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Comprehensive structural study of lanthanide(III) chloride hydrates: [$RECl_3 \cdot xH_2O$ (RE = La–Nd, Sm–Lu; x = 6, 7)]

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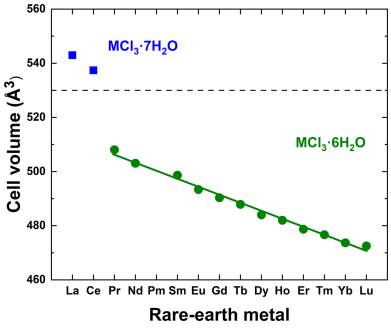
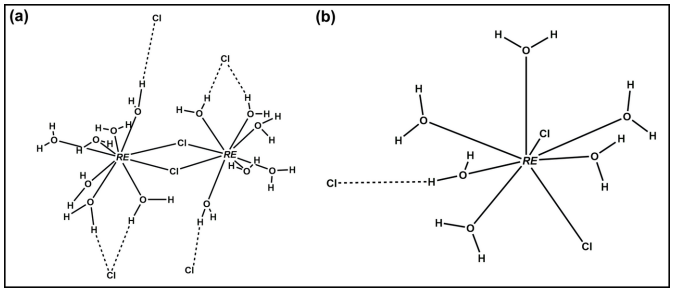
A comprehensive crystallographic study is presented of the complete series of rare-earth(III) chloride hydrates. Early lanthanides form dimeric $[(H_2O)_7RE(\mu\text{-}Cl)_2RE(H_2O)_7]^{4+}$ binuclear complexes in which each RE atom (RE = La^{3+}, Ce^{3+}) is coordinated by seven H_2O molecules and two bridging inner-sphere chloride ions. Di-μ-chlorido-bis[heptaaqualanthanide(III)] tetrachloride, $[(H_2O)_7RE(\mu\text{-}Cl)_2RE(H_2O)_7]Cl_4$, crystallizes in the triclinic space group $P\overline{1}$. Heavier lanthanides exhibit monomeric $[RECl_2(H_2O)_6]^+$ units where each RE atom (RE = Pr^{3+}, Nd^{3+}, Sm^{3+}–Lu^{3+}) is coordinated by six H_2O molecules and two inner-sphere chloride ions. Hexaaquadichloridolanthanide(III) chlorides, $[RECl_2(H_2O)_6]Cl$, adopt the monoclinic space group $P2/c$. In both structures, the cationic *inner-sphere* complex is counter-charged by the corresponding number of *outer-sphere* Cl^- anions, in which the metal ion and outer-sphere chloride ion lie on crystallographic twofold axes. Crystal structures for all compounds were determined in high quality with refined H-atom positions and were collected at the same temperature (100 K), providing a uniform structural dataset and addressing discrepancies in previous reports. The crystal structure of $[HoCl_2(H_2O)_6]Cl$ is reported for the first time.

1. Chemical context and database survey

The rare-earth trivalent metal chloride hydrates [$RECl_3 \cdot xH_2O$ (RE = La–Nd, Sm–Lu; x = 6, 7)] are commonly used as precursors in the synthesis of complex inorganic and organometallic compounds (Boyle & Steele, 2011). Most lanthanides are characterized by the presence of partially filled 4*f* orbitals, which significantly influence the chemical and physical properties of these elements and their compounds, offering a broad landscape for potential applications. For instance, lanthanide chloride salts possess catalytic (Narasimhulu *et al.*, 2007), luminescent (Hsieh *et al.*, 2013), scintillation (Boatner *et al.*, 2013), and magnetic properties (Layfield & Murugesu, 2015), to name a few. The compositional and structural aspects of the lanthanide (III) chloride hydrate chemistry are well established, with nearly the entire series of $RECl_3 \cdot xH_2O$ compositions identified (Boyle *et al.*, 2010; Cotton & Harrowfield, 2011). However, our database survey indicates that while most of the compounds presented in this work are listed in the ICSD database (Release 2024.1; Zagorac *et al.*, 2019), structural data for $HoCl_3 \cdot 6H_2O$ and $TmCl_3 \cdot 6H_2O$ are missing from the ICSD, and for $HoCl_3 \cdot 6H_2O$, from the CSD (Release 2024.2; Groom *et al.*, 2016) databases (Bakakin *et al.*, 1975; Bel'skii & Struchkov, 1965; Boyle *et al.*, 2010; Habenschuss & Spedding, 1979, 1980*a*,*b*,*c*,*d*, 1978; Hsieh *et al.*, 2013; Kepert *et al.*, 1983; Knopf *et al.*, 2015; Levason & Webster, 2002; Louer *et al.*, 1989; Marezio *et al.*, 1961; Narasimhulu *et al.*, 2007;



