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## The Crystal and Absolute Molecular Structure of (+)<sub>546</sub>-*cis*- $\alpha$ -Sodium Carbonato[(2*S*,2'*S*)-1,1'-ethylenedi-2-pyrrolidinecarboxylato(2-)]cobaltate(III) Trihydrate

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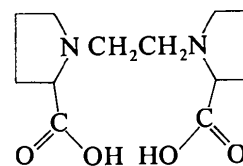
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## Abstract

Monoclinic crystals of the title compound, Na[Co(C<sub>12</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>)(CO<sub>3</sub>)]·3H<sub>2</sub>O, C<sub>13</sub>H<sub>18</sub>CoN<sub>2</sub>O<sub>7</sub>·Na<sup>+</sup>·3H<sub>2</sub>O, space group *P*2<sub>1</sub>, have *a* = 7.845 (4), *b* = 7.760 (2), *c* = 14.922 (10) Å,  $\beta$  = 106.51 (3)° and *Z* = 2. Refinement with 2463 diffractometer data measured with Mo *K* $\alpha$  radiation converged at *R* = 0.059. The structure consists of [Co(pren)(CO<sub>3</sub>)]<sup>-</sup> complex anions linked into double layers parallel to the (001) planes by O–Na–O and O–H<sub>2</sub>O–H<sub>2</sub>O–O bridges. The distorted octahedral complex anion has the *cis*- $\alpha$  geometrical arrangement and its absolute configuration is  $\Delta$ (OC–6–13–C). The Na<sup>+</sup> ions have approximate NaO<sub>6</sub> octahedral coordination.

## Introduction

The quadridentate ligand (2*S*,2'*S*)-1,1'-ethylenedi-2-pyrrolidinecarboxylic acid (1), abbreviated as H<sub>2</sub>-pren, has been used recently to prepare a series of cobalt(III) complexes including Na[Co(pren)(CO<sub>3</sub>)]·3H<sub>2</sub>O (Woon & O'Connor, 1979).



(1)

<sup>13</sup>C NMR and absorption spectral measurements indicated that this and related compounds have the symmetrical *cis*- $\alpha$  structure in aqueous solution. A strong negative circular dichroism band under the <sup>1</sup>A<sub>1g</sub> → <sup>1</sup>T<sub>1g</sub> cubic absorption band and the presence of a negative Cotton effect in the visible region of the optical rotatory dispersion spectrum in aqueous solution were used to predict that the complex anion [Co(pren)(CO<sub>3</sub>)]<sup>-</sup> has the  $\Delta$  absolute configuration (IUPAC Commission on Inorganic Chemical Nomenclature, 1971). The present study was carried out to confirm these predictions.

## Experimental

The title compound was prepared by the method of Woon & O'Connor (1979), and purple tabular crystals

were obtained by slow crystallization from water. Weissenberg photographs revealed the crystal symmetry and space group; accurate cell parameters were determined by a least-squares fit of  $2\theta$  values measured for 20 high-angle reflections on a four-circle diffractometer with Mo  $K\alpha$  radiation ( $\lambda = 0.7107 \text{ \AA}$ ). The crystal density was determined by flotation in a xylene/bromofrom mixture.

### Crystal data

C<sub>13</sub>H<sub>18</sub>CoN<sub>2</sub>O<sub>7</sub>·Na<sup>+</sup>·3H<sub>2</sub>O,  $M_r = 450.3$ , monoclinic,  $P2_1$ ,  $a = 7.845 (4)$ ,  $b = 7.760 (2)$ ,  $c = 14.922 (10) \text{ \AA}$ ,  $\beta = 106.51 (3)^\circ$ ,  $U = 871 (1) \text{ \AA}^3$ .  $D_m = 1.71 (3)$ ,  $D_c = 1.717 \text{ Mg m}^{-3}$ ,  $Z = 2$ ,  $F(000) = 468$ ,  $\mu(\text{Mo } K\alpha) = 1.12 \text{ mm}^{-1}$ .

