Table 3. *Distances* (Å) *from least-squares planes*

| I | | II | | III | |
|---|---|---|---|---|---|
| C(1) | 0·009 (4) | C(5) | 0·034 (4) | C(5) | −0·002 (4) |
| C(2) | −0·008 (4) | Cl(2) | −0·009 (1) | N(2) | 0·005 (9) |
| C(3) | 0·008 (4) | N(1) | −0·013 (3) | C(6) | −0·001 (6) |
| C(4) | −0·009 (4) | N(2) | −0·012 (3) | C(9) | −0·001 (6) |
| Cl(1)* | 0·025 (1) | C(4)* | 0·375 (4) | | |
| O(1)* | −0·033 (4) | | | | |
| O(2)* | 0·063 (4) | | | | |
| N(1)* | 0·089 (3) | | | | |

Angles between planes (°): I–II 50 (1)
II–III 5 (1)

* Atoms not used in the definition of the least-squares plane.

50 (1)° with the amidine group. This rotation is necessary to avoid repulsion between Cl(2) and O(2). The observed distance is 3·286 (6) Å and corresponds to the sum of the van der Waals radii of Cl and O. The angle between the cyclobutene and amidine groups results from torsion angles C(3)–C(4)–N(1)–C(5) of −37 (1)° and C(4)–N(1)–C(5)–Cl(2) of −24 (1)°. This conformation allows an almost equal contribution of the N(1) $\pi$ electron to the neighbouring $\pi$ systems. C(5) has a small amount of pyramidal character (Table 3).

In the crystal structure there is an intermolecular contact distance of 3·440 (4) Å between Cl(1) and Cl(2) (symmetry code: $x$, $1-y$, $-\frac{1}{2}+z$). No other intermolecular distances are shorter than the sum of the van der Waals radii of the constituent atoms.

### References


BLESSING, R. H., COPPENS, P. & BECKER, P. (1974). *J. Appl. Cryst.* **7**, 488–492.

*International Tables for X-ray Crystallography* (1974). Vol. IV. Birmingham: Kynoch Press.

MAIN, P., WOOLFSON, M. M., LESSINGER, L., GERMAIN, G. & DECLERCQ, J.-P. (1974). *MULTAN 74. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

RIED, W., DIETSCHMANN, H. & ERLE, H.-E. (1981). *Synthesis.* In the press.

STEWART, J. M., KRUGER, G. J., AMMON, H. L., DICKINSON, C. & HALL, S. R. (1972). The XRAY system – version of June 1972. Tech. Rep. TR-192. Computer Science Center, Univ. of Maryland, College Park, Maryland.

STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.


# Notes and News

*Acta Cryst.* (1981). B**37**, 2250

## ICSD—Inorganic Crystal Structure Data Base

Complementary to the well known Cambridge Crystallographic Data File, a similar file for inorganic substances has been established at the University of Bonn (G. Bergerhoff and I. D. Brown). The current file contains information on 9000 structures: chemical name, chemical formula, mineral name, unit cell, space group, coordinates, temperature factors, references, remarks. More detailed information will be given in a paper to be published in *Acta Crystallographica*. The data base will be made available by Fachinformationszentrum Energie Physik Mathematik GmbH (Dr H. Behrens), D-7514 Eggenstein-Leopoldshafen, Federal Republic of Germany, from 1982 on, in three versions:

(1) On-line access *via* telecommunications systems (Euronet, Datex-P, *etc.*).

(2) Leasing the up-to-date data base and retrieval programs (IBM–FORTRAN) at an annual rate.

(3) Leasing only the up-to-date data base at an annual rate.

Detailed conditions are available on request from Dr Behrens at the address given above.