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Chemotherapeutic Agents. The Structure of 1-(2-Chloroethyl)-3-(4-carbamoylpyrazol-3-yl)-Δ^2-1,2,3-triazolinium Chloride*

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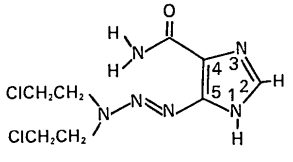
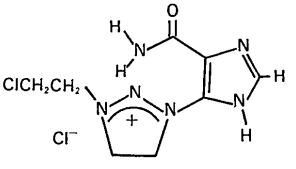
A number of nitrogen mustards have shown significant activity in experimental tumors; however, many of them exhibit erratic behavior in clinical tests. The nitrogen mustard 5-[3,3-bis(2-chloroethyl)-1-triazeno]-pyrazole-4-carboxamide was found to undergo a spontaneous ring closure to form the compound 1-(2-chloroethyl)-3-(4-carbamoylpyrazol-3-yl)-Δ^2-1,2,3-triazolinium chloride, $[ClON_6C_8H_{12}]^+Cl^-$, which shows no *in vivo* activity in experimental tumors. The structure of this ionic compound was determined by single-crystal X-ray diffraction techniques, using 1253 independent counter-collected reflections. A full-matrix least-squares refinement yielded a conventional R value of 0·0497. The space group is *Pbca* and the cell dimensions are $a = 14{\cdot}151$ (5), $b = 16{\cdot}990$ (5) and $c = 10{\cdot}344$ (10) Å. The observed density of 1·489 g.cm^{-3} is consistent with 8 molecules per unit cell, $d_c = 1{\cdot}490$ g.cm^{-3}. The molecule contains a positively charged triazolinium ring with the chloride ion almost symmetrically located above the ring. The planes of the pyrazole and triazolinium rings make an angle of 50° while the amide group makes an angle of 22° with the pyrazole ring. The amide oxygen atom interacts with the triazolinium ring but on the side opposite to the chloride ion. Both pyrazole tautomers are present in the crystal.

Introduction

Several nitrogen mustards have exhibited antitumor activity and recently there has been considerable interest in 5-[3,3-bis(2-chloroethyl)-1-triazeno]-imidazole-4-carboxamide, compound (I) (NSC-82196). This compound showed significant activity in experimental tumors (Shealy & Krauth, 1966); however, it has been disappointing in many clinical trials (Cancer Chemother. Rept., 1969–71). Oral administration of compound (I) showed that gastrointestinal absorption was erratic and that almost all of the absorbed material can be recovered from the urine as the ionic product (II) (Loo, Stasswender, Jardine & Frei, 1967; Luce, Thurman, Isaacs & Talley, 1970). Compound (I) is transformed rapidly to the ionic product at 37°C *in vitro* (Vogel, Denham, Waalkes & DeVita, 1970) and more slowly even in the solid state (Shealy, Krauth, Holum & Fitzgibbon, 1968). The crystal structure of compound (II) has been reported (Abraham, Rutherford & Rosenstein, 1969).



I



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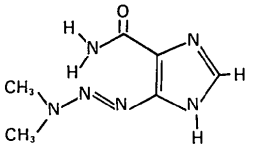

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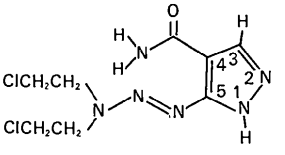

IV

The compound 5-(dimethyltriazeno)-imidazole-4-carboxamide, (III) (NSC-45388), is also absorbed erratically in the gastrointestinal tract (Loo *et al.*, 1967; Loo, Luce, Jardine & Frei, 1968), but it is clinically more useful than compound (I) in inducing temporary remission of malignant melanoma (Shealy, Montgomery & Lafter, 1962; Loo, 1971). Many authors have assumed that the mechanism of the anticancer activity of these compounds is similar to the mechanism of carcinogenesis of aryltriazenes proposed by Preussman, von Hodenberg & Hengy (1969). These workers suggested that the aryl-triazenes ultimately degrade to a carbonium ion plus other products with the carbonium ion being responsible for the alkylating properties of these compounds. However, as the authors point out, *in vitro* metabolism occurs only with lung and liver microsomal fractions and never with brain, neurogenic tissue or kidney, where the tumors are observed to occur. Although they offer several rationalizations to explain why the site of alkylating agent generation is different from the site of tumor activity, there is some doubt about the actual mechanism of carcinogenesis. Hansch (1971) has reported that the mechanism for the antitumor activity of compound (I) is probably different from that of the other disubstituted triazene compounds.

