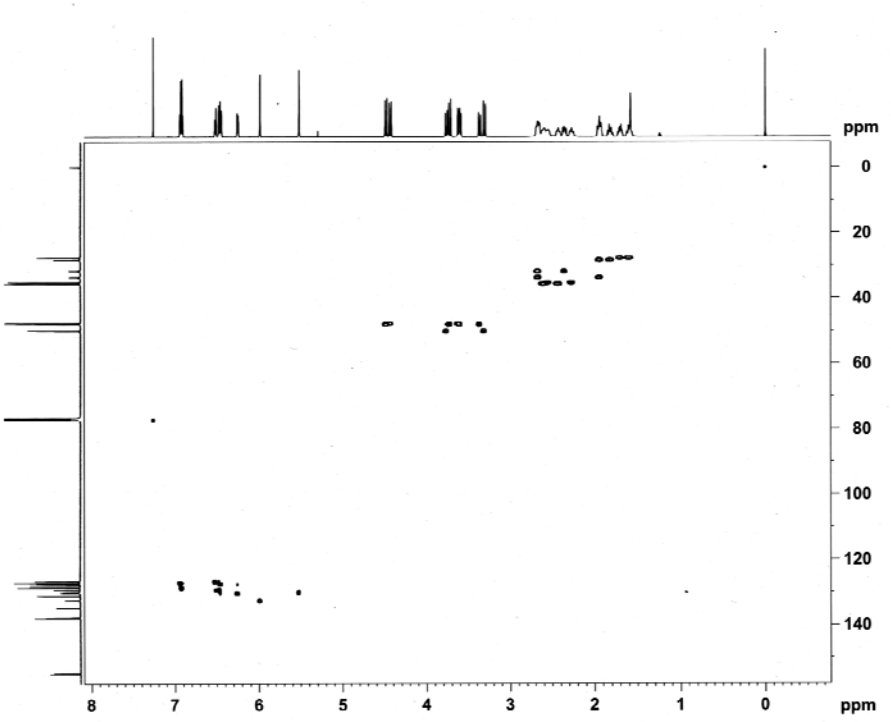


Figure S15. HSQC spectrum of three-layered [3.3]PCP-dione **7**.

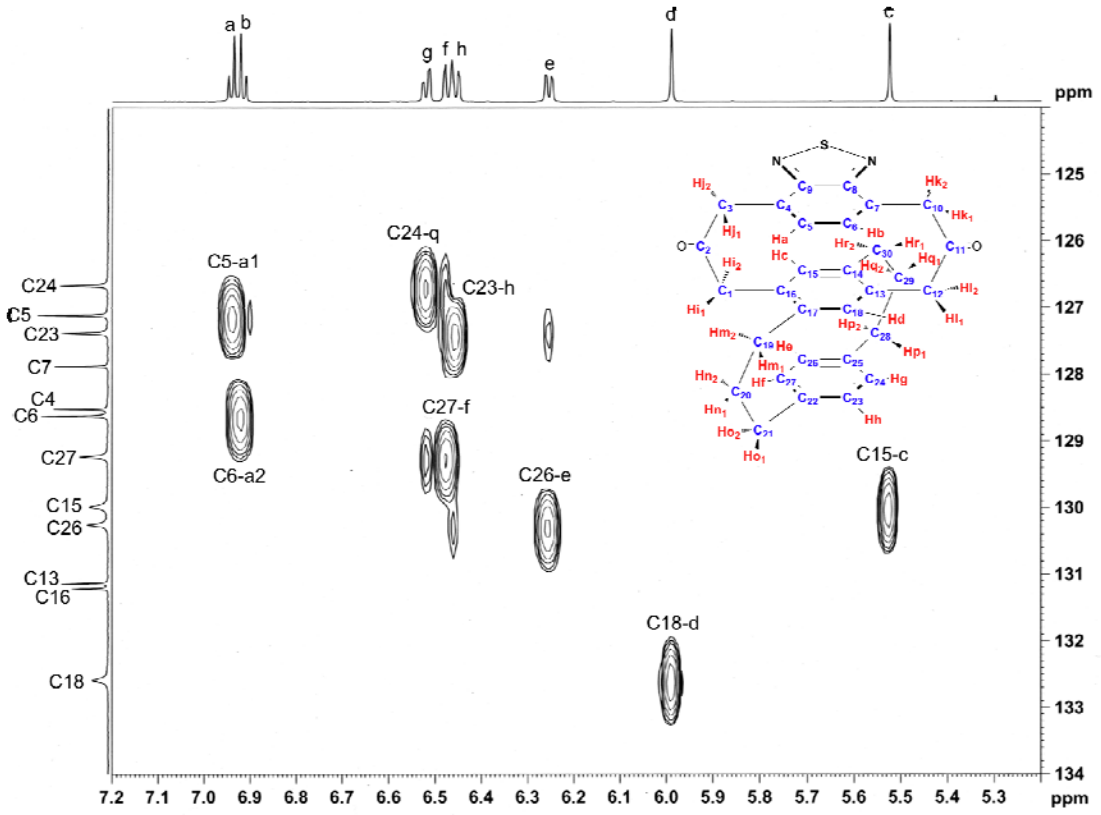


Figure S16. Selected HSQC spectrum of three-layered [3.3]PCP-dione **7**.

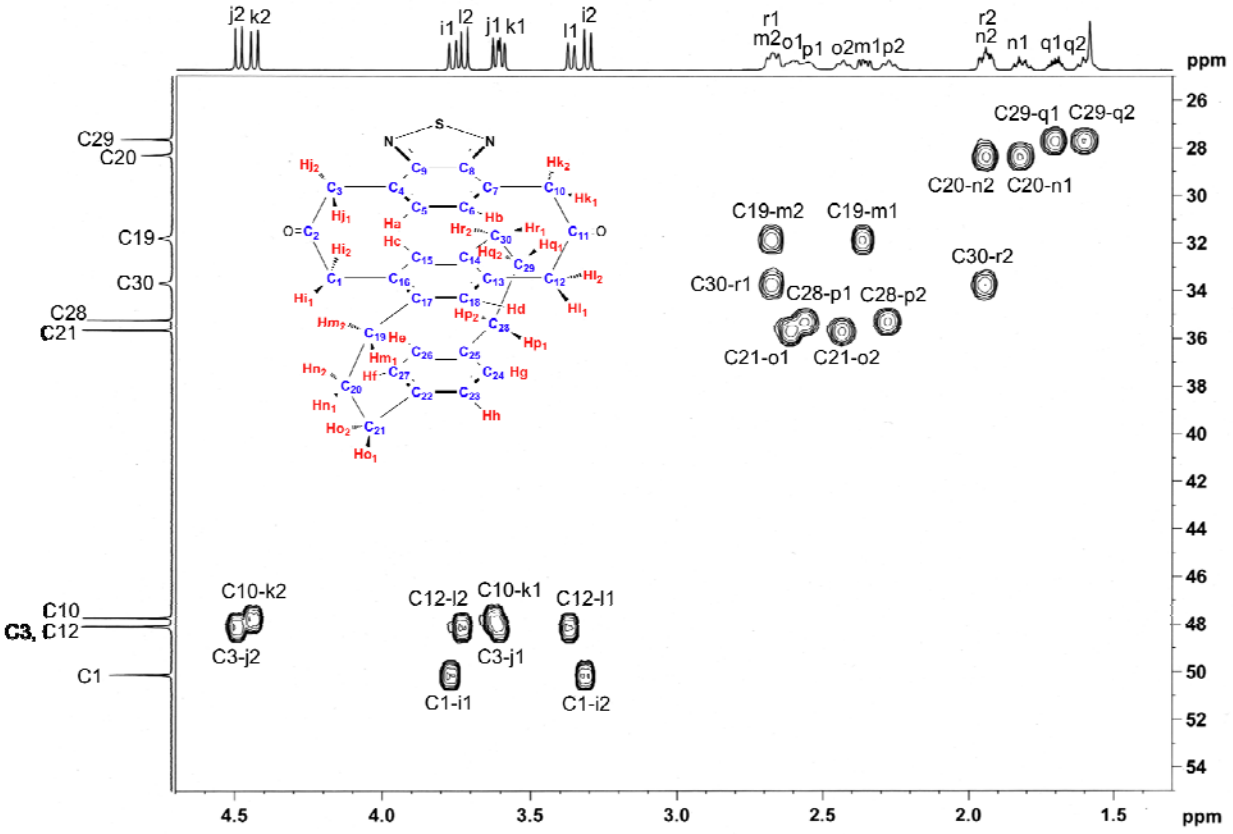


Figure S17. Selected HSQC spectrum of three-layered [3.3]PCP-dione **7**.

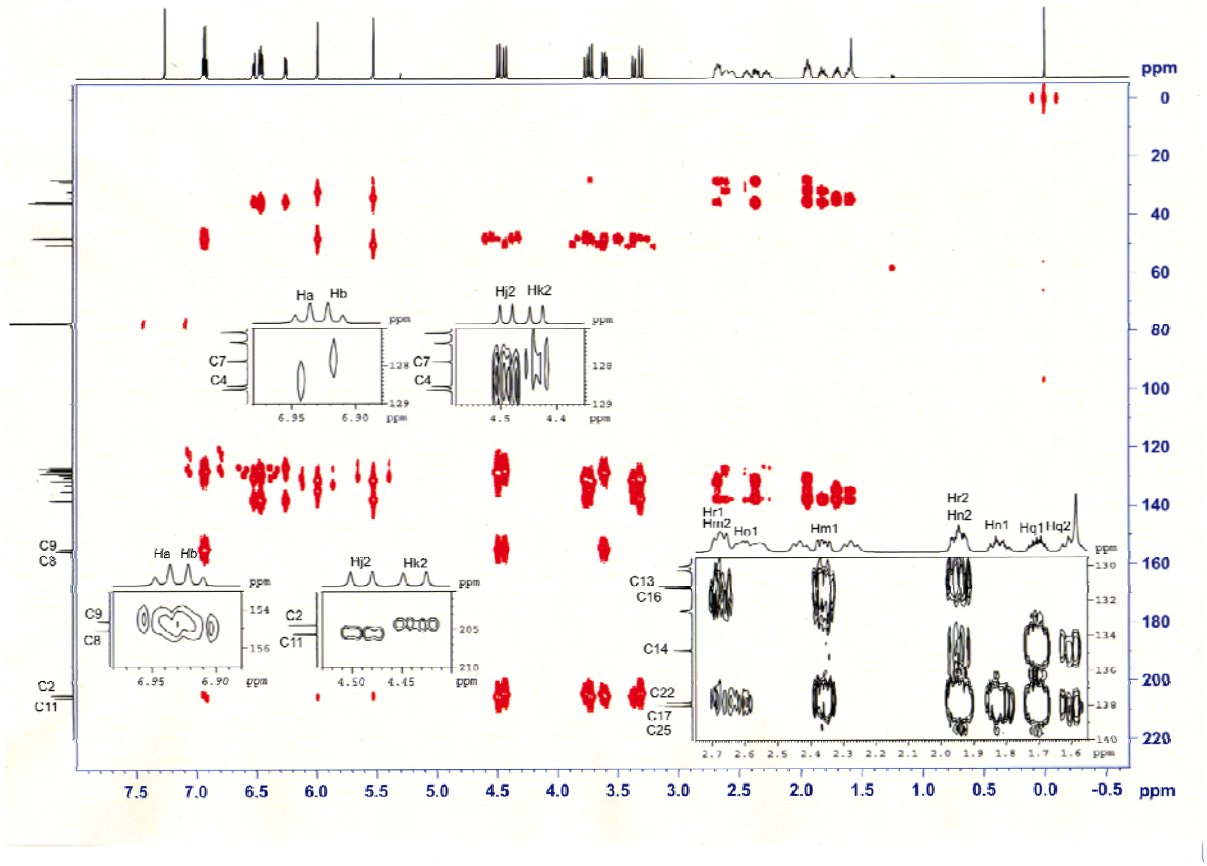


Figure S18. HMBC spectrum of three-layered [3.3]PCP-dione **7**.

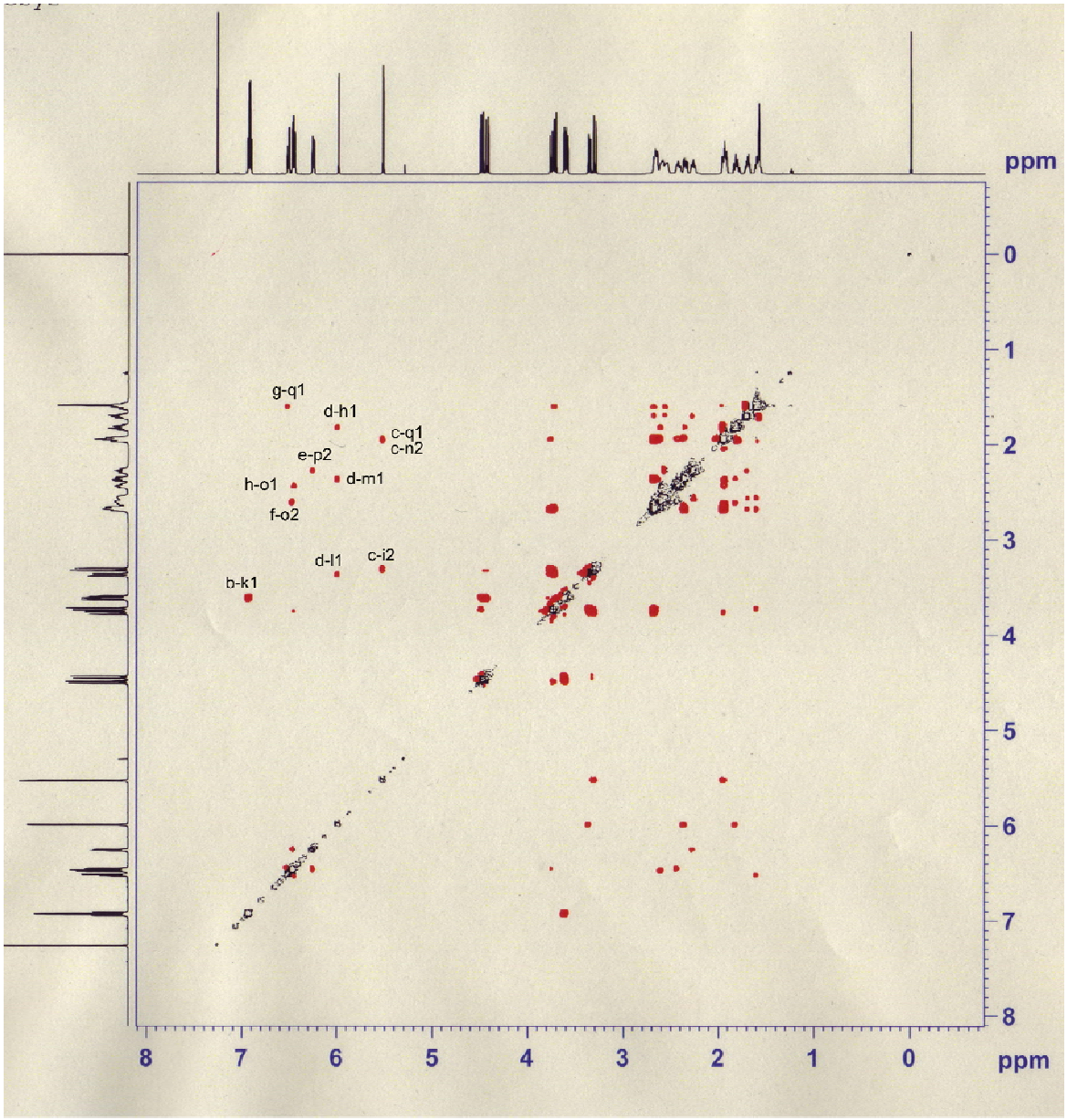
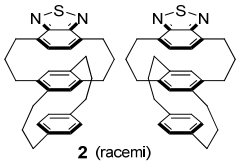


Figure S19. NOESY spectrum of three-layered [3.3]PCP-dione **7**.



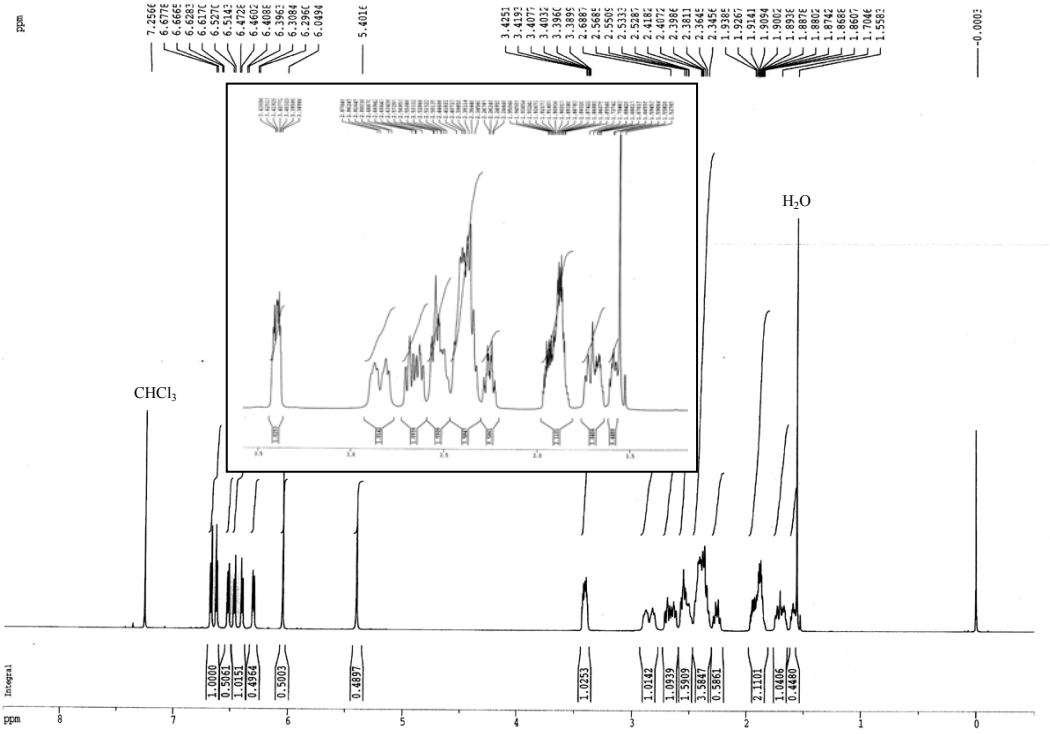


Figure S20. ^{1}H NMR spectrum of three-layered [3.3]PCP **2**.

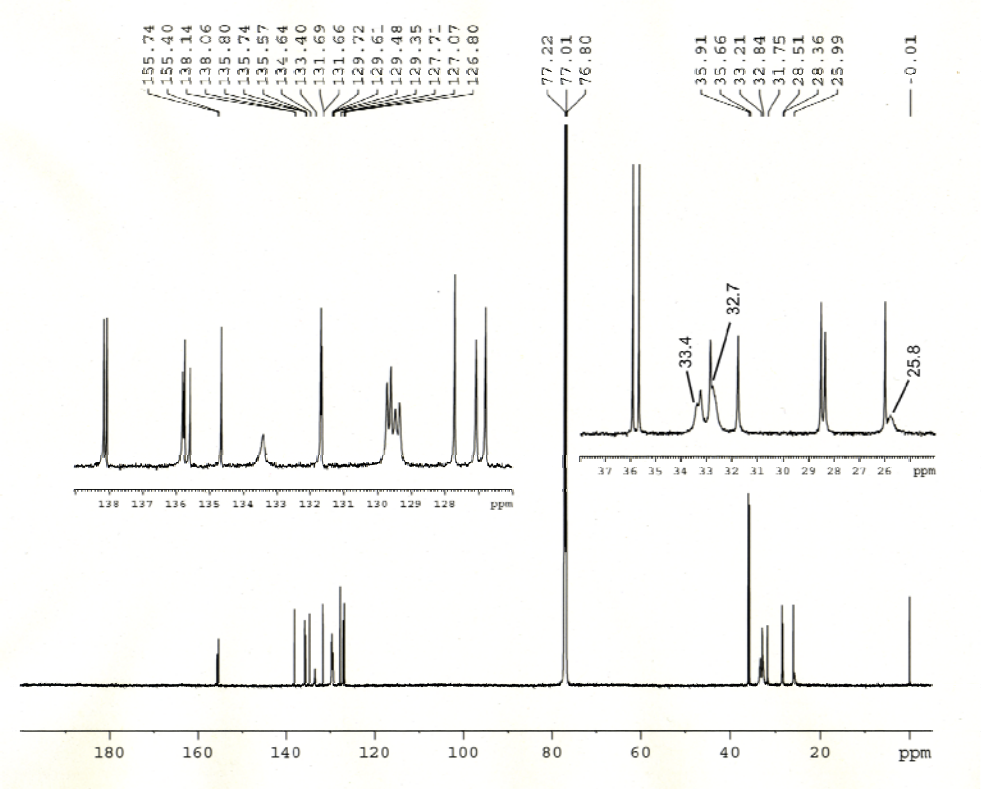


Figure S21. ^{13}C NMR spectrum of three-layered [3.3]PCP **2**.

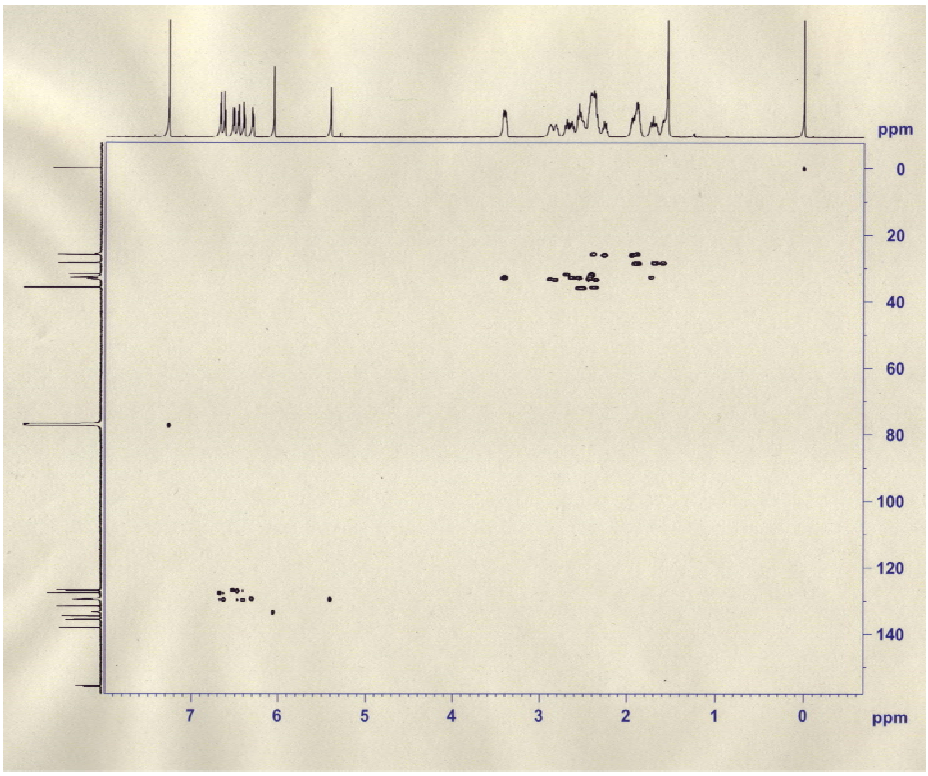


Figure S22. HSQC spectrum of three-layered [3.3]PCP **2**.

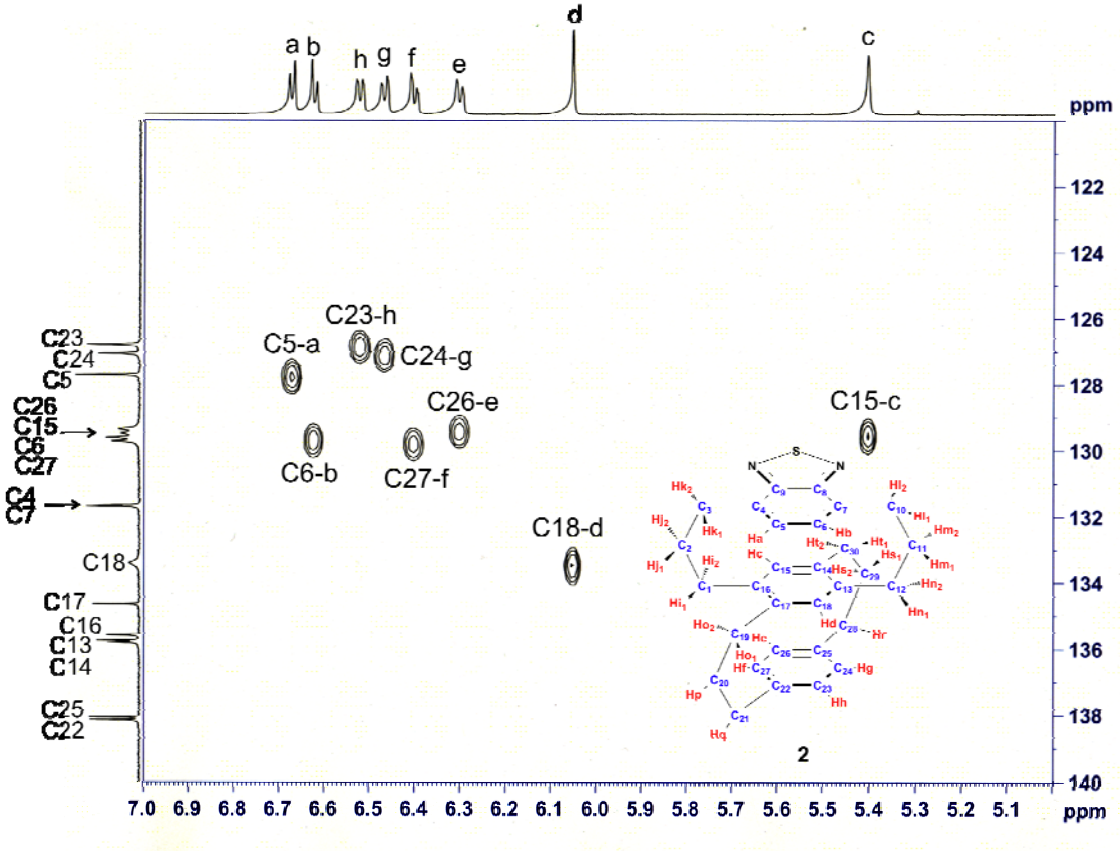


Figure S23. Selected HSQC spectrum of three-layered [3.3]PCP **2**.

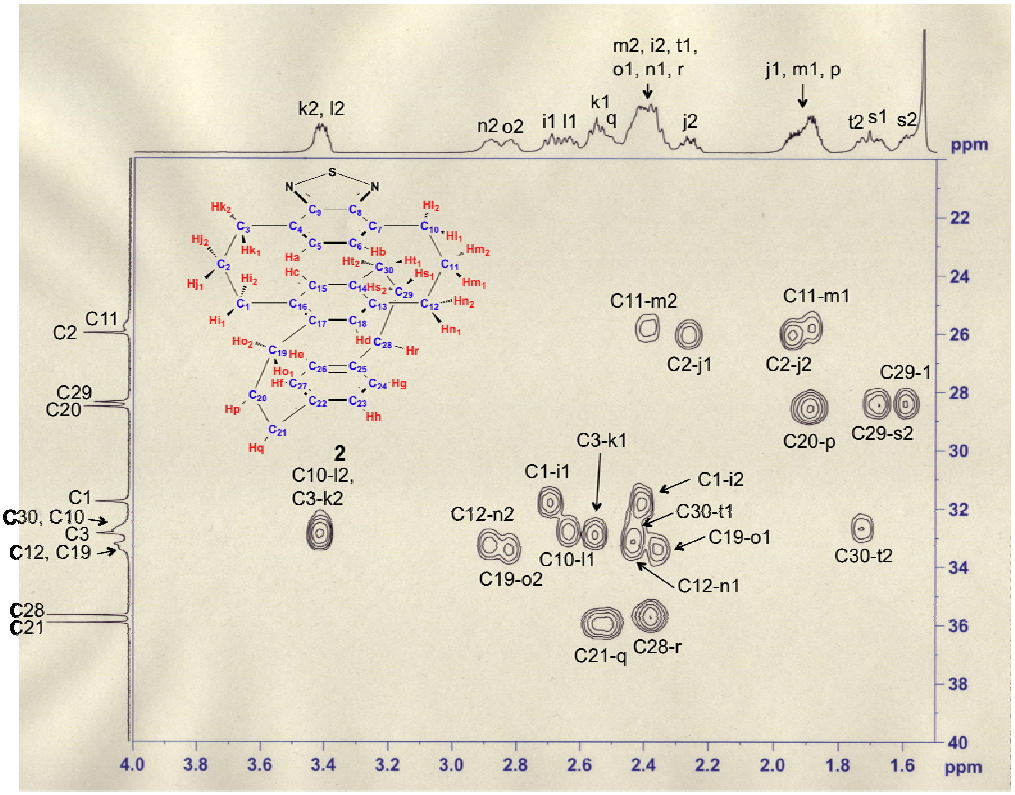


Figure S24. Selected HSQC COSY spectrum of three-layered [3.3]PCP **2**.

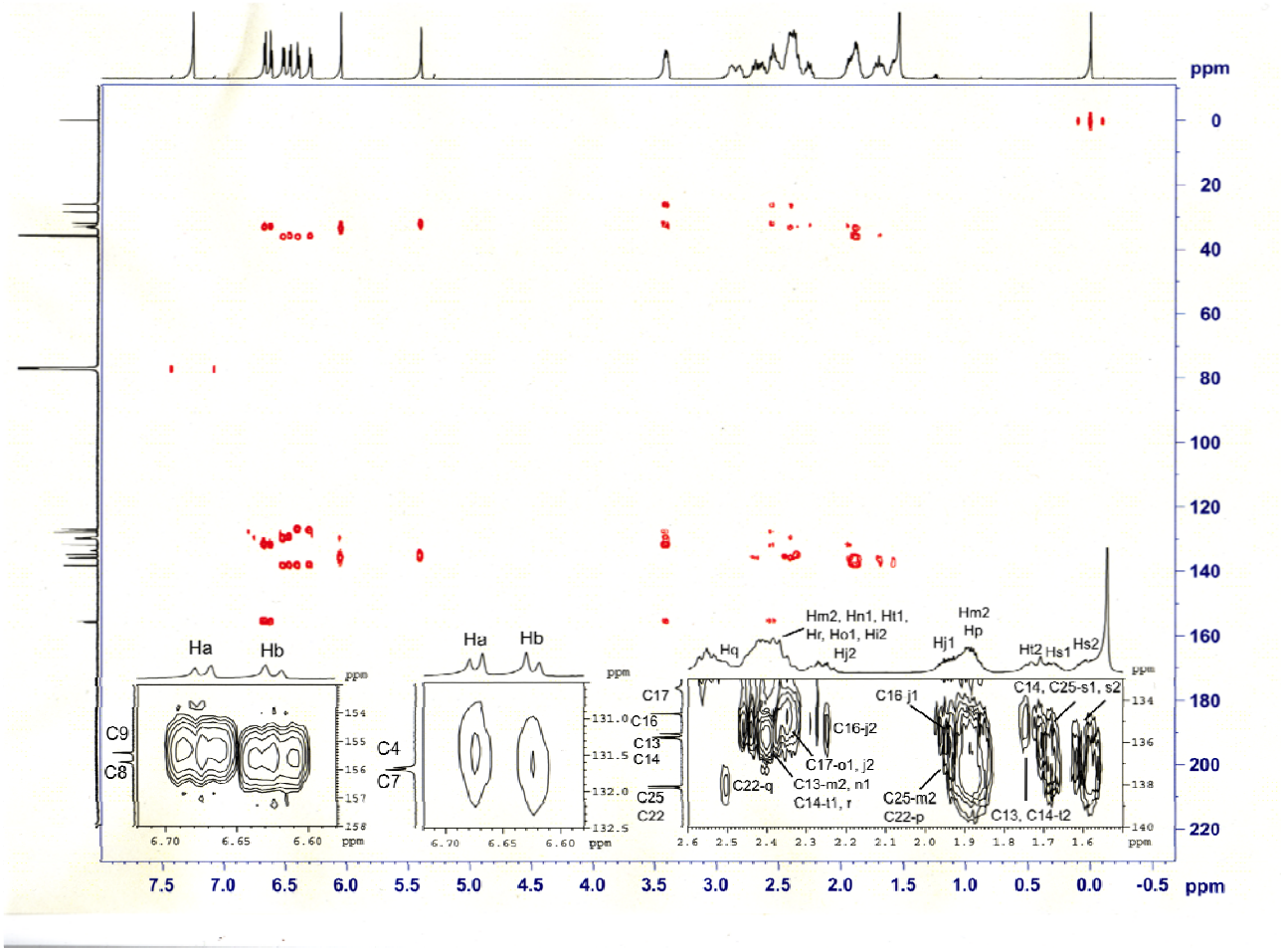


Figure S25. Selected HMBC spectrum of three-layered [3.3]PCP **2**.

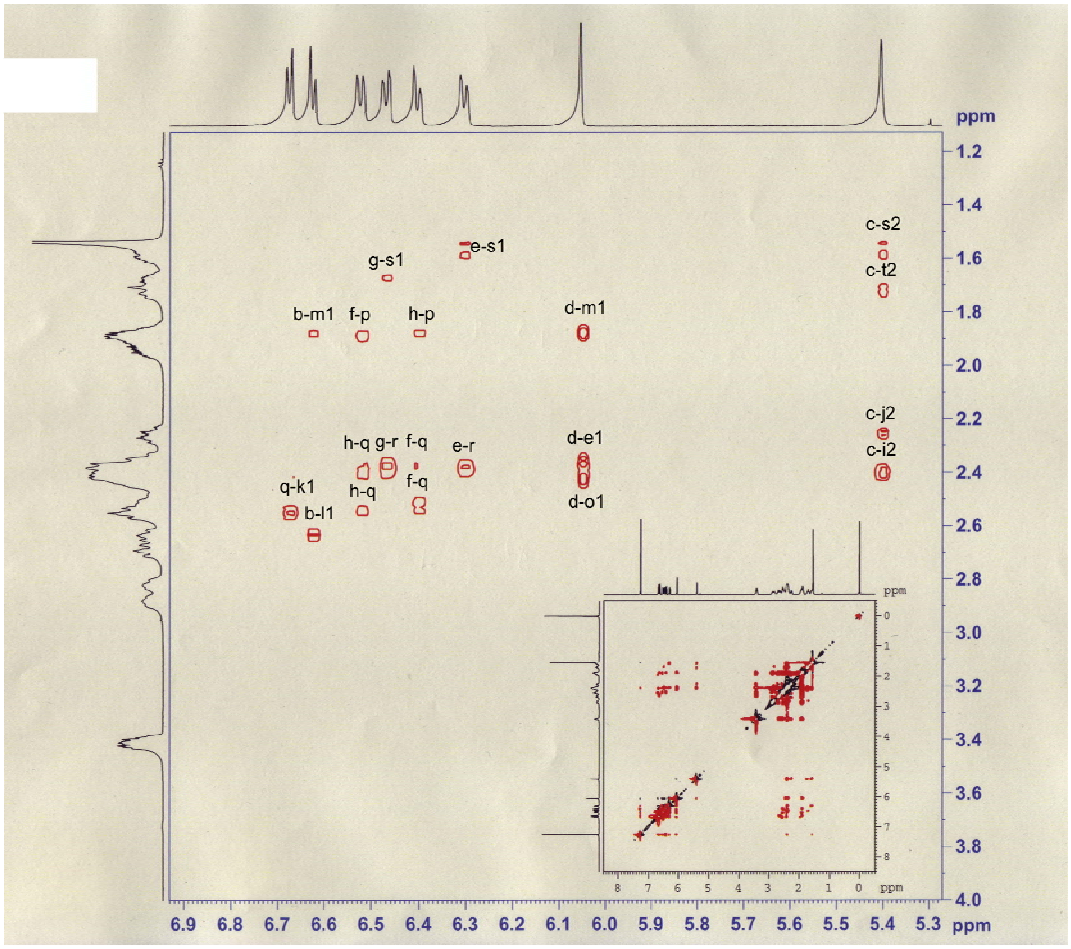


Figure S26. NOESYspectrum of three-layered [3.3]PCP **2**.