Peterson *et al.*, 1979; Reuter *et al.*, 1994; Reuter & Frenzen, 1994; Rheingold & King, 1989; Tambornino *et al.*, 2014; Wegner *et al.*, 2018; Chen *et al.*, 1991).



In addition, most of the reported datasets are of standard quality, lacking refined hydrogen atoms, which complicates the unambiguous interpretation of hydrogen bonding and the crystal packing. Another inconsistency involves data collection temperatures, which vary across the series in the previous reports. This study presents a comprehensive crystallographic analysis by providing a uniform structural dataset for the complete series of rare-earth metal(III) chloride hydrates except for radioactive promethium.

2. Structural commentary

The rare-earth metal(III) chloride hydrates [$RECl_3{\cdot}xH_2O$ (*RE* = La–Nd, Sm–Lu; x = 6, 7)] adopt two different structure types, with the rare-earth metal being coordinated by seven (for *RE* = La, Ce) or six (for *RE* = Pr, Nd, Sm–Lu) water molecules. The degree of hydration is likely influenced by steric effects and aligns well with the decreasing trend of the atomic radii within the lanthanide series (Fig. 5). Metal–ligand bond distances for the La and Ce phases are listed in Tables 1 and 2, respectively, and the metal–ligand distances for the hexahydrates are summarized in Table 3. The hydrogen-bond geometrical data for the complete series (La–Lu) are listed in Table 4 to 17.

Table 1
Selected bond lengths (Å) for La.

La1—Cl1	2.9187 (5)	La1—O4	2.5873 (13)
La1—O1	2.5443 (13)	La1—O5	2.5233 (14)
La1—O2	2.5504 (13)	La1—O6	2.5413 (15)
La1—O3	2.5315 (13)	La1—O7	2.5643 (13)

Table 2
Selected bond lengths (Å) for Ce.

Ce1—Cl1	2.8986 (2)	Ce1—O4	2.5580 (7)
Ce1—O1	2.5276 (7)	Ce1—O5	2.5018 (7)
Ce1—O2	2.5229 (7)	Ce1—O6	2.5214 (7)
Ce1—O3	2.5076 (8)	Ce1—O7	2.5397 (8)

The early rare-earth metal (*RE* = La–Pr) chloride hydrates adopt the [$LaCl_3(H_2O)_7$] structure type and crystallize in the triclinic space group $P\overline{1}$, although there are a few reports on $RECl_3(H_2O)_3$ trihydrates (*RE* = La, Ce) crystallizing in the hexagonal space group $P\overline{6}2m$ or the orthorhombic space group *Pnma* (Reuter *et al.*, 1994; Reuter & Frenzen, 1994). This structure type is characterized by the Wyckoff sequence i^{11} (excluding H atoms) and the Pearson Symbol *aP*50, with 11 atomic sites occupying general positions. The crystal structure of [$RECl_3(H_2O)_7$] (*RE* = La, Ce, Pr) is better described as a dimeric [$(H_2O)_7RE(\mu\text{-}Cl)_2RE(H_2O)_7]Cl_4$ molecule in which each *RE* atom is coordinated by seven water molecules and the two lanthanide ions are linked by the two *inner-sphere* bridging chloride (μ-Cl) anions (Fig. 1). This complex $[(H_2O)_7RE(\mu\text{-}Cl)_2RE(H_2O)_7]^{4+}$ *inner-sphere* cation is charge-balanced by four Cl^- anions located in the *outer-sphere*. While we identified the La- and Ce-bearing analogs, we did not find a Pr-containing compound within this structure type.

