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The Crystal and Molecular Structure of Mono-(*N*,*N*-diethylnicotinamide)cadmium Dithiocyanate

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Crystals of mono-(*N*,*N*-diethylnicotinamide)cadmium dithiocyanate are monoclinic, space group $P2_1/c$ with unit-cell constants: $a=9·735$ (7), $b=16·202$ (10), $c=10·640$ (9) Å; $\beta=105·2$ (1)°, $Z=4$. The structure has been determined from three-dimensional intensity data, measured on an automated diffractometer ($R=0·036$). The structure consists of a three-dimensional network of octahedral metal complexes held together by bridges of thiocyanato anions and nicotinamide molecules. The thiocyanato anion is practically linear. In the organic ligand, the pyridine ring as a whole does not lie in the same plane, but part of it is planar and therefore the ring is slightly bent into a boat shape. The bonds radiating from the carbon atom of the carbonyl group are planar, whereas those from the amide nitrogen are not; the dihedral angle between the best planes through these two groups is 8·1°. Intramolecular repulsion between one ethyl group and the pyridine ring seems to be the cause of the distortion.

Introduction

N,*N*-Diethylnicotinamide is an important respiration stimulant. It can form crystalline compounds with thiocyanates of divalent metals (Sandri Cavicchi, 1959). We have now undertaken the study of the crystal structure of the complex mono-(*N*,*N*-diethylnicotinamide)cadmium dithiocyanate, $Cd(C_{10}H_{14}N_2O)(NCS)_2$, in order to give a contribution to the definition of the chemical properties of this nicotinamide.

Experimental

Preparation

Colorless crystals of the compound are obtained by evaporation of an aqueous solution of cadmium chloride, potassium thiocyanate and organic ligand.

Crystal data

Compound: mono-(*N*,*N*-diethylnicotinamide)cadmium dithiocyanate, $Cd(C_{10}H_{14}N_2O)(NCS)_2$. Formula weight 406·8. Crystal class: monoclinic prismatic. Unit cell: the parameters, determined from rotation and Weissenberg photographs and refined with data obtained on an automated single-crystal diffractometer (Mo $K\alpha$, $\lambda=0·71069$ Å), are: $a=9·735$ (7), $b=16·202$ (10), $c=10·640$ (9) Å; $\beta=105·2$ (1)°, $V=1619·4$ Å^3, $Z=4$. $D_x=1·668$, $D_m=1·643$ g.cm^{-3}. μ(Mo $K\alpha$)$=15·6$ cm^{-1}, $F(000)=808$. Space group: $P2_1/c$ [$C_{2h}(5)$ – No. 14] from systematic absences.

Intensity data

The intensity data 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. The crystal was aligned with its [001] axis along the φ axis of the diffractometer and all the reflexions with $2\theta \le 58°$ were collected. In this way the intensities of 4317 independent reflexions were measured; of these only 2594, having $I \ge 2\sigma(I)$, were used in the analysis.

