Electronic Supplementary Material (ESI) for RSC Advances.

Insight in the C–H····F–C hydrogen bond:- Cambridge Structural Database Analyses and Computational Studies

Sagarika Dev.,[2,≠] Sudeep Maheswari,[1,≠] Angshuman Roy Choudhury[1,*]

[1]*Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Mohali, Knowledge City, Sector 81, S. A. S. Nagar, Manauli PO, Punjab, 140306. India.*

[2]*Department of Chemistry, MCM DAV College for Women, Sector 36, Chandigarh, 160036. U.T. India.*

Electronic Supplementary Information

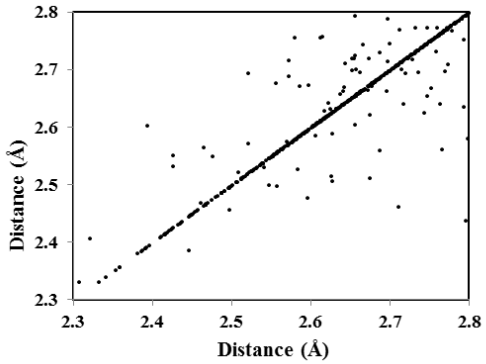


Figure 1: Scatterogram plot of two C–H···F distances in synthon1.

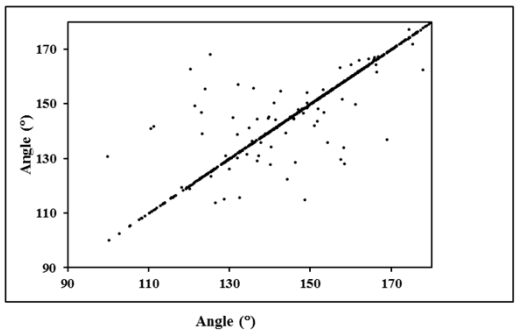


Figure 2: Scatterogram plot of two C–H···F angles in synthon1.

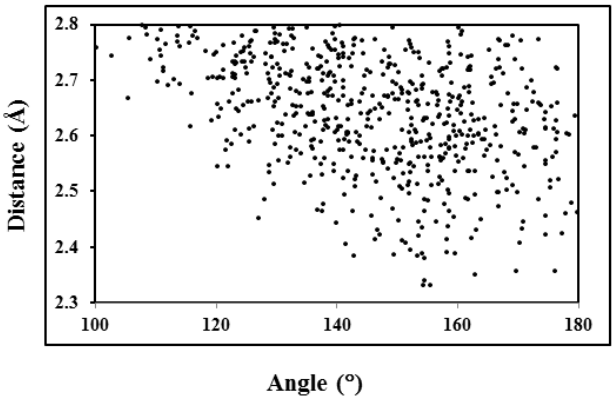


Figure 3: Scatterogram plot of one of the C–H···F distances and angles in synthon1.

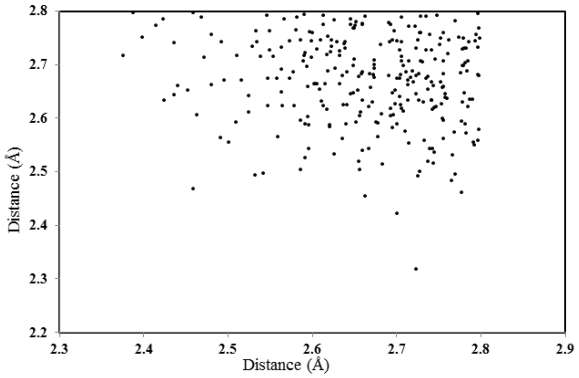


Figure 4: Scatterogram plot of two C–H···F distances in synthon 2.

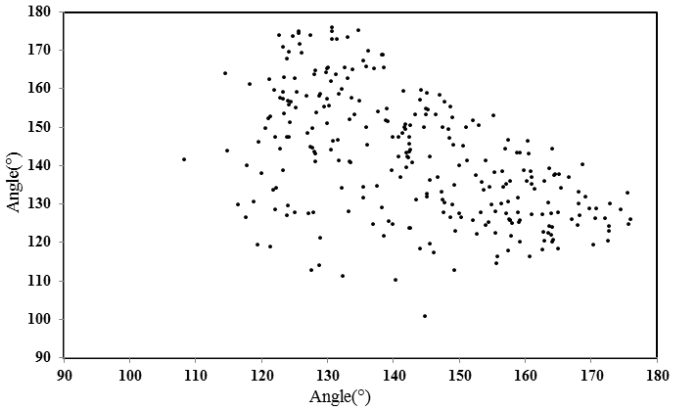


Figure 5: Scatterogram plot of two C–H···F angles in synthon 2.

