

Fig. 1. Projection de la structure de $\mathrm{K}_{2} \mathrm{~V}_{3} \mathrm{O}_{8}$ sur le plan (001).
réseau; il est environné par dix atomes d'oxygène formant un antiprisme pentagonal.

Cette structure cristalline $\operatorname{deK}_{2} \mathrm{~V}_{3} \mathrm{O}_{8}$ ou $\mathrm{K}_{2}(\mathrm{VO})\left[\mathrm{V}_{2} \mathrm{O}_{7}\right]$
est isotype de la fresnoïte $\mathrm{Ba}_{2}(\mathrm{TiO})\left[\mathrm{Si}_{2} \mathrm{O}_{7}\right]$ reportée par Massé, Grenier \& Durif (1967) et Moore \& Louisnathan (1967, 1969).

Dans $\mathrm{K}_{2} \mathrm{~V}_{3} \mathrm{O}_{8}$, le vanadium( +IV ) occupe les sites pyramidaux à base carrée [site $\mathrm{V}(1)$ ]; la liaison $\mathrm{V}(1)-\mathrm{O}(4)$ très courte, $1,582 \AA$, est typique du radical vanadyle $\mathrm{VO}^{2+}$. Le vanadium $(+\mathrm{V})$ dans les tétraèdres $\mathrm{VO}_{4}$ présente un environnement légèrement distordu, la liaison la plus longue $\mathrm{V}(2)-\mathrm{O}(3)=1,794 \AA$ étant celle qui assume le pont $\mathrm{V}-\mathrm{O}-\mathrm{V}$ dans les groupements $\left[\mathrm{V}_{2} \mathrm{O}_{7}\right]^{4-}$.

## Références

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A redetermination of the crystal structure of $\mathbf{Z n}\left(\mathbf{N O}_{3}\right)_{\mathbf{2}} \cdot \mathbf{2} \mathbf{H}_{\mathbf{2}} \mathbf{O}$. 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) $\left(0,0, \frac{1}{2}\right)$ not $2(d)\left(\frac{1}{2}, 0, \frac{1}{2}\right)$ as reported by Ribár, Nowacki, Sljukić, Šćavničar \& Gabela [Z. Kristallogr. (1969). 129, 305-317]; the structure is isotypic with that of $\mathrm{Mg}\left(\mathrm{NO}_{3}\right)_{2} .2 \mathrm{H}_{2} \mathrm{O}$.

Similar values of lattice constants and the same space group for $\mathrm{Mg}\left(\mathrm{NO}_{3}\right)_{2} .2 \mathrm{H}_{2} \mathrm{O}$ and $\mathrm{Zn}\left(\mathrm{NO}_{3}\right)_{2} .2 \mathrm{H}_{2} \mathrm{O}$ suggested isomorphism of their structures and the coordinates of the zinc compound were used as input for a structure-factor calculation of $\mathrm{Mg}\left(\mathrm{NO}_{3}\right)_{2} .2 \mathrm{H}_{2} \mathrm{O}$ (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 $2(d)\left(\frac{1}{2}, 0, \frac{1}{2}\right)$ but in $2(c)\left(0,0, \frac{1}{2}\right)$. A closer inspection revealed the mis-indexing of the data for $\mathrm{Zn}\left(\mathrm{NO}_{3}\right)_{2} .2 \mathrm{H}_{2} \mathrm{O}$ ( $h k l$ and $\bar{h} k l$ indices were exchanged because the angle $\beta$ is very close to $90^{\circ}$ ). Therefore a complete redetermination of the crystal structure of zinc nitrate dihydrate was undertaken. The unit cell has, as previously reported, $a=\cdot 5.754$ (6), $b=5.978$ (5), $c=8.557$ (5) $\AA, \beta=$ $91 \cdot 0(5)^{\circ}$; space group $P 2_{1} / c, Z=2$. The intensities were determined with a microdensitometer for layers 0-3 along $\mathbf{a}, 0-3$ along $b$ and $0-4$ along $\mathbf{c}$, by the multiple-film method with an integrating Weissenberg camera and $\mathrm{Cu} K \alpha$ radiation, spherical crystal. 459 independent non-zero reflexions were observed. Lp and absorption corrections were applied.