4. Cyclic voltammograms

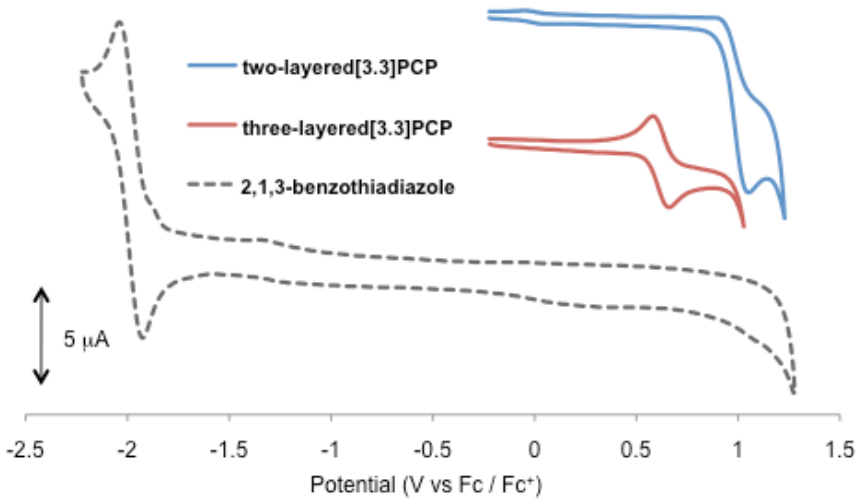


Figure S27. Cyclic voltammograms of two-and three-layered [3.3]PCPs, and 2,1,3-benzothiadiazole in CH_2Cl_2/0.1 M Bu_4NPF_6 observed at a potential scan rate of 100 mVs.

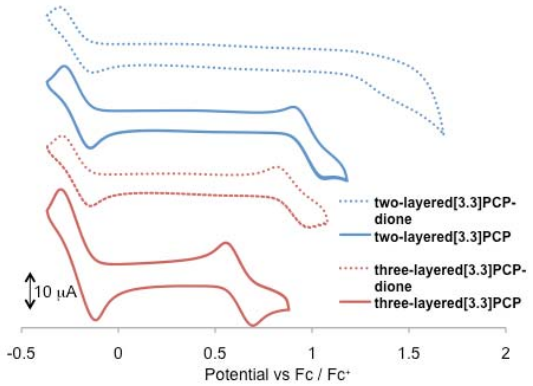


Figure S28. Cyclic voltammograms of [3.3]PCPs–TCNE complexes (0.5 mM : 0.5 mM) in CH_2Cl_2/0.1 M Bu_4NPF_6 observed at a potential scan rate of 400 mVs^{-}.

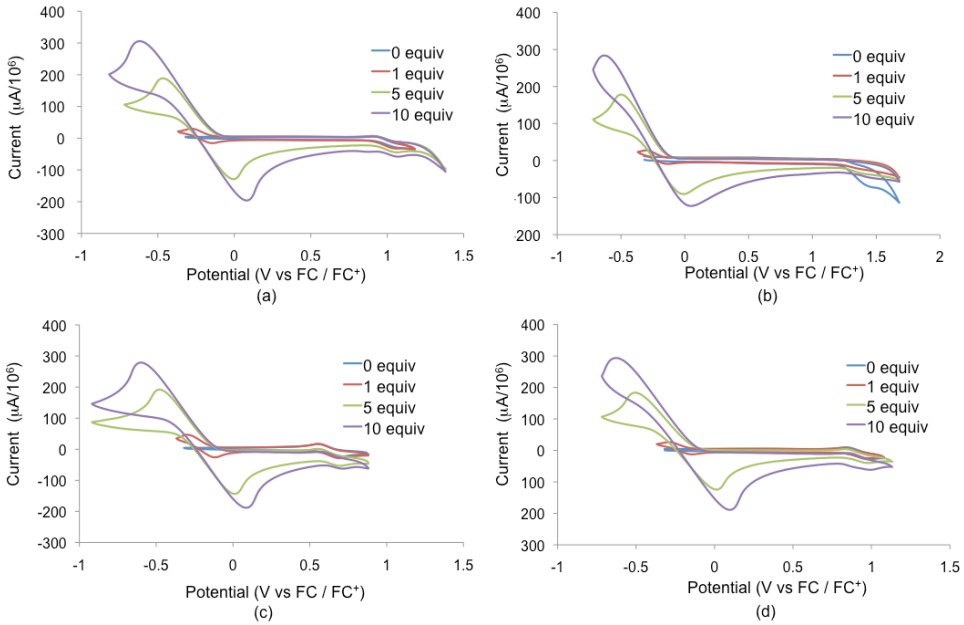


Figure S29. Cyclic voltammograms of [3.3]PCPs–TCNE complexes (0.5 mM : 0.5-5.0 mM) of (a) **1**, (b) **5**, (c) **2**, and (d) **7** in CH_2Cl_2/0.1 M Bu_4NPF_6 observed at a potential scan rate of 400 mVs^{-}

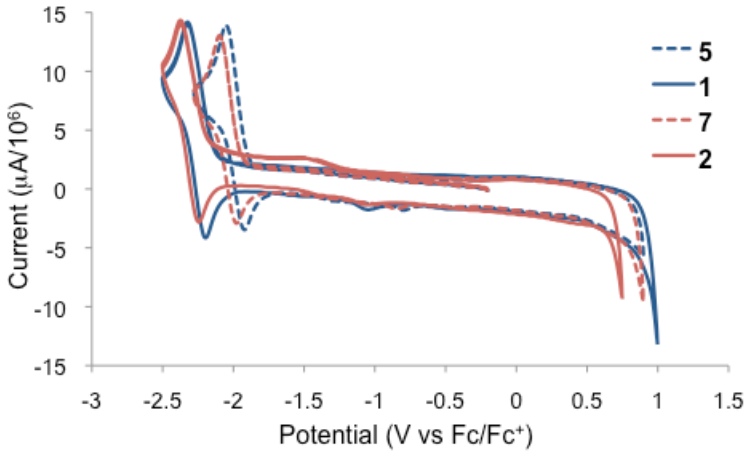


Figure S30. Cyclic voltammograms of [3.3]PCPs **1**, **2**, **5**, and **7** in THF/.0.1 M Bu_4NPF_6 observed at a potential scan rate of 100 mVs.

TABLE S3. Redox potentials of [3.3]PCPs–TCNE complexes (0.5 mM : 0.5 mM) in CH_2Cl_2 and the calculated HOMO- LUMO energies.

Compound	$^{red}E_{1/2}(I)^a$ (V vs Fc/Fc^+)	$^{ox}E_{1/2}(I)^a$ (V vs Fc/Fc^+)	LUMO[b] (eV)	HOMO[b] (eV)
[3.3]PCP-dione-TCNE	-0.20		2.43	-7.98
[3.3]PCP-TCNE	-021	0.98	3.52	-7.34
Three-layered	-0.22	0.90	2.51	-7.29
[3.3]PCP-dione-TCNE				
Three-layered	-0.21	0.63	3.37	-6.85
[3.3]PCP-TCNE				
TCNE	-0.22		-1.76	-11.71

[a]measured in CH_2Cl_2/0.1 M Bu_4NPF_6 at a potential scan rate of 400 mVs^{-1}, [b] [3.3]PCPs moieties only calculated by DFT (MP2/6-31G(d) level) calculations.

5. Electronic spectra

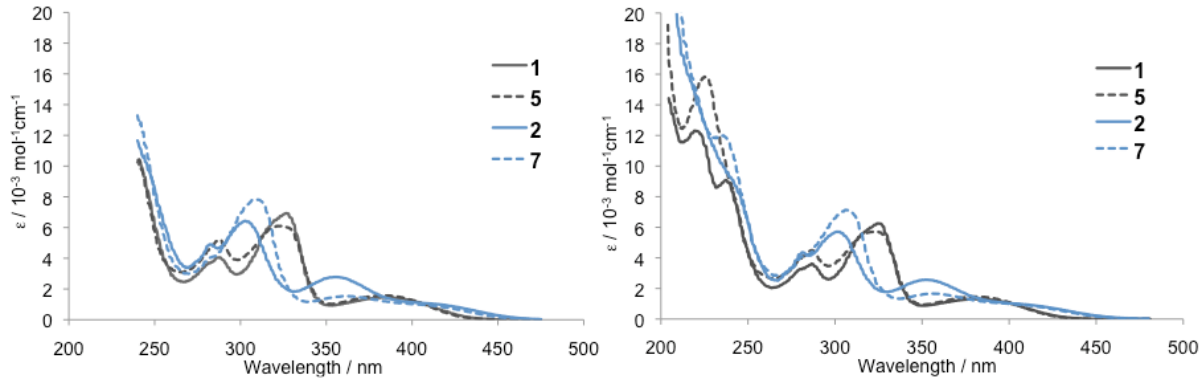


Figure S31. UV/Vis spectra of cyclophanes in (a) $CHCl_3$ (10^{-4} M) (b) MeCN (10^{-4} M).

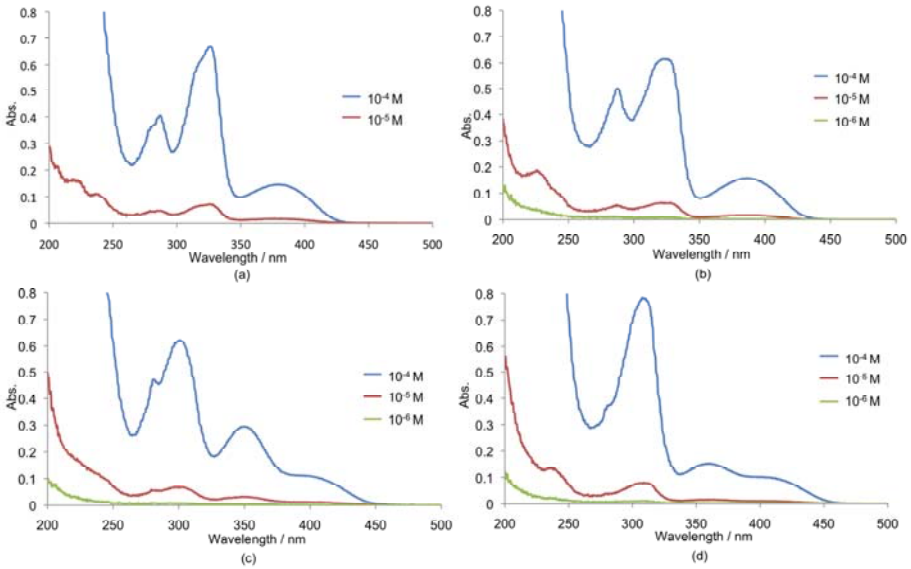


Figure S32. UV/Vis spectra of (a) **1**, (b) **5**, (c) **2**, and (d) **7** in cyclohexane (10^{-4} – 10^{-6}M).

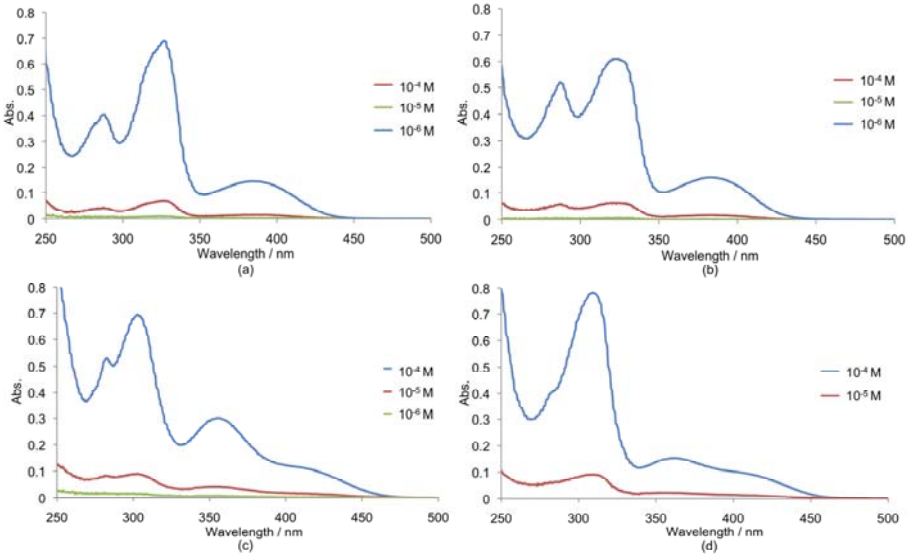


Figure S33. UV/Vis spectra of (a) **1**, (b) **5**, (c) **2**, and (d) **7** in $CHCl_3$ (10^{-4} – 10^{-6}M)

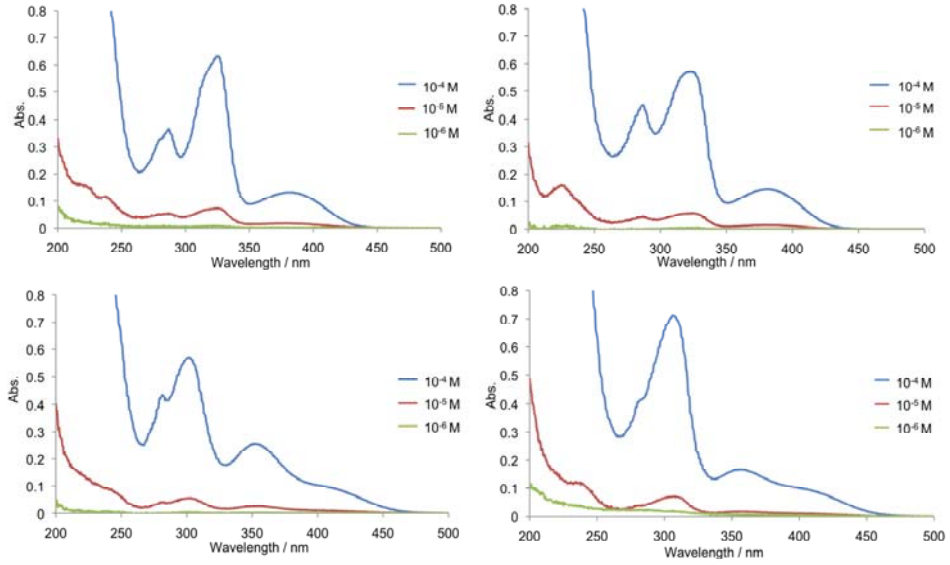


Figure S34. UV/Vis spectra of (a) **1**, (b) **5**, (c) **2**, and (d) **7** in MeCN (10^{-4} – 10^{-6}M)

Comp.	5	1	7	2	8	9	10

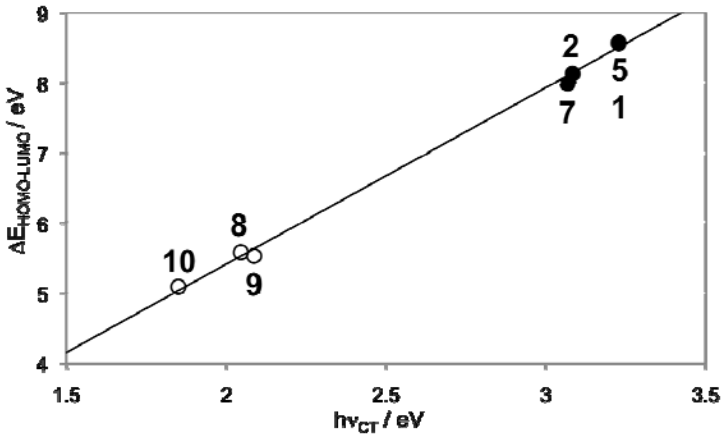


FIGURE S35. HOMO-LUMO gap ($\Delta E_{HOMO\text{-}LUMO}$) dependance on the peak position ($h\nu_{CT}$) of the CT complex. White circles: PCP-TCNE complexes (**8** - **10**); Black circles: Benzothiadiazonophanes (**1**, **2**, **5** and **7**).

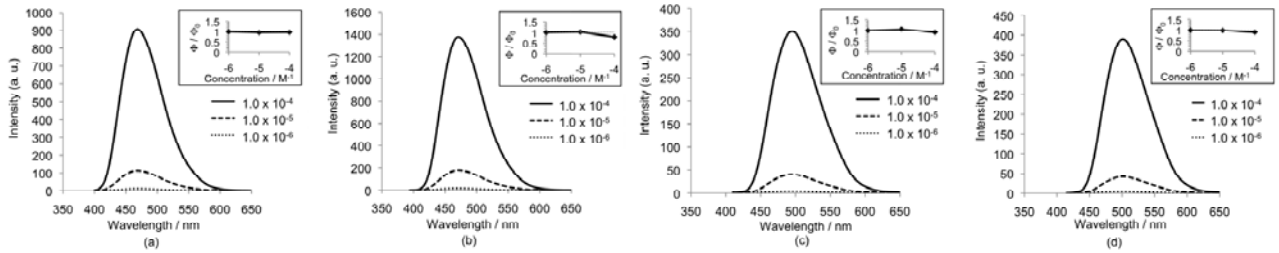


Figure S36. FL spectra of (a) **1**, (b) **5**, (c) **2**, and (d) **7** in cyclohexane (10^{-4} – 10^{-6}M)

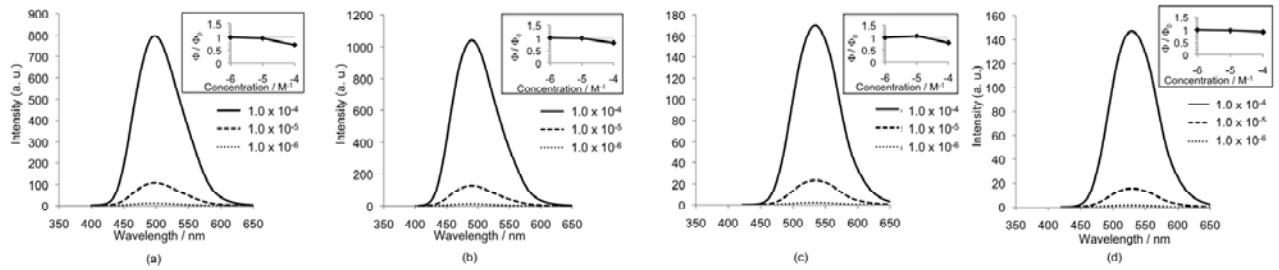


Figure S37. FL spectra of (a) **1**, (b) **5**, (c) **2**, and (d) **7** in $CHCl_3$ (10^{-4} – 10^{-6}M)

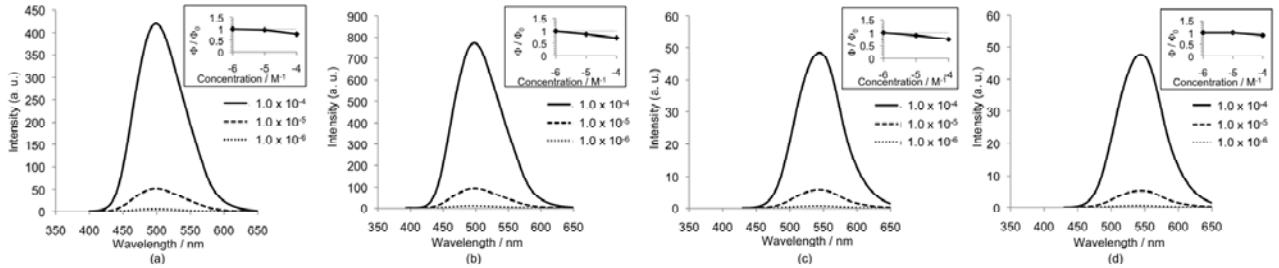


Figure S38. FL spectra of (a) **1**, (b) **5**, (c) **2**, and (d) **7** in MeCN (10^{-4} – 10^{-6}M).

6. Computational results.

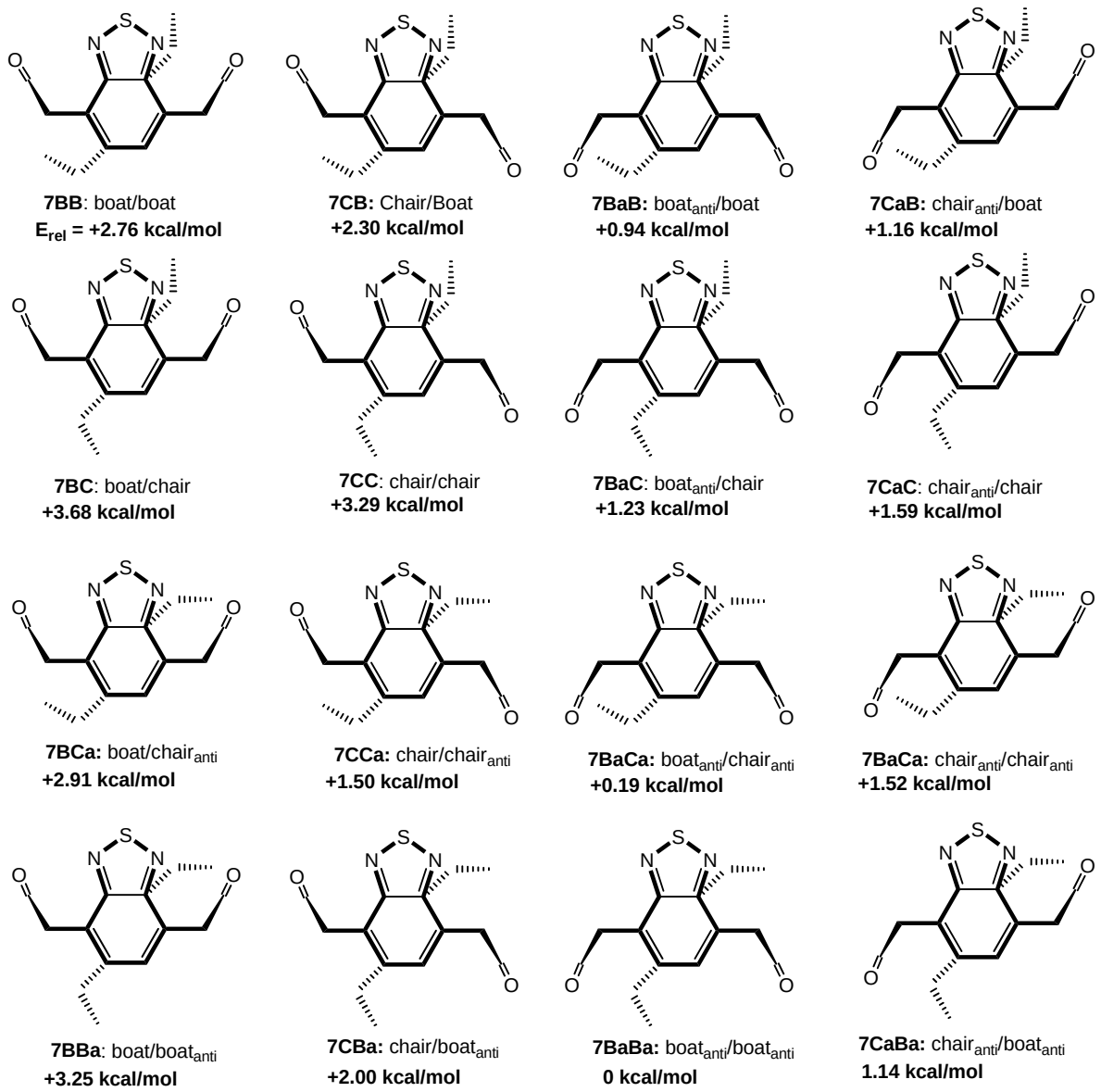
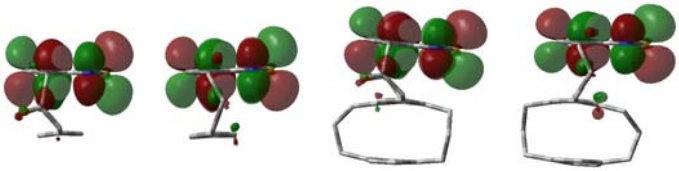
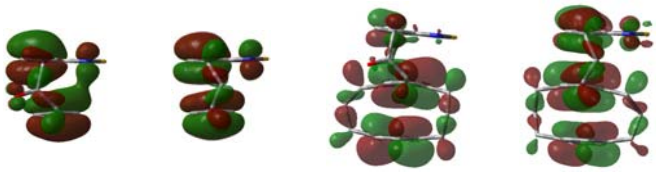
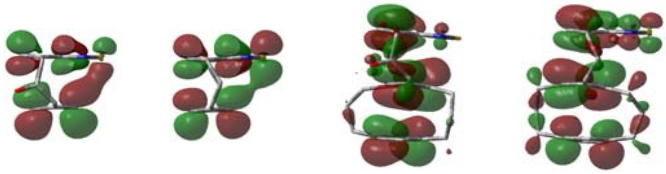
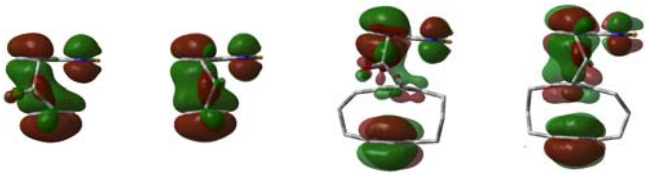
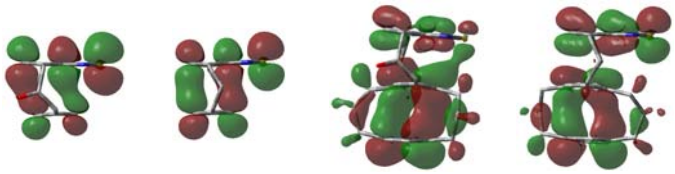
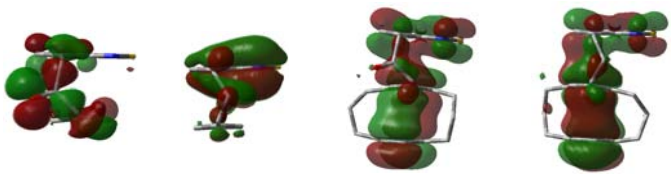
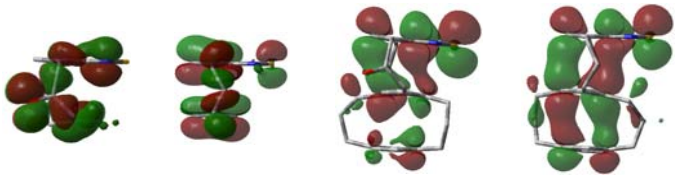


Figure S39. Possible conformers of **7** at B3LYP/6-31G(d)) level.

Table S4. HOMO and LUMO orbitals of the two- and three-layered [3.3]PCPs **1** and **2** and their diones **5** and **7** (MP2/6-31G (d)).

MOs	**5**	**1**	**7**	**2**
LUMO				
	0.43	1.04	0.53	1.11
HOMO				
	-8.15	-7.46	-7.42	-6.97
HOMO-1				
	-9.02	-8.37	-7.83	-7.36
HOMO-2				
	-9.16	--8.81	-8.60	-8.33
HOMO-3				
	-9.70	-9.49	-9.08	-8.66
HOMO-4				
	-11.22	--11.57	-9.36	-9.11
HOMO-5				
	-11.50	-11.65	-9.53	-9.44

		Excited state (contribution)	Wavelength (nm)	Excited energy (eV)	Oscillator strength (*f*)
5	B3LYP	HOMO → LUMO (0.67984)	483	2.57	0.0133
	BHandHLYP	HOMO → LUMO (0.6934)	386	3.21	0.0297
	HF	HOMO → LUMO (0.62252) HOMO -2 → LUMO (0.28373)	336	3.69	0.0792
	Exp.		384	3.23	
7	B3LYP	HOMO → LUMO (0.68404) HOMO-1 → LUMO (0.68404)	562	2.21	0.0046
	BHandHLYP	HOMO → LUMO (0.59597) HOMO -1 → LUMO (-0.32339) HOMO -2 → LUMO (-0.12650)	417	2.97	0.0114
	HF	HOMO → LUMO (-0.32346) HOMO -1 → LUMO (0.42491) HOMO -3 → LUMO (0.41046) HOMO -5 → LUMO (-0.11225)	339	3.66	0.0624
	Exp.		401	3.09	

Table S5. Theoretical calculation results (gas phase) and the observed lowest energy absorption bands in cyclohexane.

Table S6. Dipole moments of the ground state (MP2/6-31G(d)) and S1 state (BHandLYP/6-31+G(d)).

