Crystal Structure and Absolute Configuration of (+)$_{546}$-*cis*(*O*)-Triammine(sarcosinate-*N*-propionato)cobalt(III) (+)$_{546}$-(Ethylenediaminetetraacetato)cobaltate(III) Monohydrate

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The crystal structure of (+)$_{546}$-*cis*(*O*)-triammine(sarcosinate-*N*-propionato)cobalt(III) (+)$_{546}$-(ethylenediaminetetraacetato)cobaltate(III) monohydrate was solved by single crystal X-ray diffraction techniques. The crystal is orthorhombic, space group $P2_12_12_1$, with $a=10.792$, $b=26.816$, $c=8.203$ Å, and $Z=4$. The final R value was 0.054. The absolute configurations of two complex ions were determined by means of anomalous dispersion using Cu $K\alpha$ radiation. The coordinated asymmetric nitrogen atom of sarcosinate-*N*-propionate ligand takes an *R* configuration, and the (+)$_{546}$-(ethylenediaminetetraacetato)cobaltate(III) ion Δ one.

Sarcosinate-*N*-propionate ($sarmp^{2-}$) forms a five- and six-membered chelate ring by coordination of an α-amino carboxylate foot and an *N*-propionate one, respectively. *cis*(*O*)-Triammine(sarcosinate-*N*-propionato)cobalt(III) cation is a model complex, which contains only one asymmetrically coordinated nitrogen atom, and was optically resolved through its diastereomeric salt formation with (+)$_{546}$-(ethylenediaminetetraacetato)-cobaltate(III) anion, $[Co(edta)]^-$.[1] The absolute configuration of (+)$_{546}$-*cis*(*O*) isomer was presumed to be an *R* one from the consideration of its CD spectra, referring to the stereochemistry of several kinds of analogous complexes.[1-4]

This paper deals with the crystal structure of the diastereomeric salt, and the absolute configurations of (+)$_{546}$-*cis*(*O*)-$[Co(sarmp)(NH_3)_3]^+$ and (+)$_{546}$-$[Co(edta)]^-$ ions are established concurrently. A preliminary report has been presented.[5]

Experimental

Preparation of the Crystals. The diastereomer (+)$_{546}$-*cis*(*O*)-$[Co(sarmp)(NH_3)_3]\cdot$(+)$_{546}$-$[Co(edta)]\cdot H_2O$ was isolated first in the course of the study on the stereochemistry of cobalt(III) complexes with *O,N,O*-tridentate ligand.[1] Silver acetate (0.30 g) was added to a solution of 0.54 g of racemic $[Co(sarmp)(NH_3)_3]Cl$ in a small amount of water and the resulting silver chloride was filtered off. The filtrate was added to a solution of 0.375 g of (+)$_{546}$-$K[Co(edta)]\cdot 2H_2O$[6] in a minimum amount of water. After the mixed solution had been evaporated by a stream of air at room temperature, the concentrated solution was kept in a refrigerator. The violet needle crystals crystallized out as less soluble diastereomer were collected by filtration. The optically active chloride (+)$_{546}$-*cis*(*O*)-$[Co(sarmp)(NH_3)_3]Cl$ obtained from the diastereomer showed $\Delta\varepsilon_{546}=+0.35$.

Crystal Data. Preliminary Weissenberg and oscillation photographs established the fact that the crystals are orthorhombic with b axis along the needle axis. The systematic extinction restricts the space group to $P2_12_12_1$. The crystal data are listed in Table 1.

Data Collection. The intensity data were collected on a Rigaku Denki Computer-controlled four-circle diffractometer employing Mo $K\alpha$ radiation. A single crystal of size *ca.* 0.45 $\times$ 0.31 $\times$ 0.41 mm was used for the intensity measurement of 2440 independent non-zero reflections. The ω-2θ scan technique was employed with a scan speed 2° min^{-1} by ω, and the background was measured for each 10.0 seconds at the start and end points of a scan range. A scan range of ω for each reflection was calculated by the formula $\Delta\omega=0.08°+0.35°\tan\theta$. Attenuators were automatically inserted when the maximum counting rate exceeded 9000 cps. The measurement of two reference reflections (0 0 2) and (0 10 0) was repeated every thirty reflections.

