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Unit cell and space group of thallous nitrate, $TlNO_3$.

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In view of the discrepancies in the published data on the structure of orthorhombic thallous nitrate, some results we have recently obtained with single crystals of this material may be of interest.

The unit cell dimensions were found to be

$$a = 6{\cdot}22,\quad b = 12{\cdot}32,\quad c = 7{\cdot}90\ \text{Å}$$

and the space group *Pbnm* (No. 62) or $Pbn2_1$ (No. 23) from systematic absences.

The space group differs from that reported by Rivoir & Abbad (1943), but is in agreement with that determined by Ferrari & Cavalca (1950).

We find the true *c* parameter of the unit cell to be twice that found by the former workers, and though this was tentatively proposed by Ferrari & Cavalca, they suggested that it might be due to twinning.

Our single crystals were very carefully selected, including an examination under the polarizing microscope, so as to eliminate this possibility. They included specimens as received from Messrs British Drug Houses (not less than 98% purity), and also after recrystallization from aqueous solution, and needle-shaped crystals were found in each case. One was finally selected from each batch and in the crystal as received, the *c* axis was found to lie along the length of the needle, while in the recrystallized specimen the *b* axis lay in this direction. The unit-cell *c* dimension of the crystal from each growth habit, however, was found to be the same.

Oscillation photographs were taken about the three axes, using Cu $K\alpha$ radiation, and complete indexing of all observed reflexions was possible only by assigning a value to the *c* parameter of 7·90 Å.

In the oscillation photographs about the [001] axis, the alternate layer-line reflexions with *l* odd were very weak, which suggests that the true unit cell may be regarded, to a first approximation, as being equivalent to the stacking, in the direction of the *c* axis, of two smaller cells possessing *c* parameters of half the true value.

Structural changes are reported to take place in thallous nitrate at elevated temperatures (Finbak & Hassel, 1937); it is proposed to investigate these in a further study.

References

Ferrari, A. & Cavalca, L. (1950). *Gazz. chim. ital.*, **80**, 199.

Finbak, C. & Hassel, O. (1937). *Z. phys. Chem.* **35**, 25.

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Bifurcated hydrogen bonds and the structure of cycloserine hydrochloride.

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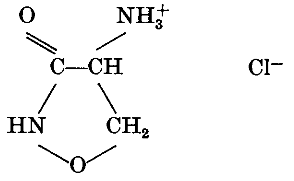
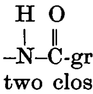
The crystal structure of the hydrochloride of 'cycloserine' (4-amino-3-isoxazolidone):



has been recently determined by Turley & Pepinsky (1956). Their discussion of the structure consists largely of the tabulation of the standard errors in the atomic positional parameter and the resulting probable errors in the interatomic distances and interbond angles, and concludes with several brief statements concerning the hydrogen bonding and the planarity of the heterocyclic ring.

In any X-ray study in which the data are not sufficiently accurate to locate the hydrogen atoms directly, the positions of these atoms can often be deduced by other considerations, among which are the requirements of molecular structure, or the formulation of a hydrogen-bonding arrangement in accord with the established geometrical properties of these bonds. The many examples where this procedure has been followed are certainly too well known to cite or enumerate here.

In the case of cycloserine hydrochloride there are four hydrogen atoms available for hydrogen bonding (three on the $-NH_3^+$ group, one on the ring imino nitrogen atom), and three atoms to serve as hydrogen-bond acceptors (chloride ion, carbonyl oxygen, and ring oxygen). The cation, however, has seven neighbors close enough to be examined in detail for possible hydrogen-bond formation.

Examining first the situation with regard to the  $\overset{\text{H}}{\underset{|}{-\text{N}}}-\overset{\text{O}}{\underset{\|}{\text{C}}}$-group, we note that the carbonyl oxygen atom has two close neighbors: an imino nitrogen at 2·89 Å, and a heterocyclic oxygen at 2·92 Å. The suggestion of Turley & Pepinsky that as a result of these two approaches 'it seems at least possible that a bifurcated hydrogen