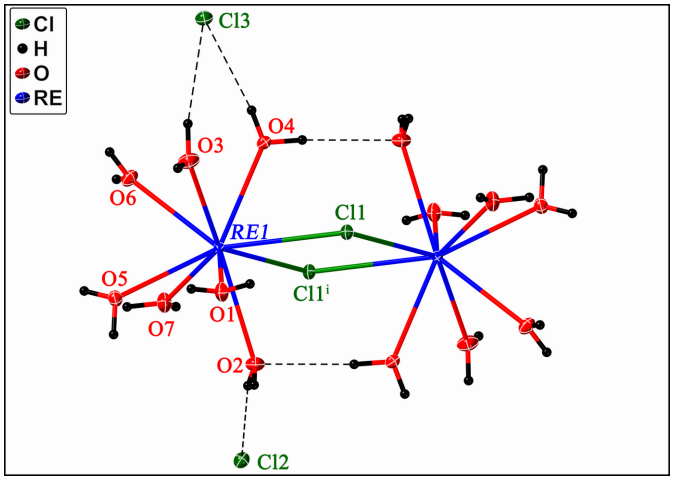


Figure 1
Molecular structure of the dimeric $[(H_2O)_7RE(\mu\text{-}Cl)_2RE(H_2O)_7]Cl_4$ compound (*RE* = La, Ce) with displacement ellipsoids drawn at 50% probability. Hydrogen bonds are shown as bold dashed lines. *RE*, Cl, O, and H atoms are represented in blue, green, red, and black, respectively. Symmetry code: (i) $-x, -y, 1-z$.

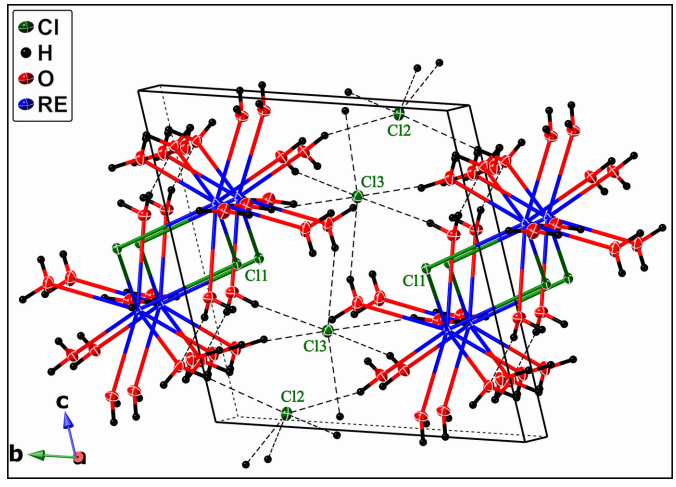


Figure 2
Schematic view of the packing diagram for the dimeric $[(H_2O)_7RE(\mu\text{-}Cl)_2RE(H_2O)_7]Cl_4$ compound (*RE* = La, Ce). Hydrogen bonds are shown as bold dashed lines, and the unit cell is outlined. *RE*, Cl, O, and H atoms are represented in blue, green, red, and black, respectively.

Table 3
Bond distances (Å) for hexahydrates.

RE	Cl1	O1	O2	O3
Pr	2.8314 (4)	2.4677 (13)	2.4818 (13)	2.4513 (12)
Nd	2.8145 (2)	2.4532 (7)	2.4629 (6)	2.4328 (7)
Sm	2.7906 (3)	2.4269 (8)	2.4349 (8)	2.4057 (8)
Eu	2.7788 (2)	2.4131 (7)	2.4206 (7)	2.3884 (7)
Gd	2.7699 (3)	2.4026 (9)	2.4101 (8)	2.3762 (8)
Tb	2.7617 (3)	2.3870 (9)	2.3940 (9)	2.3646 (9)
Dy	2.7500 (2)	2.3735 (8)	2.3795 (8)	2.3480 (8)
Ho	2.7425 (3)	2.3646 (10)	2.3705 (9)	2.3372 (9)
Er	2.7309 (3)	2.3538 (9)	2.3578 (9)	2.3239 (9)
Tm	2.7246 (2)	2.3414 (7)	2.3446 (8)	2.3142 (7)
Yb	2.7173 (3)	2.3293 (8)	2.3328 (8)	2.3003 (8)
Lu	2.7113 (4)	2.3246 (11)	2.3272 (12)	2.2917 (12)

Each unit cell consists of a single $[(H_2O)_7RE(\mu\text{-}Cl)_2\text{-}RE(H_2O)_7]Cl_4$ (*RE* = La, Ce) formula unit with $[(H_2O)_7RE(\mu\text{-}Cl)_2RE(H_2O)_7]^{4+}$ binuclear cations linked *via* O—H···Cl hydrogen bonds ranging in H···Cl length from *ca.* 2.25 Å to 2.51 Å. Two outer-sphere Cl atoms link neighboring cations *via* these hydrogen bonds (Fig. 2).

