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Absolute Configuration and Circular Dichroism Spectrum of *all-cis*(NO_2,N,O)-$(-)^{CD}_{450}$[Co(NO_2)$_2$(gly)$_2$]$^-$ Complex

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An X-Ray analysis of *all-cis*(NO_2,N,O)-$(-)^{CD}_{450}$K[Co(NO_2)$_2$(gly)$_2$]·1/2H_2O has been carried out. The crystal form is trigonal, $P3_121$, with a=10.747(1), c=18.589(4) Å and Z=6. The structure was refined by a block-diagonal least-squares method to a final R value of 0.047 for 3207 independent reflections with $|F_o|>3\sigma(|F_o|)$. The absolute configuration of the $(-)^{CD}_{450}$[Co(NO_2)$_2$(gly)$_2$]$^-$ ion has been determined to be $\Delta(R)$. By comparing the CD spectrum of $\Delta(R)$-[Co(NO_2)$_2$(gly)$_2$]$^-$ with that of a related $\Lambda(R)$-[Co(NO_2)$_2$(en)(ox)]$^-$ complex, the optical activities of these complexes have been concluded to be derived largely from helical distributions of chelate rings.

In a previous paper,[1] the CD spectrum of $\Lambda(R)$-*all-cis*(C,N,O)-$(+)^{CD}_{500}$[Co(CN)$_2$(gly)$_2$]$^-$ was reported and compared with that of $\Delta(R)$-*cis*-$(-)_{589}$[Co(CN)$_2$(ox)(en)]$^-$,[2] where the absolute configuration due to a helical ring pair is designated with Δ or Λ,[3] and the absolute configuration due to the distribution of donor atoms around a metal ion, with R or S.[4] The CD spectra of these complexes resemble each other due to the common R configuration. This result can not be anticipated from a dynamic coupling model regarding optical activity in transition metal complexes since the contribution from the chelate rings is usually evaluated by second-order perturbation[5] and that from the donor atoms by fourth-order perturbation.[6]

In order to clarify the optical activity derived from a chiral arrangement of donor atoms, we attempted to investigate the CD spectra of *all-cis*(NO_2,N,O)-[Co(NO_2)$_2$(gly)$_2$]$^-$ (N and O represent donor atoms of glycinato). This complex is composed of the same donor atoms as those of *cis*-[Co(NO_2)$_2$(ox)(en)]$^-$.[2] Since the ligand field strength of NO_2^- is weaker than that of CN^-, a CD spectral comparison between the dinitro complexes affords further information on the optical activity due to the arrangement of donor atoms. The *all-cis*(NO_2,N,O)-[Co(NO_2)$_2$(gly)$_2$]$^-$ complex has already been prepared by a reaction of [Co(NO_2)$_6$]$^{3-}$ with glycine, and resolved into optical antipodes with cinchonine by Celap et al.[7,8] However, the complex will later be prepared and optically resolved by other methods during this study. The absolute configuration of *all-cis*(NO_2,N,O)-$(-)^{CD}_{450}$[Co(NO_2)$_2$(gly)$_2$]$^-$ has been determined by an X-ray analysis in order to facilitate an analysis of the CD spectra.

Experimental

Preparation and Optical Resolution. One *cis*(NO_2) isomer of [Co(NO_2)$_2$(gly)$_2$]$^-$ has been isolated by Matsuoka et al.[9] In this study, the complex was prepared by a method described in the literature[9] with a few modification. Potassium nitrite (15 g, 0.18 mol) and glycine (15 g, 0.20 mol) were dissolved in 80 cm^3 of water. The solution was mixed with a solution containing $CoCl_2 \cdot 6H_2O$ (10 g, 0.042 mol, in 30 cm^3 H_2O) and aerated for 12 h. Deposited orange needle-like crystals were filtered, and the filtrate was diluted to 3 dm^3 with water and poured onto a column of Dowex 1-X8 resin in Cl^- form (200—400 mesh, ϕ4×25 cm). The column was washed with water and the adsorbed species were eluted with 0.05 mol dm^{-3} KCl. Two bands, corresponding to univalent species, were collected in each fraction. The isomers are labelled E1 and E2 according to the order of elution. The fractions were concentrated with simultaneous removals of the eluting agent. After additions of ethanol, the solutions were kept in a refrigerator in order to precipitate the crystals. The absorption spectrum of the orange needle-like crystals deposited from the reaction mixture was identical with that of the E1 isomer. Found for E1: C, 14.14; H, 2.43; N, 16.51%. Calcd for K[Co(NO_2)$_2$($C_2H_4O_2N$)$_2$]: C, 14.21; H, 2.38; N, 16.57%. Found for E2: C, 13.83; H, 2.61; N, 16.66%. Calcd for K[Co(NO_2)$_2$($C_2H_4O_2N$)$_2$]·0.5H_2O: C, 13.84; H, 2.59; N, 16.14%. The infrared and absorption spectra of E1 were identical with those of the known isomer.[9]