Compounds	**1**	**2**	**5**	**7**
MOs of MP2/6-31G(d) (ground state)				
Dipole moments (Debye)	1.95	2.05	3.58	3.04
MOs of BHandLYP/6-31+G(d) (excited state)				
Dipole moments (Debye)	1.71	1.81	3.70	3.12

Table S7. Coordinates of **1B**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.733970	1.450032	0.464593
2	6	0	-0.712144	-2.726319	0.052271
3	6	0	0.684017	-2.731700	0.053783
4	6	0	1.412131	-1.884210	-0.786994
5	6	0	0.691257	-1.146038	-1.737395
6	6	0	-0.702797	-1.140797	-1.739045
7	6	0	-1.431592	-1.873353	-0.790316
8	6	0	-0.721044	1.451185	0.468078
9	6	0	1.473507	0.542904	1.295885
10	6	0	0.725855	-0.176523	2.192617
11	6	0	-0.706547	-0.175608	2.195815
12	6	0	-1.457703	0.544744	1.302690
13	6	0	-2.942491	0.340011	1.117191
14	6	0	-2.926992	-1.673056	-0.622639
15	6	0	2.956243	0.334580	1.099729
16	6	0	2.909205	-1.697743	-0.616156
17	6	0	-3.363541	-0.227796	-0.265491
18	7	0	1.266179	2.324480	-0.394099
19	7	0	-1.255866	2.327007	-0.387616
20	6	0	3.361337	-0.252579	-0.279901
21	1	0	-1.247758	-3.345606	0.769220
22	1	0	1.213198	-3.354918	0.772096
23	1	0	1.223520	-0.519762	-2.450161
24	1	0	-1.228837	-0.510402	-2.452821
25	1	0	1.231791	-0.862411	2.868157
26	1	0	-1.210250	-0.861010	2.873495
27	1	0	-3.463242	1.299248	1.238830
28	1	0	-3.309224	-0.323285	1.911332
29	1	0	-3.446643	-1.942971	-1.553270
30	1	0	-3.299856	-2.364680	0.144743
31	1	0	3.330575	-0.318576	1.898700
32	1	0	3.478978	1.294833	1.202393

33	1	0	3.429948	-1.989706	-1.539531
34	1	0	3.270177	-2.381005	0.164314
35	1	0	-3.019306	0.462328	-1.043198
36	1	0	-4.460817	-0.201509	-0.299173
37	1	0	4.458475	-0.235948	-0.322748
38	1	0	3.016684	0.432040	-1.062320
39	16	0	0.004024	3.088533	-1.129771

Table S8. Coordinates of **1C**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.448590	1.578706	0.402002
2	6	0	-0.129365	-2.777122	-0.070610
3	6	0	1.231561	-2.497422	-0.185109
4	6	0	1.687841	-1.458882	-1.007692
5	6	0	0.747520	-0.830428	-1.832155
6	6	0	-0.613331	-1.124201	-1.731426
7	6	0	-1.084542	-2.044207	-0.786629
8	6	0	-0.977042	1.301769	0.499845
9	6	0	1.399041	0.848919	1.189414
10	6	0	0.862373	0.008612	2.132788
11	6	0	-0.537888	-0.276468	2.216797
12	6	0	-1.469520	0.276452	1.374123
13	6	0	-2.894319	-0.216573	1.278532
14	6	0	-2.567433	-2.179030	-0.489035
15	6	0	2.884097	0.939536	0.903368
16	6	0	3.121790	-0.968529	-0.932382
17	6	0	3.542079	-0.388791	0.443850
18	7	0	0.747365	2.523180	-0.495373
19	7	0	-1.723272	2.044995	-0.323281
20	6	0	-3.282752	-0.866504	-0.078137
21	1	0	-0.459738	-3.539523	0.632283
22	1	0	1.940345	-3.050141	0.428711
23	1	0	1.074991	-0.053662	-2.519629
24	1	0	-1.319125	-0.575029	-2.350468
25	1	0	1.529319	-0.552663	2.783551

26	1	0	-0.855905	-1.040484	2.922646
27	1	0	-3.074884	-0.932527	2.090872
28	1	0	-3.584755	0.622800	1.436139
29	1	0	-3.092233	-2.565025	-1.375070
30	1	0	-2.709018	-2.931988	0.297811
31	1	0	3.053825	1.714766	0.149048
32	1	0	3.411650	1.266695	1.809925
33	1	0	3.288560	-0.209968	-1.707707
34	1	0	3.811354	-1.794870	-1.156650
35	1	0	3.381979	-1.153036	1.215602
36	1	0	4.626206	-0.216612	0.410257
37	1	0	-3.159767	-0.118524	-0.868484
38	1	0	-4.358414	-1.082043	-0.029504
39	16	0	-0.680328	3.017474	-1.150251

Table S9. Coordinates of **1Ba**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.727764	1.469511	0.457829
2	6	0	-0.696107	-2.619035	-0.310049
3	6	0	0.696049	-2.619046	-0.310051
4	6	0	1.420807	-1.654848	-1.027824
5	6	0	0.698967	-0.798877	-1.864308
6	6	0	-0.699000	-0.798866	-1.864305
7	6	0	-1.420851	-1.654825	-1.027819
8	6	0	-0.727724	1.469525	0.457825
9	6	0	1.464314	0.564813	1.288945
10	6	0	0.715109	-0.155818	2.187152
11	6	0	-0.715112	-0.155803	2.187149
12	6	0	-1.464298	0.564843	1.288939
13	6	0	-2.950509	0.354061	1.088927
14	6	0	-2.915902	-1.487554	-0.829097
15	6	0	2.950520	0.353990	1.088933
16	6	0	2.915862	-1.487599	-0.829106
17	6	0	3.344058	-1.066093	0.601967
18	7	0	1.261193	2.339125	-0.406695

19	7	0	-1.261129	2.339162	-0.406691
20	6	0	-3.344092	-1.066012	0.601967
21	1	0	-1.227644	-3.345264	0.302127
22	1	0	1.227575	-3.345284	0.302123
23	1	0	1.231399	-0.071702	-2.473051
24	1	0	-1.231422	-0.071682	-2.473046
25	1	0	1.218384	-0.836817	2.870280
26	1	0	-1.218405	-0.836789	2.870277
27	1	0	-3.325443	1.102270	0.383000
28	1	0	-3.475326	0.529110	2.038141
29	1	0	-3.298630	-0.752991	-1.549116
30	1	0	-3.429761	-2.433641	-1.051537
31	1	0	3.325473	1.102190	0.383005
32	1	0	3.475344	0.529025	2.038145
33	1	0	3.298591	-0.753019	-1.549108
34	1	0	3.429712	-2.433683	-1.051575
35	1	0	2.966349	-1.806499	1.319467
36	1	0	4.439417	-1.131225	0.648093
37	1	0	-4.439454	-1.131100	0.648082
38	1	0	-2.966421	-1.806426	1.319479
39	16	0	0.000043	3.091957	-1.150221

Table S10. Coordinates of **5B**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.726849	1.459279	0.575158
2	6	0	-0.698357	-2.861590	0.080477
3	6	0	0.696601	-2.861753	0.081202
4	6	0	1.413736	-1.953715	-0.704004
5	6	0	0.697389	-1.145363	-1.597571
6	6	0	-0.696930	-1.145191	-1.598264
7	6	0	-1.414437	-1.953352	-0.705444
8	6	0	-0.726186	1.458513	0.575482
9	6	0	1.461730	0.511531	1.362377
10	6	0	0.717464	-0.263268	2.216211
11	6	0	-0.714135	-0.264079	2.216464

12	6	0	-1.459650	0.509909	1.362966
13	6	0	-2.944170	0.321964	1.152274
14	6	0	-2.912092	-1.765924	-0.527551
15	6	0	2.946126	0.324785	1.150096
16	6	0	2.911381	-1.767048	-0.524504
17	6	0	-3.317567	-0.310508	-0.213966
18	8	0	3.960104	0.322871	-1.025334
19	7	0	1.260403	2.371741	-0.240560
20	7	0	-1.261071	2.370522	-0.239868
21	16	0	-0.000912	3.165590	-0.940908
22	8	0	-3.962246	0.325018	-1.021155
23	6	0	3.317354	-0.310937	-0.215247
24	1	0	-1.233022	-3.532946	0.749081
25	1	0	1.230408	-3.533199	0.750401
26	1	0	1.234012	-0.460308	-2.249685
27	1	0	-1.232704	-0.459962	-2.250906
28	1	0	1.223257	-0.980534	2.858015
29	1	0	-1.218882	-0.981894	2.858467
30	1	0	-3.470241	1.280370	1.181483
31	1	0	-3.340233	-0.322036	1.948435
32	1	0	-3.461509	-2.034145	-1.436427
33	1	0	-3.265183	-2.416311	0.283330
34	1	0	3.344339	-0.316753	1.947178
35	1	0	3.471173	1.283828	1.175845
36	1	0	3.461836	-2.038829	-1.431712
37	1	0	3.262523	-2.415181	0.288997

Table S11. Coordinates of **5C**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.391943	1.674964	0.389323
2	6	0	0.098966	-2.738574	-0.122804
3	6	0	1.402650	-2.332835	-0.398868
4	6	0	1.645132	-1.250735	-1.255349
5	6	0	0.560616	-0.697279	-1.944730
6	6	0	-0.744850	-1.113906	-1.677525

7	6	0	-0.996450	-2.085348	-0.701314
8	6	0	-0.998960	1.311573	0.601309
9	6	0	1.440892	0.991490	1.084266
10	6	0	1.045683	0.088389	2.040548
11	6	0	-0.323554	-0.277422	2.238784
12	6	0	-1.351827	0.246883	1.494626
13	6	0	-2.755791	-0.311206	1.499461
14	6	0	-2.412840	-2.344509	-0.213176
15	6	0	2.890460	1.164980	0.668965
16	6	0	3.026016	-0.610987	-1.311685
17	6	0	3.456648	-0.148494	0.092645
18	7	0	0.558549	2.640065	-0.519810
19	7	0	-1.854763	2.012614	-0.146807
20	16	0	-0.947927	3.050919	-1.045084
21	8	0	4.197468	-0.840032	0.765021
22	6	0	-3.159445	-1.061111	0.202018
23	8	0	-4.090446	-0.659449	-0.463951
24	1	0	-0.070834	-3.531081	0.602807
25	1	0	2.235413	-2.801517	0.119472
26	1	0	0.728505	0.114025	-2.649033
27	1	0	-1.577790	-0.622980	-2.174895
28	1	0	1.805251	-0.450586	2.601279
29	1	0	-0.536578	-1.071398	2.950518
30	1	0	-2.861074	-1.009120	2.340741
31	1	0	-3.495918	0.485976	1.613581
32	1	0	-3.029402	-2.804243	-0.993316
33	1	0	-2.380170	-3.033539	0.640474
34	1	0	2.959727	1.969982	-0.069170
35	1	0	3.517447	1.418870	1.529169
36	1	0	3.012109	0.237785	-2.004319
37	1	0	3.785746	-1.325010	-1.647165

Table S12. Coordinates of **5Ba**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.726952	1.542783	0.592585

2	6	0	-0.696049	-2.338440	-0.769919
3	6	0	0.695757	-2.338481	-0.769925
4	6	0	1.412341	-1.298260	-1.380971
5	6	0	0.698775	-0.346809	-2.115188
6	6	0	-0.698971	-0.346767	-2.115179
7	6	0	-1.412581	-1.298178	-1.380956
8	6	0	-0.726672	1.542880	0.592545
9	6	0	1.457432	0.548671	1.317883
10	6	0	0.714974	-0.287227	2.117873
11	6	0	-0.715026	-0.287132	2.117834
12	6	0	-1.457325	0.548867	1.317802
13	6	0	-2.941634	0.347987	1.076215
14	6	0	-2.906985	-1.146239	-1.131118
15	6	0	2.941714	0.347555	1.076342
16	6	0	2.906765	-1.146391	-1.131170
17	6	0	3.193767	-1.004230	0.375310
18	7	0	1.260676	2.499236	-0.173935
19	7	0	-1.260223	2.499437	-0.173967
20	16	0	0.000300	3.328970	-0.830423
21	8	0	3.569663	-1.963040	1.021553
22	6	0	-3.193957	-1.003831	0.375348
23	8	0	-3.570013	-1.962493	1.021717
24	1	0	-1.235018	-3.109258	-0.224708
25	1	0	1.234688	-3.109327	-0.224718
26	1	0	1.233482	0.444780	-2.634217
27	1	0	-1.233637	0.444858	-2.634197
28	1	0	1.225606	-1.054409	2.694577
29	1	0	-1.225793	-1.054242	2.694513
30	1	0	-3.326398	1.175370	0.472540
31	1	0	-3.491356	0.311074	2.021545
32	1	0	-3.285282	-0.271702	-1.672163
33	1	0	-3.459818	-2.030569	-1.465637
34	1	0	3.326666	1.174934	0.472785
35	1	0	3.491390	0.310405	2.021688
36	1	0	3.285044	-0.271773	-1.672093
37	1	0	3.459575	-2.030673	-1.465858

Table S13. Coordinates of **2BB**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.790648	2.576898	1.285565
2	6	0	-0.211539	-0.005918	-1.027702
3	6	0	-3.557562	-0.858342	-1.726573
4	6	0	-4.314503	1.848063	0.858351
5	6	0	-0.169575	-1.145412	-0.214825
6	6	0	-0.565890	1.264094	-0.561417
7	6	0	-1.041626	1.362904	0.762795
8	6	0	-0.825501	0.271079	1.608787
9	6	0	-3.230748	-1.958364	-0.919289
10	6	0	-3.989316	0.340364	-1.165305
11	6	0	-4.110606	0.485040	0.225250
12	6	0	-3.940649	-0.658937	1.008943
13	6	0	-3.508521	-1.860810	0.446315
14	6	0	2.130199	3.095999	-1.132528
15	6	0	-2.499373	-3.156443	-1.490178
16	6	0	0.001794	-2.515065	-0.859644
17	6	0	-0.322720	-0.959372	1.174092
18	6	0	3.193704	-0.294653	0.454705
19	6	0	3.089197	0.808296	-0.489054
20	6	0	2.715220	-0.159391	1.801808
21	6	0	2.320291	1.103041	2.163125
22	6	0	2.216032	2.187970	1.233898
23	6	0	2.501918	2.059452	-0.100753
24	7	0	3.735409	-1.397284	-0.071864
25	7	0	3.552985	0.515636	-1.707161
26	16	0	4.088191	-1.042935	-1.643813
27	6	0	2.571497	-1.358484	2.707795
28	6	0	0.047316	-2.019812	2.196859
29	6	0	-0.420398	2.463501	-1.488451
30	6	0	-3.163211	2.859874	0.616729
31	6	0	0.991369	2.665455	-2.096324
32	6	0	-1.045191	-2.866851	-1.950265

33	6	0	1.545364	-2.423071	2.233640
34	1	0	-1.184249	3.486951	1.170390
35	1	0	-1.945420	2.457907	2.366168
36	1	0	0.032636	-0.116678	-2.083062
37	1	0	-3.412359	-0.920450	-2.803570
38	1	0	-4.468124	1.728090	1.938965
39	1	0	-5.233269	2.309234	0.468238
40	1	0	-1.073761	0.380331	2.663831
41	1	0	-4.178412	1.193850	-1.813935
42	1	0	-4.073298	-0.592736	2.086752
43	1	0	-3.314438	-2.713376	1.094123
44	1	0	1.843077	4.023131	-0.619467
45	1	0	3.005750	3.330667	-1.751705
46	1	0	-2.486442	-3.966610	-0.748993
47	1	0	-3.042132	-3.546504	-2.362850
48	1	0	0.993561	-2.584816	-1.327980
49	1	0	-0.019564	-3.299519	-0.095778
50	1	0	1.972775	1.273823	3.179201
51	1	0	1.795213	3.123856	1.594528
52	1	0	2.299629	-1.011329	3.713093
53	1	0	3.540039	-1.868081	2.798699
54	1	0	-0.530782	-2.939586	2.026506
55	1	0	-0.248434	-1.665206	3.193261
56	1	0	-0.707795	3.383357	-0.967535
57	1	0	-1.122714	2.365976	-2.329654
58	1	0	-3.507599	3.836494	0.984308
59	1	0	-3.020091	2.977933	-0.464209
60	1	0	0.908065	3.448139	-2.862254
61	1	0	1.306200	1.758547	-2.623411
62	1	0	-0.683857	-3.765929	-2.467756
63	1	0	-1.065432	-2.072015	-2.706477
64	1	0	1.637102	-3.277672	2.917652
65	1	0	1.856361	-2.785901	1.248983

Table S14. Coordinates of **2CB**

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

1	6	0	-1.817948	2.572654	1.245995
2	6	0	-0.153871	-0.016745	-0.996690
3	6	0	-3.469697	-0.877961	-1.795790
4	6	0	-4.327503	1.847488	0.735707
5	6	0	-0.130992	-1.155079	-0.175908
6	6	0	-0.526787	1.252919	-0.553219
7	6	0	-1.049228	1.357312	0.755968
8	6	0	-0.867443	0.269475	1.610663
9	6	0	-3.169332	-1.970023	-0.967839
10	6	0	-3.926564	0.323579	-1.261183
11	6	0	-4.100430	0.479157	0.122526
12	6	0	-3.958118	-0.658319	0.921173
13	6	0	-3.500771	-1.863045	0.385157
14	6	0	2.201090	3.033641	-1.212100
15	6	0	-2.413833	-3.170576	-1.501889
16	6	0	0.074744	-2.515918	-0.828989
17	6	0	-0.339771	-0.963227	1.202777
18	6	0	3.168411	-0.366175	0.408372
19	6	0	3.100741	0.729323	-0.548080
20	6	0	2.717320	-0.193852	1.759114
21	6	0	2.385536	1.090546	2.110887
22	6	0	2.303503	2.163087	1.167116
23	6	0	2.563814	2.004748	-0.170321
24	7	0	3.656551	-1.496972	-0.112064
25	7	0	3.536376	0.403081	-1.768422
26	16	0	4.006550	-1.175741	-1.690190
27	6	0	2.542728	-1.379135	2.687291
28	6	0	-0.004844	-1.991982	2.271222
29	6	0	-0.370264	2.448998	-1.484401
30	6	0	-3.166086	2.855639	0.528978
31	6	0	1.025083	2.618369	-2.137307
32	6	0	1.111203	-1.554869	3.256671
33	6	0	-0.952940	-2.874874	-1.935867
34	1	0	-1.206445	3.481505	1.149385
35	1	0	-2.010980	2.457775	2.320848
36	1	0	0.129493	-0.134901	-2.041078
37	1	0	-3.283577	-0.948000	-2.865952
38	1	0	-4.522266	1.737219	1.810740
39	1	0	-5.230076	2.306408	0.307001

40	1	0	-1.168256	0.379573	2.652177
41	1	0	-4.093614	1.171154	-1.923503
42	1	0	-4.133348	-0.584126	1.992464
43	1	0	-3.328663	-2.709944	1.046475
44	1	0	1.954323	3.978456	-0.710399
45	1	0	3.067046	3.229711	-1.857563
46	1	0	-2.933927	-3.580329	-2.379447
47	1	0	-2.410441	-3.968108	-0.747095
48	1	0	1.072378	-2.560399	-1.285971
49	1	0	0.059477	-3.312789	-0.079155
50	1	0	2.067758	1.295483	3.130471
51	1	0	1.922418	3.119072	1.519348
52	1	0	2.846583	-2.289830	2.160646
53	1	0	3.225983	-1.276282	3.542029
54	1	0	0.289014	-2.945763	1.822930
55	1	0	-0.900161	-2.203456	2.873964
56	1	0	-0.616388	3.374504	-0.951816
57	1	0	-1.102510	2.375099	-2.302461
58	1	0	-3.520363	3.834514	0.880784
59	1	0	-2.986703	2.969359	-0.546928
60	1	0	0.933027	3.397233	-2.906079
61	1	0	1.307004	1.702831	-2.667857
62	1	0	1.166919	-2.316698	4.046005
63	1	0	0.805678	-0.626116	3.755150
64	1	0	-0.577136	-3.773045	-2.444589
65	1	0	-0.964040	-2.081939	-2.694285

Table S15. Coordinates of **2BaB**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.782787	2.669227	0.991362
2	6	0	-0.088621	0.008881	-1.153116
3	6	0	-3.486868	-0.986455	-1.689643
4	6	0	-4.306009	1.851372	0.721339
5	6	0	-0.102897	-1.111635	-0.302770
6	6	0	-0.460799	1.291844	-0.752499
7	6	0	-1.012162	1.437411	0.544169

8	6	0	-0.861628	0.370732	1.427700
9	6	0	-3.178128	-2.041096	-0.818092
10	6	0	-3.937128	0.236781	-1.203731
11	6	0	-4.096630	0.452956	0.172949
12	6	0	-3.954239	-0.649970	1.018896
13	6	0	-3.502821	-1.877796	0.531120
14	6	0	2.351632	2.933195	-1.295093
15	6	0	0.891844	3.454300	-1.293727
16	6	0	-2.420417	-3.257670	-1.312615
17	6	0	0.101873	-2.488341	-0.918843
18	6	0	-0.346269	-0.883424	1.062703
19	6	0	3.150251	-0.461709	0.441916
20	6	0	3.127146	0.601829	-0.552818
21	6	0	2.707249	-0.222616	1.783474
22	6	0	2.444330	1.088928	2.093443
23	6	0	2.418628	2.132072	1.116331
24	6	0	2.656373	1.913201	-0.218265
25	7	0	3.585837	-1.631378	-0.038418
26	7	0	3.544293	0.211755	-1.761476
27	16	0	3.945031	-1.380495	-1.626585
28	6	0	2.445387	-1.363892	2.743332
29	6	0	0.971086	-1.476546	3.213679
30	6	0	-0.088711	-1.901608	2.163148
31	6	0	-0.234579	2.462803	-1.695089
32	6	0	-1.015661	-2.947513	-1.894662
33	6	0	-3.189209	2.865112	0.358611
34	1	0	-1.897237	2.636937	2.083184
35	1	0	-1.212358	3.582620	0.777524
36	1	0	0.236688	-0.132947	-2.182933
37	1	0	-3.308089	-1.100655	-2.756942
38	1	0	-4.411800	1.803097	1.813207
39	1	0	-5.251023	2.267186	0.342231
40	1	0	-1.189077	0.508793	2.457542
41	1	0	-4.104047	1.055555	-1.900800
42	1	0	-4.119326	-0.529016	2.087723
43	1	0	-3.326254	-2.695959	1.226679
44	1	0	3.010809	3.804535	-1.175078
45	1	0	2.591155	2.499608	-2.271537
46	1	0	0.668380	3.879743	-0.307869
47	1	0	0.847924	4.294752	-1.999739

48	1	0	-2.993370	-3.759317	-2.105893
49	1	0	-2.323991	-3.987285	-0.497762
50	1	0	1.039528	-2.496985	-1.488826
51	1	0	0.221752	-3.252259	-0.145190
52	1	0	2.138197	1.342141	3.106071
53	1	0	2.096510	3.117917	1.443717
54	1	0	2.759639	-2.303533	2.277153
55	1	0	3.067290	-1.238981	3.640642
56	1	0	0.943921	-2.218929	4.022795
57	1	0	0.667357	-0.524182	3.666925
58	1	0	0.213253	-2.866068	1.744549
59	1	0	-1.024535	-2.090044	2.709295
60	1	0	-1.153278	3.054521	-1.801720
61	1	0	-0.010330	2.072412	-2.696174
62	1	0	-1.120720	-2.202250	-2.693536
63	1	0	-0.655555	-3.863573	-2.382607
64	1	0	-3.541370	3.859489	0.665933
65	1	0	-3.092881	2.905719	-0.733196

Table S16. Coordinates of **2CaB**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.851310	2.645228	1.095697
2	6	0	-0.163138	0.012991	-1.086307
3	6	0	-3.523729	-0.998742	-1.689612
4	6	0	-4.346256	1.744671	0.832608
5	6	0	-0.131388	-1.098954	-0.230671
6	6	0	-0.549488	1.292314	-0.678781
7	6	0	-1.059023	1.433723	0.632651
8	6	0	-0.841061	0.379979	1.522189
9	6	0	-3.171049	-2.072973	-0.859496
10	6	0	-3.983708	0.200220	-1.153858
11	6	0	-4.107036	0.371898	0.233095
12	6	0	-3.912096	-0.751031	1.041227
13	6	0	-3.453239	-1.954822	0.503703
14	6	0	2.194236	3.010705	-1.291784
15	6	0	-2.401501	-3.256489	-1.408545

16	6	0	0.072062	-2.489271	-0.820049
17	6	0	-0.317363	-0.863605	1.144357
18	6	0	3.190032	-0.335259	0.442537
19	6	0	3.095698	0.724355	-0.551359
20	6	0	2.730659	-0.125977	1.785605
21	6	0	2.376940	1.163133	2.093534
22	6	0	2.293328	2.207042	1.118701
23	6	0	2.548218	2.006286	-0.214534
24	7	0	3.696851	-1.475081	-0.038787
25	7	0	3.532241	0.361453	-1.761157
26	16	0	4.032225	-1.202978	-1.630632
27	6	0	2.551068	-1.277974	2.743865
28	6	0	0.015958	-1.889050	2.215939
29	6	0	-0.381804	2.459950	-1.637485
30	6	0	-0.966217	-2.916390	-1.891924
31	6	0	1.500523	-2.332834	2.304867
32	6	0	0.721233	3.490339	-1.270669
33	6	0	-3.271177	2.806661	0.483661
34	1	0	-1.308111	3.574526	0.878408
35	1	0	-1.950036	2.604973	2.188788
36	1	0	0.123149	-0.127182	-2.127691
37	1	0	-3.374352	-1.079096	-2.764708
38	1	0	-4.428196	1.656280	1.924007
39	1	0	-5.311700	2.141593	0.486290
40	1	0	-1.116736	0.522528	2.566387
41	1	0	-4.190889	1.034839	-1.820819
42	1	0	-4.046259	-0.664806	2.117517
43	1	0	-3.239963	-2.789304	1.168947
44	1	0	2.831806	3.900432	-1.190342
45	1	0	2.429615	2.576838	-2.269221
46	1	0	-2.937440	-3.690778	-2.264481
47	1	0	-2.346365	-4.046091	-0.647287
48	1	0	0.072613	-3.242599	-0.025592
49	1	0	1.063752	-2.551173	-1.288231
50	1	0	2.047292	1.389583	3.104841
51	1	0	1.908516	3.169435	1.447634
52	1	0	3.504339	-1.809505	2.866290
53	1	0	2.280630	-0.878537	3.729941
54	1	0	-0.583059	-2.799870	2.070867
55	1	0	-0.290791	-1.487382	3.190922

56	1	0	-1.320372	3.021661	-1.731213
57	1	0	-0.166604	2.066225	-2.639288
58	1	0	-0.569675	-3.813411	-2.386665
59	1	0	-1.026761	-2.144524	-2.669612
60	1	0	1.550908	-3.153288	3.033578
61	1	0	1.821454	-2.755506	1.348152
62	1	0	0.640265	4.318701	-1.987469
63	1	0	0.501926	3.923744	-0.287544
64	1	0	-3.653835	3.780131	0.820059
65	1	0	-3.190609	2.877863	-0.607713

Table S17. Coordinates of **2BC**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.817653	2.691775	1.052632
2	6	0	-0.208287	-0.090385	-1.014158
3	6	0	-3.402322	-0.928740	-1.825693
4	6	0	-4.315775	1.941991	0.528620
5	6	0	-0.174727	-1.145641	-0.098996
6	6	0	-0.570457	1.220959	-0.678106
7	6	0	-1.051972	1.447729	0.625981
8	6	0	-0.832872	0.442374	1.577286
9	6	0	-3.188542	-1.986413	-0.932938
10	6	0	-3.836229	0.315851	-1.371379
11	6	0	-4.087894	0.542998	-0.012859
12	6	0	-4.035765	-0.560908	0.846714
13	6	0	-3.586480	-1.800512	0.395856
14	6	0	2.127619	2.974888	-1.423010
15	6	0	-2.448582	-3.237476	-1.362239
16	6	0	0.008249	-2.572920	-0.603183
17	6	0	-0.336503	-0.824955	1.266922
18	6	0	3.177537	-0.245116	0.492890
19	6	0	3.080725	0.760399	-0.554724
20	6	0	2.699355	0.024690	1.819514
21	6	0	2.314455	1.319695	2.054739
22	6	0	2.214919	2.307936	1.022902

23	6	0	2.497565	2.045909	-0.292888
24	7	0	3.714976	-1.396721	0.078511
25	7	0	3.546158	0.347546	-1.736880
26	16	0	4.073785	-1.199758	-1.519514
27	6	0	2.549987	-1.077568	2.840449
28	6	0	0.026594	-1.783666	2.387637
29	6	0	-0.421791	2.307206	-1.734882
30	6	0	-3.261209	2.425960	1.558540
31	6	0	0.996246	2.446599	-2.346702
32	6	0	-0.958686	-3.012053	-1.734024
33	6	0	1.523674	-2.183178	2.471794
34	1	0	-1.281728	3.194866	1.871353
35	1	0	-1.869199	3.419785	0.237243
36	1	0	0.037945	-0.301106	-2.053347
37	1	0	-3.155683	-1.054634	-2.878353
38	1	0	-5.295747	1.995016	1.024730
39	1	0	-4.359194	2.654034	-0.306196
40	1	0	-1.071348	0.656531	2.618776
41	1	0	-3.922592	1.141271	-2.075477
42	1	0	-4.279225	-0.436472	1.899921
43	1	0	-3.484053	-2.620981	1.103415
44	1	0	3.005773	3.151159	-2.057729
45	1	0	1.834215	3.946747	-1.005273
46	1	0	-2.937223	-3.682289	-2.240799
47	1	0	-2.508192	-3.989411	-0.564103
48	1	0	-0.092208	-3.279546	0.228008
49	1	0	1.031751	-2.706722	-0.980811
50	1	0	1.970323	1.592373	3.049663
51	1	0	1.799845	3.277291	1.289411
52	1	0	3.517331	-1.576768	2.985812
53	1	0	2.274976	-0.630604	3.804661
54	1	0	-0.276140	-1.337683	3.344481
55	1	0	-0.550846	-2.715398	2.299653
56	1	0	-0.716669	3.281481	-1.332049
57	1	0	-1.113600	2.106775	-2.566692
58	1	0	-3.632523	3.366614	1.987868
59	1	0	-3.222473	1.710188	2.389199
60	1	0	0.919305	3.146487	-3.189523
61	1	0	1.315652	1.490771	-2.775408
62	1	0	-0.577949	-3.960974	-2.135600

63	1	0	-0.905453	-2.294376	-2.561946
64	1	0	1.610860	-2.964203	3.239226
65	1	0	1.838498	-2.644419	1.530497

Table S18. Coordinates of **2CC**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.897299	2.709512	0.923837
2	6	0	-0.151222	-0.126494	-0.943426
3	6	0	-3.288714	-1.049110	-1.883131
4	6	0	-4.354525	1.900771	0.303663
5	6	0	-0.135073	-1.143907	0.018619
6	6	0	-0.547819	1.188980	-0.683221
7	6	0	-1.090056	1.462701	0.590629
8	6	0	-0.901382	0.502554	1.590304
9	6	0	-3.092643	-2.062173	-0.936323
10	6	0	-3.766004	0.204726	-1.502939
11	6	0	-4.079639	0.484807	-0.167566
12	6	0	-4.045148	-0.580247	0.740805
13	6	0	-3.552412	-1.828025	0.364720
14	6	0	2.173049	2.862568	-1.593257
15	6	0	-2.310018	-3.314154	-1.278338
16	6	0	0.098430	-2.581606	-0.434312
17	6	0	-0.364722	-0.768808	1.358643
18	6	0	3.166615	-0.286725	0.455832
19	6	0	3.098201	0.677488	-0.632640
20	6	0	2.700643	0.051303	1.769712
21	6	0	2.356398	1.367199	1.952660
22	6	0	2.272016	2.309408	0.879378
23	6	0	2.543638	1.983942	-0.425152
24	7	0	3.670784	-1.469288	0.087527
25	7	0	3.548889	0.203533	-1.797864
26	16	0	4.033748	-1.347353	-1.515764
27	6	0	2.531303	-1.008547	2.840030
28	6	0	1.111060	-1.094217	3.455462
29	6	0	-0.028109	-1.643571	2.555674
30	6	0	-0.395545	2.233259	-1.783396

31	6	0	-3.361155	2.441446	1.365651
32	6	0	1.000395	2.315422	-2.452709
33	6	0	-0.809462	-3.072789	-1.592330
34	1	0	-1.411857	3.255925	1.746060
35	1	0	-1.917691	3.401131	0.075920
36	1	0	0.145377	-0.379044	-1.959268
37	1	0	-2.995131	-1.215273	-2.918012
38	1	0	-5.359498	1.958572	0.746453
39	1	0	-4.363853	2.577825	-0.560758
40	1	0	-1.202104	0.752702	2.607913
41	1	0	-3.838968	0.996697	-2.245961
42	1	0	-4.336904	-0.415542	1.776075
43	1	0	-3.463665	-2.614527	1.111505
44	1	0	3.037060	2.977961	-2.260255
45	1	0	1.916841	3.863570	-1.222511
46	1	0	-2.750182	-3.805040	-2.157917
47	1	0	-2.390956	-4.033152	-0.452187
48	1	0	-0.027887	-3.270679	0.407033
49	1	0	1.140487	-2.704604	-0.759591
50	1	0	2.029007	1.698069	2.935269
51	1	0	1.878713	3.298273	1.104137
52	1	0	2.812639	-1.980530	2.421395
53	1	0	3.235899	-0.814176	3.661083
54	1	0	1.176116	-1.749367	4.334646
55	1	0	0.821948	-0.106627	3.837294
56	1	0	0.244607	-2.654980	2.239735
57	1	0	-0.916170	-1.753460	3.194614
58	1	0	-0.644165	3.228649	-1.400948
59	1	0	-1.125966	2.031610	-2.581599
60	1	0	-3.766500	3.392714	1.736979
61	1	0	-3.356005	1.760300	2.225748
62	1	0	0.904529	2.979444	-3.322089
63	1	0	1.288772	1.337191	-2.851603
64	1	0	-0.394897	-4.027261	-1.944306
65	1	0	-0.732083	-2.382701	-2.441539

Table S19. Coordinates of **2BaC**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.623278	2.739615	0.707858
2	6	0	-0.081755	-0.224450	-1.139663
3	6	0	-3.387438	-0.936432	-1.731970
4	6	0	-4.186717	2.104846	0.431112
5	6	0	-0.134270	-1.239053	-0.171088
6	6	0	-0.396756	1.111397	-0.881503
7	6	0	-0.921900	1.423899	0.393092
8	6	0	-0.789992	0.461374	1.393995
9	6	0	-3.239382	-1.949482	-0.776843
10	6	0	-3.772367	0.350178	-1.359788
11	6	0	-4.039685	0.666348	-0.023052
12	6	0	-4.055416	-0.386571	0.900167
13	6	0	-3.653115	-1.669066	0.531071
14	6	0	2.366054	2.829420	-1.537837
15	6	0	-2.570349	-3.263846	-1.131637
16	6	0	-0.023392	-2.688803	-0.624504
17	6	0	-0.333525	-0.844174	1.165346
18	6	0	3.106886	-0.436242	0.447092
19	6	0	3.085055	0.543483	-0.629434
20	6	0	2.722419	-0.073795	1.778826
21	6	0	2.508077	1.266909	1.987775
22	6	0	2.482368	2.228388	0.929548
23	6	0	2.672187	1.893806	-0.388917
24	7	0	3.484779	-1.656237	0.049612
25	7	0	3.444469	0.042427	-1.815702
26	16	0	3.791620	-1.547422	-1.564949
27	6	0	2.475433	-1.126412	2.839221
28	6	0	-0.064874	-1.736163	2.368144
29	6	0	-0.169503	2.155038	-1.962291
30	6	0	-3.035375	2.614029	1.338502
31	6	0	-1.108750	-3.141074	-1.637494
32	1	0	-1.010731	3.328395	1.407449

33	1	0	-1.705994	3.350730	-0.197580
34	1	0	0.209852	-0.494066	-2.153596
35	1	0	-3.128891	-1.132835	-2.770526
36	1	0	-5.121753	2.228705	0.995875
37	1	0	-4.269191	2.760336	-0.446080
38	1	0	-1.076101	0.729607	2.410196
39	1	0	-3.805003	1.136432	-2.111541
40	1	0	-4.313021	-0.187728	1.938860
41	1	0	-3.601791	-2.451285	1.286000
42	1	0	2.961068	3.747294	-1.434213
43	1	0	2.680297	2.358026	-2.474641
44	1	0	-3.142313	-3.771821	-1.921626
45	1	0	-2.595013	-3.932103	-0.260557
46	1	0	-0.054399	-3.367059	0.233724
47	1	0	0.951694	-2.856929	-1.099822
48	1	0	2.249452	1.611177	2.986810
49	1	0	2.205016	3.249610	1.182530
50	1	0	2.781002	-2.103514	2.450832
51	1	0	3.114008	-0.923325	3.710008
52	1	0	0.235489	-2.738980	2.050608
53	1	0	-0.991269	-1.865768	2.946972
54	1	0	-1.112405	2.668263	-2.200266
55	1	0	0.133118	1.645927	-2.886197
56	1	0	-3.320995	3.612580	1.696692
57	1	0	-2.982339	1.978919	2.231609
58	1	0	-0.809851	-4.131097	-2.008207
59	1	0	-1.088722	-2.476046	-2.509976
60	6	0	0.877384	3.254764	-1.638490
61	1	0	0.812920	4.011762	-2.431969
62	1	0	0.593036	3.765014	-0.710011
63	6	0	1.011244	-1.199417	3.347997
64	1	0	0.710058	-0.208516	3.711365
65	1	0	1.006509	-1.857331	4.227683

Table S20. Coordinates of **2CaC**

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

1	6	0	-1.743743	2.697064	0.881881
2	6	0	-0.138168	-0.147566	-1.093324
3	6	0	-3.398455	-0.950167	-1.759295
4	6	0	-4.276137	1.969258	0.542290
5	6	0	-0.140074	-1.189914	-0.158142
6	6	0	-0.494459	1.169276	-0.784185
7	6	0	-0.996936	1.423358	0.509188
8	6	0	-0.800462	0.437360	1.480427
9	6	0	-3.201685	-1.996445	-0.849666
10	6	0	-3.819746	0.306176	-1.327096
11	6	0	-4.074087	0.557929	0.026148
12	6	0	-4.035991	-0.531657	0.904792
13	6	0	-3.599697	-1.783821	0.475495
14	6	0	2.204389	2.962704	-1.437287
15	6	0	-2.489521	-3.269140	-1.264960
16	6	0	0.011094	-2.627861	-0.638458
17	6	0	-0.315526	-0.843761	1.196990
18	6	0	3.151280	-0.314254	0.447219
19	6	0	3.064959	0.696609	-0.596692
20	6	0	2.719457	-0.028425	1.785108
21	6	0	2.397284	1.282437	2.032642
22	6	0	2.322026	2.278938	1.008299
23	6	0	2.554245	2.006791	-0.316547
24	7	0	3.625402	-1.487737	0.015835
25	7	0	3.472335	0.263793	-1.793630
26	16	0	3.937577	-1.303397	-1.592916
27	6	0	2.549260	-1.124556	2.809627
28	6	0	0.015993	-1.787631	2.340506
29	6	0	-0.323382	2.253779	-1.834638
30	6	0	-3.156706	2.482323	1.486784
31	6	0	-1.015871	-3.076430	-1.711525
32	1	0	-1.161681	3.267363	1.621511
33	1	0	-1.837718	3.352800	0.009604
34	1	0	0.135715	-0.374022	-2.122505
35	1	0	-3.149803	-1.094988	-2.808855
36	1	0	-5.221636	2.033356	1.099692
37	1	0	-4.374926	2.659117	-0.306403
38	1	0	-1.053587	0.668240	2.514517
39	1	0	-3.893280	1.120983	-2.044823
40	1	0	-4.280036	-0.385254	1.955253

