7	0	-0.467542	3.074341	-0.097472
42	6	0	-1.607190	2.400887	-0.082155
43	6	0	-3.852952	1.954601	-0.059817
44	6	0	-4.754236	4.558072	-0.125426
45	6	0	-2.925518	3.018812	-0.093957
46	6	0	-5.225715	2.162745	-0.057537
47	6	0	-5.658291	3.490370	-0.091410
48	6	0	-3.359775	4.358911	-0.127678
49	1	0	-5.918467	1.329548	-0.030625
50	1	0	-6.721242	3.710726	-0.091509
51	1	0	-5.154642	5.563456	-0.150442
52	30	0	-0.255889	-0.289111	-0.053093
53	6	0	-3.225706	7.170486	-0.207254
54	1	0	-3.839058	7.258634	0.691779
55	1	0	-3.848374	7.207052	-1.103461
56	1	0	-2.522698	8.005317	-0.234978
57	6	0	-7.717182	-3.214902	0.168762
58	1	0	-7.768909	-3.802046	1.087959
59	1	0	-7.798879	-3.861970	-0.706979

60	1	0	-8.547758	-2.506374	0.158943
61	6	0	6.335256	2.048015	1.840346
62	1	0	5.547434	1.762867	2.538793
63	1	0	6.648009	3.077313	2.020408
64	1	0	7.192556	1.383929	1.967266
65	1	0	1.902059	-5.721978	-0.040839
66	6	0	7.373064	-2.497054	-1.041204
67	1	0	8.070925	-1.684609	-1.251817
68	1	0	7.026866	-2.929138	-1.981126
69	1	0	7.877910	-3.246874	-0.430580
70	16	0	-2.177625	5.676463	-0.169901
71	16	0	5.781331	1.838327	0.100230
72	16	0	5.984366	-1.720438	-0.140898
73	16	0	-6.217251	-2.175932	0.108803
74	1	0	4.125601	0.011504	-0.064938

Na-Protonated p-8a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.497276	-4.357702	-0.000005
2	6	0	-5.177463	-2.058203	-0.000001
3	6	0	-4.900854	-4.483368	-0.000005
4	6	0	-2.968269	-3.080242	-0.000002
5	6	0	-3.790486	-1.932259	0.000000
6	6	0	-5.729000	-3.338430	-0.000003
7	1	0	-6.806061	-3.448875	-0.000004
8	1	0	-5.815790	-1.181151	0.000001
9	6	0	-1.582963	-2.596167	-0.000001
10	6	0	-2.900477	-0.785384	0.000002
11	7	0	-1.595096	-1.222803	0.000001
12	7	0	-0.529261	-3.399637	-0.000003
13	6	0	0.738422	-2.983809	-0.000002
14	6	0	1.879707	-3.882712	-0.000003
15	6	0	3.032054	-3.074934	-0.000003
16	6	0	1.989687	-5.277131	-0.000005
17	1	0	1.105587	-5.905225	-0.000005
18	6	0	3.260089	-5.829859	-0.000005
19	1	0	3.405394	-6.904545	-0.000006
20	6	0	4.419324	-5.014171	-0.000005
21	6	0	4.315416	-3.614194	-0.000003
22	6	0	2.561344	-1.689048	-0.000001
23	7	0	1.184391	-1.685256	-0.000002
24	7	0	3.364081	-0.635827	-0.000001
25	6	0	2.959252	0.631270	0.000000

