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Supramolecular salts assemblied by melamine and two organic hydroxyl acids: synthesis, structure, hydrogen bonds and luminescent property

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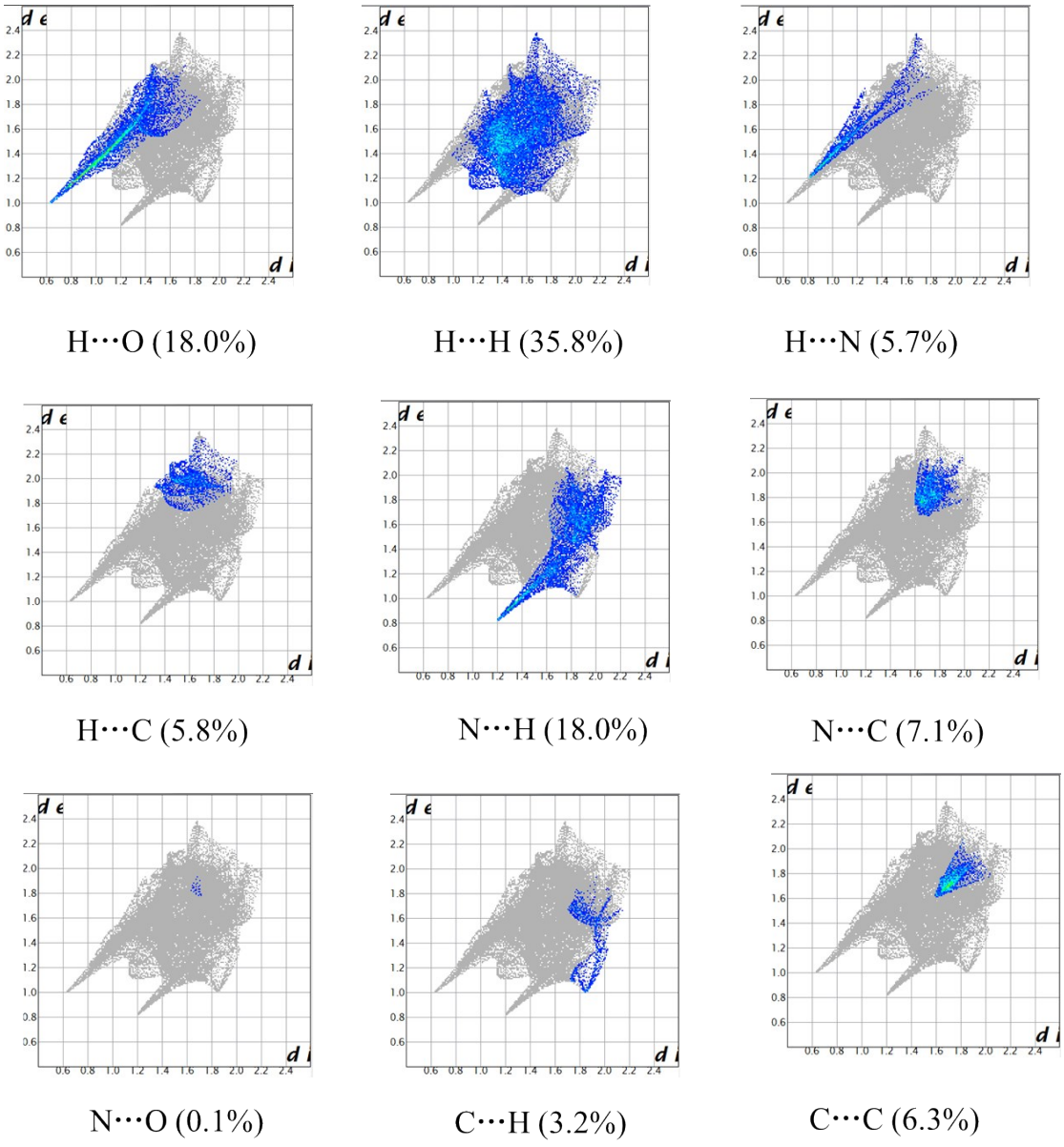

Fig S1. 2D fingerprint distribution of supramolecular salt I.

