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## The Structure of *S,S'*-Methylenebis(L-cysteine) Monohydrochloride

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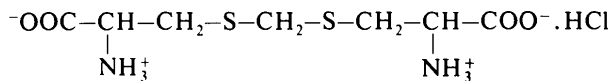
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### Abstract

The crystal structure of the title compound has been determined from diffractometer data by Patterson and Fourier methods and refined to  $R = 0.039$  for 1147 counter reflections:  $C_7H_{15}N_2O_4S_2 \cdot Cl^-$ ,  $M_r = 290.779$ ,  $a = 10.405$  (6),  $b = 5.074$  (3),  $c = 11.972$  (6) Å,  $\beta = 104.9$  (1)°,  $V = 610.81$  (65) Å<sup>3</sup>, space group  $P2_1$ ,  $Z = 2$ ,  $D_m = 1.60$ ,  $D_c = 1.58$  Mg m<sup>-3</sup>,  $F(000) = 304$ ,  $\lambda(Cu K\alpha) = 1.54178$  Å,  $\mu = 6.0203$  mm<sup>-1</sup>. The monovalent cation arranges the polar groups in such a way as to enclose the chloride ion. Packing is determined by a three-dimensional network of hydrogen bonds involving the protonated amino and carboxyl groups. In the very strong  $O_i'' \cdots O_k''$  [2.444 (8) Å] hydrogen bond, the H atom is disordered. Other contacts involve H atoms bonded to C atoms:  $C^\alpha-H \cdots O = 3.165$  (8),  $3.267$  (8) Å and  $C(\text{methylene})-H \cdots O = 3.377$  (9) Å. The two chemically equivalent parts of the molecule are not equivalent crystallographically and the most relevant difference between them is observed for the conformation around the  $C^\beta-S^p$  bond,  $\chi^2$  being  $-169.3$  (5) and  $-130.6$  (5)°.

### Introduction

As a continuation of a research programme on the conformational aspects of the sulphur-containing amino acid structures, the crystal structure analysis of *S,S'*-methylenebis(L-cysteine) monohydrochloride (djenkolic acid monohydrochloride),



has been carried out. The present study is connected with previous work on crystals of DL-homocystine itself and of its monohydrogen oxalate (Bigoli, Lanfranchi, Leporati, Nardelli & Pellinghelli, 1981).

### Experimental

Attempts to obtain single crystals of L-djenkolic hydrochloride from aqueous solutions were unsuccessful, while clear, colourless needle-like single crystals of the title compound were obtained when attempting to prepare a copper(I) complex, *i.e.* by adding commercial L-djenkolic acid to a saturated solution of CuCl in 37% hydrochloric acid. From these

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a sample  $0.2 \times 0.04 \times 0.07$  mm was used for data collection. The most significant crystal data are given in the *Abstract*. The unit-cell parameters were determined from rotation and Weissenberg photographs and from diffractometer measurements. The intensities were collected with an 'on-line' Siemens AED single-crystal diffractometer with Ni-filtered Cu  $K\alpha$  radiation and the  $\omega/2\theta$  scan mode to a limit of  $2\theta = 140^\circ$ . 1295 independent reflections were measured of which 1147, having  $I \geq 2\sigma(I)$ , were considered to be observed. Data were corrected for Lorentz and polarization factors but not for absorption or extinction effects.

### Structure determination

The structure was solved by interpreting the sharpened Patterson map to derive the positions of Cl and S and by a subsequent Fourier synthesis which revealed all the non-hydrogen atoms. Refinement was carried out by block-diagonal ( $9 \times 9$  for anisotropic,  $4 \times 4$  for

Table 1. Final atomic coordinates ( $\times 10^4$ , for H  $\times 10^3$ ) with e.s.d.'s in parentheses and  $B_{eq}$  or  $B_{iso}$  ( $\text{\AA}^2$ )

For non-hydrogen atoms  $B_{eq} = \frac{1}{3} \sum_i \sum_j B_{ij} a_i^* a_j^* a_i \cdot a_j$ .

