bases only the acceptor sites for protons are available. Thus, base–base interaction is not possible. In (I) *B* and *C*, N(1) and N(2), but not N(8), are involved in hydrogen bonds. However, in (I)*A*, N(1) and N(8) are hydrogen bonded whereas N(2) is free and does not make any contact < 3·50 Å. The ring O(4′) atom of the ribose is not involved in a hydrogen bond. Base stacking does not occur in these structures.

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(*E*)-3-Hexenedinitrile, $C_6H_6N_2$

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Abstract. $M_r = 106{\cdot}13$, $P2_1/c$, $a = 4{\cdot}033\ (2)$, $b = 14{\cdot}201\ (8)$, $c = 5{\cdot}331\ (6)$ Å, $\beta = 103{\cdot}04\ (6)°$, $V = 297{\cdot}4$ Å^3, $Z = 2$, $D_x = 1{\cdot}185$ g cm^{-3}, Mo $K\alpha$ radiation, $\lambda = 0{\cdot}7107$ Å, $\mu = 0{\cdot}82$ cm^{-1}, $F(000) = 112$, $T = 296\ (2)$ K, $R = 0{\cdot}079$ for 524 reflections. The molecule lies on a center of symmetry; it is close to planar with the cyano groups eclipsing the double bond. Bond lengths and angles are normal. The short contacts in the packing are from the nitrogen atom to the cyano carbon atom, 3·38 (1) and 3·65 (1) Å, and from the nitrogen atom to the α-carbon atom, 3·39 (1) Å, all of types found in the packing of other nitriles.

Introduction. As part of a study of Lewis-acid–Lewis-base interactions in the solid state we have determined the structure of the title compound. This structure is the third in a series where we are examining the environment of the nitrile group attached to otherwise aliphatic hydrocarbons. See also Britton & Gleason (1982–fumaronitrile) and Gleason & Britton (1982–tetramethylsuccinonitrile).

Experimental. Sample obtained from the organic chemical collection of the Department of Chemistry of the University of Minnesota, recrystallized from ethanol, crystal roughly equant, 0·2 × 0·3 × 0·3 mm, lattice parameters determined from accurate measurement of positions of eight reflections with $10 < \theta < 18°$, Hilger & Watts four-circle automatic diffractometer, systematic absences $0k0$ $k = 2n + 1$, $h0l$ $l = 2n + 1$, no absorption corrections, one quadrant of data, $0 < \theta < 26°$, h 0–4, k 0–18, l −6–6, 569 independent reflections, 524 with $I_{\rm obs} > 0$ used; two check reflections, measured every 25 data measurements, showed no significant variation with time; trial structure found

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by direct methods, refined (on F^2) with full-matrix least squares; hydrogen-atom positions found in a difference electron density map and allowed to vary in the refinement with fixed $B = 5{\cdot}0$ Å^2; $R = 0{\cdot}079$, $R_w = \sum w(|F_o|^2 - |F_c|^2)^2/\sum w|F_o|^4 = 0{\cdot}021$, $S = 2{\cdot}13$, $w = [\sigma(F^2)]^{-2}$, $\sigma(F^2)$ calculated from $\sigma^2(I) = \sigma^2(I)_{\text{counting}} + (0{\cdot}03I)^2$, largest shift/error in last cycle of refinement 0·05, atomic scattering factors from *International Tables for X-ray Crystallography* (1962), no corrections for anomalous dispersion, direct-methods calculations made using a local version of the program of Long (1965), the remaining calculations with programs described by Chow & Britton (1974).

Discussion. The final positional parameters are given in Table 1.* The thermal ellipsoids and the labelling of the atoms are shown in Fig. 1. Bond lengths and angles are given in Table 2. They are all normal within experimental error. The molecule deviates significantly but only slightly from planarity. The deviations from the best plane through the eight non-hydrogen atoms are: N +0·001 (3); C(1) +0·004 (3); C(2) −0·010 (3); C(3) +0·020 (3) Å. The torsion angle C(2)—C(3)—C(3′)—C(2′) must be 180° since the molecule lies on a center of symmetry, but the torsion angle C(1)—C(2)—C(3)—C(3′) is 4·1 (3)° rather than the 0° that would be expected for exact eclipsing of the cyano group and the double bond. This conformation is the one usually found for tetrahedral carbon atoms adjacent to double bonds.

