

## Supporting Information for the paper

Synthesis, X-ray characterization and theoretical study of all-cis 1,4:2,3:5,8:6,7-tetraepoxynaphthalenes: on the importance of through-space  $\alpha$ -effect

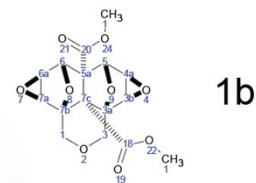
by

Anh T. Le, Van T. T. Tran, Duan T. Le, Rosa M. Gomila, Antonio Frontera, Fedor I. Zubkov

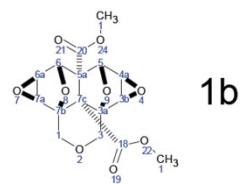
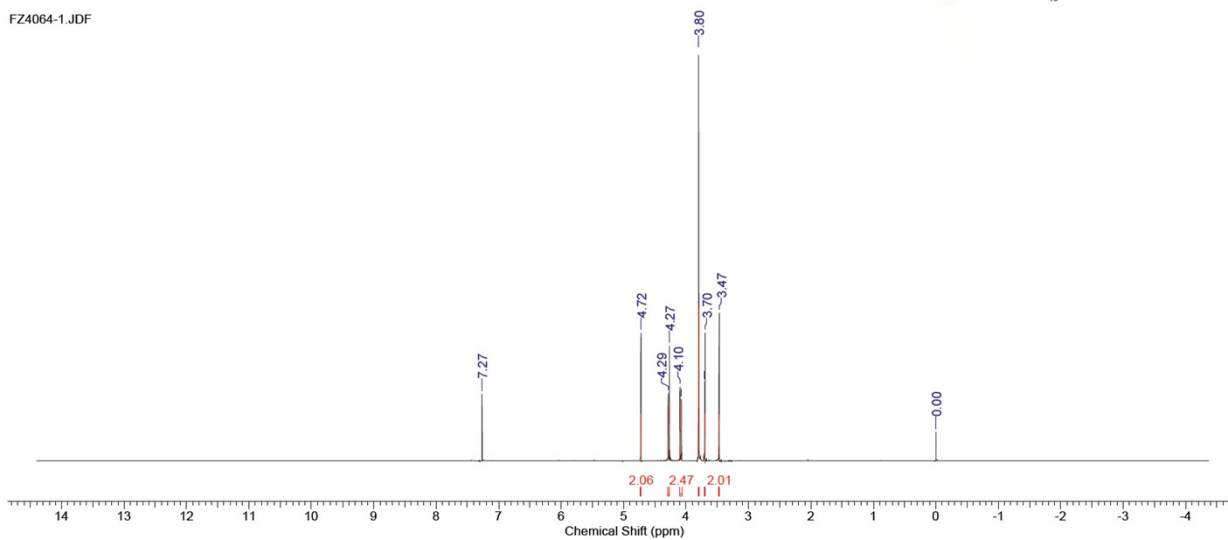
### 1. Experimental section

**General synthetic methods.** All commercially available reagents and solvents were used without further purification. Values of the melting point were measured on a capillary point apparatus equipped with a digital thermometer and were left unchanged.  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra were recorded on 600 (for  $^1\text{H}$ ) and 150.9 (for  $^{13}\text{C}$ ) MHz spectrometers with TMS ( $^1\text{H}$  and  $^{13}\text{C}$  NMR) as the internal standard, using  $\text{CDCl}_3$  and  $\text{DMSO}-d_6$  as solvents. Data for  $^1\text{H}$  NMR spectra are reported as follows: chemical shift  $\delta$  (ppm), referenced to TMS; multiplicities are indicated as the following: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; dd, doublet of doublets; coupling constants (Hz) and integration. Data for  $^{13}\text{C}$  NMR spectra are reported in terms of chemical shift  $\delta$  (ppm) relative to residual solvent peaks. IR spectra were obtained in KBr pellets or in thin films using an Infracum FT-801 IR-Fourier spectrometer. Mass spectral data were collected either on Thermo Focus DSQ II (electron ionization, 70 eV, ion source temperature 200 °C, gas chromatographic inlet with Varian FactorFour VF-5ms column) or on Thermo Trace DSQ (electron ionization, 70 eV, ion source temperature 200 °C, direct inlet probe) spectrometers. High-resolution mass spectra (HRMS) were registered on Agilent mass spectrometer, using ESI-TOF (electrospray ionization-time of flight). Analytical TLC was performed on silica plates Sorbfil (visualization in  $\text{I}_2$  vapors).

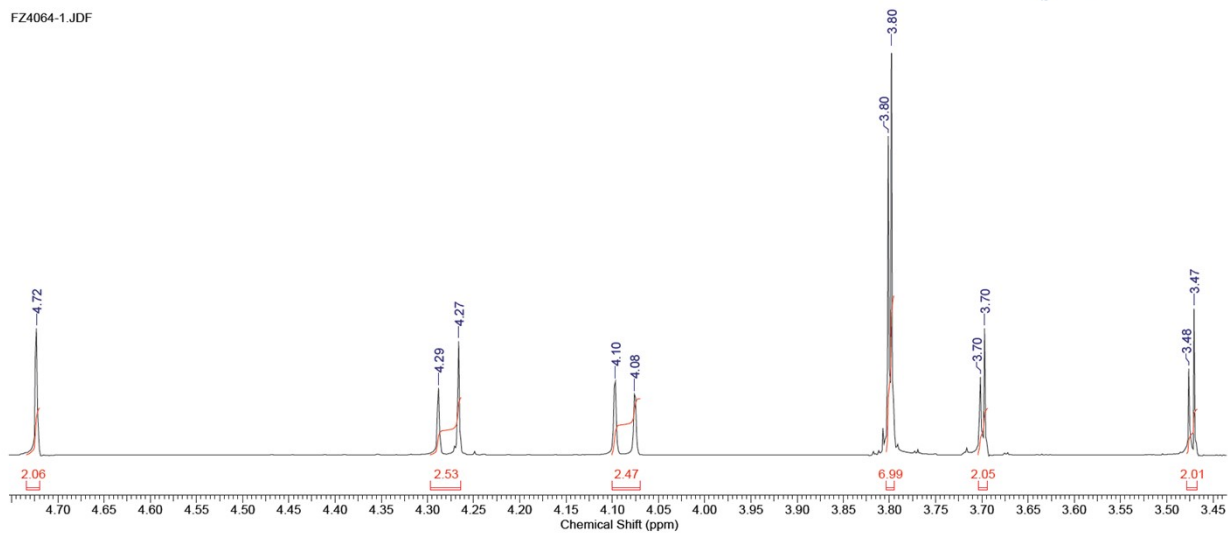
# <sup>1</sup>H-NMR and <sup>13</sup>C-NMR spectra of compounds 1b-3b:



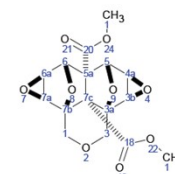
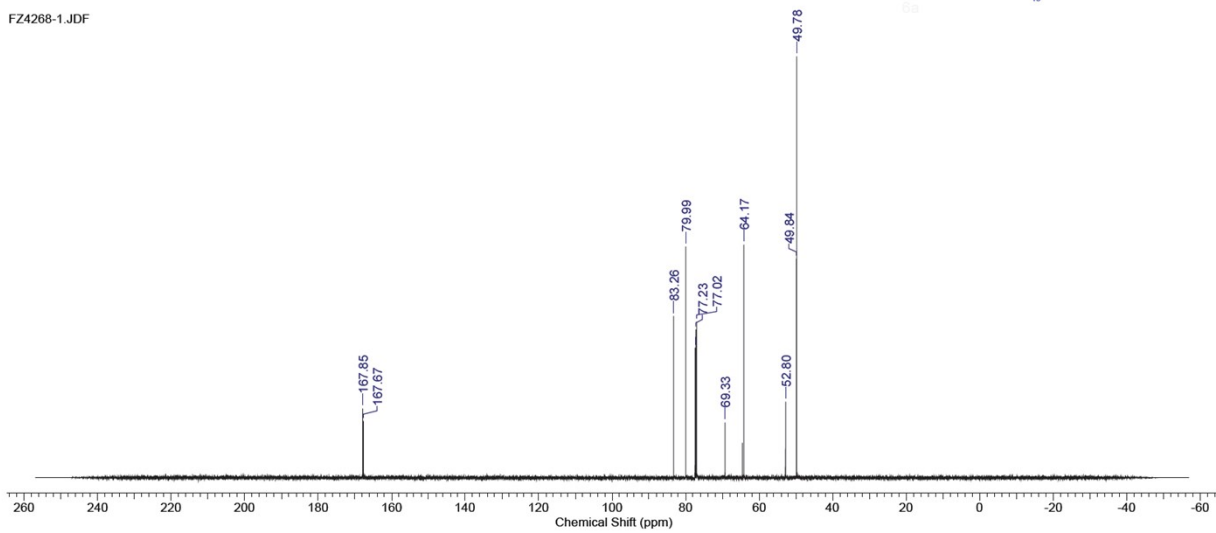
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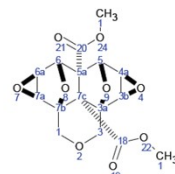
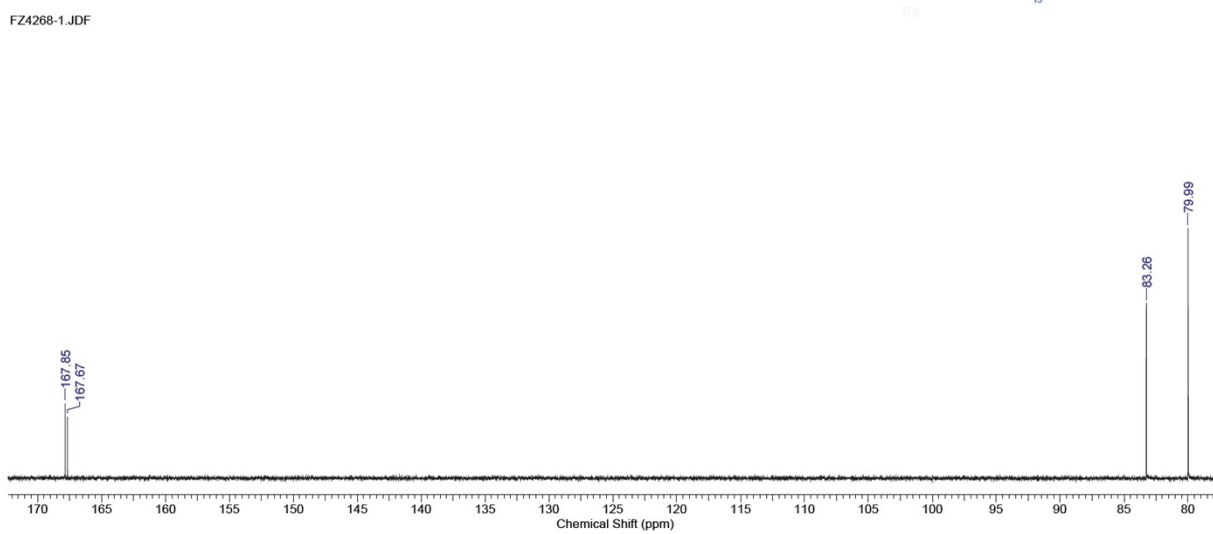