IUPAC designation	x	y	z	$B_{eq}$ or $B_{iso}$
Cl	6778 (1)	0	899 (1)	2.68 (3)
S(1)	S $_7^1$	8540 (2)	3508 (4)	2.90 (4)
S(2)	S $_k^1$	6605 (2)	7518 (4)	4065 (1)
O(1)	O $_i^1$	10302 (4)	1013 (9)	1066 (3)
O(2)	O $_i^2$	11557 (4)	2356 (11)	2790 (4)
O(3)	O $_k^1$	3647 (5)	9427 (10)	1487 (4)
O(4)	O $_i^2$	3016 (5)	8505 (12)	3088 (4)
N(1)	N $_i$	8627 (4)	5028 (12)	821 (4)
N(2)	N $_k$	5122 (4)	5071 (12)	1594 (4)
C(1)	C $_i$	10607 (5)	2618 (14)	1878 (5)
C(2)	C $_a^1$	9836 (5)	5186 (13)	1820 (5)
C(3)	C $_i^1$	9484 (6)	5967 (14)	2933 (5)
C(4)	C $_k$	3640 (5)	8011 (12)	2312 (5)
C(5)	C $_a^1$	4371 (5)	5381 (13)	2492 (5)
C(6)	C $_k^1$	5295 (6)	4998 (17)	3715 (5)
C(7)	C $_s^1$	8041 (6)	5344 (18)	4587 (5)
H(1)	H $_i^1$	1048 (6)	668 (14)	156 (5)
H(2)	H $_i^{11}$	1035 (6)	598 (16)	359 (6)
H(3)	H $_i^{22}$	891 (5)	763 (15)	285 (5)
H(4)	H $_k^1$	370 (6)	372 (16)	235 (5)
H(5)	H $_i^{11}$	460 (5)	522 (15)	417 (5)
H(6)	H $_i^{22}$	579 (7)	321 (18)	352 (6)
H(7)	H $_i^{11}$	775 (6)	357 (17)	511 (5)
H(8)	H $_i^{22}$	886 (6)	635 (14)	497 (5)
H(9)	H $_i^1$	813 (6)	343 (17)	87 (6)
H(10)	H $_i^2$	803 (6)	628 (16)	79 (6)
H(11)	H $_i^3$	890 (6)	512 (17)	21 (5)
H(12)	H $_i^4$	575 (7)	644 (17)	152 (6)
H(13)	H $_i^2$	567 (6)	348 (16)	180 (5)
H(14)	H $_i^3$	456 (6)	498 (18)	87 (6)
H(15)	H $_i^1$ †	1200 (7)	67 (18)	267 (6)
H(16)	H $_i^2$ †	240 (7)	967 (17)	300 (6)

† Calculated for an occupancy of 0.5.

isotropic atoms) least squares, first with isotropic, then with anisotropic thermal parameters. At this stage a difference synthesis revealed the positions of all the H atoms. The positional and isotropic thermal parameters of these atoms were refined in the last cycles. A plot of  $|\Delta F|$  against  $|\bar{F}_o|$  indicated that unit weights were satisfactory and a good convergence was obtained using them. The final conventional  $R(F)$  value is 0.039 (observed reflections only).<sup>\*</sup> Atomic coordinates, equivalent isotropic thermal parameters (Hamilton, 1959) and isotropic ones for H atoms are given in Table 1. No particular anisotropy in the atomic thermal motion was observed except for O(3) and O(4) which show a direction along which the r.m.s. displacement is three times greater than in the other directions. The atomic scattering factors of Cromer & Mann (1968) were used for non-hydrogen atoms and those of Stewart, Davidson & Simpson (1965) for the H atoms. All the calculations were carried out on the CDC 6600 computer of the Consorzio per la Gestione del Centro di Calcolo Elettronico Interuniversitario dell'Italia Nord-Orientale, Casalecchio, Bologna, with programs written by Immirzi (1967).

### Discussion

The unexpected feature of this structure is that the two parts of the zwitterion, which should be chemically non-equivalent, appear to be structurally equivalent, as the proton is distributed in a disordered manner between the two carboxyl groups, each with a 50% occupancy as deduced from the electron density and  $B$  values.