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

	x	*y*	*z*
Cd	0·2613 (1)	0·0893 (1)	0·0483 (1)
S(1)	−0·0177 (1)	−0·1685 (1)	0·0717 (1)
S(2)	0·6979 (2)	−0·0790 (1)	0·1851 (1)
O	0·3786 (3)	0·2179 (2)	0·1023 (3)
N(1)	0·1623 (4)	−0·0385 (2)	0·0563 (4)
N(2)	0·4784 (4)	0·0338 (2)	0·1507 (4)
N(3)	0·2185 (4)	0·3885 (2)	−0·2465 (3)
N(4)	0·5427 (3)	0·3156 (2)	0·1064 (3)
C(1)	0·0881 (4)	−0·0911 (3)	0·0637 (4)
C(2)	0·5664 (5)	−0·0131 (3)	0·1618 (4)
C(3)	0·3180 (4)	0·3523 (2)	−0·1537 (4)
C(4)	0·3005 (4)	0·3328 (2)	−0·0328 (3)
C(5)	0·1716 (4)	0·3520 (3)	−0·0073 (4)
C(6)	0·0684 (4)	0·3914 (3)	−0·1018 (4)
C(7)	0·0952 (4)	0·4092 (3)	−0·2195 (4)
C(8)	0·4105 (4)	0·2853 (2)	0·0632 (3)
C(9)	0·5838 (5)	0·4003 (3)	0·0875 (5)
C(10)	0·6957 (6)	0·4061 (3)	0·0128 (6)
C(11)	0·6492 (5)	0·2639 (4)	0·1971 (5)
C(12)	0·7151 (6)	0·2010 (4)	0·1267 (8)
H(1)	0·4140 (49)	0·3388 (28)	−0·1754 (43)
H(2)	0·1413 (47)	0·3329 (28)	0·0774 (42)
H(3)	−0·0264 (46)	0·4138 (26)	−0·0926 (41)
H(4)	0·0173 (54)	0·4248 (31)	−0·2824 (48)
H(5)	0·6222 (52)	0·4239 (30)	0·1764 (47)
H(6)	0·5000 (51)	0·4238 (28)	0·0360 (43)
H(7)	0·7178 (55)	0·4583 (34)	0·0071 (51)
H(8)	0·6400 (57)	0·3800 (33)	−0·0765 (50)
H(9)	0·7849 (56)	0·3745 (36)	0·0626 (49)
H(10)	0·5918 (58)	0·2435 (34)	0·2598 (52)
H(11)	0·7326 (51)	0·3069 (31)	0·2410 (46)
H(12)	0·6317 (61)	0·1656 (36)	0·0734 (54)
H(13)	0·7784 (56)	0·2332 (34)	0·0742 (50)
H(14)	0·7875 (61)	0·1626 (35)	0·1900 (53)

Table 2. *Thermal parameters with e.s.d.'s* (Å^2)

$B_{ij}=8\pi^2U_{ij}$ referred to a^*, b^*, c^*.

(*a*) Heavy atoms (values × 10^3)

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Cd	2941 (9)	3137 (9)	2739 (8)	−125 (10)	501 (7)	−122 (10)
S(1)	3123 (43)	3311 (45)	7024 (71)	−208 (36)	5 (44)	1106 (46)
S(2)	10887 (122)	13029 (145)	3380 (51)	8812 (118)	2873 (66)	3205 (73)
O	4168 (133)	3284 (120)	3740 (124)	−932 (102)	615 (104)	641 (99)
N(1)	3387 (152)	3227 (155)	6856 (231)	−421 (124)	377 (151)	−620 (153)
N(2)	3585 (149)	4600 (172)	3733 (153)	329 (132)	945 (124)	318 (132)
N(3)	3271 (134)	3541 (145)	2925 (125)	182 (109)	967 (107)	118 (104)
N(4)	3040 (126)	2848 (127)	3401 (134)	−494 (105)	697 (108)	204 (106)
C(1)	2848 (140)	3158 (152)	3939 (166)	329 (137)	−253 (122)	−401 (148)
C(2)	4187 (184)	5450 (227)	2425 (145)	1086 (169)	1243 (136)	1154 (146)
C(3)	3204 (152)	3120 (151)	2808 (140)	328 (125)	1066 (120)	164 (120)
C(4)	2866 (137)	2511 (134)	2539 (128)	−449 (111)	500 (107)	−129 (106)
C(5)	2744 (142)	3859 (171)	3232 (152)	−807 (129)	963 (119)	−680 (135)
C(6)	2627 (146)	4404 (208)	4419 (190)	31 (132)	1232 (138)	−329 (149)
C(7)	2809 (139)	4090 (175)	3518 (155)	46 (146)	748 (119)	− 94 (151)
C(8)	3470 (155)	3013 (150)	2242 (124)	−510 (121)	795 (114)	−114 (110)
C(9)	3721 (175)	2795 (170)	5364 (215)	−1183 (135)	1008 (157)	−974 (148)
C(10)	5437 (248)	4382 (226)	7049 (293)	−1565 (206)	2592 (226)	488 (219)
C(11)	3193 (179)	6067 (275)	5407 (243)	48 (181)	− 20 (167)	1434 (212)
C(12)	4758 (263)	5409 (287)	10959 (471)	1680 (230)	2166 (285)	1871 (301)

Table 2 (*cont.*)

(*b*) Hydrogen atoms (values × 10^2)

	B
H(1)	458 (104)
H(2)	433 (102)
H(3)	396 (94)
H(4)	579 (125)
H(5)	532 (117)
H(6)	475 (108)
H(7)	621 (127)
H(8)	618 (128)
H(9)	637 (134)
H(10)	662 (136)
H(11)	531 (117)
H(12)	728 (150)
H(13)	636 (134)
H(14)	728 (150)

Calculations

After the usual corrections for Lorentz and polarization factors the structure amplitudes were put approximately on absolute scale by Wilson's (1942) method; no correction for absorption was made.

