Crystal structure of potassium scandium (monophosphate-hydrogen-monoborate-monophosphate), KSc[BP$_2$O$_8$(OH)]

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Abstract
BHKO$_2$P$_2$Sc, triclinic, $P$1 (no. 2), $a$ = 5.2696(2) Å, $b$ = 8.2739(8) Å, $c$ = 8.3890(5) Å, $\alpha$ = 88.22(1)°, $\beta$ = 79.701(6)°, $\gamma$ = 86.67(1)°, $V$ = 359.2 Å$^3$, $Z$ = 2, $R_{	ext{int}}$ = 0.032, $wR_{	ext{ref}}(F^2)$ = 0.075, $T$ = 295 K.

Source of material
Single crystals of the title compound were obtained during the investigations of the systems $M_2O$–Sc$_2$O$_3$–B$_2$O$_3$–P$_2$O$_5$–H$_2$O ($M$ = Li, Na, K, Rb, Cs). The reaction was carried out with a mixture of 0.25 g Sc$_2$O$_3$ (ABCR, 99.9 %), 0.2769 g K$_2$B$_4$O$_7$ • 4H$_2$O (Riedel-de Haen, > 99 %) and 1.1051 g K$_2$HPO$_4$ (Merck, extra pure) in the molar ratio K:Sc:B:P = 4:1:1:1.75. 2.0 ml HQ (37 %) were added to adjust the pH value to 1. The mixture was filled in a 10 ml Teflon autoclave (filling degree 30 %) and heated at 443 K under autogenous pressure for two weeks. The reaction product was washed with water and dried in air at 333 K. The chemical composition was confirmed by chemical analysis. IR spectra are consistent with the presence of B—OH groups.

Discussion
Borophosphates have received much attention because of their variable structural chemistry and potential concerning applica-

Table 1. Data collection and handling.

| Crystal: | colorless block, size 0.125 × 0.075 × 0.060 mm |
| Wavelength: | Mo K$_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 20.77 cm$^{-1}$ |
| Diffractometer, scan mode: | Rigaku AFC-7 & Mercury CCD, $\varphi/\omega$ |
| $2\theta_{	ext{max}}$: | 63.0° |
| $N(hkl)$_{obs}$, N(hkl)$_{meas}$: | 1918, 6078 |
| Criterion for $I_{obs}$, $I_{meas}$: | $I_{obs} > 2 \sigma(I_{obs})$, 1783 |
| $N(\text{param})$_{meas}: | 131 |
| Programs: | SHELXS-97 [9], SHELXL-97 [10], DIAMOND [11] |

Table 2. Atomic coordinates and displacement parameters (in Å$^2$).

<table>
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<th>Atom</th>
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<th>$y$</th>
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* Correspondence author (e-mail: kniep@cpfs.mpg.de)
Table 3. Atomic coordinates and displacement parameters (in Å$^2$).

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References