41	1	0	-3.509164	-2.594116	1.196345
42	1	0	2.787468	3.887750	-1.327765
43	1	0	2.507525	2.517412	-2.390440
44	1	0	-3.021756	-3.739967	-2.103964
45	1	0	-2.521925	-3.991708	-0.438593
46	1	0	-0.054327	-3.317977	0.209423
47	1	0	1.012155	-2.777209	-1.065543
48	1	0	2.091006	1.566288	3.036943
49	1	0	1.965065	3.266451	1.292527
50	1	0	3.507480	-1.640902	2.957558
51	1	0	2.283988	-0.667523	3.771873
52	1	0	-0.578803	-2.709338	2.263934
53	1	0	-0.288716	-1.317126	3.284852
54	1	0	-1.283504	2.752214	-2.030405
55	1	0	-0.033095	1.783986	-2.783060
56	1	0	-3.489055	3.448781	1.889833
57	1	0	-3.082625	1.806552	2.347926
58	1	0	-0.669376	-4.040207	-2.108800
59	1	0	-0.988999	-2.376966	-2.556277
60	6	0	1.503916	-2.214618	2.449029
61	1	0	1.819670	-2.697685	1.519356
62	1	0	1.567473	-2.983388	3.231054
63	6	0	0.707800	3.364507	-1.498493
64	1	0	0.614832	4.142185	-2.268780
65	1	0	0.429908	3.843295	-0.551453

Table S21. Coordinates of **2BCa**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.721463	2.469058	1.436892
2	6	0	-0.227270	0.003998	-1.060494
3	6	0	-3.474187	-0.616328	-1.819351
4	6	0	-4.273452	1.887835	0.945917
5	6	0	-0.161453	-1.177658	-0.315458
6	6	0	-0.564656	1.249843	-0.516096
7	6	0	-1.013456	1.274291	0.818240

8	6	0	-0.786722	0.131728	1.596714
9	6	0	-3.253816	-1.796661	-1.099667
10	6	0	-3.901118	0.547794	-1.182332
11	6	0	-4.103452	0.576585	0.203337
12	6	0	-4.034028	-0.639886	0.890837
13	6	0	-3.626545	-1.808313	0.249961
14	6	0	2.106169	3.144468	-1.077769
15	6	0	-2.550989	-2.985447	-1.728326
16	6	0	-0.018419	-2.505581	-1.042800
17	6	0	-0.284984	-1.069056	1.088426
18	6	0	3.197949	-0.278644	0.411646
19	6	0	3.078116	0.846773	-0.502377
20	6	0	2.732226	-0.179639	1.766262
21	6	0	2.335467	1.071446	2.163926
22	6	0	2.221471	2.180362	1.264979
23	6	0	2.494701	2.086472	-0.075292
24	7	0	3.735853	-1.366052	-0.149908
25	7	0	3.524936	0.585500	-1.734150
26	16	0	4.062559	-0.972514	-1.717384
27	6	0	2.606066	-1.401774	2.643947
28	6	0	0.123297	-2.171314	2.052332
29	6	0	-0.443473	2.496756	-1.381999
30	6	0	-3.082201	2.870520	0.804895
31	6	0	0.947463	2.730919	-2.024810
32	6	0	-1.258177	-3.441905	-1.004000
33	6	0	1.640518	-2.496363	2.116365
34	1	0	-1.076393	3.359269	1.396008
35	1	0	-1.879248	2.267842	2.504740
36	1	0	-0.021517	-0.054346	-2.128089
37	1	0	-3.244374	-0.589460	-2.882704
38	1	0	-4.449830	1.682447	2.009986
39	1	0	-5.168195	2.414715	0.583821
40	1	0	-1.009453	0.184726	2.661784
41	1	0	-4.002283	1.463486	-1.761883
42	1	0	-4.234473	-0.660474	1.960171
43	1	0	-3.524514	-2.722578	0.830968
44	1	0	1.828241	4.060854	-0.540860
45	1	0	2.969291	3.391619	-1.709263
46	1	0	-3.227727	-3.852314	-1.750230
47	1	0	-2.318254	-2.757008	-2.776816

48	1	0	0.824605	-3.080291	-0.639911
49	1	0	0.231590	-2.305765	-2.093080
50	1	0	1.994890	1.213563	3.186764
51	1	0	1.802566	3.105995	1.653379
52	1	0	2.292533	-1.085409	3.647305
53	1	0	3.590785	-1.875860	2.755277
54	1	0	-0.388664	-3.111659	1.808247
55	1	0	-0.218712	-1.898656	3.059739
56	1	0	-0.709148	3.388022	-0.803216
57	1	0	-1.174900	2.445348	-2.202364
58	1	0	-3.385685	3.818537	1.270318
59	1	0	-2.936218	3.092244	-0.258718
60	1	0	0.835773	3.536036	-2.763383
61	1	0	1.256165	1.843667	-2.587743
62	1	0	-0.951279	-4.394076	-1.458076
63	1	0	-1.504480	-3.675700	0.038497
64	1	0	1.753895	-3.364901	2.779214
65	1	0	1.997048	-2.817452	1.133258

Table S22. Coordinates of **2CCa**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.729336	2.523458	1.379768
2	6	0	-0.163044	0.079194	-1.087142
3	6	0	-3.378688	-0.651817	-1.857402
4	6	0	-4.259188	1.885931	0.853475
5	6	0	-0.125908	-1.110096	-0.348960
6	6	0	-0.502278	1.320661	-0.540116
7	6	0	-0.994132	1.335251	0.782140
8	6	0	-0.811006	0.183523	1.553599
9	6	0	-3.187698	-1.826246	-1.120439
10	6	0	-3.817618	0.521000	-1.245091
11	6	0	-4.063402	0.565144	0.132886
12	6	0	-4.023560	-0.645622	0.833814
13	6	0	-3.602919	-1.822846	0.217213
14	6	0	2.241974	3.103197	-1.042592
15	6	0	-2.464576	-3.020700	-1.714126

16	6	0	0.052740	-2.434740	-1.073160
17	6	0	-0.299744	-1.015600	1.046633
18	6	0	3.135615	-0.411298	0.367637
19	6	0	3.068431	0.732768	-0.529263
20	6	0	2.739585	-0.295907	1.740911
21	6	0	2.447562	0.975573	2.167550
22	6	0	2.363167	2.096167	1.281670
23	6	0	2.583130	2.001612	-0.069502
24	7	0	3.566317	-1.529088	-0.227039
25	7	0	3.450077	0.455946	-1.779785
26	16	0	3.865318	-1.138973	-1.799388
27	6	0	2.560605	-1.522141	2.610842
28	6	0	0.051688	-2.139759	2.009552
29	6	0	-0.335248	2.578451	-1.382428
30	6	0	-3.083848	2.888428	0.714058
31	6	0	1.068749	2.780173	-2.007448
32	6	0	1.104696	-1.769355	3.086702
33	6	0	-1.149149	-3.414482	-0.992192
34	1	0	-1.100155	3.424638	1.342007
35	1	0	-1.904767	2.329165	2.446174
36	1	0	0.082685	0.028545	-2.146360
37	1	0	-3.115438	-0.636094	-2.913139
38	1	0	-4.445207	1.693453	1.918369
39	1	0	-5.158665	2.392239	0.473915
40	1	0	-1.084685	0.224991	2.607369
41	1	0	-3.894841	1.431165	-1.836740
42	1	0	-4.260408	-0.654934	1.895975
43	1	0	-3.525177	-2.733229	0.808534
44	1	0	2.008573	4.015324	-0.477936
45	1	0	3.117337	3.328986	-1.665809
46	1	0	-2.250922	-2.826085	-2.773389
47	1	0	-3.119042	-3.904305	-1.692859
48	1	0	0.268221	-2.231248	-2.130274
49	1	0	0.933690	-2.965979	-0.688633
50	1	0	2.167943	1.133832	3.206834
51	1	0	2.020051	3.042790	1.693180
52	1	0	2.925949	-2.400665	2.069008
53	1	0	3.186511	-1.427287	3.508885
54	1	0	0.413034	-3.015699	1.461398
55	1	0	-0.852559	-2.468840	2.542704

56	1	0	-0.580412	3.466189	-0.788733
57	1	0	-1.058415	2.567516	-2.211868
58	1	0	-3.415019	3.839281	1.154133
59	1	0	-2.918978	3.092397	-0.350643
60	1	0	0.995580	3.620412	-2.710926
61	1	0	1.342032	1.906314	-2.607956
62	1	0	1.137761	-2.594149	3.811294
63	1	0	0.757606	-0.890345	3.644631
64	1	0	-0.816785	-4.368956	-1.423200
65	1	0	-1.374944	-3.623392	0.060494

Table S23. Coordinates of **2BaCa**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.724247	2.634615	1.154760
2	6	0	-0.127351	0.043411	-1.143683
3	6	0	-3.372120	-0.780924	-1.800523
4	6	0	-4.253269	1.871476	0.796954
5	6	0	-0.115535	-1.103314	-0.335346
6	6	0	-0.465999	1.317165	-0.679300
7	6	0	-0.974826	1.416611	0.636509
8	6	0	-0.800417	0.315322	1.477702
9	6	0	-3.179328	-1.921505	-1.013853
10	6	0	-3.811597	0.416309	-1.238885
11	6	0	-4.054821	0.519923	0.136017
12	6	0	-4.013899	-0.659463	0.889029
13	6	0	-3.593895	-1.862012	0.322872
14	6	0	2.330257	2.996778	-1.241165
15	6	0	0.866481	3.503474	-1.181674
16	6	0	-2.447087	-3.134297	-1.554752
17	6	0	0.066578	-2.471567	-0.975121
18	6	0	-0.298164	-0.920409	1.048338
19	6	0	3.119221	-0.474546	0.336353
20	6	0	3.066578	0.619864	-0.621952
21	6	0	2.780253	-0.263883	1.712014
22	6	0	2.576577	1.044188	2.078167
23	6	0	2.519676	2.117866	1.136100

24	6	0	2.666472	1.934140	-0.217188
25	7	0	3.476076	-1.643251	-0.208498
26	7	0	3.383284	0.254285	-1.868481
27	16	0	3.726979	-1.354625	-1.810614
28	6	0	2.554257	-1.426747	2.653388
29	6	0	1.087388	-1.581737	3.136544
30	6	0	0.025343	-1.989312	2.081910
31	6	0	-0.261908	2.517399	-1.590014
32	6	0	-1.118666	-3.463885	-0.826449
33	6	0	-3.123861	2.899933	0.533732
34	1	0	-1.842775	2.536778	2.242181
35	1	0	-1.134775	3.548055	0.999916
36	1	0	0.144845	-0.065610	-2.192230
37	1	0	-3.107537	-0.809616	-2.855545
38	1	0	-4.371348	1.731386	1.879650
39	1	0	-5.190502	2.328400	0.446513
40	1	0	-1.085668	0.419841	2.524048
41	1	0	-3.889663	1.298844	-1.870366
42	1	0	-4.249586	-0.622974	1.950877
43	1	0	-3.514687	-2.746544	0.952039
44	1	0	2.984081	3.868065	-1.096015
45	1	0	2.548917	2.608988	-2.241393
46	1	0	0.667876	3.889819	-0.174630
47	1	0	0.797159	4.368943	-1.854714
48	1	0	-2.248051	-2.992024	-2.625096
49	1	0	-3.086248	-4.025946	-1.478420
50	1	0	0.271134	-2.332393	-2.044785
51	1	0	0.957120	-2.966939	-0.565948
52	1	0	2.350313	1.273008	3.117425
53	1	0	2.253130	3.103263	1.511837
54	1	0	2.882598	-2.351712	2.168033
55	1	0	3.181406	-1.301439	3.546641
56	1	0	1.085005	-2.352731	3.918860
57	1	0	0.773256	-0.651056	3.626065
58	1	0	0.363629	-2.907544	1.591835
59	1	0	-0.888412	-2.258981	2.631868
60	1	0	-1.184217	3.108126	-1.664984
61	1	0	-0.053931	2.157122	-2.605779
62	1	0	-0.771942	-4.434845	-1.206428
63	1	0	-1.333023	-3.618000	0.237676

64	1	0	-3.467276	3.867367	0.925487
65	1	0	-3.020533	3.037874	-0.548852

Table S24. Coordinates of **2CaCa**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.791373	2.554692	1.251274
2	6	0	-0.175421	0.016264	-1.098187
3	6	0	-3.421158	-0.786169	-1.789817
4	6	0	-4.316464	1.782491	0.884944
5	6	0	-0.111108	-1.132842	-0.298603
6	6	0	-0.548641	1.279294	-0.625355
7	6	0	-1.028128	1.358973	0.700033
8	6	0	-0.789926	0.260979	1.533989
9	6	0	-3.178237	-1.936803	-1.031490
10	6	0	-3.883730	0.385518	-1.193654
11	6	0	-4.099638	0.452660	0.188290
12	6	0	-4.006236	-0.739501	0.915041
13	6	0	-3.564339	-1.916875	0.314559
14	6	0	2.151206	3.088408	-1.220820
15	6	0	-2.428844	-3.119989	-1.613936
16	6	0	0.078813	-2.486353	-0.968467
17	6	0	-0.262666	-0.959319	1.094200
18	6	0	3.179432	-0.316940	0.368618
19	6	0	3.052932	0.772400	-0.587912
20	6	0	2.775939	-0.145512	1.734627
21	6	0	2.440440	1.135160	2.095013
22	6	0	2.330973	2.209954	1.157341
23	6	0	2.535858	2.048587	-0.189927
24	7	0	3.652566	-1.446589	-0.168772
25	7	0	3.429241	0.441047	-1.826929
26	16	0	3.913226	-1.131305	-1.765909
27	6	0	2.634261	-1.324054	2.666763
28	6	0	0.117335	-2.012082	2.125602
29	6	0	-0.413262	2.480512	-1.547998
30	6	0	1.617640	-2.402758	2.209256
31	6	0	0.666983	3.528343	-1.164816
32	6	0	-3.197435	2.828149	0.648681

33	6	0	-1.112629	-3.479484	-0.878871
34	1	0	-1.211373	3.478009	1.119611
35	1	0	-1.902641	2.426077	2.336230
36	1	0	0.070600	-0.081688	-2.154357
37	1	0	-3.179245	-0.785645	-2.850706
38	1	0	-4.432477	1.612148	1.963446
39	1	0	-5.258222	2.238416	0.545820
40	1	0	-1.038066	0.358050	2.590304
41	1	0	-4.001492	1.278879	-1.803620
42	1	0	-4.216756	-0.731533	1.982647
43	1	0	-3.445059	-2.810256	0.924228
44	1	0	2.766963	3.988667	-1.085040
45	1	0	2.386750	2.702291	-2.217919
46	1	0	-2.212412	-2.927514	-2.673022
47	1	0	-3.064867	-4.017078	-1.591447
48	1	0	0.953080	-3.004031	-0.555719
49	1	0	0.308173	-2.319197	-2.029167
50	1	0	2.150158	1.331352	3.124605
51	1	0	1.969197	3.165588	1.529526
52	1	0	3.604208	-1.828576	2.775111
53	1	0	2.357188	-0.954398	3.662585
54	1	0	-0.438800	-2.942661	1.949851
55	1	0	-0.204952	-1.658282	3.114115
56	1	0	-1.365261	3.021710	-1.621468
57	1	0	-0.196755	2.120085	-2.561950
58	1	0	1.691716	-3.232210	2.925579
59	1	0	1.957736	-2.801561	1.249856
60	1	0	0.553823	4.374749	-1.855728
61	1	0	0.452865	3.927434	-0.166266
62	1	0	-3.544935	3.779239	1.075357
63	1	0	-3.105409	3.003569	-0.429252
64	1	0	-0.759562	-4.434114	-1.292576
65	1	0	-1.343892	-3.680077	0.173558

Table S25. Coordinates of **2BBa**

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

1	6	0	1.692330	-2.562494	1.301109
2	6	0	0.219835	0.056003	-1.065665
3	6	0	3.355999	0.614139	-1.921756
4	6	0	4.227179	-2.036163	0.686465
5	6	0	0.167979	1.188244	-0.252253
6	6	0	0.550090	-1.227206	-0.602473
7	6	0	0.988306	-1.340860	0.728744
8	6	0	0.766910	-0.244702	1.578120
9	6	0	3.256875	1.770377	-1.143436
10	6	0	3.761460	-0.599089	-1.361744
11	6	0	4.077014	-0.694652	-0.003887
12	6	0	4.145280	0.499098	0.729554
13	6	0	3.743513	1.708338	0.170778
14	6	0	-2.119440	-3.071173	-1.249307
15	6	0	2.559119	3.015459	-1.657596
16	6	0	0.044413	2.559835	-0.895847
17	6	0	0.290893	0.992265	1.144623
18	6	0	-3.191804	0.268707	0.431554
19	6	0	-3.079805	-0.803812	-0.544942
20	6	0	-2.731391	0.088637	1.779427
21	6	0	-2.352313	-1.188027	2.107019
22	6	0	-2.243777	-2.244547	1.146108
23	6	0	-2.506676	-2.070474	-0.188361
24	7	0	-3.718778	1.391229	-0.067872
25	7	0	-3.521953	-0.468458	-1.760437
26	16	0	-4.045569	1.090878	-1.655616
27	6	0	-2.593479	1.258579	2.724182
28	6	0	-0.105572	2.041126	2.170954
29	6	0	0.425866	-2.395651	-1.570271
30	6	0	1.315977	3.451943	-0.838599
31	6	0	-0.980327	-2.596379	-2.191643
32	6	0	-1.620102	2.373752	2.256747
33	6	0	3.152958	-2.321989	1.769625
34	1	0	1.135325	-2.925883	2.177307
35	1	0	1.693160	-3.389918	0.584892
36	1	0	0.020285	0.182144	-2.128642
37	1	0	3.036552	0.640764	-2.961645
38	1	0	5.207302	-2.097285	1.181038
39	1	0	4.211129	-2.839861	-0.061426
40	1	0	0.969999	-0.370881	2.641302

41	1	0	3.755221	-1.498132	-1.974989
42	1	0	4.452269	0.471968	1.773331
43	1	0	3.746910	2.605093	0.787177
44	1	0	-1.825596	-4.011021	-0.764026
45	1	0	-2.988769	-3.295223	-1.881225
46	1	0	2.268000	2.863885	-2.705370
47	1	0	3.257832	3.864778	-1.655271
48	1	0	-0.242128	2.432081	-1.948040
49	1	0	-0.767182	3.134580	-0.433418
50	1	0	-2.019540	-1.392520	3.121984
51	1	0	-1.834586	-3.194505	1.482687
52	1	0	-2.280533	0.883726	3.707397
53	1	0	-3.574019	1.733701	2.864336
54	1	0	0.414450	2.989114	1.977894
55	1	0	0.236786	1.709538	3.160402
56	1	0	0.725591	-3.332211	-1.089738
57	1	0	1.128525	-2.250703	-2.404287
58	1	0	1.022934	4.447000	-1.200561
59	1	0	1.615324	3.589947	0.207466
60	1	0	-0.882362	-3.353102	-2.981577
61	1	0	-1.303490	-1.676747	-2.690624
62	1	0	-1.725832	3.204561	2.967482
63	1	0	-1.975561	2.751964	1.293715
64	1	0	3.468960	-3.221646	2.315454
65	1	0	3.163400	-1.504364	2.501624

Table S26. Coordinates of **2CBa**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.728942	2.648344	1.145503
2	6	0	-0.130938	0.017522	-1.119158
3	6	0	-3.251486	-0.680799	-1.947642
4	6	0	-4.246609	2.017979	0.561878
5	6	0	-0.128398	-1.112102	-0.296837
6	6	0	-0.470746	1.303089	-0.677519
7	6	0	-0.987016	1.423368	0.627826
8	6	0	-0.827059	0.330285	1.489845

9	6	0	-3.178943	-1.822036	-1.144944
10	6	0	-3.681137	0.540839	-1.426866
11	6	0	-4.052589	0.661139	-0.085452
12	6	0	-4.139054	-0.517816	0.670262
13	6	0	-3.710141	-1.736030	0.150864
14	6	0	2.305590	3.001561	-1.248017
15	6	0	-2.458178	-3.071066	-1.614946
16	6	0	0.043683	-2.489278	-0.915895
17	6	0	-0.331694	-0.910771	1.085814
18	6	0	3.124681	-0.407688	0.439695
19	6	0	3.093311	0.666955	-0.541307
20	6	0	2.703650	-0.184574	1.791918
21	6	0	2.424465	1.119425	2.116879
22	6	0	2.373634	2.171441	1.147978
23	6	0	2.616119	1.972664	-0.188122
24	7	0	3.549758	-1.572812	-0.060514
25	7	0	3.496658	0.291902	-1.759009
26	16	0	3.887297	-1.305817	-1.650607
27	6	0	2.487231	-1.340735	2.745211
28	6	0	1.018234	-1.530837	3.206489
29	6	0	-0.017900	-1.965402	2.137247
30	6	0	-0.268482	2.476062	-1.627585
31	6	0	-1.184549	-3.432909	-0.805363
32	6	0	1.158277	2.611521	-2.219016
33	6	0	-3.180090	2.382604	1.629237
34	1	0	-1.182590	3.078019	1.998551
35	1	0	-1.761535	3.435559	0.385843
36	1	0	0.133202	-0.115357	-2.166815
37	1	0	-2.894301	-0.726442	-2.974401
38	1	0	-5.226259	2.059932	1.059026
39	1	0	-4.262371	2.796153	-0.212623
40	1	0	-1.106158	0.456936	2.535443
41	1	0	-3.655051	1.428053	-2.056585
42	1	0	-4.485845	-0.471108	1.701030
43	1	0	-3.731556	-2.621538	0.783487
44	1	0	2.061951	3.953083	-0.757618
45	1	0	3.198582	3.178777	-1.861992
46	1	0	-2.192275	-2.960745	-2.674491
47	1	0	-3.132482	-3.937727	-1.557142
48	1	0	0.298635	-2.369107	-1.977019

49	1	0	0.898905	-3.009181	-0.463810
50	1	0	2.127938	1.359026	3.135795
51	1	0	2.036680	3.150742	1.480654
52	1	0	2.848476	-2.262126	2.276779
53	1	0	3.096585	-1.189860	3.646953
54	1	0	1.023198	-2.299272	3.991290
55	1	0	0.673459	-0.607653	3.689396
56	1	0	0.339275	-2.885301	1.663352
57	1	0	-0.938386	-2.240391	2.673081
58	1	0	-0.525785	3.419671	-1.135531
59	1	0	-0.961160	2.384889	-2.477875
60	1	0	-0.859300	-4.427019	-1.141804
61	1	0	-1.459361	-3.547229	0.250409
62	1	0	1.117018	3.390602	-2.992054
63	1	0	1.440078	1.688053	-2.735079
64	1	0	-3.523762	3.295097	2.135523
65	1	0	-3.167007	1.598365	2.396733

Table S27. Coordinates of **2BaBa**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.595548	2.702265	0.935317
2	6	0	-0.094764	-0.094246	-1.184048
3	6	0	-3.274509	-0.715767	-1.859012
4	6	0	-4.156535	2.108668	0.548818
5	6	0	-0.127694	-1.182501	-0.303973
6	6	0	-0.394373	1.218160	-0.804353
7	6	0	-0.898137	1.420619	0.497828
8	6	0	-0.757772	0.373582	1.413914
9	6	0	-3.226122	-1.826783	-1.013531
10	6	0	-3.663142	0.536838	-1.382159
11	6	0	-4.013380	0.720790	-0.042344
12	6	0	-4.119839	-0.423669	0.762306
13	6	0	-3.734439	-1.673825	0.285670
14	6	0	2.383663	2.933587	-1.353802
15	6	0	0.902691	3.395503	-1.388300

16	6	0	-2.559561	-3.117552	-1.449478
17	6	0	-0.017987	-2.595078	-0.853012
18	6	0	-0.304465	-0.903285	1.066478
19	6	0	3.086250	-0.487472	0.366002
20	6	0	3.058081	0.567165	-0.636655
21	6	0	2.760819	-0.211520	1.733294
22	6	0	2.590256	1.115534	2.045086
23	6	0	2.556872	2.150854	1.059066
24	6	0	2.695698	1.907794	-0.285894
25	7	0	3.407497	-1.687308	-0.131104
26	7	0	3.357846	0.141252	-1.868236
27	16	0	3.655042	-1.472781	-1.744759
28	6	0	2.518536	-1.331552	2.721889
29	6	0	1.048428	-1.457645	3.204234
30	6	0	-0.011456	-1.912315	2.167356
31	6	0	-0.170590	2.349838	-1.792732
32	6	0	-1.274085	-3.488244	-0.663366
33	6	0	-3.019414	2.515773	1.524129
34	1	0	-0.993382	3.208259	1.704924
35	1	0	-1.658522	3.406228	0.098542
36	1	0	0.166892	-0.282037	-2.224019
37	1	0	-2.932562	-0.811777	-2.887309
38	1	0	-5.101302	2.185219	1.105418
39	1	0	-4.216193	2.848319	-0.260752
40	1	0	-1.024289	0.557654	2.453993
41	1	0	-3.621103	1.397232	-2.047193
42	1	0	-4.450216	-0.325479	1.794927
43	1	0	-3.773514	-2.533139	0.952752
44	1	0	3.000679	3.828611	-1.194726
45	1	0	2.666493	2.528375	-2.330751
46	1	0	0.643031	3.822265	-0.411587
47	1	0	0.841510	4.223680	-2.107533
48	1	0	-2.323660	-3.061661	-2.520404
49	1	0	-3.259848	-3.957372	-1.333981
50	1	0	0.212440	-2.537928	-1.924904
51	1	0	0.830757	-3.120926	-0.395818
52	1	0	2.376029	1.392833	3.075134
53	1	0	2.317930	3.158384	1.393174
54	1	0	2.842685	-2.278706	2.278283
55	1	0	3.141333	-1.172361	3.612703

56	1	0	1.039589	-2.189167	4.023634
57	1	0	0.736609	-0.503147	3.647203
58	1	0	0.313855	-2.864632	1.736740
59	1	0	-0.934216	-2.132152	2.724462
60	1	0	-1.107211	2.898986	-1.966100
61	1	0	0.107576	1.920910	-2.763758
62	1	0	-0.993455	-4.507109	-0.964155
63	1	0	-1.520233	-3.546583	0.403993
64	1	0	-3.309902	3.471880	1.980754
65	1	0	-2.980782	1.789139	2.345512

Table S28. Coordinates of **2CaBa**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.674339	2.611496	1.075346
2	6	0	-0.147173	-0.112237	-1.120140
3	6	0	-3.321777	-0.697800	-1.863311
4	6	0	-4.229078	2.007367	0.669434
5	6	0	-0.120118	-1.210835	-0.255555
6	6	0	-0.487616	1.185971	-0.718955
7	6	0	-0.955427	1.356727	0.598020
8	6	0	-0.743052	0.305715	1.499492
9	6	0	-3.221461	-1.835560	-1.058689
10	6	0	-3.739754	0.524525	-1.334473
11	6	0	-4.065546	0.649325	0.018336
12	6	0	-4.124206	-0.526067	0.781771
13	6	0	-3.711515	-1.745549	0.253044
14	6	0	2.179114	3.039842	-1.338049
15	6	0	-2.523029	-3.089945	-1.548888
16	6	0	0.001464	-2.609143	-0.839348
17	6	0	-0.261415	-0.952245	1.127005
18	6	0	3.151727	-0.320612	0.375128
19	6	0	3.038960	0.732711	-0.622462
20	6	0	2.767197	-0.087236	1.737291
21	6	0	2.465071	1.214730	2.049760
22	6	0	2.370613	2.254752	1.071585
23	6	0	2.556793	2.035680	-0.270491

24	7	0	3.595106	-1.480437	-0.121858
25	7	0	3.393554	0.344144	-1.851307
26	16	0	3.842227	-1.235056	-1.732733
27	6	0	2.620390	-1.224071	2.720580
28	6	0	0.108355	-1.956137	2.208038
29	6	0	-0.351856	2.329719	-1.710456
30	6	0	-3.094206	2.383538	1.659378
31	6	0	-1.267831	-3.499820	-0.735242
32	6	0	1.611644	-2.330412	2.312403
33	6	0	0.678928	3.431498	-1.345392
34	1	0	-1.079517	3.100237	1.861492
35	1	0	-1.749196	3.341668	0.262799
36	1	0	0.085597	-0.279846	-2.170476
37	1	0	-2.996691	-0.746483	-2.900473
38	1	0	-5.173468	2.045988	1.230723
39	1	0	-4.300623	2.781565	-0.106100
40	1	0	-0.967568	0.474289	2.552234
41	1	0	-3.737839	1.408902	-1.968796
42	1	0	-4.435955	-0.475097	1.823460
43	1	0	-3.712053	-2.628110	0.889764
44	1	0	2.758360	3.963007	-1.197679
45	1	0	2.462978	2.641031	-2.317308
46	1	0	-3.217914	-3.941736	-1.516590
47	1	0	-2.245431	-2.963205	-2.603590
48	1	0	0.818255	-3.163219	-0.361308
49	1	0	0.279360	-2.524415	-1.898179
50	1	0	2.192077	1.458024	3.074159
51	1	0	2.036242	3.233608	1.408275
52	1	0	3.591923	-1.718920	2.857447
53	1	0	2.338105	-0.809167	3.696972
54	1	0	-0.440397	-2.897059	2.066702
55	1	0	-0.223084	-1.562031	3.178137
56	1	0	-1.321241	2.828698	-1.852196
57	1	0	-0.085057	1.915245	-2.690954
58	1	0	-3.393926	3.314930	2.159108
59	1	0	-3.042996	1.620936	2.446764
60	1	0	-0.978273	-4.505355	-1.070118
61	1	0	-1.552666	-3.606084	0.318442
62	1	0	1.692793	-3.125378	3.066090
63	1	0	1.954196	-2.768777	1.371107

64	1	0	0.561145	4.244215	-2.075084
65	1	0	0.421472	3.861912	-0.369903

Table S29. Coordinates of **7BB**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.143164	2.097196	-1.917175
2	6	0	0.260165	0.320795	0.887632
3	6	0	3.476941	-0.564064	1.955267
4	6	0	4.581602	1.350020	-1.157621
5	6	0	0.160923	-0.988421	0.396659
6	6	0	0.741951	1.387415	0.125184
7	6	0	1.280294	1.112193	-1.149047
8	6	0	1.012941	-0.145625	-1.693742
9	6	0	3.111470	-1.810901	1.425187
10	6	0	4.030395	0.424837	1.146552
11	6	0	4.238879	0.204950	-0.223776
12	6	0	4.025110	-1.087524	-0.709267
13	6	0	3.470802	-2.079309	0.101890
14	6	0	-1.932084	3.368538	0.302202
15	6	0	2.264314	-2.781127	2.224632
16	6	0	-0.162150	-2.125939	1.355561
17	6	0	0.395764	-1.177631	-0.978587
18	6	0	-3.158360	-0.237777	-0.451103
19	6	0	-3.017824	1.058494	0.191250
20	6	0	-2.627001	-0.466311	-1.764134
21	6	0	-2.133771	0.638399	-2.411875
22	6	0	-1.989291	1.912823	-1.777436
23	6	0	-2.337757	2.135573	-0.469272
24	7	0	-3.783276	-1.143846	0.305396
25	7	0	-3.540169	1.106720	1.418738
26	6	0	-2.545190	-1.863552	-2.331777
27	6	0	-0.004759	-2.450671	-1.706470
28	6	0	0.645305	2.799915	0.691664
29	6	0	3.501099	2.459525	-1.255912
30	6	0	-0.745191	3.118565	1.269502
31	6	0	0.829810	-2.278948	2.539190
32	6	0	-1.508278	-2.792264	-1.647674

33	8	0	-0.907455	3.200580	2.469258
34	8	0	-1.878367	-3.823318	-1.124978
35	16	0	-4.167626	-0.386626	1.717811
36	1	0	1.602862	3.041472	-2.080588
37	1	0	2.336718	1.690740	-2.918321
38	1	0	-0.050442	0.518146	1.911912
39	1	0	3.268648	-0.342635	3.000266
40	1	0	4.783330	0.954000	-2.161575
41	1	0	5.510534	1.837807	-0.829475
42	1	0	1.317995	-0.339254	-2.721132
43	1	0	4.249733	1.401273	1.574755
44	1	0	4.224826	-1.305034	-1.756625
45	1	0	3.249604	-3.055916	-0.324177
46	1	0	-1.643107	4.159414	-0.402051
47	1	0	-2.753284	3.731430	0.925993
48	1	0	2.202239	-3.739550	1.692813
49	1	0	2.748787	-2.994949	3.187779
50	1	0	-1.159649	-1.969839	1.788025
51	1	0	-0.226880	-3.076709	0.818634
52	1	0	-1.746920	0.530002	-3.421918
53	1	0	-1.499254	2.704915	-2.338416
54	1	0	-2.285209	-1.800133	-3.396971
55	1	0	-3.503034	-2.383186	-2.238376
56	1	0	0.514532	-3.333581	-1.318107
57	1	0	0.272842	-2.348959	-2.764427
58	1	0	0.876664	3.535022	-0.087030
59	1	0	1.353819	2.951547	1.514187
60	1	0	3.933355	3.284391	-1.838530
61	1	0	3.317994	2.863505	-0.252575
62	1	0	0.381553	-2.993943	3.241649
63	1	0	0.898808	-1.327229	3.081094

Table S30. Coordinates of **7CB**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.887939	1.613114	-2.319887

2	6	0	0.223906	0.461682	0.914462
3	6	0	3.508266	0.100468	2.032031
4	6	0	4.392560	1.242618	-1.501685
5	6	0	0.184777	-0.932258	0.753002
6	6	0	0.605728	1.337831	-0.101479
7	6	0	1.119575	0.793360	-1.299212
8	6	0	0.917474	-0.569381	-1.515508
9	6	0	3.215293	-1.258444	1.841464
10	6	0	3.971165	0.888370	0.981564
11	6	0	4.157021	0.347596	-0.299948
12	6	0	4.017654	-1.035136	-0.443215
13	6	0	3.555147	-1.825362	0.610290
14	6	0	-2.183785	3.208218	-0.193241
15	6	0	2.460351	-2.049364	2.891475
16	6	0	-0.025467	-1.807551	1.980614
17	6	0	0.382162	-1.430346	-0.547730
18	6	0	-3.159398	-0.546744	-0.182996
19	6	0	-3.092211	0.854970	0.196847
20	6	0	-2.700562	-0.977588	-1.469608
21	6	0	-2.337245	0.014445	-2.346946
22	6	0	-2.258046	1.391293	-1.967080
23	6	0	-2.543886	1.832094	-0.698482
24	7	0	-3.651019	-1.336027	0.777384
25	7	0	-3.537356	1.097020	1.432214
26	16	0	-4.010185	-0.353121	2.050910
27	6	0	-2.516609	-2.451532	-1.781625
28	6	0	-0.008707	-2.838533	-0.986867
29	6	0	0.439728	2.839618	0.111135
30	6	0	3.230281	2.217864	-1.825503
31	6	0	-0.925848	3.208759	0.715016
32	6	0	-1.045715	-2.766317	-2.120625
33	6	0	0.998073	-1.584518	3.126146
34	8	0	-1.017240	3.520200	1.884515
35	8	0	-0.706383	-2.913964	-3.279688
36	1	0	1.274171	2.449654	-2.685968
37	1	0	2.085255	0.985442	-3.198177
38	1	0	-0.060336	0.883207	1.876515
39	1	0	3.314362	0.561693	2.998562
40	1	0	4.599276	0.622504	-2.383829
41	1	0	5.290139	1.857130	-1.342711