The heavier lanthanides (*RE* = Pr, Nd, Sm–Lu) crystallize in the monoclinic crystal system with the space group *P*2/*c* (note that most of the datasets were previously reported in the unconventional space group *P*2/*n*). They adopt the $GdCl_3{\cdot}6H_2O$ structure type, characterized by the Wyckoff sequence g^4fe (excluding H atoms) and Pearson Symbol *mP*44. Each $RECl_3{\cdot}6H_2O$ formula unit consists of an $[RECl_2(H_2O)_6]^+$ *inner-sphere* monomeric cation charge-balanced by a Cl^- anion located in the *outer-sphere* (Fig. 3). The RE^{3+} cation is coordinated by six water molecules and two chloride anions in distorted square antiprism fashion and is positioned on a crystallographic twofold axis.

Each unit cell of the $RECl_2(H_2O)_6Cl$ (*RE* = Pr, Nd, Sm–Lu) structure type contains two formula units, with $[RECl_2(H_2O)_6]^+$ cations linked *via* O—H···Cl and O—H···O

Table 4
Hydrogen-bond geometry (Å, °) for La.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···Cl3^{i}	0.75 (3)	2.48 (3)	3.1947 (15)	161 (3)
O1—H1*B*···Cl2	0.79 (3)	2.38 (3)	3.1365 (16)	161 (2)
O2—H2*A*···Cl2^{ii}	0.80 (3)	2.38 (3)	3.1378 (14)	157 (3)
O2—H2*B*···Cl2^{iii}	0.79 (3)	2.26 (3)	3.0382 (13)	172 (3)
O3—H3*A*···Cl3	0.82 (3)	2.47 (3)	3.2552 (15)	160 (3)
O3—H3*B*···Cl1^{i}	0.78 (3)	2.92 (3)	3.2954 (13)	112 (2)
O3—H3*B*···Cl2	0.78 (3)	2.72 (3)	3.4160 (16)	150 (3)
O4—H4*A*···O2^{iv}	0.78 (3)	2.08 (3)	2.859 (2)	174 (3)
O4—H4*B*···Cl3	0.84 (3)	2.31 (3)	3.1488 (15)	179 (2)
O5—H5*A*···Cl3^{v}	0.80 (3)	2.34 (3)	3.1308 (14)	167 (3)
O5—H5*B*···Cl2^{vi}	0.75 (3)	2.44 (3)	3.1690 (15)	163 (3)
O5—H5*B*···O5^{vi}	0.75 (3)	2.67 (3)	2.986 (3)	108 (2)
O6—H6*A*···Cl3^{vii}	0.77 (3)	2.57 (3)	3.3288 (16)	168 (3)
O6—H6*B*···Cl1^{viii}	0.80 (3)	2.93 (3)	3.3705 (14)	117 (2)
O6—H6*B*···O4^{ix}	0.80 (3)	2.24 (3)	3.038 (2)	169 (3)

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x, -y+1, -z$; (iii) $x, y-1, z$; (iv) $-x, -y, -z+1$; (v) $x, y, z-1$; (vi) $-x+1, -y+1, -z$; (vii) $-x+1, -y+1, -z+1$; (viii) $x+1, y, z$; (ix) $-x+1, -y, -z+1$.