Table 1. Crystal data

$Co_2C_{16}H_{32}N_6O_{13}$	$M_r=634.33$	
Orthorhombic	$P2_12_12_1$	
$a=10.792(9)$Å	$b=26.816(4)$Å	$c=8.203(12)$Å
$\alpha=90.0°$	$\beta=90.0°$	$\gamma=90.0°$
$D_{calcd}=1.775$ g cm^{-3}		$Z=4$.
$D_{obsd}=1.766$ g cm^{-3} (by flotation)		

For the determination of absolute configurations of both complex ions, the intensities of pairs of reflections, *hkl* and $\bar{h}\bar{k}\bar{l}$, were measured by use of Cu $K\alpha$ radiation.

Structure Determination and Refinement. The structure was solved by the usual heavy-atom method. The positions of two cobalt atoms were determined by means of the Patterson synthesis, and all the non-hydrogen atoms were located by the subsequent Fourier synthesis. The trial structure was refined by a diagonal least-squares procedure with the positional and isotropic thermal parameters. The atomic scattering factors were taken from International Tables for X-ray Crystallography.[7] Further refinement was carried out by the least-squares method of a block-diagonal matrix approximation with the positional and anisotropic thermal parameters for all the non-hydrogen atoms (a program by Dr. T. Ashida was used). After several cycles of refinement, the R value ($R=\sum||F_o|-|F_c||/\sum|F_o|$) decreased to 0.054.

The final parameters of all atoms (except hydrogen atoms) are listed in Table 2. These positional parameters are normal within the estimated standard deviations: 0.0011 and 0.0015 Å for cobalts, 0.006—0.009 Å for oxygens, 0.008—0.010 Å for nitrogens, and 0.009—0.013 Å for carbons. Table 3 containing the observed and calculated structure factors is kept as Document No. 7841 at the Chemical Society of Japan.

Results and Discussion

Description of the Structure. The numbering schemes

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Table 2a. Final atomic parameters

Atom	*X*	*Y*	*Z*	Atom	*X*	*Y*	*Z*
Co1	0.0249(1)	0.0427(1)	0.0764(1)	N5	−0.1175(9)	0.0856(8)	0.1341(9)
Co2	0.4913(1)	0.2489(1)	0.2807(1)	N6	−0.0115(9)	−0.0100(7)	0.2447(8)
O1	0.1594(7)	0.0018(7)	0.0113(7)	C1	0.1883(11)	−0.0345(10)	0.1068(11)
O2	0.5037(7)	0.3009(6)	0.1268(6)	C2	0.1085(11)	−0.0398(12)	0.2603(10)
O3	0.4682(7)	0.1968(6)	0.4340(7)	C3	0.3773(11)	0.1769(10)	0.1043(10)
O4	0.3518(7)	0.2205(7)	0.1623(7)	C4	0.6309(10)	0.3227(10)	0.4307(11)
O5	0.4137(6)	0.2982(7)	0.4215(7)	C5	0.5378(10)	0.2863(10)	−0.0192(10)
O6	−0.0807(8)	0.0153(7)	−0.0909(7)	C6	0.6409(10)	0.2386(10)	0.5557(9)
O7	0.2754(8)	−0.0630(8)	0.0871(9)	C7	0.7444(9)	0.2529(11)	0.2884(9)
O8	0.3011(8)	0.1494(8)	0.0403(8)	C8	0.5979(10)	0.2352(9)	−0.0267(9)
O9	0.5249(8)	0.3117(7)	−0.1398(6)	C9	0.7132(9)	0.2022(10)	0.2142(10)
O10	0.5426(9)	0.1677(7)	0.6678(7)	C10	0.4907(12)	0.3320(9)	0.4704(8)
O11	0.2735(9)	0.3568(9)	0.1535(9)	C11	0.5157(10)	0.1608(9)	0.1131(9)
O12	0.4581(8)	0.3702(7)	0.5381(7)	C12	−0.1159(11)	−0.0425(11)	0.1904(10)
O13	−0.1501(8)	−0.0449(9)	−0.2483(8)	C13	−0.1089(11)	−0.0300(11)	−0.1151(10)
N1	0.1346(9)	0.0795(9)	0.2256(10)	C14	−0.0458(12)	0.0087(11)	0.4133(11)
N2	0.0747(11)	0.0894(9)	−0.0998(10)	C15	0.5457(10)	0.1980(10)	0.5571(9)
N3	0.6391(7)	0.2677(7)	0.3959(8)	C16	−0.0988(14)	−0.0673(11)	0.0234(11)
N4	0.5879(8)	0.2075(7)	0.1362(8)				

