six-membered rings adopt almost the same conformation as the (+)-8β analogue (Bernardinelli, Dunand, Flack, Yvon, Giersch & Ohloff, 1984). The main difference between the two structures occurs in the orientation of the p-bromobenzoyloxy fragment, due to the position of the acetoxy group. The values of the torsional angles C(9)—C(18)—C(19)—O(20) and C(18)—C(19)—O(20)—C(21) are respectively: 68·6 (1·3) and 173·3 (1·1)° for the α form and −174·5 (5) and 89·8 (7)° for the β form.

(II): Even with all Friedel pairs measured, the very small anomalous-dispersion contribution from the O atoms means that the absolute configuration of this molecule should be difficult to determine. This is borne out in practice by the absolute-structure parameter refining to $x = -0.6$ (2·0), a value which does not significantly select one configuration from another. More precise measurements of sensitive reflections with a longer wavelength are called for. However, the absolute configuration of (II) can be deduced from its precursors (Lucius, 1960; Ruzicka, Seidel & Engel, 1942) and corresponds to that shown in Fig. 1. Hydrogen bonds occur between O(1)···O(2^i) 2·879 (6) and O(2)···O(1^{ii}) 2·754 (6) Å and lead to the presence of two short H···H intermolecular contacts: H(131)···H(162^i) 1·98 (10) and H(101)···H(102^{ii}) 1·93 (9) Å. [Symmetry code: (i) $x-1, y, z$; (ii) $\frac{1}{2}+x, \frac{3}{2}-y, 2-z$.]

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Structure of the Hydrogen Oxalate of Formamide Oxime, CH₅N₂O⁺.C₂HO₄⁻, at 105 K

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Abstract. $M_r = 150.10$, monoclinic, *Pc*, $a = 3.530$ (1), $b = 9.642$ (3), $c = 16.706$ (6) Å, $\beta = 91.07$ (3)°, $V = 568.5$ (4) Å³ at 105 K, $Z = 4$, $D_x = 1.753$ (1), D_m(293 K) = 1.701 (5) Mg m⁻³, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 0.158$ mm⁻¹, $F(000) = 312$, final $R = 0.028$ for 2259 unique observed reflections. The crystals are built up of hydrogen oxalate ions, C₂HO₄⁻, and N^1-hydroxyformamidinium ions, H₂N⁺=CH—NHOH, the protonated form of a tautomer of formamide oxime. The anions are connected by short asymmetric OH···O bonds into infinite chains, which are interlinked by the cations. The conformation of the cation H₂N⁺=CH—NH—OH is synperiplanar. The H-bonding system includes two-, three-, and four-center bonds (*i.e.* 'linear', 'bifurcated', and 'trifurcated' H bonds).

Introduction. Formamide oxime inhibits DNA synthesis in cells and bacteria by the same mechanism as hydroxyurea, *i.e.* by inhibition of the enzyme ribonucleotide reductase, but was found to be less potent in accordance with a lower one-electron oxidizability (Kjøller Larsen, Sjöberg & Thelander, 1982). The compound has been shown to possess antitumor activity against L1210 leukemia (Flora, van't Riet & Wampler, 1978), and, together with hydroxyurea, to induce virus expression, probably *via* damage to cellular DNA (Rascati & Tennant, 1978).

In solution formamide oxime has been proposed to exist as an equilibrium between two tautomers, H₂N—CH=N—OH ⇌ HN=CH—NH—OH, but crystallizes in the amide oxime form (*cf.* Jeffrey, Ruble, McMullan, DeFrees & Pople, 1981, and references therein).

Table 1. *Fractional atomic coordinates* ($\times 10^4$, *for* H $\times 10^3$) *and isotropic thermal parameters* (Å^2)

For non-H atoms $B_{\text{eq}} = \frac{1}{3} \sum_i \sum_j B_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$.

