Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

Dicyanovinyl Terthiophene as Reaction Based Colorimetric and Ratiometric Fluorescence Probe for Cyanide Anion

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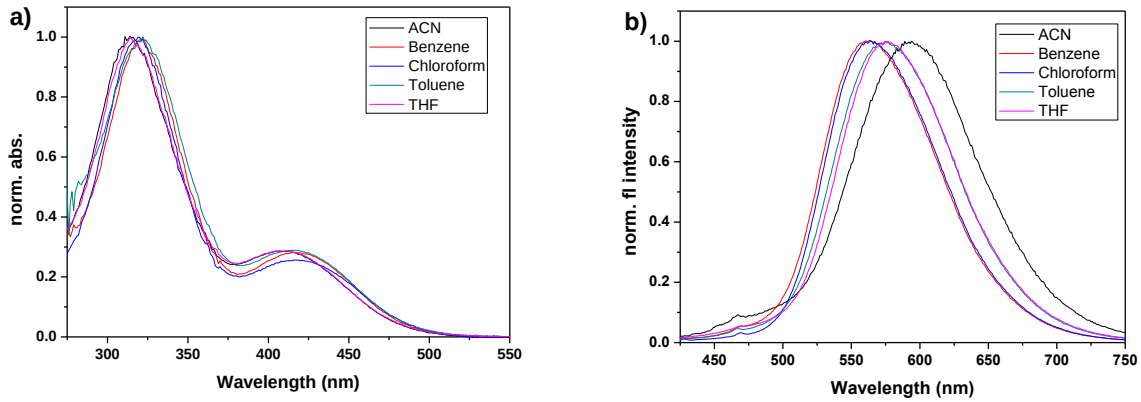

Fig. S1 Normalised absorption (a) and emission (b) spectra of compound **3** in acetonitrile, benzene, chloroform, toluene and THF.

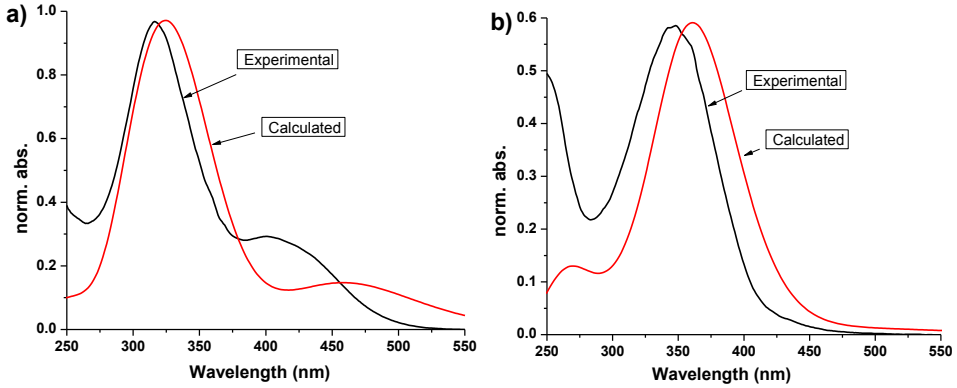

Fig. S2 Experimental and simulated UV-vis absorption spectra for **3** (a) and **3-CN**$^-$(b).

