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Abstracts



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Supramolecular Structure of 1,10-Phenanthrolin-1-ium Cation with a Tin(IV) Anion

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Single crystals of the 1,10-phenanthrolin-1-ium salt of the complex monocation, [SnCl₂(CH₂CO₂H)(CH₂CO₂H)(CH₂CO₂)] was investigated as part of a study of pseudo symmetric structures. The six coordinate tin exhibits pseudo octahedral coordination by two *cis* Cl atoms, two *trans* C atoms, and two O atoms *trans* to the Cl atoms. One proton has been transferred from the originally neutral tin dicarboxylic acid complex to form the complex anion and a phenanthrolin-1-ium monocation. The Sn-O distances for the chemically distinct oxygen atoms of the five member chelate rings of the carboxylate and carboxylic acid groups thus formed differ by more than 0.2 Å (2.306(2) and 2.519(2) Å) leading to large differences in the Cl atoms coordinated *trans* to the two O atoms (Sn-Cl distances are 2.404(1) and 2.486(1) Å).

One nitrogen atom of the 1,10-phenanthrolin-1-ium is protonated (d[N-H] = 0.78 Å) while the other nitrogen is not. Protonation of the N causes the C-N-C angle to increase (122.14° in the protonated ring vs 116.51° in the unprotonated ring). The protonated ring exhibits increased Lewis acidity and links into a network with the anions using an N-H-O (2.688 Å), a C-H-O (3.155 Å), and two C-H-Cl (3.578 and 3.876 Å) bonds. The remaining rings also participate in hydrogen bonding by forming significantly weaker C-H-O and C-H-Cl interactions. These layers are joined into a 3-dimensional network of interactions by two distinct alternating face-to-face $(\pi-\pi)$ interactions along the α axis.