42	1	0	1.183264	-0.989008	-2.483878
43	1	0	4.134992	1.951828	1.146334
44	1	0	4.201608	-1.493639	-1.412654
45	1	0	3.389266	-2.888353	0.446537
46	1	0	-1.993204	3.871153	-1.047195
47	1	0	-2.989186	3.631986	0.412462
48	1	0	2.978468	-1.978623	3.858164
49	1	0	2.460466	-3.113421	2.620291
50	1	0	-1.024800	-1.627970	2.399205
51	1	0	-0.004940	-2.867441	1.706185
52	1	0	-1.994616	-0.262250	-3.340615
53	1	0	-1.866615	2.095592	-2.697367
54	1	0	-2.850758	-3.043842	-0.924233
55	1	0	-3.103987	-2.742616	-2.658380
56	1	0	-0.424252	-3.410650	-0.153117
57	1	0	0.851498	-3.385817	-1.388047
58	1	0	0.558384	3.367060	-0.841633
59	1	0	1.192707	3.231155	0.805187
60	1	0	3.585493	2.898326	-2.611311
61	1	0	3.043025	2.846254	-0.946024
62	1	0	0.620263	-2.127269	4.002923
63	1	0	1.002897	-0.524332	3.407973

Table S31. Coordinates of **7BaB**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.643867	2.553387	1.103105
2	6	0	-0.163643	-0.001436	-1.324361
3	6	0	-3.631167	-0.823801	-1.740340
4	6	0	-4.212204	1.858099	0.905815
5	6	0	-0.185222	-1.184838	-0.565030
6	6	0	-0.472272	1.253656	-0.798786
7	6	0	-0.961464	1.323372	0.528057
8	6	0	-0.809845	0.185916	1.318001
9	6	0	-3.321788	-1.950273	-0.963833
10	6	0	-4.007753	0.375816	-1.144753

11	6	0	-4.089887	0.495901	0.250486
12	6	0	-3.951239	-0.671158	1.006667
13	6	0	-3.572886	-1.875288	0.408890
14	6	0	2.402651	2.831864	-1.251756
15	6	0	0.958435	3.341378	-1.088749
16	6	0	-2.644569	-3.156065	-1.585638
17	6	0	-0.073269	-2.519241	-1.287308
18	6	0	-0.360238	-1.047139	0.822647
19	6	0	3.125023	-0.660343	0.299063
20	6	0	3.116205	0.446987	-0.643048
21	6	0	2.735383	-0.461434	1.661886
22	6	0	2.513049	0.838855	2.046234
23	6	0	2.499646	1.926873	1.119246
24	6	0	2.710477	1.755221	-0.227541
25	7	0	3.483309	-1.825342	-0.250434
26	7	0	3.468991	0.096316	-1.883396
27	16	0	3.796676	-1.516615	-1.837061
28	6	0	2.432052	-1.638881	2.567197
29	6	0	0.925624	-1.681775	2.902521
30	6	0	-0.072974	-2.155402	1.833239
31	6	0	-0.214188	2.502203	-1.634709
32	6	0	-1.262754	-2.860606	-2.226203
33	6	0	-3.069313	2.847951	0.557829
34	8	0	0.752712	4.391430	-0.507865
35	8	0	0.535479	-1.308282	3.992421
36	1	0	-1.703147	2.444631	2.193754
37	1	0	-1.041097	3.448690	0.913154
38	1	0	0.110102	-0.069689	-2.376167
39	1	0	-3.514009	-0.865940	-2.821461
40	1	0	-4.267922	1.736123	1.995437
41	1	0	-5.154658	2.337367	0.603617
42	1	0	-1.059550	0.251066	2.374904
43	1	0	-4.179273	1.248521	-1.771706
44	1	0	-4.060606	-0.624226	2.088188
45	1	0	-3.399491	-2.749598	1.033524
46	1	0	3.054106	3.701852	-1.119195
47	1	0	2.562352	2.425787	-2.254985
48	1	0	-3.281055	-3.576294	-2.377518
49	1	0	-2.534642	-3.946390	-0.831370
50	1	0	0.830460	-2.523813	-1.910261

51	1	0	0.052662	-3.342271	-0.576786
52	1	0	2.224163	1.041052	3.074537
53	1	0	2.204163	2.906724	1.485292
54	1	0	2.745004	-2.565621	2.076419
55	1	0	2.957733	-1.547988	3.522507
56	1	0	0.327869	-3.044076	1.339265
57	1	0	-0.985414	-2.442525	2.368105
58	1	0	-1.078992	3.171777	-1.660185
59	1	0	0.014945	2.202469	-2.664602
60	1	0	-1.377861	-2.054736	-2.962215
61	1	0	-0.969503	-3.751547	-2.797904
62	1	0	-3.359848	3.832220	0.948444
63	1	0	-3.022961	2.961493	-0.532437

Table S32. Coordinates of **7CaB**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.065330	2.442436	1.276671
2	6	0	-0.222230	0.117753	-1.128548
3	6	0	-3.510304	-1.074728	-1.777930
4	6	0	-4.507185	1.423353	0.928573
5	6	0	-0.123740	-1.067130	-0.381562
6	6	0	-0.687764	1.322091	-0.597745
7	6	0	-1.211078	1.318018	0.716207
8	6	0	-0.935848	0.198253	1.500866
9	6	0	-3.099741	-2.185389	-1.025410
10	6	0	-4.044044	0.052376	-1.160796
11	6	0	-4.186683	0.113491	0.233706
12	6	0	-3.934030	-1.054124	0.958588
13	6	0	-3.401009	-2.186414	0.339155
14	6	0	1.999995	3.227381	-0.965550
15	6	0	-2.260370	-3.279146	-1.655019
16	6	0	0.178929	-2.380592	-1.088994
17	6	0	-0.335484	-0.966630	1.005031
18	6	0	3.180755	-0.251666	0.320165
19	6	0	3.023322	0.916778	-0.529805
20	6	0	2.720960	-0.236453	1.678516

21	6	0	2.289106	0.976831	2.153034
22	6	0	2.139574	2.129749	1.319559
23	6	0	2.415779	2.111406	-0.024945
24	7	0	3.735076	-1.295160	-0.303020
25	7	0	3.458746	0.731299	-1.779024
26	16	0	4.035998	-0.810844	-1.847934
27	6	0	2.621527	-1.518618	2.467575
28	6	0	0.042074	-2.075202	1.977116
29	6	0	-0.549756	2.603637	-1.411949
30	6	0	-0.867205	-2.809978	-2.152767
31	6	0	-3.491022	2.566429	0.669328
32	1	0	-1.571794	3.409590	1.128140
33	1	0	-2.160542	2.305386	2.361960
34	1	0	0.078788	0.094859	-2.174839
35	1	0	-3.351199	-1.066978	-2.854598
36	1	0	-4.592305	1.251154	2.009649
37	1	0	-5.490743	1.790113	0.600861
38	1	0	-1.226463	0.222292	2.550072
39	1	0	-4.296442	0.920334	-1.766748
40	1	0	-4.084343	-1.056701	2.036348
41	1	0	-3.148334	-3.056490	0.942195
42	1	0	2.543752	4.152235	-0.746344
43	1	0	2.226337	2.927625	-1.993445
44	1	0	-2.785993	-3.704311	-2.521853
45	1	0	-2.129880	-4.102744	-0.940895
46	1	0	0.301412	-3.190187	-0.364607
47	1	0	1.145632	-2.303553	-1.604028
48	1	0	1.953457	1.052250	3.184376
49	1	0	1.693667	3.020347	1.754712
50	1	0	3.556131	-2.085044	2.425525
51	1	0	2.408088	-1.277382	3.517702
52	1	0	-0.524824	-2.993801	1.790267
53	1	0	-0.208002	-1.741950	2.993452
54	1	0	-1.482939	3.172751	-1.456174
55	1	0	-0.256942	2.347965	-2.437303
56	1	0	-0.425408	-3.642524	-2.716181
57	1	0	-1.005391	-1.995298	-2.875448
58	1	0	-3.926819	3.489603	1.073959
59	1	0	-3.410813	2.724568	-0.413240
60	6	0	1.525557	-2.500171	1.978470

61	6	0	0.504301	3.554690	-0.810932
62	8	0	1.833841	-3.632023	1.665415
63	8	0	0.164265	4.547753	-0.193655

Table S33. Coordinates of **7BC**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.183887	2.159772	1.851552
2	6	0	-0.236027	0.337819	-0.891583
3	6	0	-3.329286	-0.412915	-2.093907
4	6	0	-4.597496	1.443921	0.996638
5	6	0	-0.170431	-0.964996	-0.386445
6	6	0	-0.726170	1.422430	-0.155802
7	6	0	-1.301226	1.170629	1.104728
8	6	0	-1.056446	-0.083969	1.674391
9	6	0	-3.074801	-1.693559	-1.586886
10	6	0	-3.889548	0.578644	-1.289664
11	6	0	-4.229818	0.321889	0.043978
12	6	0	-4.129289	-1.000523	0.493562
13	6	0	-3.555589	-1.988296	-0.305447
14	6	0	1.988324	3.344728	-0.340114
15	6	0	-2.218316	-2.682396	-2.353622
16	6	0	0.164095	-2.120056	-1.321058
17	6	0	-0.441927	-1.133373	0.987142
18	6	0	3.146706	-0.265084	0.498285
19	6	0	3.039503	1.022380	-0.167922
20	6	0	2.584413	-0.463911	1.803266
21	6	0	2.094871	0.658810	2.422417
22	6	0	1.982034	1.924025	1.764059
23	6	0	2.361255	2.119705	0.460090
24	7	0	3.774668	-1.192473	-0.229481
25	7	0	3.589407	1.042811	-1.384137
26	16	0	4.201340	-0.464022	-1.644962
27	6	0	2.468478	-1.849880	2.392161
28	6	0	-0.072832	-2.402574	1.738151
29	6	0	-0.593903	2.820225	-0.752093

30	6	0	-3.612265	1.646239	2.177690
31	6	0	0.809989	3.096522	-1.318560
32	6	0	-0.748274	-2.235130	-2.570376
33	6	0	1.425325	-2.770787	1.706941
34	8	0	0.990303	3.148654	-2.517411
35	8	0	1.784922	-3.815978	1.205529
36	1	0	-1.714169	2.428998	2.809383
37	1	0	-2.278044	3.095235	1.290196
38	1	0	0.098768	0.520141	-1.910780
39	1	0	-3.020772	-0.164138	-3.107293
40	1	0	-5.587704	1.254550	1.435137
41	1	0	-4.687405	2.384413	0.437053
42	1	0	-1.375503	-0.258552	2.701108
43	1	0	-4.011086	1.584226	-1.688039
44	1	0	-4.438650	-1.250298	1.506701
45	1	0	-3.425228	-2.991525	0.095773
46	1	0	2.824234	3.680599	-0.959378
47	1	0	1.704126	4.154008	0.344863
48	1	0	-2.650874	-2.860983	-3.348233
49	1	0	-2.226651	-3.651180	-1.837127
50	1	0	0.146032	-3.070086	-0.778958
51	1	0	1.196380	-2.014996	-1.681316
52	1	0	1.686376	0.572963	3.426151
53	1	0	1.490974	2.732304	2.300493
54	1	0	3.417978	-2.388056	2.322062
55	1	0	2.193375	-1.764256	3.451999
56	1	0	-0.365049	-2.282536	2.790249
57	1	0	-0.601021	-3.281648	1.352976
58	1	0	-0.812288	3.580273	0.005260
59	1	0	-1.290923	2.967512	-1.585473
60	1	0	-4.067365	2.374157	2.862896
61	1	0	-3.537199	0.708315	2.742057
62	1	0	-0.281498	-2.967626	-3.242016
63	1	0	-0.743368	-1.282959	-3.115407

Table S34. Coordinates of **7BC**

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	1.864401	1.279914	-2.527212
2	6	0	0.188277	0.657505	0.856378
3	6	0	3.382840	0.650675	2.022212
4	6	0	4.364539	1.111651	-1.642162
5	6	0	0.194402	-0.741015	0.934005
6	6	0	0.559835	1.365193	-0.290506
7	6	0	1.097173	0.644092	-1.376651
8	6	0	0.925544	-0.742706	-1.364300
9	6	0	3.207940	-0.736075	2.109401
10	6	0	3.828632	1.244221	0.841986
11	6	0	4.130628	0.472825	-0.286513
12	6	0	4.116073	-0.919839	-0.140396
13	6	0	3.654549	-1.512667	1.033678
14	6	0	-2.273518	3.083071	-0.747466
15	6	0	2.466035	-1.359015	3.276043
16	6	0	-0.000306	-1.408032	2.289204
17	6	0	0.414365	-1.444084	-0.267046
18	6	0	-3.127130	-0.650353	-0.125345
19	6	0	-3.103754	0.795766	0.020679
20	6	0	-2.650935	-1.270549	-1.325350
21	6	0	-2.313885	-0.423541	-2.352521
22	6	0	-2.273847	0.998460	-2.200945
23	6	0	-2.578514	1.630202	-1.020722
24	7	0	-3.598908	-1.287300	0.951022
25	7	0	-3.563450	1.222570	1.199365
26	16	0	-3.995010	-0.120903	2.046638
27	6	0	-2.416386	-2.768098	-1.394203
28	6	0	-0.923826	-3.082897	-1.621756
29	6	0	0.067940	-2.918930	-0.458646
30	6	0	0.351791	2.876159	-0.308886
31	6	0	3.310633	0.750313	-2.721608
32	6	0	-1.046021	3.296443	0.177902
33	6	0	0.977545	-0.938936	3.399317
34	8	0	-1.185458	3.826023	1.260940
35	8	0	-0.534432	-3.419046	-2.724450
36	1	0	1.329325	1.102810	-3.471759
37	1	0	1.913110	2.367623	-2.408699
38	1	0	-0.111561	1.227030	1.733804

39	1	0	3.098965	1.283615	2.860741
40	1	0	5.344400	0.806587	-2.036323
41	1	0	4.407378	2.203167	-1.530034
42	1	0	1.197802	-1.311812	-2.251207
43	1	0	3.885711	2.329239	0.778869
44	1	0	4.399287	-1.553010	-0.979001
45	1	0	3.584480	-2.597145	1.092306
46	1	0	-3.111135	3.574650	-0.245228
47	1	0	-2.079061	3.597650	-1.697521
48	1	0	2.956510	-1.086898	4.221387
49	1	0	2.525722	-2.453161	3.204222
50	1	0	0.085454	-2.495956	2.196593
51	1	0	-1.019168	-1.219785	2.653294
52	1	0	-1.960921	-0.848050	-3.288944
53	1	0	-1.896539	1.586234	-3.034379
54	1	0	-2.771565	-3.231508	-0.468581
55	1	0	-2.955296	-3.210423	-2.237964
56	1	0	-0.369857	-3.339917	0.450348
57	1	0	0.954273	-3.507634	-0.720396
58	1	0	0.494906	3.269172	-1.320595
59	1	0	1.064850	3.384174	0.350988
60	1	0	3.673312	1.147785	-3.679112
61	1	0	3.281221	-0.339775	-2.840224
62	1	0	0.602546	-1.343644	4.348904
63	1	0	0.921501	0.152196	3.496246

Table S35. Coordinates of **7BaC**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.448098	2.608235	0.914120
2	6	0	-0.134763	-0.202117	-1.331796
3	6	0	-3.502258	-0.659121	-1.806847
4	6	0	-4.055582	2.143935	0.721784
5	6	0	-0.227703	-1.322323	-0.492953
6	6	0	-0.371038	1.105189	-0.897725
7	6	0	-0.851222	1.298152	0.416908
8	6	0	-0.752810	0.213535	1.290113

9	6	0	-3.397506	-1.787228	-0.983990
10	6	0	-3.796671	0.593791	-1.272456
11	6	0	-4.012771	0.762635	0.099853
12	6	0	-4.072913	-0.390870	0.892069
13	6	0	-3.761480	-1.641833	0.360481
14	6	0	2.476262	2.800813	-1.312475
15	6	0	0.994429	3.232027	-1.307530
16	6	0	-2.825153	-3.088661	-1.515297
17	6	0	-0.222752	-2.711855	-1.112456
18	6	0	-0.380501	-1.073253	0.883919
19	6	0	3.063162	-0.685043	0.303637
20	6	0	3.079523	0.399464	-0.663689
21	6	0	2.721025	-0.437744	1.670944
22	6	0	2.563534	0.879945	2.029027
23	6	0	2.577517	1.946196	1.076505
24	6	0	2.750154	1.735439	-0.270740
25	7	0	3.352243	-1.877849	-0.227124
26	7	0	3.379742	0.004436	-1.904833
27	16	0	3.630417	-1.620395	-1.828839
28	6	0	2.407660	-1.584535	2.612138
29	6	0	0.908643	-1.588934	2.984406
30	6	0	-0.120881	-2.114356	1.971175
31	6	0	-0.083446	2.267945	-1.840265
32	6	0	-2.829260	2.486091	1.609048
33	6	0	-1.391095	-2.986769	-2.097521
34	8	0	0.688467	4.328389	-0.878895
35	8	0	0.550812	-1.143251	4.058237
36	1	0	-0.761070	3.069167	1.638674
37	1	0	-1.521852	3.330881	0.096709
38	1	0	0.117801	-0.359650	-2.379012
39	1	0	-3.281840	-0.743930	-2.869014
40	1	0	-4.949886	2.246149	1.352380
41	1	0	-4.148562	2.899926	-0.069060
42	1	0	-0.976147	0.368007	2.343488
43	1	0	-3.799103	1.465425	-1.924121
44	1	0	-4.292481	-0.303867	1.954511
45	1	0	-3.745347	-2.511405	1.014901
46	1	0	3.055936	3.707027	-1.112521
47	1	0	2.752509	2.417409	-2.300130
48	1	0	-3.469044	-3.480132	-2.316116

49	1	0	-2.838213	-3.844545	-0.718942
50	1	0	-0.240724	-3.483409	-0.335983
51	1	0	0.710602	-2.869145	-1.668715
52	1	0	2.312613	1.117662	3.059693
53	1	0	2.342442	2.948203	1.427297
54	1	0	2.691220	-2.529656	2.139350
55	1	0	2.956017	-1.479260	3.553133
56	1	0	0.247012	-3.048825	1.539064
57	1	0	-1.032658	-2.332210	2.538783
58	1	0	-0.974462	2.878797	-2.021446
59	1	0	0.249808	1.864751	-2.804140
60	1	0	-3.034032	3.452336	2.088873
61	1	0	-2.767329	1.754235	2.423979
62	1	0	-1.172252	-3.941152	-2.595272
63	1	0	-1.379788	-2.226158	-2.888279

Table S36. Coordinates of **7CaC**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.982904	2.423902	1.257214
2	6	0	-0.217461	-0.034071	-1.083620
3	6	0	-3.382325	-1.016164	-1.886180
4	6	0	-4.445141	1.577512	0.711556
5	6	0	-0.110533	-1.179318	-0.284884
6	6	0	-0.670932	1.198106	-0.603590
7	6	0	-1.158699	1.264233	0.718205
8	6	0	-0.862352	0.184896	1.555210
9	6	0	-3.090339	-2.131209	-1.090586
10	6	0	-3.890338	0.153734	-1.323246
11	6	0	-4.141861	0.246023	0.050934
12	6	0	-4.010272	-0.923127	0.810662
13	6	0	-3.486606	-2.087508	0.251387
14	6	0	1.894753	3.280240	-1.021598
15	6	0	-2.283286	-3.292532	-1.637124
16	6	0	0.164024	-2.530397	-0.931699
17	6	0	-0.285997	-1.006059	1.102397
18	6	0	3.145224	-0.176679	0.258245

19	6	0	2.941530	0.977752	-0.601118
20	6	0	2.756552	-0.141166	1.638256
21	6	0	2.339656	1.077923	2.112551
22	6	0	2.144235	2.216932	1.268830
23	6	0	2.356591	2.179673	-0.087068
24	7	0	3.671742	-1.228206	-0.375526
25	7	0	3.313149	0.772977	-1.867835
26	16	0	3.889789	-0.768685	-1.941809
27	6	0	2.727859	-1.406561	2.460921
28	6	0	0.146038	-2.054960	2.115852
29	6	0	-0.581740	2.423065	-1.505663
30	6	0	-3.399105	2.037704	1.760841
31	6	0	-0.830875	-2.935643	-2.051558
32	1	0	-1.456110	2.882934	2.106432
33	1	0	-2.068590	3.219111	0.512164
34	1	0	0.049305	-0.108755	-2.136172
35	1	0	-3.142318	-1.034580	-2.947613
36	1	0	-5.415865	1.528680	1.225555
37	1	0	-4.547050	2.352591	-0.059336
38	1	0	-1.107024	0.268434	2.613320
39	1	0	-4.037742	1.029337	-1.952651
40	1	0	-4.252291	-0.906286	1.871526
41	1	0	-3.328079	-2.959247	0.883396
42	1	0	2.351992	4.239271	-0.758818
43	1	0	2.187287	3.024688	-2.045425
44	1	0	-2.778837	-3.708169	-2.526020
45	1	0	-2.256065	-4.101632	-0.895540
46	1	0	0.186202	-3.319407	-0.174404
47	1	0	1.169530	-2.530962	-1.373312
48	1	0	2.058490	1.169579	3.158833
49	1	0	1.718300	3.113819	1.711975
50	1	0	3.675646	-1.947368	2.386205
51	1	0	2.562909	-1.142592	3.514450
52	1	0	-0.403962	-2.995236	2.000129
53	1	0	-0.069411	-1.673760	3.123140
54	1	0	-1.553130	2.910091	-1.640331
55	1	0	-0.223567	2.108557	-2.493155
56	1	0	-3.811128	2.921197	2.266528
57	1	0	-3.309346	1.263774	2.533998
58	1	0	-0.408890	-3.818377	-2.549984

59	1	0	-0.863956	-2.147570	-2.814759
60	6	0	1.639369	-2.438917	2.065332
61	6	0	0.369933	3.499161	-0.948220
62	8	0	1.967143	-3.573914	1.786110
63	8	0	-0.070537	4.514936	-0.443748

Table S37. Coordinates of **7BCa**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.118881	-1.974802	2.007536
2	6	0	0.282624	-0.292955	-0.888816
3	6	0	3.394599	0.422652	-1.981933
4	6	0	4.569147	-1.301067	1.213897
5	6	0	0.125836	1.018146	-0.425665
6	6	0	0.771816	-1.333556	-0.092378
7	6	0	1.268744	-1.019509	1.187246
8	6	0	0.954282	0.243790	1.700201
9	6	0	3.078815	1.709720	-1.529662
10	6	0	3.966858	-0.521287	-1.130266
11	6	0	4.226846	-0.215386	0.211839
12	6	0	4.057483	1.113549	0.614977
13	6	0	3.502869	2.062209	-0.242205
14	6	0	-1.827230	-3.428102	-0.386477
15	6	0	2.231172	2.653561	-2.362885
16	6	0	-0.204963	2.128124	-1.409387
17	6	0	0.319088	1.240560	0.954817
18	6	0	-3.146576	0.134646	0.398161
19	6	0	-2.960602	-1.144568	-0.264676
20	6	0	-2.663553	0.345872	1.731947
21	6	0	-2.168122	-0.761287	2.373969
22	6	0	-1.983907	-2.021331	1.721202
23	6	0	-2.286978	-2.223754	0.398300
24	7	0	-3.754864	1.048008	-0.363137
25	7	0	-3.431442	-1.172978	-1.513687
26	16	0	-4.066446	0.317795	-1.806550
27	6	0	-2.638439	1.731986	2.331011
28	6	0	-0.158567	2.503945	1.651943

29	6	0	0.741128	-2.757637	-0.636894
30	6	0	3.479970	-2.391653	1.385836
31	6	0	-0.602311	-3.128326	-1.289475
32	6	0	0.933079	3.152885	-1.676951
33	6	0	-1.684567	2.736356	1.635215
34	8	0	-0.696441	-3.215039	-2.496173
35	8	0	-2.137198	3.748679	1.141061
36	1	0	1.563919	-2.902929	2.212009
37	1	0	2.305821	-1.521726	2.989800
38	1	0	0.015901	-0.512731	-1.920597
39	1	0	3.128347	0.133361	-2.996516
40	1	0	4.779448	-0.842966	2.189276
41	1	0	5.492552	-1.816605	0.913413
42	1	0	1.221924	0.461436	2.733359
43	1	0	4.145160	-1.529670	-1.499336
44	1	0	4.301830	1.396323	1.637034
45	1	0	3.332224	3.071737	0.125744
46	1	0	-1.553311	-4.233114	0.308008
47	1	0	-2.612104	-3.789028	-1.056251
48	1	0	2.815840	3.546727	-2.627530
49	1	0	1.975996	2.166979	-3.313373
50	1	0	-1.074068	2.701983	-1.066487
51	1	0	-0.495028	1.673855	-2.365485
52	1	0	-1.813790	-0.665039	3.397130
53	1	0	-1.498321	-2.816441	2.282094
54	1	0	-2.339298	1.657713	3.385061
55	1	0	-3.627111	2.198221	2.283796
56	1	0	0.273864	3.411420	1.219797
57	1	0	0.153884	2.462729	2.704639
58	1	0	0.945817	-3.471034	0.169014
59	1	0	1.501816	-2.903876	-1.412739
60	1	0	3.900175	-3.174849	2.031411
61	1	0	3.303890	-2.867927	0.413974
62	1	0	0.505881	3.935751	-2.317240
63	1	0	1.200616	3.653974	-0.739092

Table S38. Coordinates of **7CCa**

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	-1.854235	1.834617	2.166956
2	6	0	-0.205438	0.452320	-0.984777
3	6	0	-3.385710	0.037365	-2.050857
4	6	0	-4.360317	1.452252	1.358467
5	6	0	-0.168246	-0.923786	-0.725402
6	6	0	-0.576294	1.399560	-0.026681
7	6	0	-1.095081	0.941308	1.201810
8	6	0	-0.907777	-0.408445	1.510959
9	6	0	-3.196248	-1.320755	-1.769573
10	6	0	-3.852258	0.917768	-1.075544
11	6	0	-4.129067	0.472579	0.223268
12	6	0	-4.089096	-0.907392	0.454257
13	6	0	-3.639677	-1.789877	-0.526458
14	6	0	2.238457	3.216399	-0.048821
15	6	0	-2.451994	-2.228230	-2.731178
16	6	0	0.045676	-1.898359	-1.870897
17	6	0	-0.373985	-1.332130	0.606425
18	6	0	3.127492	-0.552170	0.209338
19	6	0	3.076976	0.816809	-0.276836
20	6	0	2.697316	-0.872206	1.537016
21	6	0	2.367941	0.191549	2.340849
22	6	0	2.303717	1.535979	1.856652
23	6	0	2.571219	1.872147	0.552186
24	7	0	3.570044	-1.425230	-0.701346
25	7	0	3.486230	0.951296	-1.540808
26	16	0	3.904334	-0.553141	-2.059424
27	6	0	2.495091	-2.312809	1.967642
28	6	0	0.008125	-2.717339	1.121549
29	6	0	-0.392753	2.880480	-0.340040
30	6	0	-3.185953	2.428193	1.632091
31	6	0	0.980820	3.194114	-0.957661
32	6	0	1.010716	-2.591092	2.280418
33	6	0	-1.145436	-2.849059	-2.170661
34	8	0	1.078554	3.453206	-2.139242
35	8	0	0.635078	-2.665680	3.435166
36	1	0	-1.228296	2.682358	2.483435
37	1	0	-2.063402	1.265053	3.081410
38	1	0	0.073882	0.800942	-1.976951

39	1	0	-3.103346	0.424884	-3.027606
40	1	0	-4.586813	0.895594	2.277261
41	1	0	-5.245907	2.069453	1.149329
42	1	0	-1.177354	-0.757850	2.505721
43	1	0	-3.931305	1.977205	-1.312038
44	1	0	-4.350938	-1.291911	1.437976
45	1	0	-3.567553	-2.850154	-0.291910
46	1	0	2.064956	3.940795	0.757688
47	1	0	3.053176	3.580159	-0.680707
48	1	0	-2.222048	-1.673109	-3.650000
49	1	0	-3.098271	-3.064551	-3.034508
50	1	0	0.277176	-1.326702	-2.778672
51	1	0	0.927894	-2.525514	-1.683027
52	1	0	2.043674	-0.001113	3.360347
53	1	0	1.941456	2.302231	2.538085
54	1	0	2.851958	-2.978770	1.175886
55	1	0	3.049364	-2.529133	2.886214
56	1	0	0.444863	-3.321775	0.321667
57	1	0	-0.862153	-3.250517	1.520346
58	1	0	-0.510099	3.472900	0.574032
59	1	0	-1.136155	3.233613	-1.064361
60	1	0	-3.535662	3.156548	2.376327
61	1	0	-2.985908	3.004524	0.720497
62	1	0	-0.792749	-3.583234	-2.907622
63	1	0	-1.386643	-3.423099	-1.267329

Table S39. Coordinates of **7BaCa**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.607353	2.525479	1.237708
2	6	0	-0.205709	0.042330	-1.305385
3	6	0	-3.500270	-0.643913	-1.846304
4	6	0	-4.176929	1.865229	0.948500
5	6	0	-0.204328	-1.159464	-0.582400
6	6	0	-0.485160	1.284541	-0.729144
7	6	0	-0.940368	1.313572	0.608493
8	6	0	-0.771258	0.149768	1.361947

9	6	0	-3.316359	-1.838827	-1.142373
10	6	0	-3.870734	0.528904	-1.191115
11	6	0	-4.052358	0.552385	0.197101
12	6	0	-4.021156	-0.673884	0.872275
13	6	0	-3.668538	-1.850878	0.213455
14	6	0	2.377694	2.892308	-1.210167
15	6	0	0.933828	3.384509	-0.994729
16	6	0	-2.658237	-3.039194	-1.794028
17	6	0	-0.096115	-2.486782	-1.316616
18	6	0	-0.332468	-1.062375	0.815683
19	6	0	3.093024	-0.661859	0.191985
20	6	0	3.059574	0.474205	-0.713864
21	6	0	2.792097	-0.496159	1.581219
22	6	0	2.620199	0.796371	2.015860
23	6	0	2.579400	1.912526	1.123946
24	6	0	2.713332	1.778081	-0.237123
25	7	0	3.384633	-1.818194	-0.413691
26	7	0	3.328013	0.154059	-1.983449
27	16	0	3.607005	-1.467405	-2.007078
28	6	0	2.520886	-1.693389	2.469420
29	6	0	1.020972	-1.764500	2.830347
30	6	0	0.010055	-2.211601	1.761769
31	6	0	-0.246247	2.554563	-1.537956
32	6	0	-1.302319	-3.453592	-1.165680
33	6	0	-3.024679	2.872636	0.701560
34	8	0	0.735888	4.414310	-0.376271
35	8	0	0.646330	-1.434463	3.939295
36	1	0	-1.675534	2.363559	2.321144
37	1	0	-0.989654	3.419693	1.095230
38	1	0	0.021987	0.003500	-2.369131
39	1	0	-3.285639	-0.614325	-2.912653
40	1	0	-4.256342	1.660836	2.024270
41	1	0	-5.111419	2.372102	0.666448
42	1	0	-0.988617	0.184688	2.427491
43	1	0	-3.945336	1.452249	-1.761679
44	1	0	-4.210026	-0.698015	1.943630
45	1	0	-3.596473	-2.776366	0.781899
46	1	0	3.025497	3.760998	-1.054883
47	1	0	2.516915	2.528976	-2.232653
48	1	0	-2.515451	-2.840665	-2.864398

49	1	0	-3.321054	-3.914183	-1.731289
50	1	0	0.059738	-2.284170	-2.384198
51	1	0	0.798310	-3.032340	-0.986176
52	1	0	2.397979	0.972949	3.065256
53	1	0	2.328686	2.887224	1.534747
54	1	0	2.835710	-2.607976	1.957230
55	1	0	3.061754	-1.611211	3.416775
56	1	0	0.423169	-3.056448	1.203836
57	1	0	-0.878320	-2.557490	2.302680
58	1	0	-1.112348	3.222654	-1.530957
59	1	0	-0.036243	2.280501	-2.578960
60	1	0	-1.006527	-4.406054	-1.626148
61	1	0	-1.461909	-3.672025	-0.102844
62	1	0	-3.314274	3.821864	1.171485
63	1	0	-2.965777	3.082188	-0.373422

Table S40. Coordinates of **7CaCa**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.084460	2.356513	1.381290
2	6	0	-0.241331	0.117960	-1.105343
3	6	0	-3.385671	-0.952082	-1.880469
4	6	0	-4.520534	1.357323	0.938166
5	6	0	-0.093372	-1.077507	-0.388008
6	6	0	-0.721678	1.303486	-0.541973
7	6	0	-1.223340	1.259185	0.776890
8	6	0	-0.908750	0.126632	1.533170
9	6	0	-3.044924	-2.122503	-1.193058
10	6	0	-3.950683	0.135754	-1.217247
11	6	0	-4.177676	0.098207	0.164194
12	6	0	-3.984734	-1.125510	0.815680
13	6	0	-3.436803	-2.219618	0.148253
14	6	0	1.898458	3.307666	-0.946853
15	6	0	-2.190645	-3.194573	-1.842428
16	6	0	0.241342	-2.361325	-1.133039
17	6	0	-0.280519	-1.009043	1.008260
18	6	0	3.164508	-0.174754	0.238668