Abraham *et al.*, proposed that compound (I) may act as an inhibitor of an enzyme for which guanine or a guanine derivative might be the substrate. This was based upon the structural resemblance of compound (I) to guanine in the solid state. The compound 5-aminoimidazole-4-carboxamide is a known inhibitor of guanine (Mandel, 1957) and this enzyme system may be suitable for an *in vitro* test of the proposal of Abraham, *et al.* (1969). Compound (II) is inactive *in vivo* due to poor transport across cell membranes; however, it might be an *in vitro* inhibitor of a guanine specific enzyme.

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Because of the activity of compound (I), 5-[3,3-bis(2-chloroethyl)-1-triazeno]-pyrazole-4-carboxamide, compound (IV), was synthesized and tested (Loo, 1971; Cheng, 1971). Although the pyrazole and imidazole analogs are structurally similar, they may have different antitumor activities. The change in electron density within the five-membered ring may affect cell membrane transport, and if the activity is due to enzyme inhibition, position 7 of the imidazole ring frequently is an enzyme binding point.

The structural analysis shows that the *in vivo* tested pyrazole compound is the ionic product 1-(2-chloroethyl)-3-(4-carbamoylpyrazol-3-yl)-Δ^2-1,2,3-triazolinium chloride. Although this material is inactive *in vivo*, it is of significant interest for *in vitro* studies of enzyme inhibition. We would like to report the structure of the ionic compound and compare the structure with that of compound (II).

Experimental

A small sample of 1-(2-chloroethyl)-3-(4-carbamoylpyrazol-3-yl)-Δ^2-1,2,3-triazolinium chloride ($Cl_2ON_6C_8H_{12}$) was recrystallized from ethanol, and uniform prismatic-shaped, clear white crystals were obtained. A single crystal having the dimensions $0{\cdot}376 \times 1{\cdot}200 \times 0{\cdot}136$ mm was selected for data collection. X-ray photographs taken with zirconium-filtered Mo $K\alpha$ radiation ($\lambda = 0{\cdot}71069$ Å) indicated the crystal belonged to the orthorhombic space group *Pbca*. The unit-cell dimensions were determined at room temperature from precession and Weissenberg photographs, which were calibrated with superimposed NaCl powder lines, $a = 5{\cdot}6402$ Å.

Crystal data

$Cl_2ON_6C_8H_{12}$ M.W. 279·1
$a = 14{\cdot}151$ (5), $b = 16{\cdot}990$ (5), $c = 10{\cdot}344$ (10) Å.
Systematic absences: $hk0$, $h = 2n+1$; $0kl$, $k = 2n+1$; $h0l$, $l = 2n+1$.
(Observed on precession and Weissenberg photographs and all three-dimensional counter-collected data.)
Space group: *Pbca* (D_{2h}^{15}), $Z = 8$,
$F(000) = 1152$, $V = 2487{\cdot}0$ Å^3, $\mu = 46{\cdot}83$ cm^{-1} (Cu $K\alpha$), Cu $K\alpha$ ($\lambda = 1{\cdot}5418$ Å), $D_{obs} = 1{\cdot}489$ g.cm^{-3}, $D_{calc} = 1{\cdot}490$ g.cm^{-3}.

The errors associated with the unit-cell parameters are the average deviations calculated from measuremenst of several high-angle reflections or layer lines. The density was measured using the flotation technique with a mixture of benzene and 1,3-dibromobenzene.

Three-dimensional data were collected through the eight levels ($hk0$ to $hk8$) with a Philips Pailred diffractometer using equi-inclination Weissenberg geometry and the continuous ω-scan technique. A scan speed of 1° per min was used and background counts of 20 sec were taken at the extremes of the scan range. Cu $K\alpha$ radiation and a graphite monochromator crystal ($d_{200} = 3{\cdot}354$ Å) were used to collect the room temperature counter data. Three reference reflections were monitored throughout the data-collection period. By the time the fourth level had been collected significant crystal deterioration had occurred. When the eighth level of data was collected, the reference intensities had decreased by more than 40%. The intensity decrease was initially linear with exposure time, but significant deviations from linearity occurred by the fourth level and the crystal turned an opaque gold color. A second crystal of dimensions $0{\cdot}365 \times 1{\cdot}230 \times 0{\cdot}144$ mm was selected, and a second set of intensity data was collected in the reverse order, beginning with level $hk8$. Crystal deterioration was apparent for the lower levels although a much shorter collection period was used.