Table 5
Hydrogen-bond geometry (Å, °) for Ce.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···Cl3^{i}	0.762 (19)	2.458 (19)	3.1945 (8)	162.9 (18)
O1—H1*B*···Cl2	0.77 (2)	2.405 (19)	3.1380 (8)	160.6 (17)
O2—H2*A*···Cl2^{ii}	0.797 (19)	2.251 (19)	3.0368 (8)	168.6 (17)
O2—H2*B*···Cl2^{iii}	0.783 (19)	2.411 (19)	3.1383 (8)	155.0 (16)
O3—H3*A*···Cl3	0.79 (2)	2.50 (2)	3.2501 (9)	160.9 (18)
O3—H3*B*···Cl1^{i}	0.80 (2)	2.91 (2)	3.3040 (8)	112.9 (16)
O3—H3*B*···Cl2	0.80 (2)	2.71 (2)	3.4188 (9)	147.3 (18)
O4—H4*A*···O2^{iv}	0.800 (17)	2.068 (17)	2.8609 (11)	171.2 (16)
O4—H4*B*···Cl3	0.781 (18)	2.369 (18)	3.1466 (8)	173.7 (16)
O5—H5*A*···Cl3^{v}	0.798 (17)	2.354 (17)	3.1286 (8)	164.0 (16)
O5—H5*B*···Cl2^{vi}	0.768 (19)	2.446 (19)	3.1699 (8)	157.6 (17)
O5—H5*B*···O5^{vi}	0.768 (19)	2.601 (17)	2.9858 (15)	112.9 (15)
O6—H6*A*···Cl1^{vii}	0.82 (2)	2.936 (18)	3.3662 (8)	115.2 (14)
O6—H6*A*···O4^{viii}	0.82 (2)	2.25 (2)	3.0451 (11)	164.9 (17)
O6—H6*B*···Cl3^{ix}	0.79 (2)	2.55 (2)	3.3165 (8)	164.4 (18)

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $x, y-1, z$; (iii) $-x, -y+1, -z$; (iv) $-x, -y, -z+1$; (v) $x, y, z-1$; (vi) $-x+1, -y+1, -z$; (vii) $x+1, y, z$; (viii) $-x+1, -y, -z+1$; (ix) $-x+1, -y+1, -z+1$.

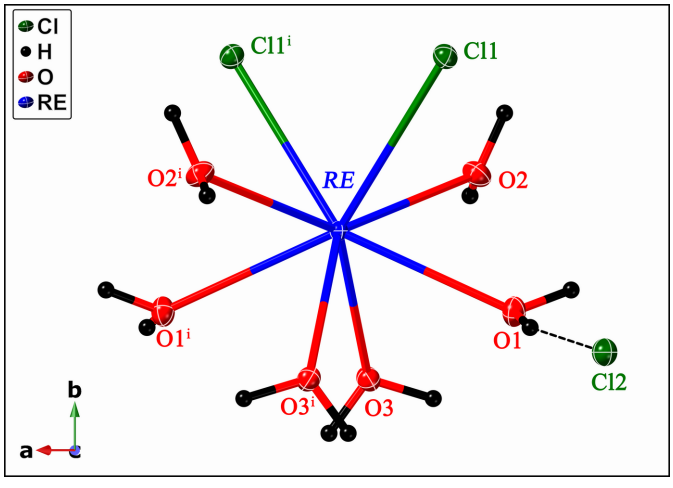


Figure 3
Molecular structure of the $RECl_2(H_2O)_6Cl$ compound (*RE* = Pr, Nd, Sm–Lu) with displacement ellipsoids drawn at 50% probability. Hydrogen bonds are shown as bold dashed lines. *RE*, Cl, O, and H atoms are represented in blue, green, red, and black, respectively. Symmetry code: (i) $1-x, y, 1/2-z$.

