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Space-group of *ortho*-phenanthroline hydrate. By MINA SEN, *X-ray Laboratory, Physics Department, Presidency College, Calcutta-700012, India*

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The space-group of *o*-phenanthroline hydrate has been determined as *P31m* on the basis of Weissenberg data together with Wilson's test for the detection of centrosymmetry.

o-Phenanthroline was crystallized from hot water and formed platy crystals. Rotation and Weissenberg photographs gave the following values for the hexagonal unit cell:

$$a = 17.67 \text{ \AA}, \quad c = 8.55 \text{ \AA}.$$

Calculated density based on 9 molecules in the unit cell = 1.28 g cm^{-3} . Observed density = 1.24 g cm^{-3} . All these data are in fairly good agreement with those given by Donnay, Donnay & Harding (1965), who also gave the space group as *P31m*.

In our study we initially observed a reflexion 0006 (in contrast to Donnay *et al.* (1965) who observed only 0003 in the series 000*l*). But a stronger exposure showed a faint 0001 showing that the space group could not be *P3₁12* or *P3₂12*. The space group must be either *P312* or *P31m*.

It was decided to apply Wilson's test for centrosymmetry. The unit cell was considered as orthohexagonal and a zero-layer Weissenberg picture was taken about the orthohexagonal axis (axial length = 30.46 \AA). The reflexions were used to plot a graph according to Wilson's method as adapted by Howells, Phillips & Rogers (1950). The spots were divided into four angular ranges of 0 to 0.1; 0.1 to

0.3; 0.3 to 0.45; and 0.45 to 0.8. Only the last three were used. Now of the two space-groups *P312* and *P31m*, the former should show a centric curve in the Wilson plot and the latter an acentric curve. The plot definitely shows an acentric distribution confirming that the space group is *P31m*. The data also satisfy the modified *N(z)* test for crystal symmetry (Hargreaves & Gogoi, 1966). This also corroborates the conclusion arrived at by Donnay *et al.* No further work is contemplated on the crystal structure of this compound.

Thanks are due to Dr B. S. Basak, Professor of Physics, Presidency College, Calcutta for guidance.

References

- DONNAY, G., DONNAY, J. D. H. & HARDING, M. J. C. (1965). *Acta Cryst.* **19**, 688–689.
 HARGREAVES, A. & GOGOI, B. N. (1966). *Acta Cryst.* **21**, 26–28.
 HOWELLS, E. R., PHILLIPS, D. C. & ROGERS, D. (1950). *Acta Cryst.* **3**, 210–214.

International Union of Crystallography

Commission on Crystallographic Computing

It is proposed to set up a bank of trial structures for testing direct methods. It is frequently found that a new method may be effective for the one or two structures to which it is first applied but that the overall pattern of success is less encouraging when a larger number of trials are made.

The bank of trial structures will cover a range of space groups and structural complexity. The structures should be those which have been difficult to solve, perhaps showing only a few atoms in the first E map, or those which direct methods failed to solve but were subsequently solved in some other way.

Any crystallographer having the data and solution for such a structure is invited to contact Professor M. M. Woolfson, Department of Physics, University of York, Heslington, York YO1 5DD, England, giving as complete a description as possible of the structural problem. If the problem seems suitable for inclusion in the bank then further information will be requested.

Forward Planning of Inter-Congress Meetings

The Executive Committee of the I.U.Cr. is anxious to encourage Inter-Congress meetings to avoid future Triennial Congresses becoming excessively large and cumbersome

to handle. A Sub-Committee on the Union Calendar has therefore been set up [see *Acta Cryst.* (1969), A25, 719] to implement this policy. Its function is to gather information on proposed or prospective meetings, coordinate the long-term planning of meetings which the Union organises or cosponsors, and actively to encourage the initiation of small or intermediate-sized meetings in fields where development is significant.

Since it is the aim of the Sub-Committee to plan at least three, and preferably more, years ahead, it is advisable to have early advice of meetings, being planned or in prospect, which might appropriately come within the category of Union sponsorship or cosponsorship in terms of their content, location, size and date. It would therefore be appreciated if bodies such as Commissions of the Union, National Committee for crystallography, regional associations and other bodies which are contemplating or have begun the planning of a future international meeting on crystallography or with a major content of crystallography would contact the Sub-Committee Chairman: Dr A. McL. Mathieson, Division of Chemical Physics, CSIRO, P.O. Box 160, Clayton, Victoria 3168, Australia.

The Sub-Committee would be pleased to receive advice of provisional details of proposed Inter-Congress meetings as soon as possible and it will also consider requests for Union cosponsorship of these meetings. Nominal financial support could be available in some cases.