Crystal structure of rubidium chromium diphosphate, $RbCrP_2O_7$

Dan Zhao* and Feifei Li

Department of Physics and Chemistry, Henan Polytechnic University, Jiaozuo 454000, Henan, P. R. China

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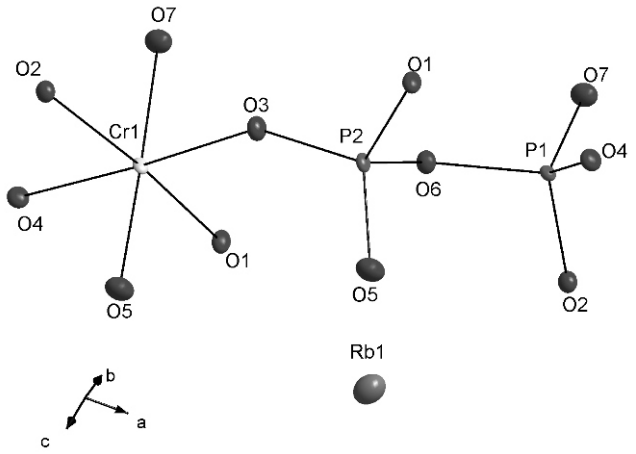

Abstract

CrO_7P_2Rb, monoclinic, $P12_1/c1$ (no. 14), a = 7.475(5) Å, b = 9.888(6) Å, c = 8.226(5) Å, β = 106.013(8)°, V = 584.4 Å^3, Z = 4, $R_{gt(F)}$ = 0.037, $wR_{ref(F^2)}$ = 0.092, T = 298 K.

Source of material

Prism-shaped colourless single crystals of $RbCrP_2O_7$ were initially obtained by the high temperature solid state reaction of $RbNO_3$, Cr_2O_3 and $NH_4H_2PO_4$, in a molar ratio of 8:1:10 (Rb:Cr:P). The reaction mixture was thoroughly ground in an agate mortar and pressed into a pellet to ensure the best homogeneity and reactivity. The pellet was put into a platinum crucible. The crucible was transferred into an furnace and heated at 1073 K in the air for 24 h, and then it was allowed to cool with a rate of 5 K min^{-1} to 673 K before switching off the furnace. After boiling in water, crystals were obtained in very low yield (about 5%).

Discussion

In recent years, inorganic metal phosphates have been part of intensive research activities both in high-temperature solid state and aqueous solution conditions, and their number has grown steadily [1-3]. The crystal chemistry of these compounds with anionic partial structures mainly built from PO_4 tetrahedral units reveals a large structural variety, which is usually accompanied by intriguing magnetism, electric, optical, and thermal expansion properties. Furthermore, chemical and thermal stability ensures their wide application in many fields. As part of this, a series of chromium double orthophosphates of alkali metals have been reported: $LiCrP_2O_7$ [4], $NaCrP_2O_7$ [5], $KCrP_2O_7$ [6] and $CsCrP_2O_7$ [7].

The title compound $RbCrP_2O_7$ is isostructural with its analogues $NaCrP_2O_7$, $KCrP_2O_7$ and $CsCrP_2O_7$. It possesses a three-dimensional $(CrP_2O_7)^-$ anionic framework with one-dimensional tunnels occupied by Rb^+ cations. The P atoms are four-connected by O atoms to form PO_4 tetrahedra. Two PO_4 groups are further connected via corner O atoms to form a P_2O_7 group. On the other hand, each CrO_6 group is connected, via Cr–O–P bonds, to five P_2O_7 groups: two corners of the CrO_6 octahedron are linked to one P_2O_7 group and the other four corners connect to four distinct P_2O_7 groups. The CrO_6 octahedra are distorted as shown by the Cr—O distances ranging from 1.935(4) Å to 1.993(4) Å. The tunnels running along [001] result from stacking of rings formed by the edges of three octahedra and four tetrahedra. The Rb^+ cations are located in these tunnels, realizing a 10-fold coordination.

Table 1. Data collection and handling.