The shape of this cation is illustrated in Fig. 1, which also shows the labelling of the atoms. A pseudo twofold symmetry axis runs through C(7) and the two polar ammonium groups are arranged in such a way as to enclose the chloride ion. Bond lengths and angles in the

<sup>\*</sup> Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36230 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

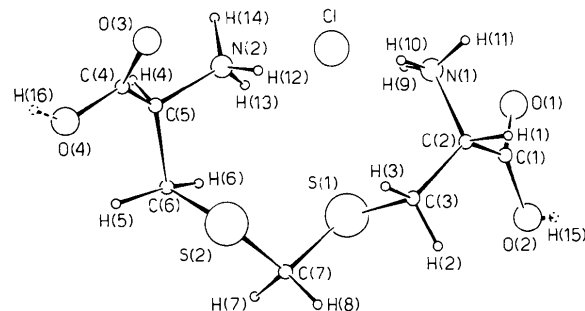


Fig. 1. Perspective view of the asymmetric unit.

two halves are compared in Table 2 and the only significant difference, if real, is observed for the  $C^\beta-S^\nu-C^\delta$  angles [101.1 (4), 98.7 (4)°]. It appears quite evident that the correlation between this angle and the C—S distances requires that the longer are the distances the narrower is the angle. Bond distances and angles involving H atoms are listed in Table 3.

Table 2. Bond distances (Å) and angles (°) in the amino acid molecule, with *e.s.d.*'s in parentheses

	Branch <i>i</i>	Branch <i>k</i>	$\Delta/\sigma^*$
C—O'	1.245 (8)	1.223 (8)	1.94
C—O''	1.277 (7)	1.288 (9)	0.96
C—C $^\alpha$	1.522 (9)	1.524 (9)	0.16
C $^\alpha$ —N	1.499 (6)	1.491 (8)	0.80
C $^\alpha$ —C $^\beta$	1.522 (9)	1.543 (8)	1.74
C $^\beta$ —S $^\nu$	1.804 (7)	1.837 (8)	3.10
S $^\nu$ —C $^\delta$	1.814 (8)	1.833 (8)	1.68
O'—C—O''	125.8 (6)	125.3 (6)	0.59
O'—C—C $^\alpha$	119.9 (5)	121.5 (6)	2.05
O''—C—C $^\alpha$	114.3 (5)	113.2 (5)	1.56
C—C $^\alpha$ —C $^\beta$	115.2 (5)	114.3 (5)	1.27
C—C $^\alpha$ —N	108.4 (5)	109.0 (5)	0.85
N—C $^\alpha$ —C $^\beta$	111.8 (5)	110.9 (5)	1.27
C $^\alpha$ —C $^\beta$ —S $^\nu$	114.0 (5)	111.9 (5)	2.97
C $^\beta$ —S $^\nu$ —C $^\delta$	101.1 (4)	98.7 (4)	4.24
S $^\nu$ —C $^\delta$ —S $^\nu$	114.9 (3)		

$$* \Delta/\sigma = |x_1 - x_2| / [\sigma^2(x_1) + \sigma^2(x_2)]^{1/2}.$$

Table 3. Bond distances (Å) and angles (°) involving hydrogen atoms, with *e.s.d.*'s in parentheses