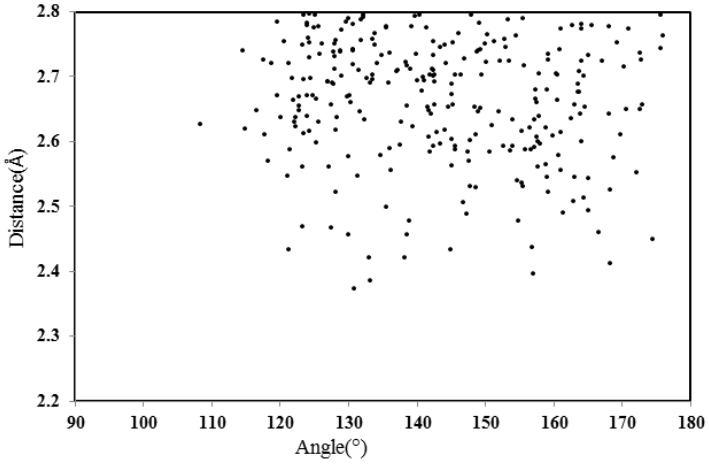


Figure 6: Scatterogram plot of one of the C–H···F distances and angles in synthon 2.

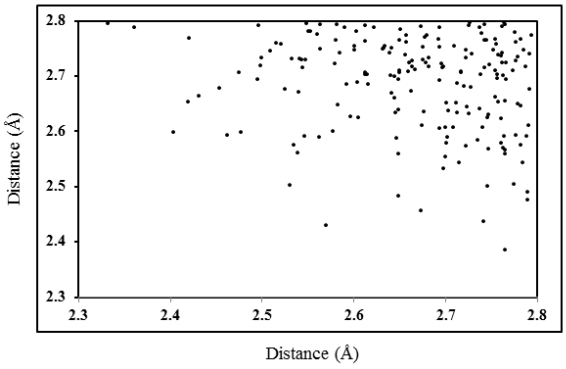


Figure 7: Scatterogram plot of two C–H···F distances in synthon 3.

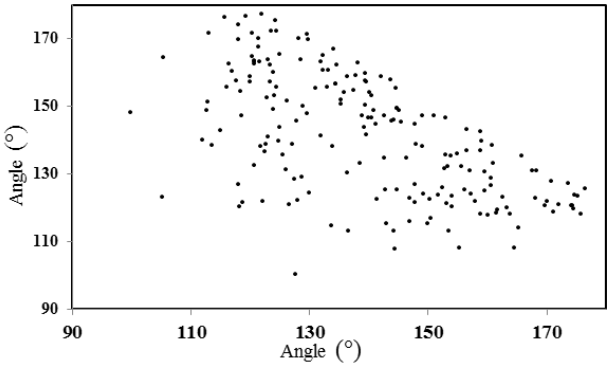


Figure 8: Scatterogram plot of two C–H···F angles in synthon 3.

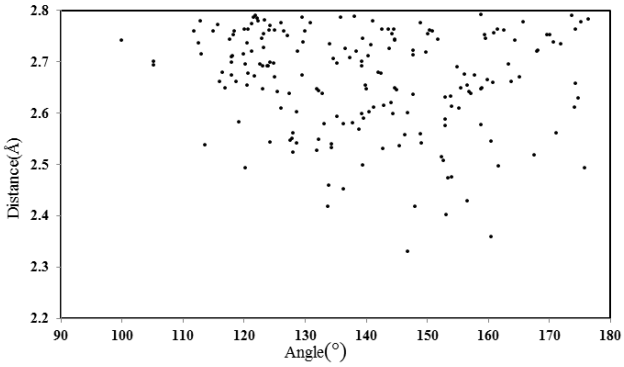


Figure 9: Scatterogram plot of one of the C–H···F distances and angles in synthon 3.