Only data collected in the linear decay regions were used, and linear correction factors were applied. The data were corrected for Lorentz and polarization factors, and the data for the two crystals were independently corrected for absorption (Stemple, 1970). The two data sets were combined, and all duplicate and equivalent reflections were averaged to provide one unique data set. A total of 1253 independent reflections were obtained and 1043 were considered to be observed, $I > 2\sigma(I)$. The levels were scaled together by comparison with reference reflections.

Standard deviations were assigned on the basis of counting statistics. Included in the standard deviation is a term for instrument instability which was chosen as 3% of the magnitude of the observed raw intensity. The standard deviation is given by

$$\sigma(F_o)^2 = \frac{A[N_S + R^2 N_B + (0{\cdot}03 I_o)^2]}{4\mathrm{Lp} I_o}$$

$$I_o = N_S - R N_B$$

where N_S is the total count obtained during a scan cycle, N_B is the total background count, R is a constant which relates the background count time to the total scan time, I_o is the number of counts for the reflection, and A is the absorption correction.

The scattering factors of Cromer & Waber (1965) were used for all nonhydrogen atoms (Cl^-, Cl, O, N, C). The scattering factors for the chlorine atom and the chloride ion were corrected for the real and complex parts of the anomalous dispersion using the values of Cromer (1965). The hydrogen scattering factors were those calculated by Stewart, Davidson & Simpson (1965).

Structure determination

The structure amplitudes were converted to $|E_h|$'s, and a program that involves a reiterative application of Sayre's relations was applied to the 125 E's > 1·69 (Long, 1965). The mode of operation was such that newly determined signs were used immediately in the determination of other signs. E–Fourier maps were

Table 1. *Atomic and thermal parameters for 1-(2-chloroethyl)-3-(4-carbamoylpyrazol-3-yl)-Δ^2-1,2,3-triazolinium chloride*

Standard deviation of the last figure is given in parentheses.

Anisotropic thermal parameters have the form

$$\exp[-0.25(B_{11}h^2a^{*2}+B_{22}k^2b^{*2}+B_{33}l^2c^{*2}+2B_{12}hka^*b^*+2B_{13}hla^*c^*+2B_{23}klb^*c^*)]\,.$$

	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Cl(17)	0·35643 (9)	0·07366 (9)	0·39826 (10)	3·96 (6)	8·98 (11)	4·16 (9)	0·94 (6)	−0·19 (5)	0·58 (5)
Cl(13)	0·1405 (1)	0·1930 (1)	−0·0992 (2)	6·02 (9)	9·99 (13)	10·04 (14)	−0·75 (8)	−2·08 (7)	2·60 (8)
C(12)	0·1133 (4)	0·1665 (5)	0·0542 (7)	3·5 (3)	12·2 (6)	10·8 (5)	−2·3 (3)	−0·4 (3)	−3·5 (4)
C(11)	0·1845 (4)	0·1119 (3)	0·1159 (4)	4·3 (2)	6·6 (4)	5·5 (3)	−2·0 (3)	−0·1 (2)	0·5 (2)
N(8)	0·2789 (3)	0·1444 (3)	0·1112 (4)	3·8 (2)	6·1 (3)	3·2 (2)	−0·2 (2)	0·1 (2)	0·4 (2)
N(7)	0·3446 (3)	0·1052 (3)	0·0577 (3)	4·3 (3)	5·9 (3)	3·0 (2)	−0·4 (2)	0·3 (2)	−0·2 (2)
N(6)	0·4225 (3)	0·1434 (3)	0·0719 (3)	4·4 (2)	5·3 (3)	3·8 (2)	−0·0 (2)	0·2 (2)	−0·9 (2)
C(9)	0·3082 (4)	0·2197 (3)	0·1694 (4)	4·1 (3)	4·6 (3)	6·0 (3)	0·3 (2)	−0·4 (2)	−1·2 (2)
C(10)	0·4121 (4)	0·2175 (4)	0·1398 (5)	4·1 (3)	6·6 (4)	7·1 (3)	−0·2 (2)	0·4 (2)	−2·9 (3)
C(5)	0·5051 (4)	0·1164 (3)	0·0133 (4)	4·5 (3)	4·7 (3)	2·6 (3)	0·3 (2)	0·4 (2)	−0·7 (2)
N(4)	0·5837 (3)	0·1126 (3)	0·0807 (3)	5·0 (2)	6·5 (3)	3·6 (2)	0·3 (2)	−0·1 (2)	−0·1 (2)
N(3)	0·6502 (3)	0·0870 (3)	−0·0013 (4)	5·3 (2)	5·6 (3)	5·1 (3)	−0·8 (2)	0·4 (2)	−1·5 (2)
C(2)	0·6138 (4)	0·0716 (3)	−0·1210 (5)	5·0 (3)	5·6 (3)	3·9 (3)	−0·0 (2)	0·4 (2)	−0·5 (2)
C(1)	0·5181 (4)	0·0899 (3)	−0·1155 (4)	4·2 (3)	4·4 (3)	4·9 (4)	−0·5 (2)	−0·6 (2)	−0·2 (2)
C(15)	0·4473 (4)	0·0946 (3)	−0·2207 (5)	3·7 (3)	4·9 (3)	4·0 (3)	−0·4 (2)	0·6 (2)	−0·2 (2)
O(16)	0·3796 (3)	0·1365 (2)	−0·2131 (3)	4·5 (2)	7·2 (2)	5·5 (2)	−0·1 (2)	−0·3 (1)	−0·4 (2)
N(14)	0·4671 (3)	0·0487 (2)	−0·3263 (4)	4·4 (2)	5·6 (3)	4·5 (2)	0·6 (2)	−0·6 (2)	0·0 (2)