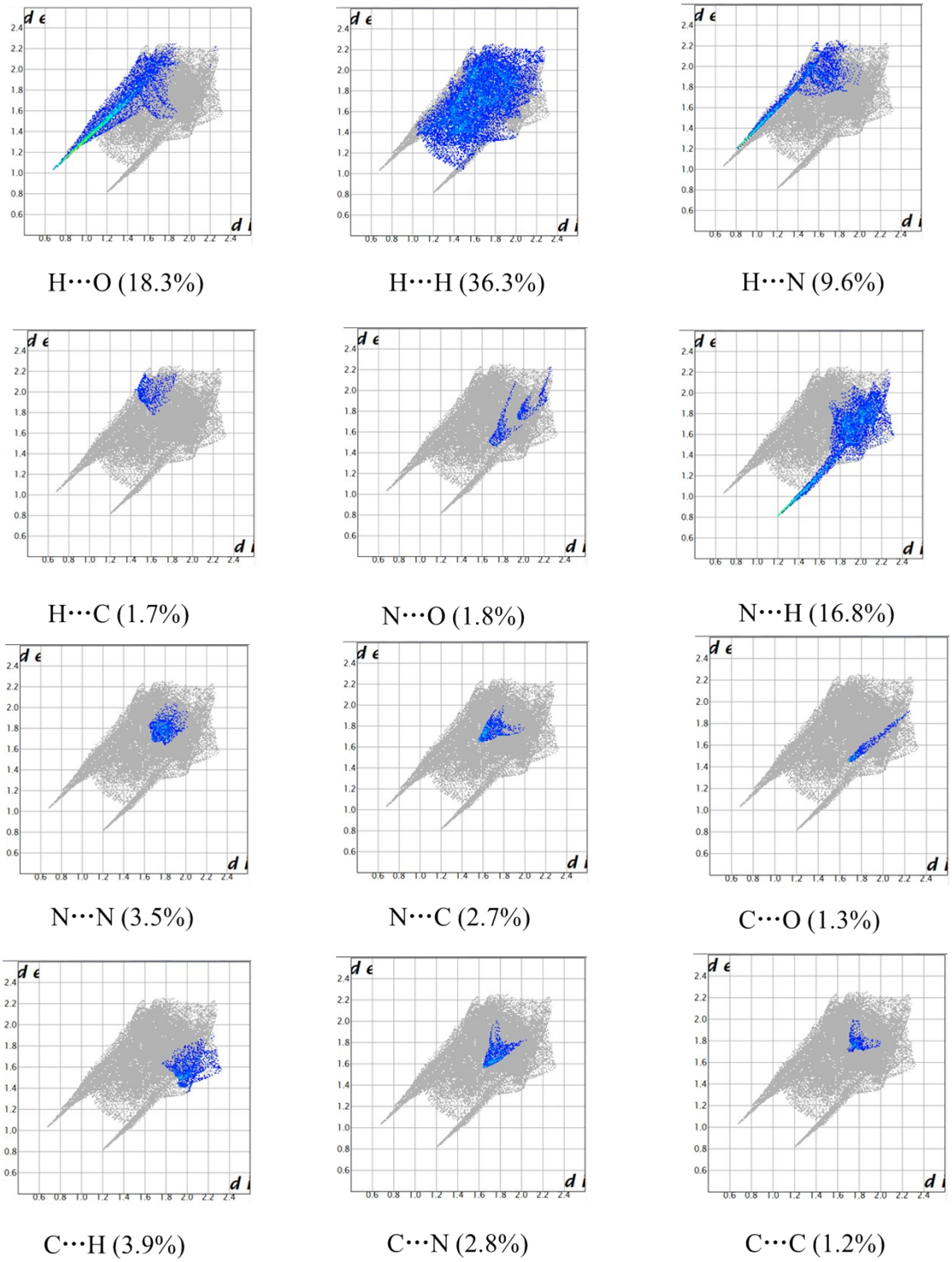

Fig S2. 2D fingerprint distribution of supramolecular salt II.

Table S1. Geometrical parameters (Bond length) and QTAIM topological parameters for bonds of interacting atoms in compound I; electron density (ρ), Laplacian electron density ($\nabla^2\rho$), electron kinetic energy density (G), electron potential energy density (V), total electron energy density (H) at bond critical point (BCP) and estimated energy of hydrogen bond (E_{HB}).

Bond type	Bond length(Å)	ρ (a.u.)	$\nabla^2\rho$ (a.u.)	G (a.u.)	V (a.u.)	H (a.u.)	E_{HB} (kJ·mol^{-1})
Structure 1							
O_3-H_3···O_2	2.606	0.008	0.029	0.006	-0.004	0.001	-5.595
N_1-H_{1B}···O_2	2.081	0.019	0.077	0.016	-0.014	0.003	-17.865
N_3-H_{3B}···O_1	1.761	0.041	0.161	0.040	-0.040	0.000	-52.987
N_6-H_{6B}···O_4	2.003	0.021	0.086	0.019	-0.015	0.003	-21.601
Structure 2							
N_5-H_{5A}···N_2	2.149	0.019	0.072	0.015	-0.012	0.003	-15.915
N_1-H_{1A}···N_4	2.307	0.014	0.047	0.010	-0.008	0.002	-9.934
N_6-H_{6A}···O_3	2.034	0.020	0.085	0.018	-0.015	0.003	-19.162

Table S2. Geometrical parameters (Bond length) and QTAIM topological parameters for bonds of interacting atoms in compound II; electron density (ρ), Laplacian electron density ($\nabla^2\rho$), electron kinetic energy density (G), electron potential energy density (V), total electron energy density (H) at bond critical point (BCP) and estimated energy of hydrogen bond (E_{HB}).

Bond type	Bond length(Å)	ρ (a.u.)	$\nabla^2\rho$ (a.u.)	G (a.u.)	V (a.u.)	H (a.u.)	E_{HB} (kJ·mol^{-1})
O_1-H_1···O_{2i}	1.79	0.036	0.153	0.037	-0.035	0.001	-46.263
O_4-H_{4A}···O_3	1.892	0.028	0.113	0.026	-0.024	0.002	-31.180
N_5-H_{5A}···O_2	1.772	0.040	0.131	0.034	-0.035	-0.001	-46.307
N_6-H_{6B}···O_3	1.951	0.026	0.100	0.022	-0.020	0.003	-26.143
N_1-H_{1B}···O_1	2.066	0.019	0.077	0.016	-0.014	0.003	-17.939
N_6-H_{6A}···N_{4ii}	2.141	0.019	0.071	0.015	-0.012	0.003	-15.887
N_3-H_{3B}···N_{2ii}	2.163	0.018	0.067	0.014	-0.011	0.003	-14.796
N_1-H_{1A}···O_4	2.070	0.018	0.078	0.016	-0.013	0.003	-17.062
O_4-H_{4B}···O_{1ii}	1.98	0.021	0.083	0.018	-0.015	0.003	-19.601