The E2 isomer was optically resolved by the following procedure: $(+)^{CD}_{520}$[Co(ox)(en)$_2$]I (1.03 g, 2.6 mmol) and silver acetate (0.434 g, 2.6 mmol) were shaken in water (6.3 cm^3) at 60 °C for 10 min. Silver iodide was filtered and washed with 2 cm^3 of hot water and crystals containing the E2 isomer (1.35 g, 3.9 mmol) were dissolved in the above-mentioned filtrate combined with the washings. Upon scratching the wall of the vessel without cooling, an orange diastereoisomeric salt was separated. The mixture was allowed to stand for 15 min at room temperature; then the crystals were filtered. The less-soluble diastereoisomeric salt was repeatedly recrystallized from hot water (50 °C) until the $\Delta\varepsilon$ value became constant. The obtained salt was converted into potassium salt by column chromatography using Dowex 50W-X8 in a K^+ form (ϕ2×5 cm). The less-soluble diastereoisomeric salt contained $(+)^{CD}_{450}$[Co(NO_2)$_2$(gly)$_2$]$^-$. The filtrate from which the less-soluble diastereoisomeric salt had been removed was also passed through a column, and a single crystal of K$(-)^{CD}_{450}$[Co(NO_2)$_2$(gly)$_2$]·0.5H_2O was obtained from the effluent and subjected to an X-ray analysis.

Spectral Measurement. Absorption and CD spectra

Table 1. Crystal Data

$K[Co(NO_2)_2(gly)_2]\cdot 1/2H_2O$	F.W.=317.2
Trigonal	Space group $P3_121$
a=10.747(1)	c=18.589(4) Å
Z=6	U=1859.3(4) Å^3
μ(Mo $K\alpha$)=1.79 mm^{-1}	D_x=1.699 g/cm^3

were recorded with a Hitachi 323 recording spectrophotometer and a JASCO J-40C automatic spectropolarimeter, respectively.

X-Ray Measurement. Crystal data are given in Table 1. Reflections were collected in a θ—2θ scan mode ($2\theta_{max}$=60°) with monochromated Mo $K\alpha$ radiation on a Rigaku AFC-5. 4187 reflections ($h \gtreqless 0$, $k \geq 0$, $l \geq 0$) were measured in which 3207 reflections, including Bijvoet pairs with $|F_o| \geq 3\sigma(|F_o|)$, were used for a structural determination. Intensities were corrected for Lp factors, but not for absorption and extinction. Calculations were carried out on a FACOM M-160F computer at Josai University with the UNICS-III program.[10] Complex atomic scattering factors were taken from tables.[11]

Structure Determination. The structure was solved by heavy-atom and Fourier methods. Potassium atoms were located at only one special position (on a twofold axis), at the beginning. This is consistent with three K atoms per unit cell. Later, the remaining cation was found at a general position with 1/2 occupancy. One of the NO_2 groups exhibited two different orientations; each orientation was weighted at 0.5. A block-diagonal least-squares refinement with anisotropic thermal parameters for non-H atoms and isotropic parameters for H atoms reduced the R value to 0.047 (R_w=0.044 with $w=1/[\sigma^2+0.02(F_o)^2]$). The absolute structure was determined by comparing Bijvoet pairs. These are given in the F_o—F_c table.[12]

