# Crystal structure of caesium iron(III) *catena*-[monohydrogenmonoborate-bis(monophosphate)], $CsFe[BP_2O_8(OH)]$

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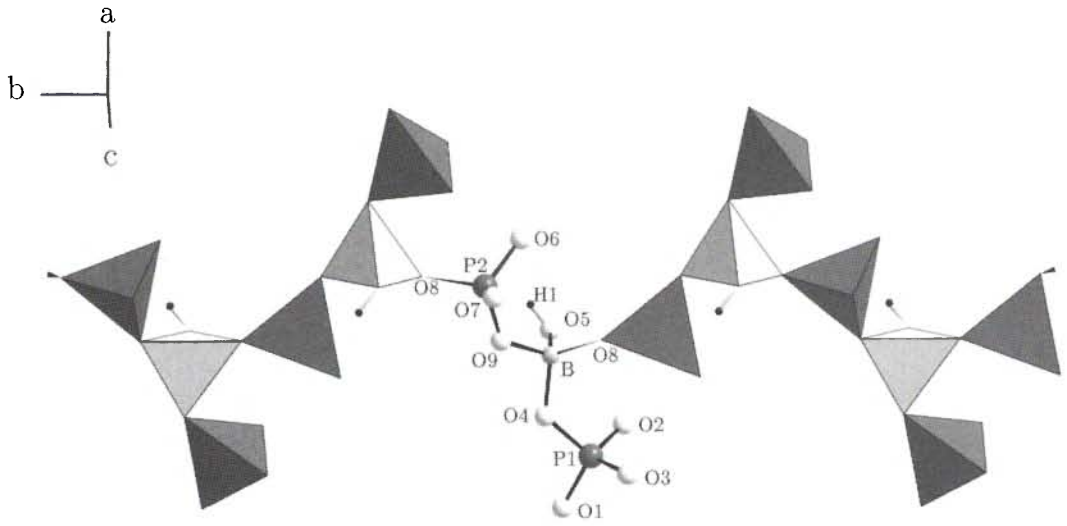


**Abstract**

$BCsFeHO_9P_2$, monoclinic, $P12_1/c1$ (No. 14), $a = 9.351(2)$ Å, $b = 8.631(4)$ Å, $c = 9.763(2)$ Å, $\beta = 102.58(2)°$, $V = 769.0$ Å$^3$, $Z = 4$, $R_{gt}(F) = 0.024$, $wR(F^2) = 0.083$, $T = 293$ K.

**Source of material**

$CsFe[BP_2O_8(OH)]$ was prepared by hydrothermal reaction of 2.78 g of a 50 wt.% aqueous solution of CsOH, 2.51 g $FeCl_3 \cdot 6H_2O$, 0.57 g $H_3BO_3$ and 2.14 g $H_3PO_4$ (85%) (molar ratio 1 : 1 : 1 : 2, conc. solution, pH 1) in teflon autoclaves at T = 433 K – 443 K for six days.

**Discussion**

The crystal structure of $CsFe[BP_2O_8(OH)]$ (hydrated borophosphate, B:P < 1; [1]) contains open-branched vierer-einfach chains $[BP_2O_8(OH)]^{4-}$, which are formed by alternating hydrogenborate and phosphate tetrahedra sharing common corners. The caesium-iron(III) compound is an isotype of $RbFe[BP_2O_8(OH)]$[2]. $Fe^{3+}$ is in an octahedral coordination ($FeO_5(OH)$) by oxygen sites of three neighbouring tetrahedral chains, while $Cs^+$ is irregularly coordinated by ten oxygen sites. Bond lengths and angles within the anionic partial structure are consistent with related borophosphates (see [1, 2] and refs. therein).

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

| | |
|---|---|
| Crystal: | amethyst-like (pale-violet), monoclinic prism, size 0.04 × 0.03 × 0.25 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| μ: | 70.68 cm$^{-1}$ |
| Diffractometer, scan mode: | Siemens P4 , ω |
| $2\theta_{max}$: | 60° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 5058, 2237 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 2056 |
| $N(param)_{refined}$: | 131 |
| Programs: | SHELXS-97 [3], SHELXL-97 [4] |

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

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(1) | 4*e* | 0.382(9) | 0.592(7) | 0.025(8) | 0.05(2) |

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**Table 3.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Cs | 4*e* | 0.19523(2) | 0.61015(3) | 0.55238(2) | 0.0247(2) | 0.0199(2) | 0.0218(2) | –0.00106(7) | 0.0020(1) | –0.00393(7) |
| Fe | 4*e* | 0.20561(5) | 0.15542(5) | 0.42773(4) | 0.0096(2) | 0.0107(2) | 0.0095(2) | –0.0003(1) | 0.0014(2) | 0.0004(1) |
| B | 4*e* | 0.3413(4) | 0.5433(4) | 0.1948(4) | 0.010(1) | 0.011(1) | 0.014(1) | 0.000(1) | –0.002(1) | –0.000(1) |
| P(1) | 4*e* | 0.07373(8) | 0.42853(9) | 0.20068(8) | 0.0087(3) | 0.0102(3) | 0.0094(3) | 0.0005(2) | 0.0013(2) | 0.0007(2) |
| P(2) | 4*e* | 0.41972(8) | 0.23297(9) | 0.21319(8) | 0.0083(3) | 0.0098(3) | 0.0111(3) | 0.0007(2) | 0.0013(2) | 0.0005(2) |
| O(1) | 4*e* | 0.0748(2) | 0.0050(3) | 0.3137(2) | 0.0097(9) | 0.018(1) | 0.018(1) | –0.0038(8) | 0.0020(8) | –0.0053(8) |
| O(2) | 4*e* | 0.0863(3) | 0.3325(3) | 0.0735(2) | 0.017(1) | 0.018(1) | 0.0102(9) | –0.0022(8) | 0.0073(8) | –0.0029(8) |
| O(3) | 4*e* | 0.1011(3) | 0.3333(3) | 0.3358(2) | 0.015(1) | 0.014(1) | 0.014(1) | 0.0041(8) | 0.0017(8) | 0.0038(8) |
| O(4) | 4*e* | 0.1940(2) | 0.5588(3) | 0.2225(2) | 0.0104(9) | 0.013(1) | 0.017(1) | –0.0010(7) | 0.0040(8) | –0.0023(8) |
| O(5) | 4*e* | 0.3236(3) | 0.5373(3) | 0.0406(2) | 0.018(1) | 0.015(1) | 0.0098(9) | –0.0040(8) | 0.0018(8) | –0.0004(8) |
| O(6) | 4*e* | 0.3411(3) | 0.1310(3) | 0.2992(3) | 0.016(1) | 0.0123(9) | 0.021(1) | –0.0012(8) | 0.0085(9) | –0.0002(8) |
| O(7) | 4*e* | 0.3601(3) | 0.2182(3) | 0.0566(2) | 0.019(1) | 0.016(1) | 0.0084(9) | 0.0041(9) | –0.0005(8) | –0.0008(8) |
| O(8) | 4*e* | 0.4206(3) | 0.4056(2) | 0.2620(2) | 0.016(1) | 0.0098(9) | 0.014(1) | 0.0023(8) | –0.0008(8) | 0.0004(7) |
| O(9) | 4*e* | 0.5845(2) | 0.1857(3) | 0.2455(3) | 0.0092(9) | 0.0114(9) | 0.020(1) | 0.0010(7) | 0.0012(8) | 0.0034(8) |

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## References

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