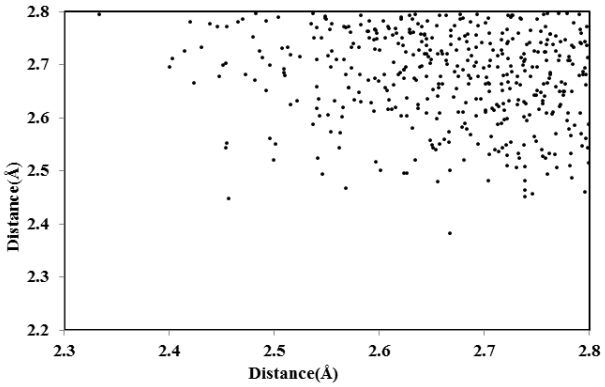


Figure 10: Scatterogram plot of two C–H···F distances in synthon 4.

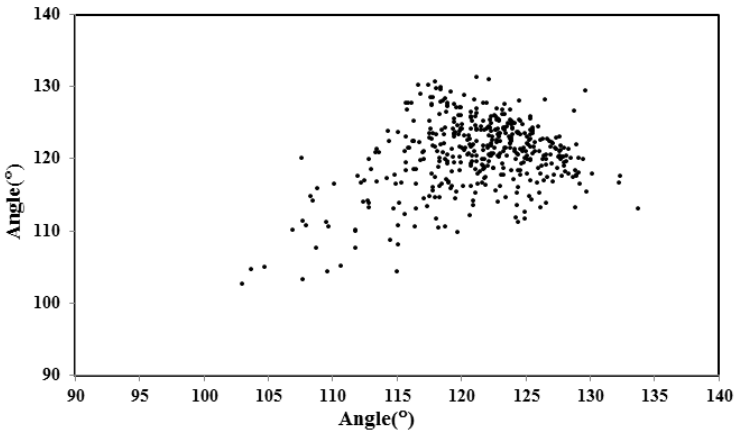


Figure 11: Scatterogram plot of two C–H···F angles in synthon 4.

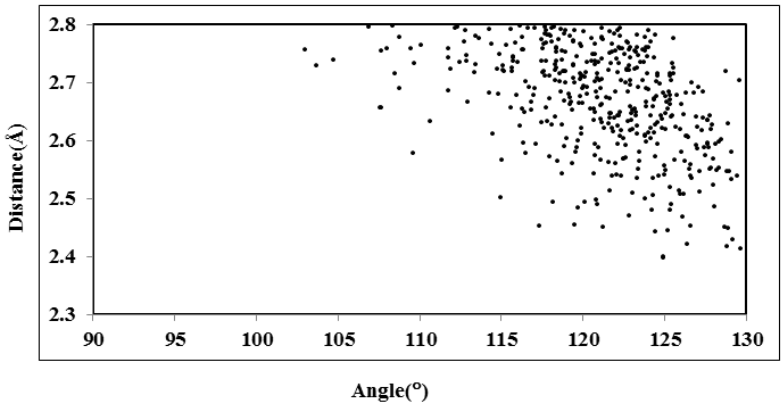


Figure 12: Scatterogram plot of one of the C–H···F distances and angles in synthon 4.

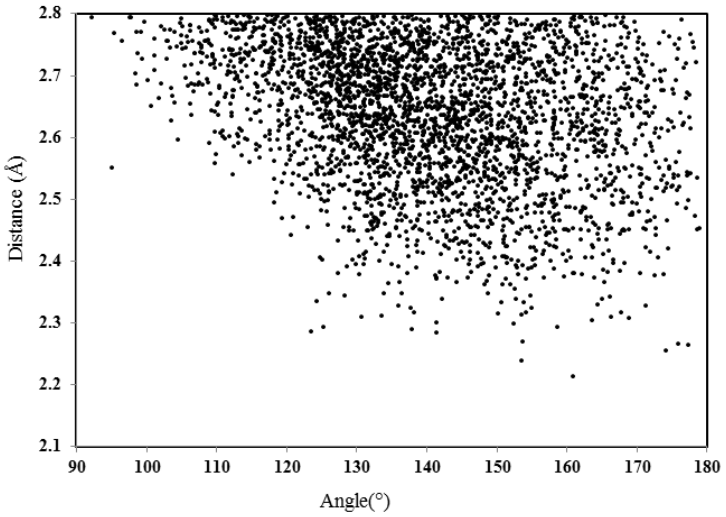
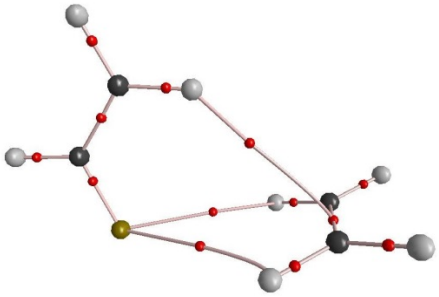


Figure 13: Scatterogram plot of the C–H···F distances and angles in synthon 5.