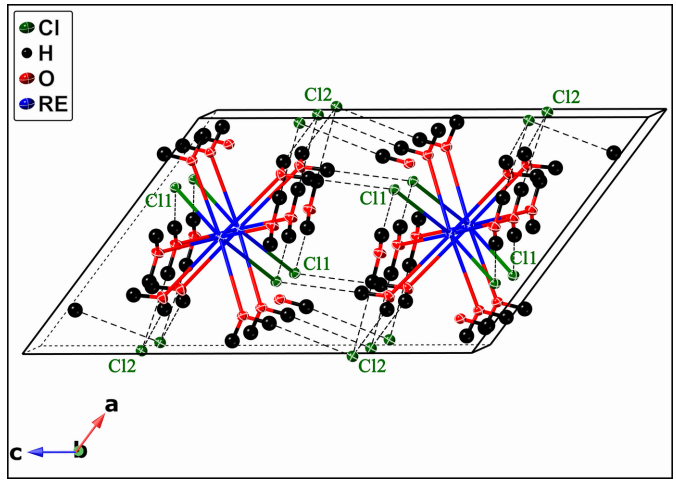


Figure 4
Schematic view of the packing diagram for the $RECl_2(H_2O)_6Cl$ compound (*RE* = Pr, Nd, Sm–Lu). Hydrogen bonds are shown as bold dashed lines, and the unit cell is outlined. *RE*, Cl, O, and H atoms are represented in blue, green, red, and black, respectively.

Table 6
Hydrogen-bond geometry (Å, °) for Pr.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···Cl1^{i}	0.75 (3)	2.42 (3)	3.1498 (14)	166 (3)
O1—H1B···Cl2^{ii}	0.78 (3)	2.40 (3)	3.1706 (13)	172 (2)
O2—H2A···Cl1^{iii}	0.76 (3)	2.40 (3)	3.1575 (13)	175 (2)
O2—H2B···Cl2^{iv}	0.77 (2)	2.49 (2)	3.2291 (14)	163 (2)
O3—H3A···Cl1^{v}	0.78 (3)	2.36 (3)	3.1303 (14)	174 (2)
O3—H3B···Cl2	0.80 (3)	2.41 (3)	3.1919 (14)	166 (2)

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

Table 7
Hydrogen-bond geometry (Å, °) for Nd.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···Cl1^{i}	0.749 (16)	2.418 (16)	3.1491 (7)	165.6 (16)
O1—H1B···Cl2^{ii}	0.722 (17)	2.451 (18)	3.1661 (8)	170.8 (15)
O2—H2A···Cl1^{iii}	0.770 (18)	2.387 (18)	3.1552 (8)	175.3 (17)
O2—H2B···Cl2^{iv}	0.760 (17)	2.490 (17)	3.2267 (8)	164.0 (15)
O3—H3A···Cl1^{v}	0.793 (16)	2.337 (17)	3.1290 (7)	176.1 (15)
O3—H3B···Cl2	0.782 (16)	2.413 (16)	3.1894 (7)	172.0 (15)

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

Table 8
Hydrogen-bond geometry (Å, °) for Sm.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···Cl1^{i}	0.693 (19)	2.484 (19)	3.1594 (10)	165 (2)
O1—H1B···Cl2^{ii}	0.79 (3)	2.39 (3)	3.1685 (9)	169.2 (19)
O2—H2A···Cl1^{iii}	0.81 (2)	2.35 (2)	3.1586 (9)	175.9 (18)
O2—H2B···Cl2^{iv}	0.78 (2)	2.48 (2)	3.2358 (10)	163.6 (17)
O3—H3A···Cl1^{v}	0.78 (2)	2.36 (2)	3.1367 (10)	176 (2)
O3—H3B···Cl2	0.794 (19)	2.41 (2)	3.1908 (9)	167.7 (18)

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

Table 9
Hydrogen-bond geometry (Å, °) for Eu.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···Cl1^{i}	0.760 (15)	2.407 (15)	3.1537 (7)	167.5 (16)
O1—H1B···Cl2^{ii}	0.766 (19)	2.407 (19)	3.1649 (8)	170.6 (14)
O2—H2A···Cl1^{iii}	0.784 (16)	2.373 (17)	3.1549 (8)	175.1 (14)
O2—H2B···Cl2^{iv}	0.759 (16)	2.500 (15)	3.2308 (7)	162.1 (14)
O3—H3A···Cl1^{v}	0.783 (16)	2.349 (16)	3.1307 (7)	175.7 (14)
O3—H3B···Cl2	0.737 (15)	2.455 (15)	3.1842 (7)	170.3 (15)

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

Table 10
Hydrogen-bond geometry (Å, °) for Gd.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···Cl1^{i}	0.79 (2)	2.39 (2)	3.1527 (9)	165 (2)
O1—H1B···Cl2^{ii}	0.75 (2)	2.43 (2)	3.1651 (9)	170.1 (19)
O2—H2A···Cl1^{iii}	0.80 (2)	2.36 (2)	3.1519 (9)	175 (2)
O2—H2B···Cl2^{iv}	0.82 (2)	2.44 (2)	3.2284 (9)	161.7 (18)
O3—H3A···Cl1^{v}	0.83 (2)	2.30 (2)	3.1290 (9)	178 (2)
O3—H3B···Cl2	0.79 (2)	2.40 (2)	3.1790 (9)	169.1 (19)

