Supporting information

Inorganic Anion Regulates the Phase Transition in Two Organic Cation Salts Containing [(4-Nitroanilinium)(18-crown-6)]+ Supramolecules

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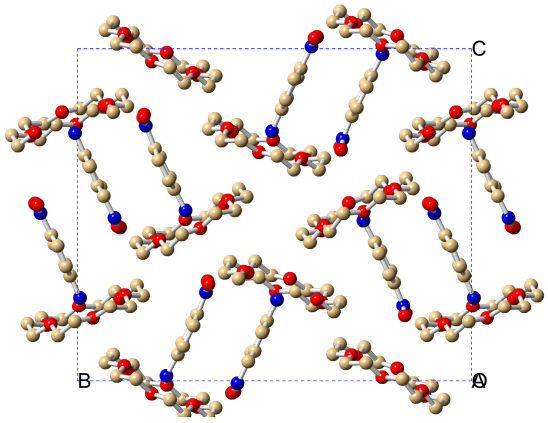

Fig.S1 the arrangement of the supramolecular cations (4-Nitroanilinium)(18-crown-6) of crystal **2** in the *bc* plane.

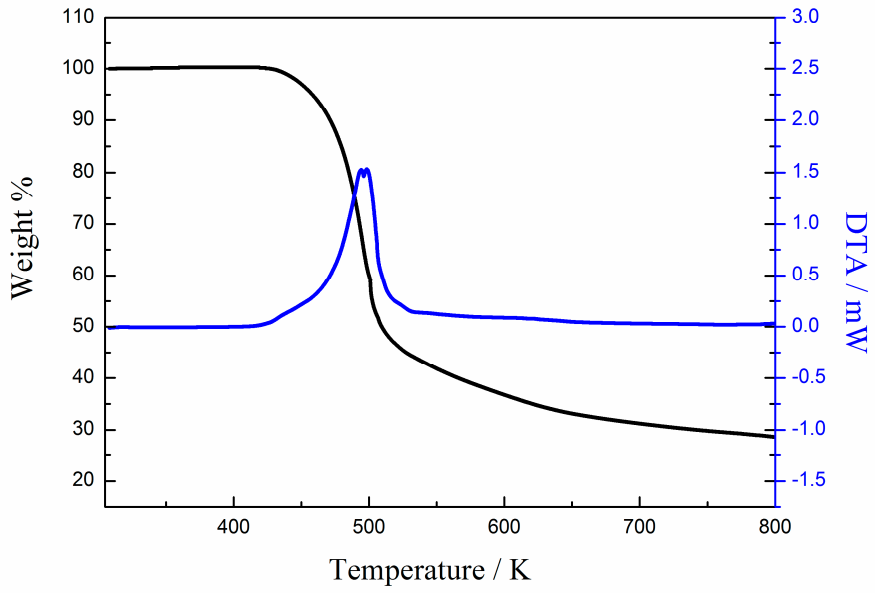

Fig S2. TG and DTA cures for inclusion compound **1**

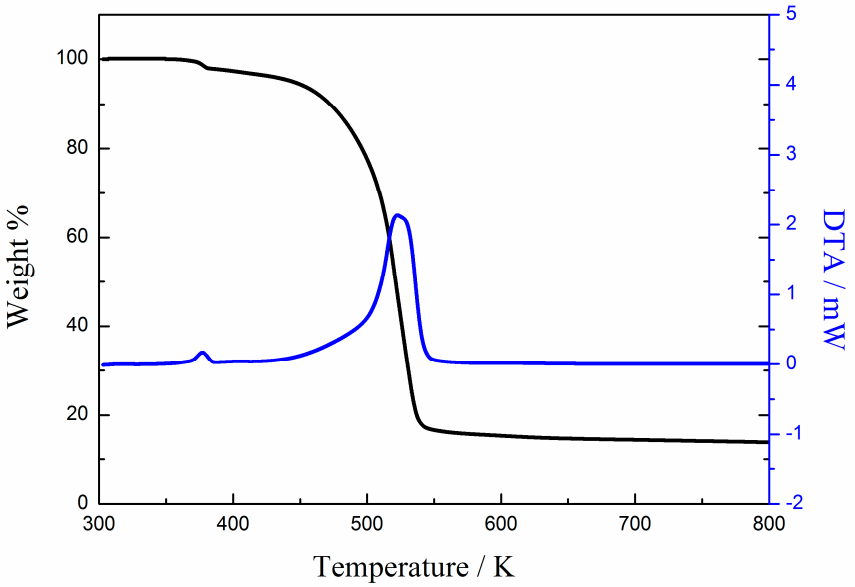

Fig S3. TG and DTA cures for inclusion compound **2**

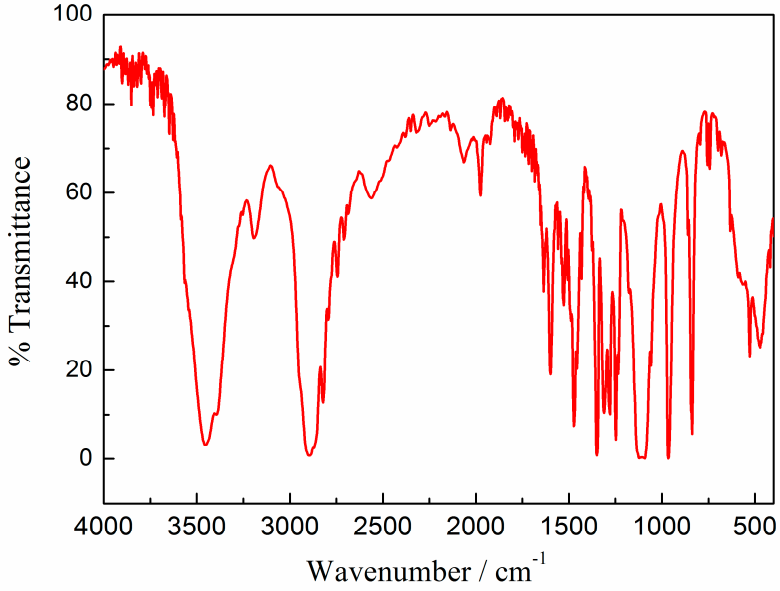

Fig. S4 IR of crystal **1**

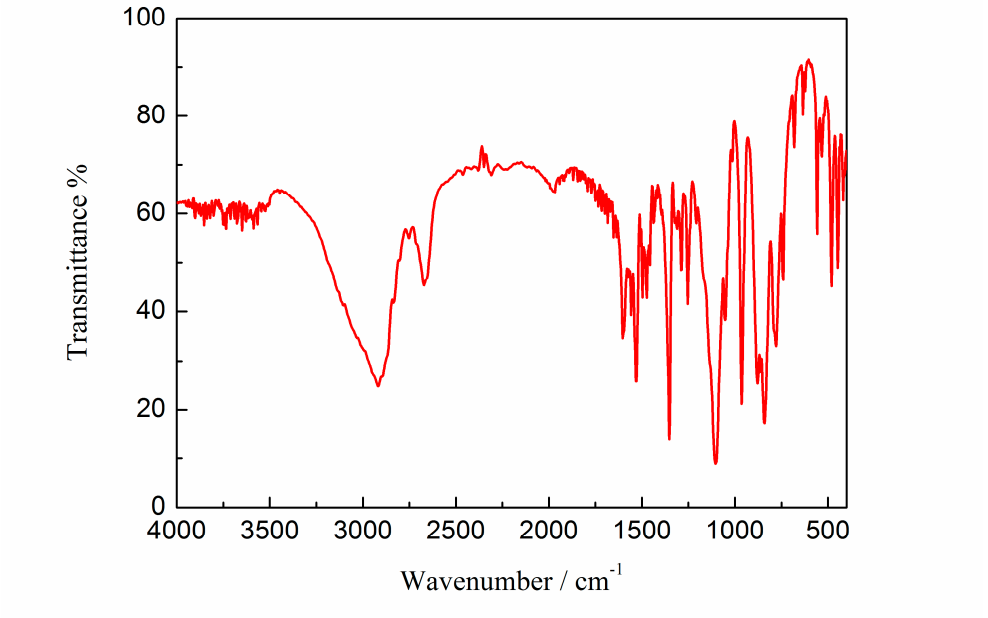

Fig. S5 IR of crystal **2**

Table S1. Hydrogen-bond geometry (Å,°) for complex **1**

D-H···A	D-H(Å)	H···A(Å)	D···A(Å)	D-H···A(°)
		100K		
N_1-H_{1WC}···O_1	0.891	2.480	2.871	107.08
N_1-H_{1WC}···O_2	0.891	2.020	2.903	171.08
N_1-H_{1WB}···O_3	0.923	2.510	2.892	105.24
