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The Crystal and Molecular Structure of Di-μ-(*N*,*N*-diethylnicotinamide-*O*,*N*-)di-isothiocyanatomanganese(II)

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Crystals of the title compound, $Mn(C_{10}H_{14}N_2O)_2(NCS)_2$ are triclinic, space group $P\bar{1}$. The unit-cell constants are: $a=9\cdot332$ (8), $b=7\cdot193$ (10), $c=11\cdot159$ (8) Å, $\alpha=113\cdot9$ (1)°, $\beta=96\cdot8$ (1)°, $\gamma=105\cdot7$ (1)°, $Z=1$. The crystal structure has been determined by X-ray diffraction and the three-dimensional intensity data have been measured on a single-crystal automated diffractometer. The structure, solved by Fourier methods and refined by least-squares methods, consists of octahedral centrosymmetric complexes: two positions of the polyhedron around the manganese atom are occupied by amidic O atoms, two by pyridine N atoms and two by isothiocyanato N atoms. Pairs of *N*,*N*-diethylnicotinamide molecules bridge two metal atoms, thus forming chains parallel to [010]. Bond distances and angles in the coordination polyhedron are compared with those obtained in the complex formed by the ligand with cadmium thiocyanate. The bond distances and angles in the organic ligand repeat those found in other determinations. The isothiocyanato group is linear.

Introduction

N,*N*-Diethylnicotinamide, a respiration stimulant, forms crystalline complexes with thiocyanates of divalent metals (Sandri Cavicchi, 1959). In order to define the chemical properties of this nicotinamide we have undertaken the determination of the crystal structures of some of the complexes. The results so far obtained in these compounds disclose various stereochemical arrangements of the ligands around the metal ion and different types of connexions between the complexes.

Experimental

Preparation

Crystals of the compound were obtained by adding an aqueous solution of manganese thiocyanate to a concentrated aqueous solution of *N*,*N*-diethylnicotinamide. This compound does not contain water molecules of crystallization, so that it is possible that it does not coincide with the dihydrate compound described by Sandri Cavicchi (1959).

Crystal data

Compound: di-μ-(*N*,*N*-diethylnicotinamide-*O*,*N*-)di-isothiocyanatomanganese(II),
$Mn(C_{10}H_{14}N_2O)_2(NCS)_2$
Formula weight 527·59
Unit cell: the parameters, determined from rotation and Weissenberg photographs and refined with data obtained on an automated single crystal diffractometer (Mo $K\alpha$, $\lambda=0\cdot71069$ Å), are:
$a=9\cdot332$ (8), $b=7\cdot193$ (10), $c=11\cdot159$ (8) Å
$\alpha=113\cdot9$ (1), $\beta=96\cdot8$ (1), $\gamma=105\cdot7$ (1)°
$V=637\cdot1$ Å^3; $Z=1$
$D_x=1\cdot375$, $D_m=1\cdot365$ g cm^{-3}
μ(Mo $K\alpha$)$=7\cdot29$ cm^{-1}; $F(000)=275$.
Space group: $P\bar{1}$ [$C_i(1)$ – No. 2] from lack of systematic absences and from structure determination.

Intensity data

The intensities were collected on a single-crystal automated Siemens diffractometer on line with a Siemens 304/P computer using Zr-filtered Mo $K\alpha$ radiation and the ω–2θ scan technique. A rather irregular crystal of approximate dimensions $0\cdot12\times0\cdot17\times0\cdot23$ mm was aligned with its [001] axis along the φ axis of the diffractometer and all the reflexions with $2\theta\le58°$ were collected. In this way the intensities of 3385 independent reflexions were measured and 1797 were used in the crystal analysis, taking as unobserved the reflexions whose intensities were less than twice their standard deviations $\{\sigma^2(I)=[\text{total counts}+(0\cdot005I)^2]\}$. Corrections for Lorentz and polarization factors were made in the usual way. No correction was made for absorption. Absolute scale factor and the mean isotropic temperature factor were obtained by Wilson's (1942) method.