Three-dimensional intensity data were measured with Mo  $K\alpha$  radiation (graphite-crystal monochromator,  $\lambda = 0.7107 \text{ \AA}$ ) on a Rigaku AFC four-circle diffractometer. For the data collection, a crystal of dimensions  $ca 0.22 \times 0.25 \times 0.18 \text{ mm}$  was wedged in a Lindemann-glass tube as the crystals reacted with adhesives normally used for crystal mounting. The intensities were recorded by an  $\omega$ - $2\theta$  scan with a scan rate of  $2^\circ \text{ min}^{-1}$ , and 10 s stationary background counts. Three reference reflections monitored every 50 reflections showed no significant variation in intensity over the data-collection period. Of the 2737 non-equivalent terms measured to a  $2\theta$  maximum of  $60^\circ$ , 2463 had values for which  $|F_o| > 2\sigma|F_o|$  and were used in the subsequent calculations. The intensities were corrected for Lorentz and polarization factors, but no corrections for absorption or extinction were made. The scattering factors for C, N and O were from Cromer & Mann (1968), for Na and Co from Doyle & Turner (1968) and for H from Stewart, Davidson & Simpson (1965). Anomalous-dispersion corrections,  $f'$  and  $f''$ , were made for the non-hydrogen atoms using the values of Cromer & Liberman (1970).

### Structure analysis

The structure was solved by the heavy-atom method. The  $x$  and  $z$  coordinates of the Co atom were derived from the vector map, and the sites of all the non-hydrogen atoms were located on a Fourier distribution phased on the Co contribution to the structure factors. Refinement with individual isotropic temperature factors given to the atoms yielded an  $R$  index of 0.11 for  $R = \sum (|F_o| - |F_c|) / \sum |F_o|$ . At this stage of the analysis it was apparent that C(4) of one of the proline residues was disordered. A difference map generated with C(4) included at only one site, C(4a), revealed a peak corresponding to the alternate site, C(4b). The structural model was adjusted to include

two positions of occupancy 0.5 for the C(4) atom. Full-matrix least-squares refinement with anisotropic temperature factors given to the non-hydrogen atoms converged at  $R = 0.059$  and  $R_w = (\sum w(|F_o| - |F_c|)^2 / \sum w|F_o|^2)^{1/2} = 0.064$ . In the final refinement cycles, the H atoms of the complex molecule were included at idealized positions; their coordinates were not refined, but they were given a refined isotropic temperature factor  $0.062 \text{ \AA}^2$ . Although several peaks in the final difference map corresponded to feasible water H atom sites, not all of the six sites could be located and so these atoms were omitted from the analysis.

The final refinements were made with the *SHELX 76* program (Sheldrick, 1976), while initial refinement and Fourier maps were calculated with the *ORFLS* (Busing, Martin & Levy, 1962) and *MUFR-3* (White, 1965) programs respectively. In the least-squares refinements, the function minimized was  $\sum w(|F_o| - |F_c|)^2$  with the terms weighted according to  $w = 1.0/[\sigma^2(F_o) + 0.016(F_o)^2]$ . Final atomic coordinates together with their estimated standard deviations are given in Table 1, and calculated H coordinates are

Table 1. Fractional atomic coordinates of non-hydrogen atoms ( $\times 10^4$ ), and their estimated standard deviations, referred to a right-handed set of axes, and equivalent isotropic thermal parameters  $B_{eq} (\text{\AA}^2)$