	x	y	z	B_{eq}/B
O(1A)	−421 (4)	2901 (1)	1946 (1)	0·87
O(2A)	2502 (4)	3247 (1)	3136 (1)	0·79
C(1A)	498 (4)	3618 (1)	2531 (1)	0·61
C(2A)	−921 (4)	5147 (1)	2534 (1)	0·60
O(3A)	−2800 (4)	5600 (1)	1965 (1)	0·91
O(4A)	45 (4)	5835 (1)	3170 (1)	0·82
H(4A)	−73 (8)	672 (3)	320 (2)	0·79
N(1B)	3773 (4)	8376 (1)	1710 (1)	0·96
C(3B)	2135 (4)	8755 (2)	1037 (1)	0·78
N(2B)	1788 (4)	10045 (1)	807 (1)	0·80
O(5B)	3704 (4)	11042 (1)	1259 (1)	0·97
H(5B)	200 (9)	1154 (3)	151 (2)	0·96
H(2B)	94 (8)	1028 (3)	35 (2)	0·79
H(3B)	107 (8)	808 (3)	67 (2)	0·77
H(11B)	467 (9)	898 (3)	205 (2)	0·92
H(12B)	413 (8)	753 (3)	181 (2)	0·92
O(1A')	10121 (4)	8587 (1)	4412 (1)	0·92
O(2A')	7501 (4)	8222 (1)	3194 (1)	0·89
C(1A')	8290 (4)	8950 (1)	3805 (1)	0·64
C(2A')	6794	10461 (1)	3786	0·60
O(3A')	7576 (4)	11235 (1)	4349 (1)	0·90
O(4A')	4798 (4)	10779 (1)	3153 (1)	0·79
H(4A')	418 (8)	1168 (3)	317 (2)	0·75
N(1B')	5721 (4)	6147 (2)	5545 (1)	0·91
C(3B')	4432 (4)	5869 (2)	4823 (1)	0·71
N(2B')	4240 (4)	4627 (1)	4521 (1)	0·78
O(5B')	5367 (4)	3535 (1)	5011 (1)	1·11
H(5B')	588 (9)	294 (3)	472 (2)	1·09
H(2B')	339 (7)	441 (3)	408 (2)	0·76
H(3B')	363 (8)	652 (3)	451 (2)	0·67
H(11B')	634 (8)	547 (3)	591 (2)	0·89
H(12B')	558 (8)	699 (3)	568 (2)	0·89

Table 2. *Bond lengths* (Å) *and angles* (°) *of ions A and B*

Hydrogen oxalate ions

	A	A'		A	A'
C(1)−O(1)	1·236 (2)	1·243 (2)	C(2)−O(3)	1·229 (2)	1·228 (2)
C(1)−O(2)	1·274 (2)	1·266 (2)	C(2)−O(4)	1·293 (2)	1·297 (2)
C(1)−C(2)	1·557 (2)	1·550 (1)	O(4)−H(4)	0·90 (3)	0·90 (3)
O(1)−C(1)−O(2)	127·2 (1)	127·2 (1)	O(3)−C(2)−O(4)	125·7 (1)	126·3 (1)
O(1)−C(1)−C(2)	116·9 (1)	117·0 (1)	O(3)−C(2)−C(1)	120·2 (1)	118·9 (1)
O(2)−C(1)−C(2)	115·9 (1)	115·8 (1)	O(4)−C(2)−C(1)	114·1 (1)	114·8 (1)
C(2)−O(4)−H(4)	117 (2)	109 (2)			

Hydroxyformamidinium ions

	B	B'		B	B'
N(1)−C(3)	1·307 (2)	1·309 (2)	N(1)−H(11)	0·87 (3)	0·92 (3)
C(3)−N(2)	1·307 (2)	1·301 (2)	N(1)−H(12)	0·84 (3)	0·85 (3)
N(2)−O(5)	1·390 (2)	1·387 (2)	C(3)−H(3)	0·97 (3)	0·86 (3)
O(5)−H(5)	0·88 (3)	0·78 (3)	N(2)−H(2)	0·85 (3)	0·82 (3)
N(1)−C(3)−N(2)	123·8 (2)	124·1 (2)	N(1)−C(3)−H(3)	121 (2)	121 (2)
C(3)−N(2)−O(5)	117·2 (1)	117·2 (1)	N(2)−C(3)−H(3)	115 (2)	115 (2)
C(3)−N(1)−H(11)	122 (2)	123 (2)	C(3)−N(2)−H(2)	123 (2)	127 (2)
H(11)−N(1)−H(12)	118 (3)	121 (3)	O(5)−N(2)−H(2)	118 (2)	116 (2)
C(3)−N(1)−H(12)	120 (2)	115 (2)	N(2)−O(5)−H(5)	108 (2)	105 (2)