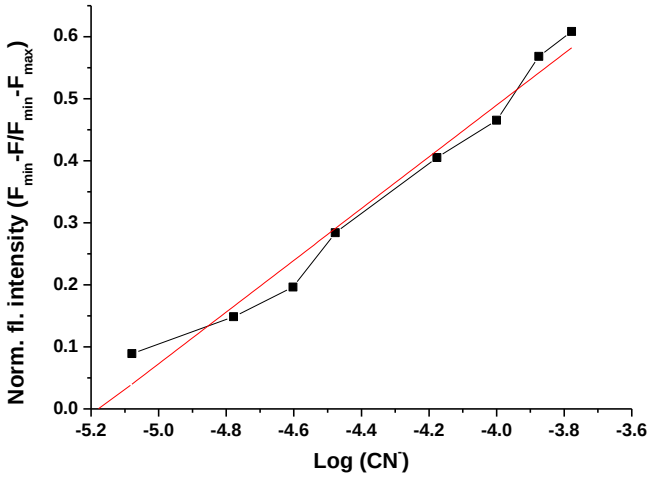

Fig. S3 Fluorescence intensity of the probe at each concentration of free cyanide anion normalized between the minimum fluorescence intensity, found at zero cyanide concentration, and the maximum fluorescence intensity, found at 660 μM free cyanide anion.

Table S1 TDDFT (B3LYP/6-31G(d)) calculated low-lying transition for **3** and **3-CN**$^{-}$

Compound	**Excitation**	**λ_{cal} (nm)**	***f***
3	H to L (96%)	461	0.1450
	H to L+1 (84%)	342	0.3795
	H-1 to L (73%)	337	0.2279
	H-3 to L (44%) H-2 to L (41%)	315	0.1542
	H-3 to L (52%)	307	0.4061
3-CN	H-1 to L (87%)	363	0.5492