Table14: Comaparison of structures at MP2/aug-cc-pVDZ and MP2/aug-cc-pVTZ level of theory.

geometry	aug-cc-pVTZ		aug-cc-pVDZ	
	Distance H-F (Å)	∠CH···F (°)	Distance H-F (Å)	∠CH···F (°)
A	2.75, 2.75	120.00, 120.03	2.75, 2.75	119.95, 119.91
B	2.78, 2.78	115.70, 115.69	2.80, 2.80	115.45, 115.45
C	2.68, 2.81 2.62	118.78, 113.70, 139.03	2.66, 2.82, 2.73	138.59, 114.02, 117.44
D	2.72, 2.72	119.93, 119.95	2.78, 2.78	119.02, 119.05
E	2.77, 2.77	119.40, 119.12	2.78, 2.77	119.10, 119.40
F	2.58, 2.72	118.55, 120.38	2.78, 2.57	116.85, 120.92
G	2.42, 2.42	158.46, 158.46	2.40, 2.40	161.64, 161.64
H	2.44, 2.44	133.44, 133.38	2.41, 2.41	138.88, 138.85
I	2.51	134.74	2.54	134.46
J	2.57	118.18	2.594	117.03
K	2.58, 2.58	118.27, 118.27	2.60, 2.60	117.49, 117.49
L	2.43, 2.35	143.93, 151.67	2.41, 2.31	150.61, 156.49
M	2.43, 2.32	168.47, 168.21	2.42, 2.30	171.16, 170.96
N	2.61, 2.74	118.35, 116.90	2.63, 2.80	117.97, 115.66
O	2.39, 2.49	156.32, 144.21	2.36, 2.45	162.10, 152.81
P	2.37, 2.48	172.80, 169.14	2.35, 2.46	176.10, 172.48
Q	2.75, 2.67	118.00, 117.65	2.80, 2.68	116.37, 117.24
R	2.45, 2.45	125.53, 125.52	2.42, 2.42	129.50, 129.51
S	2.46, 2.46	125.17, 125.17	2.44, 2.44	125.11, 125.11
T	2.36, 2.36	149.58, 149.51	2.36, 2.36	149.86, 149.95
U	2.41, 2.45	153.71, 140.20	2.38, 2.42	159.71, 148.91
V	2.39, 2.37	140.25, 149.45	2.37, 2.34	147.79, 154.65
W	2.44, 2.45	167.24, 167.20	2.42, 2.42	172.90, 172.81
X	2.44, 2.39	147.44, 154.98	2.41, 2.39	150.55, 154.35
Y	2.66, 2.66	116.58, 116.56	2.67, 2.67	115.10, 115.98

Figure 14: Molecular graphs of structures A-Y



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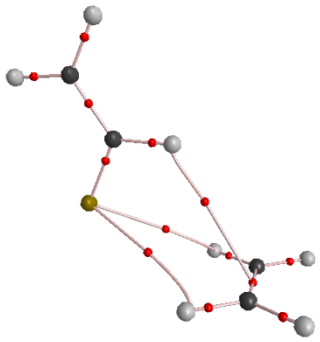

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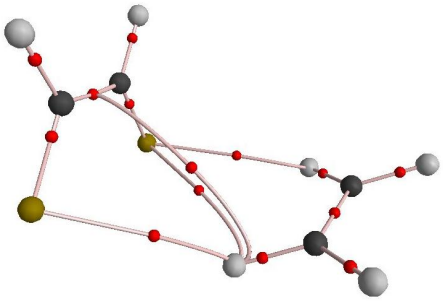

