

The Crystal Structure and Absolute Configuration of (–)-*mer*-Tris(L-alaninato)cobalt(III) Monohydrate

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(Received 13 June 1977; accepted 30 June 1977)

The crystal structure has been determined from three-dimensional X-ray data collected on a Syntex $P\bar{1}$ diffractometer. The compound forms orthorhombic crystals, with $a = 5.247$ (2), $b = 13.555$ (4), $c = 19.351$ (7) Å, $Z = 4$, in space group $P2_12_12_1$. The structure has been solved by the heavy-atom method and refined by full-matrix least-squares calculations to an R of 0.076. The crystal structure consists of molecules of complex and molecules of water. The coordination around the Co atom is distorted octahedral. The absolute configuration of the complex cation can be designated as $\Delta(\delta\delta\delta)$. The methyl groups are in equatorial positions.

Introduction

The first tris(amino acidato)cobalt(III) complex was prepared in 1909 (Ley & Winkler, 1909). In the mid-sixties, along with the development of chiroptical methods, renewed interest in the study of the isomerism of cobalt(III) amino acid complexes was shown. Dunlop & Gillard (1965) prepared the four isomers of tris(L-alaninato)cobalt(III) and tentatively assigned their absolute configurations on the basis of relative stabilities of isomers. Douglas & Yamada (1965) deduced the absolute configuration for the same isomers from circular dichroism spectra. Denning & Piper (1966) reported electronic absorption, circular dichroism and proton magnetic resonance spectra for 11 out of 12 possible isomers of Co^{III} with L-alanine, L-leucine and L-proline and assigned absolute configurations to these. A preliminary, two-dimensional X-ray structure of (+)-*mer*-tris(L-alaninato)cobalt(III) (Drew, Dunlop, Gillard & Rogers, 1966) confirmed the absolute configurations found in the work of Denning & Piper. However, apart from the work of Drew *et al.* (1966), no full crystal structure analysis has been reported for any tris(amino acid) complexes of Co^{III} . The reason might be the difficulty of obtaining good crystals for X-ray analysis.

Conformational analysis of diamine complexes with five- and six-membered rings predicted, with a high degree of certainty, the most stable conformations for these compounds (Hawkins, 1971; Niketić, Rasmussen, Woldbye & Lifson, 1976). Such an analysis of tris(amino acidato) complexes is presently lacking and experimental information on the conformation of the amino acidato chelate rings in tris complexes is needed.

The X-ray diffraction study of (–)-*mer*-[Co(L-

Ala)₃].H₂O was undertaken to determine the stereochemical features of the complex molecule.

Experimental

Crystal data

[Co(NH₂CHCH₃COO)₃].H₂O, CoC₉H₂₀N₃O₇, $M_r = 341.2$. Orthorhombic, $a = 5.247$ (2), $b = 13.555$ (4), $c = 19.351$ (7) Å, $V = 1376.2$ (8) Å³, $D_m = 1.64$, $D_x = 1.65$ g cm⁻³, $Z = 4$. Space group $P2_12_12_1$, Mo $K\alpha$ radiation, $\lambda = 0.7107$ Å, $\mu(\text{Mo } K\alpha) = 13.3$ cm⁻¹.

Dark-violet, thin prismatic and weakly diffracting crystals were obtained by slow evaporation of the aqueous solution. The unit-cell dimensions were initially determined from rotation and Weissenberg photographs and later adjusted by a least-squares refinement of a series of diffractometer-measured θ angles. From systematic absences, $h00$ with h odd, $0k0$ with k odd and $00l$ with l odd, the space group was uniquely defined as $P2_12_12_1$. The intensity data were collected from a crystal $0.13 \times 0.15 \times 0.30$ mm on a Syntex $P\bar{1}$ four-circle diffractometer, using graphite-monochromatized radiation. The ω -scanning mode was used. All the independent reflexions in the sphere with $2\theta(\text{Mo } K\alpha) \leq 55^\circ$ were measured, but, owing to the poor quality of the crystal, only 1106 had $I > 2\sigma(I)$ and were used in the calculations. The intensity of a standard reflexion, measured after every 30 reflexions, remained essentially constant throughout data collection. The values of I and $\sigma(I)$ were corrected for Lorentz–polarization effects. No absorption correction was applied.

