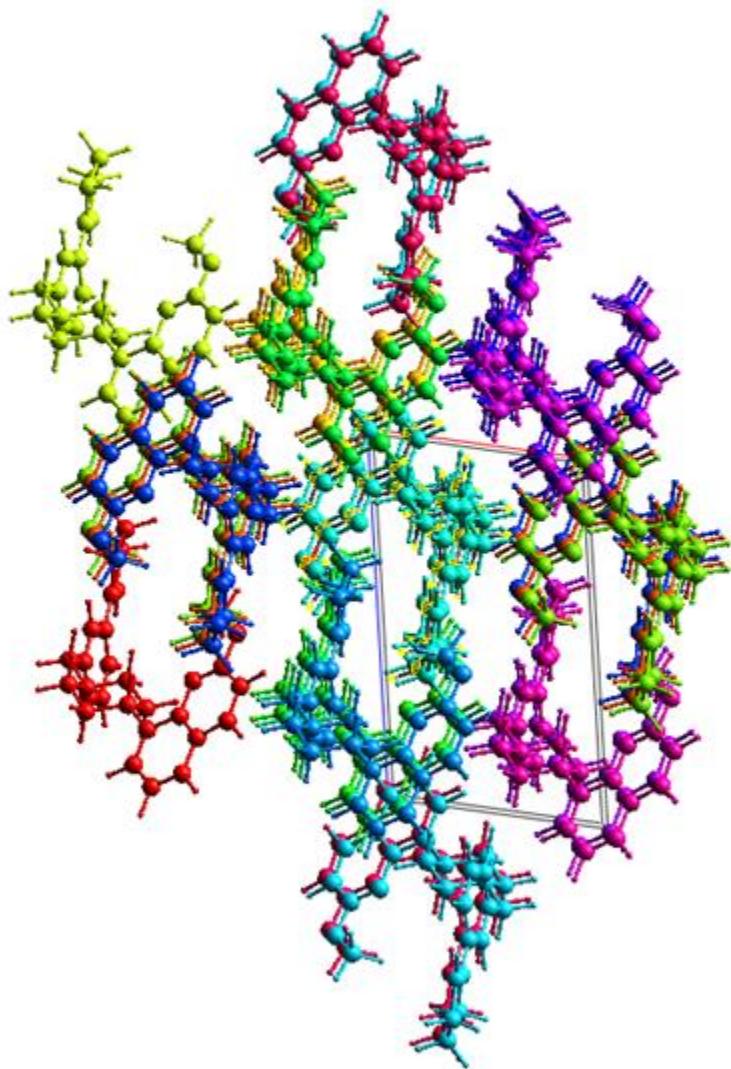


## **Supplementary file S2**

**The colour-coded interaction mappings within a radius of 6 Å of a central reference molecule for compounds (a) I, (b) II and (c) III, are given below.**

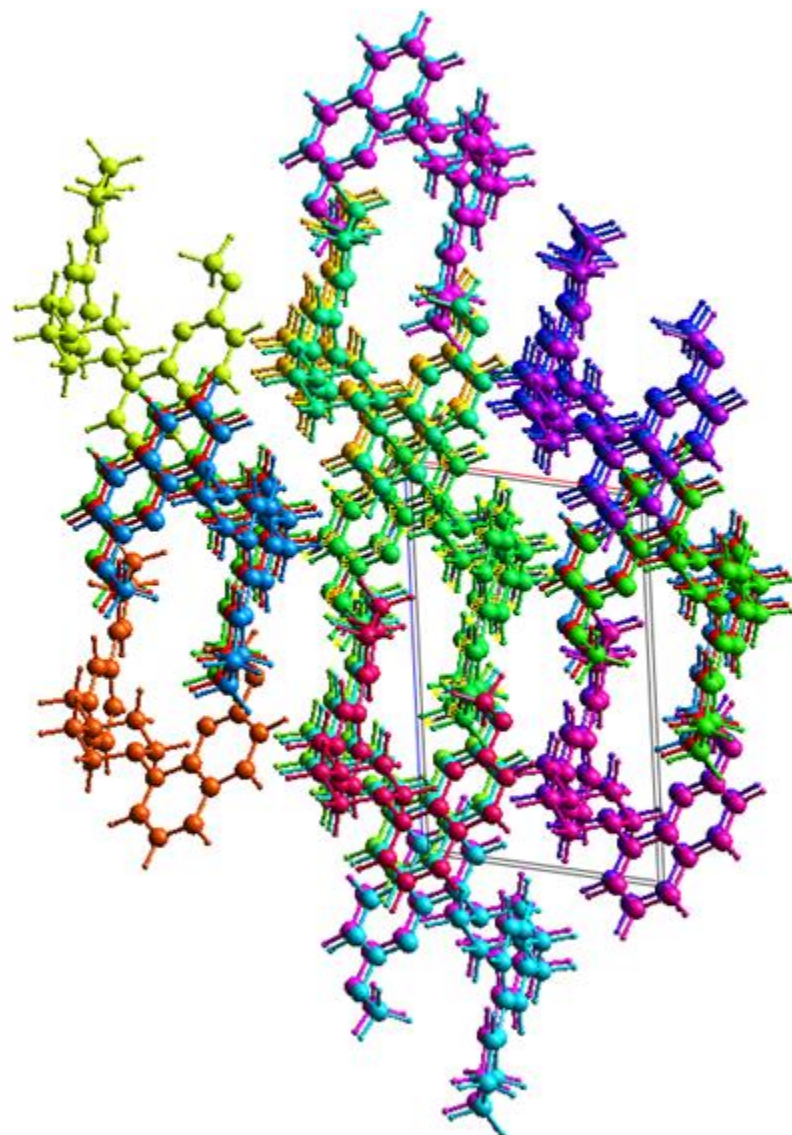
**Full details of the various contributions to the total energy ( $E_{\text{tot}}$ ) are also given.**