	Branch <i>i</i>	Branch <i>k</i>
C $^\alpha$ —H $^\alpha$	1.11 (7)	1.08 (7)
C $^\beta$ —H $^{\beta 1}$	1.03 (6)	1.02 (6)
C $^\beta$ —H $^{\beta 2}$	1.02 (7)	1.10 (9)
N—H $^1$	0.97 (8)	0.97 (8)
N—H $^2$	0.88 (7)	0.98 (7)
N—H $^3$	0.85 (7)	0.91 (6)
O'—H''	1.00 (9)	0.86 (8)
C $^\delta$ —H $^{\delta 1}$		1.18 (8)
C $^\delta$ —H $^{\delta 2}$		1.00 (6)
C—C $^\alpha$ —H $^\alpha$	104 (3)	112 (3)
N—C $^\alpha$ —H $^\alpha$	105 (3)	104 (4)
C $^\beta$ —C $^\alpha$ —H $^\alpha$	112 (3)	106 (4)
C $^\alpha$ —C $^\beta$ —H $^{\beta 1}$	108 (4)	98 (3)
C $^\alpha$ —C $^\beta$ —H $^{\beta 2}$	113 (3)	97 (4)
S $^\nu$ —C $^\beta$ —H $^{\beta 1}$	100 (4)	113 (4)
S $^\nu$ —C $^\beta$ —H $^{\beta 2}$	104 (3)	105 (4)
H $^{\beta 1}$ —C $^\beta$ —H $^{\beta 2}$	116 (6)	130 (6)
C $^\alpha$ —N—H $^1$	110 (4)	119 (5)
C $^\alpha$ —N—H $^2$	116 (5)	106 (4)
C $^\alpha$ —N—H $^3$	107 (4)	111 (4)
H $^1$ —N—H $^2$	103 (6)	104 (6)
H $^1$ —N—H $^3$	113 (6)	103 (6)
H $^2$ —N—H $^3$	108 (6)	113 (6)
S $^\nu$ —C $^\delta$ —H $^{\delta 1}$		99 (4)
S $^\nu$ —C $^\delta$ —H $^{\delta 2}$		103 (4)
S $^\nu$ —C $^\delta$ —H $^{\delta 1}$		110 (3)
S $^\nu$ —C $^\delta$ —H $^{\delta 2}$		112 (4)
H $^{\delta 1}$ —C $^\delta$ —H $^{\delta 2}$		117 (5)
C—O'—H''	105 (4)	123 (5)

The conformational properties of the amino acid are better illustrated by the Newman projections of Fig. 2; the corresponding torsion angles are listed in Table 4 together with those of some related compounds, following the IUPAC—IUB Commission on Biochemical Nomenclature (1970).

In both branches, the carboxyl-group atoms and C $^\alpha$  are coplanar, N(1) and N(2) deviating from these planes by 0.244 (5) and 0.092 (5) Å respectively, and consequently the carboxyl groups are near to being eclipsed with respect to the C $^\alpha$ —N bonds (Fig. 2a, a').

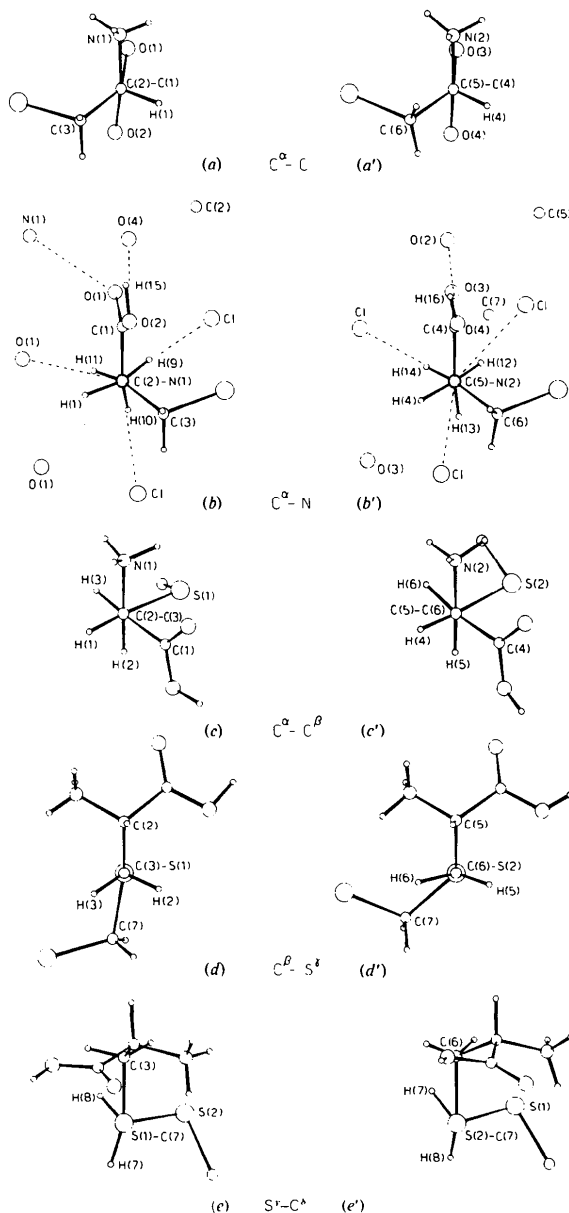


Fig. 2. Conformations about the most significant bonds. Broken lines refer to the N—H...Cl, N—H...O and O—H...O hydrogen bonds, while dotted lines refer to the C $^\alpha$ —H...O contacts.

