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Crystal structure of *catena*-[triaqua-bis(acetato-*O,O'*)gadolinium(III)] chloride, $[Gd(CH_3COO)_2(H_2O)_3]Cl$

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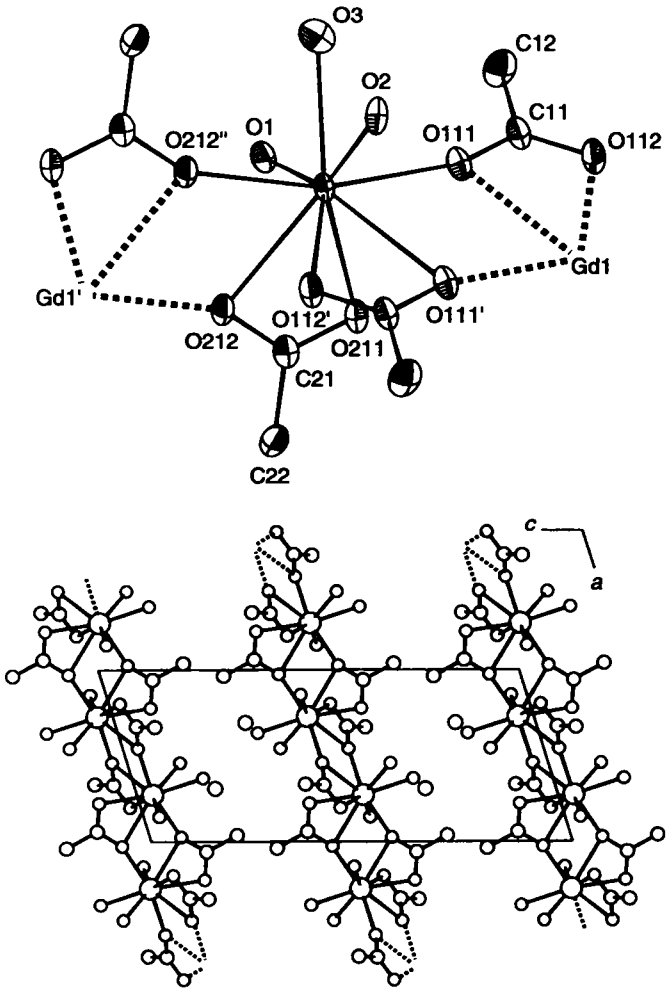

Abstract

$C_4H_{12}ClGdO_7$, monoclinic, $P12_1/c1$ (no. 14), $a = 7.8213(5)$ Å, $b = 7.8625(5)$ Å, $c = 18.100(1)$ Å, $\beta = 107.037(5)°$, $V = 1064.2$ Å^3, $Z = 4$, $R_{gt}(F) = 0.031$, $wR_{ref}(F^2) = 0.100$, $T = 150$ K.

Source of material

Colorless crystals of $[Gd(CH_3COO)_2(H_2O)_3]Cl$ crystallized unexpectedly from an ethanolic solution (80 ml) containing L-prolin (0.23 g, 2 mmol), $Mn(CH_3COO)_2 \cdot 4H_2O$ (0.49 g, 2 mmol) and $GdCl_3 \cdot 6H_2O$ (1.49 g, 4 mmol) by slow evaporation of the solvent in a beaker, sealed with a perforated foil.

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Experimental details

The methylene H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.96 Å and $U_{iso}(H) = 0.11$ Å^2. The remaining H atoms were located in a Fourier difference map and refined with O—H distances restrained to 0.82 Å.

Discussion

The *catena*-poly(triaqua-bis(acetato-*O,O'*)) chlorides of the formula $[M(CH_3COO)_2(H_2O)_3]Cl$ (M = Ce – Lu, Y) were structurally characterized by X-ray powder diffraction [1] after the crystal structure of the respective compound with M = Eu had been determined by single-crystal X-ray diffraction [2].