26	6	0	3.853922	1.770077	-0.000004
27	6	0	5.014667	4.305297	-0.000013
28	6	0	3.054090	2.935005	-0.000002
29	6	0	5.250941	1.873526	-0.000011
30	6	0	5.817305	3.134289	-0.000015
31	6	0	3.617921	4.218518	-0.000007
32	1	0	5.867696	0.981644	-0.000012
33	1	0	6.893308	3.268814	-0.000020
34	6	0	1.694147	2.442765	0.000004
35	7	0	1.653097	1.093837	0.000006
36	7	0	0.569285	3.215026	0.000006
37	6	0	-0.740937	2.853163	0.000007
38	7	0	-1.140598	1.560214	0.000004
39	7	0	-3.316637	0.478764	0.000004
40	6	0	-2.521836	1.537893	0.000005
41	6	0	-1.866302	3.755840	0.000009
42	6	0	-4.440044	4.832896	0.000012
43	6	0	-3.008603	2.915942	0.000008
44	6	0	-2.018876	5.144782	0.000011
45	6	0	-3.304440	5.677185	0.000013
46	6	0	-4.292171	3.434705	0.000010
47	1	0	-1.168384	5.821697	0.000012
48	1	0	-3.427945	6.752576	0.000015
49	30	0	0.026186	-0.085417	0.000006
50	8	0	5.711387	5.463798	-0.000018
51	8	0	-5.712952	5.279702	0.000013
52	8	0	-5.362931	-5.752488	-0.000008
53	8	0	5.588076	-5.692406	-0.000005
54	6	0	-5.966101	6.685008	0.000022
55	1	0	-5.555577	7.162983	0.896540
56	1	0	-7.050671	6.787305	0.000026
57	1	0	-5.555584	7.162992	-0.896495
58	6	0	5.002941	6.699312	-0.000016
59	1	0	4.379962	6.801199	-0.896824
60	1	0	5.764378	7.478566	-0.000020
61	1	0	4.379970	6.801200	0.896798
62	6	0	6.811286	-4.959698	-0.000002
63	1	0	6.900057	-4.334061	0.895651
64	1	0	6.900061	-4.334060	-0.895654
65	1	0	7.603918	-5.707359	-0.000001
66	6	0	-6.770864	-5.985331	-0.000008
67	1	0	-7.243496	-5.567307	0.895957
68	1	0	-6.889406	-7.068427	-0.000009
69	1	0	-7.243497	-5.567304	-0.895971
70	1	0	5.182855	-2.967020	-0.000003
71	1	0	-2.875085	-5.244965	-0.000006
72	1	0	-5.168649	2.797499	0.000009
73	1	0	3.007458	5.114456	-0.000006
74	1	0	0.737129	4.213813	0.000006

Nb-Protonated p-8b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.869875	-2.739634	0.000074
2	6	0	-2.911798	-4.804377	0.000042
3	6	0	-5.247501	-4.093954	0.000165
4	6	0	-3.517748	-2.441308	-0.000042
5	6	0	-2.530654	-3.459783	-0.000060
6	6	0	-4.267830	-5.115422	0.000150
7	6	0	-2.808547	-1.164798	-0.000146
8	6	0	-1.271526	-2.757245	-0.000180
9	7	0	-1.449548	-1.416345	-0.000222
10	7	0	-3.413298	0.014135	-0.000103
11	6	0	-2.787129	1.186298	-0.000104
12	6	0	-3.478729	2.476418	0.000063
13	6	0	-2.469401	3.463811	0.000081
14	6	0	-4.823278	2.804883	0.000210
15	1	0	-5.606003	2.055422	0.000206
16	6	0	-5.161062	4.171843	0.000366
17	6	0	-4.155386	5.164361	0.000380
18	6	0	-2.805557	4.814598	0.000245
19	6	0	-1.195820	2.761320	-0.000077
20	7	0	-1.433745	1.402704	-0.000180
21	7	0	-0.015823	3.370848	-0.000052
22	6	0	1.161227	2.749614	-0.000090
23	6	0	2.438169	3.444705	0.000049
24	6	0	5.131023	4.136469	0.000287
25	6	0	3.439246	2.455953	0.000022
26	6	0	2.779512	4.800954	0.000203
27	6	0	4.124335	5.134034	0.000314
28	6	0	4.795237	2.774054	0.000146
29	1	0	2.012614	5.567736	0.000230
30	1	0	4.447110	6.169382	0.000428
31	6	0	2.743357	1.169071	-0.000131
32	7	0	1.387335	1.392772	-0.000190
33	7	0	3.360945	-0.005947	-0.000135
34	6	0	2.747068	-1.183144	-0.000173
35	7	0	1.384494	-1.422582	-0.000227
36	7	0	-0.038769	-3.332960	-0.000179
37	6	0	1.199719	-2.761609	-0.000195
38	6	0	3.443913	-2.463140	-0.000091
39	6	0	4.169214	-5.136780	0.000065
40	6	0	2.451956	-3.471042	-0.000103
41	6	0	4.804172	-2.768133	0.000003
42	6	0	5.162572	-4.122054	0.000077
43	6	0	2.822626	-4.825884	-0.000019
44	1	0	4.506133	-6.167314	0.000125
45	30	0	-0.025365	0.010911	-0.000960
46	1	0	2.090012	-5.628692	-0.000023
47	1	0	-5.628571	-1.965901	0.000094
48	1	0	-2.035777	5.578803	0.000262
49	1	0	-2.185759	-5.613268	0.000037
50	1	0	5.543050	1.991682	0.000127

