Acta Cryst. (1956). 9, 832

The crystal structure of chloroacetamide.

By Bruce R. Penfold and W. S. Simpson, *Chemistry Department, Canterbury University College, Christchurch C. 1, New Zealand*

(*Received* 13 *June* 1956)

The approximate crystal structure of chloroacetamide has recently been reported (Dejace, 1955). The crystal structure of this compound had been determined independently in this department (Simpson, 1955) and it is of interest to compare the results of the two analyses.

With a space group $P2_1/c$ the following unit-cell dimensions were found:

$$a = 10{\cdot}25,\ b = 5{\cdot}18,\ c = 7{\cdot}49\ \text{Å}\ (\text{all}\ \pm 0{\cdot}6\%);$$
$$\beta = 102°\ (\pm 0{\cdot}5°).$$

These agree with the measurements of Dejace within experimental error, with the exception of the angle β. (Dejace reports 98° 49′.)

The structure was determined by means of Patterson projections on to (010) and (001), using eye estimated intensities from Cu $K\alpha$ radiation. Projections of the structure on (010) and (001) are shown in Fig. 1.

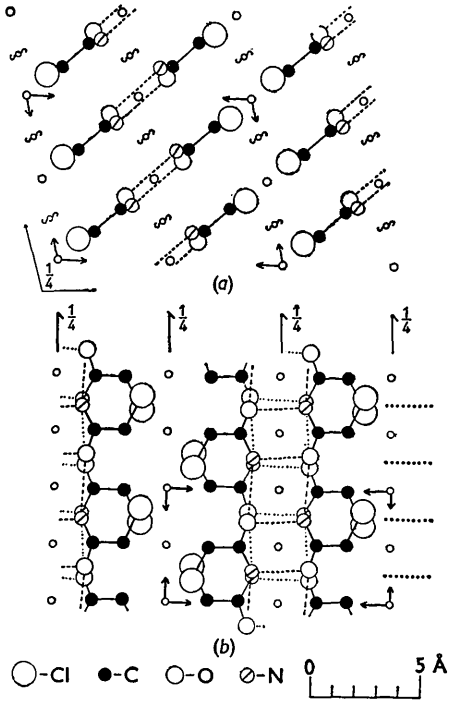

Fig. 1. Structure projected (*a*) on (010), (*b*) on (001).

Atomic coordinates derived from a succession of difference syntheses are listed in Table 1. The difference syntheses revealed that the chlorine atom had a pronounced anisotropic vibration with maximum amplitude approximately perpendicular to the C–Cl bond. Using an appropriate anisotropic temperature factor for chlorine, the listed coordinates gave R factors of 0·15 and 0·16 for the (*h*0*l*) and (*hk*0) reflexions respectively. The interatomic distances listed in Table 2 have a standard deviation of 0·027 Å, except for the C–Cl bond where the value is 0·022 Å. The two sets of N–H · · · O hydrogen bonds have lengths of 2·95 and 2·99 Å, and the closest approach distances of pairs of chlorine atoms are 3·82 and 3·96 Å. The amide group is planar within experimental error.

Table 1. *Atomic coordinates*

Atom	*X*/*a*	*Y*/*b*	*Z*/*c*
Cl	0·115	0·181	0·130
C_1	0·191	0·483	0·182
C_2	0·324	0·487	0·322
O	0·360	0·700	0·395
N	0·383	0·270	0·341

Table 2. *Bond lengths and bond angles, with values reported by Dejace in parenthesis*

Cl–C_1	1·77 Å	(1·81 Å)	Cl–C_1–C_2	108°	(116°)
C_1–C_2	1·54	(1·48)	C_1–C_2–O	118	(111)
C_2–O	1·25	(1·23)	O–C_2–N	127	(130)
C_2–N	1·29	(1·33)	C_1–C_2–N	115	(119)

The two independent analyses of this crystal structure have led to the same general result. Although Dejace does not state a standard deviation, it is to be expected that our atomic coordinates are more precise in view of the considerably better structure-amplitude agreement. It is of interest to note that the coordinates as published by Dejace do not refer to one molecule and furthermore that his Z coordinates appear to be halved with respect to the true unit cell. Only when these Z coordinates are doubled do they agree with those published here.

We wish to acknowledge a grant from the research fund of the University of New Zealand.

References

Dejace, J. (1955). *Acta Cryst.* 8, 851.
Simpson, W. S. (1955). M. Sc. Thesis, University of New Zealand.