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

hydrogen bonds (Fig. 4). Each outer-sphere chloride ion accepts six O—H···Cl contacts (*ca*. 2.36–2.48 Å for the Ho-bearing structure), thus linking six neighboring cations. The inner sphere Cl atom forms three hydrogen O—H···Cl bonds

Table 11
Hydrogen-bond geometry (Å, °) for Tb.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···Cl1^{i}	0.77 (2)	2.41 (2)	3.1527 (9)	164 (2)
O1—H1B···Cl2^{ii}	0.77 (2)	2.40 (2)	3.1661 (10)	172 (2)
O2—H2A···Cl1^{iii}	0.82 (2)	2.33 (2)	3.1524 (10)	175 (2)
O2—H2B···Cl2^{iv}	0.76 (2)	2.51 (2)	3.2283 (10)	158.8 (19)
O3—H3A···Cl1^{v}	0.81 (2)	2.33 (2)	3.1297 (10)	173.2 (19)
O3—H3B···Cl2	0.77 (2)	2.43 (2)	3.1798 (9)	166 (2)

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

Table 12
Hydrogen-bond geometry (Å, °) for Dy.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···Cl1^{i}	0.755 (19)	2.413 (19)	3.1545 (9)	167.6 (19)
O1—H1B···Cl2^{ii}	0.78 (2)	2.39 (2)	3.1655 (8)	172.6 (16)
O2—H2A···Cl1^{iii}	0.79 (2)	2.37 (2)	3.1511 (9)	175.7 (19)
O2—H2B···Cl2^{iv}	0.712 (19)	2.544 (19)	3.2303 (8)	162.7 (19)
O3—H3A···Cl1^{v}	0.787 (19)	2.342 (19)	3.1276 (8)	176.2 (18)
O3—H3B···Cl2	0.75 (2)	2.44 (2)	3.1766 (8)	167.1 (19)

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

Table 13
Hydrogen-bond geometry (Å, °) for Ho.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···Cl1^{i}	0.78 (2)	2.40 (2)	3.1589 (11)	166 (2)
O1—H1B···Cl2^{ii}	0.76 (2)	2.41 (2)	3.1678 (10)	170 (2)
O2—H2A···Cl1^{iii}	0.79 (2)	2.37 (2)	3.1546 (10)	172 (2)
O2—H2B···Cl2^{iv}	0.79 (2)	2.48 (2)	3.2320 (10)	161.6 (19)
O3—H3A···Cl1^{v}	0.79 (2)	2.35 (2)	3.1309 (10)	172 (2)
O3—H3B···Cl2	0.82 (2)	2.36 (2)	3.1765 (10)	168.9 (19)

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

Table 14
Hydrogen-bond geometry (Å, °) for Er.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···Cl1^{i}	0.78 (2)	2.39 (2)	3.1557 (10)	166 (2)
O1—H1B···Cl2^{ii}	0.76 (3)	2.41 (3)	3.1632 (10)	170 (2)
O2—H2A···Cl1^{iii}	0.76 (2)	2.39 (2)	3.1502 (10)	176 (2)
O2—H2B···Cl2^{iv}	0.79 (2)	2.47 (2)	3.2287 (10)	161 (2)
O3—H3A···Cl1^{v}	0.77 (2)	2.36 (2)	3.1286 (10)	172 (2)
O3—H3B···Cl2	0.78 (2)	2.41 (2)	3.1689 (9)	167 (2)

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

Table 15
Hydrogen-bond geometry (Å, °) for Tm.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···Cl1^{i}	0.73 (2)	2.44 (2)	3.1573 (8)	165 (2)
O1—H1B···Cl2^{ii}	0.81 (2)	2.36 (2)	3.1602 (8)	169.7 (16)
O2—H2A···Cl1^{iii}	0.78 (2)	2.38 (2)	3.1485 (8)	173.4 (19)
O2—H2B···Cl2^{iv}	0.737 (18)	2.528 (18)	3.2301 (8)	159.7 (18)
O3—H3A···Cl1^{v}	0.789 (19)	2.343 (19)	3.1280 (8)	173.4 (18)
O3—H3B···Cl2	0.75 (2)	2.43 (2)	3.1714 (8)	169.4 (17)

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

(*ca*. 2.35–2.40 Å for the Ho-bearing structure), thus linking four $[RECl_2(H_2O)_6]^+$ cations.

