

builds a pyramid on one of the rectangular faces of another trigonal prism. Also, the distribution of the prisms is such that they form rings and enclose cavities occupied by Na(1) and Na(2). These cavities are antiprisms with a triangular base. They are not linked to one another.

F(1) and F(4) are, respectively, the bases of the U(1) and Na(3), and of the Na(4) and U(2) polyhedra. They build, respectively, a pyramid on the U(2) and U(1) polyhedra and are linked to Na(1). F(2) and F(3) are, respectively, the bases of the U(2) and Na(4), and of the U(1) and Na(3) polyhedra. They build, respectively, a pyramid on the Na(3) and Na(4) polyhedra and are linked to Na(2). The F atoms are of two types: F(1) and F(4) with a charge of $-(1 + \frac{1}{2})e$ and F(2) and F(3) with a charge of $-(1 - \frac{1}{2})e$.

As can be seen in Fig. 1, each U(1) polyhedron shares three F(3)–F(4) edges with the Na(4) polyhedra, and three F(1)–F(4) edges with the U(2) polyhedra. Each U(2) polyhedron shares the above-mentioned edges with U(1) and three F(1)–F(2) edges with the Na(3) polyhedra.

Several varieties of this compound are known, but no other structural study has been made. This variety is

the most stable form (Barton, Friedman, Grimes, Insley, Moore & Thoma, 1958).

The fact that U and Na atoms occupy the same type of polyhedra is unusual, and the fact that these prisms share triangular bases and edges with their neighbours probably accounts for the particular stability of this compound.

References

- AHMED, F. R. (1976). Editor. *Crystallographic Computing Techniques*. Copenhagen: Munksgaard.
- BARTON, C. J., FRIEDMAN, H. A., GRIMES, W. R., INSLEY, H., MOORE, R. E. & THOMA, R. E. (1958). *J. Am. Chem. Soc.* **41**(2), 63–70.
- BORDERIE, B., PINAULT, J.-L. & BARRANDON, J.-N. (1977). *Analysis*, **5**, 280–283.
- BUSING, W. R., MARTIN, K. O. & LEVY, H. A. (1962). *ORFLS*. Report ORNL-TM-305. Oak Ridge National Laboratory, Tennessee.
- COUSSON, A., PAGÈS, M., COUSSEINS, J. C. & VEDRINE, A. (1977). *J. Cryst. Growth*, **40**, 157–160.
- International Tables for X-ray Crystallography* (1974). Vol. IV. Birmingham: Kynoch Press.
- MEULENAER, J. DE & TOMPA, H. (1965). *Acta Cryst.* **19**, 1014–1018.

Acta Cryst. (1979). B35, 1200–1201

The Structure of Potassium Tetrachlorozincate

BY IBRAHIM MIKHAIL* AND KARL PETERS†

Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-7000 Stuttgart 80, Federal Republic of Germany

(Received 29 September 1978; accepted 16 January 1979)

Abstract. K_2ZnCl_4 , orthorhombic, $Pna2_1$, $a = 26.778$ (6), $b = 12.402$ (2), $c = 7.256$ (2) Å, $Z = 12$, $d_o = 2.29$, $d_c = 2.36$ Mg m⁻³. Crystals prepared from aqueous solution were found to be isomorphous with high-temperature K_2CoCl_4 . The structure was refined by the full-matrix least-squares method to $R = 0.049$.

Introduction. The crystal structure of K_2CoCl_4 has been reported by Vermin, Verschoor & Ijdo (1976) to be closely related to the K_2SO_4 type, containing tetrahedral $CoCl_4^{2-}$ ions. Our crystal structure refinement of K_2ZnCl_4 is a part of the investigation of structures of the type A_2ZnCl_4 .

