C222	0.1738 (6)	−0.0524 (5)	0.5186 (4)	0.077 (2)
C223	0.1096 (5)	−0.1305 (6)	0.5632 (4)	0.077 (2)
C224	0.1693 (6)	−0.2347 (6)	0.5667 (4)	0.088 (2)
C225	0.2749 (5)	−0.2164 (6)	0.5243 (4)	0.084 (2)
C231	0.5891 (3)	−0.2100 (3)	0.2371 (3)	0.0410 (9)
C232	0.5886 (4)	−0.3248 (3)	0.2805 (3)	0.0482 (10)
C233	0.6984 (4)	−0.3770 (4)	0.2863 (3)	0.0567 (12)
C234	0.7684 (4)	−0.2964 (4)	0.2470 (3)	0.0565 (12)
C235	0.7021 (3)	−0.1947 (4)	0.2170 (3)	0.0498 (11)
C241	0.5663 (3)	−0.2652 (4)	0.0055 (3)	0.0499 (11)
C242	0.5598 (4)	−0.3772 (4)	0.0498 (3)	0.0548 (12)
C243	0.6677 (4)	−0.4343 (4)	0.0569 (4)	0.0594 (12)
C244	0.7408 (4)	−0.3585 (4)	0.0174 (3)	0.0550 (12)
C245	0.6788 (3)	−0.2547 (4)	−0.0143 (3)	0.0469 (10)
O3†	0.9070 (10)	0.5100 (8)	0.4659 (8)	0.137 (4)

† Site occupancy = 0.5.

Table 2. *Selected geometric parameters (Å, °)*

O11—C11	1.239 (6)	O21—C21	1.226 (4)
C11—C12	1.452 (6)	C21—C22	1.470 (5)
C11—C111	1.473 (6)	C21—C211	1.475 (5)
C12—C13	1.362 (6)	C22—C23	1.347 (5)
C13—C131	1.458 (5)	C23—C231	1.475 (5)
C13—C14	1.488 (6)	C23—C24	1.495 (6)
O11—C11—C12	123.5 (5)	C22—C23—C231	120.0 (4)
O11—C11—C111	119.3 (4)	C22—C23—C24	123.9 (4)
C12—C11—C111	117.2 (4)	C231—C23—C24	116.1 (4)
C13—C12—C11	128.1 (4)	C115—C111—C112	106.8 (4)
C12—C13—C131	119.8 (4)	C115—C111—C11	127.9 (4)
C12—C13—C14	124.0 (4)	C132—C131—C135	106.0 (4)
C131—C13—C14	116.1 (4)	C135—C131—C13	126.1 (4)
O21—C21—C22	124.7 (4)	C215—C211—C212	107.3 (4)
O21—C21—C211	119.7 (4)	C215—C211—C21	128.6 (4)
C22—C21—C211	115.6 (3)	C235—C231—C232	106.4 (4)
C23—C22—C21	128.4 (4)	C235—C231—C23	126.9 (4)

H-atom positions were calculated riding on the parent C atom, with C—H distances of 0.96 (cyclopentadienyl), 0.93 (methyl) and 0.90 Å (methylene), and refined with an overall $U_{\rm iso}$ of 0.07 Å^2.

Data collection: *CAD*-4 *Software* (Enraf--Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Data reduction: *CAD*-4 *Software*. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *SHELXL*93.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AB1313). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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(*trans*-1*R*,2*R*-Cyclohexanediamine-*N*,*N*′)(L-ascorbato-C^2,O^5)platinum(II)–Water (1/3)

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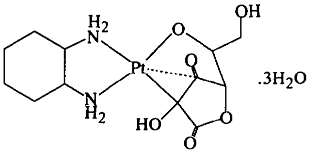
Abstract

In the title compound, $[Pt(C_6H_6O_6)(C_6H_{14}N_2)].3H_2O$, the dianionic ascorbate ligand forms a six-membered chelate ring coordinating to the Pt atom through O and C atoms. The Pt—N distance at the *trans* position of the C atom is slightly longer than that at the *trans* position of the O atom [2.093 (5) and 2.033 (5) Å, respectively]. Three water molecules link the carbonyl or hydroxyl groups of one ascorbate ligand with the amino group of another through hydrogen bonds surrounding the cyclohexane ring.