Structure determination and refinement

The whole structure, except for the hydrogen atoms, was solved from a three-dimensional Fourier map, obtained with the phases determined by putting the manganese atom on a centre of symmetry. The refinement was carried out by the block-diagonal least-squares method, at first with isotropic, then with anisotropic thermal parameters. The hydrogen atoms were located directly from a difference synthesis calculated after several cycles of least squares. Further least-squares cycles were computed including the hydrogen atoms with isotropic thermal parameters. Unit weighting factors were assumed for every reflexion in all stages of the refinement. At the end of the refinement the R value was 0·042.

Atomic scattering factors given by Cromer & Mann (1968) were used for non-hydrogen atoms and those of Stewart, Davidson & Simpson (1965) for hydrogen atoms.

All the calculations were performed on the CDC

6600 Computer of the Centro di Calcolo Elettronico Interuniversitario dell' Italia Nord-Orientale (Bologna) using programs written by Immirzi (1967).

The final atomic coordinates and the thermal parameters are given in Tables 1 and 2. A list of observed and calculated structure factors is available as Supplementary Publication No. SUP 30018 (15 pp., 1 microfiche).*

Discussion

The crystal structure consists of chains of octahedral centrosymmetric complexes, parallel to [010], held

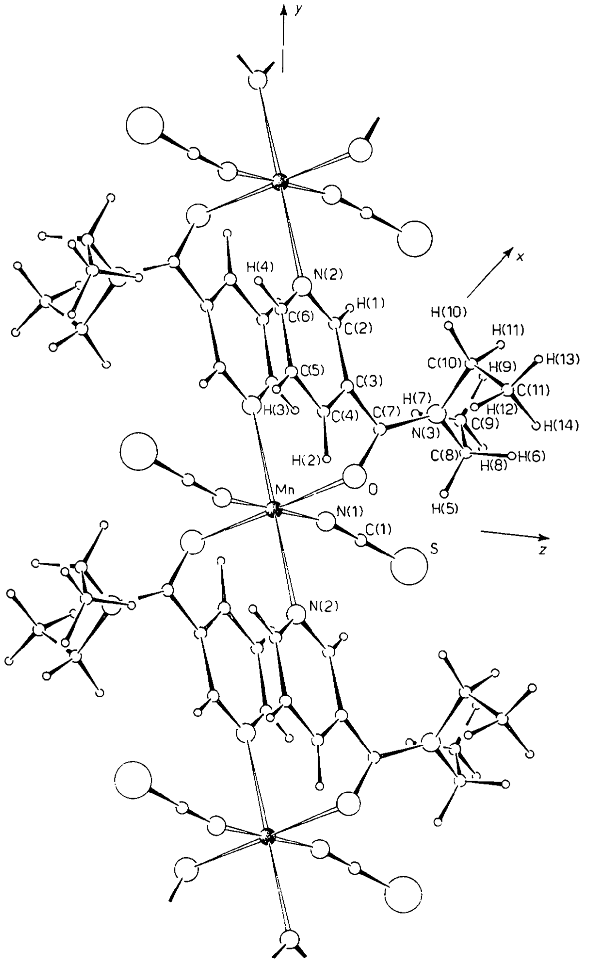

Fig. 1. Chains of centrosymmetrical octahedral complexes along [010].

Table 1. *Final fractional atomic coordinates* ($\times 10^4$) *with e.s.d.'s in parentheses*

Mn	0	0	0
S(1)	4888 (1)	−22 (2)	2109 (1)
O	362 (2)	2721 (3)	1964 (2)
N(1)	2324 (3)	185 (4)	705 (2)
N(2)	−939 (2)	7618 (3)	874 (2)
N(3)	1695 (3)	6065 (3)	3646 (2)
C(1)	3398 (3)	122 (4)	1284 (3)
C(2)	7 (3)	6955 (4)	1473 (2)
C(3)	−541 (3)	5488 (4)	1969 (2)
C(4)	−2111 (3)	4629 (5)	1821 (3)
C(5)	−3076 (3)	5349 (5)	1223 (3)
C(6)	−2441 (3)	6877 (4)	786 (3)
C(7)	561 (3)	4681 (4)	2541 (2)
C(8)	2855 (3)	5282 (5)	4108 (3)
C(9)	4253 (4)	5756 (6)	3579 (4)
C(10)	1877 (4)	8353 (4)	4493 (3)
C(11)	1106 (5)	8561 (7)	5633 (4)
H(1)	1146 (29)	7495 (41)	1541 (26)
H(2)	−2488 (32)	3409 (45)	2019 (28)
H(3)	−4180 (34)	4793 (48)	1170 (30)
H(4)	−3121 (31)	7384 (45)	368 (28)
H(5)	2373 (34)	3630 (48)	3669 (30)
H(6)	3155 (34)	6134 (48)	5196 (30)
H(7)	3918 (42)	5042 (58)	2518 (36)
H(8)	5034 (41)	5193 (58)	3914 (36)
H(9)	4803 (41)	7404 (59)	3942 (37)
H(10)	1500 (32)	9026 (46)	3970 (29)
H(11)	3087 (32)	9263 (46)	4874 (29)
H(12)	−30 (43)	7606 (59)	5085 (37)
H(13)	1182 (44)	10165 (63)	6373 (39)
H(14)	1608 (43)	7956 (61)	6226 (38)