Table 4. Internal rotation angles ( $^{\circ}$ )

	$\psi^1$	$\psi^2$	$\chi^1$	$\chi^2$	$\chi^3$	References
L-Djenkolic acid.HCl						
branch <i>i</i>	+10.7 (8)	-170.5 (5)	+67.4 (6)	-169.3 (5)	+80.5 (5)	(I)
branch <i>k</i>	+4.8 (8)	-176.7 (5)	+63.2 (6)	-130.6 (5)	+73.6 (5)	(I)
S-Carboxymethyl-L-cysteine	-39.0 (3)	+142.9 (2)	-48.8 (3)	-67.3 (2)	-158.6 (2)	(II)
L-Cysteine (monoclinic)						
molecule <i>A</i>	-3.0 (1.2)	+176.4 (8)	+72.6 (9)			(III)
molecule <i>B</i>	-36.1 (1.1)	+144.3 (9)	-170.1 (7)			(III)
L-Cysteine (orthorhombic)	-17.0 (3)	+163.6 (2)	+65.3 (3)			(IV)
5-(S-Cysteinyl)uracil.H <sub>2</sub> O	-38.3 (7)	+144.6 (5)	-55.4 (6)	-82.7 (6)		(V)
L-Cysteine.HCl.H <sub>2</sub> O	-5.9	+173.4	+65.0			(VI)

$\psi^1 = \tau[\text{N}-\text{C}^{\alpha}-\text{C}-\text{O}']$ ,  $\psi^2 = \tau[\text{N}-\text{C}^{\alpha}-\text{C}-\text{O}'']$ ,  $\chi^1 = \tau[\text{N}-\text{C}^{\alpha}-\text{C}^{\beta}-\text{S}^{\gamma}]$ ,  $\chi^2 = \tau[\text{C}^{\alpha}-\text{C}^{\beta}-\text{S}^{\gamma}-\text{C}^{\delta}]$ ,  $\chi^3 = \tau[\text{C}^{\beta}-\text{S}^{\gamma}-\text{C}^{\delta}-\text{S}]$  or  $\tau[\text{C}^{\beta}-\text{S}^{\gamma}-\text{C}^{\delta}-\text{C}]$ .

References: (I) Present work. (II) Mighell, Hubbard, Harris, Staffa & Zervos (1979). (III) Harding & Long (1968). (IV) Kerr & Ashmore (1973). (V) Williams, Varghese & Berman (1977). (VI) Ramachandra Ayyar (1968).

If the compounds quoted in this work and in the previous one on DL-homocysteine are considered, it is found that the values of  $\psi^1$  fall in the range  $-41, +41^{\circ}$ , even though most of them show negative  $\psi^1$  values, the carboxyl groups showing the tendency to be eclipsed with respect to  $\text{C}^{\alpha}-\text{H}^{\alpha}$  rather than to  $\text{C}^{\alpha}-\text{C}^{\beta}$ . The  $\alpha\text{-NH}_3^+$  groups are staggered with respect to the substituents on  $\text{C}^{\alpha}$  as shown in Fig. 2(*b, b'*), the angles being  $\varphi_i^1 = 52$  (4),  $\varphi_i^2 = 169$  (4),  $\varphi_i^3 = -71$  (5),  $\varphi_k^1 = 55$  (4),  $\varphi_k^2 = 173$  (4),  $\varphi_k^3 = -64$  (5) $^{\circ}$  (where  $\varphi_s^r = \tau[\text{C}-\text{C}^{\alpha}-\text{N}-\text{H}_s^r]$ ,  $r = 1, 2, 3$ ,  $s = i, k$ ).