	$x$	$y$	$z$	$B_{eq}^*$
Co	168 (1)	0	2672 (1)	1.31
Na	4612 (3)	138 (5)	-149 (2)	2.64
O(1)	927 (5)	788 (6)	1651 (3)	1.78
O(2)	3106 (7)	589 (8)	991 (3)	2.56
O(1')	-637 (6)	-777 (6)	3687 (3)	1.75
O(2')	-2237 (6)	208 (8)	4595 (3)	2.48
O(3)	-2220 (4)	59 (8)	1890 (2)	1.90
O(4)	-469 (5)	-2142 (5)	2035 (3)	1.89
O(5)	-3155 (6)	-2222 (7)	955 (4)	2.66
N	2702 (6)	-404 (6)	3314 (3)	1.48
N'	388 (6)	2304 (6)	3259 (3)	1.55
C(1)	2536 (7)	392 (6)	1673 (4)	1.59
C(2)	3725 (7)	-261 (7)	2598 (4)	1.81
C(3)	4553 (12)	-2017 (11)	2546 (6)	2.98
C(4a)†	3607 (13)	-3235 (12)	3006 (7)	1.21
C(4b)†	4495 (23)	-2983 (25)	3447 (12)	3.67
C(5)	3126 (10)	-2186 (10)	3751 (4)	2.25
C(6)	3218 (7)	968 (9)	4044 (4)	2.13
C(7)	-2044 (7)	-1486 (8)	1583 (4)	1.87
C(1')	-1232 (7)	443 (8)	4113 (4)	1.96
C(2')	-531 (7)	2251 (8)	4025 (4)	1.72
C(3')	-1979 (9)	3647 (9)	3783 (5)	2.60
C(4')	-2345 (10)	3845 (10)	2731 (5)	2.93
C(5')	-511 (9)	3727 (8)	2606 (5)	2.31
C(6')	2339 (8)	2637 (8)	3623 (4)	1.97
O(6)	6930 (6)	2453 (7)	427 (3)	2.74
O(7)	9528 (7)	1347 (11)	9505 (4)	3.71
O(8)	6438 (8)	-699 (8)	-1123 (4)	3.45

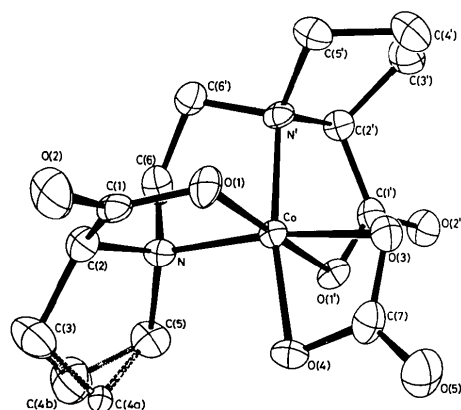
\* Calculated from the refined anisotropic thermal parameters (deposited),  $B_{eq} = 8\pi^2 U_{eq}$ .

† Calculated for an occupancy of 0.5.

Table 2. Calculated hydrogen coordinates of the complex anion ( $\times 10^3$ ) referred to a right-handed set of axes

H bonded to atom	x	y	z	H bonded to atom	x	y	z
C(2)	478	69	279	C(5 <sub>2</sub> b)*	194	-298	355
C(3 <sub>1</sub> a)*	596	-199	291	C(6 <sub>1</sub> )	276	62	464
C(3 <sub>2</sub> a)*	436	-239	183	C(6 <sub>2</sub> )	465	112	427
C(3 <sub>1</sub> b)*	380	-271	193	C(2')	37	252	471
C(3 <sub>2</sub> b)*	591	-187	252	C(3 <sub>1</sub> )	-150	484	414
C(4 <sub>1</sub> a)*	242	-373	251	C(3 <sub>2</sub> )	-316	324	396
C(4 <sub>2</sub> a)*	466	-430	332	C(4 <sub>1</sub> )	-296	507	249
C(4 <sub>1</sub> b)*	420	-433	330	C(4 <sub>2</sub> )	-319	282	236
C(4 <sub>2</sub> b)*	576	-286	398	C(5 <sub>1</sub> )	191	493	279
C(5 <sub>1</sub> a)*	423	-213	438	C(5 <sub>2</sub> )	-58	340	189
C(5 <sub>2</sub> a)*	198	-273	391	C(6 <sub>1</sub> )	260	363	415
C(5 <sub>1</sub> b)*	356	-206	450	C(6 <sub>2</sub> )	286	304	306

\* Calculated for an occupancy of 0.5.