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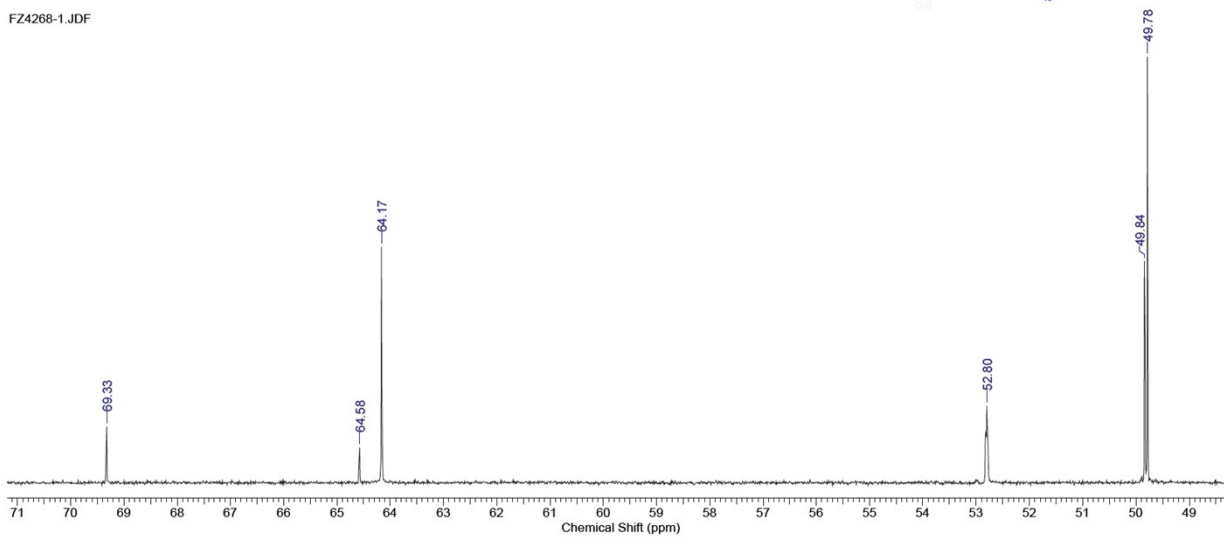
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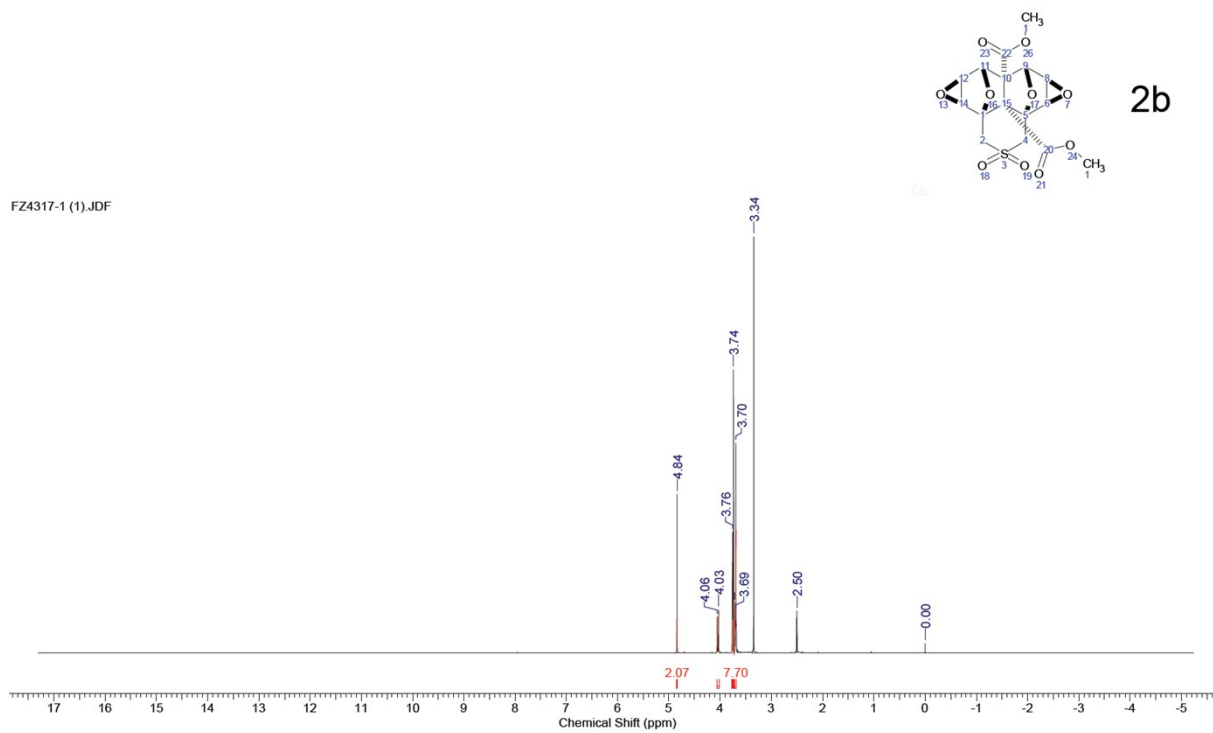


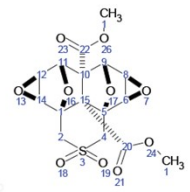
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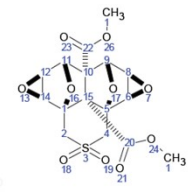
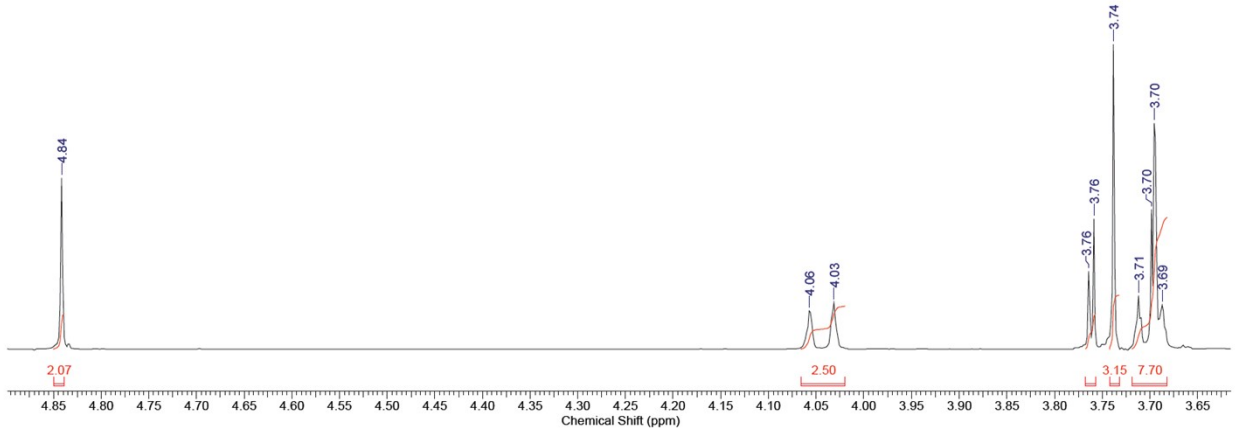
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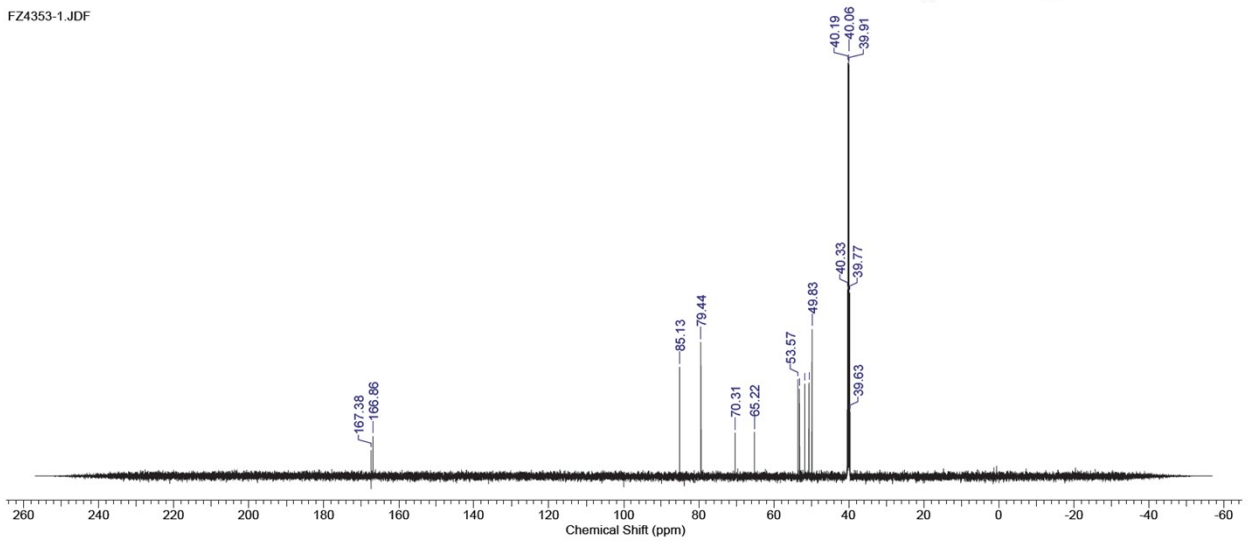
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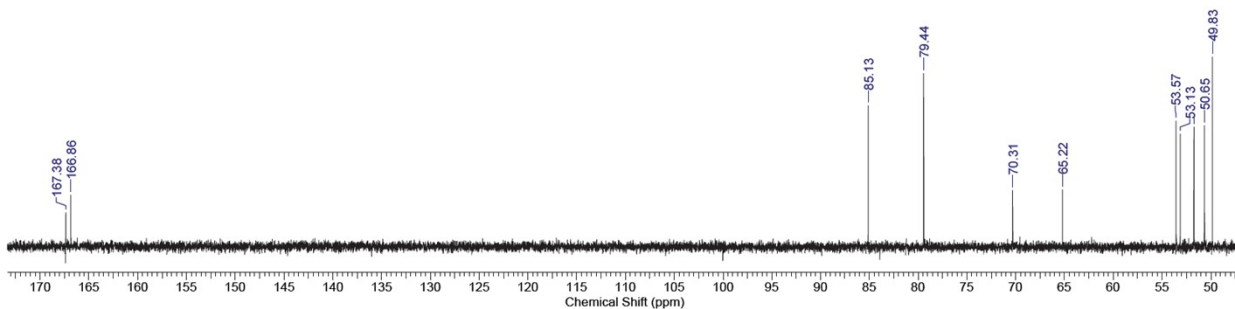
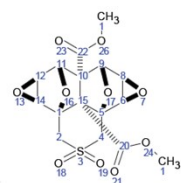