Results and Discussion

Spectral Characterization. There are five possible geometrical isomers in $[Co(NO_2)_2(gly)_2]^-$. Celap et al.[7] have isolated four isomers, except a *cis(NO₂)-trans(O)* isomer, from a reaction mixture of $[Co(NO_2)_6]^{3-}$ with glycine. Two isomers were isolated by column chromatography in this study. One isomer (E1) was identified with the *cis(NO₂)-trans(N)* isomer, and another isomer (E2) with the *all-cis(NO₂,N,O)* isomer from spectral data. The $(-)^{CD}_{450}$-*all-cis(NO₂,N,O)* isomer shows two CD peaks with opposite signs in the ${}^1A_{1g} \rightarrow {}^1T_{1g}$ (Oh) transition region (19400 cm^{-1}, $\Delta\varepsilon$=+0.3; 22400 cm^{-1}, $\Delta\varepsilon$=−1.4), as shown in Fig. 1.

Description of the Structure. Final atomic parameters are listed in Table 2. A perspective drawing of the complex anion is drawn in Fig. 2 with atomic numbering. Interatomic distances and angles are listed in Table 3. The geometrical arrangement of ligands around a cobalt ion coincides with the assignment based on spectral data; the cobalt ion is in an octahedral coordination with two bidentate glycinate ions and two unidentate nitro ions. Each of the chemically identical ligating atoms occupy cis positions on the octahedron, i.e. *all-cis(NO₂,N,O)*. The octahedral arrangement around a metal ion is much distorted, since there are discernible differences, even in the chemically identical bond distances around a metal ion. The differences, Co-N(NO_2), Co-N(gly), and Co-O are 0.025, 0.024, and 0.019 Å, respectively. The bond angles around a metal ion are spread at an octahedral face comprizing N(1), N(3), and N(4). The absolute configuration of helical chelate rings is described as Δ; accordingly the chiral arrangement of donor atoms, as R.

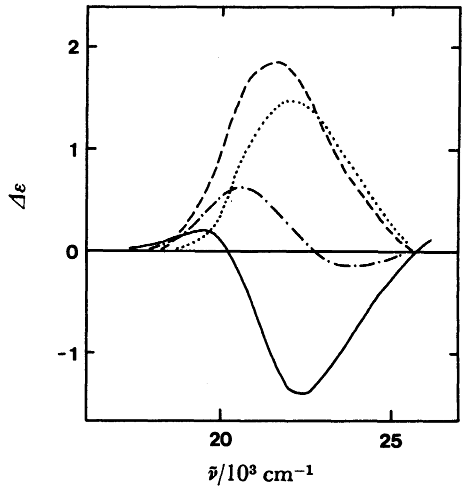

Fig. 1. CD spectra and calculated configurational curves.
a. *all-cis(NO₂,N,O)*-$\Delta(R)$-$(-)^{CD}_{450}[Co(NO_2)_2(gly)_2]^-$ (——), b. *cis*-$\Lambda(R)$-$(+)_{589}[Co(NO_2)_2(ox)(en)]^-$ (----), c. $\Delta\varepsilon(R)=[\Delta\varepsilon(a)+\Delta\varepsilon(b)]/2$ (—·—), d. $\Delta\varepsilon(\Lambda)=[\Delta\varepsilon(b)-\Delta\varepsilon(a)]/2$ (······).

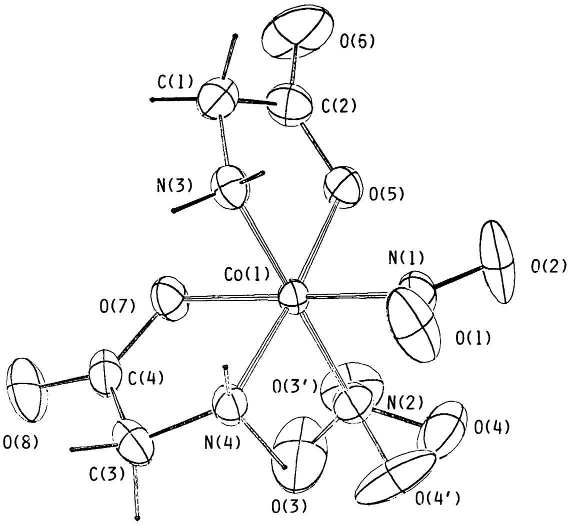

Fig. 2. Perspective view of the *all-cis(NO₂,N,O)*-$[Co(NO_2)_2(gly)_2]^-$ complex with atomic numbering.