The atomic parameters were determined from Patterson and Fourier syntheses and the structure was

refined by full-matrix least-squares calculations. The function minimized was $\Sigma w\Delta^2$, where $w = 1/\sigma^2$, $\Delta = |F_o| - |F_c|$, and $|F_o|$ and $|F_c|$ are the observed and calculated structure amplitudes. All atoms were assumed to be uncharged. Values for the atomic scattering factors and anomalous terms for Co were taken from *International Tables for X-ray Crystallography* (1974). Refinement of the positional and thermal parameters (anisotropic for Co, carbonyl O and methyl C atoms, isotropic for other non-hydrogen atoms) converged at $R = 0.088$. The final coordinates were then inverted to calculate the enantiomeric *B* configuration, and the convergence was reached at $R = 0.084$. The *B* configuration of the molecule is in accordance with the configuration deduced from a knowledge of the absolute configuration of the L-

alaninato ligand. A difference Fourier map, calculated at this stage of refinement, revealed the positions of most of the H atoms. The position of one of the water hydrogens, H(W2), was located with the least certainty. The H atoms of the complex molecule were included in the structure factor calculations in calculated, fixed positions, with fixed temperature factors. The atomic parameters of the water H atoms were not refined. Refinement converged at $R = 0.076$, $R_w = 0.075$. In the last cycle of refinement the shifts of all parameters were less than 0.3σ . The final difference Fourier map was featureless. The final atomic parameters derived from the last cycle of least-squares refinement are given in Table 1, along with standard deviations estimated from the inverse matrix.*

The main computer programs used on the CDC-3600 computer were Zalkin's *FORDAP* Fourier program, Ibers's *NUCLS* least-squares program, and the function and error program *ORFFE* of Busing, Martin & Levy.

Table 1. *The final atomic parameters (with standard deviations in parentheses)*

	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> (Å ²)
Co	0.4854 (4)	0.6247 (1)	0.1550 (1)	*
O(W)	0.9948 (25)	0.8568 (6)	0.2389 (4)	*
O(1)	0.2314 (17)	0.6746 (6)	0.0945 (4)	2.5 (2)
O(2)	0.3027 (16)	0.5071 (6)	0.1693 (4)	3.0 (2)
O(3)	0.7345 (18)	0.5754 (6)	0.2154 (5)	3.5 (2)
O(12)	0.1263 (17)	0.8056 (7)	0.0335 (4)	*
O(22)	0.221 (2)	0.3585 (7)	0.1256 (5)	*
O(32)	0.796 (2)	0.5392 (6)	0.3254 (5)	*
N(1)	0.665 (2)	0.7466 (7)	0.1353 (5)	2.5 (2)
N(2)	0.652 (2)	0.5533 (7)	0.0803 (5)	2.6 (2)
N(3)	0.312 (2)	0.6724 (7)	0.2372 (5)	2.3 (2)
C(11)	0.263 (2)	0.7667 (9)	0.0767 (7)	2.5 (2)
C(12)	0.476 (3)	0.8201 (8)	0.1138 (5)	2.3 (2)
C(13)	0.594 (2)	0.9025 (9)	0.0713 (7)	*
C(21)	0.330 (3)	0.4390 (10)	0.1236 (7)	2.9 (3)
C(22)	0.487 (3)	0.4702 (9)	0.0599 (6)	3.2 (2)
C(23)	0.629 (3)	0.3859 (12)	0.0256 (8)	*
C(31)	0.685 (3)	0.5884 (10)	0.2818 (7)	3.3 (3)
C(32)	0.489 (3)	0.6676 (8)	0.2969 (6)	2.7 (2)
C(33)	0.346 (3)	0.6571 (10)	0.3643 (6)	*
H(1)	0.765	0.770	0.180	3.5
H(2)	0.800	0.734	0.095	3.5
H(3)	0.406	0.853	0.157	3.5
H(4)	0.500	0.969	0.053	3.5
H(5)	0.767	0.923	0.090	4.0
H(6)	0.695	0.874	0.031	4.0
H(7)	0.831	0.524	0.100	3.5
H(8)	0.686	0.600	0.038	3.5
H(9)	0.366	0.494	0.022	3.5
H(10)	0.808	0.388	0.043	4.0
H(11)	0.558	0.322	0.040	4.0
H(12)	0.636	0.393	-0.025	4.0
H(13)	0.153	0.627	0.248	3.5
H(14)	0.251	0.746	0.229	3.5
H(15)	0.588	0.733	0.300	3.5
H(16)	0.247	0.596	0.364	4.0
H(17)	0.459	0.656	0.406	4.0
H(18)	0.216	0.712	0.371	4.0
H(W1)	0.100	0.860	0.280	4.0
H(W2)	0.100	-0.075	0.220	4.0

* These atoms were assigned anisotropic temperature factors (see deposition footnote).

