Table S1. Energy of dimer (AB) and each monomer (A, B), basis-set superposition error [a.u.] and interaction energy [kcal/mol].

Refcode	atoms	E(AB)	E(A)	E(B)	BSSE	E_{int}
CIWMEA10	O6···N3	–1569.8682564	–784.9308300	–784.9300827	0.0070633	–4.61
CUGCOW	O4···N1	–3474.5707741	–1737.2791733	–1737.2787861	0.0236098	–8.04
DEMSOD	O4···N2	–1736.4105624	–868.2032067	–868.2020766	0.0053334	–3.31
FIHLOY	O1(2)···N2	–1357.6044369	–678.7971005	–678.7968975	0.0144598	–6.55
FIHLOY	O5(6)···N4	–1357.8773625	–678.9336798	–678.9338929	0.0148791	–6.14
FINMAQ	O3···N1	–2524.2890052	–1262.1314832	–1262.1476164	0.0117629	–6.22
FINMAQ	O5···N2	–2524.2637981	–1262.1291333	–1262.1279284	0.0060992	–4.23
HOPKON	O1···N6	–1001.8230685	–500.9078902	–500.9046596	0.0079716	–6.60
HOPKUT	O4···N9	–923.4612149	–461.7119126	–461.7460576	0.0067248	–2.04
CCDC-875783	O1A···N2A	–1980.3483101	–990.1692187	–990.1708717	0.0063036	–5.16
CCDC-875783	O2A···N2A	–1980.3489804	–990.1713764	–990.1695165	0.0071061	–5.07