The only earlier work on thermal expansion which is of relevance for comparison with these results is that done by Ubbelohde and his collaborators. They found that in oxalic acid dihydrate (Robertson & Ubbelohde, 1939) and in Rochelle salt (Ubbelohde & Woodward, 1946) the maximum expansion lay nearly in the direction of the short hydrogen bond, and they therefore attributed the large value to a particularly large expansion of the bond itself. There is no evidence of any such large expansion in the results obtained for afwillite. It is not even possible to explain the experimental values by taking some account of the anisotropy of the electrostatic forces, and assuming that any expansion of the hydrogen bonds must be superimposed on a general large expansion perpendicular to the cleavage plane and a small one parallel to it. This also would lead to a large expansion approximately in the direction of the z axis, and not in a direction at right angles to it as has been observed. These results suggest that any simple interpretation of the total thermal expansion in terms of changes in individual bond lengths is not applicable to afwillite. The geometry of the structure as a whole must be considered, and some account taken of changes in bond angles as well as changes in the lengths of bonds.

If changes in bond angles are assumed to take place a plausible mechanism of expansion can be postulated. The three contiguous hydrogen bonds form a zigzag line very nearly in the direction of maximum expansion. If, on heating, there are changes in the bond angles of the oxygens which result in a straightening out of this line, there will be an expansion along its length, and a contraction in a direction at right angles to it. It is suggested tentatively that this is the explanation of the large expansion in a direction within the cleavage plane, and the small one perpendicular to it.

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The structure of oxamide.

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In connexion with investigations going on in this laboratory dealing with the structure and properties of the peptide bond we have redetermined the unit cell dimensions of oxamide. These dimensions,

$$a = 3{\cdot}61\ ,\ b = 5{\cdot}17,\ c = 5{\cdot}62\ \text{Å}\ ,$$

$$\alpha = 83^\circ\ 50',\ \beta = 113^\circ\ 54',\ \gamma = 115^\circ\ ,$$

agree with the results of an earlier investigation (Misch & v. d. Wijk, 1938). The cell contains one molecule (density = 1·667 g.cm.$^{-3}$). Assuming a centre of symmetry, the asymmetric unit of the molecule consists of one oxygen, one nitrogen and one carbon atom, neglecting the hydrogen atoms. All x parameters are zero; consequently the molecules are flat and form a layer structure very similar to the structure of cyanuric acid (Wiebenga & Moerman, 1938; Wiebenga, 1952). The y and z parameters are

	y	z
C	0·002	0·132
N	−0·226	0·259
O	0·217	0·219

The crystals are frequently twinned with a twinning plane (100). This same plane shows a perfect cleavage. We find a C–C distance of 1·49 Å, in contradiction with Misch & v. d. Wijk's assumption that this distance should have the abnormal length of 1·65 Å. The C–O and C–N distances are 1·25 and 1·31 Å respectively. The molecules are linked together in the plane (100) by hydrogen bonds of 2·91 and 2·96 Å. The distances between the planes (100) are van der Waals distances of the order of 3·5 Å. The C–N distance is short; however, rather short C–N distances are also found in cyanuric acid (1·345 Å) and in urea (1·345 Å) (Vaughan & Donohue, 1952). A three-dimensional refinement of the structure is in progress.

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Note added in proof, 14 *March* 1953.—We have found the positions of the hydrogen atoms in the section OYZ of the three-dimensional Fourier synthesis. Consequently, the whole molecule is flat.

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