Results and discussion

The crystal structure of $\text{Co(L-Ala)}_3 \cdot \text{H}_2\text{O}$ consists of discrete neutral molecules of the complex and molecules of water. Projections of the structure along the *a* and *b* axes are presented in Figs. 1 and 2 respectively. The complex molecules form ribbons, extending parallel to the *b* axis, the thickness of which is half a unit cell in the *z* direction. The molecules of water are sandwiched between the ribbons. Hydrogen bonds join molecules of complex and water to form sheets. There are two sheets within the repeat distance *c*; the second sheet is displaced by half the *a* axis.

The geometry of the complex molecule is given in Table 2. The coordination around Co is distorted octahedral. Each alaninato ligand is bidentate and bound to the metal atom through carboxylato O and amino N atoms in a meridional arrangement. Figs. 1 and 2 correctly represent the absolute configuration, Δ , of the complex, which is the same as that which Denning & Piper (1966) found on the basis of steric considerations.

The L-alaninato ligands form five-membered chelate rings. The geometries of the rings are very similar. There are no significant differences in the bond lengths and angles in the rings. These values are in good agreement with those found in other compounds containing five-membered amino acidato rings (Freeman, 1967) and in particular with those in closely related complexes (Watson, Johnson, Čelap & Kamberi, 1972; Herak, Prelesnik, Manojlović-Muir &

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32890 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

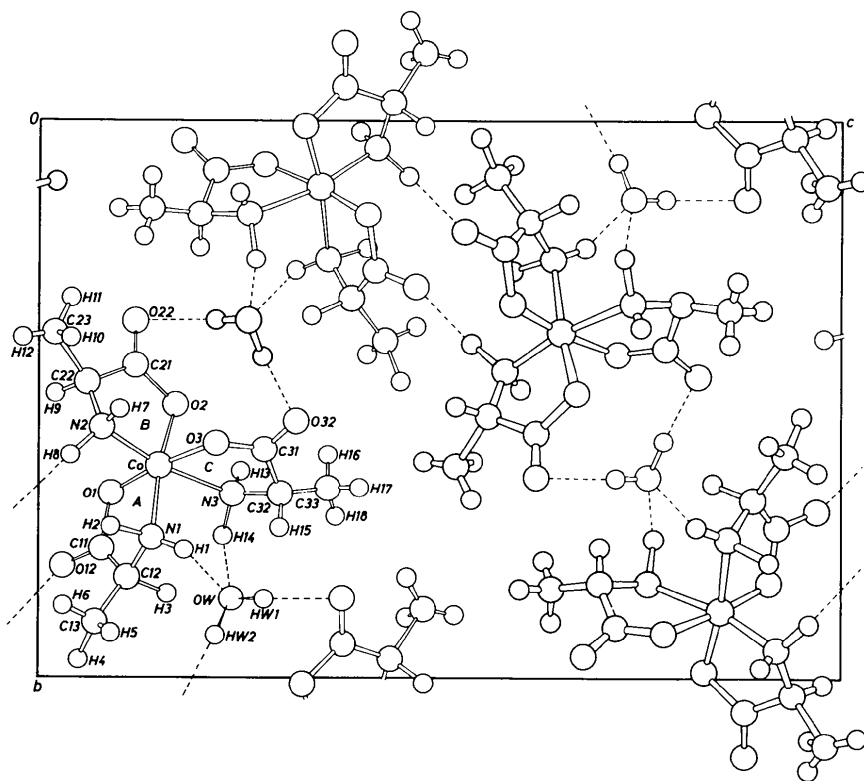


Fig. 1. View of the crystal structure down **a**. A unique set of the atoms is labelled.

