**Supporting information**

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

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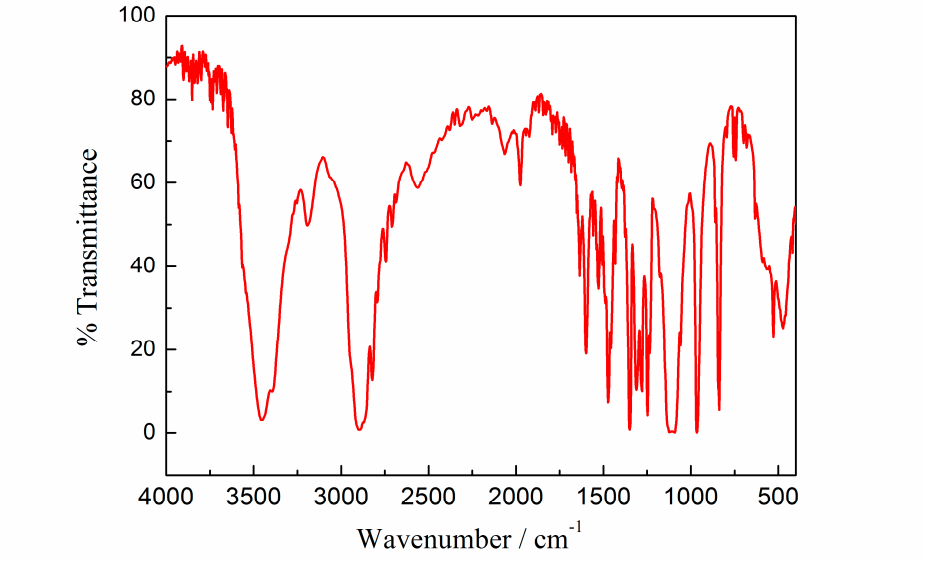