Comment

L-Ascorbic acid (H_2asc), which is one of the most important biomolecules and participates in electron-transfer systems *in vivo*, acts as a monobasic acid in general. Its crystal structure and those of the Na^+, Ca^{2+} and Tl^+ salts have already been reported (Hvoslef, 1968*a*,*b*, 1969; Hearn & Bugg, 1974; Hvoslef & Kjellevold, 1974; Hughes, 1973). The molecule may often behave as a dibasic acid (pK_1 = 4.26 and pK_2 = 11.64), however, and is oxidized by the removal of two electrons to crystallize as a dimeric form of dehydro-L-ascorbic acid (Hvoslef, 1972), with an intramolecular O6···C3 bond and an intermolecular O3···C2 bond. Although Martell (1982) proposed some structures of transition metal–ascorbate complexes chelating with the enediol group, Hollis, Amundsen & Stern (1985) synthesized and characterized [Pt(*cis*-dach)(asc-C^2,O^5)].3H_2O, (1′) (dach is 1,2-diaminocyclohexane), in which the ascorbate dianion is coordinated by the Pt atom at the C and O atoms; its structural details have not been reported. According to our different preparation procedures (Yuge & Miyamoto, 1996), we have obtained single crystals of the title compound, [Pt(*trans*-1*R*,2*R*-dach)(asc-C^2,O^5)].3H_2O, (1), which is analogous to (1′); their compositions and cell dimensions are similar [a = 6.425 (1), b = 20.542 (2), c = 6.662 (1) Å, β = 104.90 (1)° for (1′)]. The NMR spectra of aqueous solutions show that (1) and the *trans*-1*S*,2*S*-dach isomer have geometrically similar structures, but their crystal structures are quite different. The 1*S*,2*S* isomer is still being investigated owing to gradual decay during the intensity-data collection.



(I)

The most characteristic structural feature of (1) is that the ascorbate dianion coordinates to the Pt atom at the C2 atom of the five-membered lactone ring and the O5 atom of the deprotonated hydroxyl group, similar to the case in (1′) (Fig. 1). The bond distances and angles of (1) almost correspond with those of (1′) within the ranges of their standard deviations, except for those about the square-planar Pt coordination centres. In (1), the Pt—C2 and Pt—C3 bond lengths [2.130 (5) and 2.547 (6) Å, respectively] suggest a π-complex-like character of the Pt atom and the C2 and C3 atoms of the asc^{2-} ligand, whereas in (1′) the longer atomic distances do not [2.138 (7) and 2.666 (8) Å]. The Pt—C3 bond seems rather weak because atoms N1, N2, O5 and C2 form the square plane about the Pt atom, with a maximum deviation from the plane of 0.06 Å. The Pt—C2—C3 and Pt—C3—C2 angles [88.4 (3) and 56.7 (3)°, respectively] are comparable to those of (1′) [93.9 (4) and 53.2 (4)°]. In both (1) and (1′), the Pt—N1 bond appears to be influenced by the C2 atoms at the *trans* positions, resulting in this distance being longer than the Pt—N2 distance. The lactone ring is almost perpendicular to the square plane about the Pt atom [dihedral angle 73.8 (2)°]. The bond lengths for the asc^{2-} ligand are comparable to those of H_2asc and the ascorbate salts, except for those of C3—O3 and C2—C3; the former is remarkably shortened and the latter is elongated [1.233 (6) and 1.458 (9) for (1), 1.326 (3) and 1.338 (2) for H_2asc (Hvoslef, 1968*a*), and 1.287 (5) and 1.373 (6) Å for NaHasc (Hvoslef, 1969)]. The double-bond character of the C2—C3 bond is not observed from the C1—C2—C3—C4 torsion angle of −20.4 (5)°. The configurations of the asc^{2-} ligand are similar to those of NaHasc. The C3—C4—C5—C6—O6 skeleton has a *trans–trans* conformation.

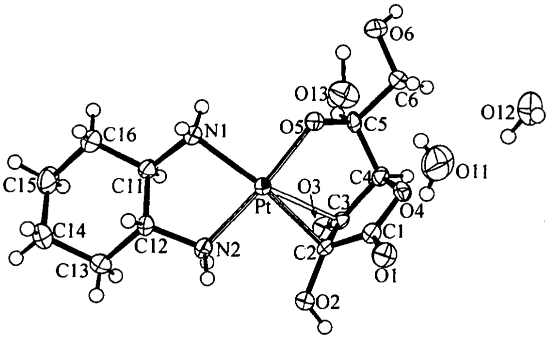


Fig. 1. The asymmetric unit of [Pt(*trans*-1*R*,2*R*-dach)(asc-C^2,O^5)].3H_2O showing the atomic notations. Displacement ellipsoids are drawn at the 50% probability level.