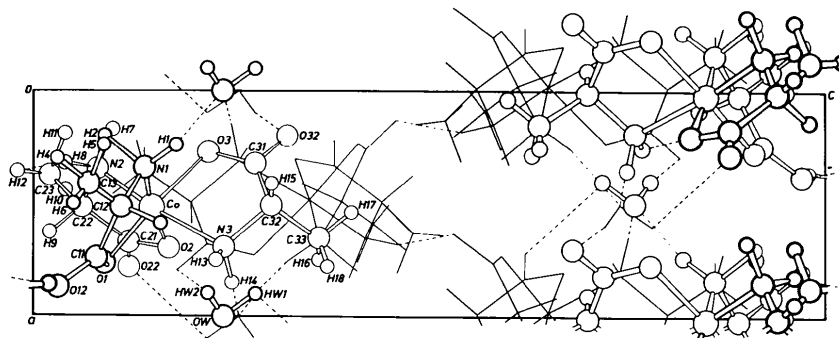


Fig. 2. View of the crystal structure down **b**.

Muir, 1974; Herak & Prelesnik, 1976; Vasić, Herak & Djurić, 1976). Rings *A* and *B* (Fig. 1) have asymmetric envelope conformations. The ring carbon atoms C(11) and C(12) lie at -0.20 and -0.56 Å respectively from the plane formed by O(1), Co and N(1) (Table 3). The corresponding deviations of C(21) and C(22) from the plane of O(2), Co and N(2) are -0.17 and -0.51 Å. In ring *C*, which has a puckered conformation, C(31) and C(32) lie respectively 0.07 Å below and 0.33 Å above the plane containing O(3), Co and N(3). All three rings could be designated as δ (IUPAC, 1970).

The position of the methyl groups with respect to the chelate rings (Table 3) is more equatorial than axial. Denning & Piper (1966) proposed an axial disposition of alkyl groups for the Δ configuration of tris(amino acidato)cobalt complexes, and an equatorial one for the Λ configuration. They tried to explain the difference in solubilities of various isomers by the position of the alkyl groups. It seems, however, that the solubility difference of various isomers of Co(L-Ala)_3 is not closely related to the position of the methyl groups.

The torsion angles in the rings are given in Table 2.

Table 2. The molecular geometry of (-)-mer-Co(L-Ala)₃·H₂O

(a) Distances (Å)

Co—O(1)	1.899 (9)	O(2)—C(21)	1.287 (14)
Co—O(2)	1.880 (8)	C(21)—C(22)	1.540 (18)
Co—O(3)	1.877 (9)	C(21)—O(22)	1.232 (14)
Co—N(1)	1.942 (10)	C(22)—N(2)	1.476 (16)
Co—N(2)	1.948 (10)	C(22)—C(23)	1.518 (19)
Co—N(3)	1.945 (10)	C(31)—O(3)	1.324 (16)
O(1)—C(11)	1.305 (13)	C(31)—C(32)	1.516 (18)
C(11)—C(12)	1.513 (17)	C(31)—O(32)	1.224 (15)
C(11)—O(12)	1.222 (14)	C(32)—N(3)	1.483 (15)
C(12)—N(1)	1.467 (15)	C(32)—C(33)	1.509 (17)
C(12)—C(13)	1.519 (15)		

(b) Angles (°)