The structure was solved from the three-dimensional Patterson function by means of the heavy atom method. A few cycles of Fourier syntheses made it possible to localize all the non-hydrogen atoms. The refinement was carried out by block-diagonal least-squares methods with anisotropic thermal parameters. Unit weighting factors were assumed. The hydrogen atoms were localized directly from a difference synthesis calculated after some cycles of least squares. The ethyl hydrogen atom maxima were very smeared, although significantly resolved. More least-squares cycles were computed including the hydrogen atoms with isotropic thermal parameters. The weighting scheme: $1/w=(A+BF_o+CF_o^2)$ with $A=1{\cdot}8496$, $B=0{\cdot}04515$, $C=0{\cdot}00027556$ was applied at this stage. At the end of the refinement the conventional residual error index R was 0·036. Atomic scattering given by Cromer & Mann (1968) were used for non-hydrogen atoms and those by Stewart, Davidson & Simpson (1965) for hydrogen atoms. All the calculations were performed on the CDC 6600 Computer of the Centro di Calcòlo Elettronico Interuniversitario dell'Italia Nord-Orientale (Bologna), using the programs written by Immirzi (1967). The final atomic coordinates are given in Table 1 and the thermal parameters in Table 2. A list of observed and calculated structure factors is available from the authors on request. The main interatomic distances and angles are quoted in Tables 3–6.

Table 3. *Bond distances and angles in the coordination polyhedron*

Cd–N(1)	2·295 (4) Å
Cd–N(2)	2·292 (6)
Cd–O	2·373 (4)
Cd–S(1^{i})	2·704 (5)
Cd–S(2^{ii})	2·621 (3)
Cd–N(3^{iii})	2·355 (4)

Asymmetric units:

i	$\bar{x}$	$\bar{y}$	$\bar{z}$
ii	$1-x$	$\bar{y}$	$\bar{z}$
iii	x	$\frac{1}{2}-y$	$\frac{1}{2}+z$
iv	$1-x$	$-\frac{1}{2}+y$	$\frac{1}{2}-z$

N(3^{iii})–Cd——N(1)	85·7 (1)°
N(3^{iii})–Cd——N(2)	89·1 (1)
N(3^{iii})–Cd——O	80·3 (1)
N(3^{iii})–Cd——S(1^{i})	91·1 (1)
S(2^{ii})—Cd——N(1)	98·5 (1)
S(2^{ii})—Cd——N(2)	94·3 (1)
S(2^{ii})—Cd——O	95·9 (1)
S(2^{ii})—Cd——S(1^{i})	85·1 (1)
N(1) —Cd——N(2)	88·4 (1)
N(2) —Cd——O	84·5 (1)
O——Cd——S(1^{i})	90·3 (1)
S(1^{i}) —Cd——N(1)	96·9 (1)
N(3^{iii})–Cd——S(2^{ii})	174·6 (1)
N(2) —Cd——S(1^{i})	174·6 (1)
N(1) —Cd——O	164·4 (1)
C(8)—O——Cd	147·3 (3)
Cd——S(1^{i}) —C(1^{i})	95·6 (2)
Cd——S(2^{ii})—C(2^{ii})	101·8 (2)
Cd——N(3^{iii})–C(3^{iii})	119·1 (3)
Cd——N(3^{iii})–C(7^{iii})	122·9 (3)
Cd——N(1) —C(1)	164·3 (4)
Cd——N(2) —C(2)	153·4 (4)

Table 4. *Bond distances and angles in the thiocyanato anion*

C(1)–N(1)	1·133 (6) Å	N(1)–C(1)–S(1)	178·5 (4)°
C(1)–S(1)	1·639 (5)	N(2)–C(2)–S(2)	177·1 (4)
C(2)–N(2)	1·128 (6)		
C(2)–S(2)	1·635 (6)		

