Charge-density distribution in hydrogen methylphosphonates of calcium and lithium.

Autorzy

Adrian Mermer

Przemysław Starynowicz

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Streszczenie

Two new crystal structures, calcium bis(hydrogen methylphosphonate), Ca(CH(3)PO(3)H)(2), and lithium hydrogen methylphosphonate, Li(CH(3)PO(3)H), have been obtained, and the experimental and theoretical charge densities, as well as their topological properties, are reported. Both compounds display layered structures. Each hydrogen methylphosphonate anion coordinates three metal cations in the calcium compound and four in the lithium one. Weak polarization of oxygen lone pairs is observed, with lithium showing somewhat stronger polarization strength than calcium. The reported topological properties from the density functional theory (DFT) and X-ray approach are consistent with each other. In both structures the P-O bonds have a significant share of ionic character. The hyperconjugation effects within the phosphonate group are quenched upon coordination of the metal cations.

Adres publiczny

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