Molecular-orbital calculations (CNDO/2 FORCE calculations) on various conformations of the two tautomers show that the amide oxime has the lower energy, and that the energy difference between the global minima of the tautomers is 76·6 kJ mol⁻¹ (Venkatesh, Srivastava & Brinn, 1979). *Ab initio* molecular-orbital calculations carried out by Jeffrey *et al.* (1981) for formamide oxime at the Hartree–Fock 3-21G level lead to similar results, *i.e.* with an energy difference of 72·2 kJ mol⁻¹ between the lowest-energy conformations of the tautomers. Structure determination of the salt of formamide oxime was undertaken in order to establish the tautomer form of the protonated molecule. The hydroxyamidine form is probably the biologically active form as this structure is analogous to the hydroxyurea structure.

Experimental. Crystals suitable for X-ray work obtained by slow evaporation from an equimolar, aqueous solution of formamide oxime (from EGA Chemie) and oxalic acid. Colourless crystals grow as rods with *a* as the needle axis. M.p. 419–421 K (decomp.). D_m measured by flotation. Crystal 0·10 × 0·15 × 0·30 mm chosen for data collection, mounted on Enraf–Nonius CAD-4 diffractometer equipped with graphite monochromator and Nonius low-temperature device. Temperature kept at about 105 K and estimated to be correct within ±5 K. Temperature kept constant within 0·5 K. Cell dimensions determined by least squares from angular settings of 18 reflections. Intensities measured using θ–2θ scan method for θ values up to 35° (h 6, k 16, l ±28). Three standard reflections measured every 100 reflections showed no significant variations. Intensities of 2942 reflections measured, 2515 of which unique ($R_{\text{int}} = 0·01$), 2259 reflections with $I_o > 2·0\sigma(I_o)$ considered observed. No absorption corrections made. Structure solved by direct methods using *MULTAN77* (Main, Lessinger, Woolfson, Germain & Declercq, 1977). Full-matrix least-squares refinement of positional parameters of all atoms, with anisotropic temperature factors for non-H atoms, and isotropic temperature factors of H atoms fixed on the values of the atoms to which they are bonded. All H atoms located in difference Fourier map, peaks of H atoms involved in very short H bonds being of lowest height ($\frac{1}{2}$ to $\frac{1}{3}$ of expected value). Quantity minimized $\sum w(|F_o| - k|F_c|)^2$, where $w = 1/\{1 + [(|F_o| - 7·5)/5·0]^2\}$. Av. and max. Δ/σ in final refinement cycle 0·2 and 0·8, respectively. Final $R = 0·028$, $wR = 0·034$, $S = 2·3$, $\Delta\rho$ fluctuations ±0·3 e Å⁻³. Scattering factors for H those of Stewart, Davidson & Simpson (1965), for O, N, and C those of Cromer & Mann (1968). Programs used in refinement from *XRAY76* (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976).

Discussion. The final atomic parameters are listed in Table 1.* Bond lengths and angles are given in Table 2, and the notation for the atoms and the conformations and packing of the ions are shown in Fig. 1.

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* Lists of structure factors, anisotropic thermal parameters and best planes of each ion have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42001 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Both symmetry-independent cations (B and B') were found to be hydroxyformamidinium ions, $H_2N^+=CH-NHOH$. The conformations of both ions are synperiplanar (sp) with torsion angles N(1)—C(3)—N(2)—O(5) of 8·5 (2) and 2·2 (2)° for ions B and B', respectively. This conformation is in accordance with the Z configuration (the so-called $anti$ isomer) of formamide oxime, which has been observed in the crystal structure ($e.g.$ Jeffrey et $al.$, 1981) and found to be the most stable by molecular-orbital calculations (Venkatesh et $al.$, 1979; Jeffrey et $al.$, 1981; Nguyen & Ha, 1982). The sp conformation is stabilized by an $intra$molecular NH···O interaction. In both cations N(1)—H(11)···O(5) is the weaker component of four-center H bonds (see below). Both ions are, with the exception of H(5), close to planar. The greatest deviations of the C, N and O atoms from the planes of the non-hydrogen atoms are −0·035 (2) and +0·008 (2) Å for ions B and B', respectively. All potent inhibitors of ribonucleotide reductase so far investigated are found to be nearly planar (Kjøller Larsen et $al.$, 1982).