Table 2b. Final atomic parameters

Atom	$B_{11}\times10^4$	$B_{22}\times10^4$	$B_{33}\times10^4$	$B_{12}\times10^4$	$B_{13}\times10^4$	$B_{23}\times10^4$
Co1	54(1)	5(0)	64(2)	−1(1)	20(3)	1(1)
Co2	35(1)	7(0)	43(1)	0(1)	1(2)	−2(1)
O1	77(7)	9(1)	74(11)	11(5)	55(16)	17(6)
O2	58(6)	7(1)	62(9)	5(4)	−14(15)	1(5)
O3	60(6)	8(1)	64(9)	−9(4)	16(16)	5(5)
O4	37(6)	10(1)	78(11)	−5(4)	−17(14)	0(6)
O5	47(6)	9(1)	67(10)	0(4)	26(15)	−11(6)
O6	103(8)	8(1)	70(11)	−5(5)	−36(18)	3(6)
O7	84(9)	15(1)	158(16)	29(6)	70(22)	21(9)
O8	72(8)	13(1)	135(15)	−30(5)	−7(18)	−22(7)
O9	93(8)	11(1)	49(9)	9(5)	−4(17)	17(5)
O10	140(11)	10(1)	47(10)	−10(6)	−4(18)	8(5)
O11	105(10)	16(1)	125(15)	24(7)	−10(21)	9(8)
O12	105(9)	8(1)	107(13)	10(5)	10(19)	−25(6)
O13	90(8)	18(2)	87(13)	−30(6)	−43(18)	−4(8)
N1	63(8)	11(1)	99(15)	−10(6)	8(21)	−11(8)
N2	122(12)	8(1)	95(15)	3(7)	60(24)	17(8)
N3	31(6)	7(1)	61(12)	−11(4)	−7(15)	6(6)
N4	46(7)	5(1)	55(11)	8(5)	−3(16)	2(6)
N5	68(9)	7(1)	109(15)	14(5)	19(20)	−4(7)
N6	57(7)	7(1)	67(11)	−5(5)	35(18)	3(6)
C1	56(9)	9(2)	106(18)	2(6)	25(22)	−3(9)
C2	60(9)	13(2)	70(15)	16(7)	9(21)	16(9)
C3	68(10)	9(1)	58(14)	−15(6)	−7(21)	10(8)
C4	47(9)	8(1)	111(17)	−8(6)	−20(24)	−10(9)
C5	39(8)	9(1)	73(14)	0(6)	−31(19)	−12(8)
C6	64(9)	10(2)	24(12)	−1(6)	−25(19)	10(7)
C7	36(7)	10(1)	54(13)	0(6)	19(17)	−2(9)
C8	66(9)	6(1)	40(13)	3(6)	−15(19)	8(6)
C9	32(8)	11(2)	71(15)	9(6)	−15(20)	−3(8)
C10	88(11)	7(1)	45(12)	5(7)	−29(23)	10(6)
C11	50(9)	6(1)	78(14)	−7(6)	9(21)	−10(7)
C12	74(10)	9(2)	77(16)	−18(7)	17(22)	14(9)
C13	58(10)	11(2)	86(17)	5(7)	4(22)	−8(8)
C14	96(12)	13(2)	55(15)	−7(8)	29(26)	−14(9)
C15	73(10)	8(1)	45(13)	4(6)	8(21)	−8(7)
C16	129(15)	8(2)	73(17)	−11(8)	−43(28)	−5(8)

Temperature factor=$\exp[-(B_{11}\times h^2+B_{22}\times k^2+B_{33}\times l^2+B_{12}\times hk+B_{13}\times hl+B_{23}\times kl)]$ or $\exp(-B(\sin\theta/\lambda)^2)$.
Estimated standard deviations are shown in parentheses.

are shown in Figs. 1 and 2. The packing mode of the complex cations, anions and the water molecules is illustrated in Fig. 3. The bond lengths and angles

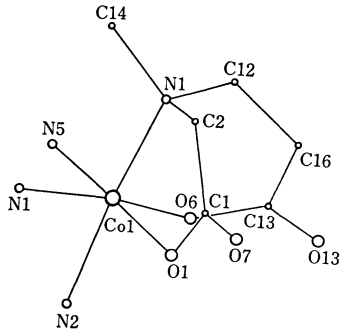

Fig. 1. Structure of *cis*(*O*)-[Co(sarmp)$(NH_3)_3$]$^+$ ion and the numbering scheme of atoms.