In $[Gd(CH_3COO)_2(H_2O)_3]Cl$, the central Gd^{III} ion is coordinated by three water molecules and by six oxygen atoms of four different acetate anions (figure, top). The acetate anions connect the central Gd^{III} ions in a tridentate-bridging manner to form one-dimensional cationic chains, $^1_\infty[Gd(CH_3COO)_2(H_2O)_3]^+$. These chains are running along the [100] direction (figure, bottom). The chloride anions, isolated between these cationic chains, complete for electroneutrality.

Table 1. Data collection and handling.

Crystal:	colorless column, size 0.05 × 0.05 × 0.40 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	64.87 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS II, ω/φ
$2\theta_{max}$:	58.72°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	15170, 2903
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2709
$N(param)_{refined}$:	143
Programs:	SIR92 [3], SHELXL-97 [4]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(12A)	4e	0.4429	0.4349	0.8936	0.11
H(12B)	4e	0.3262	0.5244	0.9394	0.11
H(12C)	4e	0.2338	0.4312	0.8614	0.11
H(22A)	4e	1.1614	0.0794	1.2154	0.11
H(22B)	4e	0.9856	0.0250	1.2340	0.11
H(22C)	4e	1.0270	0.2182	1.2264	0.11
H(1A)	4e	0.957(4)	0.300(8)	0.962(4)	0.02(2)
H(1B)	4e	0.816(9)	0.377(8)	0.923(2)	0.03(2)
H(2A)	4e	0.439(4)	–0.176(8)	0.873(4)	0.02(2)
H(2B)	4e	0.575(6)	–0.242(4)	0.855(3)	0.00(1)
H(3A)	4e	0.63(1)	0.252(4)	0.822(6)	0.07(3)
H(3B)	4e	0.557(9)	0.09(1)	0.801(4)	0.06(3)

Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Gd(1)	4*e*	0.72709(3)	0.03989(3)	0.96230(1)	0.0105(1)	0.0155(2)	0.0219(2)	0.00158(6)	0.0052(1)	0.00037(7)
O(111)	4*e*	0.4585(4)	0.1627(4)	0.9634(2)	0.014(1)	0.024(2)	0.029(2)	0.004(1)	0.006(1)	–0.001(1)
O(112)	4*e*	0.1973(4)	0.2342(5)	0.9738(2)	0.015(1)	0.022(2)	0.036(2)	0.001(1)	0.010(1)	0.006(1)
C(11)	4*e*	0.3295(6)	0.2675(6)	0.9506(3)	0.013(2)	0.018(2)	0.031(3)	0.001(2)	0.005(2)	0.003(2)
C(12)	4*e*	0.3335(8)	0.4290(7)	0.9074(4)	0.034(3)	0.022(2)	0.040(3)	0.000(2)	0.019(3)	0.008(2)
O(211)	4*e*	0.7777(4)	0.1291(5)	1.0971(2)	0.014(1)	0.023(2)	0.029(2)	–0.000(1)	0.009(1)	–0.000(1)
O(212)	4*e*	1.0267(5)	0.0612(4)	1.0739(2)	0.016(2)	0.021(2)	0.026(2)	0.003(1)	0.010(1)	0.002(1)
C(21)	4*e*	0.9409(6)	0.0991(6)	1.1224(3)	0.017(2)	0.014(2)	0.029(3)	–0.001(2)	0.008(2)	–0.001(2)
C(22)	4*e*	1.0374(7)	0.1061(8)	1.2072(3)	0.024(2)	0.038(3)	0.025(3)	–0.003(2)	0.012(2)	–0.001(2)
Cl(1)	4*e*	0.6925(2)	0.5300(1)	0.81032(8)	0.0252(6)	0.0194(5)	0.0273(6)	0.0023(4)	0.0077(5)	0.0014(4)
O(1)	4*e*	0.8556(4)	0.3211(4)	0.9627(2)	0.015(1)	0.019(2)	0.027(2)	0.003(1)	0.006(1)	0.001(1)
O(2)	4*e*	0.5429(4)	–0.1595(4)	0.8744(2)	0.016(1)	0.019(2)	0.034(2)	–0.002(1)	0.013(1)	–0.007(1)
O(3)	4*e*	0.6326(5)	0.1496(5)	0.8316(2)	0.028(2)	0.018(2)	0.031(2)	–0.005(1)	0.002(2)	0.001(1)

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