Clear, colourless crystals were obtained by slow evaporation of an aqueous solution of KCl and $ZnCl_2$ in the ratio 2:1. Since they are deliquescent, the freshly prepared crystals were immediately enclosed in thin-walled capillaries. A crystal of dimensions $0.16 \times 0.22 \times 0.20$ mm was optically centred on the Syntex P1, four-circle diffractometer. The orientation matrix and the cell parameters were determined on the basis of 15 reflections. The intensities of 3081 hkl reflections were measured according to the ω -scan technique (Mo $K\alpha$, graphite monochromator) using a scan range of 1° and a scan speed between 0.5 and $24.0^\circ \text{ min}^{-1}$ depending on the intensity of the measured reflection. In the range $3.0^\circ \leq 2\theta \leq 55.0^\circ$, 2558 reflections hkl with $I > 1.96\sigma(I)$ were obtained which were used for the structure refinement. For the evaluation the XTL system (Syntex, Nova 1200) was employed. An

* Present address: Department of Physics, Faculty of Science, El Manoufia-University, Shebien Elkoom, Egypt.

† To whom correspondence should be addressed.

Table 1. Final atomic coordinates ($\times 10^4$) and thermal parameters [$\exp(-B \sin^2\theta/\lambda^2) \times 10$]

	x	y	z	B (Å ²)
K(1)	433 (1)	814 (4)	7866 (9)	41 (2)
K(2)	3797 (1)	855 (5)	7638 (9)	49 (2)
K(3)	7106 (1)	833 (4)	7223 (7)	43 (2)
K(4)	3319 (1)	6875 (3)	7219 (6)	26 (1)
K(5)	6660 (1)	6863 (3)	7388 (6)	25 (1)
K(6)	9986 (1)	6883 (3)	7932 (6)	27 (1)
Zn(1)	721 (1)	4194 (1)	7500*	19 (1)
Zn(2)	4050 (1)	4181 (1)	7796 (2)	17 (1)
Zn(3)	7403 (1)	4177 (1)	7365 (2)	19 (1)
Cl(1)	9917 (1)	4437 (3)	6731 (6)	25 (1)
Cl(2)	1123 (1)	5756 (3)	8151 (7)	27 (1)
Cl(3)	844 (1)	3012 (3)	9795 (6)	31 (1)
Cl(4)	1111 (1)	3560 (4)	4910 (6)	28 (1)
Cl(5)	3229 (1)	4366 (3)	8129 (7)	36 (1)
Cl(6)	4439 (2)	5782 (4)	8132 (9)	45 (2)
Cl(7)	4353 (2)	3072 (5)	-4 (7)	44 (2)
Cl(8)	4306 (2)	3480 (4)	5110 (6)	48 (2)
Cl(9)	6591 (1)	4358 (3)	8044 (7)	34 (1)
Cl(10)	7794 (1)	5760 (4)	6660 (8)	30 (1)
Cl(11)	7778 (1)	3615 (3)	26 (6)	32 (1)
Cl(12)	7560 (1)	2942 (3)	5177 (6)	35 (1)

* Value fixed during the refinements.

absorption correction was applied to all intensities which was based on ψ -scan measurements. The parameters of the complete structure were refined by least-squares cycles to $R = 0.117$. Refinements of anisotropic thermal parameters yielded final index values of 0.049 and 0.064 for R and R_w respectively; $R = \sum (|F_o| - |F_c|) / \sum |F_o|$ and $R_w = \sum w^{1/2} (|F_o| - |F_c|) / \sum w^{1/2} |F_o|$ where $w = 1/\sigma^2$. The final atomic parameters and their estimated standard deviations are listed in Table 1.*

Discussion. Individual Zn-Cl and K-Cl distances and bond angles are given in Table 2.

The crystal structure of K_2ZnCl_4 is essentially the same as that of K_2CoCl_4 and the structural details of this compound were discussed by Vermin, Verschoor & IJdo (1976).

The arrangement of the significantly distorted $ZnCl_4$ tetrahedra causes a high distortion of all K-Cl coordination parameters. The wide range of K-Cl distances allows only an approximate symmetry assignment; K(5) and K(6): bicapped trigonal prism; K(4): square antiprism; K(1): trigonal prism; K(2) and K(3) have a 4,2 environment like Mn in Mn_2O_3 . With the

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34190 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. Interatomic distances (Å) and angles (°)

Standard deviations of all angles are 0.2°.