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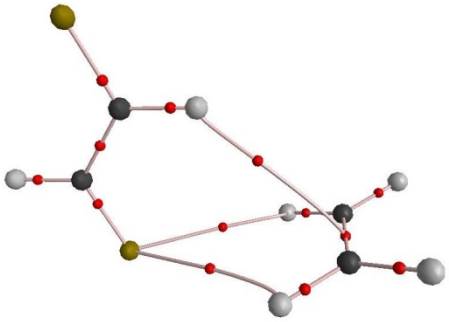

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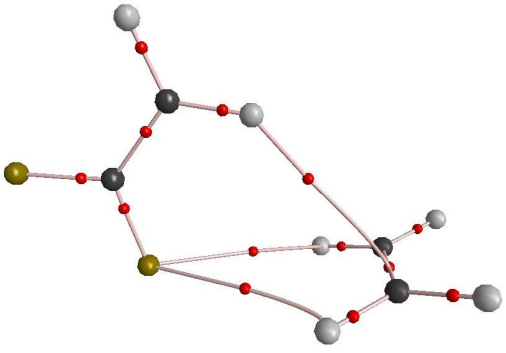

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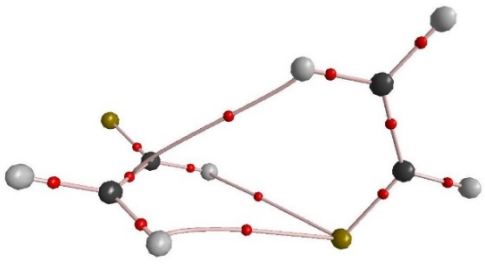

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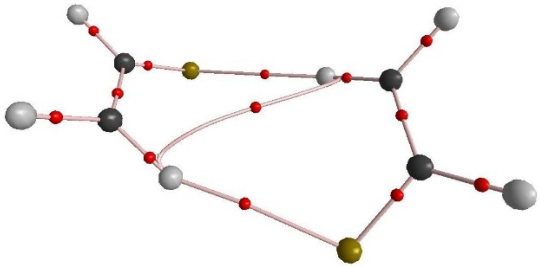

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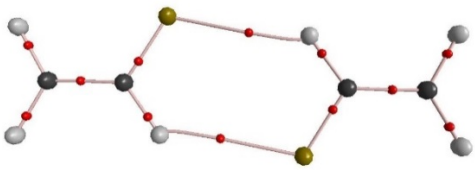

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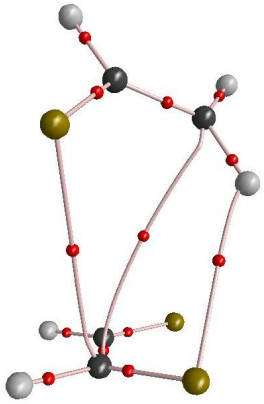

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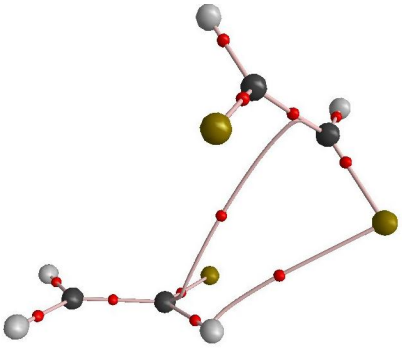

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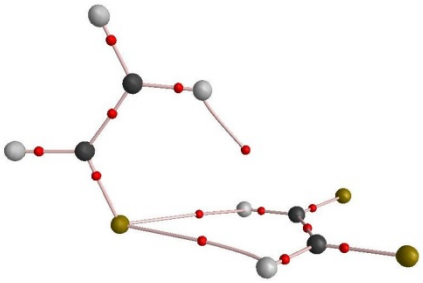

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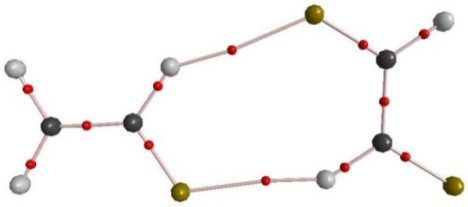

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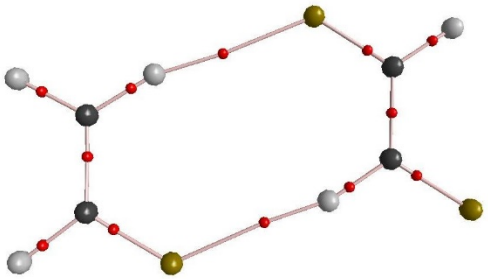