19	6	0	2.960557	1.002199	-0.588133
20	6	0	2.768480	-0.180457	1.616437
21	6	0	2.340934	1.020718	2.125015
22	6	0	2.144594	2.182223	1.313872
23	6	0	2.367432	2.184858	-0.040910
24	7	0	3.692364	-1.208394	-0.423147
25	7	0	3.335158	0.833172	-1.859502
26	16	0	3.910820	-0.705947	-1.975670
27	6	0	2.732436	-1.471821	2.394680
28	6	0	0.161286	-2.111083	1.961351
29	6	0	-0.636972	2.598764	-1.341917
30	6	0	-3.506832	2.518652	0.775182
31	6	0	-0.844209	-3.473400	-1.127306
32	1	0	-1.588579	3.328882	1.280950
33	1	0	-2.185634	2.168509	2.458305
34	1	0	0.026740	0.118067	-2.160503
35	1	0	-3.143723	-0.865360	-2.937877
36	1	0	-4.625223	1.111268	2.003122
37	1	0	-5.500281	1.740905	0.617955
38	1	0	-1.177937	0.124644	2.588447
39	1	0	-4.146721	1.050764	-1.772551
40	1	0	-4.203623	-1.203820	1.878819
41	1	0	-3.245330	-3.136650	0.702023
42	1	0	2.415130	4.244938	-0.716093
43	1	0	2.111320	3.038958	-1.986107
44	1	0	-1.996926	-2.919212	-2.887529
45	1	0	-2.739712	-4.146817	-1.875238
46	1	0	1.154483	-2.812818	-0.728428
47	1	0	0.466844	-2.105124	-2.176577
48	1	0	2.049779	1.078842	3.170922
49	1	0	1.707031	3.062313	1.778128
50	1	0	3.683803	-2.006612	2.322081
51	1	0	2.541974	-1.246869	3.452908
52	1	0	-0.372584	-3.049795	1.783998
53	1	0	-0.075640	-1.793001	2.985858
54	1	0	-1.588171	3.138075	-1.362108
55	1	0	-0.355158	2.364046	-2.375289
56	1	0	-3.947922	3.408022	1.244594
57	1	0	-3.421606	2.759673	-0.291052
58	1	0	-0.392648	-4.350848	-1.608647

59	1	0	-1.049910	-3.780779	-0.095983
60	6	0	1.657257	-2.488338	1.933682
61	6	0	0.396256	3.578529	-0.751467
62	8	0	0.035968	4.549935	-0.111727
63	8	0	1.993034	-3.614739	1.628640

Table S41. Coordinates of **7BBa**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.133030	-2.006338	1.990857
2	6	0	0.253050	-0.320351	-0.885329
3	6	0	3.258470	0.232041	-2.099122
4	6	0	4.565662	-1.427491	1.082148
5	6	0	0.132069	0.993241	-0.427578
6	6	0	0.742689	-1.369680	-0.096196
7	6	0	1.266776	-1.061325	1.171884
8	6	0	0.978848	0.210392	1.688437
9	6	0	3.070514	1.553926	-1.685775
10	6	0	3.827996	-0.715446	-1.245934
11	6	0	4.224159	-0.371648	0.049168
12	6	0	4.190028	0.986551	0.397855
13	6	0	3.625749	1.931373	-0.453599
14	6	0	-1.897580	-3.404173	-0.385541
15	6	0	2.215832	2.519443	-2.485010
16	6	0	-0.190988	2.106274	-1.409576
17	6	0	0.355934	1.217358	0.950334
18	6	0	-3.144531	0.178124	0.428843
19	6	0	-2.990872	-1.102306	-0.240231
20	6	0	-2.636527	0.377099	1.755319
21	6	0	-2.152378	-0.740990	2.387026
22	6	0	-2.000067	-2.001954	1.728227
23	6	0	-2.325917	-2.194798	0.409380
24	7	0	-3.749355	1.103798	-0.320117
25	7	0	-3.481704	-1.119023	-1.481716
26	16	0	-4.096407	0.383089	-1.760323
27	6	0	-2.575523	1.760550	2.358253

28	6	0	-0.090662	2.492303	1.646919
29	6	0	0.681026	-2.786136	-0.658791
30	6	0	0.980258	3.077462	-1.730444
31	6	0	-0.675976	-3.125257	-1.300030
32	6	0	3.574770	-1.502610	2.273670
33	6	0	-1.613136	2.749863	1.652292
34	8	0	-0.783785	-3.206984	-2.505939
35	8	0	-2.055042	3.771368	1.167345
36	1	0	1.660695	-2.182923	2.968390
37	1	0	2.202609	-2.987692	1.510162
38	1	0	-0.033154	-0.538508	-1.912142
39	1	0	2.885327	-0.082381	-3.071530
40	1	0	5.561573	-1.233314	1.505169
41	1	0	4.625242	-2.411448	0.598412
42	1	0	1.255601	0.422603	2.720585
43	1	0	3.896232	-1.752330	-1.569711
44	1	0	4.552338	1.300187	1.375132
45	1	0	3.560085	2.967669	-0.128404
46	1	0	-1.632130	-4.217519	0.302506
47	1	0	-2.696252	-3.746765	-1.048547
48	1	0	1.885998	2.032713	-3.411997
49	1	0	2.819183	3.385371	-2.794006
50	1	0	-0.537262	1.656912	-2.349121
51	1	0	-1.020474	2.720404	-1.040173
52	1	0	-1.781825	-0.653994	3.405315
53	1	0	-1.518607	-2.806598	2.278862
54	1	0	-3.555564	2.245926	2.327051
55	1	0	-2.262674	1.676574	3.407595
56	1	0	0.237542	2.453405	2.694916
57	1	0	0.349774	3.389680	1.201452
58	1	0	0.876627	-3.518852	0.130908
59	1	0	1.431735	-2.933382	-1.444307
60	1	0	0.559343	3.884262	-2.344640
61	1	0	1.320130	3.556609	-0.804075
62	1	0	4.010265	-2.180237	3.020473
63	1	0	3.521980	-0.517249	2.753742

Table S42. Coordinates of **7CBa**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.877751	1.813510	2.192581
2	6	0	-0.158441	0.533370	-0.975659
3	6	0	-3.238331	0.295329	-2.145859
4	6	0	-4.362281	1.528479	1.288771
5	6	0	-0.167500	-0.850330	-0.776749
6	6	0	-0.535171	1.452580	0.010521
7	6	0	-1.101551	0.958920	1.201471
8	6	0	-0.949340	-0.408420	1.461291
9	6	0	-3.168920	-1.087431	-1.957229
10	6	0	-3.707101	1.137419	-1.135679
11	6	0	-4.119681	0.623999	0.096631
12	6	0	-4.202690	-0.770911	0.222271
13	6	0	-3.736190	-1.610441	-0.785079
14	6	0	2.332838	3.177901	0.091381
15	6	0	-2.418350	-1.978961	-2.927699
16	6	0	0.051210	-1.782840	-1.955819
17	6	0	-0.421270	-1.308100	0.532931
18	6	0	3.113470	-0.620749	0.240381
19	6	0	3.111739	0.764681	-0.199699
20	6	0	2.639630	-0.973749	1.544621
21	6	0	2.319759	0.071081	2.376731
22	6	0	2.304959	1.432441	1.937931
23	6	0	2.613559	1.804831	0.652571
24	7	0	3.557890	-1.474208	-0.687799
25	7	0	3.558249	0.930502	-1.447189
26	16	0	3.950910	-0.566438	-2.006069
27	6	0	2.388340	-2.422019	1.920331
28	6	0	-0.086510	-2.723500	0.997701
29	6	0	-0.302352	2.937400	-0.250939
30	6	0	-1.162730	-2.673250	-2.336839
31	6	0	-3.341181	1.359559	2.445161
32	1	0	-1.368121	1.804980	3.167211
33	1	0	-1.896282	2.860070	1.870531

34	1	0	0.154409	0.915530	-1.945119
35	1	0	-2.851431	0.730169	-3.065019
36	1	0	-5.358851	1.335248	1.710341
37	1	0	-4.366572	2.576459	0.960851
38	1	0	-1.242080	-0.791590	2.437121
39	1	0	-3.683831	2.215009	-1.286499
40	1	0	-4.579410	-1.206271	1.145931
41	1	0	-3.759740	-2.687921	-0.632619
42	1	0	2.169068	3.880681	0.918781
43	1	0	3.169128	3.535771	-0.515129
44	1	0	-2.125350	-1.393951	-3.809179
45	1	0	-3.081070	-2.775451	-3.295209
46	1	0	0.336420	-1.183030	-2.829489
47	1	0	0.901750	-2.451469	-1.765359
48	1	0	1.965639	-0.146709	3.381171
49	1	0	1.947049	2.185181	2.636421
50	1	0	2.749321	-3.070069	1.115591
51	1	0	2.911970	-2.684049	2.844941
52	1	0	0.354881	-3.304570	0.183221
53	1	0	-0.979919	-3.249880	1.351551
54	1	0	-0.409322	3.506310	0.678521
55	1	0	-1.024222	3.337130	-0.973219
56	1	0	-0.809039	-3.396390	-3.084139
57	1	0	-1.465539	-3.265420	-1.464209
58	1	0	-3.714241	1.940279	3.299451
59	1	0	-3.341721	0.311449	2.769231
60	6	0	0.889470	-2.672729	2.184721
61	6	0	1.090018	3.227451	-0.837009
62	8	0	0.482650	-2.785080	3.325831
63	8	0	1.215308	3.526121	-2.006579

Table S43. Coordinates of **7BaBa**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.476915	2.533658	1.186746
2	6	0	-0.191952	-0.088852	-1.284795
3	6	0	-3.401973	-0.541129	-1.936132

4	6	0	-4.062128	2.102810	0.738356
5	6	0	-0.220620	-1.258594	-0.518159
6	6	0	-0.430731	1.184041	-0.754829
7	6	0	-0.860615	1.279615	0.584241
8	6	0	-0.713333	0.140597	1.383468
9	6	0	-3.354491	-1.718522	-1.185689
10	6	0	-3.719766	0.680998	-1.340572
11	6	0	-3.998371	0.766073	0.025912
12	6	0	-4.112459	-0.437380	0.738804
13	6	0	-3.796688	-1.655989	0.144717
14	6	0	2.382834	2.914876	-1.216247
15	6	0	0.903500	3.338536	-1.098015
16	6	0	-2.757646	-2.991794	-1.753573
17	6	0	-0.181841	-2.614005	-1.202870
18	6	0	-0.327838	-1.104401	0.878973
19	6	0	3.065713	-0.662714	0.142519
20	6	0	3.023754	0.479612	-0.754823
21	6	0	2.807964	-0.501785	1.540855
22	6	0	2.668472	0.790493	1.988229
23	6	0	2.623566	1.913517	1.104497
24	6	0	2.717827	1.787281	-0.261052
25	7	0	3.318688	-1.819831	-0.478478
26	7	0	3.245383	0.162729	-2.034373
27	16	0	3.493037	-1.463306	-2.076056
28	6	0	2.554456	-1.704740	2.428075
29	6	0	1.074389	-1.753864	2.867226
30	6	0	0.003603	-2.220245	1.867700
31	6	0	-0.201983	2.408104	-1.633459
32	6	0	-1.463492	-3.477759	-1.048192
33	6	0	-2.911020	2.347863	1.750390
34	8	0	0.621641	4.401471	-0.578046
35	8	0	0.761796	-1.386826	3.983949
36	1	0	-0.848805	2.882290	2.019020
37	1	0	-1.476445	3.353501	0.463676
38	1	0	0.010055	-0.175361	-2.350677
39	1	0	-3.114900	-0.563899	-2.985451
40	1	0	-5.005377	2.185677	1.296611
41	1	0	-4.070871	2.914247	-0.001090
42	1	0	-0.899192	0.225672	2.452470
43	1	0	-3.679481	1.590985	-1.936214

44	1	0	-4.391341	-0.414190	1.790546
45	1	0	-3.838932	-2.565419	0.741301
46	1	0	2.972666	3.809053	-0.993038
47	1	0	2.601800	2.595763	-2.240435
48	1	0	-2.553778	-2.853547	-2.823556
49	1	0	-3.486805	-3.811710	-1.684674
50	1	0	0.013631	-2.462654	-2.272383
51	1	0	0.662679	-3.209360	-0.830483
52	1	0	2.479254	0.962951	3.044742
53	1	0	2.407098	2.890460	1.529970
54	1	0	2.827444	-2.617620	1.890074
55	1	0	3.144217	-1.643651	3.347621
56	1	0	0.358870	-3.110292	1.340517
57	1	0	-0.873245	-2.500264	2.462264
58	1	0	-1.102511	3.024644	-1.724757
59	1	0	0.077945	2.071088	-2.638816
60	1	0	-1.230056	-4.474492	-1.446425
61	1	0	-1.676575	-3.621707	0.018545
62	1	0	-3.156276	3.260883	2.309117
63	1	0	-2.908942	1.534590	2.487346

Table S44. Coordinates of **7CaBa**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.925150	2.317940	1.406546
2	6	0	-0.235370	-0.031998	-1.095863
3	6	0	-3.315372	-0.832153	-1.951831
4	6	0	-4.409400	1.585774	0.795467
5	6	0	-0.080114	-1.203239	-0.348994
6	6	0	-0.679798	1.178423	-0.549968
7	6	0	-1.119009	1.185548	0.787664
8	6	0	-0.787646	0.071911	1.570269
9	6	0	-3.103730	-2.014379	-1.237581
10	6	0	-3.823866	0.307703	-1.325273
11	6	0	-4.136209	0.301972	0.036584
12	6	0	-4.082191	-0.928958	0.707271
13	6	0	-3.575724	-2.064508	0.083094

14	6	0	1.817369	3.340941	-1.007160
15	6	0	-2.304606	-3.163304	-1.823671
16	6	0	0.170867	-2.523670	-1.057756
17	6	0	-0.207958	-1.089057	1.053350
18	6	0	3.132330	-0.120008	0.184496
19	6	0	2.889315	1.040426	-0.654773
20	6	0	2.805928	-0.097595	1.580028
21	6	0	2.405977	1.115355	2.084281
22	6	0	2.174237	2.261968	1.260481
23	6	0	2.329402	2.237294	-0.103698
24	7	0	3.622057	-1.169201	-0.481795
25	7	0	3.195229	0.842773	-1.940419
26	16	0	3.757601	-0.701122	-2.053752
27	6	0	2.824233	-1.371047	2.390593
28	6	0	0.284769	-2.166812	2.006958
29	6	0	-0.654869	2.433446	-1.414560
30	6	0	-3.351206	1.925498	1.878626
31	6	0	-1.015346	-3.528179	-1.041919
32	1	0	-1.392422	2.698431	2.290011
33	1	0	-1.992679	3.168214	0.723121
34	1	0	-0.020453	-0.069705	-2.162080
35	1	0	-3.007215	-0.775291	-2.993926
36	1	0	-5.381975	1.522034	1.304091
37	1	0	-4.487123	2.423115	0.089709
38	1	0	-0.992479	0.114009	2.639421
39	1	0	-3.907101	1.234702	-1.889439
40	1	0	-4.380393	-0.984744	1.752493
41	1	0	-3.489878	-2.988973	0.650828
42	1	0	2.262732	4.305807	-0.745831
43	1	0	2.078678	3.104864	-2.043951
44	1	0	-2.924587	-4.070877	-1.858327
45	1	0	-2.045175	-2.932898	-2.865414
46	1	0	1.031155	-3.041117	-0.618204
47	1	0	0.439376	-2.317239	-2.102051
48	1	0	2.168176	1.195676	3.142186
49	1	0	1.764165	3.153533	1.728743
50	1	0	3.799590	-1.863157	2.329268
51	1	0	2.628592	-1.124871	3.443076
52	1	0	-0.194290	-3.134021	1.825942
53	1	0	0.035379	-1.865285	3.033550

54	1	0	-1.643236	2.897820	-1.493701
55	1	0	-0.332359	2.156828	-2.425495
56	1	0	-3.739022	2.771915	2.461113
57	1	0	-3.280582	1.083310	2.579163
58	1	0	-0.635397	-4.469635	-1.460190
59	1	0	-1.286399	-3.753483	-0.003402
60	6	0	1.800877	-2.455082	1.964450
61	6	0	0.292207	3.522343	-0.874298
62	8	0	2.197463	-3.565078	1.672507
63	8	0	-0.152136	4.520663	-0.339012

Table S45. Coordinates of **1B at MP2/6-31G(d)**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.716975	1.284089	0.552329
2	6	0	-0.696836	-2.546838	-0.094773
3	6	0	0.698299	-2.546604	-0.094800
4	6	0	1.418866	-1.656433	-0.896835
5	6	0	0.698460	-0.852232	-1.794940
6	6	0	-0.697668	-0.852434	-1.794883
7	6	0	-1.417762	-1.656962	-0.896822
8	6	0	-0.717811	1.284059	0.552614
9	6	0	1.458581	0.388266	1.360953
10	6	0	0.708359	-0.365141	2.251381
11	6	0	-0.708552	-0.365226	2.251592
12	6	0	-1.459003	0.387525	1.360809
13	6	0	-2.945259	0.236801	1.186272
14	6	0	-2.914567	-1.526039	-0.752699
15	6	0	2.944931	0.237967	1.186547
16	6	0	2.915588	-1.524796	-0.752667
17	6	0	-3.380601	-0.151620	-0.241136
18	7	0	1.266963	2.173752	-0.330802
19	7	0	-1.268223	2.173131	-0.330841
20	6	0	3.380845	-0.150231	-0.240750
21	1	0	-1.233715	-3.212787	0.580155
22	1	0	1.235432	-3.212314	0.580163
23	1	0	1.234458	-0.191385	-2.476320

24	1	0	-1.233909	-0.191837	-2.476315
25	1	0	1.226409	-1.055466	2.916715
26	1	0	-1.226294	-1.056097	2.916600
27	1	0	-3.440464	1.184477	1.437462
28	1	0	-3.309583	-0.513203	1.901275
29	1	0	-3.399553	-1.705514	-1.722084
30	1	0	-3.278762	-2.309944	-0.075025
31	1	0	3.309313	-0.511979	1.901582
32	1	0	3.439833	1.185749	1.437961
33	1	0	3.400681	-1.703666	-1.722109
34	1	0	3.280223	-2.308710	-0.075240
35	1	0	-3.045242	0.629116	-0.929990
36	1	0	-4.478440	-0.138971	-0.263672
37	1	0	4.478688	-0.137138	-0.262908
38	1	0	3.045417	0.630405	-0.929669
39	16	0	-0.000796	2.902886	-1.060014

Table S46. Coordinates of **5Ba at MP2/6-31G(d)**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.717043	1.148420	-0.886205
2	6	0	0.696462	-1.786644	1.085926
3	6	0	-0.696408	-1.786648	1.085924
4	6	0	-1.409078	-0.675135	1.555306
5	6	0	-0.698989	0.365053	2.168043
6	6	0	0.699031	0.365058	2.168043
7	6	0	1.409126	-0.675128	1.555311
8	6	0	0.716997	1.148443	-0.886208
9	6	0	-1.450368	0.088760	-1.463585
10	6	0	-0.706855	-0.890657	-2.113362
11	6	0	0.706870	-0.890635	-2.113363
12	6	0	1.450353	0.088800	-1.463579
13	6	0	2.939143	-0.014578	-1.253720
14	6	0	2.904642	-0.581440	1.315704
15	6	0	-2.939156	-0.014660	-1.253728
16	6	0	-2.904597	-0.581446	1.315710
17	6	0	-3.210029	-1.001650	-0.117048

18	7	0	-1.269545	2.232038	-0.257617
19	7	0	1.269467	2.232075	-0.257617
20	16	0	-0.000052	3.123765	0.253591
21	8	0	-3.592041	-2.142314	-0.368782
22	6	0	3.210045	-1.001599	-0.117073
23	8	0	3.592081	-2.142248	-0.368845
24	1	0	1.236709	-2.629906	0.659352
25	1	0	-1.236650	-2.629914	0.659350
26	1	0	-1.239869	1.206502	2.598058
27	1	0	1.239906	1.206512	2.598056
28	1	0	-1.233496	-1.721599	-2.581700
29	1	0	1.233535	-1.721567	-2.581693
30	1	0	3.347768	0.973784	-1.016869
31	1	0	3.433955	-0.411466	-2.145501
32	1	0	3.239040	0.447768	1.490723
33	1	0	3.465219	-1.254209	1.974752
34	1	0	-3.347817	0.973696	-1.016913
35	1	0	-3.433951	-0.411596	-2.145497
36	1	0	-3.238985	0.447770	1.490696
37	1	0	-3.465170	-1.254186	1.974790

Table S47. Coordinates of **2BB at MP2/6-31G(d)**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.844665	2.565652	1.288816
2	6	0	-0.222001	-0.079552	-0.902316
3	6	0	-3.274202	-1.021839	-1.756426
4	6	0	-4.234226	1.597483	0.852174
5	6	0	-0.082486	-1.156414	-0.018813
6	6	0	-0.646530	1.192090	-0.499921
7	6	0	-1.067862	1.355079	0.834080
8	6	0	-0.758315	0.339077	1.744629
9	6	0	-2.864598	-2.098215	-0.955989
10	6	0	-3.773382	0.147291	-1.181804
11	6	0	-3.864305	0.280922	0.212590
12	6	0	-3.566837	-0.837317	0.997655
13	6	0	-3.072670	-2.007692	0.423581

14	6	0	1.801880	3.099167	-1.380472
15	6	0	-2.104997	-3.261207	-1.535648
16	6	0	0.204908	-2.543813	-0.562621
17	6	0	-0.207037	-0.887590	1.361381
18	6	0	2.990661	-0.113531	0.385961
19	6	0	2.792078	0.897841	-0.612074
20	6	0	2.633007	0.104569	1.739897
21	6	0	2.206521	1.388889	2.042623
22	6	0	2.002169	2.384021	1.055696
23	6	0	2.224827	2.155608	-0.292781
24	7	0	3.512268	-1.279648	-0.109577
25	7	0	3.150912	0.508967	-1.874177
26	16	0	3.698799	-1.024471	-1.715329
27	6	0	2.664149	-1.012596	2.745193
28	6	0	0.220892	-1.876343	2.416887
29	6	0	-0.672679	2.311416	-1.518526
30	6	0	-3.217844	2.727514	0.608166
31	6	0	0.660540	2.539367	-2.251058
32	6	0	-0.620529	-2.943886	-1.799774
33	6	0	1.727774	-2.189976	2.411042
34	1	0	-1.267400	3.486709	1.120673
35	1	0	-1.996520	2.498191	2.374793
36	1	0	-0.013852	-0.238159	-1.960618
37	1	0	-3.169638	-1.087839	-2.839753
38	1	0	-4.360744	1.450558	1.933150
39	1	0	-5.208131	1.932918	0.469690
40	1	0	-0.972618	0.504353	2.802602
41	1	0	-4.060468	0.980524	-1.823764
42	1	0	-3.667715	-0.771851	2.080236
43	1	0	-2.804993	-2.849302	1.062368
44	1	0	1.488494	4.050130	-0.928744
45	1	0	2.656472	3.315742	-2.034527
46	1	0	-2.168335	-4.116628	-0.849697
47	1	0	-2.563080	-3.581328	-2.481121
48	1	0	1.270444	-2.632724	-0.812458
49	1	0	0.021873	-3.288469	0.222048
50	1	0	1.935664	1.617863	3.072876
51	1	0	1.586029	3.343562	1.362611
52	1	0	2.407976	-0.604978	3.732478
53	1	0	3.686115	-1.408392	2.817018

54	1	0	-0.327241	-2.823565	2.305503
55	1	0	-0.058441	-1.480197	3.403033
56	1	0	-0.959521	3.253064	-1.037207
57	1	0	-1.449358	2.102104	-2.269448
58	1	0	-3.661691	3.666036	0.968111
59	1	0	-3.081109	2.846577	-0.471864
60	1	0	0.480935	3.255240	-3.064420
61	1	0	1.004292	1.613740	-2.723150
62	1	0	-0.159537	-3.841152	-2.234544
63	1	0	-0.552335	-2.166519	-2.569238
64	1	0	1.913947	-2.979194	3.152241
65	1	0	2.021978	-2.596800	1.439781

Table S48. Coordinates of **7BaBa at MP2/6-31G(d)**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.725541	2.637425	0.913762
2	6	0	-0.054900	-0.142870	-1.628717
3	6	0	-3.182876	0.150536	-1.745546
4	6	0	-3.318711	2.613603	1.141857
5	6	0	-0.324928	-1.296977	-0.881782
6	6	0	-0.022968	1.137548	-1.057837
7	6	0	-0.446999	1.290875	0.278170
8	6	0	-0.545086	0.131702	1.053203
9	6	0	-3.377141	-1.078448	-1.106891
10	6	0	-3.244259	1.347662	-1.033515
11	6	0	-3.504028	1.353307	0.340600
12	6	0	-3.810815	0.132747	0.959481
13	6	0	-3.754703	-1.064426	0.245131
14	6	0	2.876408	2.545068	-1.020894
15	6	0	1.492455	3.161972	-1.233708
16	6	0	-3.154888	-2.375848	-1.845710
17	6	0	-0.566603	-2.622426	-1.560586
18	6	0	-0.423612	-1.151626	0.516901
19	6	0	2.581940	-1.027264	0.387209
20	6	0	2.825178	0.068135	-0.503738
21	6	0	2.384068	-0.819013	1.769496

22	6	0	2.495146	0.493950	2.215298
23	6	0	2.728194	1.575342	1.334393
24	6	0	2.821637	1.402717	-0.043123
25	7	0	2.578952	-2.250976	-0.228862
26	7	0	2.996145	-0.307754	-1.809135
27	16	0	2.859036	-1.934739	-1.806801
28	6	0	1.928081	-1.951942	2.649320
29	6	0	0.399062	-1.962884	2.719410
30	6	0	-0.390697	-2.332158	1.472037
31	6	0	0.397218	2.326394	-1.893766
32	6	0	-1.971084	-3.207742	-1.322132
33	6	0	-1.950027	2.678329	1.846169
34	8	0	1.278375	4.318295	-0.876709
35	8	0	-0.173739	-1.624675	3.753270
36	1	0	0.156519	2.957397	1.488160
37	1	0	-0.856662	3.398895	0.137606
38	1	0	0.123226	-0.241218	-2.700860
39	1	0	-2.931104	0.167880	-2.805257
40	1	0	-4.104540	2.699982	1.903896
41	1	0	-3.420652	3.485485	0.482077
42	1	0	-0.745198	0.221685	2.119065
43	1	0	-3.050324	2.290227	-1.545620
44	1	0	-4.061710	0.115728	2.020233
45	1	0	-3.976316	-2.003174	0.753719
46	1	0	3.520677	3.350093	-0.653353
47	1	0	3.268914	2.181717	-1.978343
48	1	0	-3.003947	-2.163515	-2.912599
49	1	0	-4.058434	-2.997211	-1.778910
50	1	0	-0.411668	-2.496842	-2.641431
51	1	0	0.173374	-3.364671	-1.229670
52	1	0	2.367282	0.698090	3.277989
53	1	0	2.763955	2.586218	1.740036
54	1	0	2.294833	-2.903154	2.246025
55	1	0	2.291996	-1.824965	3.673602
56	1	0	0.076598	-3.195779	0.985432
57	1	0	-1.397978	-2.612578	1.804967
58	1	0	-0.438255	3.009199	-2.094495
59	1	0	0.775088	1.961375	-2.858513
60	1	0	-2.005748	-4.192366	-1.808086
61	1	0	-2.115747	-3.390613	-0.251859

62	1	0	-1.906386	3.620075	2.409186
63	1	0	-1.892259	1.877903	2.592336

Table S49. Coordinates of **[3.3]paracyclophane-boat at MP2/6-31G(d)**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.410872	1.549819	-0.124959
2	6	0	0.588160	1.624764	-1.255289
3	6	0	-0.800813	1.634881	-1.132970
4	6	0	-1.410917	1.549802	0.125038
5	6	0	-0.588205	1.624574	1.255379
6	6	0	0.800767	1.634713	1.133061
7	6	0	1.410916	-1.549802	-0.125035
8	6	0	0.800814	-1.634847	1.132974
9	6	0	-0.588160	-1.624728	1.255294
10	6	0	-1.410872	-1.549819	0.124964
11	6	0	-0.800768	-1.634747	-1.133055
12	6	0	0.588203	-1.624611	-1.255374
13	6	0	-2.896844	1.311556	0.246768
14	6	0	-2.896805	-1.311608	0.246715
15	6	0	2.896804	1.311611	-0.246718
16	6	0	2.896843	-1.311557	-0.246777
17	6	0	3.379647	0.000019	0.402001
18	6	0	-3.379644	-0.000020	-0.402013
19	1	0	1.039520	1.614103	-2.246999
20	1	0	-1.415553	1.639501	-2.032821
21	1	0	-1.039564	1.613765	2.247087
22	1	0	1.415506	1.639198	2.032914
23	1	0	1.415553	-1.639437	2.032827
24	1	0	-1.039516	-1.614039	2.247006
25	1	0	-1.415509	-1.639262	-2.032906
26	1	0	1.039564	-1.613830	-2.247082
27	1	0	-3.447390	2.139630	-0.220779
28	1	0	-3.178807	1.313441	1.308150
29	1	0	-3.447336	-2.139678	-0.220858

30	1	0	-3.178759	-1.313540	1.308099
31	1	0	3.447335	2.139676	0.220862
32	1	0	3.178755	1.313553	-1.308103
33	1	0	3.447391	-2.139629	0.220771
34	1	0	3.178799	-1.313446	-1.308161
35	1	0	3.097331	-0.000010	1.461730
36	1	0	4.477724	0.000037	0.379122
37	1	0	-3.097319	0.000008	-1.461741
38	1	0	-4.477720	-0.000037	-0.379142

Table S50. Coordinates of **[3.3]paracyclophane-dione-boat at MP2/6-31G(d)**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.367181	1.592410	-0.336340
2	6	0	0.388600	1.659679	-1.334971
3	6	0	-0.965719	1.663816	-1.003657
4	6	0	-1.367282	1.592376	0.336470
5	6	0	-0.388700	1.659443	1.335112
6	6	0	0.965618	1.663620	1.003799
7	6	0	1.367281	-1.592373	-0.336468
8	6	0	0.965718	-1.663823	1.003658
9	6	0	-0.388601	-1.659687	1.334972
10	6	0	-1.367183	-1.592412	0.336342
11	6	0	-0.965621	-1.663614	-1.003797
12	6	0	0.388698	-1.659435	-1.335111
13	6	0	-2.819876	1.317645	0.672249
14	6	0	-2.819782	-1.317758	0.672169
15	6	0	2.819782	1.317757	-0.672169
16	6	0	2.819876	-1.317644	-0.672250
17	1	0	0.684999	1.646924	-2.383044
18	1	0	-1.718848	1.640849	-1.789768
19	1	0	-0.685099	1.646505	2.383182
20	1	0	1.718747	1.640504	1.789905
21	1	0	1.718847	-1.640861	1.789769
22	1	0	-0.685000	-1.646939	2.383045
23	1	0	-1.718749	-1.640492	-1.789904

24	1	0	0.685097	-1.646491	-2.383181
25	1	0	-3.481254	2.093277	0.271343
26	1	0	-2.950336	1.269743	1.759585
27	1	0	-3.481134	-2.093404	0.271247
28	1	0	-2.950213	-1.269917	1.759512
29	1	0	3.481135	2.093407	-0.271254
30	1	0	2.950208	1.269912	-1.759512
31	1	0	3.481255	-2.093280	-0.271353
32	1	0	2.950329	-1.269736	-1.759586
33	6	0	3.226093	0.000051	-0.018141
34	6	0	-3.226093	-0.000051	0.018142
35	8	0	3.789786	0.000038	1.075104
36	8	0	-3.789775	-0.000038	-1.075109

Table S51. Coordinates of **three-layered [3.3]paracyclophane-boat-boat at MP2/6-31G(d)**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.050717	0.577159	-1.332445
2	6	0	2.847673	1.700834	-0.532826
3	6	0	2.894605	1.608058	0.861264
4	6	0	3.264546	0.379449	1.427784
5	6	0	3.467959	-0.744872	0.627020
6	6	0	3.299953	-0.676086	-0.764835
7	6	0	0.122403	-1.223210	0.404687
8	6	0	0.292317	-1.194540	-0.994307
9	6	0	0.000094	0.000122	-1.661966
10	6	0	-0.292039	1.194795	-0.994299
11	6	0	-0.122624	1.223335	0.404751
12	6	0	-0.000086	0.000050	1.067150
13	6	0	-2.894811	-1.608229	0.860959
14	6	0	-2.846985	-1.700822	-0.533115
15	6	0	-3.049917	-0.577133	-1.332735
16	6	0	-3.299746	0.675997	-0.765127
17	6	0	-3.468612	0.744585	0.626635
18	6	0	-3.265291	-0.379754	1.427406
19	6	0	-0.767252	2.400775	-1.765329

20	6	0	-3.334163	1.917522	-1.622597
21	6	0	0.109924	-2.499295	1.220825
22	6	0	-2.440499	-2.760573	1.717548
23	6	0	-1.013723	-2.584293	2.271321
24	6	0	-2.171605	2.894200	-1.366957
25	6	0	2.440278	2.760446	1.717789
26	6	0	-0.110156	2.499382	1.220944
27	6	0	1.013457	2.584289	2.271481
28	6	0	0.767473	-2.400509	-1.765381
29	6	0	3.334411	-1.917561	-1.622383
30	6	0	2.171748	-2.894156	-1.366928
31	1	0	2.953986	0.663816	-2.413853
32	1	0	2.604960	2.655909	-0.998451
33	1	0	3.357916	0.293359	2.510751
34	1	0	3.725744	-1.696561	1.092693
35	1	0	0.000253	0.000175	-2.754093
36	1	0	-0.000364	0.000030	2.156097
37	1	0	-2.603835	-2.655806	-0.998699
38	1	0	-2.952492	-0.663642	-2.414093
39	1	0	-3.726811	1.696182	1.092267
40	1	0	-3.359357	-0.293821	2.510325
41	1	0	-0.064364	3.239104	-1.647529
42	1	0	-0.769271	2.156597	-2.836535
43	1	0	-4.273781	2.460403	-1.450414
44	1	0	-3.334909	1.625181	-2.681181
45	1	0	0.021130	-3.368273	0.557620
46	1	0	1.072942	-2.610522	1.741876
47	1	0	-2.484398	-3.689369	1.132943
48	1	0	-3.123419	-2.892324	2.567696
49	1	0	-0.798810	-3.442888	2.922075
50	1	0	-0.991274	-1.700495	2.919026
51	1	0	-2.376056	3.816093	-1.928908
52	1	0	-2.175713	3.172746	-0.307830
53	1	0	3.123146	2.892155	2.567983
54	1	0	2.484286	3.689235	1.133177
55	1	0	-0.021345	3.368390	0.557788
56	1	0	-1.073176	2.610596	1.742003
57	1	0	0.990893	1.700482	2.919171
58	1	0	0.798587	3.442905	2.922214
59	1	0	0.064452	-3.238740	-1.647704

60	1	0	0.769627	-2.156250	-2.836568
61	1	0	3.335307	-1.625159	-2.680951
62	1	0	4.273983	-2.460498	-1.450119
63	1	0	2.376145	-3.816022	-1.928939
64	1	0	2.175719	-3.172796	-0.307829

