

Microsymposium

MS15.O06

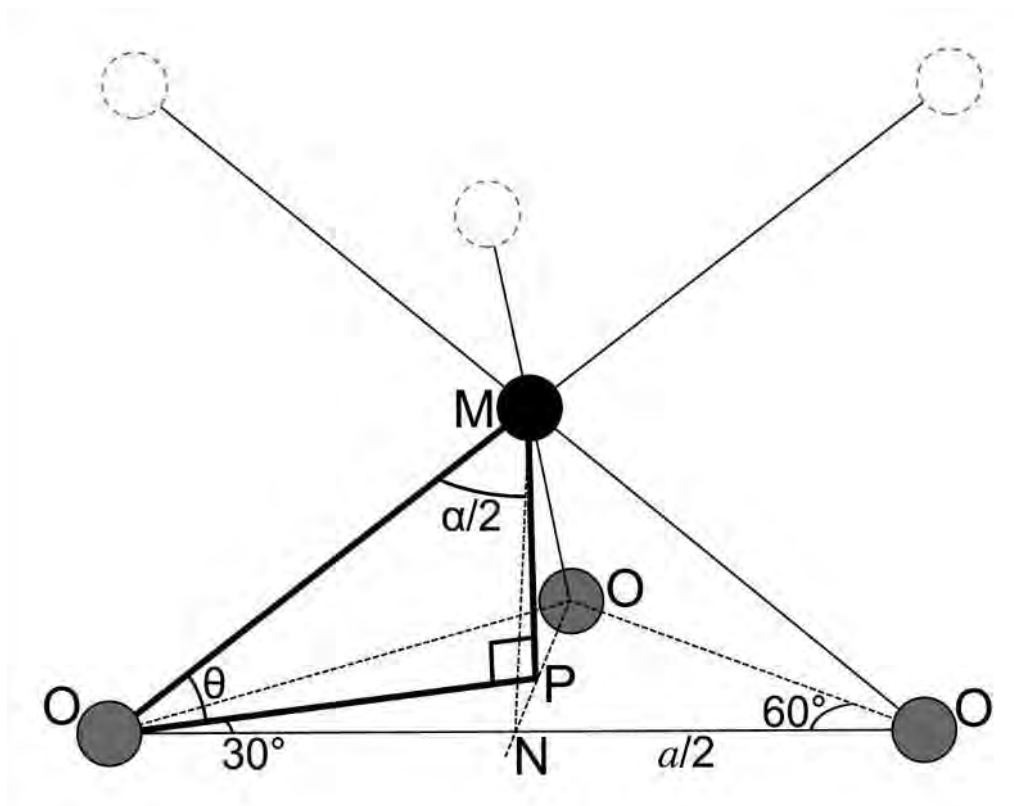
Crystal chemistry of layered single and double hydroxides

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Layered double hydroxides (LDH) are derived from layered single hydroxides by the substitution of a fraction (x) of the divalent metal cations by trivalent cations, with the charge balanced by anions in the space between the main hydroxide layers. LDH phases can have a range of metal cations and interlayer anions and the value of x can vary quite widely. Straightforward crystal-chemical and geometrical reasoning has resulted in new yet fundamental information about these phases [1, 2]. In particular: (1) It is now possible to calculate x from the 'a' parameter of the unit cell or vice versa (whichever is known with the most confidence) for LDH phases that are based on Mg, Ni, Zn or Co; (2) The phase at $x = 0$ is shown to be an alpha form of $M(OH)_2$ rather than the beta polymorph; (3) The extent to which the metal-oxygen octahedra in the main layer of LDH phases are squashed is now known to be independent of the type of the interlayer anions or the type of trivalent ion, which also has no substantial effect on the reduction in layer spacing that occurs as x increases; (4) It is now easy to create reliable structural models for hydrotalcite- and takovite-type LDH phases that have any trivalent ion (or ions) and any value of x ; (5) The ordered distributions of trivalent cations that are possible in LDH phases have been clarified and a plausible explanation provided for the observed variation in the lower solid-solution limit [3]; (6) A reliable model for the crystal structure of beta-Zn(OH)₂.

[1] I.G. Richardson, *Acta Cryst.*, 2013, B69, 150–162., [2] I.G. Richardson, *Acta Cryst.*, 2013, B69, 414–417., [3] I.G. Richardson, *Acta Cryst.*, 2013, B69, 629–633.



Keywords: Layered double hydroxides, Ionic radii, Hexagonal ordered distributions