Unit cells and space groups of a series of N -( $\omega$-dimethylaminoalkyl)-phthalimide methiodides.* By James E. Weidenborner $\dagger$ and L. Edward Godycki $\ddagger$, Chemistry Department, St. Louis University, St. Louis, Missouri, U.S.A.

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Pharmacologic tests have shown that the curare-like activity of a series of monoquaternary $N$-( $\omega$-dialkylamino-alkyl)-phthalimides of general formula,

is a function of the methylene chain length. Paralyzing activity rises as $n$ increases, reaches a maximum at $n=7,8$, and 9 , then drops off as the chain length is further increased.

In an attempt to establish the structure-activity relationship, three compounds in a series of N -( $\omega$-di-methylaminoalkyl)-phthalimide methiodides with $n=6$, 10 and 11 were selected for X-ray diffraction studies. Crystals prepared ly recrystallization from isopropyl alcohol were obtained from Seiwald (1954) of this laboratory. Examination under a microscope showed the crystals to have the shape of elongated and flattened parallelepipeds with six well-developed faces parallel to the ( 100 ), ( 010 ), and ( 001 ) planes.

The Weissenberg technique and, to a lesser extent,

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Table 1. Crystallographic data for
N -( $\omega$-dimethylaminoalkyl)-phthalimide methiodides

| Crystal data | 6 | Chain length 10 | 11 |
| :---: | :---: | :---: | :---: |
| $a(\AA)$ | $19.62 \mp 0.06$ | $31.6 \mp 0 \cdot 1$ | $33 \cdot 9 \mp 0 \cdot 1$ |
| $b$ ( $\AA$ ) | $10.27 \mp 0.04$ | $7.55 \mp 0.03$ | $9.52 \mp 0.03$ |
| $c$ ( $\AA$ ) | $9.86 \mp 0.03$ | $9.67 \mp 0.03$ | $7.55 \mp 0.03$ |
| $\alpha\left({ }^{\circ}\right)$ | $106.9 \mp 0.5$ | 90 | 90 |
| $\beta\left({ }^{\circ}\right)$ | $94.1 \mp 0.5$ | $92.6 \mp 0.4$ | 90 |
| $\gamma\left({ }^{\circ}\right)$ | $96.3 \mp 0.5$ | 90 | 90 |
| $D_{m}\left(\mathrm{~g} . \mathrm{cm} .^{-3}\right)^{*}$ | $1.46 \mp 0.01$ | $1.35 \mp 0.01$ | $1.32 \mp 0.01$ |
| $D_{x}\left(\mathrm{~g} . \mathrm{cm} .^{-3}\right) \dagger$ | $1 \cdot 47 \mp 0.01$ | $1 \cdot 36 \mp 0.01$ | $1.326 \mp 0.01$ |
| Diffraction symbol | $\overline{\mathrm{l}}$ P- | $2 / m C$ - - | $m m m P n-$ |
| Probable space group | $P \overline{1}$ | C2 | $P_{m n 2}{ }_{1}$ |

* Determined by flotation.
$\dagger$ Based on four formula weights per unit cell.
the oscillation method were used to obtain the diffraction photographs. Unit cell dimensions were measured from oscillation photographs and zero-level Weissenberg photographs, using Mo $K \alpha$ and $\mathrm{Cu} K \alpha$ radiation. Diffraction symbols were obtained from the level symmetries of the Weissenberg photographs and the observed systematic extinctions. Probable space groups were deduced by a study of molecular models. The results are given in Table 1.


## Reference

Serwald, R. J. (1954). Ph.D. Dissertation, St. Louis University, St. Louis.

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## The crystal structure of iridiohexacyanides of divalent cations. By Adolfo Ferrari, Maria Eleo- <br> nora Tant and Emanuele Morisi, Institute of Chemistry, University of Parma, Italy

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The crystalline structures of the iridiohexacyanides of divalent cations having the formula $M e_{3}^{\mathrm{II}}\left[\operatorname{Ir}(\mathrm{CN})_{6}\right]_{2} .12 \mathrm{H}_{2} \mathrm{O}$, where $M e^{\mathrm{II}}=\mathrm{Cr}, \mathrm{Mn}, \mathrm{Fe}, \mathrm{Co}, \mathrm{Ni}, \mathrm{Cu}, \mathrm{Zn}, \mathrm{Cd}$ have been determined. $\mathrm{Cu} K \alpha$ radiation was used ( $\lambda=1,5418 \AA$ ).

The compounds were prepared for the first time in this Institute. They are isotypic with the salts of the correspondent series of ferrihexacyanides, cobaltihexacyanides (Ferrari, Tani \& Magnano, 1959) and rhodiohexacyanides.

The probable space groups are: $\mathrm{O}_{h}(5)-F m 3 m$ and $T_{a}(2)-F \overline{4} 3 \mathrm{~m}$. The unit cell containing two molecules has the following constants:

| $\mathrm{Cr}_{3}\left[\operatorname{Ir}(\mathrm{CN})_{6}\right]_{2} .12 \mathrm{H}_{2} \mathrm{O}, a=10.452 \pm 0.02 \AA$, | $d_{c}=3.113 \mathrm{g.cm} .^{-3}$ |
| :---: | :---: |
| $\mathrm{Mn}_{3}\left[\operatorname{Ir}(\mathrm{CN})_{6}\right]_{2} .12 \mathrm{H}_{2} \mathrm{O}, \quad a=10.708 \pm 0.02$ | $d_{c}=2.907$ |
| $\mathrm{Fe}_{3}\left[\operatorname{Ir}(\mathrm{CN})_{6}\right]_{2} .12 \mathrm{H}_{2} \mathrm{O}, a=10.593 \pm 0.02$ | $d_{c}=3.023$ |
| $\mathrm{Co}_{3}\left[\operatorname{Ir}(\mathrm{CN})_{6}\right]_{2} .12 \mathrm{H}_{2} \mathrm{O}, a=10.540 \pm 0.03$ | $d_{c}=3.094$ |
| $\mathrm{Ni}_{3}\left[\operatorname{Ir}(\mathrm{CN})_{6}\right]_{2} .12 \mathrm{H}_{2} \mathrm{O}, \quad a=10.361 \pm 0.01$ | $d_{c}=3.255$ |
| $\mathrm{Cu}_{3}\left[\operatorname{Ir}(\mathrm{CN})_{6}\right]_{2} .12 \mathrm{H}_{2} \mathrm{O}, \quad a=10 \cdot 298 \pm 0.02$ | $d_{c}=3.362$ |
| $\mathrm{Zn}_{3}\left[\operatorname{Ir}(\mathrm{CN})_{6}\right]_{2} .12 \mathrm{H}_{2} \mathrm{O}, a=10.483 \pm 0.02$ | $d_{c}=3.207$ |
| $\mathrm{Cd}_{3}\left[\operatorname{Ir}(\mathrm{CN})_{6}\right]_{2} .12 \mathrm{H}_{2} \mathrm{O}, a=10.878 \pm 0.01$ | $d_{c}=3.229$ |

The water contained is of zeolitic nature because it can be eliminated without any change in the lattice.

## Reference

Ferrari, A., Tani, M. E. \& Magnano, G. (1959). Gazz. Chim. Ital. 89, 2512.