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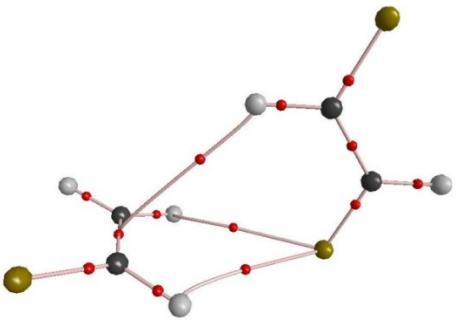

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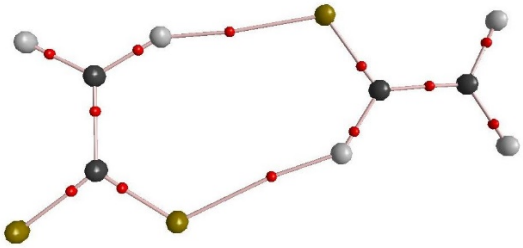

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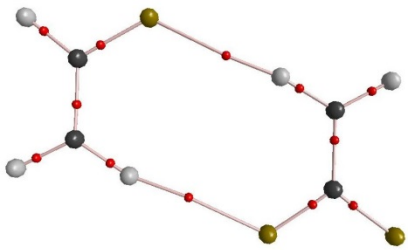

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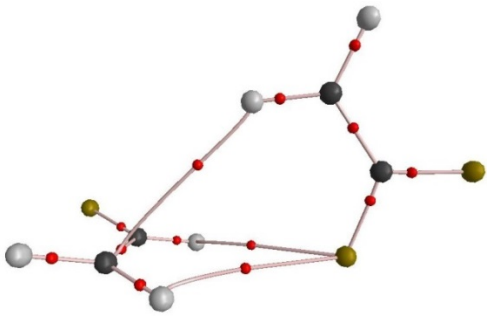

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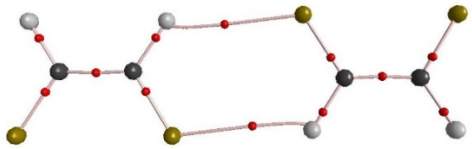

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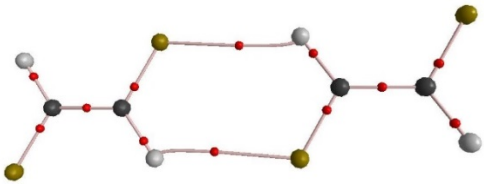

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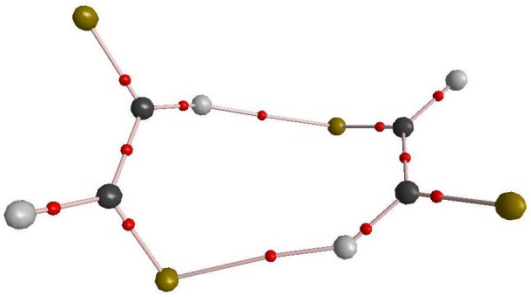

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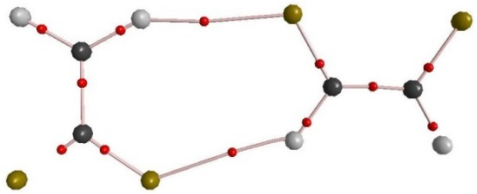

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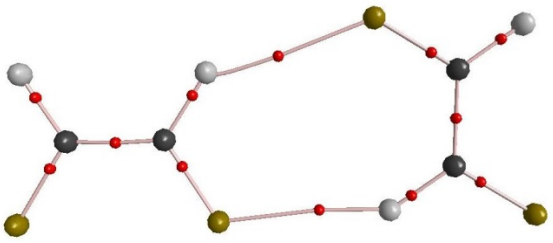

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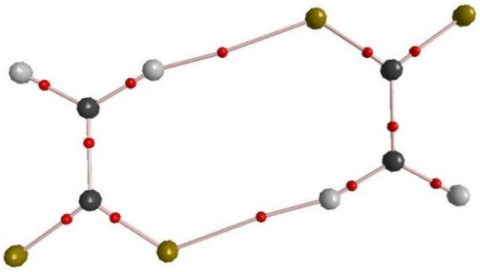

