structure (solids and liquids)

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Refinement of the CsYP2O7 Crystal Structure by the Rietveld Method. — The structure of the title compound, characterized by the powder XRD data, is refined by the Rietveld method. CsYP2O7, prepared from a stoichiometric mixture of Cs2CO3, Y2O3 and (NH4)2HPO4 at 740 °C, crystallizes in the monoclinic space group P21/c with Z = 4. The structure which is isotypic with M(I)M(III)P2O7 (M(I): K, Rb, Cs; M(III): Fe, V, Mo, Ti) consists of layers of M(III)P2O11 units, composed of diphosphate groups linked to M(III)O6 octahedra, forming a three- dimensional framework. The large size of the Cs+ and Y3+ cations has a significant influence on the distortions of the CsO10 and P2O7 polyhedra and thus explains the lower thermal stability of CsYP2O7 as compared to RbYP2O7. — (AKRIM, A.; ZAMBON, D.; METIN, J.; COUSSEINS, J.-C.; C. R. Acad. Sci., Ser. II: Mec., Phys., Chim., Astron. 318 (1994) 10, 1319-1324; Lab. Chim. Solides, Univ. Blaise-Pascal, F-63177 Aubiere, Fr.; FR)