The bond distances and angles do not deviate more than three e.s.d.'s between the two symmetry-independent hydroxyformamidinium ions ($cf.$ Table 2). The two C—N bonds of each ion are almost identical, average 1·304 (2) Å, indicating π-electron delocalization over the region N(1)—C(3)—N(2), with an estimated π-bond order (Norrestam, Mertz & Crossland, 1983) of about 0·8. This means that the

positive charge of both cations is shared between the two N atoms, $H_2N^{(+)} \underset{\cdots}{=} CH \underset{\cdots}{=} N^{(+)}HOH$, and that the ion can be described as a hydroxyformamidinium ion or as an oximinium ion with the proton attached not to the amino but to the oxime N atom. The last is in agreement with the findings of Endres & Schendzielorz (1984) for the mono- and di-protonated oxamide dioxime molecule in two salts. The length of the N—O bond [average 1·389 (2) Å] is near to the average for this bond [1·391 (4) Å] in the series of hydroxamic acids (hydroxyurea analogues) earlier investigated (Larsen, Sjöberg & Thelander, 1982). The angle between the two C—N bonds is significantly smaller than the corresponding angle in formamide oxime [126·21 (3)°]. The C—N—O angle [average 117·2 (1)°] is within the range (113·9–121·3°) found for this angle in similar compounds (Larsen et $al.$, 1982).

The geometry of the hydrogen oxalate ions is in agreement with that observed in other hydrogen oxalate structures ($cf.$ Thomas & Renne, 1975). The dihedral angle between the two COO planes is 1·7 (1) and 2·3 (1)° for ions A and A', respectively. Twists of up to 12·9 (1)° have been observed and completely flat oxalate ions are very uncommon (Thomas & Renne, 1975). The bond lengths and angles also seem to be normal.

The crystal structure is stabilized by a network of H bonds, in which all H atoms of both ions take part ($cf.$ Fig. 1 and Table 3). Most of the H bonds are two-centered ('linear'), others are three-centered ('bifurcated'), and two of the H atoms [H(11B) and H(11B')] are involved in four-centered ('trifurcated') H bonding, which is very seldom observed (Taylor, Kennard & Versichel, 1984). The dimensions of these bonds are within the arbitrary limits given by Taylor et $al.$ (1984), but the H-atom positions have not been 'normalized' (Taylor et $al.$, 1984). In both cases an $intra$molecular NH···O bond is a weak component of the four-center bond. The N atom involved is positvely charged as in the other known cases of four-center bonding (Taylor et $al.$, 1984).

The hydrogen oxalate ions are linked into infinite chains by short, asymmetric OH···O bonds [2·471 (2) and 2·514 (2) Å]. Similar H-bonded ion chains are normally observed in hydrogen oxalate structures (Thomas & Renne, 1975). The anion chains are interlinked by the cations, which are the H donors to 15 different H bonds ($cf.$ Table 3), including the three- and four-center bonds mentioned above. Each of these systems consists of one strong and one or two weak bonds. In addition, some other short distances are observed ($cf.$ Table 3). Short distances, $i.e.$ less than the sum of the van der Waals radii, are observed between the C-bonded H atoms and the nearest O atoms. These should probably also be described as H bonds, as all the conditions for C—H···X bonds, defined by Taylor & Kennard (1982), are fulfilled.
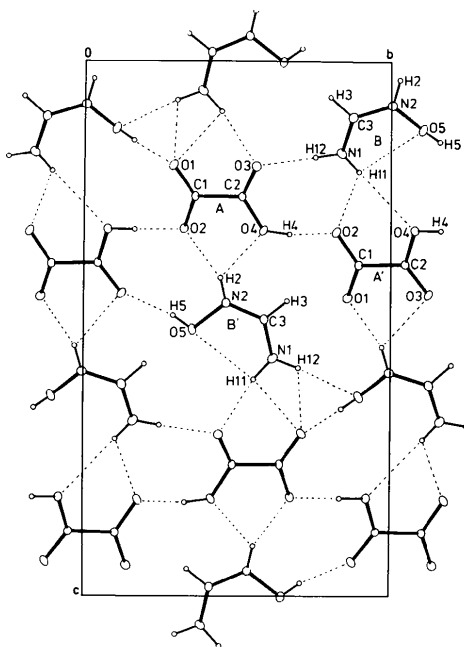

Fig. 1. H bonding of the hydrogen oxalate of formamide oxime. The structure is viewed along the a^* axis and drawn by $ORTEP$ (Johnson, 1970).