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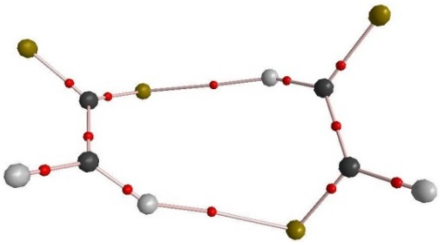

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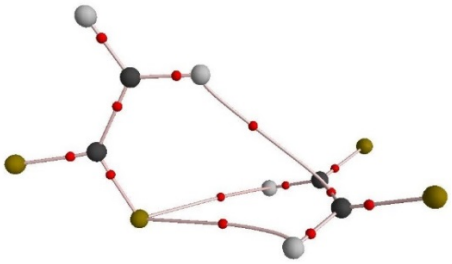

Y

Table 15: Energy decomposition by LMOEDA

	Elect Energy (kcal/mole)	Ex. Energy (kcal/mole)	Rep Energy (kcal/mole)	Pol. Energy (kcal/mole)	Dispersion Energy (kcal/mole)	Total (ΔE) (kcal/mole)
A	-1.37	-2.51	4.59	-1.7	-1.73	-2.71
B	-1.52	-2.43	4.36	-1.52	-1.51	-2.63
C	-1.72	-4.61	7.66	-0.23	-1.29	-0.18
D	-2.66	-5.03	8.48	-0.49	-0.87	-0.58
E	-1.37	-2.59	4.75	-1.53	-1.7	-2.44
F	-1.78	-2.29	4.27	-1.95	-1.65	-3.4
G	-1.74	-2.64	4.93	-2.34	-2.17	-3.96
H	-2.47	-2.05	3.88	-2.17	-1.33	-4.14
I	-1.55	-3.26	5.96	-2.05	-2.59	-3.49
J	-1.98	-3.72	6.67	-2.02	-2.47	-3.52
K	-2.33	-2.38	4.51	-2.28	-1.55	-4.03
L	-2.58	-2.24	4.28	-2.41	-1.45	-4.39
M	-2.38	-2.21	4.27	-2.53	-1.69	-4.54
N	-1.76	-2.48	4.65	-2.02	-1.65	-3.27
O	-1.88	-1.87	3.61	-1.97	-1.5	-3.61
P	-1.74	-1.85	3.59	-2.08	-1.72	-3.8
Q	-1.3	-2.26	4.22	-1.67	-1.69	-2.7
R	-2.79	-2.02	3.83	-2.11	-1.18	-4.28
S	-2.2	-1.88	3.59	-1.99	-1.4	-3.87
T	-2.33	-3.09	5.79	-2.58	-2.13	-4.34
U	-1.94	-1.87	3.6	-1.94	-1.43	-3.58
V	-2.66	-2.25	4.3	-2.38	-1.39	-4.37
W	-1.29	-1.59	3.1	-1.68	-1.65	-3.11
X	-1.62	-2.5	4.73	-2.11	-2.12	-3.63
Y	-1.37	-2.24	4.27	-1.87	-1.7	-2.92

Table 16: Computed thermochemistry parameters at aug-cc-pVDZ.

	ΔG (kcal/mol)	ΔH (kcal/mol)	ΔS (Kcal/mol/K)
A	5.56	-1.32	-0.02
B	4.95	-1.35	-0.02
C	5.24	-1.42	-0.02
D	5.28	-1.70	-0.02
E	5.41	-1.38	-0.02
F	5.09	-1.76	-0.02
G	5.26	-1.64	-0.02
H	4.77	-1.92	-0.02
I	5.43	-2.16	-0.02
J	5.20	-2.51	-0.03
K	4.80	-2.19	-0.02
L	5.00	-2.05	-0.02
M	4.49	-1.92	-0.02
N	5.19	-1.82	-0.02
O	5.12	-1.53	-0.02
P	4.89	-1.45	-0.02
Q	5.21	-1.48	-0.02
R	4.37	-2.19	-0.02
S	4.73	-1.75	-0.02
T	5.08	-2.30	-0.02
U	4.95	-1.60	-0.02
V	4.89	-2.11	-0.02
W	5.03	-1.14	-0.02
X	5.25	-1.77	-0.02
Y	4.85	-1.60	-0.02