Geometric Analysis of Tartrate Coordination Modes from Crystallographic Data

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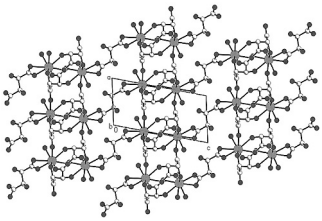
Tartaric acid is a small organic molecule [$C_4H_4O_6$] with a bewildering array of ligation (or binding) possibilities to metal centers. We are interested in using these in crystal engineering applications, especially in the formation of chiral solids. We present the results of a geometric analysis 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-TAR)$_3$(H_2O)$_2$] using μ^4, κ^6 and μ^2, κ^4 binding modes

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