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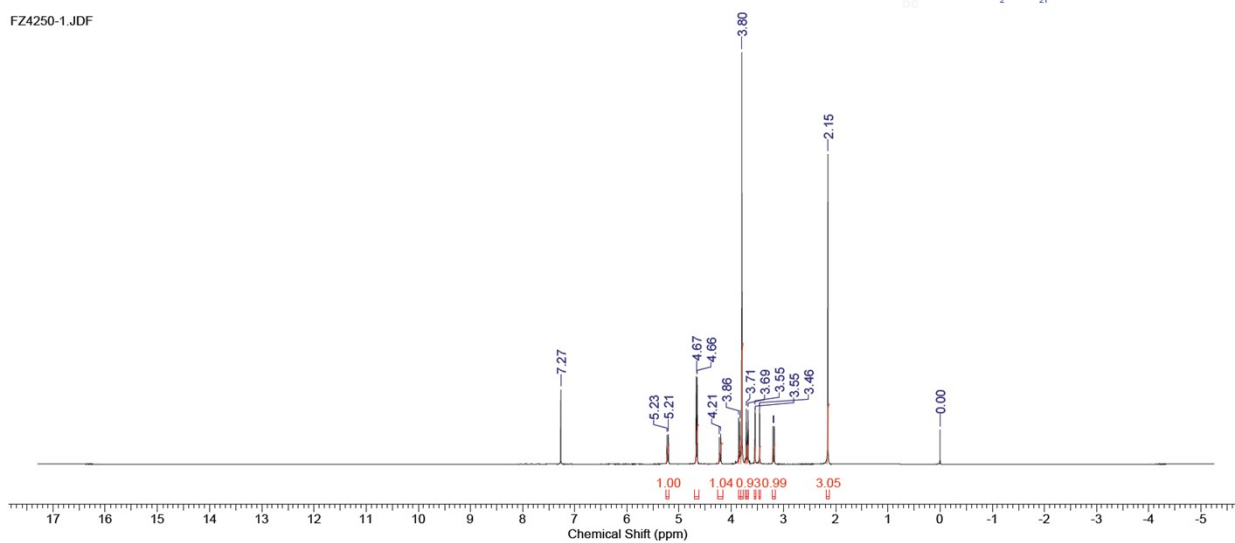
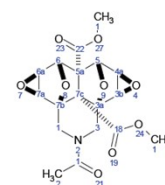
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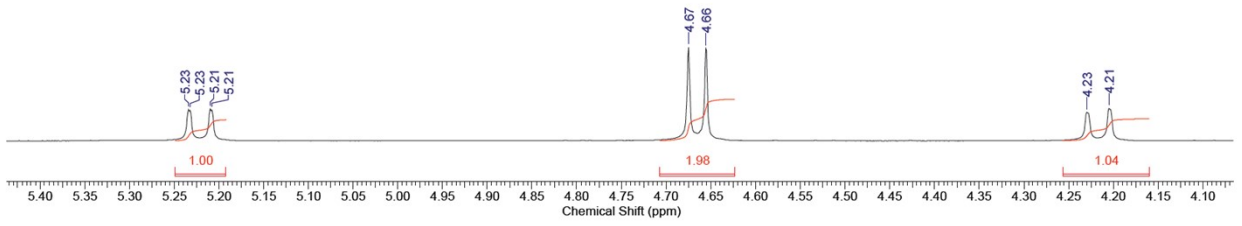
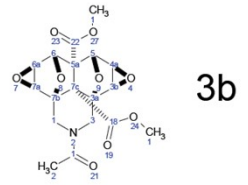
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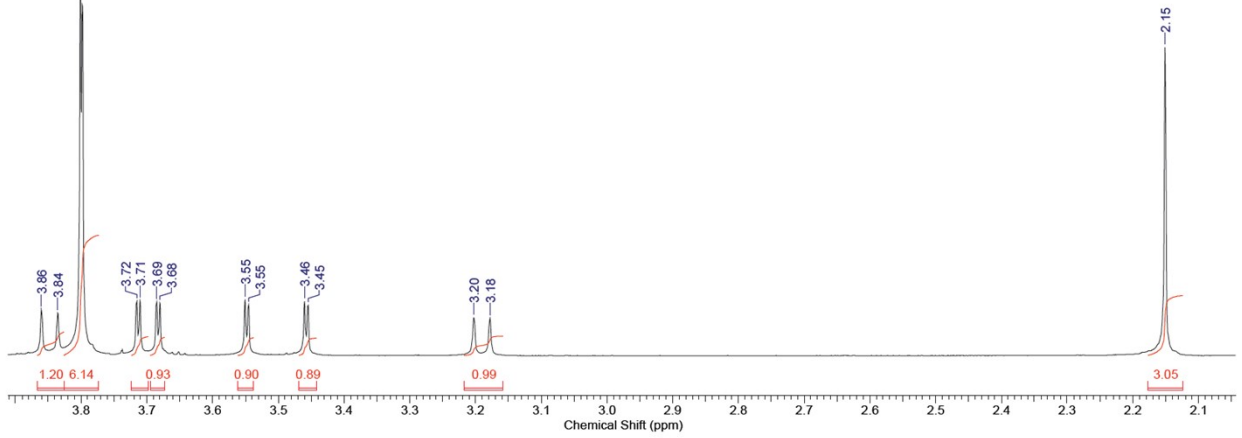
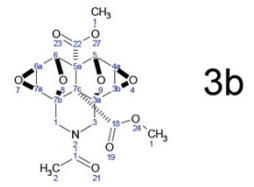
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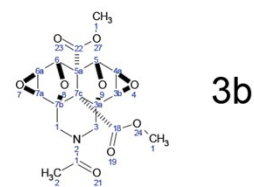
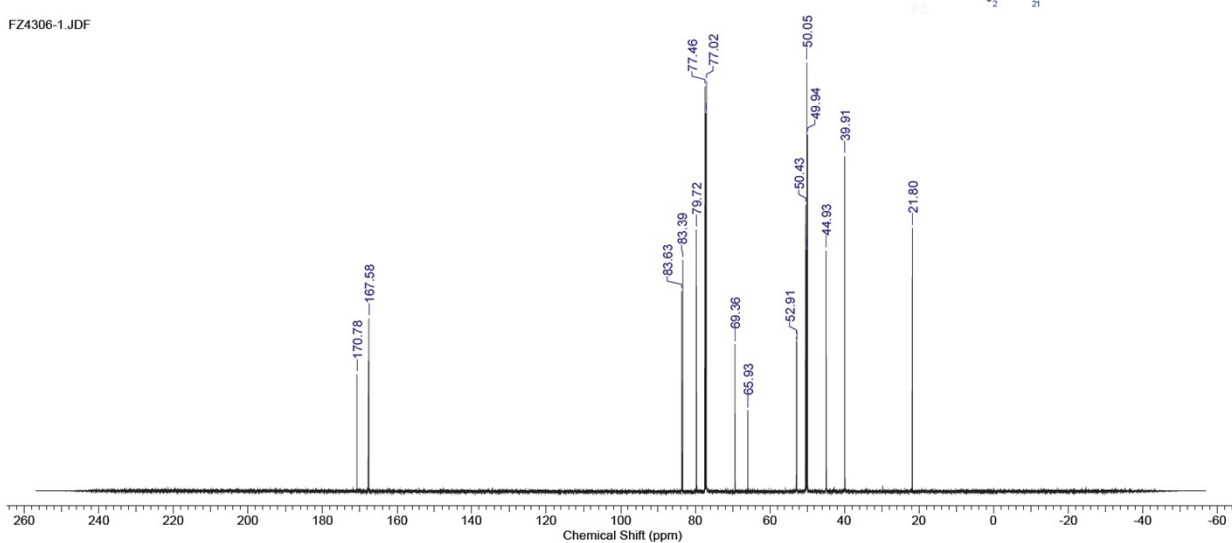
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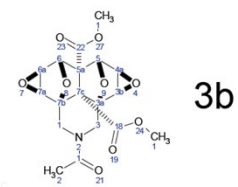
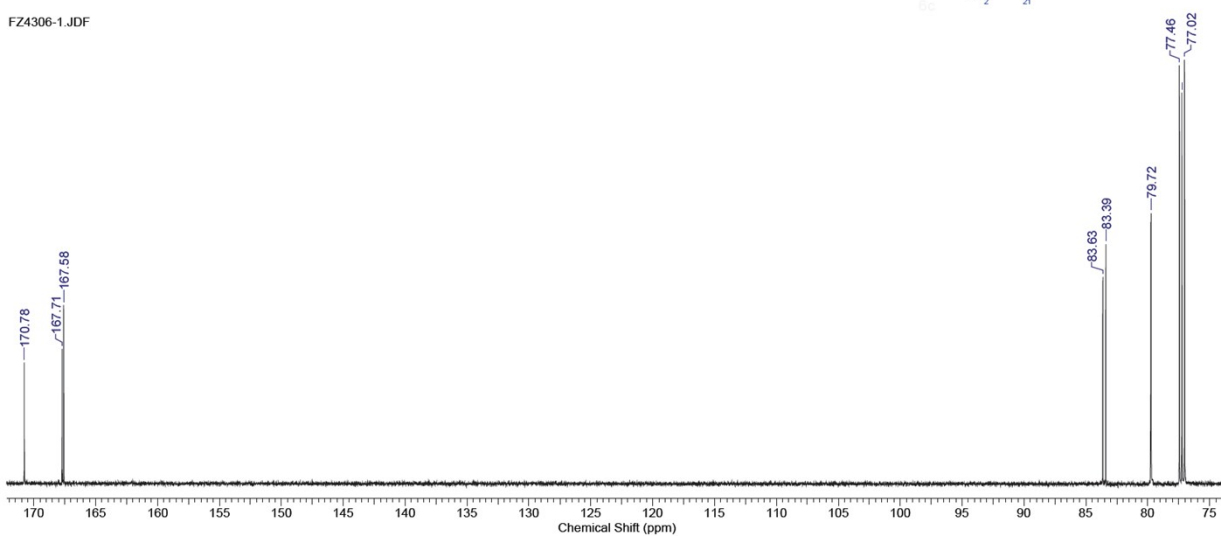
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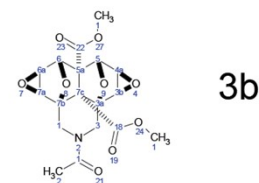
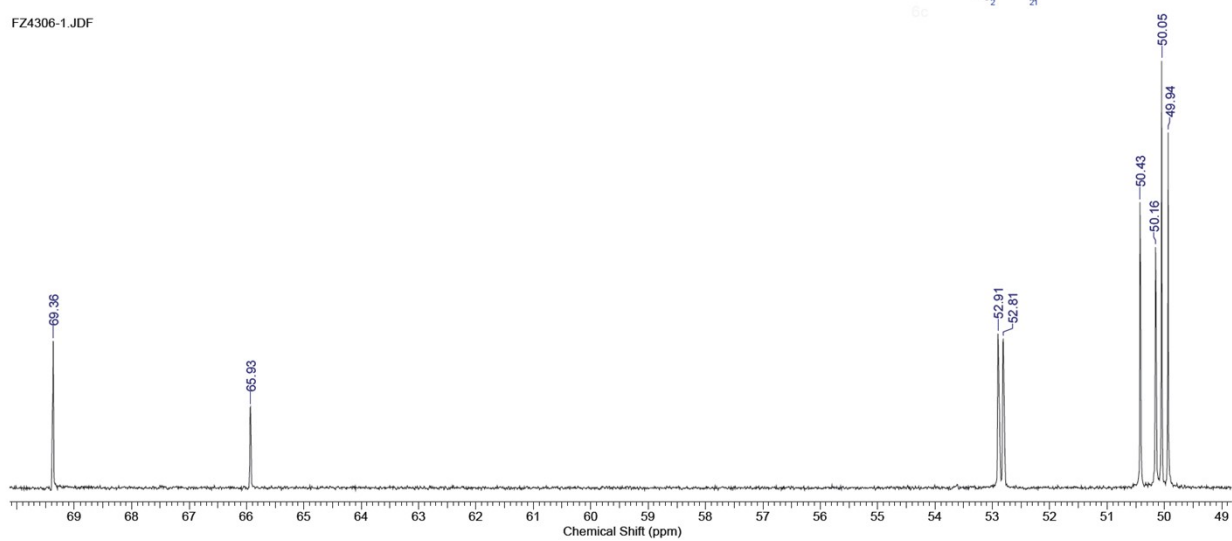


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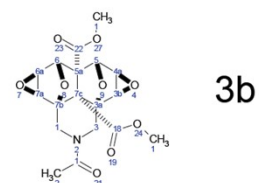
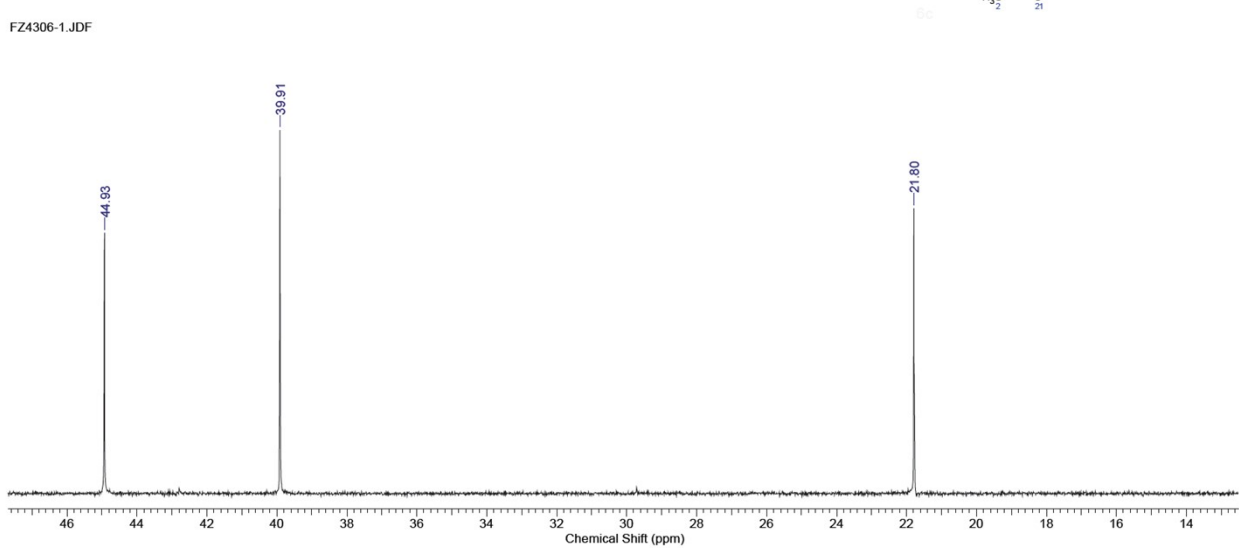




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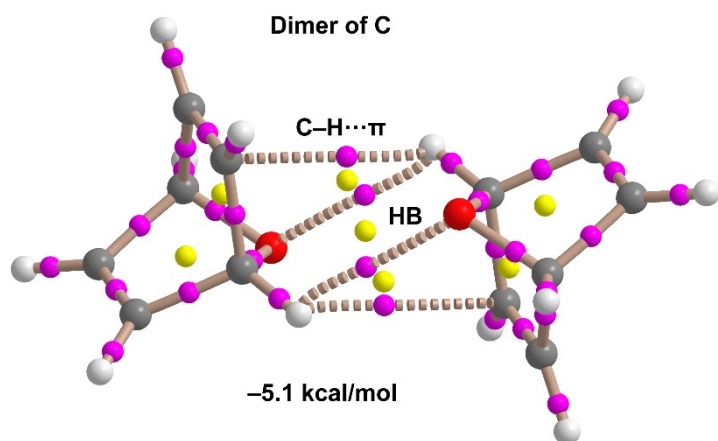