Fig. 1. ORTEP diagram of the absolute structure of the complex anion  $[\text{Co}(\text{pren})(\text{CO}_3)]^-$ . Hydrogen atoms are omitted.

given in Table 2.\* Fig. 1, which illustrates the structure of the complex anion, was prepared from the output of ORTEP (Johnson, 1965).

### Results and discussion

A perspective view of the complex anion,  $[\text{Co}(\text{pren})(\text{CO}_3)]^-$ , including the numbering system, is given in Fig. 1. The Co atom is bonded to the quadridentate (2*S*,2'*S*)-1,1'-ethylenedi-2-pyrrolidine-carboxylate ligand in the *symmetrical cis-α* geometric configuration with the carboxylate O atoms in *trans* positions. The Co—O(1) and Co—O(1') bond lengths (see Table 3) are similar to those found in

\* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35258 (27 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 3. Interatomic distances (Å) and angles (°) in the complex anion with their estimated standard deviations in parentheses

Co—N	1.971 (5)	C(2)—N	1.512 (7)
Co—N'	1.977 (5)	C(2')—N'	1.515 (7)
Co—O(1)	1.888 (4)	C(2)—C(3)	1.521 (10)
Co—O(1')	1.897 (5)	C(2')—C(3')	1.537 (9)
Co—O(3)	1.905 (3)	C(3)—C(4a)	1.485 (13)
Co—O(4)	1.909 (4)	C(3)—C(4b)	1.551 (20)
C(7)—O(3)	1.305 (8)	C(3')—C(4')	1.521 (10)
C(7)—O(4)	1.329 (7)	C(5)—C(4a)	1.510 (12)
C(7)—O(5)	1.225 (8)	C(5)—C(4b)	1.421 (20)
C(1)—O(1)	1.290 (7)	C(5')—C(4')	1.505 (11)
C(1')—O(1')	1.299 (8)	C(5)—N	1.525 (9)
C(1)—O(2)	1.232 (7)	C(5')—N'	1.509 (8)
C(1')—O(2')	1.222 (7)	C(6)—N	1.494 (8)
C(1)—C(2)	1.517 (8)	C(6')—N'	1.494 (8)
C(1')—C(2')	1.526 (9)	C(6)—C(6')	1.517 (9)
O(1)—Co—N	86.4 (2)	C(2')—N'—C(5')	105.8 (4)
O(1)—Co—N'	93.3 (2)	N'—C(5')—C(4')	104.6 (5)
O(1')—Co—N	94.6 (2)	C(5')—C(4')—C(3')	102.4 (6)
O(1')—Co—N'	86.6 (2)	C(4')—C(3')—C(2')	102.9 (6)
O(3)—Co—N'	101.3 (2)	C(3')—C(2')—N'	106.4 (5)
O(1')—Co—O(3)	90.2 (2)	N'—C(6')—C(6)	107.5 (5)
O(4)—Co—O(1')	91.2 (2)	C(6')—C(6)—N	108.0 (5)
O(4)—Co—N	100.9 (2)	C(5')—N'—Co	114.2 (4)
O(1)—Co—O(4)	88.8 (2)	Co—N'—C(6')	105.6 (3)
O(4)—Co—O(3)	69.1 (2)	C(6)—N—Co	105.5 (3)
N—Co—N'	88.8 (2)	Co—O(1)—C(1)	115.7 (4)
O(1)—Co—O(3)	88.8 (2)	O(1)—C(1)—C(2)	116.5 (5)
O(1)—Co—O(1')	179.0 (2)	O(1)—C(1)—O(2)	122.1 (5)
N'—Co—O(4)	170.2 (2)	O(2)—C(1)—C(2)	121.3 (5)
N—Co—O(3)	169.0 (2)	C(1)—C(2)—N	110.8 (4)
Co—O(4)—C(7)	89.6 (3)	C(2)—N—Co	108.0 (3)
Co—O(3)—C(7)	90.5 (4)	N—C(2)—C(3)	106.9 (5)
O(3)—C(7)—O(4)	110.5 (5)	C(2)—C(3)—C(4a)	105.7 (7)
O(4)—C(7)—O(5)	124.5 (6)	C(2)—C(3)—C(4b)	105.7 (9)
O(3)—C(7)—O(5)	125.0 (6)	C(3)—C(4a)—C(5)	105.0 (8)
Co—O(1')—C(1')	114.0 (4)	C(3)—C(4b)—C(5)	106.1 (12)
O(1')—C(1')—C(2')	116.1 (5)	C(4a)—C(5)—N	104.1 (6)
C(2')—C(1')—O(2')	119.8 (5)	C(4b)—C(5)—N	110.6 (9)
O(1')—C(1')—O(2')	124.1 (6)	C(5)—N—C(2)	105.9 (4)
C(1')—C(2')—N'	110.5 (5)	C(5)—N—Co	114.8 (4)
C(2')—N'—Co	108.0 (3)		

