

MS14-05 | THE STRUCTURE OF THE LANTHANUM OXONITRIDOPHOSPHATE La₂₁P₄₀O₄₆N₅₇

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High-pressure metathesis is a successful method for syntheses of intriguing nitridophosphates, e.g. LiNdP₄N₈ or LiPr₂P₄N₇O₃ [1]. The reaction of LiPN₂ and LaCl₃ at either 7 GPa and 750 °C or 9 GPa and 950 °C yields the new oxonitrodophosphate La₂₁P₄₀O₄₆N₅₇ if water is present, e.g. by hydrolysis of LaCl₃ or the used BN crucible. The microcrystalline product was characterized by single-crystal structure determination using microfocussed synchrotron radiation after preselecting suitable crystallites by transmission electron microscopy and electron diffraction. The compound crystallizes in the monoclinic space group $P2_1/n$ with a c lattice parameter of ca. 41.4 Å. Its complicated structure is built up from vertex-sharing P(O,N)₄ tetrahedra forming loop-branched chains with *dreier* ring branches. Lanthanum atoms are embedded between these loops. The chains are built up by *21er* units. These units are interconnected either by vertex- or by edge-sharing tetrahedra; alternatively, the chain can interrupt. These different variants are described by disordered tetrahedra. An additional split position involving La and N/O atoms leads to eight different local structure variants. Tentative structure refinements in lower-symmetric space groups such as Pn , taking into account twinning where appropriate, do not result in ordered models and thus confirm the disorder.

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[1] S. D. Kloß, W. Schnick, *Angew. Chem. Int. Ed.* **2019**, *58*, 2-14.