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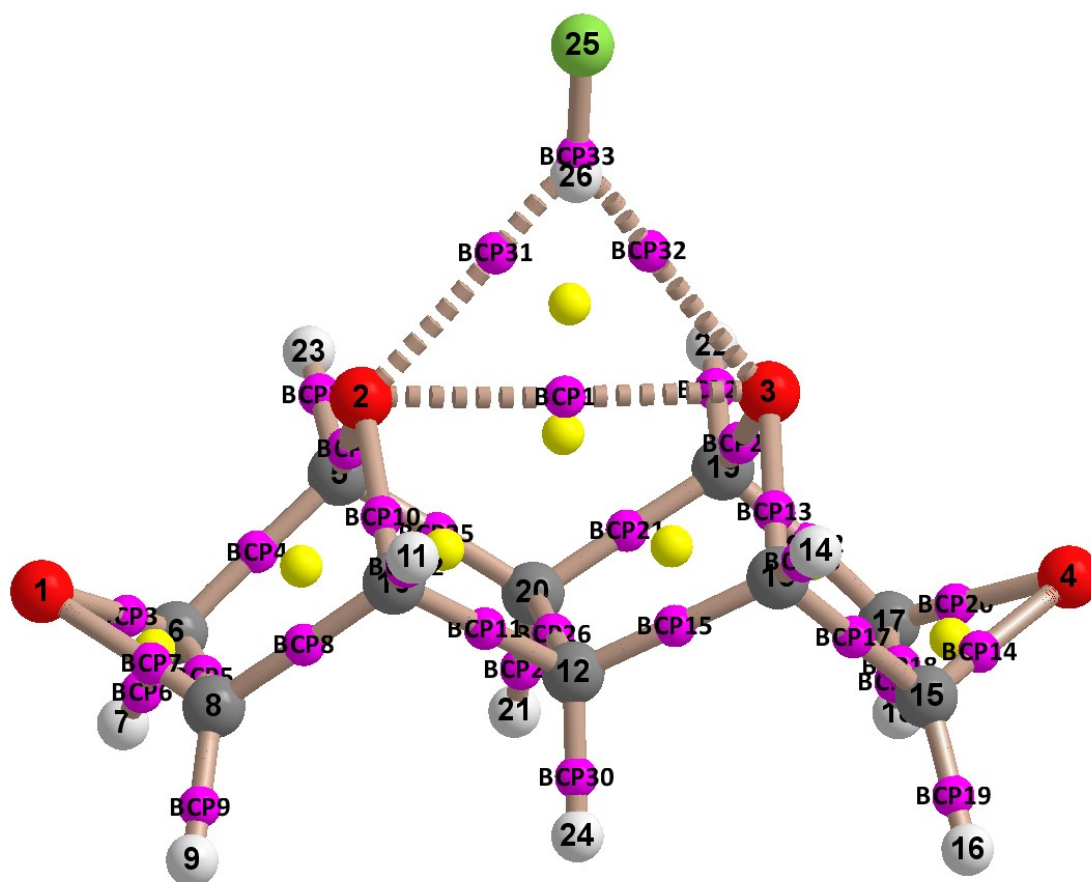
## 1. Theoretical section

### Dimer of compound C (Figure S1)



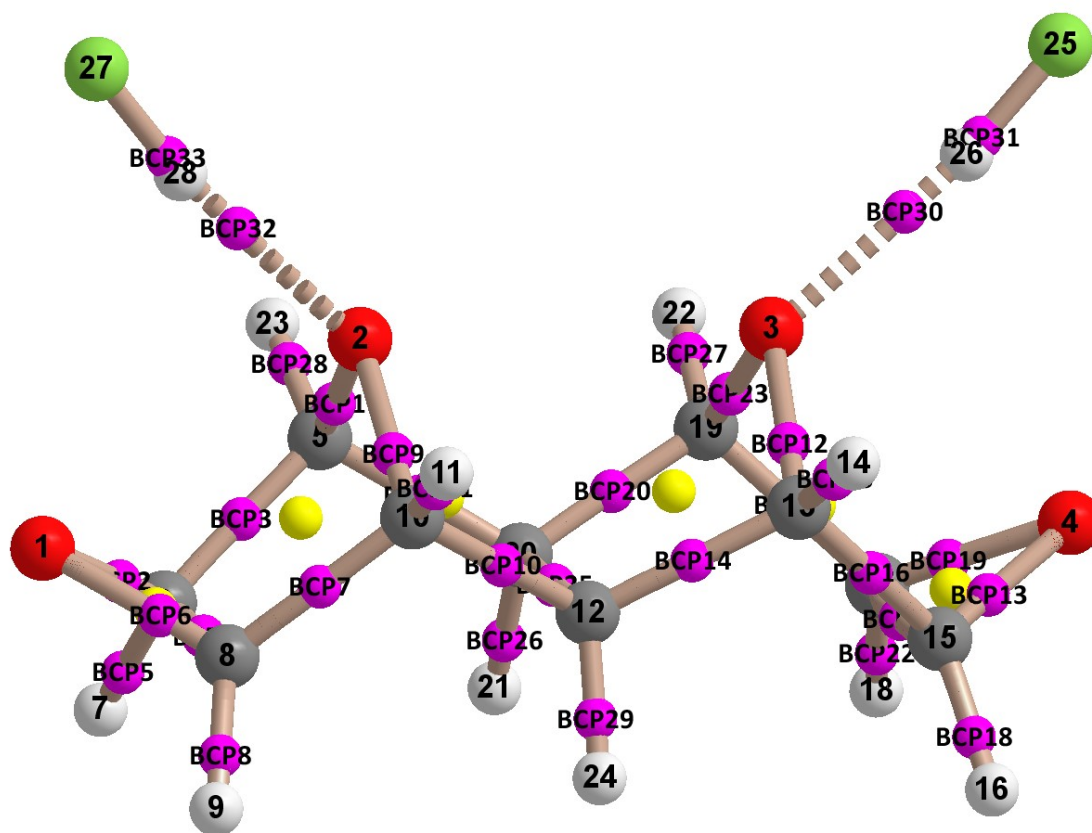
**Figure S1** QTAIM (bond CPs in fuchsia and ring CP in yellow) for the dimers of model C. The dimerization energies are also indicated.

QTAIM data:



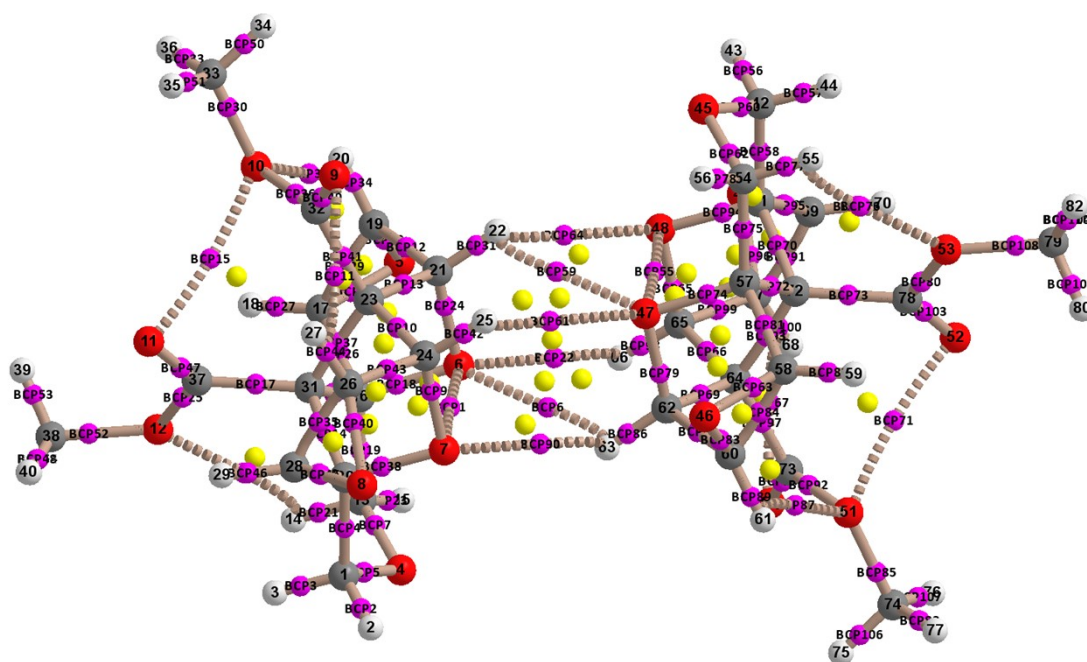
BCP #	Name	Atoms	Rho	DelSqRho	Ellipticity	V	G
1	BCP1	O2 - O3	0.014729	+0.071406	0.458001	-0.012571	+0.015211
2	BCP2	O2 - C5	0.265317	-0.612641	0.057420	-0.559669	+0.203254
3	BCP3	O1 - C6	0.262746	-0.413816	0.644907	-0.580008	+0.238277
4	BCP4	C5 - C6	0.255531	-0.654362	0.086390	-0.283274	+0.059842

5	BCP5	C6 - C8	0.266192	-0.608676	0.301204	-0.362272	+0.105052
6	BCP6	C6 - H7	0.287703	-1.038845	0.037867	-0.329758	+0.035023
7	BCP7	O1 - C8	0.262746	-0.413816	0.644907	-0.580008	+0.238277
8	BCP8	C8 - C10	0.255531	-0.654362	0.086390	-0.283274	+0.059842
9	BCP9	C8 - H9	0.287703	-1.038845	0.037867	-0.329758	+0.035023
10	BCP10	O2 - C10	0.265317	-0.612641	0.057420	-0.559669	+0.203254
11	BCP11	C10 - C12	0.247536	-0.611328	0.022779	-0.270992	+0.059080
12	BCP12	C10 - H11	0.288571	-1.047438	0.026728	-0.328060	+0.033100
13	BCP13	O3 - C13	0.265317	-0.612641	0.057420	-0.559669	+0.203254
14	BCP14	O4 - C15	0.262746	-0.413816	0.644907	-0.580008	+0.238277
15	BCP15	C12 - C13	0.247536	-0.611328	0.022779	-0.270992	+0.059080
16	BCP16	C13 - H14	0.288571	-1.047438	0.026728	-0.328060	+0.033100
17	BCP17	C13 - C15	0.255531	-0.654362	0.086390	-0.283274	+0.059842
18	BCP18	C15 - C17	0.266192	-0.608676	0.301204	-0.362272	+0.105052
19	BCP19	C15 - H16	0.287703	-1.038845	0.037867	-0.329758	+0.035023
20	BCP20	O4 - C17	0.262746	-0.413816	0.644907	-0.580008	+0.238277
21	BCP21	C19 - C20	0.247536	-0.611328	0.022779	-0.270992	+0.059080
22	BCP22	C17 - C19	0.255531	-0.654362	0.086390	-0.283274	+0.059842
23	BCP23	C17 - H18	0.287703	-1.038845	0.037867	-0.329758	+0.035023
24	BCP24	O3 - C19	0.265317	-0.612641	0.057420	-0.559669	+0.203254
25	BCP25	C5 - C20	0.247536	-0.611328	0.022779	-0.270992	+0.059080
26	BCP26	C12 - C20	0.227529	-0.500075	0.037591	-0.240778	+0.057880
27	BCP27	C20 - H21	0.279421	-0.964634	0.000569	-0.323128	+0.040985
28	BCP28	C19 - H22	0.288571	-1.047438	0.026728	-0.328060	+0.033100
29	BCP29	C5 - H23	0.288571	-1.047438	0.026728	-0.328060	+0.033100
30	BCP30	C12 - H24	0.279421	-0.964634	0.000569	-0.323128	+0.040985
31	BCP31	O2 - H26	0.017309	+0.069135	0.196885	-0.012400	+0.014842
32	BCP32	O3 - H26	0.017309	+0.069135	0.196885	-0.012400	+0.014842
33	BCP33	F25 - H26	0.347758	-2.611463	0.000501	-0.812370	+0.079752



BCP #	Name	Atoms	Rho	DelSqRho	Ellipticity	V	G
1	BCP1	O2 - C5	0.260781	-0.583540	0.056311	-0.553877	+0.203996
2	BCP2	O1 - C6	0.263458	-0.419137	0.632758	-0.582112	+0.238664
3	BCP3	C5 - C6	0.255579	-0.654402	0.086744	-0.283052	+0.059726
4	BCP4	C6 - C8	0.265810	-0.605657	0.307502	-0.361606	+0.105096

