

**Table 1** Interaction energies of respective dimers in kJ/mol. Symmetry codes are defined in the legend to Figure 5. In the first column the respective Cg-Cg distances and the numbers of F..F < 2.94 Å contacts (N) within a dimer are given. When calculated, the dispersion contributions to the interaction energy are given after slashes, avTZ= aug-cc-pvTZ, TZVPP= def2-TZVPP.

	Cg-Cg/ N	B3LYP/ avTZ	PBE0/ avTZ	PBE0-D2/ avTZ	b97d/ TZVPP	TPSSH- D3/ TZVPP	M062X/ avTZ	SCS- MP2/ avTZ
M-M <sup>iv</sup>	5.11/2	0.79	-3.51	-17.11/-	-21.88/-	-15.94/-	-12.93	-21.92
				13.60	28.37	12.01		
M-M <sup>ix</sup> , M-M <sup>x</sup>	5.714/3	3.56	-0.38	-13.31/-	-16.23/-	-8.54/-	-10.71	-16.65
				12.93	26.94	11.55		
M-M <sup>v</sup> ,M-M <sup>vii</sup>	6.674/2	3.60	0.79	-7.07/-	-8.95/-	-4.23/-	-5.23	-8.58
				7.87	16.36	6.74		
M-M <sup>i</sup> ,M-M <sup>viii</sup>	6.93/2	2.30	-0.08	-6.15/-	-7.91/-	-5.23/-	-3.89	-7.70
				6.07	12.76	3.89		
M-M <sup>ii</sup> ,M-M <sup>vi</sup>	7.095/2	2.30	0.21	-6.23/-	-7.74/-	-4.27/-	-3.51	-7.61
				6.44	13.43	5.69		
M-M <sup>iii</sup>	7.782/1	0.63	-0.84	-4.48/-	-6.61/-	-4.10/-	-2.80	-5.73
				3.64	7.57	3.39		
M-M <sup>xii</sup> ,M-M <sup>xii</sup>	7.247/0	0.38	-1.17	-5.40/-	-8.49/-	-5.23/-	-3.31	-6.82
				4.23	8.74	3.89		