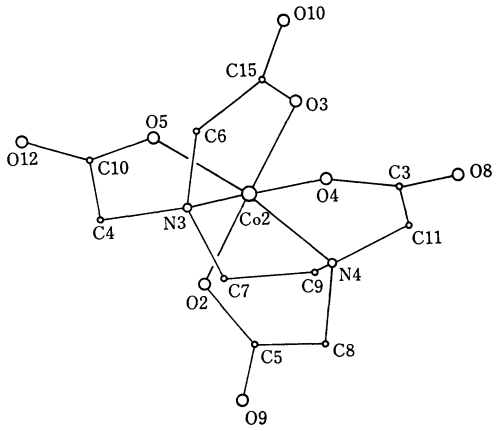

Fig. 2. Structure of [Co(edta)]$^-$ ion and the numbering scheme of atoms.

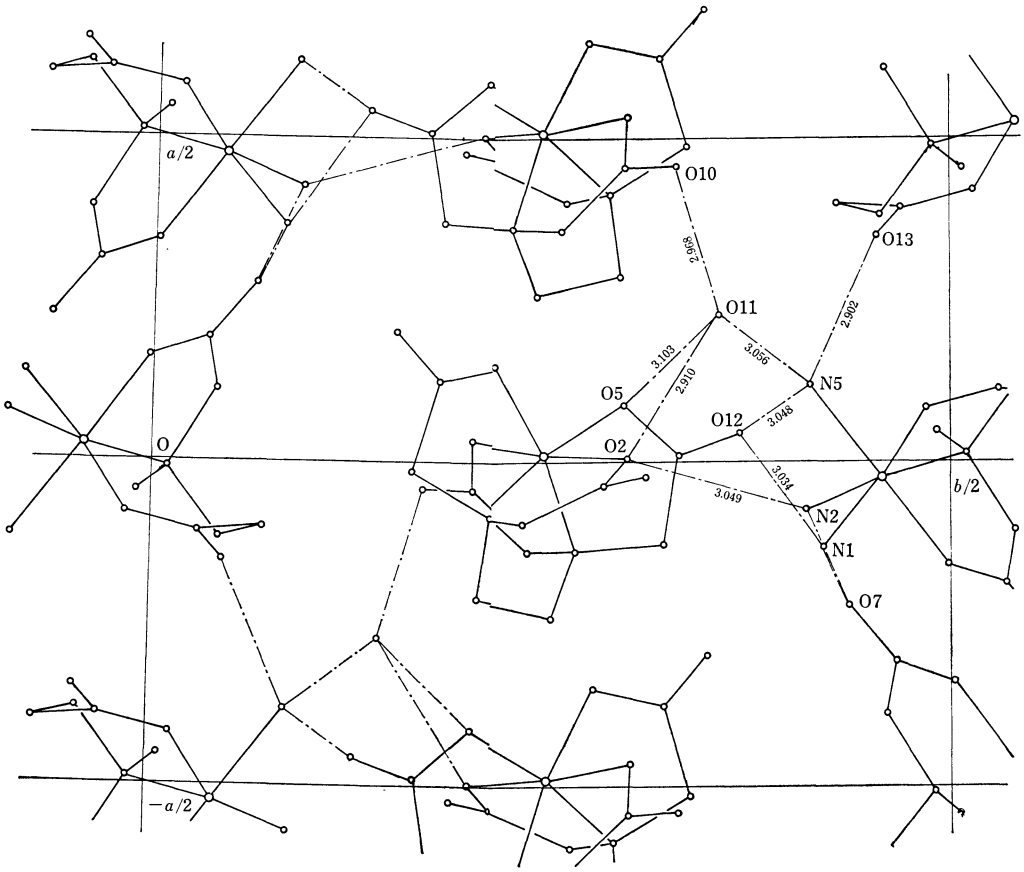

Fig. 3. A projection of the crystal packing viewed along c axis.

