

monoclinic crystals, providing that the line PQ (Fig. 1(c)) is marked out in intervals of λ/b (corresponding to the distance OO_1 in Fig. 1(a)), rather than in intervals of b^* .

In the Reciprocal-Axis Setting, the b^* axis is chosen to coincide with the axis of the φ circle (Fig. 1(b)). The ($h0l$) reflexions now no longer have a χ setting of zero. In this case it is convenient to construct the projection of the ($h0l$) net on the plane perpendicular to b^* . This projection (a_1^*, c_1^*) is then used in place of the reciprocal-lattice net in the computer. The angle φ is given by the angle between P_1O and the a_1^* axis and is computed in the manner described by Arndt & Phillips (1957). The angle χ is measured if the distance PB_1 (Fig. 1(c)) is made to correspond to the distance PP_1 (Fig. 1(b)). This is done by providing a scale, free to move along PQ (Fig. 1(c)) and marked out in units of b^* , which is displaced by an amount PD corresponding to the distance (Fig. 1(b)) $P_1P_0 = ha^* \cos \gamma^* + lc^* \cos \alpha^*$. This displacement is found by means of a two-sided rule marked out on one side in units of $a^* \cos \gamma^*$ and on the other in units of $c^* \cos \alpha^*$, each measured from a common origin. It will be observed that all reflexions on a row parallel to b^* can then be found with one setting of the scale PQ , and that these will also all have the same φ setting.

The Real-Axis Setting is most suitable for the collection of data from the ($h0l$) layer, since in this setting the angle χ is always zero, and only φ and θ need to be computed.

In computing the settings for other levels, the reciprocal-lattice net has to be shifted for each level, and no other class of reflexions will, in general, have the same φ or χ setting. The Reciprocal-Axis Setting is more suitable for the collection of three-dimensional data, since reflexions on central zones will have the same φ setting (cf. Furnas & Harker's zone diffractometer) and all reflexions in rows of these zones parallel to b^* will have the same setting of the computer scale PQ . These two triclinic settings also, of course, allow monoclinic crystals to be mounted about axes other than their unique axis on occasions when it may be advantageous to do this.

I should like to thank Dr D. C. Phillips for his encouragement and assistance in this work, the Managers of the Royal Institution for permission to use the Davy Faraday Research Laboratory, and the Department of Scientific and Industrial Research for a maintenance grant.

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Note on the hydrogen bonding in the crystal structure of hydroxylamine. By BODIL JERSLEV, *The Royal Danish School of Pharmacy, Copenhagen, Denmark*

(Received 20 January 1958)

In the crystal structure of hydroxylamine (Meyers & Lipscomb, 1955) the molecules are associated by two different hydrogen bonds between oxygen and nitrogen in neighbouring molecules; the lengths of these hydrogen bonds are 2.74 and 3.07 Å respectively. Since the hydrogen atoms did not show up in the structure determination, the authors refrain from deciding between the three possible arrangements of the hydrogen atoms:

- (a) the 2.74 Å bond is O-H...N, the 3.07 Å bond is O...H-N.
 (b) the 3.07 Å bond is O-H...N, the 2.74 Å bond is O...H-N.
 (c) both the 2.74 Å bond and the 3.07 Å bond are O...H-N.

From a consideration of the crystal structures of five different oximes published so far it has been inferred, that the hydrogen bonds between oxygen and nitrogen, by which the molecules in all the structures are associated, are of the type O-H...N (Jerslev, 1957). In two of the oxime structures, *anti-p*-chlorobenzaldoxime and formamidoxime, the hydrogen bonds result in the formation of chains $\cdots \rangle N-O-H \cdots \rangle N-O-H \cdots$, the

geometry of which is very similar to one of two chains similarly formed by identical hydrogen bonds in the crystal structure of hydroxylamine.

	<i>anti</i> - <i>p</i> -chloro- benzald- oxime	Form- amid- oxime	Hydroxyl- amine	Hydroxyl- amine
$\angle N-O \cdots N'$	109°	100°	101°	129°
$\angle O-N \cdots O'$	112°	122°	111°	83°
$O \cdots N' = N \cdots O'$	2.82 Å	2.81 Å	2.74 Å	3.07 Å

It would seem very likely that a hydrogen bond between oxygen and nitrogen in the hydroxylamine crystal structure is of the same type as that found with the oximes; and both the angles connected with the hydrogen bonds and the lengths of these favour among the systems of hydrogen bonding the one designated by (a).

References

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