Fig. S1 IR of crystal **1**

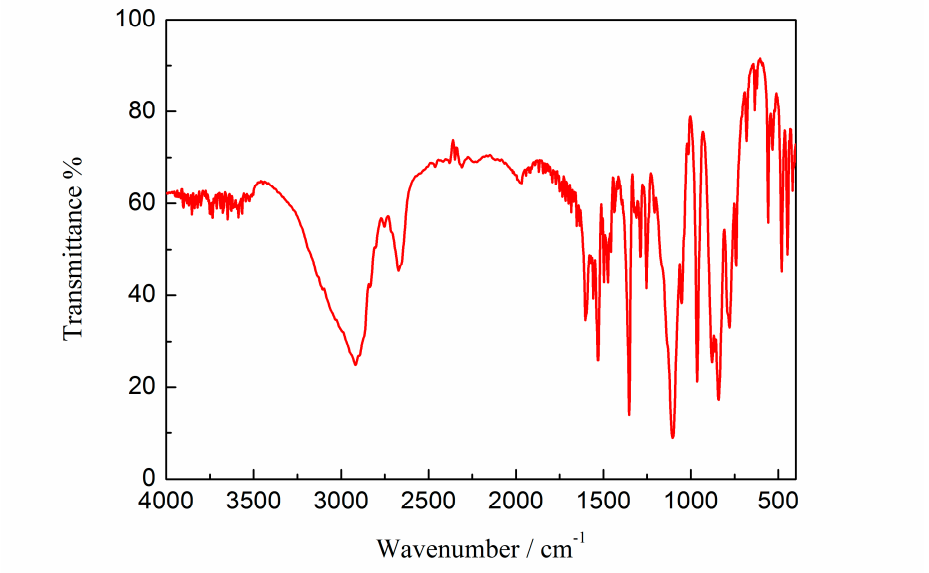


Fig. S2 IR of crystal **2**

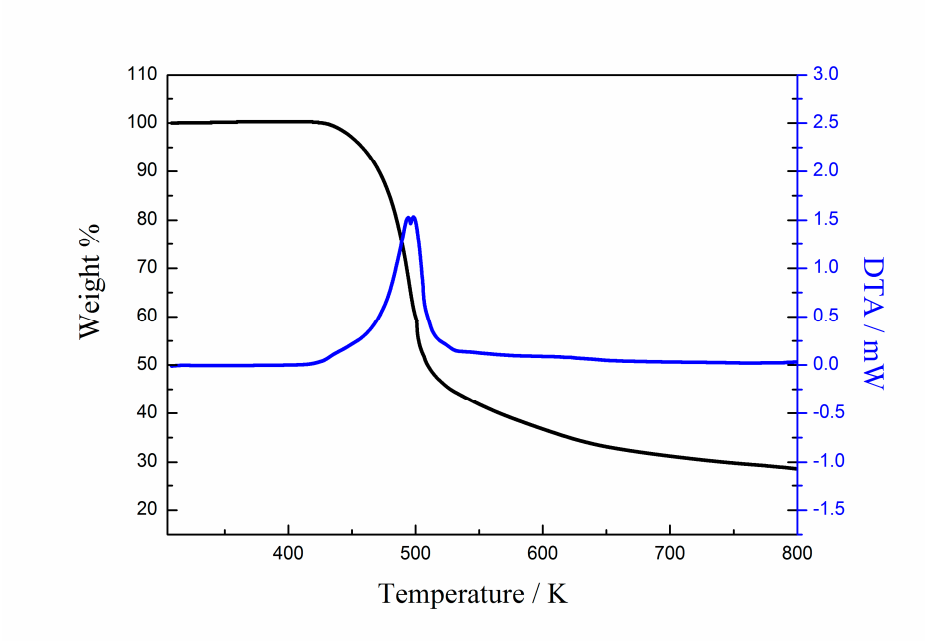


Fig S3. TG and DTA cures for inclusion compound **1**

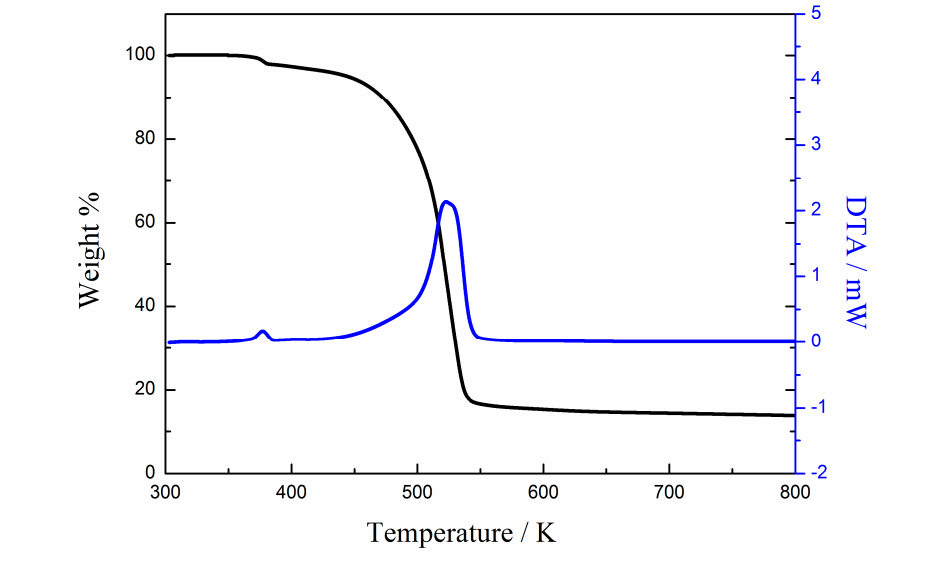


Fig S4. TG and DTA cures for inclusion compound **2**

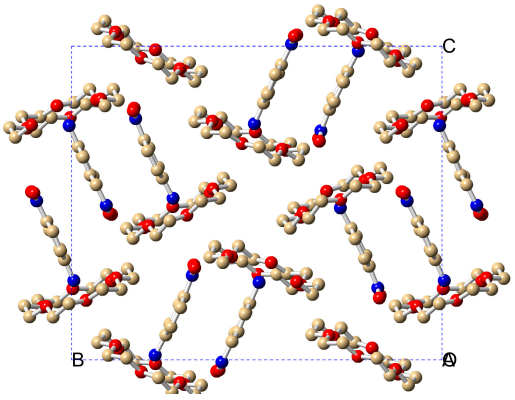


Fig.S5 the arrangement of the supramolecular cations (4-Nitroanilinium)(18-crown-6) of crystal **2** in the *bc* plane.

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. 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 |