Table 1. *Crystallographic data*

| Compound | $a$ (Å) | $b$ (Å) | $c$ (Å) | $\alpha$ | $\beta$ | $\gamma$ | Space group | Density (g.cm.$^{-3}$) obs. | calc. | $n$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Silver dibenzyl phosphate | 14·5 | 5·77 | 9·03 | — | 112° 50′ | — | $P2_1$ or $P2_1/m$ | > 1·595 | 1·83 | 2 |
| Dibenzyl phosphoric acid | 12·7 | 5·72 | 28·6 | — | 136° 35′ | — | $P2_1/c$ | 1·30 | 1·30 | 4 |
| Cupric diethyl phosphate | 5·02 | 14·9 | 14·2 | 129° 12′ | 92° 24′ | 91° 42′ | $P1$ or $P\bar{1}$ | 1·51 | 1·45 | 2 |
| Silver diethyl phosphate | 20·3 | 14·4 | 5·88 | — | — | — | $Pccn$ | > 1·495 | 2·01 | 8 |
| Zinc diethyl phosphate | 22·1 | 8·07 | 9·15 | — | 96° 45′ | — | $Cc$ or $C2/c$ | 1·54 | 1·50 | 4 |
| Magnesium diethyl phosphate | 22·3 | 8·02 | 9·33 | — | 97° 10′ | — | $Cc$ or $C2/c$ | 1·35 | 1·35 | 4 |

acetate with a small amount of water. Zinc and silver diethyl phosphate were crystallized from water. All crystallizations were carried out by slow evaporation at room temperature. The possibility that these crystals contain solvent of crystallization has not been excluded.

Mo $K\alpha$ and Cu $K\alpha$ precession photographs, both zero- and upper-level, were used to obtain the crystallographic data in Table 1. Densities were determined by the sink-or-float method with appropriate liquid mixtures.

The magnesium and zinc salts appear isomorphous and the investigation of their crystal structure is proceeding. Neither compound gives a piezoelectric test and thus the space group is probably $C2/c$.

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## Simplified formula for calculating interplanar spacings in the rhombohedral system.

By William R. McMillan, *Westinghouse Research Laboratories, East Pittsburgh, Pa., U.S.A.*

(*Received* 12 *July* 1954)

It is apparently not common knowledge that the formula (*International Tables*, 1935) for calculating interplanar spacings in the rhombohedral system:

$$\frac{a^2}{d^2} = \frac{\cos^2 \alpha/2}{\sin \alpha/2 \,.\, \sin 3\alpha/2} \times [(h^2+k^2+l^2)-(1-\tan^2\alpha/2)(hk+kl+lh)]$$

can be simplified by the use of half-angle formulas. When this is done, the coefficient of the bracket becomes

$$\frac{1+\cos \alpha}{1+\cos \alpha - 2\cos^2 \alpha}.$$

This is an advantage because one has to look up only one trigonometric function instead of three.

One can make a similar but trivial simplification of the tangent term.

### Reference

*International Tables for the Determination of Crystal Structures* (1935). Berlin: Borntraeger.

# Notes and News

*Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the British Co-editor (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).*

## *Dictionary of Values of Molecular Constants*

The editors have received a copy of Volume I of the above publication. This work is to contain the numerical values of quantities such as the energies, coefficients and charges of the electron levels in a large number of molecules of interest to chemists. The values have been gathered together by Dr Daudel in Paris and Prof. Coulson in Oxford. Both the valence-bond approximation of Pauling and the molecular-orbital approximation of Hund, Mulliken and Lennard-Jones have been used, so that comparisons are possible. When complete the dictionary will consist of approximately four volumes, each containing some 50–100 pages. A limited number of copies are available. Enquiries should be addressed to Dr R. Daudel, Centre de Chimie Théorique de France, 5 avenue de l'Observatoire, Paris VI, France.

## *Publicaciones del Departamento de Cristalografia y Mineralogia*

The editors have received Parts 1 and 2 (October 1953 and May 1954) of Volume 1 of the above new publication. Each part contains about 55 small pages and carries some six articles in the fields of morphology, crystal chemistry, structure analysis and instrumentation. Abstracts are in English and the articles in Spanish. All enquiries should be addressed to the Department of Crystallography and Mineralogy, University of Barcelona, Spain.