calculated for the four solutions having the highest self-consistency indexes (C),

$$C=\langle|E_A\sum_{A=B+C}E_BE_C|\rangle/\langle|E_A\sum_{A=B+C}|E_B|\,|E_C|\rangle.$$

The correct structure could be seen in the E maps associated with the three highest consistency indexes. The peaks in the E map of highest consistency index (92·6%) were of uniform height and no spurious peaks of comparable magnitude were present. In the other two maps the correct peaks were of variable height and several spurious peaks were of comparable magnitude; however, it is probable that the correct structure could have been obtained from any of these maps.

A full-matrix least-squares isotropic refinement of the parameters of seventeen nonhydrogen atoms with all 1043 observed reflections yielded $R=0{\cdot}120$. All hydrogen atoms were located in a difference-Fourier map; however, the hydrogen positional parameters were calculated assuming C–H and N–H distances of 0·97 and 0·90 Å. The inclusion of these parameters in a structure-factor calculation reduced R to 0·101. This is significant at the $\alpha=0{\cdot}005$ level based on Hamilton's significance test (Hamilton, 1965). Anisotropic refinement of all nonhydrogen atoms reduced R to 0·068 which is significant at the $\alpha=0{\cdot}005$ level. The hydrogen positions were not refined, but their contributions to the structure factors were included in each least-squares calculation. New hydrogen atom positions were determined after each set of least-squares calculations.

Since the compound is ionic, a positive charge is spread over the three nitrogen atoms in the triazoline ring. To accommodate this loss of one electron, the three nitrogen atoms were assigned occupancy factors of 0·952 per nitrogen. A final full-matrix least-squares refinement of the model with all observed reflections yielded $R=0{\cdot}0497$. The function minimized in the refinement is $\sum w(k|F_o|-|F_c|)^2$ where $w=[1/\sigma(F_o)]^2$.

Table 1 (*cont.*)

	x	y	z	B
H(12)	0·1063	0·2133	0·1071	2·0
H(12′)	0·0514	0·1421	0·0557	2·0
H(11)	0·1835	0·0616	0·0717	2·0
H(11′)	0·1668	0·1023	0·2051	2·0
H(9)	0·2989	0·2176	0·2622	2·0
H(9′)	0·2791	0·2628	0·1228	2·0
H(10)	0·4477	0·2157	0·2199	2·0
H(10′)	0·4281	0·2605	0·0822	2·0
H(4)	0·5921	0·1247	0·1647	2·0
H(3)*	0·7114	0·0807	0·0199	2·0
H(2)	0·6480	0·0517	−0·1954	2·0
H(14)	0·5211	0·0163	−0·3231	2·0
H(14′)	0·4259	0·0453	−0·3992	2·0

* Position of hydrogen in tautomer N(3)–H.