Table 2. Atomic Parameters. Positional Parameters are Multiplied by 10^4 (10^5 for Co). Thermal Parameters are Given by the Equivalent Temperature Factors (Å^2)

Atom	*X*	*Y*	*Z*	B_{EQV}
Co(1)	53117(8)	21979(8)	11783(4)	1.57(0.02)
K$^+$(1)	0	2488(2)	1667	3.58(0.22)
K$^+$(2)	670(4)	1038(4)	3648(2)	4.28(0.11)
O (1)	7943(6)	3313(7)	1803(3)	5.04(0.19)
O (2)	7048(7)	4658(6)	1944(3)	5.34(0.18)
O (3)	5345(18)	3156(14)	−176(6)	7.44(0.48)
O (3′)	4841(12)	3816(13)	154(5)	3.90(0.34)
O (4)	6823(13)	4774(11)	450(5)	4.79(0.33)
O (4′)	6961(11)	4245(15)	142(6)	5.50(0.39)
N (1)	6962(6)	3561(6)	1700(3)	2.67(0.12)
N (2)	5825(7)	3560(6)	400(3)	2.60(0.22)
O (5)	4112(5)	2814(5)	1638(2)	2.39(0.12)
O (6)	2138(7)	1941(7)	2291(4)	6.31(0.16)
N (3)	4704(6)	800(6)	1959(3)	2.26(0.15)
C (1)	3339(8)	592(8)	2233(4)	2.73(0.15)
C (2)	3150(8)	1841(8)	2044(4)	3.04(0.14)
O (7)	3668(5)	822(5)	663(2)	2.38(0.14)
O (8)	2964(6)	−701(6)	−255(3)	3.98(0.18)
N (4)	6335(6)	1401(6)	689(3)	2.48(0.19)
C (3)	5398(9)	404(9)	100(4)	3.38(0.21)
C (4)	3898(8)	119(7)	164(3)	2.49(0.17)
W (1)	101(25)	−2623(19)	1435(6)	6.54(0.57)
W (2)	−2247(12)	−559(12)	3941(7)	4.47(0.34)

Atomic Parameters.
Positional Parameters are Multiplied by 10^3

Atom	*X*	*Y*	*Z*	*B*
H(N31)	527(6)	102(6)	227(3)	1.3(0.9)
H(N32)	469(7)	3(7)	180(3)	3.2(1.2)
H(C11)	328(7)	55(8)	273(3)	3.4(1.1)
H(C12)	262(6)	−18(6)	201(3)	1.9(1.1)
H(N41)	738(7)	225(6)	48(3)	1.8(1.0)
H(N42)	682(12)	95(12)	120(5)	10.2(2.2)
H(C31)	540(8)	−53(7)	9(3)	3.4(1.4)
H(C32)	584(9)	73(9)	−40(4)	4.9(1.6)

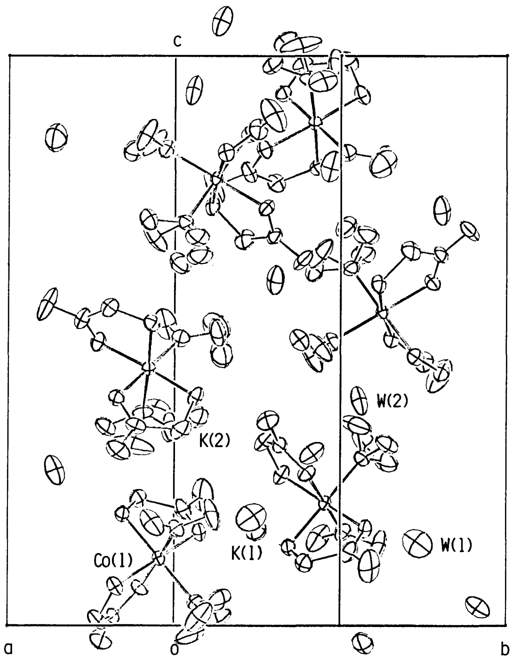

Fig. 3. Crystal packing diagram viewed down a*.