The packing is shown in Fig. 2. The molecules are nearly parallel, tilted 20 °, to $(10\bar{1})$. The nitrile group is involved in two close contacts. The N atom is 3·38 (1) Å from the C(1) atom in the molecule related by a *c* glide at $(x,\frac{1}{4},z)$, and it is 3·39 (1) Å from the C(2) atom in the molecule related by a $[\bar{1}0\bar{1}]$ translation. There is also a longer contact of 3·65 (1) Å from the N atom to the C(1) atom in the molecule related by a $[\bar{1}00]$ translation. The 3·38 and 3·65 Å contacts are similar in direction and magnitude to contacts found in muconodinitrile and 2-butynedinitrile (Filippakis, Leiserowitz & Schmidt, 1967), and in fumaronitrile (Britton & Gleason, 1982). The 3·39 Å contact is similar in orientation to those found in methyl tetracyanide (Britton, 1974), but is longer.

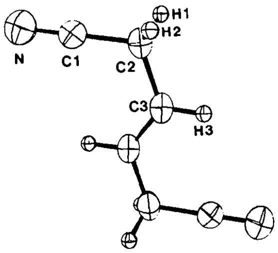

Fig. 1. Numbering of the atoms plus the thermal ellipsoids at the 50% probability contour (H atoms shown with arbitrary radius).

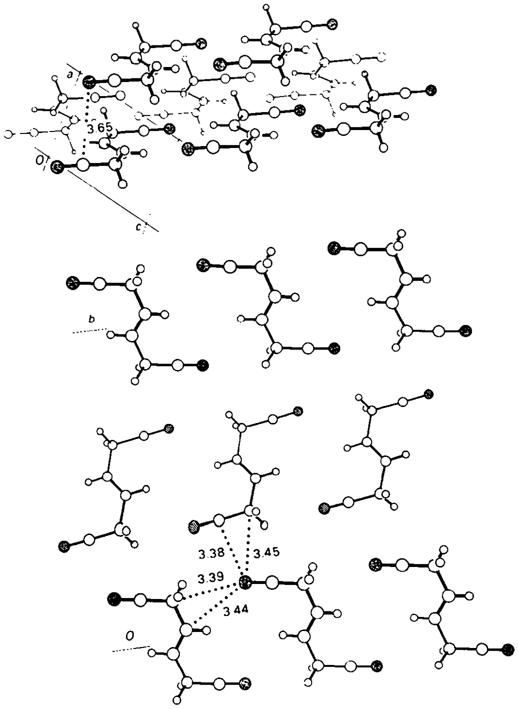

Fig. 2. The structure of 3-hexenedinitrile. Top: view along **b**. Bottom: view normal to $(10\bar{1})$. Short intermolecular contacts are shown as dotted lines with distances in Å.

Table 1. *Atomic coordinates* ($\times 10^4$) *and average isotropic thermal parameters* (Å^2)

$$B_{\text{eq}} = \tfrac{1}{3}\sum_i\sum_j B_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq} or B_{iso}
N	−317 (7)	1578 (2)	1058 (5)	4·8
C(1)	1398 (7)	1451 (2)	3043 (5)	3·4
C(2)	3624 (8)	1293 (2)	5570 (6)	3·5
C(3)	5168 (7)	324 (2)	5886 (5)	3·2
H(1)	5404 (99)	1776 (22)	5845 (67)	5·0
H(2)	2178 (98)	1386 (22)	6865 (71)	5·0
H(3)	6446 (95)	228 (27)	7574 (74)	5·0

Table 2. *Bond lengths* (Å) *and angles* (°)

C(3)—C(3′)	1·304 (5)	C(3′)—C(3)—C(2)	126·3 (3)
C(2)—C(3)	1·504 (4)	C(3)—C(2)—C(1)	113·4 (2)
C(1)—C(2)	1·458 (4)	C(2)—C(1)—N	179·3 (3)
C(1)—N	1·140 (4)	C(3′)—C(3)—H(3)	122 (2)
C(2)—H(1)	0·98 (4)	H(1)—C(2)—H(2)	109 (3)
C(2)—H(2)	1·01 (5)		
C(3)—H(3)	0·94 (4)		