Table 2. *Thermal parameters with e.s.d.'s*

The anisotropic temperature factors are in the form $\exp[-0\cdot25(h^2a^{*2}B_{11}+\ldots 2klb^*c^*B_{23})]$.

Heavy atoms

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Mn	2·275 (20)	2·117 (19)	2·433 (21)	0·931 (16)	0·099 (16)	1·132 (17)
S(1)	3·837 (37)	5·922 (46)	6·533 (51)	2·041 (34)	−0·522 (34)	3·254 (41)
O	5·143 (98)	2·391 (70)	3·011 (79)	1·704 (69)	0·508 (70)	1·093 (62)
N(1)	2·916 (95)	3·787 (104)	4·627 (118)	1·323 (82)	0·305 (84)	2·199 (93)
N(2)	2·994 (88)	2·546 (82)	2·993 (88)	1·055 (71)	0·566 (70)	1·491 (72)
N(3)	3·691 (99)	2·548 (83)	2·861 (91)	1·178 (75)	0·041 (75)	1·036 (73)
C(1)	2·843 (105)	2·898 (102)	3·550 (117)	0·965 (86)	0·655 (88)	1·673 (92)
C(2)	3·078 (105)	2·512 (92)	2·633 (99)	1·215 (82)	0·490 (82)	1·232 (79)
C(3)	3·177 (106)	2·176 (89)	2·335 (97)	1·031 (80)	0·394 (80)	0·855 (78)
C(4)	3·578 (122)	3·718 (120)	3·703 (124)	1·157 (100)	1·065 (99)	2·097 (103)
C(5)	3·289 (123)	4·684 (145)	4·981 (151)	1·436 (112)	0·983 (111)	2·779 (127)
C(6)	3·024 (112)	3·720 (120)	3·689 (123)	1·446 (96)	0·619 (94)	1·847 (102)
C(7)	3·111 (104)	2·519 (91)	2·352 (94)	1·110 (82)	1·008 (80)	1·388 (79)
C(8)	3·957 (146)	4·285 (137)	4·369 (147)	1·709 (117)	−0·331 (114)	2·170 (120)
C(9)	4·188 (158)	6·960 (211)	7·928 (231)	2·755 (153)	1·963 (156)	4·255 (190)
C(10)	5·116 (151)	2·642 (107)	3·560 (130)	1·292 (105)	0 (111)	0·599 (96)
C(11)	8·401 (251)	7·015 (220)	4·676 (177)	4·198 (199)	2·369 (173)	2·046 (164)

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* This table has been deposited with the National Lending Library, England. Copies may be obtained through the Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 2 (*cont.*)

Hydrogen atoms

	B
H(1)	3·59 (58)
H(2)	4·67 (68)
H(3)	5·34 (73)
H(4)	4·50 (66)
H(5)	5·41 (74)
H(6)	5·33 (73)
H(7)	7·97 (99)
H(8)	7·79 (97)
H(9)	8·00 (99)
H(10)	4·72 (68)
H(11)	4·72 (68)
H(12)	8·00 (99)
H(13)	8·89 (108)
H(14)	8·47 (104)