Table 3. Distances (*l*/Å) and Angles (*ϕ*/°) within the Complex Anion

Co(1)–N(1)	1.906(5)	N(1)–O(1)	1.225(11)
Co(1)–N(2)	1.931(5)	N(1)–O(2)	1.223(10)
Co(1)–O(5)	1.920(6)	N(2)–O(3)	1.174(12)
Co(1)–N(3)	1.951(5)	N(2)–O(4)	1.209(10)
Co(1)–O(7)	1.901(4)	N(2)–O(3′)	1.303(17)
Co(1)–N(4)	1.927(7)	N(2)–O(4′)	1.168(12)
N(3)–C(1)	1.461(11)	N(4)–C(3)	1.511(9)
C(1)–C(2)	1.495(14)	C(3)–C(4)	1.487(13)
C(2)–O(5)	1.286(7)	C(4)–O(7)	1.294(9)
C(2)–O(6)	1.234(13)	C(4)–O(8)	1.228(8)
N(1)–Co(1)–N(2)	89.7(2)	O(5)–Co(1)–N(3)	84.9(3)
N(1)–Co(1)–O(5)	92.0(3)	O(5)–Co(1)–N(3)	88.3(2)
N(1)–Co(1)–N(3)	92.2(2)	O(5)–Co(1)–N(4)	174.1(2)
N(1)–Co(1)–O(7)	179.4(3)	N(3)–Co(1)–O(7)	87.3(2)
N(1)–Co(1)–N(4)	93.6(3)	N(7)–Co(1)–N(4)	93.1(3)
N(2)–Co(1)–O(5)	93.4(3)	O(7)–Co(1)–N(4)	86.0(2)
N(2)–Co(1)–N(3)	177.4(3)		
N(2)–Co(1)–O(7)	90.8(2)		
N(2)–Co(1)–N(4)	88.5(3)		
Co(1)– N(1)–O(1)	118.9(5)		
Co(1)– N(1)–O(2)	121.5(6)		
O(1)– N(1)–O(2)	119.6(6)		
Co(1)– N(2)–O(3)	119.8(7)	Co(1)0N(2)–O(3′)	118.0(5)
Co(1)– N(2)–O(4)	121.6(6)	Co(1)–N(2)–O(4′)	126.8(9)
O(3)– N(2)–O(4)	117.2(8)	O(3′)–N(2)–O(4′)	115.1(10)
Co(1)– N(3)–C(1)	107.5(5)	Co(1)–N(4)–C(3)	109.3(6)
Co(1)– O(5)–C(2)	112.7(6)	Co(1)–O(7)–C(4)	116.1(4)
N(3)– C(1)–C(2)	110.9(5)	N(4)–C(3)–C(4)	110.9(7)
C(1)– C(2)–O(5)	117.0(8)	C(3)–C(4)–O(7)	116.2(6)
C(1)– C(2)–O(6)	120.8(6)	C(3)–C(4)–O(8)	120.6(7)
O(5)– C(2)–O(6)	122.2(9)	O(7)–C(4)–O(8)	123.2(8)

One nitro group which occupies the site trans to the oxygen atom of glycinate ion ligates with a particular orientation. However, the other nitro group trans to the nitrogen atom of glycinate ion exhibits two different orientations in disorder. The geometry of the former nitro group is normal compared with related compounds,[13–15] while the bond angle, ∠ONO, of the latter group is somewhat smaller than that of the former group. The geometry of the glycinato groups is very similar to that observed in related complexes.[16] The bite angles of glycinate ions are 84.9 and 86.0°, and the dispositions of Co atom from mean planes of glycinate ions are 0.496(8) and 0.226(0) Å, respectively.