*unsymmetrical cis-β*-(*R*)-1,2-diaminopropane(*N,N'*-ethylenediaminediacetato)cobalt(III) chloride monohydrate (Halloran, Caputo, Willett & Legg, 1975) and in the five-membered chelate rings in lithium [(*S,S*)-*N,N'*-ethylenediaminedisuccinato]cobaltate(III) trihydrate (Pavelčík & Majer, 1978). The Co—N and Co—N' bonds have lengths similar to the mean Co—N bond length in several complexes involving the coordination of the pyrrolidiny N to a Co<sup>III</sup> ion (Freeman, 1978).

The carbonato moiety is coordinated to the cobalt ion as a *cis*-bidentate ligand. The Co—O and other bond lengths and angles within the group are as expected (Geue & Snow, 1971; Toriumi & Saito, 1975; Loehlin & Fleischer, 1976). The small bite angle of the bidentate carbonato group [ $69.1(1)^\circ$ ] necessarily leads to a distorted-octahedral arrangement of the  $\text{N}_2\text{O}_4$  coordination sphere of the cobalt ion.

Table 4. Equations of the mean planes and deviations ( $\text{\AA} \times 10^3$ ) of atoms from these planes, with their estimated standard deviations in parentheses

Each plane equation is of the form  $AX + BY + CZ + D = 0$ , with  $X, Y, Z$  expressed in  $\text{\AA}$ , referred to orthogonal axes.

	$A (\times 10^4)$	$B (\times 10^4)$	$C (\times 10^4)$	$D (\times 10^4)$
Plane 1	5942	3707	-7138	33739
Plane 2	6203	3942	-6782	33950
Plane 3	-791	-9318	-3542	13496
Plane 4	-7868	1576	-5968	15644
Plane 5	-5242	-6631	-5344	31175

	Plane 1	Plane 2	Plane 3
Co	50 (1)	O(3)	2 (4)
O(3)	-50 (4)	O(4)	2 (4)
O(4)	-52 (4)	Co*	182 (1)
C(7)	4 (4)	C(7)	-6 (6)
O(5)	48 (5)	O(5)	2 (5)

	Plane 4	Plane 5	
Co	71 (1)	N'	5 (5)
N'	-89 (5)	C(2')	-5 (6)
C(2')	74 (6)	C(4')*	622 (8)
O(1')	-56 (5)	C(3')	3 (7)
		C(5')	-3 (7)

\* Atom omitted from mean-plane calculation.

The complex anion has, as previously predicted (Woon & O'Connor, 1979), the  $\Delta$  absolute configuration (IUPAC Commission on Inorganic Chemical Nomenclature, 1971). Such an arrangement is a consequence of the  $S$  absolute configuration of atoms C(2) and C(2'). The overall description of the dissymmetric complex anion is OC-6-13-C (Brown, Cook & Sloan, 1975) and the coordinated N atoms have the  $R$  absolute configuration.

