structure B, in which the sites with C.N. 16 are completely occupied by niobium, gave much the better agreement with observation. The scattering factors used were those of Thomas & Umeda (1957), and a complex correction for dispersion was made (Dauben & Templeton, 1955).

The coordinates of the ordered structure B were then refined by difference methods. An overall isotropic temperature factor of 0·25 Å^2 was applied, and, with the final parameters shown in Table 1, the R value was 0·13.

To discover the effect of varying the degree of ordering between the D_1 and D_2 sites, calculations were carried out with the other arrangements given in Table 2. The results given there show that the residual steadily diminished as the niobium not accommodated in the a and c sites was increasingly concentrated in the D_1 site, until a minimum of 0·12 was reached when niobium was almost entirely absent from D_2. With this structure, the R value computed over all the observed reflexions was 0·22.

Table 2. *Ordering of sites*

Structure	Sites a and c	Ratio of Nb : Re		R value
		Site D_1	Site D_2	
A				0·24
B	Nb	2·25 : 21·75	2·25 : 21·75	0·13
C	Nb	1·5 : 22·5	3 : 21	0·14
D	Nb	3 : 21	1·5 : 22·5	0·13
E	Nb	3·75 : 20·25	0·75 : 23·25	0·12
F	Nb	4·5 : 19·5	0 : 24	0·12

Distribution of Nb and Re is random in structure A.

We are grateful to Dr Knapton of A.E.I., Aldermaston, for supplying the specimens, and to the Department of Scientific and Industrial Research for a grant for equipment.

References

Bradley, A. J. & Thewlis, J. (1927). *Proc. Roy. Soc.* A, **115**, 456.
Dauben, C. H. & Templeton, D. H. (1955). *Acta Cryst.* **8**, 841.
Farquhar, M. C. M. & Lipson, H. (1946). *Proc. Phys. Soc.* **58**, 200.
Greenfield, P. & Beck, P. A. (1956). *J. Metals, N.Y.* **8**, 265.
Knapton, A. G. (1958). *J. Inst. Met.* **87**, 28.
Niemiec, J. & Trzebiatowski, W. (1956). *Bull. Acad. Polon. Sci.* **4**, 601.
Rogers, D. & Moffett, R. H. (1956). *Acta Cryst.* **9**, 1037.
Thomas, L. H. & Umeda, K. (1957). *J. Chem. Phys.* **26**, 293.

Acta Cryst. (1964). **17**, 63

Crystallographic data for 1,2-dichloronaphthalene.

By James Trotter, *Department of Chemistry University of British Columbia, Vancouver 8, B. C., Canada*

(*Received* 17 *June* 1963)

Crystal data previously reported for 1,2-dichloronaphthalene (Trotter, 1960) actually corresponded to the 1,3-derivative (Trotter, 1961). The data for the 1,2-derivative have now been determined from precession films; crystals of 1,2-dichloronaphthalene are thick colourless plates, with (100) well developed, and smaller {011} forms.

Crystal data (λ, Mo $K\alpha = 0{\cdot}7107$ Å)

1,2-Dichloronaphthalene, $C_{10}H_6Cl_2$; M, 197·1; m.p., 37 °C.

Monoclinic,

$$a = 7{\cdot}26 \pm 0{\cdot}02,\ b = 8{\cdot}96 \pm 0{\cdot}02,\ c = 13{\cdot}72 \pm 0{\cdot}03\ \text{Å};\ \beta = 104{\cdot}2^\circ \pm 0{\cdot}1^\circ.$$

Volume of the unit cell: 865 Å^3.
D_m (flotation in aqueous KI): 1·51 g.cm^{-3},
D_x (with $Z = 4$): 1·51 g.cm^{-3}.
Absent reflexions: $h0l$ when l is odd, $0k0$ when k is odd. Space group is $P2_1/c(C_{2h}^5)$.
No further work on this compound is planned.

The author is indebted to Dr Wolfgang Strehlow for suggesting measurement of these data and for the crystal sample, and to the National Research Council of Canada for financial support.

References

Trotter, J. (1960). *Acta Cryst.* **13**, 276.
Trotter, J. (1961). *Canad. J. Chem.* **39**, 1964.