Discussion

The whole structure consists of a three-dimensional network of octahedral complexes held together by bridges of thiocyanato anions and nicotinamide molecules (Fig. 1). The octahedron around Cd is slightly deformed (Fig. 2); the corners of the coordination polyhedron are occupied by 2N from NCS, 2S from NCS, 1 N (pyridine) and 1 O (amide) from the organic ligand. The two Cd–NCS bonds, Cd–N(1) = 2·295 (4) and Cd–N(2) = 2·292 (6) Å, are equal to one another, although the angles Cd–N(1)–C(1) = 164·3 (4)° and Cd–N(2)–C(2) = 153·4 (4)° are not. The Cd–SCN bonds are significantly different, Cd–S(1$^{\mathrm{i}}$) = 2·704 (5) and Cd–S(2$^{\mathrm{ii}}$) = 2·621 (3) Å, and the angles as well, Cd–S(1$^{\mathrm{i}}$)–C(1$^{\mathrm{i}}$) = 95·6 (2)° and Cd–S(2$^{\mathrm{ii}}$)–C(2$^{\mathrm{ii}}$) = 101·8 (2)°. These bonds between cadmium and bridging

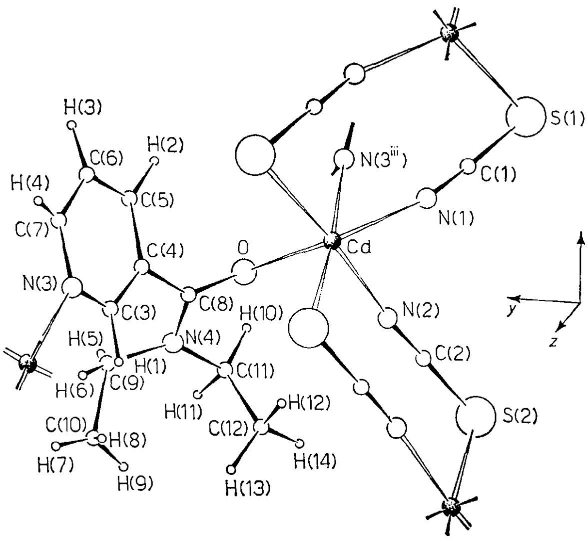


Fig. 1. Clinographic projection of the network of complexes.

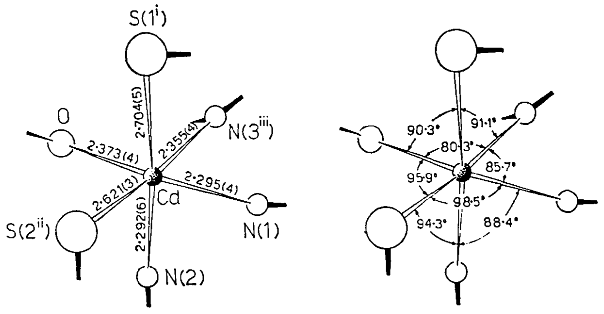


Fig. 2. Coordination around cadmium atom.

Table 5. *Bond distances and angles in the organic molecule*

(*a*) Distances

N(3)—C(3)	1·325 (5) Å	C(3)—H(1)	1·04 (5) Å
N(3)—C(7)	1·348 (7)	C(5)—H(2)	1·07 (4)
C(3)—C(4)	1·378 (5)	C(6)—H(3)	1·02 (5)
C(4)—C(5)	1·387 (7)	C(7)—H(4)	0·91 (5)
C(5)—C(6)	1·378 (6)	C(9)—H(5)	1·00 (5)
C(6)—C(7)	1·735 (6)	C(9)—H(6)	0·94 (5)
C(4)—C(8)	1·486 (5)	C(10)–H(7)	0·88 (6)
C(8)—O	1·237 (5)	C(10)–H(8)	1·05 (5)
C(8)—N(4)	1·341 (6)	C(10)–H(9)	1·03 (6)
N(4)—C(9)	1·458 (6)	C(11)–H(10)	1·03 (6)
C(9)—C(10)	1·510 (9)	C(11)–H(11)	1·08 (5)
N(4)—C(11)	1·478 (7)	C(12)–H(12)	1·03 (6)
C(11)–C(12)	1·504 (9)	C(12)–H(13)	1·07 (6)
		C(12)–H(14)	1·04 (6)