With starting coordinates as given by Ribár, Nowacki, Šljukić, Šćavničar \& 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 $\left(\AA^{2}\right)$

|  | $x$ | $y$ | $z$ | $B$ |
| :--- | :--- | :--- | :--- | :--- |
|  | $x$ | 0 | 0.5 | $2 \cdot 12(3)$ |
| Zn | 0 | $0.0540(12)$ | $0.3676(12)$ | $0.2338(9)$ |
| $\mathrm{O}(1)$ | $0.0546(12)$ | $0.16(12)$ |  |  |
| $\mathrm{O}(2)$ | $0.426(12)$ | $0.4165(13)$ | $0.2465(9)$ | $2.33(12)$ |
| $\mathrm{O}(3)$ | $0.2565(14)$ | $0.2221(12)$ | $0.4224(9)$ | $2.03(12)$ |
| N | $0.2480(13)$ | $0.3385(13)$ | $0.2984(9)$ | $1.49(12)$ |
| $\mathrm{O}_{w}$ | $0.2461(12)$ | $-0.2452(12)$ | $0.5120(9)$ | $1.92(12)$ |

Table 2. Bond distances $(\AA)$ and angles $\left({ }^{\circ}\right)$

| Symmetry code <br> $-x, y-\frac{1}{2}, \frac{1}{2}-z$ |  |  |  |
| :--- | :--- | :--- | ---: |
| $\mathrm{Zn}-\mathrm{O}_{w}$ | $2.039(9)(2 \times)$ | $\mathrm{O}(1)-\mathrm{N}$ | $1.25(2)$ |
| $\mathrm{Zn}-\mathrm{O}(3)$ | $2.102(10)(2 \times)$ | $\mathrm{O}(2)-\mathrm{N}$ | $1.22(2)$ |
| $\mathrm{Zn}-\mathrm{O}\left(1^{\mathrm{i}}\right)$ | $2.169(9)(2 \times)$ | $\mathrm{O}(3)-\mathrm{N}$ | $1.27(2)$ |
| $\mathrm{O}_{w}-\mathrm{Zn}-\mathrm{O}(3)$ | $88.8(4)$ | $\mathrm{O}(1)-\mathrm{N}-\mathrm{O}(2)$ | $122.5(1.5)$ |
| $\mathrm{O}(3)-\mathrm{Zn}-\mathrm{O}\left(1^{\mathrm{i}}\right)$ | $91.7(4)$ | $\mathrm{O}(1)-\mathrm{N}-\mathrm{O}(3)$ | $117.8(1 \cdot 4)$ |
| $\mathrm{O}\left(1^{1}\right)-\mathrm{Zn}-\mathrm{O}_{w}$ | $82.6(4)$ | $\mathrm{O}(2)-\mathrm{N}-\mathrm{O}(3)$ | $119.7(1 \cdot 4)$ |

ment with isotropic thermal-motion factors was carried out on a Varian 73 computer of the University of Novi Sad. The final value of $R$ was 0.076 for the observed reflexions.

The zinc atoms are surrounded by a distorted octahedron composed of four oxygen atoms belonging to the nitrate ions and of two oxygen atoms belonging to two water molecules. The octahedra are linked together by common nitrate groups in a layer parallel to (100). The structure of $\mathrm{Zn}\left(\mathrm{NO}_{3}\right)_{2} \cdot 2 \mathrm{H}_{2} \mathrm{O}$ is isotypic with that of $\mathrm{Mg}\left(\mathrm{NO}_{3}\right)_{2} .2 \mathrm{H}_{2} \mathrm{O}$ (Ribár, Gabela, Herak \& Prelesnik, 1973). The atomic
parameters are reported in Table 1; the bond distances and angles are listed in Table 2.

## References

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