O(1)—Co—O(2)	92.0 (4)	C(11)—C(12)—C(13)	113.4 (10)
O(1)—Co—O(3)	179.5 (4)	O(1)—C(11)—O(12)	121.2 (12)
O(1)—Co—N(1)	85.2 (4)	O(12)—C(11)—C(12)	115.3 (11)
O(1)—Co—N(2)	92.0 (4)	Co—O(2)—C(21)	116.8 (8)
O(1)—Co—N(3)	93.3 (4)	O(2)—C(21)—C(22)	114.3 (11)
O(2)—Co—O(3)	87.8 (4)	C(21)—C(22)—N(2)	108.1 (10)
O(2)—Co—N(1)	176.9 (4)	C(22)—N(2)—Co	108.2 (8)
O(2)—Co—N(2)	85.3 (4)	O(2)—C(21)—O(22)	124.1 (13)
O(2)—Co—N(3)	85.6 (4)	O(22)—C(21)—C(22)	121.2 (12)
O(3)—Co—N(1)	94.9 (4)	N(2)—C(22)—C(23)	113.6 (13)
O(3)—Co—N(2)	88.4 (4)	C(21)—C(22)—C(23)	113.9 (10)
O(3)—Co—N(3)	86.3 (4)	Co—O(3)—C(31)	114.9 (9)
N(1)—Co—N(2)	93.4 (4)	O(3)—C(31)—C(32)	114.5 (12)
N(1)—Co—N(3)	96.0 (4)	C(31)—C(32)—N(3)	107.9 (9)
N(2)—Co—N(3)	169.6 (4)	C(32)—N(3)—Co	109.2 (8)
Co—N(1)—C(12)	107.8 (7)	O(3)—C(31)—O(32)	120.1 (13)
N(1)—C(12)—C(11)	108.0 (9)	O(32)—C(31)—C(32)	125.4 (12)
C(12)—C(11)—O(1)	115.3 (11)	N(3)—C(32)—C(33)	115.6 (12)
C(11)—O(1)—Co	114.4 (8)	C(31)—C(32)—C(33)	115.8 (10)
N(1)—C(12)—C(13)	112.2 (11)		

(c) Torsion angles (°)

Co—N(1)—C(12)—C(11)	31.9 (10)
N(1)—C(12)—C(11)—O(1)	26.4 (14)
C(12)—C(11)—O(1)—Co	7.0 (13)
C(11)—O(1)—Co—N(1)	9.9 (8)
O(1)—Co—N(1)—C(12)	24.0 (7)
Co—N(2)—C(22)—C(21)	28.4 (12)
N(2)—C(22)—C(21)—O(2)	23.7 (16)
C(22)—C(21)—O(2)—Co	6.5 (15)
C(21)—O(2)—Co—N(2)	8.7 (9)
O(2)—Co—N(2)—C(22)	21.4 (8)
Co—N(3)—C(32)—C(31)	25.3 (11)
N(3)—C(32)—C(31)—O(3)	29.4 (15)
C(32)—C(31)—O(3)—Co	19.1 (14)
C(31)—O(3)—Co—N(3)	2.9 (9)
O(3)—Co—N(3)—C(32)	13.7 (8)

The dihedral angles between the corresponding N—C(2)—C(1) and C(2)—C(1)—O planes are 26, 24 and 29° for rings *A*, *B* and *C* respectively. The X-ray structural studies have shown that these angles are between 0 and 30°, in accordance with energy-minimization calculations (Hawkins, 1971).

The best least-squares planes containing the atoms of the carboxylato groups (Table 3) show that they

Table 3. Equations of least-squares mean planes through selected groups of atoms

The equation of the plane is expressed as $AX + BY + CZ - D = 0$.

	<i>A</i>	<i>B</i>	<i>C</i>	<i>D</i>
Plane (1)				
Co, O(1), N(1)	0.46	-0.44	-0.77	-4.87
Plane (2)				
Co, O(2), N(2)	0.70	-0.31	0.63	1.05
Plane (3)				
Co, O(3), N(3)	0.50	0.86	-0.06	8.39
Plane (4)				
O(1), C(11), O(12), C(12)	0.64	-0.28	-0.72	-3.10
Plane (5)				
O(2), C(21), O(22), C(22)	0.81	-0.36	0.45	0.29
Plane (6)				
O(3), C(31), O(32), C(32)	0.72	0.69	0.05	8.35
Displacements (Å) of atoms from the planes				
Plane				
(1)	C(11) -0.203	C(12) -0.566	C(13) -0.135	
(2)	C(21) -0.173	C(22) -0.508	C(23) -0.041	
(3)	C(31) -0.060	C(32) 0.331	C(33) -0.243	
(4)	O(1) -0.002	C(11) 0.005	O(12) -0.002	
	C(12) -0.001	Co 0.196	N(1) 0.608	
(5)	O(2) -0.012	C(21) 0.037	O(22) -0.014	
	C(22) -0.010	Co 0.059	N(2) 0.463	
(6)	O(3) 0.001	C(31) -0.003	O(32) 0.001	
	C(32) 0.001	Co -0.542	N(3) -0.680	

