

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) π electron to the neighbouring π 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

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Notes and News

Acta Cryst. (1981). **B37**, 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 Fachinformati-

zentrum 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.