(a) I



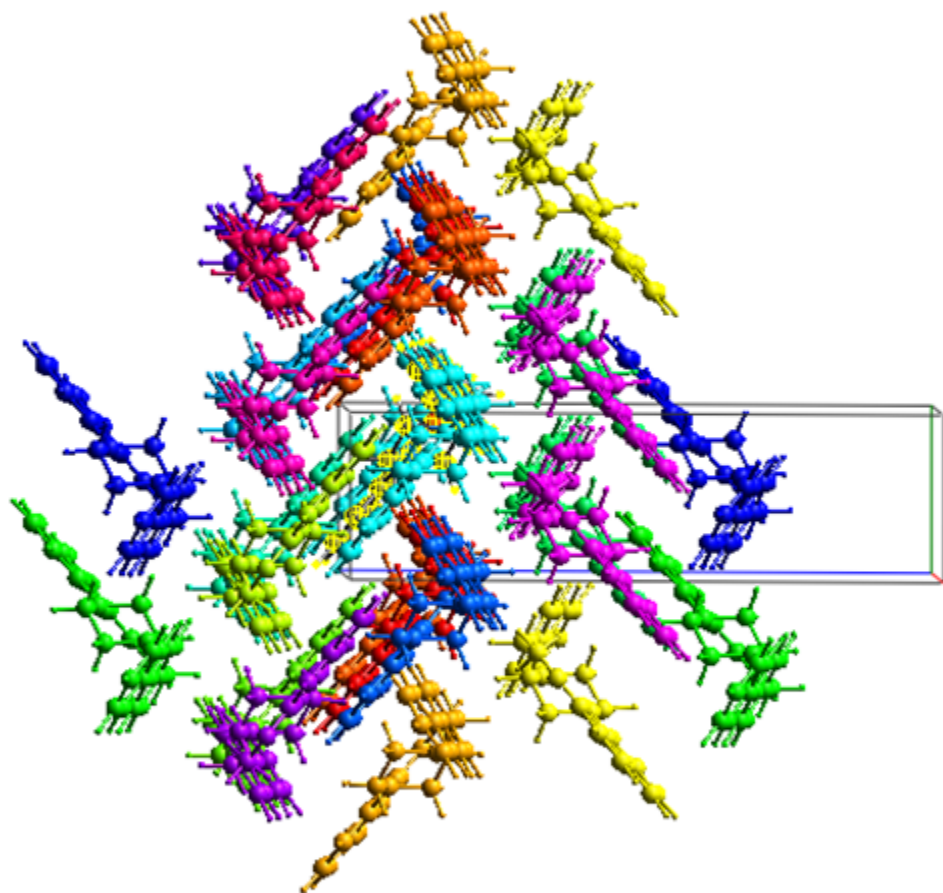
	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-x, -y, -z	11.24	HF/3-21G	-1.1	-0.2	-4.2	0.5	-4.6
	2	x, y, z	7.71	HF/3-21G	-3.2	-0.7	-30.6	12.9	-20.8
	1	-x, -y, -z	15.76	HF/3-21G	-6.6	-1.2	-16.3	7.4	-16.2
	1	-x, -y, -z	7.74	HF/3-21G	-2.7	-3.1	-53.2	20.4	-36.1
	1	-x, -y, -z	19.71	HF/3-21G	0.6	-0.0	-0.5	0.0	0.1
	2	x, y, z	14.50	HF/3-21G	-7.4	-2.2	-19.4	9.4	-18.9
	1	-x, -y, -z	6.88	HF/3-21G	-5.4	-1.8	-45.5	18.6	-32.7
	1	-x, -y, -z	11.23	HF/3-21G	-0.2	-0.0	-1.5	0.0	-1.6
	1	-x, -y, -z	10.79	HF/3-21G	-8.3	-2.7	-56.5	22.0	-43.3
	2	x, y, z	11.28	HF/3-21G	-4.9	-1.8	-38.1	15.5	-27.9
	2	x, y, z	17.27	HF/3-21G	0.0	-0.2	-5.6	2.7	-2.9
	1	-x, -y, -z	20.98	HF/3-21G	0.1	-0.0	-0.6	0.0	-0.5
	2	x, y, z	12.78	HF/3-21G	0.1	-0.0	-0.9	0.0	-0.7
	1	-x, -y, -z	7.87	HF/3-21G	-17.1	-4.1	-64.7	34.9	-50.1
	1	-x, -y, -z	15.07	HF/3-21G	0.1	-0.0	-1.3	0.0	-1.1
	1	-x, -y, -z	9.33	HF/3-21G	0.3	-0.0	-2.9	0.0	-2.3
	1	-x, -y, -z	12.31	HF/3-21G	-0.8	-0.1	-5.3	0.3	-5.3
	1	-x, -y, -z	13.41	HF/3-21G	-5.9	-1.9	-39.4	12.1	-32.9
	2	x, y, z	12.95	HF/3-21G	-0.2	-0.0	-0.8	0.0	-0.9

