Bis(S-(-)-1-phenylethylammonium) tetrabromidocuprate(II): another step in the sequential breakdown of the A2CuX4 layer perovskite structure

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The A2CuX4 layer perovskite structure is well represented in halidocuprates in which monopositive A cations form bilayers with ammonium head groups directed outward into interleaving layers of corner-sharing Cu(X4/2)X2 octahedra (X = Cl or Br). In these structures the A cations typically are protonated primary amines or anilines that have a narrow enough cross section to pack together in a bilayer without disrupting the 2-D inorganic structure. Our laboratory has previously reported (Bond & Nalla ACA Annual Meeting (2013) abstract T-52) the structures of bis(4-chloro-2,6-dimethylanilinium)- and bis((R,S)-1-phenylethylammonium)-tetrachloridocuprate(II) in which the bulkier A cations now force the 2-D inorganic structure to break apart into 1-D chains or 0-D complexes, respectively, while still maintaining the organic bilayer. The title structure consists of 0-D CuBr42-complexes that, by virtue of their larger size, force the organic bilayer to spread out and lead to its partial collapse. In contrast to both the racemic and enantiomeric bis(1-phenylethylammonium) structures (the latter of which is also presented) which both crystallize in polar space groups (orthorhombic Aea2 and monoclinic C2, respectively) with one symmetrically unique organic cation, the title structure crystallizes in orthorhombic P212121 with two symmetrically inequivalent organic cations. The sequential breakdown of the aristotype K2NIF4 2-D structure (I4/mmm) to these 1- and 0-D structures is followed through descent of symmetry.

Figure 1