The intermolecular space is filled up by three crystallographically independent water molecules, which form hydrogen bonds with themselves, the carbonyl and the hydroxyl groups of the asc^{2-} ligand and the amino groups of the dach ligand (Fig. 2). The water molecules thus connect adjacent molecules of (1) through hydrogen-bond formation to support the three-dimensional crystal structure; the interatomic distances for possible hydrogen bonds are summarized in Table 3.

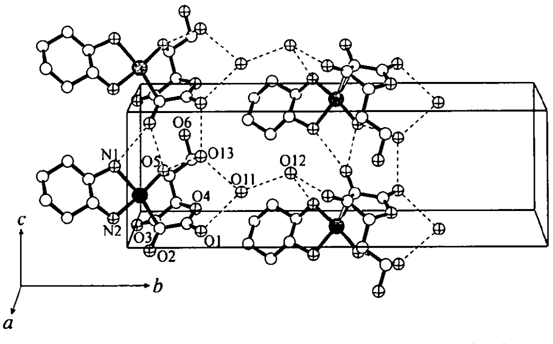


Fig. 2. Packing diagram of [Pt(*trans*-1*R*,2*R*-dach)(asc-C^2,O^5)].3H_2O. O and N atoms are shown by crossed circles and hydrogen bonds are shown by broken lines. H atoms have been omitted for clarity.

Experimental

The title compound was obtained from an aqueous solution containing H_2asc and [Pt(*trans*-1*R*,2*R*-dach)$(OH)_2$] in a 1:1 molar ratio according to the procedures described by Yuge & Miyamoto (1996). Single crystals were prepared by recrystallization from water.

Crystal data

$[Pt(C_6H_6O_6)(C_6H_{14}N_2)]$.-
$3H_2O$
$M_r = 537.44$
Monoclinic
$P2_1$
$a = 6.245\ (2)$ Å
$b = 20.797\ (2)$ Å
$c = 6.7034\ (14)$ Å
$\beta = 105.42\ (2)°$
$V = 839.3\ (3)$ Å^3
$Z = 2$
$D_x = 2.127$ Mg m^{-3}
$D_m = 2.128$ Mg m^{-3}
D_m measured by flotation in $CHBr_3/CCl_4$ solution

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 17.29–19.20°$
$\mu = 8.492$ mm^{-1}
$T = 293$ K
Prism
$0.20 \times 0.10 \times 0.10$ mm
Yellow

Data collection

Rigaku AFC-7*R* diffractometer
$\omega/2\theta$ scans
Absorption correction: empirical *via* ψ scans (North, Phillips & Mathews, 1968)
$T_{\min} = 0.824$, $T_{\max} = 1.000$
6671 measured reflections
6068 independent reflections

5654 observed reflections $[I > 2\sigma(I)]$
$R_{\rm int} = 0.0237$
$\theta_{\max} = 32.5°$
$h = -9 \rightarrow 9$
$k = -31 \rightarrow 31$
$l = -10 \rightarrow 10$
3 standard reflections monitored every 150 reflections intensity decay: 3.2%

Refinement

Refinement on F^2
$R(F) = 0.028$
$wR(F^2) = 0.064$
$S = 1.188$
6068 reflections
319 parameters
All H-atom parameters refined except for H(C5) (only H-atom *U*'s refined)
$w = 1/[\sigma^2(F_o^2) + 4.622P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 1.766$ e Å^{-3}
$\Delta\rho_{\min} = -2.609$ e Å^{-3}

