

**Structural Phase Transition in Paramagnetic Molecular Conductors
 β'' -(BEDT-TTF)₄(H₃O)[Fe(C₂O₄)₃]·G with different guest solvent molecules G**

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X-ray diffraction studies of the isostructural series of conducting radical cation salts β'' -(BEDT-TTF)₄(H₃O⁺)[Fe(C₂O₄)₃]·G, where G is a guest solvent molecule: PhCl (**1**), [(PhCl)_{0.66}(PhCN)_{0.34}] (**2**), PhBr (**3**), [(PhBr)_x(PhCN)_{1-x}] (**4**) and PhF(**5**), have revealed the presence of a structural phase transition to a lower symmetry around 240-250 K in the salts **1-4**. For instance, the unit cell parameters for the crystal **2** are: $a = 10.2758(3) \text{ \AA}$, $b = 20.0034(7) \text{ \AA}$, $c = 35.242(1) \text{ \AA}$, $\beta = 93.023(3)^\circ$, $V = 7233.9(3) \text{ \AA}^3$, sp. gr. $C2/c$, $Z = 4$ at 300K, and $a = 10.2413(4) \text{ \AA}$, $b = 11.1675(4) \text{ \AA}$, $c = 35.127(1) \text{ \AA}$, $\alpha = 88.537(3)^\circ$, $\beta = 86.680(3)^\circ$, $\gamma = 62.704(4)^\circ$, $V = 3564.1(2) \text{ \AA}^3$, sp. gr. $P\bar{1}$, $Z=2$ at 150 K. The transition was also confirmed by DC electrical conductivity measurements. Phase transition in the brombenzene derivative has been detected earlier by X-ray diffraction and by the thermal variation of the heat capacity [1], but in this work the unit cell parameters and crystal structure of low temperature phase have not been determined. In our work we report the room temperature monoclinic and the low temperature triclinic crystal structures of the listed compounds, as well as discuss the effect of the transition on their structures and conducting properties. The salt **2** is an organic superconductor with $T_c = 6 \text{ K}$, while superconducting transitions were not observed in the case of the **1** and **3-5** salts.

[1] E. Coronado, S. Curreli, C. Gimenez-Saiz, C.J. Gomez-Garcia. *J. Mater. Chem.* (2005) 15, 1429.