Table 5 (*cont.*)

(*b*) Angles

C(7)–N(3)—C(3)	118·0 (3)°	N(3)—C(7)—H(4)	122·1 (3·3)°
N(3)–C(3)—C(4)	123·5 (4)	N(4)—C(9)—H(5)	106·1 (2·8)
C(3)–C(4)—C(5)	118·1 (3)	C(10)–C(9)—H(5)	109·4 (3·0)
C(3)–C(4)—C(8)	121·1 (3)	N(4)—C(9)—H(6)	103·6 (2·9)
C(5)–C(4)—C(8)	120·5 (3)	C(10)–C(9)—H(6)	107·7 (2·9)
C(4)–C(5)—C(6)	119·0 (4)	H(5)—C(9)—H(6)	116·8 (4·0)
C(5)–C(6)—C(7)	119·1 (4)	C(9)—C(10)–H(7)	108·6 (3·6)
C(6)–C(7)—N(3)	122·3 (4)	C(9)—C(10)–H(8)	100·3 (3·1)
C(4)–C(8)—O	119·3 (3)	C(9)—C(10)–H(9)	109·0 (3·0)
C(4)–C(8)—N(4)	120·0 (3)	H(7)—C(10)–H(8)	113·7 (4·5)
N(4)–C(8)—O	120·7 (3)	H(7)—C(10)–H(9)	109·0 (4·8)
C(8)–N(4)—C(9)	124·8 (3)	H(8)—C(10)–H(9)	115·6 (4·3)
C(8)–N(4)—C(11)	117·5 (3)	N(4)—C(11)–H(10)	101·4 (3·1)
C(9)–N(4)—C(11)	116·9 (4)	C(12)–C(11)–H(10)	118·7 (3·1)
N(4)–C(9)—C(10)	113·1 (4)	N(4)—C(11)–H(11)	103·7 (2·7)
N(4)–C(11)–C(12)	112·1 (5)	C(12)–C(11)–H(11)	106·4 (2·7)
N(3)–C(3)—H(1)	116·8 (2·5)	H(10)–C(11)–H(11)	113·6 (4·0)
C(4)–C(3)—H(1)	119·7 (2·5)	C(11)–C(12)–H(12)	105·8 (3·4)
C(4)–C(5)—H(2)	124·5 (2·5)	C(11)–C(12)–H(13)	108·0 (3·0)
C(6)–C(5)—H(2)	116·2 (2·5)	C(11)–C(12)–H(14)	112·7 (3·1)
C(5)–C(6)—H(3)	126·9 (2·4)	H(12)–C(12)–H(13)	117·5 (4·3)
C(7)–C(6)—H(3)	113·9 (2·4)	H(12)–C(12)–H(14)	108·9 (4·5)
C(6)–C(7)—H(4)	114·2 (3·3)	H(13)–C(12)–H(14)	104·1 (4·4)

thiocyanato can be compared with the situation found in the ethylenethiourea complex Cdetu_2(NCS)$_2$ (Cavalca, Nardelli & Fava, 1960). The main difference concerns the cadmium–nitrogen bond which is much longer (2·53 Å) in the ethylenethiourea complex. The distance between cadmium and pyridine nitrogen, Cd–N(3^{iii}) = 2·355 (4) Å, is longer than the Cd–N(1) and Cd–N(2) bonds, in accordance with electrostatic attracting power of the negative charge born by the anionic N. The cadmium–oxygen bond length, Cd–O = 2·373 (4) Å is only slightly longer than that between cadmium and pyridine nitrogen.