A final three-dimensional difference-Fourier map contained no peak larger than 0·6 e.Å^{-3}. The estimated standard deviations of the parameters were calculated from the inverse of the normal-equations matrix of the last least-squares cycle. All shifts of the parameters during the final cycle were less than 0·1 of the estimated standard deviation of the parameters. The final positional and thermal parameters are listed in Table 1, and the squares of the calculated and observed structure factors are listed in Table 2. Bond lengths, angles and some intermolecular distances are listed in Table 3. C–H and N–H distances of 1·07 and 1·00 Å were used in calculating inter- and intramolecular distances involving hydrogen atoms.

Discussion

The projection of the unit cell contents onto the *ac* plane is shown in Fig. 1 and bond lengths, angles and the numbering system used in the tables and figures

are shown in Fig. 2. Fig. 3 shows the interaction distances between the triazolinium ring and the chloride ion and amide oxygen.

A unit-weighted least-squares plane fitted to the triazolinium ring gives the equation $0{\cdot}169x-0{\cdot}468y+0{\cdot}867z=0{\cdot}513$ with an average deviation of 0·004 Å and a maximum deviation of 0·006 Å. A least-squares plane fitted to the pyrazole ring gives the equation of $0{\cdot}207x+0{\cdot}939y-0{\cdot}276z=3{\cdot}285$ with an average deviation of 0·008 Å and atoms N(1) and C(2) out of the plane by 0·012 and 0·010 Å respectively. The triazolinium and pyrazole rings may be considered to be planar. The planes of the two rings make an angle of 50° and the amide group makes an angle of 22° with the pyrazole ring. In the imidazole analog, the two rings, the amide group and the α-carbon of the chloroethyl group are roughly coplanar.

Peaks corresponding to hydrogen atom positions on the pyrazole ring were located readily in the difference-Fourier map. Apparently, both tautomers are present in the crystal with an N(4)H/N(3)H tautomer ratio of about 4/1. The ratio was estimated from a series of structure-factor calculations and difference-Fourier maps. The hydrogen position corresponding to the N(4)H tautomer was used in the refinement. Structural studies on pyrazole indicate that the π electrons are delocalized, which results in a symmetric set of bond lengths (Larsen, Lehmann, Sotofte & Rasmussen, 1970; Berthou, Elguero & Rérat, 1970); however, different substituents and variations in hydrogen bonding affect the bond lengths in the present structure. For tautomer N(3)H the intermolecular H–Cl(17) distance of 2·12 Å and the N(3)HCl(17) angle of 170° indicate a strong hydrogen bond. This strong interaction probably determines the packing and conformation of both tautomers in the solid state. The hydrogen of the other tautomer is not involved in hydrogen bonding.

Table 2. *Squares of the observed and calculated structure factors*

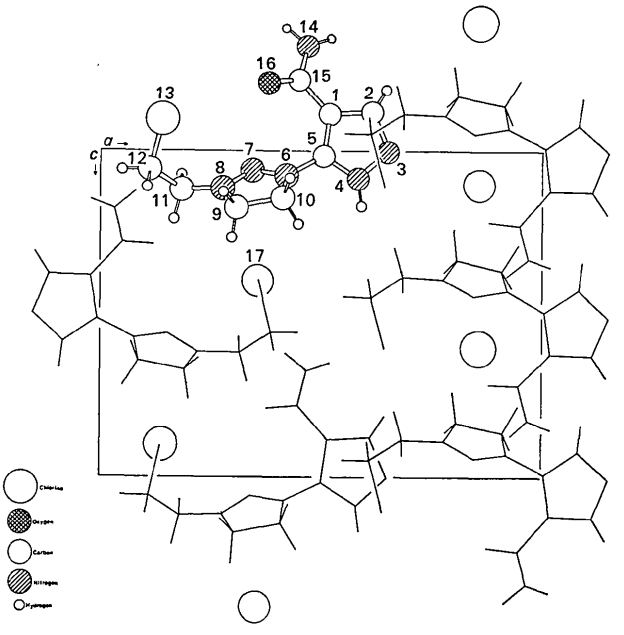

Fig. 1. Projection of the unit cell contents onto the *ac* plane. The atoms corresponding to the coordinates in Table 1 are labeled. All ionic chlorine atoms are shown as spheres.