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38611 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of *N*-Cyano-*N*′-methyl-*N*″-(2-{[(5-methyl-1*H*-imidazol-4-yl)methyl]thio}ethyl)guanidine (Cimetidine) Monohydrochloride Monohydrate, $C_{10}H_{17}N_6S^+.Cl^-.H_2O$

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Abstract. $M_r = 306{\cdot}82$, monoclinic, $P2_1/c$, $a = 11{\cdot}542\ (3)$, $b = 10{\cdot}859\ (3)$, $c = 11{\cdot}632\ (3)$ Å, $\beta = 91{\cdot}09\ (2)°$, $V = 1457{\cdot}5\ (7)$ Å^3, $Z = 4$, $D_m = 1{\cdot}391\ (1)$, $D_x = 1{\cdot}398$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 2{\cdot}362$ mm^{-1}, $F(000) = 648$, $T = 293$ K, final $R = 0{\cdot}046$ for 2478 independent reflections. Both N atoms of the imidazole ring are protonated and hydrogen-bonded to a Cl^- ion and an N atom of the cyano group of an adjacent molecule, respectively. The Cl^- ion is further linked with the N atom of the neighboring guanidine group by a hydrogen bond, consequently forming a 20-membered ring consisting of two cimetidine molecules and two Cl^- ions related by a center of symmetry, respectively.

Introduction. Cimetidine monohydrochloride is a specific histamine H_2-receptor antagonist which inhibits the secretion of the histamine-stimulated gastric acid. It is utilized in the treatment of peptic ulcer by injection, and has been widely investigated for its stability (Walker *et al.,* 1981; Yuhas, Loften, Baldinus & Mayron, 1981; Rosenberg, Dougherty, Mayron & Baldinus, 1980). Comparing the four kinds of cimetidine crystalline structures (forms *A*, *B*, *C* and *D*) with their inhibitory effects for peptic ulceration in rats, we previously proposed that the relative orientation of the cyanoguanidine group with respect to the imidazole ring is an important factor for the effective binding to the histamine H_2-receptor (Shibata, Kokubo, Morimoto, Morisaka, Ishida & Inoue, 1983). On the other hand, the conformation of cimetidine may change depending upon the environment, acidic or basic, because it has an imidazole ring capable of being isomerized and shows a weak inhibitory effect of peptic ulceration. In order to obtain the conformational characteristics of cimetidine under an acidic environment, we carried out the X-ray analysis of the crystal structure of cimetidine monohydrochloride.

Experimental. Cimetidine monohydrochloride was crystallized as the monohydrate by the slow evaporation of an aqueous solution of 1*M* HCl saturated with cimetidine. D_m measured by flotation in C_6H_6/CCl_4. Single crystal $0{\cdot}2 \times 0{\cdot}3 \times 0{\cdot}5$ mm; cell parameters determined by least-squares methods on the basis of 20 independent 2θ values; intensity data collected on a Rigaku four-circle diffractometer, graphite-monochromated Cu $K\alpha$, $\sin\theta/\lambda \le 0{\cdot}588$ Å^{-1}, h: $-13 \rightarrow 13$, k: $0 \rightarrow 12$, l: $0 \rightarrow 13$; four standards measured every 100 reflections: no significant variation; of 2494 reflections measured by ω–2θ scan mode, 2478 had $I \ge 2\sigma(I)$ and were subsequently used for structure refinement; Lorentz and polarization corrections applied, but absorption ignored. Structure solved by direct methods with *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978). An *E* map, computed with the 200 phase set ($|E| \ge 1{\cdot}72$) having the highest combined figure of merit, gave reasonable positions for all non-H atoms. Refinement by block-diagonal least squares with anisotropic thermal parameters for all non-H atoms. Positional parameters of all H atoms obtained from a difference Fourier map and refined with isotropic thermal parameters. The quantity minimized was $\sum w(|F_o| - |F_c|)^2$; $w = 1{\cdot}0$ for $0 < F_o \le 15{\cdot}0$ and $w = 1{\cdot}0/[1{\cdot}0 + 0{\cdot}398\ (F_o - 15{\cdot}0)]$ for $F_o > 15{\cdot}0$; final $R = 0{\cdot}046$, $R_w = 0{\cdot}059$. Ratio of maximum least-squares shift to error: for non-H atoms ~0·008, for H atoms ~0·06. Maximum and minimum

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