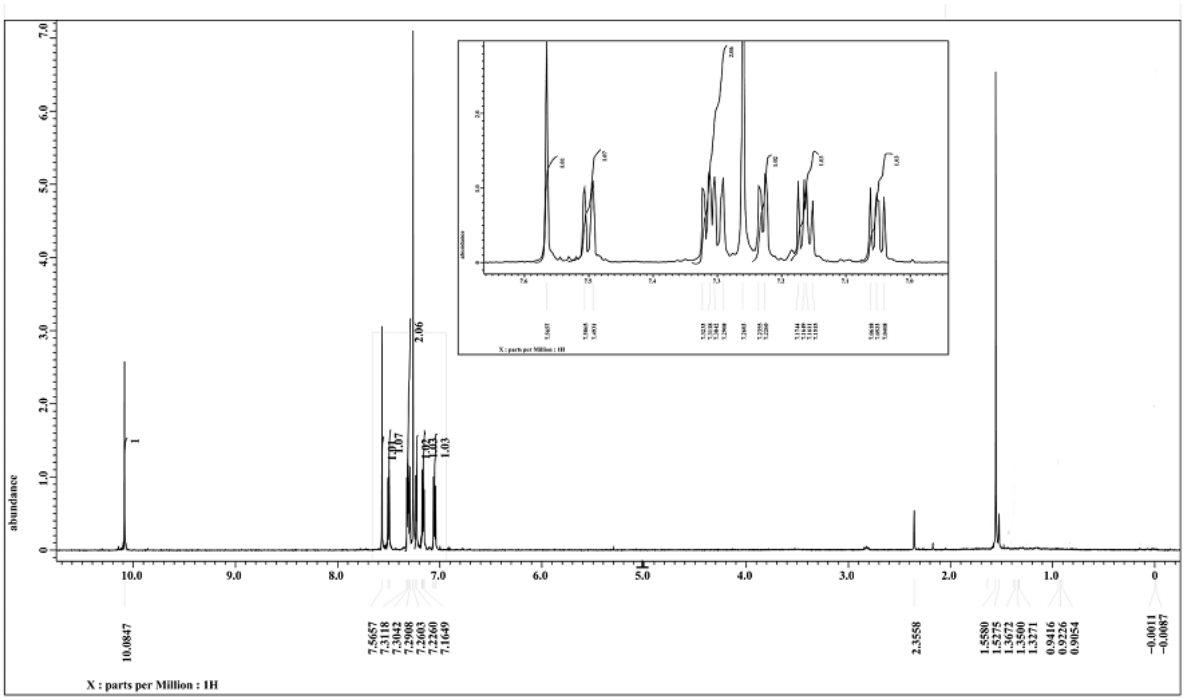

Fig. S4 ^{1}H NMR of compound **2**

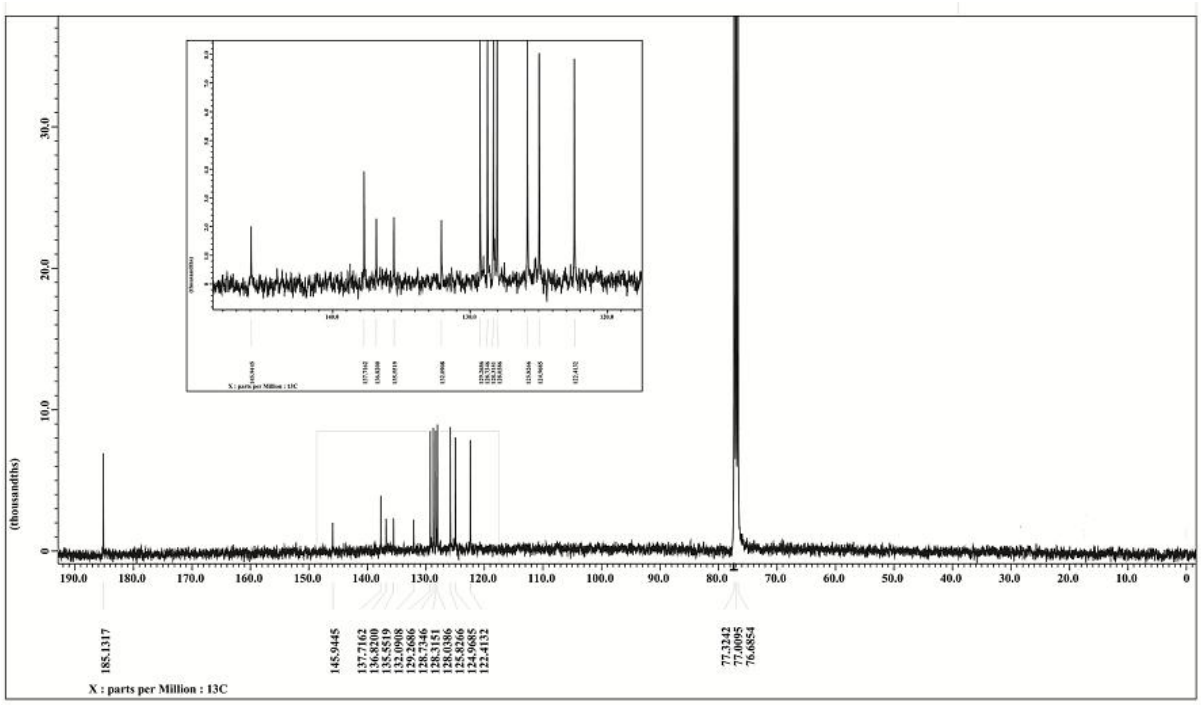

Fig. S5 ^{13}C NMR of compound **2**

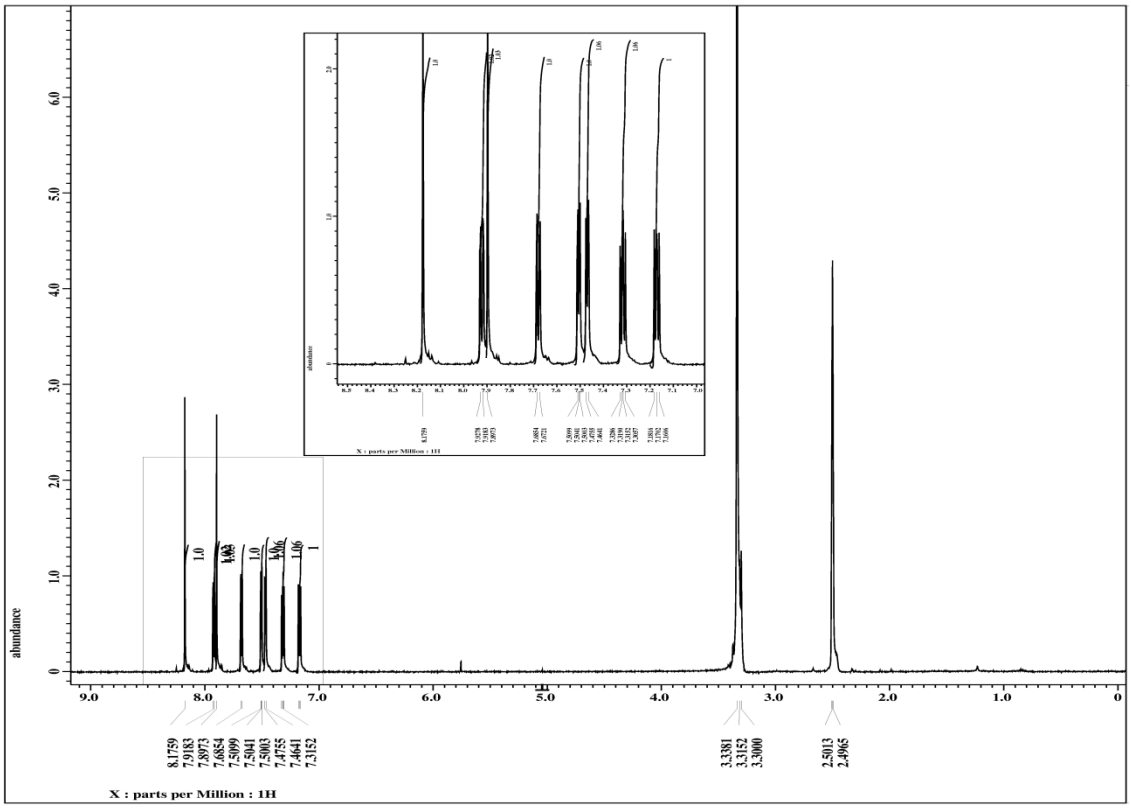

Fig. S6 ^{1}H NMR of compound **3**

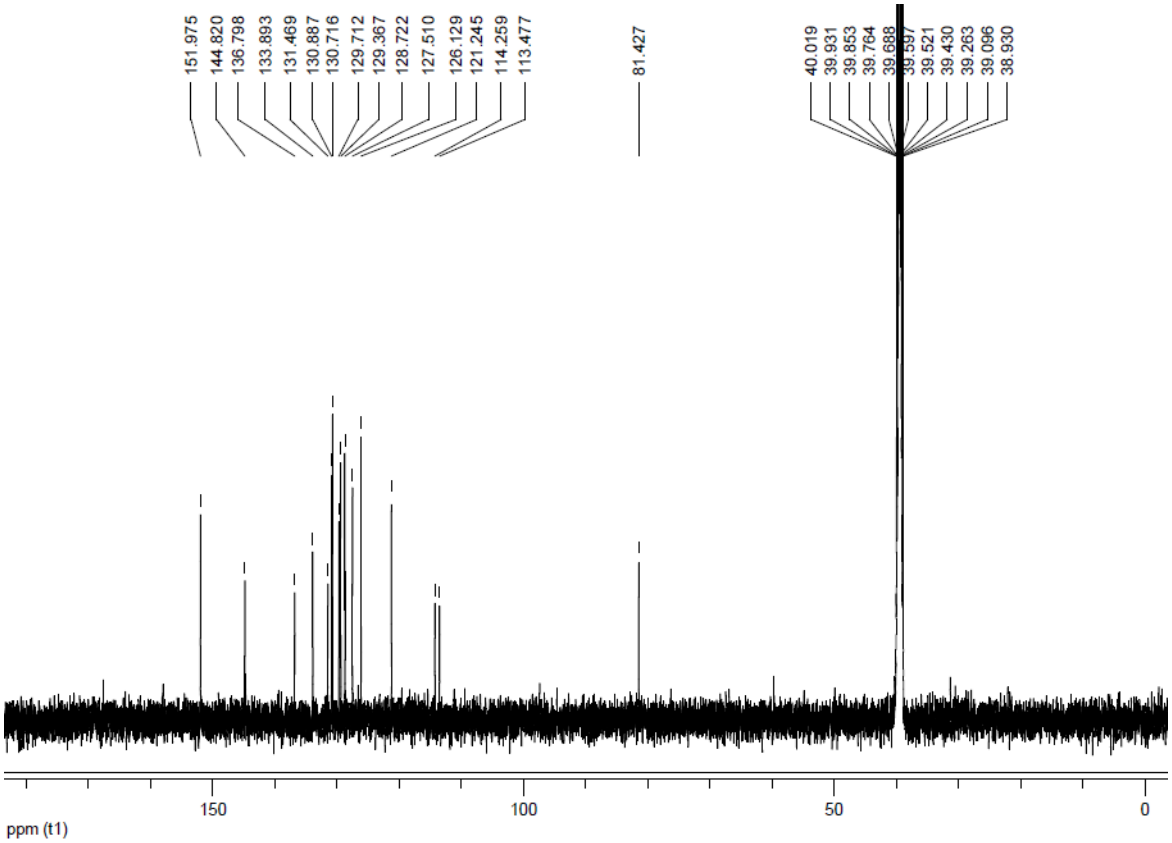

Fig. S7 ^{13}C NMR of compound **3**

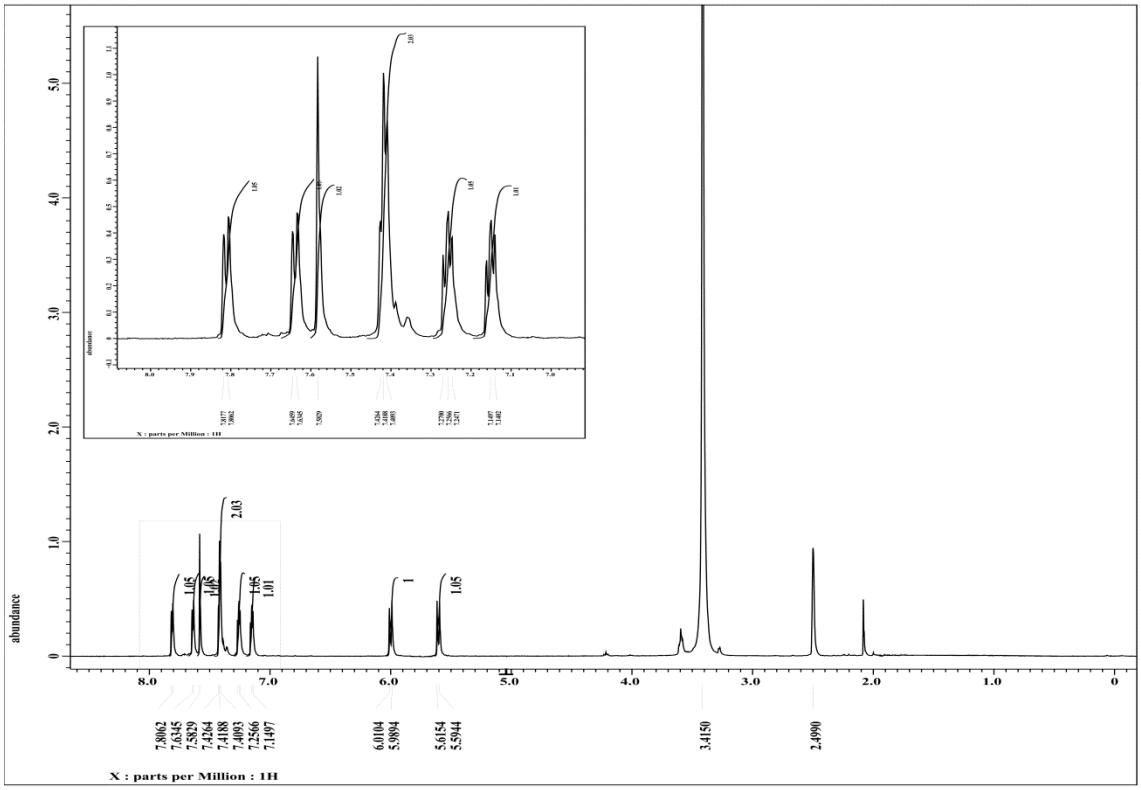

Fig. S8 ^{1}H NMR of compound **3-CN**

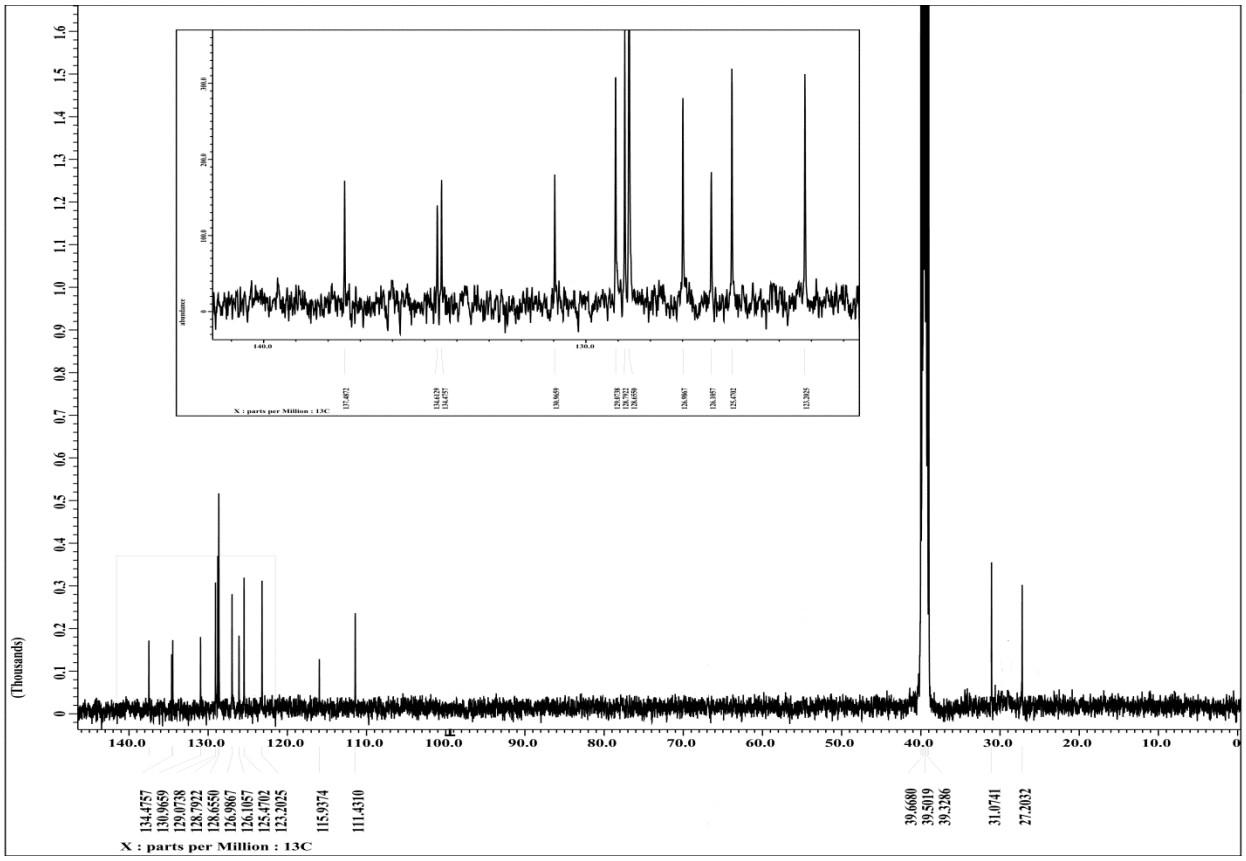

Fig. S9 ^{13}C NMR of compound **3-CN**

Coordinates of **3**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.568317	-0.063602	0.000325