The positive charge in the triazolinium ring is delocalized over the three nitrogen atoms and the two N–N bonds of 1·289 (7) and 1·272 (6) Å are statistically equivalent. The chloride ion lies above the ring and slightly skewed towards N(8) and C(9). The distances between the chloride ion and the ring are N(8)–Cl = 3·386 (4), N(7)–Cl = 3·567 (4), N(6)–Cl = 3·698 (4), C(9)–Cl = 3·497 (5) and C(10)–Cl = 3·707 (6) Å. The triazolinium ring is tilted so that the amide oxygen is located on the opposite side of the ring from the chloride ion and N(6)–O(16) = 3·013 (5), N(7)–O(16) = 2·894 (5) and N(8)–O(16) = 3·648 (5) Å. The oxygen and nitrogen atoms of the amide group were identified by the bond lengths, temperature factors and the two amide hydrogen atoms observed in the difference-Fourier map. The amide hydrogens form no strong hydrogen bonds. In the imidazole analog (Abraham *et al.*, 1969), the bond lengths in the triazolinium ring are equivalent to those reported in this work, and the chloride ion also lies above the ring but at a slightly greater distance. The triazolinium ring, imidazole ring and amide group are held in a coplanar conformation by a weak interaction between the amide hydrogen and N(7).

The chloroethyl group is in the *gauche* conformation

Table 3. *Inter- and intramolecular distances and bond angles*

C(1)—C(2)	1·390 (8) Å	C(10)—O(16)*	2·946 (7) Å
C(2)—N(3)	1·367 (7)	C(9)—O(16)*	2·910 (6)
N(3)—N(4)	1·339 (6)	H(9)—O(16)*	2·743
N(4)—C(5)	1·314 (6)	H(9′)—O(16)*	2·806
C(5)—C(1)	1·418 (6)	H(10)–O(16)*	2·778
C(5)—N(6)	1·395 (7)	H(10′)–O(16)*	2·837
N(6)—N(7)	1·289 (7)	Cl(17)–H(12′)*	2·932
N(7)—N(8)	1·272 (6)	Cl(17)–H(3)*	2·125†
N(8)—C(9)	1·473 (7)	Cl(17)–H(11)*	2·872
C(9)—C(10)	1·503 (7)	N(14)–H(11)*	2·990
C(10)–N(6)	1·448 (8)	H(14′)–H(11)	2·315
N(8)—C(11)	1·446 (7)	C(1)—C(2)—N(3)	106·7 (4)°
C(11)–C(12)	1·510 (9)	C(2)—N(3)—N(4)	111·8 (4)
C(12)–Cl(13)	1·694 (7)	N(3)—N(4)—C(5)	105·9 (4)
C(1)—C(15)	1·481 (7)	N(4)—C(5)—C(1)	111·9 (4)
C(15)–N(14)	1·371 (6)	C(5)—C(1)—C(2)	103·7 (4)
C(15)–O(16)	1·197 (6)	C(5)—C(1)—C(15)	125·8 (5)
Cl(17)–N(6)	3·698 (4)	C(2)—C(1)—C(15)	129·8 (4)
Cl(17)–N(7)	3·567 (4)	C(1)—C(15)–N(14)	114·6 (9)
Cl(17)–N(8)	3·386 (4)	C(1)—C(15)–O(16)	121·7 (4)
Cl(17)–C(9)	3·497 (5)	N(14)–C(15)–O(16)	123·7 (4)
Cl(17)–C(10)	3·707 (6)	C(1)—C(5)—N(6)	128·5 (4)
N(8)—O(16)	3·648 (5)	N(4)—C(5)—N(6)	119·6 (4)
N(7)—O(16)	2·894 (5)	C(5)—N(6)—N(7)	120·0 (4)
N(6)—O(16)	3·013 (5)	C(5)—N(6)—N(10)	125·6 (5)
N(6)—C(1)	2·533 (6)	N(6)—N(7)—N(8)	108·2 (4)
Cl(13)–N(7)	3·634 (5)	N(7)—N(8)—C(9)	115·3 (4)
Cl(13)–N(8)	3·042 (4)	N(8)—C(9)—C(10)	100·0 (4)
Cl(17)–H(9)	2·891	C(9)—C(10)–N(6)	102·7 (4)
Cl(17)–H(10)	3·271	C(10)—N(6)—N(7)	114·0 (4)
		N(7)—N(8)—C(11)	119·4 (5)
		C(9)—N(8)—C(11)	125·3 (4)
		N(8)—C(11)–C(12)	111·6 (5)
		C(11)—C(12)–Cl(13)	114·1 (4)