Extinction correction: *SHELXL*93 (Sheldrick, 1993)
Extinction coefficient: 0.0062 (3)
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
Absolute configuration: Flack (1983)
Flack parameter = −0.024 (9)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	*y*	*z*	$U_{\rm eq}$
Pt	0.05413 (3)	0.00000 (2)	0.13784 (2)	0.01912 (5)
N1	0.1731 (10)	−0.0592 (2)	0.3960 (8)	0.0249 (9)
N2	0.2394 (8)	−0.0598 (2)	0.0111 (8)	0.0217 (9)
C11	0.2253 (10)	−0.1222 (3)	0.3117 (9)	0.0228 (10)
C12	0.3671 (10)	−0.1061 (3)	0.1644 (9)	0.0228 (11)
C13	0.4322 (13)	−0.1673 (3)	0.0686 (10)	0.0328 (14)
C14	0.5424 (15)	−0.2159 (4)	0.2319 (12)	0.040 (2)
C15	0.3970 (15)	−0.2307 (3)	0.3752 (13)	0.040 (2)
C16	0.3322 (13)	−0.1707 (3)	0.4747 (11)	0.0300 (12)
O1	0.0779 (8)	0.1561 (2)	−0.1371 (8)	0.0322 (10)
O2	0.0349 (8)	0.0242 (2)	−0.3007 (7)	0.0269 (8)
O3	−0.3992 (8)	−0.0212 (2)	−0.2192 (7)	0.0301 (9)
O4	−0.2313 (7)	0.1356 (2)	−0.0438 (7)	0.0256 (8)
O5	−0.1158 (7)	0.0548 (2)	0.2924 (6)	0.0246 (8)
O6	−0.4312 (11)	0.1026 (3)	0.4999 (8)	0.0461 (15)
C1	−0.0582 (10)	0.1169 (3)	−0.1138 (9)	0.0236 (10)
C2	−0.0662 (10)	0.0465 (2)	−0.1537 (8)	0.0204 (9)
C3	−0.2901 (10)	0.0272 (3)	−0.1514 (8)	0.0224 (10)
C4	−0.3708 (10)	0.0812 (3)	−0.0326 (8)	0.0223 (10)
C5	−0.3423 (9)	0.0643 (2)	0.1929 (9)	0.0222 (10)
C6	−0.4330 (12)	0.1205 (3)	0.2970 (10)	0.0296 (12)
O11	0.1339 (18)	0.2601 (3)	0.1844 (16)	0.068 (2)
O12	0.1075 (11)	0.3837 (3)	0.3239 (11)	0.0432 (13)
O13	0.1500 (10)	0.1574 (3)	0.4653 (10)	0.0411 (12)

Table 2. *Geometric parameters (Å, °)*

Pt—N1	2.093 (5)	O1—C1	1.217 (7)
Pt—N2	2.033 (5)	O2—C2	1.384 (7)
Pt—C2	2.130 (5)	O3—C3	1.233 (6)
Pt—O5	2.020 (4)	O4—C1	1.345 (7)
Pt—C3	2.547 (6)	O4—C4	1.442 (7)
N1—C11	1.495 (7)	O5—C5	1.408 (7)
N2—C12	1.477 (8)	O6—C6	1.408 (8)
C11—C16	1.507 (8)	C1—C2	1.488 (8)
C11—C12	1.529 (9)	C2—C3	1.458 (9)
C12—C13	1.528 (9)	C3—C4	1.537 (8)
C13—C14	1.515 (10)	C4—C5	1.515 (8)
C14—C15	1.519 (12)	C5—C6	1.545 (8)
C15—C16	1.519 (10)		
C2—Pt—N1	170.7 (2)	O1—C1—C2	128.8 (6)
C2—Pt—N2	89.7 (2)	O1—C1—O4	120.4 (5)
C2—Pt—O5	96.3 (2)	O2—C2—C3	122.4 (5)
O5—Pt—N1	91.6 (2)	O2—C2—C1	117.2 (5)
O5—Pt—N2	174.0 (2)	O3—C3—C2	131.2 (5)
C3—Pt—N1	143.4 (2)	O3—C3—C4	124.2 (6)
C3—Pt—N2	106.1 (2)	O4—C4—C5	108.8 (4)
C3—Pt—O5	79.2 (2)	C3—C4—C5	112.3 (4)
C3—Pt—C2	34.9 (2)	C4—C5—C6	108.3 (4)
N1—Pt—N2	82.5 (2)	C5—C6—O6	109.0 (5)
Pt—C2—C1	107.2 (4)	C4—C5—O5	110.0 (5)
Pt—C2—C3	88.4 (3)	O5—C5—C6	109.6 (5)
Pt—C2—O2	112.6 (4)	N1—C11—C16	114.3 (5)
Pt—C3—C2	56.7 (3)	N1—C11—C12	106.0 (5)
Pt—O5—C5	115.7 (3)	N2—C12—C13	113.9 (5)
Pt—N1—C11	105.5 (4)	N2—C12—C11	107.1 (5)
Pt—N2—C12	111.7 (4)	C16—C11—C12	113.2 (5)
C1—C2—C3	104.8 (5)	C11—C12—C13	110.7 (5)
C2—C3—C4	104.6 (5)	C12—C13—C14	111.9 (6)
C3—C4—O4	105.1 (5)	C13—C14—C15	111.1 (6)
C1—O4—C4	110.2 (4)	C14—C15—C16	112.7 (6)
O4—C1—C2	110.8 (5)	C11—C16—C15	110.5 (6)

