

Copper(II) hydrogenphosphate, CuHPO₄Christiane Günther,^a Helmar Görls^b and Dörte Stachel^{a*}^aOtto-Schott-Institut, Friedrich-Schiller-Universität Jena, Frauenhoferstrasse 6, 07745 Jena, Germany, and ^bInstitute of Inorganic and Analytical Chemistry, Friedrich-Schiller-Universität Jena, August-Bebel-Strasse 2, D-07743 Jena, Germany
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Key indicators: single-crystal X-ray study; $T = 183$ K; mean $\sigma(\text{P}-\text{O}) = 0.004$ Å; R factor = 0.026; wR factor = 0.066; data-to-parameter ratio = 12.6.

The title compound, CuHPO₄, has been synthesized from a mixture of phosphoric acid and copper oxide. It has the same composition as MHPO₄ ($M = \text{Ca}, \text{Ba}, \text{Pb}, \text{Sr}$ or Sn), but adopts a rhombohedral structure with all atoms on general positions. The structure features distorted PO₄ tetrahedra linked by copper, forming 12-membered rings. The Cu^{II} atom is coordinated by five O atoms in a distorted square-pyramidal manner. O—H...O hydrogen bonding leads to an additional stabilization of the structure.

Related literature

For the structure of CaHPO₄, see: Smith *et al.* (1955); MacLennan & Beevers (1955). For a report about BaHPO₄ and PbHPO₄, see: Bengtsson (1941). For the structure of SnHPO₄, see: Berndt & Lamberg (1971). For information about SrHPO₄, see: Boudjada *et al.* (1978). For a report about CuHPO₄·H₂O, see: Boudjada (1980). For information about CuHPO₄·0.5 H₂O see: Sierra *et al.* (2003). For the structure of α -Cu₂P₂O₇, see: Lukaszewicz (1966). For information about β -Cu₂P₂O₇, see: Robertson & Calvo (1968). For a report about Cu₂P₄O₁₂, see: Laügt *et al.* (1972).

Experimental

Crystal data

CuHPO ₄	$Z = 6$
$M_r = 159.52$	Mo $K\alpha$ radiation
Rhombohedral, $R\bar{3}$	$\mu = 6.92$ mm ⁻¹
$a = 9.5145$ (4) Å	$T = 183$ K
$\alpha = 114.678$ (2)°	$0.05 \times 0.03 \times 0.03$ mm
$V = 495.88$ (6) Å ³	

Data collection

Nonius KappaCCD diffractometer	755 independent reflections
Absorption correction: none	654 reflections with $I > 2\sigma(I)$
3338 measured reflections	$R_{\text{int}} = 0.045$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$	60 parameters
$wR(F^2) = 0.066$	All H-atom parameters refined
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.62$ e Å ⁻³
755 reflections	$\Delta\rho_{\text{min}} = -0.66$ e Å ⁻³

Table 1

Selected bond lengths (Å).

Cu1—O1	1.925 (2)	P1—O4	1.515 (2)
Cu1—O4 ⁱ	1.932 (2)	P1—O1	1.530 (2)
Cu1—O3 ⁱⁱ	1.971 (2)	P1—O3	1.541 (2)
Cu1—O3 ⁱⁱⁱ	1.992 (2)	P1—O2	1.571 (2)
Cu1—O4 ^{iv}	2.360 (2)		

Symmetry codes: (i) $z, x - 1, y - 1$; (ii) $-z + 2, -x + 2, -y + 1$; (iii) $-x + 2, -y + 1, -z + 1$; (iv) $y, z, x - 1$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H2...O1 ⁱⁱ	0.87 (5)	1.93 (5)	2.800 (3)	176 (5)

Symmetry code: (ii) $-z + 2, -x + 2, -y + 1$.

Data collection: COLLECT (Nonius, 1998); cell refinement: DENZO (Otwinowski & Minor 1997); data reduction: DENZO; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 2006); software used to prepare material for publication: SHELXL97.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2089).

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