together by pairs of bridging *N,N*-diethylnicotinamide molecules (Fig. 1). The *N,N*-diethylnicotinamide molecules are bound to the metal atom through pyridinic nitrogen and amidic oxygen atoms; in this respect the type of bonding between metal and *N,N*-diethylnicotinamide is the same as that found in μ-(*N,N*-diethylnicotinamide)-di-μ-dithiocyanatocadmium (Bigoli, Braibanti, Pellinghelli & Tiripicchio, 1972), except that in the latter only one single molecule bridges the metal atoms. The difference between manganese and cadmium complexes stems mainly from the different role played by the thiocyanato group rather than that of nicotinamide. In the cadmium compound both thiocyanato bridging groups are bound to the metal through N and S, with pairs N,N and S,S in *cis* position in the coordination octahedron. In the present compound the thiocyanato group is bound to manganese only through N. Therefore the manganese compound can be classified as an isothiocyanate. This different behaviour probably depends on the different (*a*) and (*b*) character of the two metals, according to the classification of Ahrland (1966). In this classification manganese (II) is of (*a*) type and cadmium of (*b*) type.

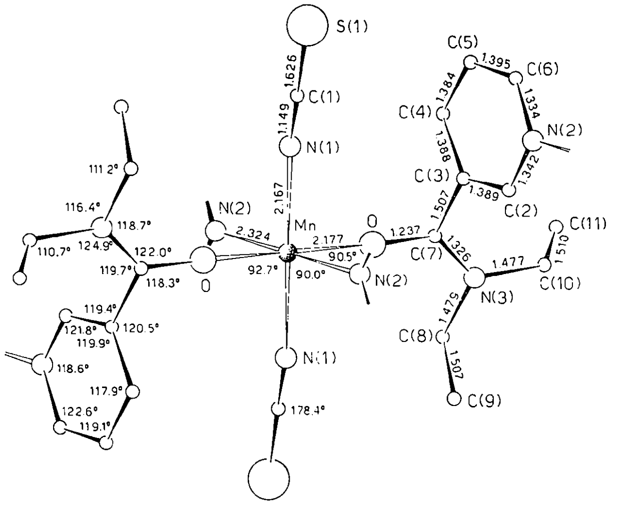


Fig. 2. Bond distances and angles in the complex.

The bond distances and angles in the coordination polyhedron are given in Table 3. In the octahedron around Mn (Fig. 2) two corners are occupied by nitrogen atoms of thiocyanato groups, two by pyridinic nitrogen atoms, and two by amidic oxygen atoms of nicotinamide molecules, each pair of equal atoms being in *trans* positions. The octahedron is only slightly distorted as shown by L–M–L (L ≡ donor atom) angles which are in the range 88–92°. The M–L bonds are rather more irregular than the angles, and disclose further differences between manganese and cadmium complexes. In fact the bond length M–N (NCS) = 2·167 Å is comparable to Cd–N = 2·295–2·292 Å if the difference in ionic radii is taken into account; the bond length Mn–O (amidic) = 2·177 Å is shorter than the corresponding distance in the cadmium compound, again in accordance with the trend in ionic radii; the bond length Mn–N (pyr) = 2·324 Å is, however, longer than the corresponding distance in the cadmium compound and even longer than any manganese–oxygen or manganese–nitrogen bonds (Mn–O = 2·172–2·253 Å, Glick & Dahl, 1966; Mn–O = 2·138–2·248 Å, Mn–N = 2·189–2·208 Å, Braibanti, Tiripicchio, Manotti Lanfredi & Camellini, 1967; Mn–O = 2·135–2·219 Å, Kay, Almodovar & Kaplan, 1968). This implies a particularly weak bond between the basic site of the pyridine ring and Mn^{+2}, even weaker than that between the same ion Mn^{+2} and the amidic O atom. The only conceivable cause of this weak interaction must be searched for in steric and packing factors, combined with the directed valence orbitals, *i.e.* regular octahedral angles, of the manganous ion.

Table 3. *Bond distances and angles*

(*a*) In the coordination polyhedron

Mn–N(1)	2·167 (4) Å	N(2^{i})–Mn—O	89·5 (1)°
Mn–N(2^{i})	2·324 (4)	N(2^{i})–Mn—N(1)	90·0 (1)
Mn–O	2·177 (4)	N(1)–Mn—O	87·3 (1)
		Mn—N(1)–C(1)	163·6 (2)

(*b*) In the thiocyanato anion

C(1)–N(1)	1·149 (5) Å	N(1)–C(1)–S(1)	178·4 (3)°
C(1)–S(1)	1·626 (4)		

Asymmetric unit: see Table 5.