(b) II



	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x, y, z	7.91	HF/3-21G	-4.2	-0.9	-30.8	14.2	-21.1
	1	-x, -y, -z	11.36	HF/3-21G	-1.1	-0.1	-3.6	0.3	-4.2
	1	-x, -y, -z	15.47	HF/3-21G	-7.5	-1.4	-18.1	10.0	-16.7
	1	-x, -y, -z	7.66	HF/3-21G	-5.6	-3.1	-57.6	23.3	-40.8
	1	-x, -y, -z	19.58	HF/3-21G	0.6	-0.0	-0.5	0.0	0.1
	1	-x, -y, -z	6.81	HF/3-21G	-7.1	-2.4	-47.7	20.5	-35.1
	2	x, y, z	14.32	HF/3-21G	-6.6	-2.0	-18.4	8.5	-17.7
	2	x, y, z	10.91	HF/3-21G	-9.7	-3.3	-39.2	16.7	-33.8
	1	-x, -y, -z	10.76	HF/3-21G	-0.3	-0.0	-1.7	0.0	-1.8
	1	-x, -y, -z	10.81	HF/3-21G	-7.3	-2.4	-54.1	19.0	-42.3
	2	x, y, z	17.28	HF/3-21G	0.1	-0.2	-5.7	2.8	-2.9
	2	x, y, z	12.58	HF/3-21G	0.1	-0.0	-0.9	0.0	-0.7
	1	-x, -y, -z	7.96	HF/3-21G	-14.7	-2.9	-58.0	32.1	-43.1
	1	-x, -y, -z	14.85	HF/3-21G	-0.3	-0.0	-1.3	0.0	-1.5
	1	-x, -y, -z	9.43	HF/3-21G	0.3	-0.1	-3.0	0.0	-2.5
	1	-x, -y, -z	12.00	HF/3-21G	-0.8	-0.1	-5.5	0.4	-5.5
	2	x, y, z	12.89	HF/3-21G	-0.2	-0.0	-0.8	0.0	-1.0
	1	-x, -y, -z	13.53	HF/3-21G	-4.7	-1.6	-33.5	7.4	-29.9
	1	-x, -y, -z	20.62	HF/3-21G	0.1	-0.0	-0.7	0.0	-0.6

(c) III



	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x, y, z	5.69	HF/3-21G	-8.0	-4.0	-68.9	26.3	-51.5
	2	x, y, z	19.84	HF/3-21G	0.7	-0.5	-8.2	3.2	-4.4
	2	x, y, z	22.16	HF/3-21G	0.2	-0.0	-0.3	0.0	-0.0
	2	-x+1/2, y+1/2, -z+1/2	11.54	HF/3-21G	-0.6	-0.0	-1.7	0.0	-2.2
	1	-x, -y, -z	6.19	HF/3-21G	-16.0	-5.6	-72.4	36.8	-55.3
	1	-x, -y, -z	21.36	HF/3-21G	0.5	-0.0	-0.4	0.0	0.2
	2	x+1/2, -y+1/2, z+1/2	17.54	HF/3-21G	-0.0	-0.0	-0.6	0.0	-0.5
	2	-x+1/2, y+1/2, -z+1/2	8.27	HF/3-21G	-4.6	-2.1	-44.4	20.4	-29.5
	1	-x, -y, -z	19.49	HF/3-21G	-0.3	-0.1	-1.8	0.0	-1.9
	2	x, y, z	19.01	HF/3-21G	-7.2	-1.8	-9.8	6.1	-12.4
	1	-x, -y, -z	5.16	HF/3-21G	-3.9	-4.5	-69.9	29.9	-45.7
	2	x, y, z	19.84	HF/3-21G	0.1	-0.0	-0.4	0.0	-0.3
	2	x+1/2, -y+1/2, z+1/2	11.87	HF/3-21G	0.2	-0.0	-1.0	0.0	-0.7
	1	-x, -y, -z	8.93	HF/3-21G	-1.5	-0.1	-3.1	0.0	-4.3
	1	-x, -y, -z	10.71	HF/3-21G	-0.5	-0.0	-2.0	0.0	-2.4
	2	-x+1/2, y+1/2, -z+1/2	14.53	HF/3-21G	-6.1	-2.5	-31.3	12.3	-26.1
	1	-x, -y, -z	20.20	HF/3-21G	-0.7	-0.1	-1.4	0.0	-2.0
	1	-x, -y, -z	21.47	HF/3-21G	0.3	-0.0	-0.9	0.0	-0.6