51	1	0	5.537184	-1.971937	0.000016
52	8	0	6.397138	4.611229	0.000405
53	8	0	6.431849	-4.579842	0.000163
54	6	0	7.479957	3.684913	0.000413
55	1	0	7.463055	3.052961	-0.895297
56	1	0	8.386828	4.289052	0.000530
57	1	0	7.462919	3.052818	0.896020
58	6	0	7.505002	-3.638824	0.000187
59	1	0	8.418241	-4.232802	0.000257
60	1	0	7.478557	-3.008380	-0.895835
61	1	0	7.478461	-3.008317	0.896161
62	1	0	-4.568239	-6.155384	0.000225
63	8	0	-6.576743	-4.322876	0.000271
64	6	0	-7.060539	-5.666515	0.000339
65	1	0	-8.146974	-5.586578	0.000386
66	1	0	-6.735359	-6.206205	-0.896122
67	1	0	-6.735278	-6.206143	0.896808
68	1	0	-4.428194	6.212181	0.000495
69	8	0	-6.486725	4.435850	0.000486
70	6	0	-6.928793	5.792501	0.000793
71	1	0	-6.586576	6.322978	0.896595
72	1	0	-6.586869	6.323289	-0.894937
73	1	0	-8.017468	5.747041	0.000961
74	1	0	-0.040217	-4.345917	-0.000136

Nc-Protonated p-8c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.865704	-5.088304	0.000481
2	6	0	-4.839713	-3.022992	0.000356
3	6	0	-4.213812	-5.394668	0.000730
4	6	0	-2.491276	-3.735033	0.000138
5	6	0	-3.479464	-2.724673	0.000080
6	6	0	-5.203537	-4.376844	0.000671
7	1	0	-4.554044	-6.424086	0.000984
8	6	0	-1.235302	-3.028819	-0.000178
9	6	0	-2.777469	-1.444645	-0.000255
10	7	0	-1.413753	-1.690991	-0.000393
11	7	0	0.000040	-3.605431	-0.000112
12	6	0	1.235370	-3.028792	-0.000173
13	6	0	2.491361	-3.734979	0.000117
14	6	0	3.479528	-2.724597	0.000071
15	6	0	2.865819	-5.088242	0.000428
16	1	0	2.136021	-5.893515	0.000479

17	6	0	4.213935	-5.394575	0.000663
18	1	0	4.554189	-6.423986	0.000894
19	6	0	5.203638	-4.376730	0.000618
20	6	0	4.839784	-3.022886	0.000331
21	6	0	2.777503	-1.444583	-0.000237
22	7	0	1.413791	-1.690960	-0.000360
23	7	0	3.385552	-0.270071	-0.000237
24	6	0	2.768260	0.910269	-0.000331
25	6	0	3.457001	2.187244	-0.000050
26	6	0	4.128667	4.886502	0.000456
27	6	0	2.461036	3.182258	-0.000084
28	6	0	4.811292	2.540115	0.000259
29	6	0	5.133967	3.886828	0.000495
30	6	0	2.768771	4.540070	0.000180
31	1	0	5.585147	1.780308	0.000303
32	1	0	6.166788	4.217614	0.000720
33	6	0	1.176397	2.479932	-0.000390
34	7	0	1.408375	1.127663	-0.000524
35	7	0	-0.000036	3.099806	-0.000369
36	6	0	-1.176454	2.479905	-0.000402
37	7	0	-1.408400	1.127631	-0.000526
38	7	0	-3.385545	-0.270148	-0.000262
39	6	0	-2.768280	0.910205	-0.000355
40	6	0	-2.461109	3.182200	-0.000120
41	6	0	-5.134055	3.886707	0.000415
42	6	0	-3.457050	2.187164	-0.000094
43	6	0	-2.768875	4.540005	0.000130
44	6	0	-4.128779	4.886405	0.000385
45	6	0	-4.811348	2.540003	0.000193
46	1	0	-6.166884	4.217469	0.000622
47	30	0	0.000003	-0.260240	-0.002212
48	1	0	-5.585185	1.780178	0.000229
49	1	0	-2.135887	-5.893561	0.000543
50	1	0	5.569581	-2.223686	0.000302
51	1	0	-5.569527	-2.223809	0.000320
52	8	0	6.473707	-4.828110	0.000868
53	8	0	-6.473597	-4.828252	0.000941
54	6	0	-7.544406	-3.882897	0.000918
55	1	0	-7.515600	-3.253164	-0.895277
56	1	0	-8.459142	-4.474378	0.001150
57	1	0	-7.515353	-3.252842	0.896879
58	6	0	7.544495	-3.882730	0.000875
59	1	0	8.459244	-4.474191	0.001104
60	1	0	7.515683	-3.252980	-0.895309
61	1	0	7.515419	-3.252694	0.896848
62	1	0	1.979857	5.280979	0.000163
63	1	0	-1.979978	5.280932	0.000118
64	8	0	4.593762	6.155395	0.000708
65	8	0	-4.593904	6.155287	0.000619
66	6	0	3.659242	7.232093	0.000682
67	1	0	3.027540	7.210041	0.896271
68	1	0	4.257161	8.143004	0.000880
69	1	0	3.027823	7.210244	-0.895113
70	6	0	-3.659409	7.232007	0.000618