In both branches C and N are  $-\text{synclinal}$  and  $+\text{synclinal}$  with respect to the  $\text{S}^{\gamma}$  atoms (Fig. 2*c, c'*) as in (III, molecule *A*), (IV) and (VI), while C and N are  $-\text{antiperiplanar}$  and  $-\text{synclinal}$  in (II) and (V), and  $+\text{synclinal}$  and  $-\text{antiperiplanar}$  in (III, molecule *B*). The most significant difference between the two branches is observed in the  $\chi^2$  torsion angle; in fact the  $\text{C}^{\delta}$  atom is  $-\text{antiperiplanar}$  with respect to  $\text{C}_i^{\alpha}$  and  $-\text{anticlinal}$  with respect to  $\text{C}_k^{\alpha}$  (Fig. 2*d, d'*). These two conformations differ also from those found in (II) and (V) where they are  $-\text{synclinal}$ . The  $\chi_k^2$  torsion angle ( $-\text{anticlinal}$ ) could justify the relevant distortion from the theoretical value of  $109.5^{\circ}$  observed for the  $\text{H}_k^{\beta 1}-\text{C}_k^{\beta}-\text{H}_k^{\beta 2}$  angle ( $130^{\circ}$ ), the distortion being produced to eliminate any eclipsing of  $\text{C}(6)-\text{H}(6)$  with  $\text{S}(2)-\text{C}(7)$ . The two  $\text{C}-\text{S}-\text{C}-\text{S}$  torsion angles ( $\chi^3$ , Fig. 2*e, e'*) show a  $+\text{synclinal}$  conformation which differs from that found in (II) as a consequence of the substitution of a C by a S atom.

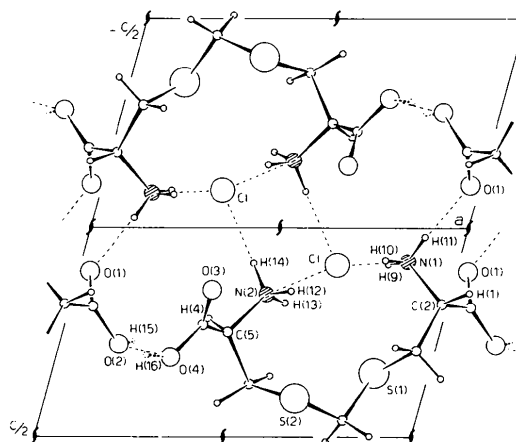
The arrangement of the molecules in the crystal lattice is determined by hydrogen bonds  $\text{N}-\text{H}\cdots\text{Cl}$ ,  $\text{N}-\text{H}\cdots\text{O}$  and  $\text{O}-\text{H}\cdots\text{O}$  (Table 5) which form layers running parallel to (001). Packing is shown in Fig. 3. Worthy of notice is the hydrogen bond formed by the  $\text{O}''$  carboxyl oxygens which is very strong and involves the disordered H atom. This hydrogen bond seems to belong to the symmetric double-minimum potential function class (Ibers, 1965; Speakman, 1972). Additional linkage is provided by  $\text{C}^{\alpha}-\text{H}\cdots\text{O}'$  contacts

 Table 5. Hydrogen-bond distances ( $\text{\AA}$ ) and angles ( $^{\circ}$ ) and  $\text{C}-\text{H}\cdots\text{O}$  contacts

$D-\text{H}\cdots A$	$D\cdots A$	$\text{H}\cdots A$	$\angle \text{H}-D\cdots A$	$\angle D-\text{H}\cdots A$
Hydrogen bonds				
$\text{N}(1)-\text{H}(9)\cdots\text{Cl}$	3.211 (6)	2.24 (8)	4 (4)	174 (6)
$\text{N}(1)-\text{H}(10)\cdots\text{Cl}^i$	3.189 (6)	2.32 (8)	7 (5)	170 (6)
$\text{N}(1)-\text{H}(11)\cdots\text{O}(1^{\text{vi}})$	2.809 (7)	1.97 (7)	8 (5)	168 (8)
$\text{N}(2)-\text{H}(12)\cdots\text{Cl}^i$	3.264 (6)	2.32 (8)	11 (4)	164 (6)
$\text{N}(2)-\text{H}(13)\cdots\text{Cl}$	3.320 (6)	2.50 (8)	28 (3)	141 (5)
$\text{N}(2)-\text{H}(14)\cdots\text{Cl}^v$	3.128 (6)	2.22 (6)	2 (6)	177 (8)
$\text{O}(2)-\text{H}(15)\cdots\text{O}(4^{\text{iv}})$	2.444 (8)	1.52 (8)	17 (4)	152 (7)
$\text{O}(4)-\text{H}(16)\cdots\text{O}(2^{\text{iii}})$	2.444 (8)	1.61 (8)	10 (5)	165 (8)
C-H...O contacts				
$\text{C}(2)-\text{H}(1)\cdots\text{O}(1^{\text{i}})$	3.165 (8)	2.27 (7)	30 (4)	136 (5)
$\text{C}(5)-\text{H}(4)\cdots\text{O}(3^{\text{ii}})$	3.267 (8)	2.41 (8)	31 (4)	136 (5)
$\text{C}(7)-\text{H}(7)\cdots\text{O}(4^{\text{vi}})$	3.377 (9)	2.48 (7)	34 (4)	131 (5)