Table 4. Bond lengths in [Co(sarmp)$(NH_3)_3$]$^+$ ion

Bond	Length	e.s.d.	Bond	Length	e.s.d.
Co1–N1	1.968 Å	0.008 Å	O1–C1	1.288 Å	0.013 Å
Co1–N2	1.987	0.011	O6–C13	1.267	0.014
Co1–N5	1.978	0.009	O7–C1	1.222	0.014
Co1–N6	2.013	0.009	O13–C13	1.246	0.014
Co1–O1	1.896	0.008	N6–C2	1.526	0.014
Co1–O6	1.928	0.008	N6–C12	1.492	0.014
			N6–C14	1.516	0.015

Table 5. Angles in $[Co(sarmp)(NH_3)_3]^+$ ion

Angle	Degree	e.s.d.	Angle	Degree	e.s.d.
O1–Co1–O6	91.83°	0.34°	C2–N6–Cl4	107.66°	0.82°
O1–Co1–N1	90.27	0.36	C12–N6–C14	106.30	0.82
O1–Co1–N2	87.26	0.39	O1–C1–O7	125.38	1.05
O6–Co1–N2	83.21	0.40	O1–C1–C2	115.66	0.94
O6–Co1–N5	86.15	0.37	O7–C1–C2	118.90	1.01
N1–Co1–N2	88.46	0.42	N6–C2–C1	111.11	0.89
N1–Co1–N5	91.50	0.39	N6–C12–C16	115.43	0.95
N2–Co1–N5	90.98	0.42	O6–C13–C16	119.83	1.04
O6–Co1–N6	96.09	0.40	O13–C13–C16	118.01	1.05
Co1–O1–C1	116.81	0.69	C12–C16–C13	111.86	1.06
Co1–O6–C13	128.15	0.75	C2–N6–C12	111.12	0.82
Co1–N6–C12	110.57	0.60			

Table 6. Bond lengths in $[Co(edta)]^-$ ion

Bond	Length	e.s.d	Bond	Length	e.s.d
Co2–N3	1.921 Å	0.008 Å	O12–C10	1.216 Å	0.015 Å
Co2–N4	1.929	0.008	N3–C4	1.505	0.014
Co2–O2	1.887	0.007	N3–C6	1.526	0.013
Co2–O3	1.897	0.007	N3–C7	1.492	0.013
Co2–O4	1.946	0.007	N4–C8	1.532	0.013
Co2–O5	1.945	0.007	N4–C9	1.503	0.013
O2–C5	1.313	0.012	N4–C11	1.486	0.013
O3–C15	1.311	0.012	C3–C11	1.556	0.015
O4–C3	1.292	0.013	C4–C10	1.568	0.017
O5–C10	1.299	0.014	C5–C8	1.518	0.014
O8–C3	1.222	0.014	C6–C15	1.497	0.014
O9–C5	1.210	0.013	C7–C9	1.526	0.015
O10–C15	1.219	0.014			

Table 7. Angles in $[Co(edta)]^-$ ion

Angle	Degree	e.s.d.	Angle	Degree	e.s.d.
O2–Co2–O4	90.61°	0.30°	C4–N3–C7	114.69°	0.78°
O2–Co2–O5	85.72	0.30	C6–N3–C7	111.22	0.74
O2–Co2–N3	94.35	0.32	C8–N4–C9	110.68	0.74
O2–Co2–N4	88.64	0.32	C8–N4–C11	109.49	0.73
O3–Co2–O4	86.59	0.30	C9–N4–C11	116.56	0.75
O3–Co2–O5	92.89	0.29	O4–C3–O8	124.11	1.01
O3–Co2–N3	88.66	0.31	O4–C3–C11	115.93	0.89
O3–Co2–N4	93.10	0.31	O8–C3–C11	119.92	0.96
O4–Co2–O5	103.21	0.29	N3–C4–C10	104.57	0.86
O4–Co2–N4	83.47	0.31	O2–C5–O9	122.97	0.92
O5–Co2–N3	83.53	0.31	O2–C5–C8	115.30	0.84
N3–Co2–N4	90.28	0.33	O9–C5–C8	111.82	0.80
Co2–O2–C5	114.09	0.62	N3–C6–C15	111.70	0.80
Co2–O3–C15	114.08	0.62	N3–C7–C9	107.72	0.82
Co2–O4–C3	111.93	0.65	N4–C8–C5	111.82	0.80
Co2–O5–C10	112.52	0.68	N4–C9–C7	106.54	0.80
Co2–N3–C4	107.58	0.61	O5–C10–O12	123.07	1.08
Co2–N3–C6	107.39	0.57	O5–C10–C4	116.41	0.97
Co2–N3–C7	105.77	0.59	O12–C10–C4	120.46	1.04
Co2–N4–C8	107.18	0.58	N4–C11–C3	106.05	0.79
Co2–N4–C9	106.16	0.58	O6–C13–O13	122.09	1.05
Co2–N4–C11	116.56	0.75	O3–C15–O10	122.63	0.98
C4–N3–C6	109.80	0.75	O3–C15–C6	116.74	0.87
			O10–C15–C6	120.62	0.97