71	1	0	-4.257350	8.142904	0.000816
72	1	0	-3.027721	7.209962	0.896218
73	1	0	-3.027975	7.210182	-0.895166
74	1	0	0.000051	-4.618323	0.000069

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.340968	-2.156463	0.000525
2	6	0	3.628642	-4.427565	0.000405
3	6	0	5.869547	-3.458414	0.001087
4	6	0	3.957651	-2.015150	-0.000117
5	6	0	3.096239	-3.139332	-0.000186
6	6	0	5.011913	-4.583420	0.001020
7	6	0	3.065902	-0.870873	-0.000705
8	6	0	1.733808	-2.638243	-0.000786
9	7	0	1.773931	-1.250246	-0.001080
10	7	0	3.456231	0.432773	-0.000585
11	6	0	2.703996	1.570903	-0.000650
12	6	0	3.214822	2.917055	0.000021
13	6	0	2.067539	3.743155	-0.000007
14	6	0	4.496940	3.490877	0.000731
15	1	0	5.402738	2.889156	0.000789
16	6	0	4.597406	4.869648	0.001367
17	1	0	5.565009	5.359934	0.001916
18	6	0	3.442584	5.696357	0.001348
19	6	0	2.159274	5.133184	0.000668
20	6	0	0.907564	2.858813	-0.000681
21	7	0	1.352879	1.548057	-0.001050
22	7	0	-0.346158	3.287230	-0.000631
23	6	0	-1.420857	2.504466	-0.000794
24	6	0	-2.787024	2.995107	-0.000249
25	6	0	-5.558105	3.254749	0.000874
26	6	0	-3.622014	1.861991	-0.000271
27	6	0	-3.339384	4.280962	0.000365
28	6	0	-4.719759	4.398112	0.000899
29	6	0	-5.010513	1.962488	0.000301
30	1	0	-2.704428	5.160927	0.000413
31	1	0	-5.200835	5.370675	0.001364
32	6	0	-2.736107	0.696274	-0.000853
33	7	0	-1.435139	1.125192	-0.001142
34	7	0	-3.176101	-0.559974	-0.000779
35	6	0	-2.387767	-1.629841	-0.000873
36	7	0	-1.016069	-1.658697	-0.001252
37	7	0	0.656879	-3.409556	-0.000739
38	6	0	-0.598977	-2.972015	-0.000861
39	6	0	-2.891984	-3.005219	-0.000210
40	6	0	-3.194004	-5.752524	0.001146
41	6	0	-1.761000	-3.842450	-0.000212

42	6	0	-4.189046	-3.510186	0.000476
43	6	0	-4.331641	-4.906722	0.001146
44	6	0	-1.909209	-5.233764	0.000495
45	1	0	-3.367094	-6.823650	0.001689
46	30	0	0.147103	-0.060490	-0.003988
47	1	0	-1.042770	-5.887031	0.000531
48	1	0	6.036124	-1.321708	0.000612
49	1	0	1.259126	5.734935	0.000660
50	1	0	2.973958	-5.292985	0.000385
51	8	0	3.699459	7.019860	0.002030
52	6	0	2.605587	7.937440	0.002189
53	1	0	3.055961	8.930030	0.002863
54	1	0	1.987699	7.814400	-0.895027
55	1	0	1.987147	7.813430	0.898892
56	1	0	-5.624224	1.070433	0.000300
57	1	0	-5.038752	-2.839074	0.000486
58	8	0	-6.882318	3.524691	0.001447
59	8	0	-5.518000	-5.553712	0.001839
60	6	0	-7.807656	2.440720	0.001459
61	1	0	-7.690718	1.819701	0.897891
62	1	0	-8.797194	2.898466	0.001942
63	1	0	-7.691352	1.820223	-0.895417
64	6	0	-6.721099	-4.789421	0.001951
65	1	0	-7.532333	-5.517841	0.002591
66	1	0	-6.791665	-4.161471	0.898392
67	1	0	-6.792350	-4.162289	-0.895007
68	1	0	5.430608	-5.582423	0.001465
69	8	0	7.218422	-3.530143	0.001679
70	6	0	7.851846	-4.810304	0.002270
71	1	0	8.922492	-4.605386	0.002673
72	1	0	7.588464	-5.382492	0.899438
73	1	0	7.589225	-5.382943	-0.894834
74	1	0	4.459927	0.580296	-0.000229