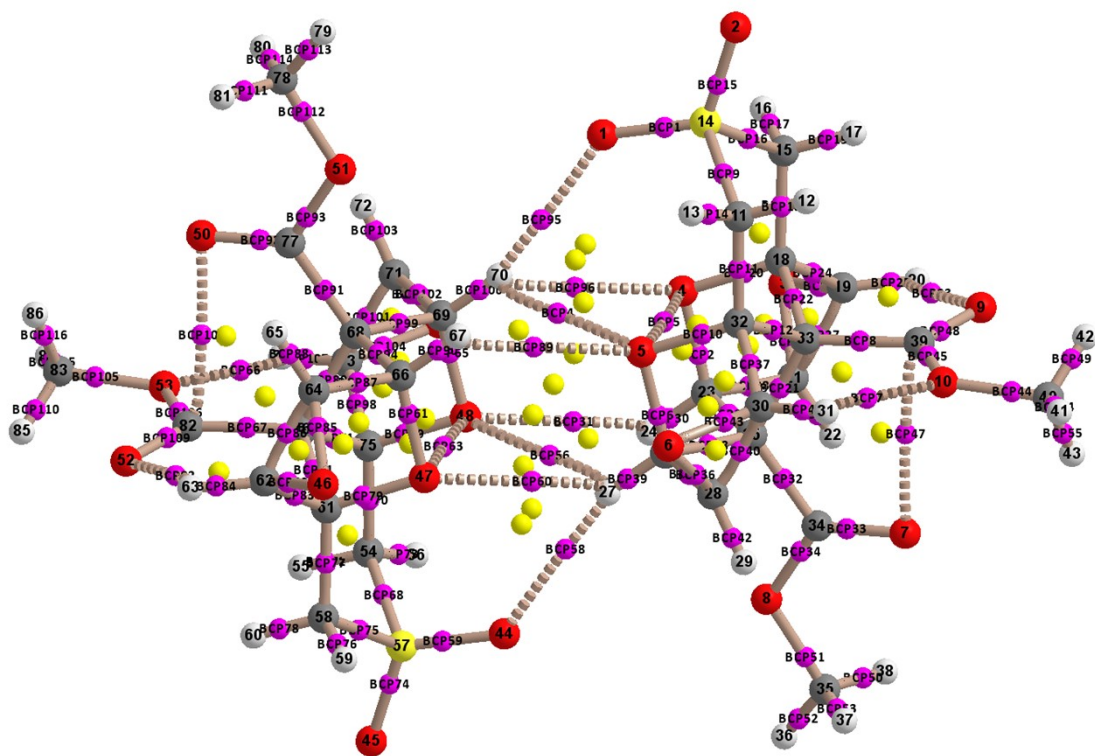
5	BCP5	C6 - H7	0.288219	-1.043905	0.036668	-0.330148	+0.034586
6	BCP6	O1 - C8	0.263458	-0.419137	0.632758	-0.582112	+0.238664
7	BCP7	C8 - C10	0.255579	-0.654402	0.086744	-0.283052	+0.059726
8	BCP8	C8 - H9	0.288219	-1.043905	0.036668	-0.330148	+0.034586
9	BCP9	O2 - C10	0.260781	-0.583540	0.056311	-0.553877	+0.203996
10	BCP10	C10 - C12	0.248765	-0.618943	0.022455	-0.273044	+0.059154
11	BCP11	C10 - H11	0.289265	-1.053614	0.026854	-0.328516	+0.032556
12	BCP12	O3 - C13	0.260781	-0.583540	0.056311	-0.553877	+0.203996
13	BCP13	O4 - C15	0.263458	-0.419137	0.632758	-0.582112	+0.238664
14	BCP14	C12 - C13	0.248765	-0.618943	0.022455	-0.273044	+0.059154
15	BCP15	C13 - H14	0.289265	-1.053614	0.026854	-0.328516	+0.032556
16	BCP16	C13 - C15	0.255579	-0.654402	0.086744	-0.283052	+0.059726
17	BCP17	C15 - C17	0.265810	-0.605657	0.307502	-0.361606	+0.105096
18	BCP18	C15 - H16	0.288219	-1.043905	0.036668	-0.330148	+0.034586
19	BCP19	O4 - C17	0.263458	-0.419137	0.632758	-0.582112	+0.238664
20	BCP20	C19 - C20	0.248765	-0.618943	0.022455	-0.273044	+0.059154
21	BCP21	C17 - C19	0.255579	-0.654402	0.086744	-0.283052	+0.059726
22	BCP22	C17 - H18	0.288219	-1.043905	0.036668	-0.330148	+0.034586
23	BCP23	O3 - C19	0.260781	-0.583540	0.056311	-0.553877	+0.203996
24	BCP24	C5 - C20	0.248765	-0.618943	0.022455	-0.273044	+0.059154
25	BCP25	C12 - C20	0.227415	-0.499771	0.033753	-0.240543	+0.057800
26	BCP26	C20 - H21	0.280154	-0.969859	0.000177	-0.323720	+0.040627
27	BCP27	C19 - H22	0.289265	-1.053614	0.026854	-0.328516	+0.032556
28	BCP28	C5 - H23	0.289265	-1.053614	0.026854	-0.328516	+0.032556
29	BCP29	C12 - H24	0.280154	-0.969859	0.000177	-0.323720	+0.040627
30	BCP30	O3 - H26	0.042617	+0.115333	0.043410	-0.043680	+0.036256
31	BCP31	F25 - H26	0.338773	-2.472817	0.000449	-0.787953	+0.084874
32	BCP32	O2 - H28	0.042617	+0.115333	0.043410	-0.043680	+0.036256
33	BCP33	F27 - H28	0.338773	-2.472817	0.000449	-0.787953	+0.084874



BCP #	Name	Atoms	Rho	DelSqRho	Ellipticity	V	G
1	BCP1	O6 - O7	0.019410	+0.093470	0.073041	-0.018015	+0.020691
2	BCP2	C1 - H2	0.355843	-1.530214	0.049196	-0.498550	+0.057998
3	BCP3	C1 - H3	0.353164	-1.496621	0.051209	-0.502890	+0.064368
4	BCP4	C1 - C30	0.256184	-0.670704	0.056163	-0.282783	+0.057553
5	BCP5	C1 - O4	0.258026	-0.574085	0.044422	-0.535404	+0.195941
6	BCP6	O6 - H63	0.008392	+0.035086	0.104048	-0.005152	+0.006962
7	BCP7	O4 - C13	0.250412	-0.546427	0.051054	-0.495588	+0.179491
8	BCP8	O5 - C17	0.246966	-0.345577	0.660065	-0.479715	+0.196660
9	BCP9	O7 - C24	0.255021	-0.574212	0.045245	-0.496465	+0.176456
10	BCP10	C23 - C24	0.230898	-0.533891	0.043337	-0.238536	+0.052532

11	BCP11	O9 - H27	0.012563	+0.057401	2.087307	-0.009177	+0.011764
12	BCP12	C19 - C21	0.245799	-0.605682	0.085146	-0.264192	+0.056386
13	BCP13	C21 - C23	0.225228	-0.504053	0.030190	-0.231933	+0.052960
14	BCP14	C30 - C31	0.225540	-0.501470	0.024795	-0.234009	+0.054321
15	BCP15	O10 - O11	0.011241	+0.054891	0.419505	-0.008177	+0.010950
16	BCP16	C16 - C31	0.232770	-0.538971	0.036205	-0.243223	+0.054240
17	BCP17	C31 - C37	0.254062	-0.655204	0.081479	-0.284114	+0.060157
18	BCP18	O6 - C16	0.258266	-0.593363	0.063885	-0.494473	+0.173066
19	BCP19	C13 - C16	0.259159	-0.686943	0.053277	-0.288868	+0.058566
20	BCP20	O12 - H14	0.009853	+0.042229	0.925241	-0.006538	+0.008547
21	BCP21	C13 - H14	0.355392	-1.514893	0.050178	-0.503523	+0.062400
22	BCP22	O6 - H66	0.007041	+0.028603	0.090501	-0.004082	+0.005616
23	BCP23	C13 - H15	0.356185	-1.532833	0.050246	-0.499618	+0.058205
24	BCP24	O6 - C21	0.257577	-0.583656	0.044364	-0.507809	+0.180947
25	BCP25	O12 - C37	0.307283	-0.656354	0.041784	-0.809041	+0.322477
26	BCP26	C16 - C17	0.247022	-0.609330	0.088516	-0.267596	+0.057632
27	BCP27	C17 - H18	0.345100	-1.453167	0.046684	-0.470078	+0.053393
28	BCP28	O5 - C19	0.243549	-0.329099	0.679934	-0.473302	+0.195514
29	BCP29	C17 - C19	0.261280	-0.599949	0.244049	-0.345271	+0.097642
30	BCP30	O10 - C33	0.228370	-0.381176	0.032394	-0.489966	+0.197336
31	BCP31	C21 - H22	0.353563	-1.539408	0.025432	-0.475885	+0.045517
32	BCP32	O10 - H20	0.018971	+0.081705	0.218685	-0.014577	+0.017502
33	BCP33	C33 - H36	0.360258	-1.556423	0.067350	-0.519353	+0.065124
34	BCP34	C19 - H20	0.347701	-1.477271	0.042289	-0.471425	+0.051054
35	BCP35	C26 - C28	0.258541	-0.587467	0.243143	-0.339053	+0.096093
36	BCP36	O10 - C32	0.317311	-0.623924	0.044020	-0.872938	+0.358478
37	BCP37	C23 - C31	0.222528	-0.479177	0.045405	-0.231632	+0.055919
38	BCP38	O7 - C30	0.264030	-0.623250	0.067263	-0.515025	+0.179606
39	BCP39	C28 - C30	0.247341	-0.609779	0.089075	-0.268483	+0.058019
40	BCP40	O8 - C26	0.239523	-0.309836	0.688811	-0.454493	+0.188517
41	BCP41	C23 - C32	0.253096	-0.652544	0.066036	-0.280057	+0.058461
42	BCP42	C24 - H25	0.352925	-1.531320	0.029208	-0.476430	+0.046800
43	BCP43	C24 - C26	0.247938	-0.617145	0.088082	-0.267715	+0.056714
44	BCP44	C26 - H27	0.347496	-1.481193	0.041106	-0.469450	+0.049576
45	BCP45	O8 - C28	0.246435	-0.348408	0.626377	-0.474485	+0.193691
46	BCP46	C28 - H29	0.346331	-1.464080	0.045463	-0.472341	+0.053161
47	BCP47	O11 - C37	0.427077	-0.195230	0.124353	-1.512586	+0.731889
48	BCP48	C38 - H40	0.360752	-1.558533	0.060349	-0.518308	+0.064337
49	BCP49	O9 - C32	0.423747	-0.241951	0.122329	-1.486130	+0.712821
50	BCP50	C33 - H34	0.361870	-1.567838	0.060028	-0.520961	+0.064500
51	BCP51	C33 - H35	0.361744	-1.567919	0.059172	-0.518916	+0.063468
52	BCP52	O12 - C38	0.229657	-0.384121	0.027843	-0.495877	+0.199923
53	BCP53	C38 - H39	0.361574	-1.565712	0.059387	-0.519513	+0.064042
54	BCP54	C38 - H41	0.360450	-1.558471	0.066257	-0.518533	+0.064458
55	BCP55	O47 - O48	0.019412	+0.093478	0.073011	-0.018017	+0.020693
56	BCP56	C42 - H43	0.355898	-1.530677	0.049198	-0.498706	+0.058018
57	BCP57	C42 - H44	0.353104	-1.496125	0.051200	-0.502711	+0.064340
58	BCP58	C42 - C71	0.256201	-0.670799	0.056153	-0.282818	+0.057559
59	BCP59	H22 - O47	0.008391	+0.035081	0.104080	-0.005152	+0.006961
60	BCP60	C42 - O45	0.258011	-0.574043	0.044430	-0.535296	+0.195893
61	BCP61	H25 - O47	0.007041	+0.028602	0.090501	-0.004082	+0.005616
62	BCP62	O45 - C54	0.250410	-0.546403	0.051051	-0.495592	+0.179496
63	BCP63	O46 - C58	0.246967	-0.345571	0.660055	-0.479707	+0.196657
64	BCP64	H22 - O48	0.007266	+0.030371	0.127431	-0.004310	+0.005951
65	BCP65	O48 - C65	0.255021	-0.574220	0.045236	-0.496461	+0.176453
66	BCP66	C64 - C65	0.230898	-0.533890	0.043338	-0.238536	+0.052532
67	BCP67	O50 - H68	0.012561	+0.057399	2.096240	-0.009177	+0.011763
68	BCP68	C60 - C62	0.245842	-0.605902	0.085140	-0.264274	+0.056399
69	BCP69	C62 - C64	0.225242	-0.504118	0.030198	-0.231959	+0.052965
70	BCP70	C71 - C72	0.225539	-0.501466	0.024791	-0.234008	+0.054321
71	BCP71	O51 - O52	0.011241	+0.054890	0.419094	-0.008177	+0.010950
72	BCP72	C57 - C72	0.232769	-0.538970	0.036206	-0.243223	+0.054240
73	BCP73	C72 - C78	0.254091	-0.655353	0.081477	-0.284177	+0.060169
74	BCP74	O47 - C57	0.258266	-0.593366	0.063880	-0.494473	+0.173066
75	BCP75	C54 - C57	0.259158	-0.686940	0.053274	-0.288868	+0.058566
76	BCP76	O53 - H55	0.009853	+0.042228	0.925233	-0.006538	+0.008547
77	BCP77	C54 - H55	0.355392	-1.514904	0.050174	-0.503520	+0.062397
78	BCP78	C54 - H56	0.356209	-1.533035	0.050242	-0.499686	+0.058214
79	BCP79	O47 - C62	0.257578	-0.583662	0.044380	-0.507805	+0.180945
80	BCP80	O53 - C78	0.307233	-0.656604	0.041793	-0.808675	+0.322262