Table 6. *Shortest intermolecular distances*

N(1)···N(1^{i})	3·315 (9) Å
N(1)···C(1^{i})	3·217 (7)
N(1)···C(7^{iii})	3·365 (6)
C(1)···C(1^{i})	3·504 (7)
S(1) ···C(5^{i})	3·319 (5)
N(2)···C(3^{iii})	3·447 (7)
O ·····C(3^{iii})	3·031 (6)
S(2) ···C(5^{iv})	3·512 (5)
N(2)···N(2^{ii})	3·517 (6)
C(2)···N(2^{ii})	3·255 (7)
C(2)···C(2^{ii})	3·372 (7)

The thiocyanato anion is almost linear, having N(1)–C(1)–S(1) = 178·5 (4)° and N(2)–C(2)–S(2) = 177·1 (4)°. The bond lengths between carbon and nitrogen, C(1)–N(1) = 1·133 (6), and C(2)–N(2) = 1·128 (6) Å, agree very well with the distance found in bis(hydrazine)zinc isothiocyanate, Zn(N_2H_4)$_2$(NCS)$_2$ (Ferrari, Braibanti, Bigliardi & Lanfredi, 1965) where N–C = 1·128 (14) Å; though, in the latter compound, the isothiocyanato anion is not acting as a bridge. Also the carbon–sulphur bonds, C(1)–S(1) = 1·639 (5) and C(2)–S(2) = 1·635 (6) Å, agree very well with those found in Zn(N_2H_4)$_2$(NCS)$_2$ were C–S = 1·655 (12) Å. The angles Cd–N–C fall in the range of values already found in isothiocyanates for angles M–N–C (Cavalca, Nardelli & Fava, 1960; Owston & Rowe, 1960; Ferrari, Braibanti, Bigliardi & Lanfredi, 1965; Nardelli, Fava Gasparri, Giraldi Battistini & Domiano, 1966; Garaj, 1969).

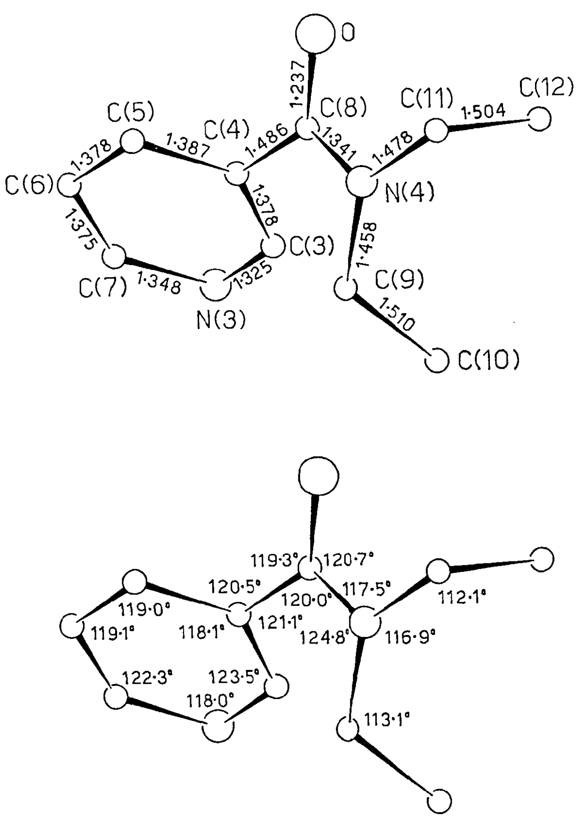


Fig. 3. Bond distances and angles in the organic molecule.

Distances and angles in the organic ligand (Fig. 3) repeat those found in other works on nicotinic acid (Wright & King, 1953), nicotinamide (Wright & King, 1954) and metal nicotinate (Biagini, Domiano, Guastini, Musatti & Nardelli, 1971). In the ring, the carbon–carbon bond lengths are C–C = 1·378, 1·378, 1·387, 1·375 Å with C–C_{av} = 1·379 (3) Å, and the carbon–nitrogen bond lengths are C(3)–N(3) = 1·325 (5) and C(7)–N(3) = 1·348 (7) with C–N_{av} = 1·333 (4) Å. The analysis of the planarities (Table 7) shows how the hexatomic ring is not exactly planar and can be assigned a boat form, with atom N(3) ($\Delta = +0·021$ Å) and its opposite C(5) ($\Delta = +0·015$ Å) a little above the plane of the others.