Table 4. Interatomic distances (Å) and angles (°) involving hydrogen atoms

<i>A</i> —H... <i>B</i>	<i>A</i> — <i>B</i>	<i>A</i> —H	H... <i>B</i>	∠ <i>A</i> —H... <i>B</i>
O(<i>W</i> ⁱ)—H(<i>W</i> 1)...O(22 ⁱⁱ)	2.86	0.97	2.48	102
O(<i>W</i> ⁱⁱⁱ)—H(<i>W</i> 2)...O(32 ^{iv})	2.98	1.13	1.86	166
N(1)—H(1)...O(<i>W</i>)	3.04	1.07	2.03	157
N(1 ⁱ)—H(2 ⁱ)...O(1)	3.22	1.07	2.40	132
N(2)—H(7)...O(3)	2.67	1.07	2.43	90
N(2)—H(8)...O(12)	2.92	1.05	1.91	160
N(3)—H(13)...O(2)	2.60	1.06	2.36	91
N(3)—H(14)...O(<i>W</i> ⁱ)	3.00	1.06	2.02	152

Symmetry code

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

are planar. The displacements of Co from these planes are different, ranging from 0.06 to 0.54 Å. The angles between the planes of rings *A* and *B*, *A* and *C* and *B* and *C* are 73.0, 76.5 and 68.9° respectively.

Interatomic distances involving H atoms are listed in Table 4. The water molecule is a donor for two hydrogen bonds to molecules of the complex in adjacent ribbons. There are two kinds of amine hydrogens — axial and equatorial. The equatorial ones

are free to form hydrogen bonds and, in the crystal structure of (-)-*mer*-[Co(L-Ala)₃].H₂O, H(1) and H(14) participate in the bonds connecting molecules of the complex and molecules of water in one sheet. The connexion between the adjacent sheets is realized through an N(2)—H(8)···O(12) interaction. It is considered that the conformation of the chelate rings and the ability of the axial H atoms to form hydrogen bonds are mutually dependent (Raymond, Corfield & Ibers, 1967). The hydrogen-bond interactions of axial amine H atoms in the crystal structure of Co(L-Ala)₃.H₂O, if they exist, are too weak to affect the conformation of the chelate rings.

It is a pleasure to thank Professor M. B. Čelap for providing the sample of the complex and for his continuous interest and encouragement, and Dr S. R. Niketić for valuable discussions.

This work was supported by the Scientific Council of the Republic of Serbia.

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The Crystal and Molecular Structure of Trichloro(1*H*⁺-thiocarbonohydrazidium-*N,S*)-copper(II) Monohydrate

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(Received 8 June 1977; accepted 9 July 1977)

CH₃Cl₃CuN₄OS is triclinic, space group *P* $\bar{1}$, with $a = 8.188$ (7), $b = 8.778$ (7), $c = 7.219$ (7) Å, $\alpha = 93.0$ (1), $\beta = 96.5$ (1), $\gamma = 117.3$ (1)°, $Z = 2$. The structure was refined to $R = 0.067$ for 1535 counter reflexions. It consists of Cu complexes, CuCl₃(NH₂NHCSNHN⁺H₃), where one monoprotonated thiocarbonohydrazide molecule acts as a chelating ligand, and water molecules which link the complexes by hydrogen bonding. The Cu coordination polyhedron is a square pyramid whose base is formed by two Cl [Cu—Cl(1) = 2.257, Cu—Cl(2) = 2.342 Å], one S (Cu—S = 2.263 Å) and one N [Cu—N(2) = 2.052 Å] from the ligand, which is in a *cis-cis* conformation. The apex of the pyramid is occupied by a third Cl atom [Cu—Cl(3) = 2.628 Å].

Introduction

In crystals thiocarbonohydrazide (tcz), SC(NHNH₂)₂, and its protonated species can assume either a *cis-trans* (I,II) or a *cis-cis* conformation (III,IV). The *cis-*

trans conformation (I) has been found in the neutral molecule (Braibanti, Tiripicchio & Tiripicchio Camellini, 1969, 1972) and its metal chelates (*N,S*) (Bigoli, Braibanti, Manotti Lanfredi, Tiripicchio & Tiripicchio Camellini, 1971; Bigoli, Pellinghelli, Tiripicchio & Tiripicchio Camellini, 1975; Bigoli, Pellinghelli & Tiripicchio, 1975) and conformation II is found when

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