The isothiocyanato group is linear; the bonds C–N = 1·149 and C–S = 1·626 Å agree well with values found previously in the same group and quoted by Bigoli, Braibanti, Pellinghelli & Tiripicchio (1972).

The organic ligand (Table 4 and Fig. 2) presents the same structure as found in the cadmium complex. The distances and angles in the pyridine ring are practically the same as those found in the cadmium compound. The average carbon–carbon bond is here C–C$_{av}$ = 1·389 (2) Å against 1·379 (3) Å in the cadmium compound; in the ring, the carbon–nitrogen bond lengths are C(2)–N(2) = 1·342 (4) and C(6)–N(2) = 1·334 (4) Å with C–N$_{av}$ = 1·338 (3) Å against 1·333 (4) Å in the cadmium compound. The hexatomic ring is not exactly planar (Table 6) and even the four central atoms, C(2), C(3), C(5), C(6), form a slightly puckered structure; nevertheless the extreme opposite atoms C(4) and N(2) both lie on the same side with respect to the average plane through the other atoms, thus maintaining the boat shape already found in the cadmium compound.

The bonds radiating from C(7), the carbon atom of the amidic group, are exactly planar in accordance with the results in the other amides, such as 4-diethylcarbamoyl-1-cyclohexene-5-carboxylic acid, DDCA (Pedone, Benedetti, Immirzi & Allegra, 1970) and the amidoxalato anion (Braibanti, Pellinghelli, Tiripicchio & Tiripicchio Camellini, 1971; Pellinghelli, Tiripicchio & Tiripicchio Camellini, 1972). C(7) is therefore in sp^2 configuration, as is also confirmed by the angles, which are each close to 120°.

The carbon–carbon bond between amidic group and pyridine ring, C(3)–C(7) = 1·507 Å corresponds to the value (1·50 Å) accepted for a typical C_{sp^2}–C_{sp^2} bond.

The bonds from the amide nitrogen atom, N(3), lie practically in the same plane, a result which is not exactly the same as that found in DDCA (Pedone, Benedetti, Immirzi & Allegra, 1970) and in the cadmium compound and suggests some degree of flexibility of the amide group in different compounds. The angle between the average planes through C(7) and N(3) is 7·4°. The carbon–nitrogen bond, C(7)–N(3) = 1·326 Å agrees very well with values found in the amidoxalato anion (1·315 Å) and in DDCA (1·343 Å).

The carbon–nitrogen bonds between amidic nitrogen and ethyl groups, N(3)–C(8) = 1·479 and N(3)–C(10) = 1·477 Å indicate that these bonds are the same as those found in amines.

It is a pleasure to thank Professors L. Cavalca and M. Nardelli for kindly permitting us to use the equipment of the Centro di Strutturistica Diffrattometrica del C.N.R. and the programs of the computer library.

Table 4. *Bond distances and angles in the organic molecule*

N(2)—C(2)	1·342 (4) Å	C(2)—H(1)	1·01 (3) Å
N(2)—C(6)	1·334 (4)	C(4)—H(2)	0·98 (4)
C(2)—C(3)	1·389 (5)	C(5)—H(3)	0·98 (3)
C(3)—C(4)	1·388 (4)	C(6)—H(4)	0·97 (4)
C(4)—C(5)	1·384 (6)	C(8)—H(5)	1·02 (3)
C(5)—C(6)	1·395 (5)	C(8)—H(6)	1·07 (3)
C(3)—C(7)	1·507 (5)	C(9)—H(7)	1·05 (4)
C(7)—O	1·237 (4)	C(9)—H(8)	1·03 (5)
C(7)—N(3)	1·326 (4)	C(9)—H(9)	1·03 (4)
N(3)—C(8)	1·479 (5)	C(10)–H(10)	0·99 (4)
C(8)—C(9)	1·507 (5)	C(10)–H(11)	1·07 (3)
N(3)—C(10)	1·477 (4)	C(11)–H(12)	1·04 (3)
C(10)–C(11)	1·510 (6)	C(11)–H(13)	1·09 (4)
		C(11)–H(14)	1·06 (5)

