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Structure cristalline de $K_2V_3O_8$ ou $K_2(VO)[V_2O_7]$

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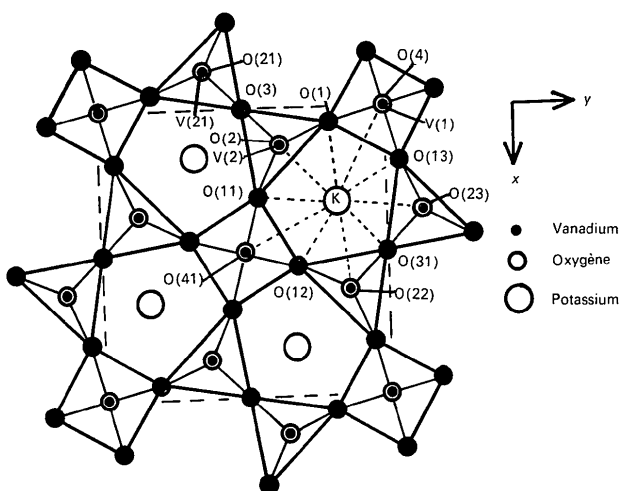


Fig. 1. Projection de la structure de $K_2V_3O_8$ sur le plan (001).

réseau; il est environné par dix atomes d'oxygène formant un antiprisme pentagonal.

Cette structure cristalline de $K_2V_3O_8$ ou $K_2(VO)[V_2O_7]$

est isotype de la fresnoïte $Ba_2(TiO)[Si_2O_7]$ reportée par Massé, Grenier & Durif (1967) et Moore & Louisnathan (1967, 1969).

Dans $K_2V_3O_8$, le vanadium(+IV) occupe les sites pyramidaux à base carrée [site V(1)]; la liaison V(1)–O(4) très courte, 1,582 Å, est typique du radical vanadyle VO^{2+} . Le vanadium(+V) dans les tétraèdres VO_4 présente un environnement légèrement distordu, la liaison la plus longue V(2)–O(3) = 1,794 Å étant celle qui assume le pont V–O–V dans les groupements $[V_2O_7]^{4-}$.

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A redetermination of the crystal structure of $Zn(NO_3)_2 \cdot 2H_2O$. By D. PETROVIĆ and B. RIBÁR, *Faculty of Science, Physics Department, University of Novi Sad, 21000 Novi Sad, Ilije Djuričića 4, Yugoslavia*

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Zn is in $2(c)$ $(0,0,\frac{1}{2})$ not $2(d)$ $(\frac{1}{2},0,\frac{1}{2})$ as reported by Ribár, Nowacki, Šljukić, Ščavničar & Gabela [*Z. Kristallogr.* (1969). **129**, 305–317]; the structure is isotypic with that of $Mg(NO_3)_2 \cdot 2H_2O$.

Similar values of lattice constants and the same space group for $Mg(NO_3)_2 \cdot 2H_2O$ and $Zn(NO_3)_2 \cdot 2H_2O$ suggested isomorphism of their structures and the coordinates of the zinc compound were used as input for a structure-factor calculation of $Mg(NO_3)_2 \cdot 2H_2O$ (Ribár, Gabela, Herak & Prelesnik, 1973). However, the three-dimensional Fourier and difference Fourier syntheses showed that the location of the magnesium atom is not in $2(d)$ $(\frac{1}{2},0,\frac{1}{2})$ but in $2(c)$ $(0,0,\frac{1}{2})$. A closer inspection revealed the mis-indexing of the data for $Zn(NO_3)_2 \cdot 2H_2O$ (hkl and $\bar{h}kl$ indices were exchanged because the angle β is very close to 90°). Therefore a complete redetermination of the crystal structure of zinc nitrate dihydrate was undertaken. The unit cell has, as previously reported, $a = 5.754$ (6), $b = 5.978$ (5), $c = 8.557$ (5) Å, $\beta = 91.0$ (5)°; space group $P2_1/c$, $Z = 2$. The intensities were determined with a microdensitometer for layers 0–3 along a , 0–3 along b and 0–4 along c , by the multiple-film method with an integrating Weissenberg camera and $Cu K\alpha$ radiation, spherical crystal. 459 independent non-zero reflexions were observed. L_p and absorption corrections were applied.

With starting coordinates as given by Ribár, Nowacki, Šljukić, Ščavničar & Gabela (1969), but with $x = 0$, $y = 0$, $z = \frac{1}{2}$ for the zinc atom, diagonal-matrix least-squares refine-

Table 1. *Fractional coordinates and isotropic thermal parameters (Å^2)*

	x	y	z	B
Zn	0	0	0.5	2.12 (3)
O(1)	0.0540 (12)	0.3676 (12)	0.2338 (9)	2.16 (12)
O(2)	0.4260 (12)	0.4165 (13)	0.2465 (9)	2.33 (12)
O(3)	0.2565 (14)	0.2221 (12)	0.4224 (9)	2.03 (12)
N	0.2480 (13)	0.3385 (13)	0.2984 (9)	1.49 (12)
O_w	0.2461 (12)	–0.2452 (12)	0.5120 (9)	1.92 (12)

Table 2. *Bond distances (Å) and angles (°)*

	Symmetry code		
	i	$-x, y - \frac{1}{2}, \frac{1}{2} - z$	
Zn— O_w	2.039 (9) (2×)	O(1)—N	1.25 (2)
Zn—O(3)	2.102 (10) (2×)	O(2)—N	1.22 (2)
Zn—O(1 ⁱ)	2.169 (9) (2×)	O(3)—N	1.27 (2)
O_w —Zn—O(3)	88.8 (4)	O(1)—N—O(2)	122.5 (1.5)
O(3)—Zn—O(1 ⁱ)	91.7 (4)	O(1)—N—O(3)	117.8 (1.4)
O(1 ⁱ)—Zn— O_w	82.6 (4)	O(2)—N—O(3)	119.7 (1.4)