Poster Presentation

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The phase transition in bis(methyl(2-phenylethyl)ammonium) tetrabromidocuprate(II)

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Bis(methyl(2-phenylethyl)ammonium) tetrachloridocuprate(II) is a well-known thermochromic compound that exhibits an abrupt color change (from green to yellow) at 353 K that is caused by a change in coordination geometry from square planar to flattened tetrahedral [1]. As part of a reinvestigation of established thermochromic chloridocuprate(II) and their related compounds, the bromide analog [bis(methyl(2-phenylethyl)ammonium) tetrabromidocuprate(II)] has been studied anew. The structure redetermination at ambient temperature agrees with the original [2] (CSD refcode: FUTTIX), i.e. alternating layers of flattened tetrahedral tetrabromidocuprate(II) complexes and of organic cations stacked along the a-axis of the monoclinic C2/c unit cell. A DSC scan from ambient temperature to 183 K reveals an exothermic peak (and corresponding endothermic peak upon heating) at 215 K. Single crystal structures, determined from ambient temperature to 120 K in steps of ~20 K, track a steady increase in b-axis length on cooling to the transition temperature. Across the transition temperature abrupt 1.1% and 0.74% increases in lengths of the b- and c-axes, respectively. and a 0.23% decrease in the a-axis length are observed with no change in space group. Slight changes of the organic cation phenyl group conformation are observed across the transition temperature that cause the organic layer to spread out and become thinner so that neighbouring layers are stacked more closely together along a. However, the flattened tetrahedral geometry of the tetrabromidocuprate(II) complex remains essentially unchanged across the transition.

[1] *Harlow, R. L., Wells, W. J., Watt, G. W., et al., Inorg. Chem., 1974, 13, 2106-2111.,* ***[2]*** *Place, H., Willett, R. D., Acta Cryst., 1988, C44, 34-38.*

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