Crystal packing (viewed down a*) is illustrated in Fig. 3, and intermolecular distances are listed in

Table 4. Intermolecular Distances in a Unit Cell (Å)

	Symmetry operations:			i)	$-y$,	$x-y$,	$1/3+z$;
ii)	y,	x,	$-z$;	iii)	$-x$,	$-x+y$,	$1/3-z$;
iv)	$x-y$,	$-y$,	$2/3-z$;	v)	$-1+x$,	y,	z;
vi)	$-x+y$,	$-y$,	$-1+z$;	vii)	$1-x$,	$1-x+y$,	$1/3-z$;
viii)	$1-y$,	$x-y$,	$1/3+z$;	ix)	$1+y$,	x,	$-z$;
x)	$1+x$,	$1+y$,	z;	xi)	$1-x+y$,	$1-x$,	$2/3+z$;
xii)	$-x$,	$-x+y$,	$4/3-z$;	xiii)	$-x+y$,	$1-x$,	$-1/3+z$;
xiv)	$-x+y$,	$-x$,	$-1/3+z$,	xv)	y,	x,	$1-z$;
xvi)	$-x$,	$1-x+y$,	$4/3-z$;	xvii)	$1-x$,	$-x+y$,	$1/3-z$.

K(1)···O(6)	2.885(9)	K(2)···O(6)	2.874(8)
K(1)···O(8)$^{\mathrm{i}}$	2.846(5)	K(2)···W(2)	2.773(2)
K(1)···O(8)$^{\mathrm{ii}}$	2.846(5)	K(2)···O(8)$^{\mathrm{i}}$	3.000(10)
K(1)···O(6)$^{\mathrm{iii}}$	2.885(8)	K(2)···O(7)$^{\mathrm{i}}$	3.144(10)
K(1)···W(2)$^{\mathrm{iv}}$	2.776(12)	K(2)···W(1)$^{\mathrm{i}}$	2.868(15)
K(1)···O(1)$^{\mathrm{v}}$	2.775(8)	K(2)···O(6)$^{\mathrm{iv}}$	3.272(10)
K(1)···W(2)$^{\mathrm{vi}}$	2.776(16)	K(2)···W(2)$^{\mathrm{iv}}$	2.884(17)
K(1)···O(1)$^{\mathrm{vii}}$	2.775(7)	K(2)···C(4)$^{\mathrm{i}}$	3.461(13)
O(1)···O(3)$^{\mathrm{viii}}$	2.786(12)	O(4′)···O(2)$^{\mathrm{xiii}}$	3.389(15)
O(1)···O(8)$^{\mathrm{ix}}$	3.331(18)	O(4′)···N(1)$^{\mathrm{xiii}}$	3.496(13)
O(2)···W(1)$^{\mathrm{x}}$	3.258(18)	O(4′)···N(3)$^{\mathrm{xiii}}$	3.337(15)
O(2)···O(3)$^{\mathrm{viii}}$	3.405(21)	O(4′)···C(1)$^{\mathrm{xiii}}$	3.370(16)
O(2)···O(4)$^{\mathrm{viii}}$	3.389(14)	O(4′)···O(8)$^{\mathrm{ix}}$	3.423(18)
O(2)···N(3)$^{\mathrm{vii}}$	3.157(12)	O(4′)···C(3)$^{\mathrm{ix}}$	3.293(15)
O(2)···C(1)$^{\mathrm{vii}}$	3.403(14)	O(5)···N(2)$^{\mathrm{xiv}}$	3.040(17)
O(2)···O(7)$^{\mathrm{vii}}$	3.417(10)	O(5)···N(3)$^{\mathrm{vii}}$	3.132(10)
O(2)···C(4)$^{\mathrm{vii}}$	3.278(12)	O(5)···N(4)$^{\mathrm{vii}}$	3.279(10)
O(3)···N(1)$^{\mathrm{xi}}$	3.057(15)	O(6)···O(8)$^{\mathrm{i}}$	3.289(13)
O(3)···N(3)$^{\mathrm{xi}}$	3.008(14)	O(6)···W(2)$^{\mathrm{xiv}}$	3.208(15)
O(3)···W(2)$^{\mathrm{xii}}$	2.994(20)	O(6)···C(3)$^{\mathrm{vii}}$	3.494(11)
O(3′)···N(3)$^{\mathrm{xiii}}$	3.206(10)	O(7)···W(2)$^{\mathrm{iii}}$	3.193(16)
O(3′)···W(2)$^{\mathrm{xiv}}$	3.053(19)	O(8)···N(4)$^{\mathrm{xv}}$	2.875(7)
O(3′)···N(2)$^{\mathrm{ii}}$	3.254(18)	O(8)···W(2)$^{\mathrm{xvi}}$	3.097(21)
O(4)···C(1)$^{\mathrm{xiii}}$	3.420(13)	N(4)···C(2)$^{\mathrm{xvii}}$	3.413(14)
O(4)···N(3)$^{\mathrm{vii}}$	3.161(17)	C(4)···W(2)$^{\mathrm{iii}}$	3.323(20)
O(4)···C(1)$^{\mathrm{vii}}$	3.009(18)		