Table 5. *Shortest intermolecular distances*

O······N(1)*	2·999 (5) Å
O······N(1^{ii})*	3·142 (7)
O······N(2^{i})*	3·170 (6)
N(2)····O^{iii}*	3·198 (4)
N(2)····N(1^{iii})*	3·177 (5)
N(1)····N(2^{i})*	3·177 (5)
N(1)····C(4^{ii})	3·400 (7)
C(1)····C(4^{ii})	3·511 (8)
N(1)····C(2^{i})	3·185 (6)
C(1)····C(2^{i})	3·449 (6)
C(6)····N(1^{iii})	3·164 (6)
C(7)····N(2^{iii})	3·593 (5)
C(2)····C(2^{iii})	3·346 (6)
C(11)···O^{iv}	3·480 (6)

Asymmetric units:

i	x,	$-1+y$,	z
ii	$\bar{x}$,	$\bar{y}$,	$\bar{z}$
iii	$\bar{x}$,	$1-y$,	$\bar{z}$
iv	$\bar{x}$,	$1-y$,	$1-z$

* Edge of the coordination octahedron.

Table 4 (*cont.*)

C(6)–N(2)—C(2)	118·6 (2)°	N(2)—C(6)—H(4)	118·4 (18)°
N(2)–C(2)—C(3)	121·8 (2)	N(3)—C(8)—H(5)	106·8 (19)
C(2)–C(3)—C(4)	119·9 (3)	N(3)—C(8)—H(6)	105·5 (19)
C(2)–C(3)—C(7)	119·4 (2)	C(9)—C(8)—H(5)	105·6 (18)
C(4)–C(3)—C(7)	120·5 (3)	C(9)—C(8)—H(6)	110·8 (17)
C(3)–C(4)—C(5)	117·9 (3)	H(5)—C(8)—H(6)	117·0 (27)
C(4)–C(5)—C(6)	119·1 (3)	C(8)—C(9)—H(7)	109·5 (22)
C(5)–C(6)—N(2)	122·6 (3)	C(8)—C(9)—H(8)	109·4 (22)
C(3)–C(7)—O	118·3 (2)	C(8)—C(9)—H(9)	111·5 (21)
C(3)–C(7)—N(3)	119·7 (3)	H(7)—C(9)—H(8)	111·6 (31)
N(3)–C(7)—O	122·0 (3)	H(7)—C(9)—H(9)	108·2 (33)
C(7)–N(3)—C(8)	118·7 (2)	H(8)—C(9)—H(9)	106·6 (32)
C(7)–N(3)—C(10)	124·9 (3)	N(3)—C(10)–H(10)	113·3 (18)
C(8)–N(3)—C(10)	116·4 (2)	N(3)—C(10)–H(11)	107·3 (18)
N(3)–C(8)—C(9)	111·2 (3)	C(11)–C(10)–H(10)	110·4 (18)
N(3)–C(10)–C(11)	110·7 (3)	C(11)–C(10)–H(11)	111·4 (16)
N(2)–C(2)—H(1)	119·4 (18)	H(10)–C(10)–H(11)	103·5 (26)
C(3)–C(2)—H(1)	118·7 (18)	C(10)–C(11)–H(12)	100·6 (21)
C(3)–C(4)—H(2)	118·3 (18)	C(10)–C(11)–H(13)	119·4 (23)
C(5)–C(4)—H(2)	123·1 (18)	C(10)–C(11)–H(14)	108·5 (22)
C(4)–C(5)—H(3)	117·3 (22)	H(12)–C(11)–H(13)	110·9 (32)
C(6)–C(5)—H(3)	123·5 (22)	H(12)–C(11)–H(14)	114·0 (34)
C(5)–C(6)—H(4)	119·0 (18)	H(13)–C(11)–H(14)	103·8 (32)

Table 6. *Analysis of planarity of groups of atoms. The plane of best fit is defined by atoms with an asterisk. X, Y, Z are orthogonal coordinates in* Å