* Intermolecular distances.
† Distance to hydrogen in N(3)–H tautomer.

with the angle between the C(11)–Cl bond and the triazolinium ring being 55°. The C–N and C–C distances of 1·446 (7) and 1·510 (9) Å are equivalent to those reported for the imidazole structure. The C–Cl distance of 1·694 (7) is significantly shorter than the corresponding distance of 1·81 Å; however, no correction has been made for the relatively large thermal motion.

In solution the conformations of the pyrazole and imidazole compounds are probably the same. Differences in antitumor activity must be associated with the locations of the nitrogen atoms in the five-membered pyrazole and imidazole rings. The geometries of the ring systems essentially are identical, but the distribution of charge densities may affect transport across cell membranes or enzyme binding. N(7) of the imidazole ring is frequently an enzyme binding point in guanine-like substrates. A careful comparative study of the activity of compounds of this type is of interest.

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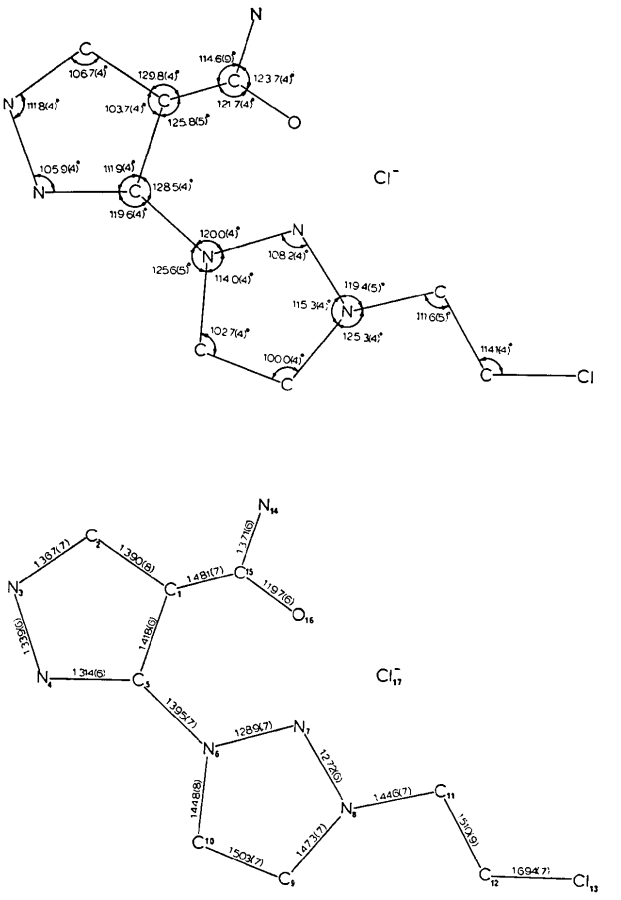

Fig. 2. Bond lengths, bond angles and numbering system for 1-(2-chloroethyl)-3-(4-carbamoylpyrazol-3-yl)-Δ^2-1,2,3-triazolinium chloride.

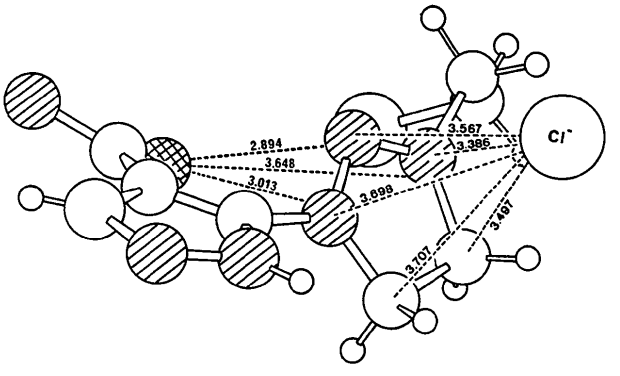

Fig. 3. Interaction distances between the triazolinium ring and the chloride ion and amide oxygen atom.