Table 4. The crystal comprises potassium cations, complex anions and water molecules in a complicated three-dimensional network of ionic and hydrogen bonds. Potassium ions are accomodated in two different environments in disorder. Half ions, K(1), are surrounded by eight oxygen atoms in a square prism while the remaining ions, K(2), by seven oxygen atoms in a monocapped octahedron. The low occupation of K(2) may be due to the short distance between the equivalent K(2) ions (2.58 Å). The K(1) ion exists near the O(1) atoms, as shown in Table 4, and an ionic bond is suggested to exist between them. On the other hand, there is no favorable atom near the oxygen atoms of the nitro group which ligates the site trans to the nitrogen atom of the glycinate ion. This is the reason for the disorder of the orientation in the nitro group.

Optical Activity of *all-cis(NO$_2$,N,O)*-[Co(NO$_2$)$_2$(gly)$_2$]$^-$. Two optical sources can be considered for the isomer as in *all-cis(C,N,O)*-[Co(CN)$_2$(gly)$_2$]$^-$;[1] a helical chelate rings and a chiral arrangement of donor atoms. The *cis*-[Co(NO$_2$)$_2$(ox)(en)]$^-$ complex also has two sources of optical activity. Since the absolute configuration of $(+)_{589}$[Co(NO$_2$)$_2$(ox)(en)]$^-$ has been assigned to $\Lambda(R)$,[2] the $\Delta(R)$-[Co(NO$_2$)$_2$(gly)$_2$]$^-$ isomer is pseudo-diastereoisomeric with the $\Lambda(R)$-[Co(NO$_2$)$_2$(ox)(en)]$^-$ isomer, judging from a description of the absolute configurations. Therefore, the contribution curve due to the *R* configuration can be formally evaluated by adding the two observed CD curves, as shown in Fig. 1. The resultant curve shows positive and negative peaks from the lower frequency, the positive one being dominant. The contribution curve due to the Λ configuration, which is calculated by subtraction (curve d in Fig. 1), exhibits a positive peak. The peak is twice as intense as the dominant peak in the *R* configurational contribution curve. Therefore, the helical ring pair is a more important optical source than the chiral arrangement of donor atoms in dinitro complexes.

The obtained result disagrees with that for the *all-cis(C,N,O)*-[Co(C)$_2$(N)$_2$(O)$_2$]-type complex in which most of the optical activity is derived from a chiral arrangement of donor atoms. These findings can be explained as follows; the difference in the ligand field strength between the cyano and the N donor atoms of glycinato is very large, while the difference between the nitro and the N donor atoms of glycinato is small. Consequently, the asymmetric field due to the donor atoms in dinitro complexes becomes weaker than that in dicyano complexes.

Atoh et al.[17] have found that *trans(P,N)*-[Co(acac)(edpp)$_2$]$^{2+}$ and [Co(acac)(en)(dppe)]$^{2+}$, which have two possibilities for the sources of optical activity (like the present complexes), exhibit CD spectra that are different from each other (edpp=(2-aminoethyl)diphenylphosphine; dppe=1,2-bis(diphenylphosphino)ethane). They concluded that the chiral arrangement of donor atoms is not the dominant source of the optical activity in the phosphine complexes. This fact can also be attributed to the ligand field strength of phosphine, similar to that of ethylenediamine.

Mason[6] has applied a dynamic coupling model to the optical activity of complexes with chiral arrangements of donor atoms. However, his application is incompatible with the present results. Though the dynamic coupling model demands that the optical activity is intimately related to polarizabilities of the donor atoms, the present results show that the optical activity derived from a chiral arrangement of donor atoms is intimately related to crystal field strengths of donor atoms rather than polarizabilities.

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