Chiral and Racemic Structures of Tartrate Salts

Terry Threlfall, Thomas Gelbrich, Mike Hursthouse, Susanne Hutt, Eva Seeger

University of Southampton, United Kingdom, University of Leipzig, Germany t.threlfall@soton.ac.uk

As part of a programme to try to understand why molecules pack as they do and why polymorphs form, we are exploring chiral relationships¹. The extent to which racemic compounds and racemic mixtures may have related structures² cannot be answered from existing crystal structure data. For example, in the Cambridge Crystallographic Data Base there are many examples of alkali metal (+) tartrates, but hardly any alkali metal (+/-) tartrates (racemates) structures, so no comparison can be made. We have therefore made sets of closely related compounds to explore these relationships. The crystal structures of the alkali metal mono and ditartrates and mesotartrates plus the ammonium and other amine tartrates have been determined. They show polymorphism, isostructurality sets, mixed crystals and cross seeding phenomena. We have the structure of a lithium tartrate trihydrate which was reported to have disappeared in 1867³. Of particular interest is the relationship between the enantiomers and racemates of the alkali metal hydrogen tartrates. The close similarity of the layer structures raises questions about the mechanism of nucleation and crystal growth⁴, which appear irresolvable within established models of crystal formation.

References

- 1. Gelbrich et al. Z. anorg. Chem. in press
- 2. Jacques, Collet and Wilen, Enantiomers, Racemates and Resolutions, Wiley New York 1981
- 3. Sacchi, Gazz. 1867
- 4. Gervais, Beilles, Cardinael, Petit and Coquerel J. Phys. Chem 2002, 106B, 646-652