within the $[Co(sarmp)(NH_3)_3]^+$ ion are given in Tables 4 and 5. In the complex cation, the sarcosinate-*N*-propionate tridentate ligand coordinates facially giving a *cis*(*O*) configuration of the CoN_4O_2 octahedron. It is interesting that the bond length from cobalt to the coordinated nitrogen atom of this ligand, 2.013 Å, is the longest of all the Co–N bonds; the other three Co–NH_3 bonds are in the range 1.968—1.987 Å. Furthermore, this Co–N bond is significantly longer than that of an analogous *O,N,O*-tridentate ligand, iminodiacetate, which makes two five-membered chelate rings.[8] The bond lengths and angles in the six-membered chelate ring differ markedly from those in the five-membered chelate ring. This is in line with the tendency known for several α- and β-amino carboxylato complexes.[9-11] Though the bond lengths and angles of the five-membered chelate ring are similar to those of simple α-amino carboxylato or *O,N,O*-tridentato complexes, the bond angles of the six-membered chelate ring differ significantly from those

Table 8. Selected pairs of reflections demonstrating the absolute configuration of $(+)_{546}$-*cis*(*O*)-$[Co(sarmp)(NH_3)_3]\cdot(+)_{546}$-$[Co(edta)]\cdot H_2O$

h	*k*	*l*	$F_c(hkl)$	Obsd	$F_c(\bar{h}kl)$	*h*	*k*	*l*	$F_c(hkl)$	Obsd	$F_c(\bar{h}kl)$
1	11	1	25	>	1	3	3	4	89	>	74
1	15	1	15	<	31	3	11	4	35	>	23
1	1	2	63	>	46	4	6	2	78	>	65
1	9	2	35	<	54	4	14	3	21	>	10
1	20	2	12	<	26	5	5	1	73	<	88
2	3	1	79	<	96	5	9	1	30	<	45
2	6	1	18	>	4	5	12	2	36	>	30
2	13	1	49	<	61	5	16	2	30	>	17
2	2	2	43	>	24	5	3	3	33	<	52
2	4	2	58	>	45	5	10	3	64	>	45
2	1	3	38	>	21	5	11	4	28	<	45
2	15	3	23	>	8	6	2	1	26	<	38
2	18	3	30	<	44	6	1	2	53	>	40
3	1	1	69	>	53	6	2	2	82	>	62
3	4	1	57	>	42	6	4	2	49	>	34
3	1	2	43	<	58	6	3	3	38	>	24
3	6	2	39	<	53	6	2	4	4	<	25
3	17	3	34	<	45	8	2	2	43	>	30

Table 9. Displacements of atoms from the chelate ring plane

$(+)_{546}$-*cis*(*O*)-*R*-$[Co(sarmp)(NH_3)_3]^+$ ion

Plane 1. [Co1, O6, N6] (six-membered chelate ring)

$0.7642X-0.5469Y-0.3419Z+0.6349=0$

Co1	0.0000	O6	0.0000	N6	0.0000	O13	0.7519	C12	−0.2322	C13	0.4996
C16	0.7422										

Plane 2. [Co1, O1, N6] (five-membered chelate ring)

$-0.5951X-0.4712Y-0.6510Z+1.1066=0$

Co1	0.0000	O1	0.0000	N6	0.0000	O7	−0.3309	C1	−0.2365	C2	−0.4777

$(+)_{546}$-Δ-$[Co(edta)]^-$ ion

Plane 3. [Co2, N3, N4] (ethylenediamine chelate ring)

$-0.1218X-0.7756Y+0.6193Z+4.3964=0$

Co2	0.0000	N3	0.0000	N4	0.0000	C7	−0.3768	C9	0.3414		

Plane 4. [Co2, O3, N3] (out-of-plane)

