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Hydrogen bonding in crystalline hydroxylamine. By JERRY DONOHUE, *Department of Chemistry, University of Southern California, Los Angeles 7, California, U.S.A.*

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Although it is obviously desirable that the hydrogen atoms in crystalline hydroxylamine be located directly either by neutron diffraction or by refinement of complete and highly accurate X-ray data, it is still possible to arrive at some interesting conclusions on the basis of the reported structure (Meyers & Lipscomb, 1955) and the well-known geometrical properties of hydrogen bonds.

In the preceding note, Jerslev concludes, after comparison of the hydroxylamine structure with those of two other oximes, that of the three different possibilities suggested for hydroxylamine by Meyers & Lipscomb, their (a) is the correct one, to wit, that the hydroxylamine molecule forms two hydrogen bonds, $\text{NH} \cdots \text{O}$ of length 3.07 Å with angle $\text{O}-\text{NH} \cdots \text{O}$ of 83° , and $\text{OH} \cdots \text{N}$ of length 2.74 Å with angle $\text{N}-\text{OH} \cdots \text{N}$ of 101° .

Since it is rather unlikely that only one of the two hydrogen atoms of the amino group would be involved in hydrogen bond formation, the consequences of choosing (a) must be examined. Following Meyers & Lipscomb, an observed $\text{N} \cdots \text{O}$ distance of 3.11 Å is eliminated as a possible hydrogen bond because of the unacceptably large angles ($\text{O}-\text{N} \cdots \text{O}$ and $\text{N} \cdots \text{O}-\text{N}$ are both 144°). Accepting the only other short $\text{N} \cdots \text{O}$ distance of 3.18 Å as a hydrogen bond, we arrive at the following possibilities:

	$\text{NH} \cdots \text{O}$	$\angle \text{O}-\text{NH} \cdots \text{O}$	$\angle \text{O} \cdots \text{HNH} \cdots \text{O}$
(a)	3.07 Å, 3.18 Å	$83^\circ, 100^\circ$	158°
(b)	2.74 3.18	111 100	85
(c)	2.74 3.07	111 83	114

	$\text{OH} \cdots \text{N}$	$\angle \text{N}-\text{OH} \cdots \text{N}$
(a)	2.74 Å	101°
(b)	3.07	129
(c)	3.18	101

Both (b) and (c) are clearly preferable to (a), with a slight bias, perhaps, in favor of (c).

Although both Meyers & Lipscomb (1955) and Jerslev (private communication) reject the 3.18 Å distance as a hydrogen bond, the fact remains that the third hydrogen atom of the molecule must be somewhere, and it seems more reasonable to assume that it is placed so that it forms a weak interaction with one of the neighboring oxygen atoms, with the other two, stronger, hydrogen bonds largely determining the molecular arrangement. Such a situation has also been observed in *p*-aminophenol (Brown, 1951), hydroxy-L-proline (Donohue & Trueblood, 1952), L-leucyl-L-prolyl-glycine (Leung & Marsh, 1958), and N,N'-diglycylcystine (Yakel & Hughes, 1954), where $\text{N} \cdots \text{O}$ distances of 3.18, 3.17, 3.18, and 3.31 Å respectively have been discussed in terms of hydrogen bonding in structures in which other stronger such bonds are also present. The meaningful comparison to make, of course, is not with an expected $\text{N} \cdots \text{O}$ van der Waals contact of 3.1 Å, but with the predicted $\text{N} \cdots \text{O}$ distance of 3.6 Å in a situation $\text{N}-\text{H} \cdots \text{O}$ where no interaction whatever existed.

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Notes and News

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In accordance with Statute 6.2 of the Union, the Executive Committee approved the appointment of Professor R. W. Asmussen (Denmark) as Technical Editor of *Acta Crystallographica*. Professor Asmussen was appointed by the Editor of the journal to succeed Dr R. C. Evans, who resigned recently after rendering his services to the Union, and in particular to its journal *Acta Crystallographica*, during a period of more than ten years. Begin-

ning in 1947 Dr Evans played an important rôle in the establishment of the Union, of which he became the first General Secretary, and of its publications. Since then his work with respect to *Acta Crystallographica* has been painstaking and without a break, and it is largely due to his efforts that the technical quality of the journal has been outstanding from the beginning. The Executive Committee wishes to take this opportunity to express to Dr Evans on behalf of the Union its appreciation and gratitude for his efforts devoted to the business of the Union and to *Acta Crystallographica*.