Table S52. Coordinates of **three-layered [3.3]paracyclophane-dione-boat-chair at MP2/6-31G(d)**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.370534	0.295078	0.457648
2	6	0	-3.161094	0.299424	-0.929048
3	6	0	-2.869028	-0.910857	-1.567814
4	6	0	-2.653433	-2.072442	-0.826041
5	6	0	-2.732366	-2.046349	0.569850
6	6	0	-3.143525	-0.862728	1.198913
7	6	0	-0.137113	1.244677	0.613839
8	6	0	-0.237680	1.432884	-0.780398
9	6	0	0.101439	0.374327	-1.627259
10	6	0	0.445724	-0.897569	-1.150523
11	6	0	0.262528	-1.143630	0.224641
12	6	0	0.072140	-0.053959	1.080536
13	6	0	2.887271	1.467719	1.033424
14	6	0	2.985298	1.776364	-0.328889
15	6	0	3.256259	0.783815	-1.268713
16	6	0	3.468490	-0.541974	-0.877590
17	6	0	3.529132	-0.818713	0.495326
18	6	0	3.239087	0.171485	1.435200
19	6	0	0.913359	-1.964620	-2.111694
20	6	0	3.506157	-1.649661	-1.898930
21	6	0	2.400129	2.499704	2.026070
22	6	0	-0.180063	2.385947	1.598666
23	6	0	0.307102	-2.541819	0.819254
24	6	0	-2.167619	-3.173095	1.399806
25	6	0	-0.847829	2.692624	-1.353549
26	6	0	-3.206389	1.596634	-1.714640
27	6	0	-2.340970	2.660485	-1.045322
28	6	0	-0.784046	-2.727147	1.868112
29	8	0	-0.573913	-2.458351	3.049381

30	8	0	-2.837721	3.425096	-0.218201
31	6	0	2.290598	-2.589874	-1.811060
32	6	0	1.108525	3.231681	1.616403
33	1	0	-3.640165	1.221546	0.961853
34	1	0	-2.743806	-0.932857	-2.649531
35	1	0	-2.378861	-2.995765	-1.335761
36	1	0	-3.230102	-0.836279	2.284587
37	1	0	0.126218	0.552041	-2.704370
38	1	0	0.056566	-0.232412	2.155615
39	1	0	2.783574	2.789390	-0.673293
40	1	0	3.251242	1.033694	-2.329301
41	1	0	3.758753	-1.829264	0.834565
42	1	0	3.221981	-0.083217	2.494658
43	1	0	0.939157	-1.533469	-3.121793
44	1	0	0.173054	-2.778479	-2.152760
45	1	0	3.560950	-1.215805	-2.906201
46	1	0	4.412724	-2.256856	-1.770601
47	1	0	2.243144	2.013764	2.998402
48	1	0	3.181045	3.256742	2.185274
49	1	0	-1.027800	3.049015	1.389700
50	1	0	-0.344455	1.974219	2.603389
51	1	0	1.266901	-2.722073	1.320311
52	1	0	0.182521	-3.291409	0.030779
53	1	0	-2.090582	-4.091872	0.804817
54	1	0	-2.768013	-3.375030	2.292442
55	1	0	-0.439363	3.609735	-0.918147
56	1	0	-0.690529	2.721693	-2.439527
57	1	0	-4.225075	1.999130	-1.756618
58	1	0	-2.862226	1.412727	-2.739209
59	1	0	2.442799	-3.410720	-2.525396
60	1	0	2.281014	-3.048568	-0.817274
61	1	0	0.952145	4.058395	2.322201
62	1	0	1.250964	3.697579	0.634448

Table S53. Coordinates of **2,1,3-benzothiadiazole at MP2/6-31G(d)**

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

1	6	0	-2.414470	-0.710532	-0.000033
2	6	0	-2.414469	0.710533	0.000007
3	6	0	-1.239308	1.436540	0.000073
4	6	0	-0.023122	0.717185	0.000020
5	6	0	-0.023123	-0.717185	-0.000076
6	6	0	-1.239308	-1.436540	-0.000053
7	7	0	1.228250	1.270309	-0.000094
8	16	0	2.257567	-0.000001	-0.000006
9	7	0	1.228248	-1.270308	0.000139
10	1	0	-3.366349	-1.236317	0.000070
11	1	0	-3.366347	1.236317	0.000040
12	1	0	-1.230540	2.522939	0.000108
13	1	0	-1.230540	-2.522939	-0.000066

Table S54. Coordinates of **tetracyanoethylene at MP2/6-31G(d)**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.686495
2	6	0	0.000000	0.000000	-0.686495
3	6	0	0.000000	1.226232	-1.422491
4	6	0	0.000000	-1.226232	-1.422491
5	6	0	0.000000	-1.226232	1.422491
6	6	0	0.000000	1.226232	1.422491
7	7	0	0.000000	2.242545	2.033920
8	7	0	0.000000	2.242545	-2.033920
9	7	0	0.000000	-2.242545	2.033920
10	7	0	0.000000	-2.242545	-2.033920

Table S55. CIF data of **1.**

data_General _audit_creation_date 'Tue Dec 30 21:14:20 2008' _audit_creation_method 'by teXsan' _audit_update_record ?
PROCESSING SUMMARY (IUCr Office Use Only)
_journal_date_recd_electronic ? _journal_date_from_coeditor ? _journal_date_accepted ? _journal_coeditor_code ?
#---------- # SUBMISSION DETAILS
_publ_contact_author_name ' ENTER NAME' _publ_contact_author_address ; ENTER ADDRESS ; _publ_contact_author_email ' ENTER EMAIL ADDRESS ' _publ_contact_author_fax ' ENTER FAX NUMBER ' _publ_contact_author_phone ' ENTER PHONE NUMBER ' _publ_contact_letter ; ENTER TEXT OF LETTER ; _publ_requested_journal ' ENTER JOURNAL NAME HERE' _publ_requested_category ' CHOOSE FI FM FO CI CM CO or AD' _publ_requested_coeditor_name ? #---------- # TITLE AND AUTHOR LIST _publ_section_title ; ENTER SECTION TITLE ; _publ_section_title_footnote ; ENTER FOOTNOTE TO TITLE OF PAPER ; loop_ _publ_author_name _publ_author_footnote _publ_author_address ' FIRST AUTHORS NAME ' ; FIRST AUTHORS FOOTNOTES ; ; FIRST AUTHORS ADDRESS ; _publ_section_synopsis ; ENTER SYNOPSIS ; #---------- # TEXT _publ_section_abstract ; ENTER ABSTRACT ; _publ_section_comment ; ENTER TEXT ; _publ_section_acknowledgements ; ENTER ACKNOWLEDGEMENTS ; _publ_section_references ; ENTER OTHER REFERENCES Molecular Structure Corporation, Rigaku Corporation. (2000). teXsan. Single Crystal Structure Analysis Software. Version 1.11. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA. Rigaku, 3-9-12 Akishima, Tokyo, Japan. ; _publ_section_figure_captions ; ENTER FIGURE CAPTIONS ; _publ_section_exptl_prep ; ENTER COMPOUND PREPARATION DETAILS ; _publ_section_exptl_refinement ; ENTER SPECIAL DETAILS OF THE REFINEMENT ; #---------- data_2BA #---------- # CHEMICAL DATA _chemical_formula_sum 'C18 H18 N2 S ' _chemical_formula_moiety 'C18 H18 N2 S ' _chemical_formula_weight 294.41 _chemical_melting_point ? #---------- # CRYSTAL DATA _symmetry_cell_setting monoclinic _symmetry_space_group_name_H-M 'P 1 21/n

1' _symmetry_Int_Tables_number
14 loop_ _symmetry_equiv_pos_as_xyz x,y,z 1/2-x,1/2+y,1/2-z -x,-y,-z 1/2+x,1/2-y,1/2+z _cell_l
ength_a 7.1034(2) _cell_length_b
14.6592(3) _cell_length_c 13.7707(3) _cell_angle_alpha
90 _cell_angle_beta 93.5768(7) _cell_angle_gamma
90 _cell_volume 1431.15(5) _cell_formula_units_Z
4 _cell_measurement_reflns_used 17896 _cell_measurement_theta_min
1.5 _cell_measurement_theta_max 27.4 _cell_measurement_temperature
113.2 #---------- _exptl_crystal_description
'prism' _exptl_crystal_colour 'yellow' _exptl_crystal_size_max
1.000 _exptl_crystal_size_mid 0.600 _exptl_crystal_size_min
0.200 _exptl_crystal_size_rad ? _exptl_crystal_density_diffrn
1.366 _exptl_crystal_density_meas ? _exptl_crystal_density_method 'not
measured' _exptl_absorpt_coefficient_mu 0.220 _exptl_absorpt_correction_type
multi-scan _exptl_absorpt_process_details '(Higashi,
1995)' _exptl_absorpt_correction_T_min 0.786 _exptl_absorpt_correction_T_max
0.957 #---------- # EXPERIMENTAL DATA
_diffrn_radiation_type 'Mo K¥a' _diffrn_radiation_wavelength
0.7107 _diffrn_measurement_device_type 'Rigaku RAXIS-RAPID Imaging
Plate' _diffrn_measurement_method ¥w _diffrn_detector_area_resol_mean
10.00 _diffrn_reflns_number 13125 _diffrn_reflns_av_R_equivalents
0.030 _diffrn_reflns_theta_max 27.44 _diffrn_measured_fraction_theta_max
0.9981 _diffrn_reflns_theta_full 27.44 _diffrn_measured_fraction_theta_full
0.9981 _diffrn_reflns_limit_h_min -9 _diffrn_reflns_limit_h_max
9 _diffrn_reflns_limit_k_min -19 _diffrn_reflns_limit_k_max
18 _diffrn_reflns_limit_l_min -17 _diffrn_reflns_limit_l_max
17 #---------- # REFINEMENT DATA
_refine_special_details ; Refinement using reflections with F^2^ > -10.0 sigma(F^2^). The
weighted R-factor (wR) and goodness of fit (S) are based on F^2^. R-factor (gt) are based on F.
The threshold expression of F^2^ > 2.0 sigma(F^2^) is used only for calculating R-factor
(gt). ; _reflns_number_total 3252 _reflns_number_gt
2984 _reflns_threshold_expression
F^2^>2.0¥s(F^2^) _refine_ls_structure_factor_coef Fsqd _refine_ls_R_factor_gt
0.0433 _refine_ls_wR_factor_ref 0.1382 _refine_ls_hydrogen_treatment
refall _refine_ls_number_reflns 3252 _refine_ls_number_parameters
262 _refine_ls_goodness_of_fit_ref 1.849 _refine_ls_weighting_scheme
calc _refine_ls_weighting_details 'w = 1/[¥s^2^(Fo^2^) + (0.06500(Max(Fo^2^,0) +
2Fc^2^)/3)^2^]' _refine_ls_shift/su_max 0.0003 _refine_diff_density_max
0.28 _refine_diff_density_min -0.48 _refine_ls_extinction_method
none _refine_ls_extinction_coef ? _refine_ls_abs_structure_details ? _refine_

ls_abs_structure_Flack ? loop_ _atom_type_symbol _atom_type_description _atom_type_scat_dispersion_real _atom_type_scat_dispersion_imag _atom_type_scat_source 'C' 'C' 0.003 0.002 ;International Tables for Crystallography (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1) ; 'H' 'H' 0.000 0.000 ;International Tables for Crystallography (1992, Vol. C, Table 6.1.1.2) ; 'N' 'N' 0.006 0.003 ;International Tables for Crystallography (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1) ; 'S' 'S' 0.125 0.123 ;International Tables for Crystallography (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1) ; #---------- # ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS loop_ _atom_site_label _atom_site_type_symbol _atom_site_fract_x _atom_site_fract_y _atom_site_fract_z _atom_site_U_iso_or_equiv _atom_site_adp_type _atom_site_occupancy _atom_site_calc_flag _atom_site_refinement_flags _atom_site_disorder_assembly _atom_site_disorder_group S(1) S -0.13902(6) 0.14168(2) 0.74726(3) 0.0246(1) Uani 1.00 d . . . N(1) N -0.1605(2) 0.25115(9) 0.73799(8) 0.0215(3) Uani 1.00 d . . . N(2) N -0.0745(2) 0.11536(8) 0.63994(9) 0.0227(3) Uani 1.00 d . . . C(1) C 0.4398(2) 0.1607(1) 0.5025(1) 0.0277(4) Uani 1.00 d . . . C(2) C 0.2733(2) 0.09333(10) 0.4963(1) 0.0237(3) Uani 1.00 d . . . C(3) C 0.0885(2) 0.12679(10) 0.4441(1) 0.0225(3) Uani 1.00 d . . . C(4) C -0.0039(2) 0.20455(9) 0.49424(10) 0.0181(3) Uani 1.00 d . . . C(5) C -0.0193(2) 0.29055(9) 0.45657(10) 0.0193(3) Uani 1.00 d . . . C(6) C -0.0733(2) 0.36786(9) 0.5122(1) 0.0192(3) Uani 1.00 d . . . C(7) C -0.1118(2) 0.36233(8) 0.6080(1) 0.0175(3) Uani 1.00 d . . . C(8) C -0.1166(2) 0.27226(9) 0.64733(10) 0.0172(3) Uani 1.00 d . . . C(9) C -0.0655(2) 0.19445(9) 0.59057(10) 0.0172(3) Uani 1.00 d . . . C(10) C -0.1388(2) 0.44461(9) 0.6717(1) 0.0216(3) Uani 1.00 d . . . C(11) C 0.0153(2) 0.45702(9) 0.7547(1) 0.0214(3) Uani 1.00 d . . . C(12) C 0.2172(2) 0.47561(9) 0.7253(1) 0.0222(3) Uani 1.00 d . . . C(13) C 0.3056(2) 0.39704(10) 0.67409(10) 0.0187(3) Uani 1.00 d . . . C(14) C 0.3711(2) 0.4068(1) 0.5809(1) 0.0222(3) Uani 1.00 d . . . C(15) C 0.4235(2) 0.3312(1) 0.5282(1) 0.0236(3) Uani 1.00 d . . . C(16) C 0.4129(2) 0.2434(1) 0.5657(1) 0.0218(3) Uani 1.00 d . . . C(17) C 0.3664(2) 0.23500(10) 0.6624(1) 0.0212(3) Uani 1.00 d . . . C(18) C 0.3145(2) 0.30997(9) 0.7158(1) 0.0197(3) Uani 1.00 d . . . H(1) H 0.548(3) 0.124(1) 0.529(2) 0.048(6) Uiso 1.00 calc . . . H(2) H 0.461(3) 0.177(1) 0.436(1) 0.040(5) Uiso 1.00 calc . . . H(3) H 0.244(3) 0.074(1) 0.564(1) 0.029(5) Uiso 1.00 calc . . . H(4) H 0.314(2) 0.038(1) 0.465(1) 0.023(4) Uiso 1.00 calc . . . H(5) H 0.004(2) 0.070(1) 0.437(1) 0.025(4) Uiso 1.00 calc . . . H(6) H 0.102(3) 0.143(1) 0.379(2) 0.038(5) Uiso 1.00 calc . . . H(7) H 0.020(3) 0.302(1) 0.394(1) 0.029(5) Uiso 1.00 calc . . . H(8) H -0.069(2) 0.430(1) 0.482(1) 0.021(4) Uiso 1.00 calc . . . H(9) H -0.145(2) 0.500(1) 0.634(1) 0.014(4) Uiso 1.00 calc . . . H(10) H -0.261(2) 0.441(1) 0.701(1) 0.025(4) Uiso 1.00 calc . . . H(11) H -0.021(3) 0.510(1) 0.797(1) 0.036(5) Uiso 1.00 calc . . . H(12) H 0.020(2) 0.405(1) 0.794(1) 0.021(4) Uiso 1.00 calc . . . H(13) H 0.225(2) 0.530(1) 0.683(1) 0.021(4) Uiso 1.00 calc . . . H(14) H 0.295(3) 0.488(2) 0.799(2)

0.063(7) Uiso 1.00 calc . . . H(15) H 0.366(2) 0.469(1) 0.552(1) 0.024(4) Uiso 1.00 calc . . . H(16) H 0.464(3) 0.337(1) 0.458(1) 0.037(5) Uiso 1.00 calc . . . H(17) H 0.369(3) 0.175(1) 0.693(1) 0.031(5) Uiso 1.00 calc . . . H(18) H 0.273(3) 0.300(1) 0.780(1) 0.025(5) Uiso 1.00 calc . . . loop_ _atom_site_aniso_label _atom_site_aniso_U_11 _atom_site_aniso_U_22 _atom _site_aniso_U_33 _atom_site_aniso_U_12 _atom_site_aniso_U_13 _atom_site_aniso_U_23 S(1) 0.0339(3) 0.0191(2) 0.0215(2) -0.0060(1) 0.0068(2) 0.0029(1) N(1) 0.0202(6) 0.0224(6) 0.0223(6) -0.0036(5) 0.0049(5) 0.0001(4) N(2) 0.0280(7) 0.0175(5) 0.0225(6) -0.0040(5) 0.0019(5) -0.0001(5) C(1) 0.0228(8) 0.0324(8) 0.0279(8) 0.0044(6) 0.0031(6) -0.0071(6) C(2) 0.0293(8) 0.0193(6) 0.0226(7) 0.0051(6) 0.0028(6) -0.0033(5) C(3) 0.0288(8) 0.0203(6) 0.0183(7) 0.0006(6) 0.0013(6) -0.0039(5) C(4) 0.0169(6) 0.0183(6) 0.0185(6) -0.0020(5) -0.0030(5) -0.0018(5) C(5) 0.0196(7) 0.0221(7) 0.0160(6) -0.0023(5) -0.0006(5) 0.0002(5) C(6) 0.0186(7) 0.0160(6) 0.0226(7) -0.0019(5) -0.0022(5) 0.0022(5) C(7) 0.0128(6) 0.0169(6) 0.0227(7) -0.0001(5) -0.0004(5) -0.0007(5) C(8) 0.0140(6) 0.0178(6) 0.0198(6) -0.0029(5) 0.0017(5) -0.0008(5) C(9) 0.0154(6) 0.0164(6) 0.0195(6) -0.0029(5) -0.0009(5) -0.0010(5) C(10) 0.0221(7) 0.0178(6) 0.0253(7) 0.0026(5) 0.0044(6) -0.0012(5) C(11) 0.0285(8) 0.0177(6) 0.0184(6) 0.0002(6) 0.0057(5) -0.0037(5) C(12) 0.0268(8) 0.0186(6) 0.0212(7) -0.0040(5) 0.0003(6) -0.0016(5) C(13) 0.0149(6) 0.0222(6) 0.0188(6) -0.0033(5) -0.0019(5) -0.0019(5) C(14) 0.0179(7) 0.0261(7) 0.0225(7) -0.0058(5) 0.0000(5) 0.0028(5) C(15) 0.0172(7) 0.0344(8) 0.0194(7) -0.0044(6) 0.0025(5) -0.0006(6) C(16) 0.0138(6) 0.0276(7) 0.0239(7) 0.0008(5) 0.0009(5) -0.0042(6) C(17) 0.0165(7) 0.0241(7) 0.0224(7) 0.0016(5) -0.0040(5) 0.0007(5) C(18) 0.0176(7) 0.0238(7) 0.0172(6) -0.0014(5) -0.0015(5) 0.0000(5)

#---------- _computing_data_collection 'PROCESS-AUTO' _computing_cell_refinement 'PROCESS-AUTO' _computing_data_reduction 'teXsan Ver. 1.11' _computing_structure_solution SIR97 _computing_structure_refinement 'teXsan Ver. 1.10' _computing_publication_material 'teXsan Ver. 1.11' _computing_molecular_graphics ? #---------- ---------- _geom_special_details ; ? ; loop_ _geom_bond_atom_site_label_1 _geom_bond_ato m_site_label_2 _geom_bond_distance _geom_bond_site_symmetry_1 _geom_bond_site_symmetr y_2 _geom_bond_publ_flag S(1) N(1) 1.616(1) . . yes S(1) N(2) 1.621(1) . . yes N(1) C(8) 1.342(2) . . yes N(2) C(9) 1.347(2) . . yes C(1) C(2) 1.539(2) . . yes C(1) C(16) 1.512(2) . . yes C(2) C(3) 1.537(2) . . yes C(3) C(4) 1.505(2) . . yes C(4) C(5) 1.365(2) . . yes C(4) C(9) 1.430(2) . . yes C(5) C(6) 1.434(2) . . yes C(6) C(7) 1.365(2) . . yes C(7) C(8) 1.429(2) . . yes C(7) C(10) 1.511(2) . . yes C(8) C(9) 1.442(2) . . yes C(10) C(11) 1.543(2) . . yes C(11) C(12) 1.539(2) . . yes C(12) C(13) 1.508(2) . . yes C(13) C(14)

1.400(2) . . yes C(13) C(18) 1.399(2) . . yes C(14) C(15) 1.387(2) . . yes C(15) C(16) 1.391(2) . . yes C(16) C(17) 1.397(2) . . yes C(17) C(18) 1.385(2) . . yes #---------- loop_ _geom_angle_atom_site_label_1 _geom_angle_atom_site_label_2 _geom_angle_atom_site_label_3 _geom_angle _geom_angle_site_symmetry_1 _geom_angle_site_symmetry_2 _geom_angle_site_symmetry_3 _geom_angle _publ_flag N(1) S(1) N(2) 101.24(6) . . . yes S(1) N(1) C(8) 106.04(9) . . . yes S(1) N(2) C(9) 106.27(10) . . . yes C(2) C(1) C(16) 115.0(1) . . . yes C(1) C(2) C(3) 116.9(1) . . . yes C(2) C(3) C(4) 114.3(1) . . . yes C(3) C(4) C(5) 123.5(1) . . . yes C(3) C(4) C(9) 121.0(1) . . . yes C(5) C(4) C(9) 115.2(1) . . . yes C(4) C(5) C(6) 123.0(1) . . . yes C(5) C(6) C(7) 123.1(1) . . . yes C(6) C(7) C(8) 115.6(1) . . . yes C(6) C(7) C(10) 123.6(1) . . . yes C(8) C(7) C(10) 120.7(1) . . . yes N(1) C(8) C(7) 125.4(1) . . . yes N(1) C(8) C(9) 113.8(1) . . . yes C(7) C(8) C(9) 120.8(1) . . . yes N(2) C(9) C(4) 125.7(1) . . . yes N(2) C(9) C(8) 112.7(1) . . . yes C(4) C(9) C(8) 121.5(1) . . . yes C(7) C(10) C(11) 114.5(1) . . . yes C(10) C(11) C(12) 117.1(1) . . . yes C(11) C(12) C(13) 114.2(1) . . . yes C(12) C(13) C(14) 121.5(1) . . . yes C(12) C(13) C(18) 121.0(1) . . . yes C(14) C(13) C(18) 117.4(1) . . . yes C(13) C(14) C(15) 120.9(1) . . . yes C(14) C(15) C(16) 121.5(1) . . . yes C(1) C(16) C(15) 121.1(1) . . . yes C(1) C(16) C(17) 121.6(1) . . . yes C(15) C(16) C(17) 117.2(1) . . . yes C(16) C(17) C(18) 121.5(1) . . . yes C(13) C(18) C(17) 120.9(1) . . . yes #---------- loop_ _geom_torsion_atom_site_label_1 _geom_torsion_atom_site_label_2 _geom_torsion_atom_site_label_3 _geom_torsion_atom_site_label_4 _geom_torsion _geom_torsion_site_symmetry_1 _geom_torsion_site_symmetry_2 _geom_torsion_site_symmetry_3 _geom_torsion_site_symmetry_4 _geom_torsion_publ_flag S(1) N(1) C(8) C(7) -178.2(1) . . . . yes S(1) N(1) C(8) C(9) -0.5(1) . . . . yes S(1) N(2) C(9) C(4) 176.3(1) . . . . yes S(1) N(2) C(9) C(8) -0.7(1) . . . . yes N(1) S(1) N(2) C(9) 0.4(1) . . . . yes N(1) C(8) C(7) C(6) -176.6(1) . . . . yes N(1) C(8) C(7) C(10) 6.2(2) . . . . yes N(1) C(8) C(9) N(2) 0.8(2) . . . . yes N(1) C(8) C(9) C(4) -176.3(1) . . . . yes N(2) S(1) N(1) C(8) 0.0(1) . . . . yes N(2) C(9) C(4) C(3) -10.2(2) . . . . yes N(2) C(9) C(4) C(5) 175.7(1) . . . . yes N(2) C(9) C(8) C(7) 178.7(1) . . . . yes C(1) C(2) C(3) C(4) -65.2(2) . . . . yes C(1) C(16) C(15) C(14) 170.0(1) . . . . yes C(1) C(16) C(17) C(18) -170.2(1) . . . . yes C(2) C(1) C(16) C(15)

-122.3(2) . . . . yes C(2) C(1) C(16) C(17) 54.2(2) . . . . yes C(2) C(3) C(4) C(5) 112.5(2) . . . . yes C(2) C(3) C(4) C(9) -61.2(2) . . . . yes C(3) C(2) C(1) C(16) 67.3(2) . . . . yes C(3) C(4) C(5) C(6) -167.4(1) . . . . yes C(3) C(4) C(9) C(8) 166.5(1) . . . . yes C(4) C(5) C(6) C(7) 0.8(2) . . . . yes C(4) C(9) C(8) C(7) 1.6(2) . . . . yes C(5) C(4) C(9) C(8) -7.6(2) . . . . yes C(5) C(6) C(7) C(8) -7.0(2) . . . . yes C(5) C(6) C(7) C(10) 170.0(1) . . . . yes C(6) C(5) C(4) C(9) 6.6(2) . . . . yes C(6) C(7) C(8) C(9) 5.7(2) . . . . yes C(6) C(7) C(10) C(11) -113.6(1) . . . . yes C(7) C(10) C(11) C(12) 64.0(2) . . . . yes C(8) C(7) C(10) C(11) 63.3(2) . . . . yes C(9) C(8) C(7) C(10) -171.4(1) . . . . yes C(10) C(11) C(12) C(13) -66.3(2) . . . . yes C(11) C(12) C(13) C(14) 122.2(1) . . . . yes C(11) C(12) C(13) C(18) -53.8(2) . . . . yes C(12) C(13) C(14) C(15) -169.4(1) . . . . yes C(12) C(13) C(18) C(17) 169.2(1) . . . . yes C(13) C(14) C(15) C(16) 0.1(2) . . . . yes C(13) C(18) C(17) C(16) 0.4(2) . . . . yes C(14) C(13) C(18) C(17) -7.0(2) . . . . yes C(14) C(15) C(16) C(17) -6.6(2) . . . . yes C(15) C(14) C(13) C(18) 6.7(2) . . . . yes C(15) C(16) C(17) C(18) 6.4(2) . . . . yes C(15) C(16) C(17) C(18) 6.4(2) . . . . yes #---------- loop_ _geom_contact_atom_site_label_1 _geom_contact_atom_site_label_2 _geom_contact_distance _geom_contact_site_symmetry_1 _geom_contact_site_symmetry_2 _geom_contact_publ_flag S(1) C(10) 3.507(1) . 2_446 ? N(1) C(17) 3.463(2) . 1_455 ? C(7) C(15) 3.443(2) . 1_455 ? C(8) C(16) 3.485(2) . 1_455 ? #---------- #----------

Table S56. CIF data of **2**

data_3ba _audit_creation_method SHELXL-97 _chemical_name_systematic ; ? ; _chemical_name_common ? _chemical_melting_point ? _chemical_formula_moiety ? _chemical_formula_sum 'C30 H32 N2 S' _chemical_formula_weight 452.64 loop_ _atom_type_symbol _atom_type_description _atom_type_scat_dispersion_real _atom_type_scat_dispersion_imag _atom_type_scat_source 'C' 'C' 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' 'H' 'H' 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' 'N' 'N' 0.0061 0.0033 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' 'S' 'S' 0.1246 0.1234 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' _symmetry_cell_setting orthorhombic _symmetry_space_group_name_H-M

'Aba2' loop_ _symmetry_equiv_pos_as_xyz 'x, y, z' '-x, -y, z' '-x+1/2, y+1/2, z' 'x+1/2, -y+1/2, z' 'x, y+1/2, z+1/2' '-x, -y+1/2, z+1/2' '-x+1/2, y+1, z+1/2' 'x+1/2, -y+1, z+1/2'
_cell_length_a 21.208(4) _cell_length_b 16.936(2)
_cell_length_c 13.147(3) _cell_angle_alpha 90.00
_cell_angle_beta 90.00 _cell_angle_gamma 90.00
_cell_volume 4722.1(16) _cell_formula_units_Z 8
_cell_measurement_temperature 123(2) _cell_measurement_reflns_used 23144
_cell_measurement_theta_min 3.08 _cell_measurement_theta_max 27.43
_exptl_crystal_description prism _exptl_crystal_colour yellow
_exptl_crystal_size_max 0.80 _exptl_crystal_size_mid 0.60
_exptl_crystal_size_min 0.13 _exptl_crystal_density_meas ?
_exptl_crystal_density_diffrn 1.273 _exptl_crystal_density_method 'not measured'
_exptl_crystal_F_000 1936 _exptl_absorpt_coefficient_mu 0.159
_exptl_absorpt_correction_type ? _exptl_absorpt_correction_T_min 1.0000
_exptl_absorpt_correction_T_max 1.0000 _exptl_absorpt_process_details ?
_exptl_special_details ; ? ; _diffrn_ambient_temperature 123(2)
_diffrn_radiation_wavelength 0.71075 _diffrn_radiation_type MoK¥a
_diffrn_radiation_source 'fine-focus sealed tube' _diffrn_radiation_monochromator graphite _diffrn_measurement_device_type ? _diffrn_measurement_method ?
_diffrn_detector_area_resol_mean ? _diffrn_standards_number ?
_diffrn_standards_interval_count ? _diffrn_standards_interval_time ?
_diffrn_standards_decay_% ? _diffrn_reflns_number 23275
_diffrn_reflns_av_R_equivalents 0.0335 _diffrn_reflns_av_sigmaI/netI 0.0321
_diffrn_reflns_limit_h_min -27 _diffrn_reflns_limit_h_max 25
_diffrn_reflns_limit_k_min -21 _diffrn_reflns_limit_k_max 21
_diffrn_reflns_limit_l_min -16 _diffrn_reflns_limit_l_max 17
_diffrn_reflns_theta_min 3.08 _diffrn_reflns_theta_max 27.43
_reflns_number_total 5361 _reflns_number_gt 5173
_reflns_threshold_expression >2sigma(I) _computing_data_collection ?
_computing_cell_refinement ? _computing_data_reduction ?
_computing_structure_solution 'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics ? _computing_publication_material ?
_refine_special_details ; Refinement of F^2^ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2^, conventional R-factors R are based on F, with F set to zero for negative F^2^. The threshold expression of F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2^ are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger. ; _refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type full _refine_ls_weighting_scheme calc

_refine_ls_weighting_details 'calc w=1/[¥s^2^(Fo^2^)+(0.1493P)^2^+6.3637P] where P=(Fo^2^+2Fc^2^)/3' _atom_sites_solution_primary direct _atom_sites_solution_secondary difmap _atom_sites_solution_hydrogens geom _refine_ls_hydrogen_treatment mixed _refine_ls_extinction_method none _refine_ls_extinction_coef ? _refine_ls_abs_structure_details 'Flack H D (1983), Acta Cryst. A39, 876-881' _refine_ls_abs_structure_Flack 0.45(11) _refine_ls_number_reflns 5361 _refine_ls_number_parameters 374 _refine_ls_number_restraints 1 _refine_ls_R_factor_all 0.0735 _refine_ls_R_factor_gt 0.0720 _refine_ls_wR_factor_ref 0.2054 _refine_ls_wR_factor_gt 0.2032 _refine_ls_goodness_of_fit_ref 1.053 _refine_ls_restrained_S_all 1.053 _refine_ls_shift/su_max 0.000 _refine_ls_shift/su_mean 0.000 loop_ _atom_site_label _atom_site_type_symbol _atom_site_fract_x _atom_site_fract_y _atom_site_fract_z _atom_site_U_iso_or_equiv _atom_site_adp_type _atom_site_occupancy _atom_site_symmetry_multiplicity _atom_site_calc_flag _atom_site_refinement_flags _atom_site_disorder_assembly _atom_site_disorder_group C1 C 0.70591(14) 0.15345(16) 0.2837(2) 0.0255(6) Uani 1 1 d . . . H1 H 0.6904(16) 0.101(2) 0.251(3) 0.016(8) Uiso 1 1 d . . . H2 H 0.7025(16) 0.144(2) 0.355(3) 0.013(7) Uiso 1 1 d . . . C2 C 0.77534(14) 0.16637(18) 0.2536(3) 0.0301(7) Uani 1 1 d . . . H3 H 0.801(2) 0.120(3) 0.278(4) 0.041(11) Uiso 1 1 d . . . H4 H 0.7920(18) 0.214(2) 0.294(3) 0.024(9) Uiso 1 1 d . . . C3 C 0.78917(17) 0.17250(19) 0.1389(3) 0.0355(7) Uani 1 1 d . . . H5 H 0.772(3) 0.117(3) 0.102(4) 0.055(14) Uiso 1 1 d . . . H6 H 0.834(3) 0.169(4) 0.150(5) 0.08(2) Uiso 1 1 d . . . C4 C 0.76016(15) 0.24363(18) 0.0876(2) 0.0293(6) Uani 1 1 d . . . C5 C 0.77599(14) 0.32139(18) 0.1211(2) 0.0269(6) Uani 1 1 d . . . C6 C 0.74044(14) 0.38928(16) 0.0862(2) 0.0256(6) Uani 1 1 d . . . C7 C 0.69050(15) 0.38125(19) 0.0149(2) 0.0287(6) Uani 1 1 d . . . C8 C 0.68137(15) 0.3072(2) -0.0230(2) 0.0326(7) Uani 1 1 d . . . H7 H 0.645(2) 0.299(3) -0.082(4) 0.041(11) Uiso 1 1 d . . . C9 C 0.71498(16) 0.23995(19) 0.0137(3) 0.0328(7) Uani 1 1 d . . . H8 H 0.705(3) 0.184(4) -0.020(6) 0.079(19) Uiso 1 1 d . . . C10 C 0.64719(17) 0.4496(2) -0.0080(3) 0.0378(7) Uani 1 1 d . . . H9 H 0.6724 0.4929 -0.0382 0.045 Uiso 1 1 calc R . . H10 H 0.6160 0.4326 -0.0596 0.045 Uiso 1 1 calc R . . C11 C 0.6125(3) 0.4813(3) 0.0817(5) 0.0715(15) Uani 1 1 d . . . H11 H 0.6446 0.5028 0.1289 0.086 Uiso 1 1 calc R . . H12 H 0.5874 0.5268 0.0573 0.086 Uiso 1 1 calc R . . C12 C 0.5695(2) 0.4312(2) 0.1436(4) 0.0489(11) Uani 1 1 d . . . H13 H 0.5348 0.4129 0.0991 0.059 Uiso 1 1 calc R . . H14 H 0.5505 0.4647 0.1972 0.059 Uiso 1 1 calc R . . C13 C 0.59857(14) 0.35960(18) 0.1941(3) 0.0318(7) Uani 1 1 d . . . C14 C 0.58261(13) 0.2845(2) 0.1571(3) 0.0304(6) Uani 1 1 d . . . H15 H 0.5535(18) 0.291(2) 0.113(3) 0.018(8) Uiso 1 1 d . . . C15 C 0.61158(13) 0.21596(16) 0.1919(2) 0.0241(5) Uani 1 1 d . . . C16 C 0.66275(13) 0.22264(16) 0.2585(2) 0.0211(5) Uani 1 1 d . . . C17 C 0.67433(13) 0.29584(16) 0.3032(2) 0.0223(5) Uani 1 1 d . . . H16 H 0.709(2) 0.303(2) 0.346(3) 0.030(10) Uiso 1 1 d . . . C18 C 0.64066(14) 0.36439(17) 0.2764(2) 0.0266(6) Uani 1 1 d . . . C19 C 0.58635(16) 0.1368(2) 0.1553(3) 0.0330(7) Uani 1 1 d . . . H17 H 0.622(3) 0.107(4) 0.132(5) 0.072(18) Uiso 1 1 d . . . H18 H 0.5504(18) 0.142(2) 0.102(3) 0.024(9) Uiso 1 1 d . . . C20 C 0.55624(17) 0.0857(2) 0.2397(3) 0.0377(8) Uani 1 1 d . . . H19 H 0.545(3) 0.042(4) 0.199(6) 0.081(18) Uiso 1 1 d . . . H20 H 0.580(2) 0.087(3) 0.299(4) 0.046(12) Uiso