$0.5368X-0.6151Y-0.5775Z+2.5890=0$

Co2	0.0000	O3	0.0000	N3	0.0000	C6	−0.2667	C15	−0.1552	O10	−0.1981

Plane 5. [Co2, O2, N4] (out-of-plane)

$-0.8396X-0.3179Y-0.4405Z+7.5876=0$

Co2	0.0000	O2	0.0000	N4	0.0000	C5	0.3443	C8	0.2614	O9	0.6800

Plane 6. [Co2, O4, N4] (in-plane)

$-0.0468X-0.7493Y+0.6606Z+3.7280=0$

Co2	0.0000	O4	0.0000	N4	0.0000	C3	0.5489	C11	0.8488	O8	0.7919

Plane 7. [Co2, O5, N3] (in-plane)

$-0.179X-0.7095Y+0.6814Z+4.1183=0$

Co2	0.0000	O5	0.0000	N3	0.0000	C4	−0.8364	C10	−0.5193	O12	−0.8041

The *X*, *Y*, and *Z* coordinates in Å are referred to the crystallographic axis.

of simple β-amino carboxylato complexes: *e.g.*, <O6–Co1–N6=96.1° (90° for $[Co^{II}(\beta\text{-alaninato})_2(H_2O)_2]$,[10] and 93.4° for *trans*-dinitro(β-alaninato)(1,3-propanediamine)cobalt(III),[11] <Co1–N6–C12=110.6° (115 and 116.2°, *vide ante*), and <N6–C12–C16=115.4° (111 and 113°, *vide ante*).

The bond lengths and angles within the $[Co(edta)]^-$ ion (Tables 6 and 7) agree well with the data for ammonium and rubidium salts.[12]

The oxygen atom O11 of the water molecule seems to have four nearest neighbor atoms, N5, O2, O5, and O10 (Fig. 3). Several hydrogen bonds are recognized between the complex ions; *e.g.*, N5–O13, N5–O12, N1–O12, and so on.

Absolute Configuration. The absolute configuration was determined by anomalous dispersion. The atomic scattering factors were taken from literature;[7] those of cobalt atoms were collected for real and imaginary parts of anomalous dispersion: $\Delta f' = -2.2$ and $\Delta f'' = 3.8$.

The intensities of the reflections, $|F_c(hkl)|$ and $|F_c(\bar{h}\bar{k}\bar{l})|$, were calculated by use of both sets of atomic parameter values given in Table 2, (X, Y, Z) and $(X, -Y, Z)$. The values calculated by $(X, -Y, Z)$ fit the observation satisfactorily (Table 8). Thus, it is confirmed that the nitrogen atom of the tridentate ligand takes *R* configuration in the $(+)_{546}$-*cis*(*O*)-[Co(sarmp)$(NH_3)_3$]$^+$ ion, which is in line with the assignment from its CD spectra.[1] This shows that the nitrogen atom has the same absolute configuration as the stereospecifically coordinated *R* nitrogen atom of *cis*(*O*)-*R*-triammine(L-prolinate-*N*-propionato)cobalt(III) ion. On the other hand, the absolute configuration of $(+)_{546}$-$[Co(edta)]^-$ ion can be designated as Δ. The complex ion has been assigned to this configuration from a comparison of its ORD[13] and CD[9] spectra with those of Δ-$(+)_{546}$-(*R*-propylenediaminetetraacetato)-cobaltate(III) formed stereospecifically.

Conformation of the Chelate Rings. In order to examine the conformation of chelate rings, the displacements of relevant atoms from the chelate ring plane, which is defined by the central cobalt atom and the two coordinating atoms in the chelate ring, were calculated. The results are given in Table 9. It is concluded that the six-membered chelate ring in the cation has an asymmetric skew-boat form with δ conformation taking C13 and C16 on the same side of the O6–Co–N6 plane. This type of conformation has been recognized in a few cobalt(III) complexes with β-alaninate.[11,14] The five-membered chelate ring in the present complex cation has an asymmetric envelope form with λ conformation.

The diamine chelate ring in the anion has an asymmetric gauche form with λ conformation. This is in line with the case of diamines such as ethylenediamine.[9] One of the two out-of-plane glycinate chelate rings has a strained asymmetric envelope form with λ conformation, and the other δ one. Both of the in-plane glycinate chelate rings have an asymmetric envelope form with δ conformation.

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