Table 3. *Contact distances (Å)*

O11···O12	2.755 (10)	O2···O5$^{\rm i}$	2.715 (6)
O11···O13	2.830 (11)	O6···O13$^{\rm ii}$	2.806 (8)
O1···O11	3.008 (10)	O3···O12$^{\rm iii}$	2.899 (8)
O5···O13	2.762 (8)	N1···O2$^{\rm iv}$	2.970 (8)
O1···O13$^{\rm i}$	2.819 (8)	N2···O12$^{\rm iii}$	2.921 (8)

Symmetry codes: (i) $x, y, z - 1$; (ii) $x - 1, y, z$; (iii) $-x, y - \frac{1}{2}, -z$; (iv) $x, y, 1 + z$.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993*a*). Cell refinement: *MSC/AFC Diffractometer Control Software*. Data reduction: *TEXSAN PROCESS* (Molecular Structure Corporation, 1993*b*). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP*II (Johnson, 1976).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AB1376). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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An Oxo-Centered Trinuclear Cobalt(II)–Diiron(III) Acetate–Aqua Complex

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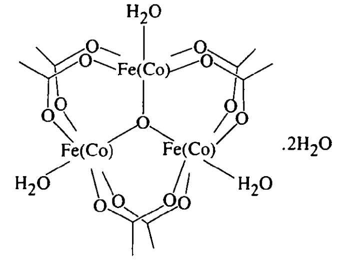
Abstract

The structure of hexakis-μ-acetato-1:2κ^4*O*:*O*′;2:3κ^4-*O*:*O*′;1:3κ^4*O*:*O*′-triaqua-1κ*O*,2κ*O*,3κ*O*-μ_3-oxo-cobalt(II)-diiron(III) dihydrate, $[CoFe_2O(C_2H_3O_2)_6(H_2O)_3].2H_2O$, is reported. The compound is isostructural with the related mixed-valence trinuclear iron(II,III,III) acetate–aqua complex, $[Fe_3O(C_2H_3O_2)_6(H_2O)_3].2H_2O$. The coordination geometries around the three metal atoms of the cobalt–iron complex are almost identical to those of the trinuclear iron complex, and the Co and Fe atoms cannot be distinguished.

Comment

The structures of oxo-centered trinuclear metal–carboxylate complexes have been reported for various combinations of transition metal atoms (isometal mixed-valence and mixed-metal complexes) (see Cannon & White, 1988, and references therein). In many isometal mixed-valence complexes, the symmetry of the molecules is strongly related to the mixed-valence states of the metal atoms (localized or delocalized). The structures of the mixed-metal complexes of $[M^{II}M'^{III}_2O(C_2H_3O_2)_6(\text{pyridine})_3]$.solvent ($M^{II}M'^{III}_2$ = $CoMn_2$, $CoFe_2$, $NiRu_2$, $CoRu_2$) have been reported in the same space group (*R*32) (Cannon *et al.*, 1993; Jang *et al.*, 1990; Ohta, Sasaki & Ito, 1994). These mixed-metal molecules have imposed D_{3h} symmetry and different kinds of metal atoms are indistinguishable.

We reported recently the structure of a mixed-valence trinuclear iron acetate–aqua complex, $[Fe_3O(C_2H_3O_2)_6(H_2O)_3].2H_2O$ (Sato *et al.*, 1996). ^{57}Fe Mössbauer spectroscopic data of this compound indicate that thermally induced intramolecular electron transfer takes place between the Fe atoms. The structural data are consistent with the results of ^{57}Fe Mössbauer spectroscopy. The coordination geometries around the three Fe atoms show good equivalence. The bond distances between the central O atom and the Fe atoms are 1.867 (4) (for Fe1), 1.904 (4) (for Fe2) and 1.906 (4) Å (for Fe3) at 293 K. Here, the structure of the corresponding trinuclear cobalt–iron acetate–aqua complex, (I), is reported.



(I)

The structure of a $[CoFe_2O(CH_3CO_2)_6(H_2O)_3]$ molecule is shown in Fig. 1. This compound is isostructural with the trinuclear iron acetate–aqua complex. Although ^{57}Fe Mössbauer data indicate that the Fe atoms are in an Fe^{III} state at room temperature, the three metal sites are almost equivalent in terms of geometry. Bond distances and angles in the molecule are almost identical to those found in the trinuclear iron acetate–aqua complex. The three Fe(Co) atoms form a near equilateral triangle. The central O4 atom is in the Fe(Co) triangular plane