## Key to symmetry operations

- |                      |                                 |
|----------------------|---------------------------------|
| (i) $x, 1+y, z$      | (v) $1-x, \frac{1}{2}+y, z$     |
| (ii) $x, -1+y, z$    | (vi) $1-x, -\frac{1}{2}+y, 1-z$ |
| (iii) $-1+x, 1+y, z$ | (vii) $2-x, \frac{1}{2}+y, z$   |
| (iv) $1+x, -1+y, z$  |                                 |


 Fig. 3. Projection of the structure along *b*.

along **b** (the shortest parameter) with H...O distances less than the sum of the van der Waals radii. Similar contacts have been observed in DL-homocystine and DL-homocystine monohydrogen oxalate. Also, the methylene group (C<sup>δ</sup>H<sub>2</sub>) is involved in a short intermolecular C—H...O contact and the value of the H—C...O'' angle falls in the range 22–59° observed by Sutor (1962) for this kind of interaction.

The N atoms around Cl form a distorted square-pyramidal arrangement with the chloride ion displaced by 0.349 (2) Å towards the top of the pyramid, the base of which is formed by N(1), N(1<sup>ii</sup>), N(2), N(2<sup>ii</sup>). The additional long contact Cl...S(1) = 3.618 (3) Å makes the environment severely distorted octahedral.

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## Structures of *E,E*-3-(*p*-Tolylimino)-2-butanone Oxime and *E,Z*-4-(*p*-Tolylimino)-2,3-pentanedione 3-Oxime. An X-ray Crystallographic Investigation on Bonding in Oximes

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#### Abstract

Single-crystal X-ray analyses of *E,E*-3-(*p*-tolylimino)-2-butanone oxime (HIB) and *E,Z*-4-(*p*-tolylimino)-2,3-pentanedione 3-oxime (HIOP) are reported. HIB (C<sub>11</sub>H<sub>14</sub>N<sub>2</sub>O, *M<sub>r</sub>* = 190.25) crystallizes in space group *B*2<sub>1</sub>/*c* with *a* = 19.539 (4), *b* = 19.673 (4), *c* = 11.242 (3) Å, β = 92.80 (3)°, *Z* = 16, *D<sub>c</sub>* = 1.17 Mg m<sup>-3</sup>, μ(Cu *K*α) = 0.537 mm<sup>-1</sup>. HIOP (C<sub>12</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>, *M<sub>r</sub>* = 218.26) is orthorhombic, *P*2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>, with *a* = 7.296 (2), *b* = 14.747 (3), *c* = 11.177 (3) Å, *Z* = 4, *D<sub>c</sub>* = 1.20 Mg m<sup>-3</sup>, μ(Cu *K*α) = 0.600 mm<sup>-1</sup>. The structures were refined from diffractometer data and final *R* values were 0.045 (2610 observed reflections)

and 0.048 (1004 observed reflections) for HIB and HIOP respectively. Both molecules display the group Ar—N=C(*R*)—C(*R'*)=N—OH and the structure analyses show that they have opposite configurations at the two centres of *syn/anti* isomerism and differ in conformation as far as the rotation around the C—C single bond is concerned. The different conformations are discussed in terms of balance of π-bond delocalization and nonbonded intramolecular potential energies. A comparison of the present data with those of the literature allows a classification of hydrogen bonds in crystals of oximes, and a possible relation between hydrogen bonding and N—O bond distances is suggested.