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The crystal structure of metanatroautunite, $Na[(UO_2)(PO_4)](H_2O)_3$, from the Lake Boga Granite, Victoria, Australia

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Abstract

Metanatroautunite, $Na[(UO_2)(PO_4)](H_2O)_3$, from the Lake Boga granite, Victoria, Australia, has tetragonal symmetry, space group *P*4/*ncc*, with the unit-cell parameters: $a = 6.9935(7)$, $c = 17.5101(12)$ Å, $V = 856.40(13)$ Å^3, and $Z = 4$. The crystal structure has been solved and refined to $R_1 = 0.0398$ for 368 unique reflections [$F > 4\sigma(F)$] and 0.0456 for all 496 unique reflections. Metanatroautunite has an almost identical corrugated polyhedral sheet to meta-autunite-group minerals, consisting of corner-sharing uranyl square pyramids and phosphate tetrahedra. Hydrogen bonds (and cation-oxygen bonds) link the water molecules in the interlayer into square-planar sets, which are connected together creating 8-membered arrays. Metanatroautunite is identical to synthetic $Na[(UO_2)(PO_4)](H_2O)_3$.

Keywords: Meta-autunite, metanatroautunite, uranium, phosphate, Lake Boga, crystal structure