81	BCP81	C57 - C58	0.246985	-0.609144	0.088515	-0.267528	+0.057621
82	BCP82	C58 - H59	0.345164	-1.453679	0.046681	-0.470255	+0.053418
83	BCP83	O46 - C60	0.243536	-0.329007	0.680114	-0.473237	+0.195493
84	BCP84	C58 - C60	0.261291	-0.600015	0.243994	-0.345291	+0.097644
85	BCP85	O51 - C74	0.228371	-0.381189	0.032426	-0.489968	+0.197336
86	BCP86	C62 - H63	0.353508	-1.538957	0.025431	-0.475739	+0.045500
87	BCP87	O51 - H61	0.018972	+0.081711	0.218656	-0.014578	+0.017503
88	BCP88	C74 - H77	0.360230	-1.556184	0.067349	-0.519266	+0.065110
89	BCP89	C60 - H61	0.347702	-1.477272	0.042291	-0.471428	+0.051055
90	BCP90	O7 - H63	0.007266	+0.030371	0.127459	-0.004310	+0.059551
91	BCP91	C67 - C69	0.258543	-0.587510	0.243044	-0.339047	+0.096085
92	BCP92	O51 - C73	0.317338	-0.623758	0.044019	-0.873126	+0.358593
93	BCP93	C64 - C72	0.222495	-0.479025	0.045407	-0.231572	+0.055908
94	BCP94	O48 - C71	0.264013	-0.623156	0.067272	-0.514925	+0.179568
95	BCP95	C69 - C71	0.247341	-0.609784	0.089048	-0.268482	+0.058018
96	BCP96	O49 - C67	0.239478	-0.309571	0.689097	-0.454264	+0.188436
97	BCP97	C64 - C73	0.253098	-0.652553	0.066037	-0.280057	+0.058459
98	BCP98	C65 - H66	0.352925	-1.531322	0.029206	-0.476429	+0.046799
99	BCP99	C65 - C67	0.247937	-0.617143	0.088074	-0.267713	+0.056714
100	BCP100	C67 - H68	0.347534	-1.481507	0.041107	-0.469552	+0.049588
101	BCP101	O49 - C69	0.246430	-0.348406	0.626155	-0.474430	+0.193664
102	BCP102	C69 - H70	0.346319	-1.463990	0.045446	-0.472304	+0.053153
103	BCP103	O52 - C78	0.427094	-0.194996	0.124352	-1.512723	+0.731987
104	BCP104	C79 - H81	0.360787	-1.558834	0.060350	-0.518416	+0.064354
105	BCP105	O50 - C73	0.423747	-0.241958	0.122326	-1.486127	+0.712819
106	BCP106	C74 - H75	0.361871	-1.567838	0.060029	-0.520962	+0.064501
107	BCP107	C74 - H76	0.361744	-1.567924	0.059171	-0.518915	+0.063467
108	BCP108	O53 - C79	0.229691	-0.384208	0.027817	-0.496047	+0.199998
109	BCP109	C79 - H80	0.361482	-1.564932	0.059371	-0.519234	+0.064001
110	BCP110	C79 - H82	0.360385	-1.557915	0.066245	-0.518338	+0.064429

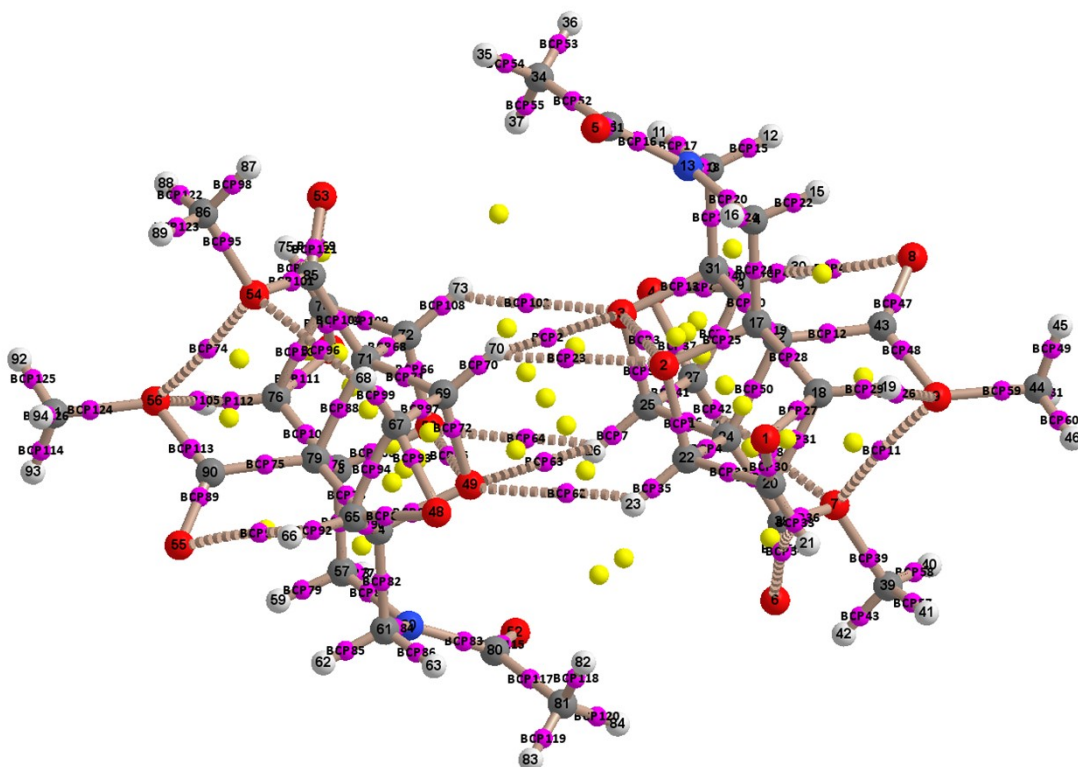


BCP #	Name	Atoms	Rho	DelSqRho	Ellipticity	V	G
1	BCP1	O1 - S14	0.312188	+1.003258	0.039160	-1.000885	+0.625850
2	BCP2	O4 - C23	0.253050	-0.562721	0.052681	-0.476591	+0.167955
3	BCP3	O3 - C19	0.240510	-0.300690	0.745877	-0.450845	+0.187836
4	BCP4	O5 - H70	0.006267	+0.026547	0.139486	-0.003679	+0.005158
5	BCP5	O4 - O5	0.019722	+0.094247	0.035256	-0.018313	+0.020937
6	BCP6	O5 - C26	0.253783	-0.564909	0.042953	-0.493082	+0.175927
7	BCP7	O10 - H31	0.022827	+0.099658	0.160849	-0.018591	+0.021753
8	BCP8	C33 - C39	0.246877	-0.621295	0.061428	-0.267230	+0.055953



9	BCP9	C11 - S14	0.211431	-0.459810	0.026556	-0.211246	+0.048147
10	BCP10	O5 - C32	0.261580	-0.615189	0.084173	-0.489872	+0.168037
11	BCP11	C11 - C32	0.252373	-0.642512	0.023216	-0.280986	+0.060179
12	BCP12	C32 - C33	0.221381	-0.485276	0.027166	-0.222650	+0.050665
13	BCP13	C11 - H12	0.346311	-1.427572	0.019210	-0.493672	+0.068389
14	BCP14	C11 - H13	0.346284	-1.434066	0.011707	-0.489316	+0.065400
15	BCP15	O2 - S14	0.308600	+0.931304	0.049612	-0.975934	+0.604380
16	BCP16	S14 - C15	0.207971	-0.439407	0.024855	-0.204733	+0.047441
17	BCP17	C15 - H16	0.346301	-1.436840	0.012774	-0.487895	+0.064343
18	BCP18	C15 - C18	0.248182	-0.621996	0.023818	-0.272755	+0.058628
19	BCP19	C15 - H17	0.347401	-1.439439	0.019695	-0.493576	+0.066858
20	BCP20	O4 - C18	0.263538	-0.627550	0.085382	-0.499864	+0.171488
21	BCP21	C25 - C33	0.220120	-0.469197	0.044624	-0.227191	+0.054946
22	BCP22	C18 - C33	0.226703	-0.511220	0.032370	-0.231028	+0.051612
23	BCP23	O9 - H20	0.022517	+0.095776	0.275104	-0.017971	+0.020957
24	BCP24	C18 - C19	0.248402	-0.617698	0.086114	-0.270127	+0.057851
25	BCP25	C19 - H20	0.350101	-1.504373	0.044941	-0.473502	+0.048704
26	BCP26	O3 - C21	0.242140	-0.309426	0.707346	-0.455874	+0.189259
27	BCP27	C19 - C21	0.266389	-0.630118	0.224018	-0.354872	+0.098671
28	BCP28	C21 - C23	0.258565	-0.668994	0.086192	-0.288798	+0.060775
29	BCP29	C21 - H22	0.345426	-1.456815	0.043295	-0.471435	+0.053616
30	BCP30	C23 - H24	0.353677	-1.536499	0.028329	-0.478431	+0.047153
31	BCP31	H24 - O48	0.006640	+0.027093	0.065026	-0.003802	+0.005288
32	BCP32	C25 - C34	0.262846	-0.704047	0.079305	-0.300046	+0.062017
33	BCP33	O7 - C34	0.416221	-0.319776	0.122446	-1.431822	+0.675939
34	BCP34	O8 - C34	0.316986	-0.659880	0.052292	-0.858904	+0.346967
35	BCP35	C23 - C25	0.231497	-0.534239	0.035249	-0.242678	+0.054559
36	BCP36	O6 - C28	0.233972	-0.254187	0.803661	-0.420858	+0.178656
37	BCP37	C30 - C32	0.244677	-0.598904	0.082250	-0.263117	+0.056695
38	BCP38	C25 - C26	0.227749	-0.517102	0.035885	-0.236518	+0.053621
39	BCP39	C26 - H27	0.355465	-1.561339	0.025904	-0.478714	+0.044190
40	BCP40	C28 - C30	0.269992	-0.653782	0.201883	-0.360468	+0.098512
41	BCP41	C26 - C28	0.255383	-0.653926	0.085213	-0.282268	+0.059393
42	BCP42	C28 - H29	0.345843	-1.464140	0.041274	-0.470885	+0.052425
43	BCP43	O6 - C30	0.242050	-0.310346	0.697872	-0.450171	+0.186292
44	BCP44	O10 - C40	0.232887	-0.356458	0.032668	-0.533325	+0.222105
45	BCP45	O10 - C39	0.315770	-0.665192	0.046943	-0.852072	+0.342887
46	BCP46	C30 - H31	0.348576	-1.486105	0.045558	-0.471796	+0.050135
47	BCP47	O7 - C39	0.015563	+0.062429	0.886364	-0.011048	+0.013328
48	BCP48	O9 - C39	0.426594	-0.208492	0.115968	-1.508284	+0.728081
49	BCP49	C40 - H42	0.362183	-1.569350	0.058403	-0.519381	+0.063522
50	BCP50	C35 - H38	0.362386	-1.572324	0.059924	-0.521868	+0.064393
51	BCP51	O8 - C35	0.225586	-0.370844	0.026780	-0.481116	+0.194203
52	BCP52	C35 - H36	0.360538	-1.560759	0.065583	-0.515303	+0.062556
53	BCP53	C35 - H37	0.361461	-1.565236	0.061454	-0.519970	+0.064331
54	BCP54	C40 - H41	0.360014	-1.553817	0.068471	-0.519198	+0.065372
55	BCP55	C40 - H43	0.361910	-1.570366	0.062515	-0.519576	+0.063492
56	BCP56	H27 - O48	0.006268	+0.026548	0.139459	-0.003680	+0.005158
57	BCP57	O8 - O44	0.001845	+0.007467	0.115901	-0.000840	+0.001353
58	BCP58	H27 - O44	0.006393	+0.026275	0.018872	-0.003481	+0.005025
59	BCP59	O44 - S57	0.312225	+1.004008	0.039148	-1.001136	+0.626069
60	BCP60	H27 - O47	0.006373	+0.027127	0.089672	-0.003745	+0.005263
61	BCP61	O47 - C66	0.253051	-0.562738	0.052694	-0.476592	+0.167954
62	BCP62	O46 - C62	0.240515	-0.300681	0.746049	-0.450867	+0.187849
63	BCP63	O47 - O48	0.019719	+0.094233	0.035227	-0.018310	+0.020934
64	BCP64	O1 - O51	0.001845	+0.007468	0.115813	-0.000840	+0.001353
65	BCP65	O48 - C69	0.253781	-0.564912	0.042956	-0.493059	+0.175916
66	BCP66	O53 - H74	0.022826	+0.099647	0.160762	-0.018589	+0.021750
67	BCP67	C76 - C82	0.246877	-0.621294	0.061431	-0.267229	+0.055953
68	BCP68	C54 - S57	0.211441	-0.459860	0.026565	-0.211265	+0.048150
69	BCP69	O48 - C75	0.261544	-0.614975	0.084178	-0.489664	+0.167960
70	BCP70	C54 - C75	0.252373	-0.642507	0.023212	-0.280986	+0.060179
71	BCP71	C75 - C76	0.221381	-0.485280	0.027160	-0.222648	+0.050664
72	BCP72	C54 - H55	0.346364	-1.428001	0.019214	-0.493826	+0.068413
73	BCP73	C54 - H56	0.346216	-1.433521	0.011705	-0.489120	+0.065370
74	BCP74	O45 - S57	0.308584	+0.930990	0.049632	-0.975830	+0.604288
75	BCP75	S57 - C58	0.207944	-0.439277	0.024853	-0.204680	+0.047430
76	BCP76	C58 - H59	0.346301	-1.436844	0.012775	-0.487896	+0.064343
77	BCP77	C58 - C61	0.248182	-0.621997	0.023815	-0.272757	+0.058629
78	BCP78	C58 - H60	0.347401	-1.439448	0.019697	-0.493576	+0.066857