N_1-H_{1WB}···O_4	0.923	1.935	2.842	167.27
N_1-H_{1WA}···O_5	0.880	2.534	2.912	106.75
N_1-H_{1WA}···O_6	0.880	1.945	2.821	173.97
O_{11}-H_{11C}···O_{10}	0.863	1.785	2.647	175.77
		296K		
N_1-H_{1WC}···O_1	0.848	2.518	2.877	106.52
N_1-H_{1WC}···O_2	0.848	2.024	2.867	172.97
N_1-H_{1WA}···O_3	0.845	2.487	2.927	113.37
N_1-H_{1WA}···O_4	0.845	2.039	2.875	169.73
N_1-H_{1WB}···O_5	0.850	2.562	2.880	103.44
N_1-H_{1WB}···O_6	0.850	2.082	2.907	163.63
O_{11}-H_{11C}···O_{10}	0.842	1.823	2.657	170.13

Table S2. The occupation factor of oxygen atoms in $-NO_2$ group for 296K

Oxygen atom	O_{14A}	O_{14B}	O_{15A}	O_{15B}	O_{16A}	O_{16B}	O_{17A}	O_{17B}
occupation factor	0.612(15)	0.388(15)	0.51(2)	0.49(2)	0.63(2)	0.37(2)	0.68(2)	0.32(2)

Table S3. Hydrogen-bond geometry (Å,°) for complex **2**

D-H···A	D-H(Å)	H···A(Å)	D···A(Å)	D-H···A(°)
		100K		
N_1-H_{1D}···O_7	0.891	2.048	2.867	152.26
N_1-H_{1E}···O_8	0.889	2.284	2.908	127.10