Bond lengths and angles of the pyrrolidine moieties are similar to those found in compounds containing pyrrolidiny groups as part of a quadridentate ligand (Freeman, 1978). An interesting difference, however, is the disorder of the C(4) atom in one of the pyrrolidine rings in which the alternate sites C(4a) and C(4b) are separated by 0.83  $\text{\AA}$ . A similar observation has been made in the structure of the cyclic hexapeptide *cyclo*-(Gly-L-Pro-D-Ala)<sub>2</sub> (Kostansek, Lipscomb & Thiessen, 1979). The second pyrrolidine residue in the present compound shows no such disorder. It has an envelope conformation with C(4') 0.622 (8)  $\text{\AA}$  above the mean plane containing N', C(2'), C(3') and C(5'). Data for this and other planes within the complex anion are given in Table 4. The coordinated N'-C(6')-C(6)-N group has the  $\delta$  conformation (IUPAC Commission on Inorganic Chemical Nomenclature, 1971) and the angle between the N'-C(6')-C(6) and N-C(6)-C(6') planes is 55.1 (1)°.

Each Na<sup>+</sup> cation is surrounded by six O atoms in an approximately octahedral arrangement. Three water O

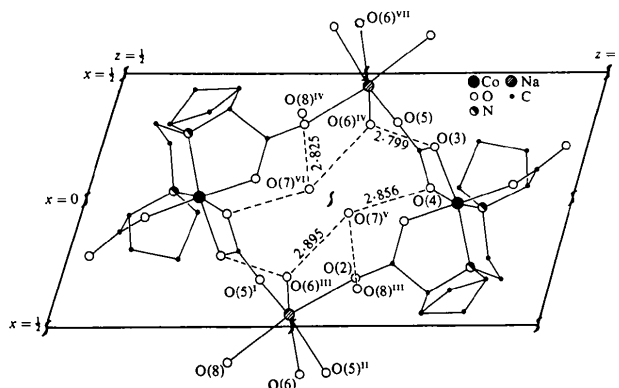


Fig. 2. Projection of the unit-cell contents viewed down the  $b$  axis, showing some intermolecular contacts ( $\text{\AA}$ ). The symmetry code refers to that given in Tables 5 and 6.

Table 5. Interatomic distances ( $\text{\AA}$ ) and angles ( $^\circ$ ) involving the six-coordinate sodium cation

The estimated standard deviations are in parentheses.

Na-O(2)	2.357 (6)	Na-O(5) <sup>I</sup>	2.738 (6)
Na-O(6)	2.527 (6)	Na-O(5) <sup>II</sup>	2.484 (7)
Na-O(8)	2.402 (7)	Na-O(6) <sup>III</sup>	2.386 (6)
O(8)-Na-O(2)	169.9 (3)		
O(6)-Na-O(6) <sup>III</sup>	163.8 (2)		
O(5) <sup>I</sup> -Na-O(5) <sup>II</sup>	166.1 (2)		

Symmetry code

- (I)  $-x, \frac{1}{2} + y, -z$   
 (II)  $1 + x, y, z$   
 (III)  $1 - x, -\frac{1}{2} + y, -z$

Table 6. Intermolecular contacts ( $\text{\AA}$ ) less than 3.30  $\text{\AA}$

The estimated standard deviations are in parentheses.