Zn(1)-Cl(1)	2.245 (3)	K(5)-Cl(2)	3.330 (5)
-Cl(2)	2.265 (4)	-Cl(5)	3.459 (7)
-Cl(3)	2.243 (5)	-Cl(7)	3.220 (5)
-Cl(4)	2.289 (4)	-Cl(8)	3.283 (6)
		-Cl(9)	3.149 (5)
Zn(2)-Cl(5)	2.222 (3)	-Cl(10)	3.372 (5)
-Cl(6)	2.256 (5)	-Cl(11)	3.149 (5)
-Cl(7)	2.258 (5)	-Cl(12)	3.202 (5)
-Cl(8)	2.242 (5)		
Zn(3)-Cl(9)	2.240 (3)	K(6)-Cl(1)	3.161 (5)
-Cl(10)	2.284 (5)	-Cl(1)	3.217 (6)
-Cl(11)	2.286 (4)	-Cl(2)	3.354 (4)
-Cl(12)	2.246 (5)	-Cl(3)	3.184 (5)
		-Cl(4)	3.315 (5)
K(1)-Cl(3)	3.257 (7)	-Cl(6)	3.248 (5)
-Cl(6)	3.452 (9)	Cl(7)	3.138 (6)
-Cl(6)	3.323 (6)	-Cl(8)	3.164 (6)
-Cl(7)	3.560 (6)		
-Cl(8)	3.394 (7)	Cl(1)-Zn(1)-Cl(2)	113.1
-Cl(9)	3.109 (4)	Cl(1)-Zn(1)-Cl(3)	114.4
		Cl(1)-Zn(1)-Cl(4)	106.2
K(2)-Cl(1)	3.093 (5)	Cl(2)-Zn(1)-Cl(3)	109.6
-Cl(2)	3.266 (8)	Cl(2)-Zn(1)-Cl(4)	104.4
-Cl(4)	3.299 (8)	Cl(3)-Zn(1)-Cl(4)	108.5
-Cl(7)	3.563 (8)		
-Cl(10)	3.424 (6)	Cl(5)-Zn(2)-Cl(6)	110.7
-Cl(11)	3.298 (6)	Cl(5)-Zn(2)-Cl(7)	110.0
		Cl(5)-Zn(2)-Cl(8)	116.0
K(3)-Cl(2)	3.357 (5)	Cl(6)-Zn(2)-Cl(7)	107.1
-Cl(4)	3.237 (5)	Cl(6)-Zn(2)-Cl(8)	107.1
-Cl(5)	3.089 (5)	Cl(7)-Zn(2)-Cl(8)	105.6
-Cl(10)	3.232 (8)		
-Cl(11)	3.194 (7)	Cl(9)-Zn(3)-Cl(10)	114.1
-Cl(12)	3.243 (6)	Cl(9)-Zn(3)-Cl(11)	105.8
		Cl(9)-Zn(3)-Cl(12)	113.9
K(4)-Cl(3)	3.178 (5)	Cl(10)-Zn(3)-Cl(11)	104.4
-Cl(4)	3.241 (5)	Cl(10)-Zn(3)-Cl(12)	110.0
-Cl(5)	3.190 (5)	Cl(11)-Zn(3)-Cl(12)	107.9
-Cl(6)	3.357 (5)		
-Cl(9)	3.402 (6)		
-Cl(10)	3.279 (5)		
-Cl(11)	3.396 (5)		
-Cl(12)	3.192 (5)		

Zn-Cl tetrahedra the 8-polyhedra share one vertex, two edges and one face and the 6-polyhedra share two vertices and two edges.

We would like to thank Mrs E.-M. Peters for her valuable help in the computation procedures on the data. Our work was supported by the Deutsche Forschungsgemeinschaft.

Reference

VERMIN, W. J., VERSCHOOR, G. C. & IJDO, D. J. W. (1976). *Acta Cryst.* B32, 3325-3328.