2	6	0	-5.280058	-1.407611	0.000836
3	6	0	-3.878070	-1.657679	0.000302
4	6	0	-3.133566	-0.492988	-0.000152
5	16	0	-4.148652	0.896157	-0.000350
6	1	0	-6.551881	0.386768	0.000219
7	1	0	-6.027607	-2.192492	0.001456
8	1	0	-3.451646	-2.654832	0.000166
9	6	0	-1.671824	-0.381637	-0.000322
10	6	0	-0.927467	0.767547	-0.000754
11	16	0	-0.664390	-1.766532	0.000150
12	6	0	0.496165	0.547408	-0.000253
13	1	0	-1.389742	1.733085	-0.001278
14	6	0	0.784675	-0.844138	-0.000026
15	6	0	2.017513	-1.680093	-0.000040
16	6	0	1.966847	-3.065735	0.000198
17	16	0	3.669605	-1.175160	-0.000211
18	6	0	3.245481	-3.691238	-0.000152
19	1	0	1.041484	-3.630334	0.000494
20	6	0	4.267713	-2.779258	-0.000193
21	1	0	3.385367	-4.765868	-0.000451
22	1	0	5.328927	-2.989037	-0.000103
23	6	0	1.548347	1.589072	0.000095
24	1	0	2.535532	1.166136	0.000518
25	6	0	1.637746	2.953250	0.000097
26	6	0	2.975606	3.478263	0.000616
27	7	0	4.064281	3.886501	0.001032
28	6	0	0.662660	4.005705	-0.000276
29	7	0	0.016270	4.972291	-0.000496

Coordinates of **3-CN**$^{-}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.676369	-0.054059	0.263814