79	BCP79	O47 - C61	0.263537	-0.627531	0.085388	-0.499866	+0.171492
80	BCP80	C68 - C76	0.220099	-0.469102	0.044621	-0.227154	+0.054939
81	BCP81	C61 - C76	0.226703	-0.511223	0.032369	-0.231028	+0.051611
82	BCP82	O52 - H63	0.022517	+0.095772	0.275107	-0.017971	+0.020957
83	BCP83	C61 - C62	0.248438	-0.617886	0.086099	-0.270196	+0.057862
84	BCP84	C62 - H63	0.350035	-1.503829	0.044935	-0.473320	+0.048682
85	BCP85	O46 - C64	0.242141	-0.309378	0.707556	-0.455873	+0.189264
86	BCP86	C62 - C64	0.266414	-0.630257	0.223972	-0.354927	+0.098681
87	BCP87	C64 - C66	0.258566	-0.668993	0.086192	-0.288799	+0.060776
88	BCP88	C64 - H65	0.345456	-1.457055	0.043294	-0.471519	+0.053628
89	BCP89	O5 - H67	0.006640	+0.027092	0.065006	-0.003802	+0.005287
90	BCP90	C66 - H67	0.353628	-1.536099	0.028323	-0.478296	+0.047135
91	BCP91	C68 - C77	0.262891	-0.704288	0.079310	-0.300139	+0.062034
92	BCP92	O50 - C77	0.416220	-0.319770	0.122461	-1.431823	+0.675940
93	BCP93	O51 - C77	0.316936	-0.660170	0.052315	-0.858545	+0.346751
94	BCP94	C66 - C68	0.231466	-0.534089	0.035252	-0.242623	+0.054551
95	BCP95	O1 - H70	0.006393	+0.026276	0.018860	-0.003481	+0.005025
96	BCP96	O4 - H70	0.006373	+0.027127	0.089659	-0.003745	+0.005263
97	BCP97	O49 - C71	0.233945	-0.253968	0.804207	-0.420742	+0.178625
98	BCP98	C73 - C75	0.244662	-0.598825	0.082247	-0.263088	+0.056691
99	BCP99	C68 - C69	0.227747	-0.517096	0.035899	-0.236516	+0.053621
100	BCP100	C69 - H70	0.355466	-1.561347	0.025902	-0.478716	+0.044189
101	BCP101	C71 - C73	0.270018	-0.653939	0.201790	-0.360518	+0.098517
102	BCP102	C69 - C71	0.255383	-0.653925	0.085211	-0.282269	+0.059394
103	BCP103	C71 - H72	0.345844	-1.464143	0.041274	-0.470884	+0.052424
104	BCP104	O49 - C73	0.242053	-0.310344	0.697862	-0.450156	+0.186285
105	BCP105	O53 - C83	0.232858	-0.356442	0.032681	-0.533163	+0.222026
106	BCP106	O53 - C82	0.315770	-0.665194	0.046945	-0.852069	+0.342885
107	BCP107	C73 - H74	0.348535	-1.485773	0.045554	-0.471685	+0.050121
108	BCP108	O50 - C82	0.015563	+0.062429	0.886506	-0.011048	+0.013328
109	BCP109	O52 - C82	0.426594	-0.208498	0.115970	-1.508284	+0.728080
110	BCP110	C83 - H85	0.362135	-1.568954	0.058393	-0.519235	+0.063498
111	BCP111	C78 - H81	0.362304	-1.571620	0.059918	-0.521627	+0.064361
112	BCP112	O51 - C78	0.225629	-0.370897	0.026790	-0.481366	+0.194321
113	BCP113	C78 - H79	0.360550	-1.560861	0.065587	-0.515346	+0.062565
114	BCP114	C78 - H80	0.361481	-1.565399	0.061459	-0.520039	+0.064345
115	BCP115	C83 - H84	0.360050	-1.554129	0.068475	-0.519306	+0.065387
116	BCP116	C83 - H86	0.361992	-1.571067	0.062518	-0.519818	+0.063525





BCP #	Name	Atoms	Rho	DelSqRho	Ellipticity	V	G
1	BCP1	O2 - C22	0.256295	-0.578104	0.047296	-0.500411	+0.177942
2	BCP2	O3 - H70	0.009747	+0.040429	0.101886	-0.006133	+0.008120
3	BCP3	O2 - O3	0.020027	+0.095317	0.050036	-0.018711	+0.021270
4	BCP4	C22 - C24	0.233501	-0.546246	0.043651	-0.243586	+0.053512
5	BCP5	O6 - H21	0.013817	+0.062433	1.216797	-0.010238	+0.012923
6	BCP6	C24 - C25	0.229960	-0.526939	0.032132	-0.240870	+0.054568
7	BCP7	C25 - H26	0.354383	-1.543503	0.025957	-0.478191	+0.046158
8	BCP8	O7 - H28	0.014423	+0.062706	0.250249	-0.010398	+0.013037
9	BCP9	O3 - C25	0.252792	-0.557877	0.045480	-0.486430	+0.173480
10	BCP10	C31 - C32	0.234880	-0.551178	0.037785	-0.245614	+0.053910
11	BCP11	O7 - O9	0.011082	+0.053362	0.249666	-0.007886	+0.010613
12	BCP12	C32 - C43	0.256974	-0.670990	0.071964	-0.289542	+0.060897
13	BCP13	O3 - C31	0.255629	-0.581293	0.068367	-0.485240	+0.169958
14	BCP14	C10 - C31	0.257313	-0.675887	0.044124	-0.286585	+0.058806
15	BCP15	C10 - H12	0.353308	-1.496923	0.042358	-0.499449	+0.062609
16	BCP16	N13 - C33	0.323840	-1.038799	0.162069	-0.712025	+0.226163
17	BCP17	C10 - H11	0.352347	-1.490195	0.035314	-0.497035	+0.062243
18	BCP18	C10 - N13	0.255007	-0.614608	0.046017	-0.392438	+0.119393
19	BCP19	C17 - C32	0.225033	-0.500346	0.024954	-0.232364	+0.053639
20	BCP20	N13 - C14	0.260440	-0.649851	0.035230	-0.419166	+0.128352
21	BCP21	C14 - C17	0.257791	-0.676812	0.051685	-0.289007	+0.059902
22	BCP22	C14 - H15	0.350489	-1.469965	0.048647	-0.502281	+0.067395
23	BCP23	O2 - H70	0.008009	+0.033246	0.151501	-0.004798	+0.006555
24	BCP24	C14 - H16	0.355079	-1.524273	0.031636	-0.493342	+0.056137
25	BCP25	O2 - C17	0.259041	-0.597443	0.068408	-0.488300	+0.169470
26	BCP26	O9 - H19	0.014780	+0.063913	0.302557	-0.010717	+0.013348
27	BCP27	O1 - C18	0.245225	-0.331269	0.685023	-0.469077	+0.193130
28	BCP28	C17 - C18	0.251123	-0.629840	0.087115	-0.275409	+0.058974
29	BCP29	C18 - H19	0.346100	-1.460986	0.046341	-0.471345	+0.053049
30	BCP30	O1 - C20	0.244533	-0.333214	0.673296	-0.475337	+0.196017
31	BCP31	C18 - C20	0.262384	-0.605897	0.243464	-0.347754	+0.098140
32	BCP32	C20 - C22	0.252101	-0.638145	0.087954	-0.275800	+0.058132
33	BCP33	C20 - H21	0.347861	-1.480078	0.041864	-0.471277	+0.050629
34	BCP34	C24 - C38	0.257633	-0.675846	0.066877	-0.289958	+0.060498
35	BCP35	C22 - H23	0.353021	-1.530023	0.029073	-0.477380	+0.047437
36	BCP36	O7 - C38	0.319855	-0.612888	0.045745	-0.889594	+0.368186
37	BCP37	O4 - C27	0.247500	-0.349165	0.665712	-0.493689	+0.203199
38	BCP38	C27 - C29	0.260864	-0.594879	0.259091	-0.345561	+0.098421
39	BCP39	O7 - C39	0.227124	-0.373199	0.031746	-0.488620	+0.197660
40	BCP40	C29 - C31	0.245114	-0.600623	0.089928	-0.263290	+0.056567
41	BCP41	C25 - C27	0.249361	-0.623683	0.086147	-0.270588	+0.057333
42	BCP42	C27 - H28	0.347966	-1.480631	0.041542	-0.472214	+0.051028
43	BCP43	C39 - H42	0.361692	-1.567659	0.060134	-0.518514	+0.063300
44	BCP44	O4 - C29	0.248291	-0.351424	0.676185	-0.491354	+0.201749
45	BCP45	O8 - H30	0.012917	+0.058344	1.193031	-0.009408	+0.011997
46	BCP46	C29 - H30	0.346888	-1.471625	0.046264	-0.470397	+0.051245
47	BCP47	O8 - C43	0.424366	-0.231874	0.120504	-1.491472	+0.716752
48	BCP48	O9 - C43	0.312956	-0.651747	0.046181	-0.841104	+0.339083
49	BCP49	C44 - H45	0.361989	-1.569106	0.058508	-0.519408	+0.063566
50	BCP50	C24 - C32	0.218076	-0.457984	0.043440	-0.224662	+0.055083
51	BCP51	O5 - C33	0.403186	-0.492607	0.103551	-1.326652	+0.601750
52	BCP52	C33 - C34	0.257786	-0.667951	0.052237	-0.296112	+0.064562
53	BCP53	C34 - H36	0.346556	-1.420901	0.016425	-0.517002	+0.080888
54	BCP54	C34 - H35	0.352211	-1.473463	0.019776	-0.513949	+0.072792
55	BCP55	C34 - H37	0.349040	-1.442244	0.015436	-0.516955	+0.078197
56	BCP56	O6 - C38	0.418132	-0.308771	0.122452	-1.444027	+0.683417
57	BCP57	C39 - H41	0.361842	-1.567675	0.059818	-0.520282	+0.064182
58	BCP58	C39 - H40	0.360973	-1.562834	0.067503	-0.520136	+0.064714
59	BCP59	O9 - C44	0.227836	-0.378439	0.029256	-0.488718	+0.197054
60	BCP60	C44 - H46	0.360367	-1.557935	0.066935	-0.518065	+0.064291
61	BCP61	C44 - H47	0.361189	-1.562610	0.062216	-0.520205	+0.064776
62	BCP62	H23 - O49	0.008046	+0.032586	0.076005	-0.004764	+0.006455
63	BCP63	H26 - O49	0.011155	+0.046258	0.080962	-0.007181	+0.009373
64	BCP64	H26 - O50	0.008337	+0.034885	0.178199	-0.005086	+0.006904
65	BCP65	O49 - O50	0.019760	+0.094015	0.050908	-0.018362	+0.020933
66	BCP66	O50 - C72	0.255826	-0.576860	0.045438	-0.496311	+0.176048
67	BCP67	H37 - O53	0.003313	+0.013127	0.234162	-0.001621	+0.002451
68	BCP68	C71 - C72	0.232601	-0.541768	0.043514	-0.242061	+0.053310
69	BCP69	O53 - H75	0.013383	+0.061768	3.402860	-0.010101	+0.012771