Crystal:	colourless prism, size 0.05 × 0.05 × 0.20 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	107.65 cm^{-1}
Diffractometer, scan mode:	Rigaku Mercury70 CCD, ω
$2\theta_{max}$:	54.96°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4351, 1342
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1150
$N(param)_{refined}$:	100
Programs:	SHELXS-97, SHELXL-97, SHELXTL [9], PLATON [10]

Table 2. 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}
Rb(1)	4*e*	0.81363(7)	0.31147(6)	0.45068(6)	0.0157(3)	0.0169(3)	0.0176(3)	0.0005(2)	0.0018(2)	–0.0025(2)
Cr(1)	4*e*	0.2373(1)	0.39948(8)	0.26034(9)	0.0056(4)	0.0015(4)	0.0071(4)	0.0005(3)	0.0027(3)	0.0005(3)
P(1)	4*e*	0.8691(2)	0.5958(1)	0.1678(2)	0.0057(5)	0.0030(6)	0.0055(5)	0.0006(4)	0.0023(4)	0.0006(4)
O(1)	4*e*	0.4443(5)	0.2809(3)	0.2409(4)	0.007(1)	0.004(1)	0.013(1)	–0.001(1)	0.004(1)	–0.001(1)
P(2)	4*e*	0.5659(2)	0.6328(1)	0.3122(2)	0.0057(5)	0.0029(6)	0.0082(5)	–0.0010(4)	0.0031(4)	–0.0001(4)
O(2)	4*e*	0.0101(4)	0.4978(4)	0.2743(4)	0.008(1)	0.006(1)	0.009(1)	0.001(1)	0.004(1)	–0.001(1)
O(3)	4*e*	0.3710(5)	0.5748(4)	0.2678(4)	0.009(1)	0.007(1)	0.012(1)	–0.002(1)	0.003(1)	–0.001(1)

* Correspondence author (e-mail: iamzd1996@163.com)

Table 2. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(4)	4*e*	0.0868(5)	0.2368(3)	0.2579(4)	0.010(1)	0.004(1)	0.011(1)	0.001(1)	0.003(1)	0.000(1)
O(5)	4*e*	0.3199(5)	0.3949(4)	0.5101(5)	0.016(1)	0.012(2)	0.010(1)	–0.001(1)	0.002(1)	0.001(1)
O(6)	4*e*	0.6707(5)	0.5532(3)	0.1932(4)	0.008(1)	0.007(1)	0.010(1)	–0.000(1)	0.004(1)	–0.001(1)
O(7)	4*e*	0.8529(5)	0.5890(4)	–0.0165(4)	0.013(1)	0.012(1)	0.010(1)	0.002(1)	0.004(1)	0.000(1)

References

1. Dogan, L.; Emirdag-Eanes, M.: Crystal structure of distrontium manganese(III) tetraoxophosphate heptaoxodiphosphate, $Sr_2Mn[PO_4][P_2O_7]$. Z. Kristallogr. NCS **222** (2007) 89-90.
2. Mao, S. Y.; Mao, Y. P.; Batchelor, R. J.; Guo, H. Y.; Ye, Z. G.; Xie, Z. X.; Zheng, L. S.: Polymorphic structures and properties of lead chromium phosphate $Pb_3Cr_2(PO_4)_4$. J. Mater. Chem. **19** (2009) 6034-6041.
3. Zhao, D.; Li, F. F.; Zhang, A. Y.: Crystal structure of calcium tin phosphate(V), $CaSn_4(PO_4)_6$. Z. Kristallogr. NCS **225** (2010) 627-628.
4. Ivashkevich, L. S.; Selevich, K. A.; Lesnikovich, A. I.; Selevich, A. F.: X-ray powder diffraction study of $LiCrP_2O_7$. Acta Crystallogr. **E63** (2007) i70-i72.
5. Bohaty, L.; Liebertz, J.; Froehlich, R.: Die Kristallstruktur von $NaCrP_2O_7$. Z. Kristallogr. **161** (1982) 53-59.
6. Gentil, S.; Andreica, D.; Lujan, M.; Rivera, J. P.; Kubel, F.; Schmid, H.: Synthesis, structure and magnetic susceptibility of $KCrP_2O_7$, a potential antiferromagnetic magnetoelectric. Ferroelectrics **204** (1997) 35-44.
7. Linde, S. A.; Gorbunova, Yu. E.: Crystal structure of cesium chromium pyrophosphate $CsCrP_2O_7$. Izv. Akad. Nauk SSSR, Neorg. Mater. **18** (1982) 464-467.
9. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112-122.
10. Spek, A. L.: Single-crystal structure validation with the program PLATON. J. Appl. Crystallogr. **36** (2003) 7-13.