2	6	0	5.462223	-1.410977	0.165497
3	6	0	4.065864	-1.717775	0.081726
4	6	0	3.294762	-0.577341	0.120121
5	16	0	4.237334	0.797530	0.252875
6	1	0	6.647306	0.431340	0.340328
7	1	0	6.242378	-2.174194	0.151571
8	1	0	3.683061	-2.736532	-0.001652
9	6	0	1.756995	-0.529964	0.052085
10	6	0	0.986026	0.610598	0.090495
11	16	0	0.814334	-1.904685	-0.080872
12	6	0	-0.410290	0.304011	0.005243
13	1	0	1.368872	1.629268	0.174609
14	6	0	-0.624636	-1.052883	-0.092512
15	6	0	-1.998692	-1.739819	-0.200627
16	6	0	-2.212957	-3.096759	-0.298381
17	16	0	-3.437629	-0.888075	-0.212429
18	6	0	-3.609323	-3.403441	-0.382462
19	1	0	-1.432883	-3.860069	-0.311700
20	6	0	-4.380310	-2.262904	-0.344847
21	1	0	-3.992212	-4.422194	-0.465490
22	1	0	-5.466916	-2.229328	-0.393290
23	6	0	-1.531648	1.359431	0.020917
24	1	0	-2.094393	1.295433	-0.886894
25	6	0	-0.912697	2.764257	0.143245
26	6	0	-2.034113	3.819596	0.160131
27	7	0	-2.878816	4.614527	0.172851
28	6	0	0.016743	3.022021	-1.057296
29	7	0	0.716841	3.216181	-1.961599
30	6	0	-2.462023	1.102132	1.220834
31	7	0	-3.162825	0.908322	2.124667