70	BCP70	C69 - H70	0.354026	-1.540278	0.026107	-0.477696	+0.046313
71	BCP71	C69 - C71	0.231262	-0.533022	0.031713	-0.243334	+0.055039
72	BCP72	O49 - C69	0.253320	-0.560500	0.045178	-0.488435	+0.174155
73	BCP73	C64 - C79	0.233348	-0.543934	0.037710	-0.242750	+0.053383
74	BCP74	O54 - O56	0.011071	+0.053369	0.175771	-0.007890	+0.010616
75	BCP75	C79 - C90	0.257472	-0.673322	0.074266	-0.290755	+0.061212
76	BCP76	C78 - C79	0.224195	-0.496248	0.024056	-0.231069	+0.053503
77	BCP77	C57 - H58	0.355224	-1.524857	0.031762	-0.494168	+0.056477
78	BCP78	C57 - C78	0.257936	-0.677377	0.051617	-0.289257	+0.059956
79	BCP79	C57 - H59	0.350242	-1.468546	0.048007	-0.500686	+0.066775
80	BCP80	C57 - N60	0.259765	-0.645744	0.025604	-0.415193	+0.126878
81	BCP81	O49 - C64	0.254590	-0.575539	0.066888	-0.480412	+0.168264
82	BCP82	C61 - C64	0.256528	-0.671815	0.043282	-0.285234	+0.058640
83	BCP83	N60 - C80	0.326298	-1.052167	0.155710	-0.726883	+0.231920
84	BCP84	N60 - C61	0.253023	-0.601652	0.040256	-0.383305	+0.116446
85	BCP85	C61 - H62	0.353316	-1.498257	0.041711	-0.498306	+0.061871
86	BCP86	C61 - H63	0.353218	-1.497893	0.035600	-0.499267	+0.062397
87	BCP87	O48 - C65	0.247952	-0.351679	0.664502	-0.489335	+0.200707
88	BCP88	C71 - C79	0.216957	-0.453127	0.043891	-0.222513	+0.054616
89	BCP89	O55 - C90	0.420003	-0.284547	0.121233	-1.458683	+0.693773
90	BCP90	C64 - C65	0.246275	-0.606479	0.089146	-0.265491	+0.056936
91	BCP91	O55 - H66	0.012303	+0.056293	2.306415	-0.008998	+0.011536
92	BCP92	C65 - H66	0.346717	-1.470518	0.045724	-0.469858	+0.051114
93	BCP93	O48 - C67	0.245662	-0.339090	0.674971	-0.483268	+0.199248
94	BCP94	C65 - C67	0.260495	-0.593865	0.255547	-0.344415	+0.097974
95	BCP95	O54 - C86	0.228662	-0.375475	0.031814	-0.496548	+0.201340
96	BCP96	O54 - H68	0.013695	+0.059357	0.239421	-0.009714	+0.012277
97	BCP97	C67 - C69	0.251351	-0.633548	0.086314	-0.274527	+0.058070
98	BCP98	C86 - H87	0.361963	-1.569611	0.059423	-0.519240	+0.063419
99	BCP99	C67 - H68	0.347739	-1.478106	0.042088	-0.472316	+0.051395
100	BCP100	C74 - C76	0.262393	-0.606462	0.241605	-0.347582	+0.097983
101	BCP101	O54 - C85	0.318586	-0.625827	0.046921	-0.878769	+0.361156
102	BCP102	O3 - H73	0.008956	+0.036380	0.065270	-0.005403	+0.007249
103	BCP103	O51 - C74	0.242340	-0.319516	0.691759	-0.463312	+0.191717
104	BCP104	C71 - C85	0.259409	-0.684922	0.067080	-0.293650	+0.061210
105	BCP105	O56 - H77	0.014561	+0.062926	0.280859	-0.010506	+0.013119
106	BCP106	O50 - C78	0.260728	-0.606489	0.066307	-0.494789	+0.171583
107	BCP107	C76 - C78	0.250927	-0.628795	0.086706	-0.275083	+0.058942
108	BCP108	C72 - H73	0.352722	-1.528755	0.028682	-0.475670	+0.046741
109	BCP109	C72 - C74	0.252182	-0.638655	0.087650	-0.275944	+0.058140
110	BCP110	C74 - H75	0.347648	-1.478145	0.041835	-0.471188	+0.050826
111	BCP111	O51 - C76	0.246118	-0.338030	0.663029	-0.471514	+0.193503
112	BCP112	C76 - H77	0.346290	-1.462349	0.046086	-0.472087	+0.053250
113	BCP113	O56 - C90	0.314573	-0.644481	0.047853	-0.852342	+0.345611
114	BCP114	C91 - H93	0.361965	-1.568804	0.059237	-0.520081	+0.063940
115	BCP115	O52 - C80	0.397609	-0.554684	0.104645	-1.283823	+0.572576
116	BCP116	O6 - H82	0.003988	+0.015895	0.216675	-0.002002	+0.002988
117	BCP117	C80 - C81	0.262360	-0.691433	0.052662	-0.305864	+0.066503
118	BCP118	C81 - H82	0.349092	-1.442751	0.014515	-0.517930	+0.078621
119	BCP119	C81 - H83	0.347533	-1.427599	0.016676	-0.519534	+0.081317
120	BCP120	C81 - H84	0.352269	-1.473129	0.019756	-0.514768	+0.073243
121	BCP121	O53 - C85	0.421045	-0.273319	0.121898	-1.466075	+0.698872
122	BCP122	C86 - H88	0.361460	-1.564346	0.059840	-0.519408	+0.064161
123	BCP123	C86 - H89	0.360512	-1.558672	0.067174	-0.518964	+0.064648
124	BCP124	O56 - C91	0.228496	-0.376473	0.030382	-0.494551	+0.200217
125	BCP125	C91 - H92	0.360691	-1.560634	0.066950	-0.518982	+0.064412
126	BCP126	C91 - H94	0.361622	-1.566192	0.061183	-0.520591	+0.064521

**Cartesian coordinates (Dimers 1b-3b are retrieved from the X-ray, the coordinates can be extracted from cif files)**

**A**

8	0.000000	3.491556	-0.113662
8	0.000000	1.406273	1.261051
8	-0.000000	-1.406273	1.261051
8	-0.000000	-3.491556	-0.113662
6	1.069022	1.310843	0.338736

6	0.729032	2.412338	-0.666035
1	1.343855	2.613367	-1.537095
6	-0.729032	2.412338	-0.666035
1	-1.343855	2.613367	-1.537095
6	-1.069022	1.310843	0.338736
1	-2.022464	1.379461	0.860389
6	-0.783915	0.000000	-0.413970
6	-1.069022	-1.310843	0.338736
1	-2.022464	-1.379461	0.860389
6	-0.729032	-2.412338	-0.666035
1	-1.343855	-2.613367	-1.537095
6	0.729032	-2.412338	-0.666035
1	1.343855	-2.613367	-1.537095
6	1.069022	-1.310843	0.338736
6	0.783915	-0.000000	-0.413970
1	1.224527	-0.000000	-1.414291
1	2.022464	-1.379461	0.860389
1	2.022464	1.379461	0.860389
1	-1.224527	0.000000	-1.414291

**B**

8	-1.369528	0.000000	1.235186
8	1.369528	-0.000000	1.235186
6	-1.320224	1.057574	0.290754
6	-2.430971	0.664347	-0.671200
6	-2.430971	-0.664347	-0.671200
6	-1.320224	-1.057574	0.290754
1	-1.393066	-2.025262	0.785414
6	0.000000	-0.778063	-0.473788
6	1.320224	-1.057574	0.290754
1	1.393066	-2.025262	0.785414
6	2.430971	-0.664347	-0.671200
6	2.430971	0.664347	-0.671200
6	1.320224	1.057574	0.290754
6	0.000000	0.778063	-0.473788
1	0.000000	1.234973	-1.463346
1	1.393066	2.025262	0.785414
1	-1.393066	2.025262	0.785414
1	-0.000000	-1.234973	-1.463346
1	-3.004891	1.339788	-1.290443
1	-3.004891	-1.339788	-1.290443
1	3.004891	1.339788	-1.290443
1	3.004891	-1.339788	-1.290443

**C**

8	0.000000	0.000000	1.294868
6	0.000000	1.052173	0.332267
6	-1.238005	0.661983	-0.497120
6	-1.238005	-0.661983	-0.497120
6	-0.000000	-1.052173	0.332267
1	0.000000	-2.031315	0.805660
6	1.238005	-0.661983	-0.497120
6	1.238005	0.661983	-0.497120
1	0.000000	2.031315	0.805660
1	-1.896602	1.349792	-1.006644
1	-1.896602	-1.349792	-1.006644
1	1.896602	1.349792	-1.006644
1	1.896602	-1.349792	-1.006644

**dimer\_C**

8	-0.979398	0.503349	-1.607679
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6	-0.973247	-0.152648	-2.875723
6	-0.051114	-1.345568	-2.557710
6	0.839401	-0.862875	-1.704450
6	0.445143	0.612783	-1.515683
1	0.754438	1.088552	-0.589258
6	0.743370	1.332330	-2.841758
6	-0.146981	0.852981	-3.696926
1	-1.981037	-0.374426	-3.219644
1	-0.116397	-2.327025	-3.004065
1	1.691713	-1.339033	-1.243513
1	-0.258793	1.044647	-4.754001
1	1.556667	2.022439	-3.011485
8	0.979398	-0.503349	1.607679
6	-0.445143	-0.612783	1.515683
6	-0.839401	0.862875	1.704450
6	0.051114	1.345568	2.557710
6	0.973247	0.152648	2.875723
1	1.981037	0.374426	3.219644
6	0.146981	-0.852981	3.696926
6	-0.743370	-1.332330	2.841758
1	-0.754438	-1.088552	0.589258
1	-1.691713	1.339033	1.243513
1	0.116397	2.327025	3.004065
1	-1.556667	-2.022439	3.011485
1	0.258793	-1.044647	4.754001
<b>A ··· HF_bifurcated</b>			
8	0.412590	3.487759	0.000000
8	-0.928984	1.384068	0.000000
8	-0.928646	-1.383922	-0.000000
8	0.413460	-3.487529	-0.000000
6	-0.002066	1.304268	1.072639
6	0.982930	2.419271	0.728952
1	1.849387	2.632831	1.345568
6	0.982930	2.419271	-0.728952
1	1.849387	2.632831	-1.345568
6	-0.002066	1.304268	-1.072639
1	-0.527921	1.367789	-2.023866
6	0.759122	0.000165	-0.784898
6	-0.001749	-1.304128	-1.072600
1	-0.527609	-1.367747	-2.023820
6	0.983533	-2.418906	-0.728950
1	1.850045	-2.632273	-1.345565
6	0.983533	-2.418906	0.728950
1	1.850045	-2.632273	1.345565
6	-0.001749	-1.304128	1.072600
6	0.759122	0.000165	0.784898
1	1.757988	0.000309	1.227519
1	-0.527609	-1.367747	2.023820
1	-0.527921	1.367789	2.023866
1	1.757988	0.000309	-1.227519
9	-3.414411	-0.001698	0.000000
1	-2.482676	0.002406	0.000000
<b>A ··· (HF) 2</b>			
8	-0.423878	3.767497	-0.000000
8	-1.321363	1.437067	-0.000000
8	-0.724865	-1.297337	0.000000
8	1.038535	-3.051899	0.000000
6	-0.401142	1.543645	1.069479
6	0.346625	2.833231	0.729193
1	1.153751	3.215513	1.345124
6	0.346625	2.833231	-0.729193

1	1.153751	3.215513	-1.345124
6	-0.401142	1.543645	-1.069479
1	-0.925530	1.499227	-2.022623
6	0.613811	0.422878	-0.784674
6	0.163287	-1.014337	-1.077130
1	-0.337673	-1.195388	-2.026267
6	1.368164	-1.886147	-0.729040
1	2.259115	-1.909909	-1.346699
6	1.368164	-1.886147	0.729040
1	2.259115	-1.909909	1.346699
6	0.163287	-1.014337	1.077130
6	0.613811	0.422878	0.784674
1	1.591788	0.633297	1.224172
1	-0.337673	-1.195388	2.026267
1	-0.925530	1.499227	2.022623
1	1.591788	0.633297	-1.224172
9	-2.170723	-3.485372	0.000000
1	-1.582783	-2.751003	0.000000