The amide group as a whole is not planar; C(8), however, is planar while N(4) is not exactly so, in accordance with findings of Pedone, Benedetti, Immirzi & Allegra (1970) in 4-diethylcarbamoyl-1-cyclohexene-5-carboxylic acid (DDCA) which is an *N,N*-diethylamide. The average plane of N(4) is rotated 8·1° with respect to that of C(8) The role of the interatomic repulsion between the non-bonded atoms C(3) of the pyridine ring and C(9) in determining this rotation is shown by the short distance C(3)···C(9) = 3·226 (8) Å. The carbon–carbon bond between amide group and pyridine ring, C(4)–C(8) = 1·486 (5) Å, is very close to the value (1·50 Å) accepted for the bond between two sp^2 carbon atoms. The carbon–oxygen bond, C(8)–O = 1·237 (5) Å is practically the same as that found in amidoxalato anion (1·244 (5) Å: Braibanti, Pellinghelli, Tiripicchio & Tiripicchio Camellini, 1971) and in the *N,N*-diethylmonoamide DDCA (1·241 Å: Pedone, Benedetti, Immirzi & Allegra, 1970); the carbon–nitrogen bond, C(8)–N(4) = 1·341 (6) Å, also agrees with values in the amidoxalato anion (1·315 Å) and in DDCA (1·343 Å). The two bonds between nitrogen and the carbon atoms of the ethyl groups, N(4)–C(9) = 1·458 (6) and N(4)–C(11) = 1·478 (7) Å, are comparable with C–N = 1·470, 1·493 Å in DDCA. These values agree with single bond lengths in amines. The angles around nitrogen, C(8)–N(4)–C(11) = 117·5 (3)°, C(11)–N(4)–C(9) = 116·9 (4)° and C(8)–N(4)–C(9) = 124·8 (3)°, indicate that actually the nitrogen atom is not exactly trigonal in accordance

Table 7. *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.

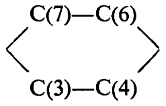
Transformation matrix from fractional to orthogonal coordinates $\begin{pmatrix} a & 0 & c\cos\beta \\ 0 & b & 0 \\ 0 & 0 & c\sin\beta \end{pmatrix}$

(1) Equation of the plane through C(3), C(4), C(6), C(7) of the pyridine ring:

$$-0\cdot2916X-0\cdot8903Y-0\cdot3495Z-5\cdot5610=0$$

	$\Delta\times10^4$ (Å)	$\sigma\times10^4$ (Å)
*C(3)	23	38
*C(4)	−20	35
*C(6)	30	45
*C(7)	−32	44
N(3)	201	32
C(5)	162	41
C(8)	1044	37

Plane-determining atoms



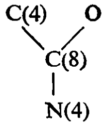
$\sum_4 (\Delta/\sigma)^2=1\cdot67$

(2) Equation of the plane of the carbonyl carbon C(8)

$$0\cdot4782X-0\cdot4592Y-0\cdot7485Z-0\cdot7815=0$$

	$\Delta\times10^4$ (Å)	$\sigma\times10^4$ (Å)
*C(4)	0	35
*C(8)	− 2	36
*O	0	28
*N(4)	0	32
C(3)	10270	37
C(5)	−9729	39
C(9)	−2684	46
C(11)	624	52

Plane-determining atoms



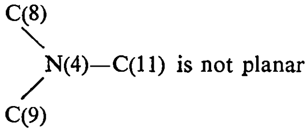
$\sum_4 (\Delta/\sigma)^2=0\cdot01$

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

$$0\cdot5009X-0\cdot3316Y-0\cdot7993Z-0\cdot1247=0$$

	$\Delta\times10^4$ (Å)	$\sigma\times10^4$ (Å)
*C(8)	−134	36
*N(4)	535	32
*C(9)	−196	47
*C(11)	−204	52
C(4)	1170	35
O	−1823	28

Plane-determining atoms



$\sum_4 (\Delta/\sigma)^2=326\cdot15$

with the results in DDCA. It is also worth mentioning that the distance between the two coordinating sites of the same amide molecule is N(3)···O=4·562 (5) Å.

The mean carbon–hydrogen distance is C–H= 1·02 (1) Å and the angles calculated from the coordinates of the hydrogen atoms lie approximately around values proper to trigonal and tetrahedral carbon atoms.

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