N_1-H_{1E}···O_9	0.889	2.032	2.847	151.87
N_1-H_{1C}···O_{10}	0.890	2.330	2.956	127.40
N_1-H_{1C}···O_{11}	0.890	1.998	2.821	153.24
N_1-H_{1D}···O_{12}	0.891	2.302	2.942	128.66
N_4-H_{4D}···O_1	0.891	2.460	2.920	112.58
N_4-H_{4D}···O_2	0.891	2.030	2.905	167.30
N_4-H_{4C}···O_3	0.891	2.508	2.949	111.18
N_4-H_{4C}···O_4	0.891	2.029	2.914	172.42
N_4-H_{4E}···O_5	0.891	2.478	2.906	114.51
N_4-H_{4E}···O_6	0.891	1.975	2.853	168.38
		296K		
N_1-H_{1A}···O_7	0.890	2.038	2.924	173.33
N_1-H_{1A}···O_8	0.890	2.653	2.960	101.35
N_1-H_{1C}···O_9	0.890	2.039	2.916	168.41
N_1-H_{1C}···O_{10}	0.890	2.590	2.913	102.33
N_1-H_{1B}···O_{11}	0.889	1.971	2.851	179.01
N_1-H_{1B}···O_{12}	0.889	2.596	2.953	104.93
N_4-H_{4C}···O_1	0.891	2.347	2.942	124.23
N_4-H_{4A}···O_2	0.890	1.970	2.816	158.02
N_4-H_{4A}···O_3	0.890	2.384	2.966	123.00
N_4-H_{4B}···O_4	0.889	2.034	2.873	156.89
N_4-H_{4B}···O_5	0.889	2.338	2.915	122.67
N_4-H_{4C}···O_6	0.891	2.018	2.867	156.5