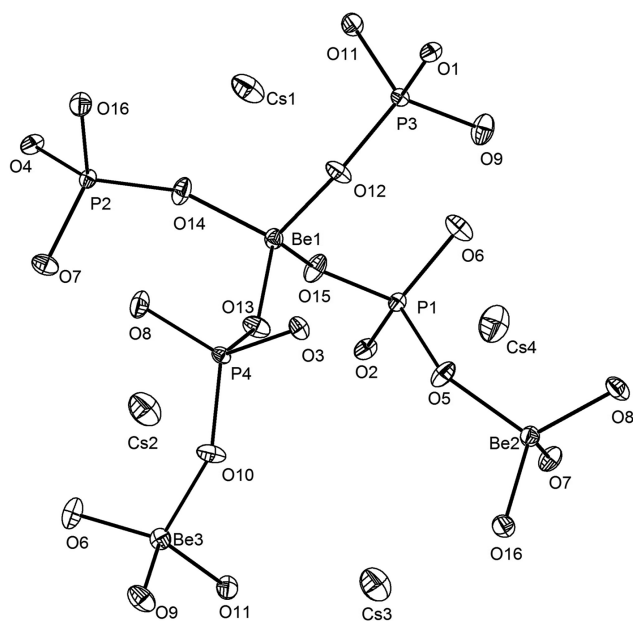


Wang Fang* and Chen Yigang

Crystal structure of cesium beryllophosphate, $\text{Be}_3\text{Cs}_2\text{P}_4\text{O}_{14}$

**Table 1:** Data collection and handling.

Crystal:	Colourless block
Size:	0.28 × 0.15 × 0.10 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	62.2 cm ⁻¹
Diffractometer, scan mode:	Xcalibur Eos Gemini, ω scans
2 θ_{max} , completeness:	56.6°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	44175, 3365, 0.051
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2998
$N(\text{param})_{\text{refined}}$:	221
Programs:	SHELX [1, 2], OLEX2 [3], CryAlis ^{PRO} [4]

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Abstract

$\text{Be}_3\text{Cs}_2\text{P}_4\text{O}_{14}$, orthorhombic, $Pnma$ (no. 62), $a = 15.0612(3)$ Å, $b = 11.0386(2)$ Å, $c = 15.5316(3)$ Å, $V = 2582.19(8)$ Å³, $Z = 8$, $R_{\text{gt}}(F) = 0.0229$, $wR_{\text{ref}}(F^2) = 0.0594$, $T = 293(2)$ K.

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The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of materials

All reagents and solvents employed were commercially available and used as received without further purification. The raw materials BeO (1.5 mmol, 0.037 g), LiF (2 mmol, 0.052 g),

$\text{NH}_4\text{H}_2\text{PO}_4$ (7 mmol, 0.805 g), Cs_2CO_3 (1.5 mmol, 0.489 g), and Y_2O_3 (0.3 mmol, 0.068 g) were ground in an agate mortar, pressed into a pellet, placed in a Pt crucible and preheated in a muffle furnace at 773 K for 10 h to eliminate the water and gas. And then, it was reground thoroughly, placed in a Pt crucible and heated at 1223 K for 20 h to homogenize the solution, and slowly cooled to 873 K at a rate of 3 K · h⁻¹ before the furnace was turned off. Colorless block crystals were then obtained.

Comment

Beryllium phosphate crystals have attracted intensive attention ascribed to many important applications such as laser hosts, phosphors, electrode materials, birefringent optics and nonlinear optical materials [5–8]. Different from structural diversity of borates [9–12], beryllium phosphates only possess the PO_4 or BeO_4 tetrahedra having more opportunities to form ordered arrangements such as infinite chains, rings, and isolated clusters [13]. However, there has been little research in the combination of the PO_4 and BeO_4 tetrahedra. Hence, preparation and study of new beryllophosphate compounds are interesting to crystal chemistry and materials science.

The title compound crystallizes in an orthorhombic space group and its asymmetric unit contains two Cs atoms, four P atoms, three Be atoms, and fourteen O atoms. It features a novel $[\text{Be}_3\text{P}_4\text{O}_{14}]^{2-}$ three-dimensional network composed of the PO_4 and BeO_4 tetrahedra with the P–O and Be–O bond lengths of 1.496(18)–1.617(11) Å and 1.602(4)–1.637(4) Å, respectively. The structure along the b axis can be viewed as a

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Cs1	0.64319(2)	0.2500	1.01594(2)	0.01977(8)
Cs2	0.84235(2)	0.2500	0.73987(2)	0.02377(9)
Cs3	0.63719(2)	0.2500	0.51783(2)	0.02293(8)
Cs4	0.62556(2)	0.7500	0.74636(2)	0.02529(9)
P1	0.58748(4)	0.38411(6)	0.78149(4)	0.00710(13)
P2	0.89228(4)	0.38285(6)	0.97422(4)	0.00708(13)
P3	0.61584(4)	0.61397(6)	0.97915(4)	0.00700(13)
P4	0.88237(4)	0.61673(6)	0.78097(4)	0.00714(13)
O1	0.62116(18)	0.7500	1.01745(16)	0.0095(5)
O2	0.58445(19)	0.2500	0.74146(16)	0.0105(5)
O3	0.83999(17)	0.7500	0.79052(16)	0.0098(5)
O4	0.89389(18)	0.2500	1.01692(16)	0.0104(5)
O5	0.58799(13)	0.46634(17)	0.70407(11)	0.0133(4)
O6	0.50494(13)	0.39707(18)	0.83622(12)	0.0151(4)
O7	0.46248(13)	0.38324(17)	0.59597(11)	0.0121(4)
O8	0.45512(13)	0.60956(17)	0.65109(12)	0.0137(4)
O9	0.53086(13)	0.60503(17)	0.92828(12)	0.0154(4)
O10	0.91640(13)	0.60730(17)	0.69073(12)	0.0141(4)
O11	0.61784(12)	0.53286(17)	1.05737(11)	0.0117(4)
O12	0.69795(13)	0.59961(17)	0.92378(12)	0.0132(4)
O13	0.80469(13)	0.53309(17)	0.79677(11)	0.0122(4)
O14	0.79980(12)	0.40005(18)	0.93982(12)	0.0134(4)
O15	0.67130(13)	0.39248(17)	0.83389(12)	0.0131(4)
Be1	0.7437(2)	0.4848(3)	0.8744(2)	0.0087(6)
Be2	0.5222(2)	0.4992(3)	0.6251(2)	0.0095(6)
O16	0.91163(13)	0.46618(17)	1.04817(11)	0.0123(4)
Be3	0.9604(2)	0.5157(3)	0.6208(2)	0.0099(6)

layered stacking, and each layer consists of a [Be₃P₄O₂₀]^{14−} fundamental unit further interconnected by O-sharing. The adjacent layers are bridged *via* O atoms from the PO₄ tetrahedra, and the Cs cations reside between the layers and maintain the charge balance.

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