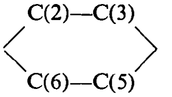
Transformation matrix from fractional to orthogonal coordinates

$$\begin{pmatrix} a\sin\gamma & 0 & -c\sin\alpha\cos\beta^* \\ a\cos\gamma & b & c\cos\alpha \\ 0 & 0 & c\sin\alpha\,\sin\beta^* \end{pmatrix}.$$

(1) Equation of the plane through C(2), C(3), C(5), C(6) of the pyridine ring

$$0{\cdot}1213X-0{\cdot}4355Y-0{\cdot}8920Z=-3{\cdot}2363\,.$$

	$\Delta.10^4$ (Å)	$\sigma.10^4$ (Å)
C(2)*	72	22
C(3)*	−74	22
C(5)*	138	32
C(6)*	−137	30
N(2)	202	21
C(4)	236	32

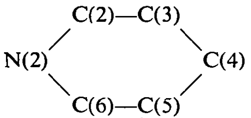


$\sum_4 (\Delta/\sigma)^2=61{\cdot}48$

(2) Equation of the plane of the pyridine ring

$$0{\cdot}1221X-0{\cdot}4378Y-0{\cdot}8907Z=-3{\cdot}2383\,.$$

	$\Delta.10^4$ (Å)	$\sigma.10^4$ (Å)
N(2)*	102	21
C(2)*	8	22
C(3)*	−111	22
C(4)*	190	32
C(5)*	56	32
C(6)*	−246	30

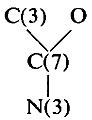


$\sum_6 (\Delta/\sigma)^2=154{\cdot}74$

(3) Equation of the plane of the carbonyl carbon [C(7)]

$$0{\cdot}7690X+0{\cdot}2830Y-0{\cdot}5731Z=-0{\cdot}9805\,.$$

	$\Delta.10^4$ (Å)	$\sigma.10^4$ (Å)
C(3)*	−15	26
C(7)*	42	26
O*	−11	20
N(3)*	−17	25



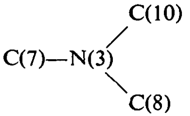
$\sum_4 (\Delta/\sigma)^2=3{\cdot}71$

Table 6 (*cont.*)

(4) Equation of the plane of the amide nitrogen [N(3)]

$$0{\cdot}7285X+0{\cdot}4044Y-0{\cdot}5529Z=-0{\cdot}6640\,.$$

	$\Delta.10^4$ (Å)	$\sigma.10^4$ (Å)
C(7)*	−27	26
N(3)*	94	25
C(8)*	−28	31
C(10)*	−39	34



$\sum_4 (\Delta/\sigma)^2=17{\cdot}35$

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The Crystal and Molecular Structure of 1,2-Benzisothiazol-3-yl Methyl Ketoxime

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Crystals of 1,2-benzisothiazol-3-yl methyl ketoxime are orthorhombic, space group *Pbca*. The unit cell constants are $a=19{\cdot}613$ (8), $b=24{\cdot}192$ (9), $c=7{\cdot}550$ (3) Å, $Z=16$. The crystal structure has been determined by X-ray diffraction. Three-dimensional intensity data have been measured on a single-crystal automated diffractometer. The structure has been solved by direct methods and refined by least-squares methods (final $R=4{\cdot}3$%). There are two independent molecules in the asymmetric unit. They are practically equal as far as distances, angles and configuration are concerned. The oxime group, =N–OH, is oriented *cis* with respect to the methyl group, *i.e.* the compound is the *anti*-1,2-benzisothiazol-3-yl methyl ketoxime. The whole molecule is nearly planar. Significant differences in bond distances and angles are found in the isothiazole ring of this compound and that of derivatives of 1,2-benzisothiazolin-3-one. The molecules are held together by a network of hydrogen bonds –OH···N, *i.e.* between the hydroxyl of the oxime group (OH) and the nitrogen atom of the isothiazole ring.

Introduction

1,2-Benzisothiazole derivatives form a class of compounds of pharmaceutical importance for their anaesthetic, antihistaminic and antifungal activities (Ponci, Vitali & Bertaccini, 1968; Vitali, Mossini, Bertaccini & Impicciatore, 1968; Vitali, Mossini, Mingiardi, Gaetani & Plazzi, 1971).