Table 3. *Hydrogen-bond distances* (Å) *and angles* (°)

X–H⋯Y	X⋯Y	H⋯Y	$\angle X$–H⋯Y
O(4A)–H(4A)⋯O(2A')	2·471 (2)	1·58 (3)	173 (3)
O(4A')–H(4A')⋯O(2A")	2·514 (2)	1·62 (3)	172 (3)
O(5B)–H(5B)⋯O(1A''')	2·591 (2)	1·73 (3)	163 (3)
O(5B')–H(5B')⋯O(3A''')	2·604 (2)	1·86 (3)	161 (3)
N(2B)–H(2B)⋯O(1A''')	2·732 (2)	1·93 (3)	159 (3)
N(2B)–H(2B)⋯O(3A''')	3·087 (2)	2·50 (3)	127 (2)
N(2B')–H(2B')⋯O(2A')	2·729 (2)	1·96 (3)	158 (3)
N(2B')–H(2B')⋯O(4A')	2·919 (2)	2·35 (3)	127 (2)
N(1B)–H(11B)⋯O(2A'')	2·789 (3)	2·26 (3)	119 (2)
N(1B)–H(11B)⋯O(5B')	2·679 (2)	2·41 (3)	99 (2)
N(1B)–H(11B)⋯O(4A'')	3·358 (2)	2·53 (3)	159 (3)
N(1B)–H(12B)⋯O(3A'')	2·965 (2)	2·17 (3)	158 (3)
N(1B')–H(11B')⋯O(3A''')	2·948 (2)	2·06 (3)	163 (3)
N(1B')–H(11B')⋯O(5B'')	2·674 (2)	2·42 (3)	96 (2)
N(1B')–H(11B')⋯O(1A'''')	2·838 (3)	2·59 (3)	96 (2)
N(1B')–H(12B')⋯O(5B''''')	3·051 (2)	2·24 (3)	162 (3)
N(1B')–H(12B')⋯O(1A'''')	2·838 (3)	2·52 (3)	103 (2)

Other short distances

O(5B)–H(5B)⋯O(1A''')	2·957 (2)	3·06 (3)	75 (2)
C(3B)–H(3B)⋯O(5B'')	3·031 (2)	2·45 (3)	118 (2)
C(3B')–H(3B')⋯O(1A')	3·101 (2)	2·35 (3)	146 (3)

Symmetry code

(i) $x - 1, y, z$
(ii) $x, y + 1, z$
(iii) $x, y - 1, z$
(iv) $x - 1, 2 - y, z - 0·5$
(v) x, y, z

(vi) $x + 1, y, z$
(vii) $x + 1, 1 - y, z + 0·5$
(viii) $x, 2 - y, z + 0·5$
(ix) $x + 1, y + 1, z$
(x) $x, 1 - y, z - 0·5$

Upon storage at room temperature for about a year the crystals of the hydrogen oxalate of formamide oxime undergo solid-state transformation into a new crystalline form. Several crystal modifications, including the above-mentioned, have been observed during the crystallization work, all with a short needle axis of about 3·5 Å.

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Structure of N^1-(2,6-Dimethyl-4-pyrimidinyl)sulphanilamide (Sulfisomidine),* $C_{12}H_{14}N_4O_2S$

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Abstract. $M_r = 278·3$, orthorhombic, $Pca2_1$, $a = 12·614$ (5), $b = 11·278$ (4), $c = 9·374$ (8) Å, $V = 1333·6$ (2) Å³, $Z = 4$, $D_m = 1·378$ (5), $D_x = 1·386$ (5) Mg m⁻³, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0·238$ mm⁻¹, $F(000) = 584$, $T = 293$ K. Final $R = 0·037$ for 2006 observed reflections. The angle of twist between the planes of the two rings is 78·6 (2)°. The benzene ring is planar while the pyrimidine ring is slightly folded about the C(12)–N(15) axis. The geometry around the sulphur atom is distorted from the

* 4-Amino-N-(2,6-dimethyl-4-pyrimidinyl)benzenesulphonamide.