1 1 d . . . C21 C 0.49502(18) 0.1169(3) 0.2882(4) 0.0467(10) Uani 1 1 d . . . H21 H 0.470(3) 0.119(3) 0.244(5) 0.061(17) Uiso 1 1 d . . . H22 H 0.475(2) 0.070(2) 0.326(3) 0.028(10) Uiso 1 1 d . . . C22 C 0.50334(15) 0.1915(2) 0.3497(3) 0.0337(7) Uani 1 1 d . . . C23 C 0.47166(16) 0.2607(3) 0.3266(3) 0.0424(8) Uani 1 1 d . . . H23 H 0.439(2) 0.264(2) 0.268(3) 0.033(10) Uiso 1 1 d . . . C24 C 0.48806(17) 0.3314(2) 0.3727(3) 0.0438(9) Uani 1 1 d . . . H24 H 0.4654 0.3779 0.3556 0.053 Uiso 1 1 calc R . . C25 C 0.53612(17) 0.3360(2) 0.4422(3) 0.0379(8) Uani 1 1 d . . . C26 C 0.56293(16) 0.2653(2) 0.4752(3) 0.0332(7) Uani 1 1 d . . . H25 H 0.5932(19) 0.266(2) 0.517(3) 0.024(9) Uiso 1 1 d . . . C27 C 0.54677(15) 0.1949(2) 0.4306(3) 0.0334(7) Uani 1 1 d . . . H26 H 0.5709(15) 0.147(2) 0.450(2) 0.013(7) Uiso 1 1 d . . . C28 C 0.5638(2) 0.4148(2) 0.4791(4) 0.0519(10) Uani 1 1 d . . . H27 H 0.5290 0.4458 0.5097 0.062 Uiso 1 1 calc R . . H28 H 0.5942 0.4031 0.5341 0.062 Uiso 1 1 calc R . . C29 C 0.5950(3) 0.4644(3) 0.4060(5) 0.0685(13) Uani 1 1 d . . . H29 H 0.6099 0.5114 0.4439 0.082 Uiso 1 1 calc R . . H30 H 0.5619 0.4832 0.3588 0.082 Uiso 1 1 calc R . . C30 C 0.64946(19) 0.43810(18) 0.3406(3) 0.0402(8) Uani 1 1 d . . . H31 H 0.6863 0.4294 0.3856 0.048 Uiso 1 1 calc R . . H32 H 0.6603 0.4822 0.2943 0.048 Uiso 1 1 calc R . . N1 N 0.82055(12) 0.33903(16) 0.1900(2) 0.0322(6) Uani 1 1 d . . . N2 N 0.76014(13) 0.45724(16) 0.1293(2) 0.0319(6) Uani 1 1 d . . . S1 S 0.81679(4) 0.43397(4) 0.20632(8) 0.0353(2) Uani 1 1 d . . . loop_ _atom_site_aniso_label _atom_site_aniso_U_11 _atom_site_aniso_U_22 _atom_site_aniso_U_33 _atom_site_aniso_U_23 _atom_site_aniso_U_13 _atom_site_aniso_U_12 C1 0.0256(13) 0.0185(12) 0.0325(15) 0.0041(11) 0.0018(11) 0.0021(10) C2 0.0253(14) 0.0210(13) 0.0440(18) 0.0050(12) 0.0020(12) 0.0064(10) C3 0.0377(17) 0.0244(14) 0.0445(19) -0.0004(13) 0.0177(14) 0.0075(12) C4 0.0329(16) 0.0238(13) 0.0311(14) -0.0027(11) 0.0127(12) -0.0007(11) C5 0.0268(13) 0.0263(13) 0.0277(14) 0.0010(11) 0.0075(11) -0.0002(11) C6 0.0296(15) 0.0245(13) 0.0225(12) 0.0031(10) 0.0049(11) -0.0008(10) C7 0.0306(14) 0.0313(15) 0.0242(13) 0.0038(11) 0.0056(11) -0.0019(12) C8 0.0342(16) 0.0390(17) 0.0246(14) -0.0026(13) 0.0068(11) -0.0073(12) C9 0.0384(16) 0.0285(14) 0.0316(15) -0.0076(12) 0.0143(13) -0.0067(12) C10 0.0378(17) 0.0420(17) 0.0336(16) 0.0124(14) 0.0006(13) 0.0053(14) C11 0.070(3) 0.063(3) 0.082(4) 0.020(3) 0.001(3) 0.015(2) C12 0.045(2) 0.045(2) 0.057(2) 0.0230(18) 0.0123(18) 0.0250(16) C13 0.0258(13) 0.0299(13) 0.0396(16) 0.0140(13) 0.0115(12) 0.0116(11) C14 0.0165(12) 0.0451(18) 0.0296(14) 0.0074(12) 0.0021(11) 0.0028(11) C15 0.0215(11) 0.0255(13) 0.0253(13) 0.0009(11) 0.0052(10) -0.0040(9) C16 0.0207(12) 0.0189(11) 0.0238(13) 0.0045(9) 0.0047(10) -0.0001(9) C17 0.0186(12) 0.0209(12) 0.0275(14) 0.0006(10) 0.0027(10) -0.0023(9) C18 0.0241(13) 0.0214(12) 0.0344(14) 0.0019(11) 0.0102(11) 0.0017(10) C19 0.0322(15) 0.0337(16) 0.0332(15) -0.0107(13) 0.0036(12) -0.0091(12) C20 0.0351(16) 0.0314(15) 0.0466(19) -0.0106(14) 0.0126(14) -0.0162(13) C21 0.0271(16) 0.051(2) 0.061(2) -0.0201(19) 0.0131(17) -0.0173(15) C22 0.0232(13) 0.0397(17) 0.0383(17) -0.0069(13) 0.0108(12) -0.0067(12) C23 0.0243(14) 0.057(2) 0.0456(19) -0.0017(17) 0.0053(14) -0.0007(14) C24 0.0323(17) 0.0445(19) 0.054(2) 0.0041(17) 0.0156(16) 0.0110(14) C25 0.0399(17) 0.0341(16) 0.0397(17) -0.0048(13) 0.0201(14) 0.0023(13) C26 0.0351(16) 0.0390(17) 0.0255(14) 0.0033(13) 0.0081(13) -0.0040(13) C27 0.0315(14) 0.0331(15) 0.0356(17) 0.0044(13) 0.0103(13) -0.0033(12) C28 0.068(3) 0.0319(17) 0.055(2) -0.0112(17) 0.024(2) 0.0023(18) C29 0.081(3) 0.059(3) 0.066(3) -0.004(2) 0.009(3) 0.014(3) C30 0.0462(19) 0.0182(13) 0.056(2)

-0.0045(13) 0.0132(16) 0.0003(12) N1 0.0309(12) 0.0251(12) 0.0405(16) -0.0005(11) -0.0001(11) 0.0022(9) N2 0.0357(14) 0.0227(11) 0.0374(14) 0.0031(11) -0.0015(11) 0.0000(10) S1 0.0366(4) 0.0272(4) 0.0420(4) -0.0044(3) -0.0067(3) 0.0004(3) _geom_special_details ; All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes. ; loop_ _geom_bond_atom_site_label_1 _geom_bond_atom_site_label_2 _geom_bond_distance _geom_bond_site_symmetry_2 _geom_bond_publ_flag C1 C16 1.524(4) . ? C1 C2 1.540(4) . ? C2 C3 1.540(5) . ? C3 C4 1.511(5) . ? C4 C9 1.367(5) . ? C4 C5 1.429(4) . ? C5 N1 1.342(4) . ? C5 C6 1.450(4) . ? C6 N2 1.349(4) . ? C6 C7 1.421(4) . ? C7 C8 1.363(5) . ? C7 C10 1.508(5) . ? C8 C9 1.428(5) . ? C10 C11 1.489(7) . ? C11 C12 1.489(7) . ? C12 C13 1.514(4) . ? C13 C14 1.403(5) . ? C13 C18 1.406(5) . ? C14 C15 1.391(4) . ? C15 C16 1.399(4) . ? C15 C19 1.521(4) . ? C16 C17 1.394(4) . ? C17 C18 1.408(4) . ? C18 C30 1.518(4) . ? C19 C20 1.545(5) . ? C20 C21 1.540(5) . ? C21 C22 1.510(5) . ? C22 C23 1.386(5) . ? C22 C27 1.409(5) . ? C23 C24 1.386(6) . ? C24 C25 1.372(6) . ? C25 C26 1.395(5) . ? C25 C28 1.536(5) . ? C26 C27 1.372(5) . ? C28 C29 1.438(7) . ? C29 C30 1.507(7) . ? N1 S1 1.624(3) . ? N2 S1 1.620(3) . ? loop_ _geom_angle_atom_site_label_1 _geom_angle_atom_site_label_2 _geom_angle_atom_site_label_3 _geom_angle _geom_angle_site_symmetry_1 _geom_angle_site_symmetry_3 _geom_angle_publ_flag C16 C1 C2 114.1(2) . . ? C3 C2 C1 116.3(3) . . ? C4 C3 C2 114.4(3) . . ? C9 C4 C5 115.2(3) . . ? C9 C4 C3 124.5(3) . . ? C5 C4 C3 120.1(3) . . ? N1 C5 C4 125.3(3) . . ? N1 C5 C6 113.8(3) . . ? C4 C5 C6 120.8(3) . . ? N2 C6 C7 126.1(3) . . ? N2 C6 C5 112.5(3) . . ? C7 C6 C5 121.4(3) . . ? C8 C7 C6 115.8(3) . . ? C8 C7 C10 123.2(3) . . ? C6 C7 C10 120.8(3) . . ? C7 C8 C9 122.7(3) . . ? C4 C9 C8 123.6(3) . . ? C11 C10 C7 114.8(3) . . ? C12 C11 C10 122.0(5) . . ? C11 C12 C13 116.5(3) . . ? C14 C13 C18 118.2(3) . . ? C14 C13 C12 118.4(3) . . ? C18 C13 C12 123.4(3) . . ? C15 C14 C13 122.4(3) . . ? C14 C15 C16 118.7(3) . . ? C14 C15 C19 118.5(3) . . ? C16 C15 C19 122.8(3) . . ? C17 C16 C15 118.2(2) . . ? C17 C16 C1 119.1(3) . . ? C15 C16 C1 122.7(2) . . ? C16 C17 C18 122.6(3) . . ? C13 C18 C17 117.8(3) . . ? C13 C18 C30 123.6(3) . . ? C17 C18 C30 118.5(3) . . ? C15 C19 C20 114.4(3) . . ? C21 C20 C19 117.0(4) . . ? C22 C21 C20 114.2(3) . . ? C23 C22 C27 116.6(3) . . ? C23 C22 C21 122.3(4) . . ? C27 C22 C21 121.0(4) . . ? C22 C23 C24 120.9(4) . . ? C25 C24 C23 121.8(3) . . ? C24 C25 C26 117.5(3) . . ? C24 C25 C28 122.9(4) . . ? C26 C25 C28 119.5(4) . . ? C27 C26 C25 120.8(3) . . ? C26 C27 C22 121.4(3) . . ? C29 C28 C25 118.2(4) . . ? C28 C29 C30 124.2(4) . . ? C29 C30 C18 117.8(4) . . ? C5 N1 S1 106.0(2) . . ? C6 N2 S1 106.5(2) . . ? N2 S1 N1 101.21(15) . . ? loop_ _geom_torsion_atom_site_label_1 _geom_torsion_atom_site_label_2 _geom_torsion_atom_site_label_3 _geom_torsion_atom_site_label_4 _geom_torsion _geom_torsion_site_symmetry_1 _geom_torsion_site_symmetry_2 _geom_torsion_site_symmetry_3 _geom_torsion_site_symmetry_4 _geom_torsion_publ_flag C16 C1 C2 C3 -66.1(4) . . . . ? C1 C2 C3 C4 65.0(4) . . . . ? C2 C3 C4 C9 -115.8(4) . . . . ? C2 C3 C4 C5 59.3(4) . . . . ? C9 C4 C5 N1

-177.3(3) . . . . ? C3 C4 C5 N1 7.2(4) . . . . ? C9 C4 C5 C6 6.9(4) . . . . ? C3 C4 C5 C6 -168.6(3) . . . . ? N1 C5 C6 N2 0.9(4) . . . . ? C4 C5 C6 N2 177.1(3) . . . . ? N1 C5 C6 C7 -178.7(3) . . . . ? C4 C5 C6 C7 -2.5(4) . . . . ? N2 C6 C7 C8 176.2(3) . . . . ? C5 C6 C7 C8 -4.2(4) . . . . ? N2 C6 C7 C10 -9.5(5) . . . . ? C5 C6 C7 C10 170.0(3) . . . . ? C6 C7 C8 C9 6.3(4) . . . . ? C10 C7 C8 C9 -167.8(3) . . . . ? C5 C4 C9 C8 -5.1(4) . . . . ? C3 C4 C9 C8 170.2(3) . . . . ? C7 C8 C9 C4 -1.7(5) . . . . ? C8 C7 C10 C11 115.0(4) . . . . ? C6 C7 C10 C11 -58.8(5) . . . . ? C7 C10 C11 C12 -59.1(6) . . . . ? C10 C11 C12 C13 60.1(7) . . . . ? C11 C12 C13 C14 -109.5(5) . . . . ? C11 C12 C13 C18 70.7(5) . . . . ? C18 C13 C14 C15 -6.7(4) . . . . ? C12 C13 C14 C15 173.5(3) . . . . ? C13 C14 C15 C16 -6.6(4) . . . . ? C13 C14 C15 C19 173.7(3) . . . . ? C14 C15 C16 C17 12.9(4) . . . . ? C19 C15 C16 C17 -167.4(3) . . . . ? C14 C15 C16 C1 -167.1(3) . . . . ? C19 C15 C16 C1 12.6(4) . . . . ? C2 C1 C16 C17 -61.1(4) . . . . ? C2 C1 C16 C15 118.9(3) . . . . ? C15 C16 C17 C18 -6.4(4) . . . . ? C1 C16 C17 C18 173.6(3) . . . . ? C14 C13 C18 C17 13.0(4) . . . . ? C12 C13 C18 C17 -167.2(3) . . . . ? C14 C13 C18 C30 -164.1(3) . . . . ? C12 C13 C18 C30 15.6(5) . . . . ? C16 C17 C18 C13 -6.8(4) . . . . ? C16 C17 C18 C30 170.5(3) . . . . ? C14 C15 C19 C20 -113.9(3) . . . . ? C16 C15 C19 C20 66.4(4) . . . . ? C15 C19 C20 C21 66.5(4) . . . . ? C19 C20 C21 C22 -66.9(5) . . . . ? C20 C21 C22 C23 120.4(4) . . . . ? C20 C21 C22 C27 -56.1(5) . . . . ? C27 C22 C23 C24 7.8(5) . . . . ? C21 C22 C23 C24 -168.8(3) . . . . ? C22 C23 C24 C25 0.3(6) . . . . ? C23 C24 C25 C26 -8.1(5) . . . . ? C23 C24 C25 C28 167.9(3) . . . . ? C24 C25 C26 C27 7.5(5) . . . . ? C28 C25 C26 C27 -168.6(3) . . . . ? C25 C26 C27 C22 0.7(5) . . . . ? C23 C22 C27 C26 -8.3(5) . . . . ? C21 C22 C27 C26 168.3(3) . . . . ? C24 C25 C28 C29 -63.8(6) . . . . ? C26 C25 C28 C29 112.1(5) . . . . ? C25 C28 C29 C30 -55.8(8) . . . . ? C28 C29 C30 C18 54.3(7) . . . . ? C13 C18 C30 C29 67.0(5) . . . . ? C17 C18 C30 C29 -110.1(4) . . . . ? C4 C5 N1 S1 -176.5(2) . . . . ? C6 C5 N1 S1 -0.5(3) . . . . ? C7 C6 N2 S1 178.7(3) . . . . ? C5 C6 N2 S1 -0.9(3) . . . . ? C6 N2 S1 N1 0.6(2) . . . . ? C5 N1 S1 N2 0.0(2) . . . . ? _diffrn_measured_fraction_theta_max 0.997 _diffrn_reflns_theta_full 27.43 _diffrn_measured_fraction_theta_full 0.997 _refine_diff_density_max 1.903 _refine_diff_density_min -0.525 _refine_diff_density_rms 0.089

Table S57. CIF data of **5**.

data_General _audit_creation_date 'Tue Oct 21 17:55:44 2008' _audit_creation_method 'by teXsan' _audit_update_record ? #---------- # PROCESSING SUMMARY (IUCr Office Use Only) _journal_date_recd_electronic ? _journal_date_from_coeditor ? _journal_date_accepted ? _journal_coeditor_code ? #---------- # SUBMISSION DETAILS _publ_contact_author_name ' ENTER NAME' _publ_contact_author_address ; ENTER ADDRESS ; _publ_contact_author_email ' ENTER EMAIL ADDRESS ' _publ_contact_author_fax ' ENTER FAX NUMBER ' _publ_contact_author_phone ' ENTER PHONE NUMBER ' _publ_contact_letter ; ENTER TEXT OF

LETTER ; _publ_requested_journal ' ENTER JOURNAL NAME HERE' _publ_requested_category 'CO' _publ_requested_coeditor_name ? #---------- # TITLE AND AUTHOR LIST _publ_section_title ; ENTER SECTION TITLE ; _publ_section_title_footnote ; ENTER FOOTNOTE TO TITLE OF PAPER ; loop_ _publ_author_name _publ_author_footnote _publ_author_address ' FIRST AUTHORS NAME ' ; FIRST AUTHORS FOOTNOTES ; ; FIRST AUTHORS ADDRESS ; _publ_section_synopsis ; ENTER SYNOPSIS ; #---------- # TEXT _publ_section_abstract ; ENTER ABSTRACT ; _publ_section_comment ; ENTER TEXT ; _publ_section_acknowledgements ; ENTER ACKNOWLEDGEMENTS ; _publ_section_references ; ENTER OTHER REFERENCES Molecular Structure Corporation, Rigaku Corporation. (2000). teXsan. Single Crystal Structure Analysis Software. Version 1.11. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA. Rigaku, 3-9-12 Akishima, Tokyo, Japan. ; _publ_section_figure_captions ; ENTER FIGURE CAPTIONS ; _publ_section_exptl_prep ; ENTER COMPOUND PREPARATION DETAILS ; _publ_section_exptl_refinement ; ENTER SPECIAL DETAILS OF THE REFINEMENT ; #---------- # CHEMICAL DATA _chemical_formula_sum 'C18 H14 N2 O2 S ' _chemical_formula_moiety 'C18 H14 N2 O2 S ' _chemical_formula_weight 322.38 _chemical_melting_point ? #---------- # CRYSTAL DATA _symmetry_cell_setting orthorhombic _symmetry_space_group_name_H-M 'P 21/n 21/m 21/a' _symmetry_Int_Tables_number
62 loop_ _symmetry_equiv_pos_as_xyz x,y,z 1/2+x,1/2-y,1/2-z -x,1/2+y,-z 1/2-x,-y,1/2+z -x,-y,-z 1/2-x,1/2+y,1/2+z x,1/2-y,z 1/2+x,y,1/2-z _cell_length_a
9.288(5) _cell_length_b 14.087(7) _cell_length_c
11.250(7) _cell_angle_alpha 89 _cell_angle_beta
89 _cell_angle_gamma 90 _cell_volume
1471(2) _cell_formula_units_Z 4 _cell_measurement_reflns_used
12304 _cell_measurement_theta_min 3.2 _cell_measurement_theta_max
27.4 _cell_measurement_temperature
123.2 #---------- _exptl_crystal_description
'needle' _exptl_crystal_colour 'yellow' _exptl_crystal_size_max
1.300 _exptl_crystal_size_mid 0.260 _exptl_crystal_size_min
0.070 _exptl_crystal_size_rad ? _exptl_crystal_density_diffrn
1.455 _exptl_crystal_density_meas ? _exptl_crystal_density_method 'not measured' _exptl_absorpt_coefficient_mu 0.231 _exptl_absorpt_correction_type none #---------- # EXPERIMENTAL DATA

_diffrn_radiation_type 'Mo K¥a' _diffrn_radiation_wavelength 0.7107 _diffrn_measurement_device_type ? _diffrn_reflns_number 14435 _diffrn_reflns_av_R_equivalents 0.032 _diffrn_reflns_theta_max 27.44 _diffrn_measured_fraction_theta_max 0.9954 _diffrn_reflns_theta_full 27.44 _diffrn_measured_fraction_theta_full 0.9954 _diffrn_reflns_limit_h_min -12 _diffrn_reflns_limit_h_max 9 _diffrn_reflns_limit_k_min -18 _diffrn_reflns_limit_k_max 17 _diffrn_reflns_limit_l_min -14 _diffrn_reflns_limit_l_max 14 #---------- # REFINEMENT DATA _refine_special_details ; Refinement using reflections with F^2^ > -10.0 sigma(F^2^). The weighted R-factor (wR) and goodness of fit (S) are based on F^2^. R-factor (gt) are based on F. The threshold expression of F^2^ > 2.0 sigma(F^2^) is used only for calculating R-factor (gt). ; _reflns_number_total 1742 _reflns_number_gt 1368 _reflns_threshold_expression F^2^>2.0¥s(F^2^) _refine_ls_structure_factor_coef Fsqd _refine_ls_R_factor_gt 0.0364 _refine_ls_wR_factor_ref 0.1049 _refine_ls_hydrogen_treatment refall _refine_ls_number_reflns 1742 _refine_ls_number_parameters 134 _refine_ls_goodness_of_fit_ref 1.099 _refine_ls_weighting_scheme calc _refine_ls_weighting_details 'w = 1/[¥s^2^(Fo^2^) + (0.05000(Max(Fo^2^,0) + 2Fc^2^)/3)^2^]' _refine_ls_shift/su_max 0.0002 _refine_diff_density_max 0.22 _refine_diff_density_min -0.23 _refine_ls_extinction_method none _refine_ls_extinction_coef ? _refine_ls_abs_structure_details ? _refine_ls_abs_structure_Flack ? loop_ _atom_type_symbol _atom_type_description _atom_type_scat_dispersion_real _atom_type_scat_dispersion_imag _atom_type_scat_source 'C' 'C' 0.003 0.002 ;International Tables for Crystallography (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1) ; 'H' 'H' 0.000 0.000 ;International Tables for Crystallography (1992, Vol. C, Table 6.1.1.2) ; 'O' 'O' 0.011 0.006 ;International Tables for Crystallography (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1) ; 'N' 'N' 0.006 0.003 ;International Tables for Crystallography (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1) ; 'S' 'S' 0.125 0.123 ;International Tables for Crystallography (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.1) ; #---------- # ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS loop_ _atom_site_label _atom_site_type_symbol _atom_site_fract_x _atom_site_fract_y _atom_site_fract_z _atom_site_U_iso_or_equiv _atom_site_adp_type _atom_site_occupancy _atom_site_calc_flag _atom_site_refinement_flags _atom_site_disorder_assembly _atom_site_disorder_group S(1) S 0.33504(6) 0.2500 0.06134(6) 0.0302(2) Uani 1.00 d S . . O(1) O 0.8586(1) -0.01394(9) -0.1531(1) 0.0389(3) Uani 1.00 d . . . N(1) N 0.4109(1) 0.16126(9) -0.0051(1) 0.0269(3) Uani 1.00 d . . . C(1) C 0.7927(2) 0.0435(1) 0.0387(2) 0.0262(4) Uani 1.00 d . . . C(2) C 0.7650(1) 0.01959(10) -0.0918(1) 0.0256(4) Uani 1.00 d . . . C(3) C 0.6172(1) 0.0413(1) -0.1456(2) 0.0261(4) Uani

1.00 d . . . C(4) C 0.5961(1) 0.1469(1) -0.1617(1) 0.0234(3) Uani 1.00 d . . . C(5) C 0.6736(1) 0.1992(1) -0.2412(1) 0.0267(4) Uani 1.00 d . . . C(6) C 0.5025(1) 0.19895(10) -0.0855(1) 0.0221(3) Uani 1.00 d . . . C(7) C 0.9100(1) 0.2005(1) -0.0098(2) 0.0270(4) Uani 1.00 d . . . C(8) C 0.8098(1) 0.1503(1) 0.0573(1) 0.0226(3) Uani 1.00 d . . . C(9) C 0.7205(1) 0.2001(1) 0.1344(1) 0.0240(4) Uani 1.00 d . . . H(1) H 0.889(2) 0.006(1) 0.061(2) 0.040(5) Uiso 1.00 calc . . . H(2) H 0.717(2) 0.021(1) 0.094(2) 0.036(5) Uiso 1.00 calc . . . H(3) H 0.611(2) 0.007(1) -0.222(2) 0.034(4) Uiso 1.00 calc . . . H(4) H 0.542(2) 0.019(1) -0.092(2) 0.030(4) Uiso 1.00 calc . . . H(5) H 0.735(2) 0.170(1) -0.294(2) 0.032(4) Uiso 1.00 calc . . . H(6) H 0.975(2) 0.169(1) -0.060(1) 0.031(4) Uiso 1.00 calc . . . H(7) H 0.655(2) 0.167(1) 0.188(2) 0.034(4) Uiso 1.00 calc . . . loop_ _atom_site_aniso_label _atom_site_aniso_U_11 _atom_site_aniso_U_22 _atom _site_aniso_U_33 _atom_site_aniso_U_12 _atom_site_aniso_U_13 _atom_site_aniso_U_23 S(1) 0.0291(3) 0.0311(3) 0.0303(4) 0.0000 0.0116(2) 0.0000 O(1) 0.0281(5) 0.0472(7) 0.0414(8) 0.0073(5) 0.0030(5) -0.0147(6) N(1) 0.0236(5) 0.0307(6) 0.0264(7) -0.0017(5) 0.0034(5) -0.0016(6) C(1) 0.0253(7) 0.0243(7) 0.0290(9) 0.0011(5) -0.0023(7) -0.0003(7) C(2) 0.0220(6) 0.0211(7) 0.0336(9) 0.0002(5) 0.0005(7) -0.0032(7) C(3) 0.0225(6) 0.0288(7) 0.0270(9) -0.0002(5) -0.0005(6) -0.0050(7) C(4) 0.0176(5) 0.0312(7) 0.0214(8) 0.0009(5) -0.0044(6) -0.0043(7) C(5) 0.0198(6) 0.0376(8) 0.0227(8) 0.0023(5) 0.0013(6) -0.0042(7) C(6) 0.0174(5) 0.0300(7) 0.0189(7) -0.0011(5) -0.0027(6) -0.0003(6) C(7) 0.0217(6) 0.0295(8) 0.0299(9) 0.0029(6) 0.0025(7) -0.0019(7) C(8) 0.0204(6) 0.0265(7) 0.0210(8) 0.0004(5) -0.0048(6) 0.0000(6) C(9) 0.0236(6) 0.0291(7) 0.0192(8) -0.0015(5) -0.0012(6) 0.0017(7)

#---------- _computing_data_collection '.' _computing_cell_refinement '.' _computing_data_reduction 'teXsan Ver. 1.11' _computing_structure_solution SIR97 _computing_structure_refinement 'teXsan Ver. 1.10' _computing_publication_material 'teXsan Ver. 1.11' _computing_molecular_graphics ? #---------- ---------- _geom_special_details ; ? ; loop_ _geom_bond_atom_site_label_1 _geom_bond_atom_site_label_2 _geom_bond_distance _geom_bond_site_symmetry_1 _geom_bond_site_symmetry_2 _geom_bond_publ_flag S(1) N(1) 1.618(1) . . yes S(1) N(1) 1.618(1) . 7_555 yes O(1) C(2) 1.206(2) . . yes N(1) C(6) 1.350(2) . . yes C(1) C(2) 1.528(2) . . yes C(1) C(8) 1.527(2) . . yes C(2) C(3) 1.531(2) . . yes C(3) C(4) 1.511(2) . . yes C(4) C(5) 1.364(2) . . yes C(4) C(6) 1.423(2) . . yes C(5) C(5) 1.431(3) . 7_555 yes C(6) C(6) 1.438(3) . 7_555 yes C(7) C(7) 1.395(3) . 7_555 yes C(7) C(8) 1.391(2) . . yes C(8) C(9) 1.390(2) . . yes C(9) C(9) 1.405(3) . 7_555 yes #---------- loop_ _geom_angle_atom_site_lab

el_1 _geom_angle_atom_site_label_2 _geom_angle_atom_site_label_3 _geom_angle _geom_angle_site_symmetry_1 _geom_angle_site_symmetry_2 _geom_angle_site_symmetry_3 _geom_angle_publ_flag N(1) S(1) N(1) 101.15(9) . . 7_555 yes S(1) N(1) C(6) 106.27(10) . . . yes C(2) C(1) C(8) 111.5(1) . . . yes O(1) C(2) C(1) 121.0(1) . . . yes O(1) C(2) C(3) 119.9(2) . . . yes C(1) C(2) C(3) 119.1(1) . . . yes C(2) C(3) C(4) 111.1(1) . . . yes C(3) C(4) C(5) 122.8(1) . . . yes C(3) C(4) C(6) 121.0(1) . . . yes C(5) C(4) C(6) 116.0(1) . . . yes C(4) C(5) C(5) 122.67(9) . . 7_555 yes N(1) C(6) C(4) 125.8(1) . . . yes N(1) C(6) C(6) 113.16(8) . . 7_555 yes C(4) C(6) C(6) 120.99(8) . . 7_555 yes C(7) C(7) C(8) 120.54(9) 7_555 . . yes C(1) C(8) C(7) 119.7(1) . . . yes C(1) C(8) C(9) 121.4(1) . . . yes C(7) C(8) C(9) 118.8(1) . . . yes C(8) C(9) C(9) 120.32(8) . . 7_555 yes #---------- loop_ _geom_torsion_atom_site_label_1 _geom_torsion_atom_site_label_2 _geom_torsion_atom_site_label_3 _geom_torsion_atom_site_label_4 _geom_torsion _geom_torsion_site_symmetry_1 _geom_torsion_site_symmetry_2 _geom_torsion_site_symmetry_3 _geom_torsion_site_symmetry_4 _geom_torsion_publ_flag S(1) N(1) C(6) C(4) 177.7(1) . . . . yes S(1) N(1) C(6) C(6) 0.06(10) . . . 7_555 yes S(1) N(1) C(6) C(4) -177.7(1) . 7_555 7_555 7_555 yes S(1) N(1) C(6) C(6) -0.06(10) . 7_555 7_555 . yes O(1) C(2) C(1) C(8) 104.6(2) . . . . yes O(1) C(2) C(3) C(4) -106.6(2) . . . . yes N(1) S(1) N(1) C(6) 0.1(1) . . 7_555 7_555 yes N(1) C(6) C(4) C(3) -9.4(2) . . . . yes N(1) C(6) C(4) C(5) 176.3(1) . . . . yes N(1) C(6) C(6) N(1) 0.0 . . 7_555 7_555 yes N(1) C(6) C(6) C(4) 177.8(1) . . 7_555 7_555 yes C(1) C(2) C(3) C(4) 71.7(2) . . . . yes C(1) C(8) C(7) C(7) 168.57(9) . . . 7_555 yes C(1) C(8) C(9) C(9) -168.51(10) . . . 7_555 yes C(2) C(1) C(8) C(7) -53.7(2) . . . . yes C(2) C(1) C(8) C(9) 121.9(2) . . . . yes C(2) C(3) C(4) C(5) 67.5(2) . . . . yes C(2) C(3) C(4) C(6) -106.5(2) . . . . yes C(3) C(2) C(1) C(8) -73.7(2) . . . . yes C(3) C(4) C(5) C(5) -167.90(10) . . . 7_555 yes C(3) C(4) C(6) C(6) 168.13(9) . . . 7_555 yes C(4) C(5) C(5) C(4) 0.0 . . 7_555 7_555 yes C(4) C(6) C(6) C(4) 0.0 . . 7_555 7_555 yes C(5) C(4) C(6) C(6) -6.2(1) . . . 7_555 yes C(5) C(5) C(4) C(6) -6.3(1) . 7_555 7_555 7_555 yes C(7) C(7) C(8) C(9) 7.1(2) . 7_555 7_555 7_555 yes C(7) C(8) C(9) C(9) 7.1(2) . . . 7_555 yes C(8) C(7) C(7) C(8) 0.0 . . 7_555 7_555 yes C(8) C(9) C(9) C(8) 0.0 . . 7_555 7_555 yes C(8) C(9) C(9) C(8) 0.0 . . 7_555 7_555

yes #---------- loop_ _geom_contact_atom_site_label_1 _geom_contact_atom_site_label_2 _geom_contact_distance _geom_contact_site_symmetry_1 _geom_contact_site_symmetry_2 _geom_contact_publ_flag O(1) C(3) 3.392(2) . 8_554 ? O(1) C(1) 3.510(2) . 5_755 ? N(1) C(2) 3.217(2) . 5_655 ? N(1) C(3) 3.330(2) . 5_655 ? N(1) C(1) 3.470(2) . 5_655 ? #---------- #----------