crystal X-ray diffraction at 270 K and the unit cell was found to be triclinic instead of orthorhombic, as reported before[1]. Hydrogen L-malate anions form infinite head-to-tail chains via O-H…O interactions and can be used as structural building blocks in solid state crystal engineering. The neutral malic acid molecules establish links between neighbouring chains. Further structural and physical properties characterization of a similar compound, in which potassium is partially substituted by rubidium, is in progress.

[1] Van Havere W.K.L., Deukrskens P.T., Lenstra T.H., Crystall. J., *Spect. Res.*, 1985, **15**, 45.
**Keywords: pyroelectricity, crystal structure analysis, optical activity**

P.09.06.4
Geometric Analysis of Tartrate Coordination Modes from Crystallographic Data
Herman H-Y. Sung, John A.K. Cha, Samadara Thushari, Ian D. Williams, *Department of Chemistry, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China*. E-mail: hermans@ust.hk

Tartaric acid is a small organic molecule [$C_4H_4O_6$] with a bewildering array of ligation (or binding) possibilities to metal centers. We are interested in using these in crystal engineering applications, especially in the formation of chiral solids. We present the results of a geometric analysis of the binding of tartrate to lanthanide metal ions. Using different stereo-chemical configurations R,R-, R,S- or R,R-/S,S- mixtures these can give different 3D arrangements incorporating a wide number of Ln-TAR binding modes. The computed minima for binding can be compared with experimental results and the energetic implications of our findings will be discussed. Finally the μκ notation set used to describe the binding modes will be introduced and explained.
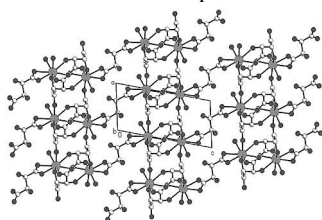
Chiral Network solid [$Er_2(L\text{-}TAR)_3(H_2O)_2$] using μ^4, κ^6 and μ^2, κ^4 binding modes
Keywords: inorganic carboxylates, crystal engineering, chiral compounds

P.09.07.1
Crystal Packing: Molecular Shape and Intermolecular Interactions
Elna Pidcock, W.D. Sam Motherwell, *Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, England*. E-mail: pidcock@ccdc.cam.ac.uk

The Box Model of crystal packing describes unit cells and their contents in terms of "packing patterns".[1] The packing patterns were derived from a consideration of the ways in which boxes of unequal dimensions can be stacked with faces touching and edges aligned. The resulting arrays of boxes have the same total volume but different surface areas. An examination of thousands of experimental structures contained within the Cambridge Structural Database[2] has shown that these packing patterns are a viable description of crystal structures and that molecular dimensions are related to unit cell dimensions in a systematic way. The packing patterns are not populated equally by experimental structures; packing patterns characterised by low surface area and most equal dimensions are preferred. Thus molecular shape appears to be of primary importance in crystal packing.

However, high surface area packing patterns do exist and a possible explanation is that these structures contain strong, "structure-determining" hydrogen bond interactions. Subsets of structures containing strong motifs have been examined within the context of the Box Model. Changes in populations of packing patterns are observed and these changes can be rationalised in terms of the symmetry requirements of the motif. However, the presence of hydrogen bond motifs does not appear to greatly perturb the principal of the Box Model - that minimum surface area is preferred.

[1] Pidcock E., Motherwell W.D.S., *Crystal Growth Des.*, 2004, **4**, 611. [2] Allen F.H. , *Acta Cryst.*, 2002, **B58**, 380.
Keywords: crystal packing, hydrogen bond, databases

P9