O(2) ... O(6) <sup>III</sup>	3.220 (7)	O(1) ... O(7) <sup>VI</sup>	3.108 (7)
O(3) ... O(6) <sup>IV</sup>	2.799 (7)	O(2) ... O(7) <sup>VI</sup>	3.100 (8)
O(4) ... O(7) <sup>V</sup>	2.856 (8)	O(5) ... O(6) <sup>VII</sup>	3.101 (7)
O(5) ... O(8) <sup>IV</sup>	3.248 (8)	O(6) ... O(7) <sup>VIII</sup>	2.895 (8)
		O(7) ... O(8) <sup>IX</sup>	2.825 (9)

Symmetry code

- (III)  $1 - x, -\frac{1}{2} + y, -z$  (VI)  $-1 + x, y, -1 + z$   
 (IV)  $-1 + x, y, z$  (VII)  $-x, -\frac{1}{2} + y, -z$   
 (V)  $1 - x, -\frac{1}{2} + y, 1 - z$  (VIII)  $x, y, -1 + z$   
 (IX)  $x, y, 1 + z$

atoms are so involved, while the carbonyl O atoms of two carbonate groups symmetry-related by a screw axis and the carbonyl O of the carboxylate group bonded to C(2) complete the octahedron. The six-coordinate nature of the Na<sup>+</sup> cation is illustrated in Fig. 2. The Na-O distances, which are in the range 2.36-2.74  $\text{\AA}$ , are given in Table 5 together with some O-Na-O angles. These values are consistent with

those found in structures involving similar coordination of the Na<sup>+</sup> cation (Fallon & Gatehouse, 1976; Hedman, 1977; Chapuis, Zalkin & Templeton, 1977).

In the crystal, the complex anions are linked into double layers parallel to the (001) planes by O—Na—O and O—H<sub>2</sub>O—H<sub>2</sub>O—O bridges (see Fig. 2), the layers being held together along *c* by van der Waals interactions. Short intermolecular contacts between the O atoms are given in Table 6. Those within the range 2.8–2.9 Å are normal for values indicative of hydrogen bonding (Hamilton & Ibers, 1968), and involve all the water molecules as expected.

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## Détermination Structurale de [(+) $\text{Co}(\text{en})_3$ (-) $\text{Cr}(\text{en})_3$ ](SCN)<sub>6</sub>, Forme Orthorhombique

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### Abstract

The active racemate crystal [(+) $\text{Co}(\text{en})_3$ (-) $\text{Cr}(\text{en})_3$ ](SCN)<sub>6</sub> is dimorphous. Its first form, previously published, is monoclinic and isomorphous with the more stable form of ( $\pm$ ) $\text{Cr}(\text{en})_3$ (SCN)<sub>3</sub>, while its second form, presently studied, is orthorhombic and isomorphous with ( $\pm$ ) $\text{Co}(\text{en})_3$ (SCN)<sub>3</sub>. The structure of orthorhombic [(+) $\text{Co}(\text{en})_3$ (-) $\text{Cr}(\text{en})_3$ ](SCN)<sub>6</sub> has been determined by single-crystal analysis ( $R = 0.09$ , 3600 *hkl*). The space group is  $P2_12_12_1$  and the lattice constants are  $a = 14.595$  (8),  $b = 14.254$  (8),  $c = 17.37$  (1) Å,  $Z = 4$ ,  $V = 3614$  Å<sup>3</sup>,  $D_c = 1.506$  Mg m<sup>-3</sup>. Unlike its monoclinic form, the two independent

complex ions (+)[ $\text{Co}(\text{en})_3$ ]<sup>3+</sup> and (-)[ $\text{Cr}(\text{en})_3$ ]<sup>3+</sup> of the orthorhombic form have the same conformation, *lel lel lel*. The dimorphism of this active racemate compound can be explained by the structural analogies which exist between the racemate crystals of orthorhombic (+) $\text{Co}(\text{en})_3$ (SCN)<sub>3</sub> and monoclinic ( $\pm$ ) $\text{Cr}(\text{en})_3$ (SCN)<sub>3</sub>.

### Introduction

Les études antérieures (Brouty, Spinat, Whuler & Herpin, 1976, 1977) ont montré que, dans la série des thiocyanates complexes, les racémiques ( $\pm$ ) $\text{Co}(\text{en})_3$ (SCN)<sub>3</sub> et ( $\pm$ ) $\text{Cr}(\text{en})_3$ (SCN)<sub>3</sub> ne sont pas