An analysis of unit-cell volumes across the La–Lu series indicates a gradual decrease (Fig. 5), which is expected due to the decreasing trend for atomic radii of the lanthanides. This

Table 16
Hydrogen-bond geometry (Å, °) for Yb.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···Cl1^{i}	0.74 (2)	2.43 (2)	3.1570 (9)	168 (2)
O1—H1B···Cl2^{ii}	0.74 (2)	2.44 (2)	3.1623 (9)	167 (2)
O2—H2A···Cl1^{iii}	0.72 (2)	2.44 (2)	3.1486 (9)	175 (2)
O2—H2B···Cl2^{iv}	0.795 (19)	2.472 (19)	3.2287 (9)	159.5 (16)
O3—H3A···Cl1^{v}	0.720 (19)	2.409 (19)	3.1273 (9)	175.4 (19)
O3—H3B···Cl2	0.84 (2)	2.33 (2)	3.1643 (8)	168.8 (17)

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

Table 17
Hydrogen-bond geometry (Å, °) for Lu.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···Cl1^{i}	0.77 (3)	2.42 (3)	3.1591 (13)	163 (3)
O1—H1B···Cl2^{ii}	0.76 (3)	2.40 (3)	3.1625 (12)	171 (2)
O2—H2A···Cl1^{iii}	0.73 (3)	2.42 (3)	3.1517 (13)	175 (3)
O2—H2B···Cl2^{iv}	0.82 (3)	2.45 (3)	3.2327 (13)	160 (3)
O3—H3A···Cl1^{v}	0.79 (3)	2.34 (3)	3.1290 (13)	174 (3)
O3—H3B···Cl2	0.77 (3)	2.41 (3)	3.1653 (12)	167 (3)

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

reduction in atomic size for heavier *RE* leads to smaller unit cell volumes in their crystal structures. The notably larger unit-cell volumes of the La- and Ce-bearing compounds are explained by the higher number of coordinated water molecules and different structural arrangements. The variations of other parameters are shown in Fig. 6.

3. Synthesis and crystallization

Single-crystal X-ray diffraction (SCXRD) data collections were performed using commercially available chemicals supplied by Edgetech Industries LLC without further purification. However, large single crystals suitable for property measurements can also be obtained by recrystallization, as reported elsewhere (Chen *et al.*, 1991, Peterson *et al.*, 1979).

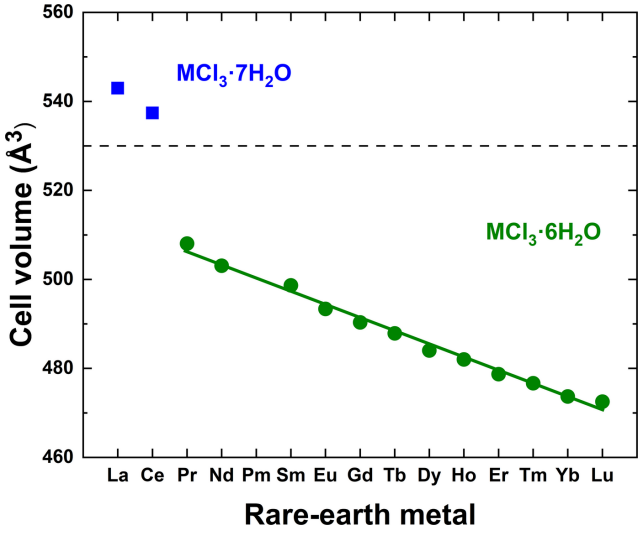


Figure 5
Variation of unit-cell volumes for $RECl_3{\cdot}xH_2O$ (*RE* = La–Nd, Sm–Lu; x = 6, 7) as determined from single-crystal X-ray diffraction experiments.

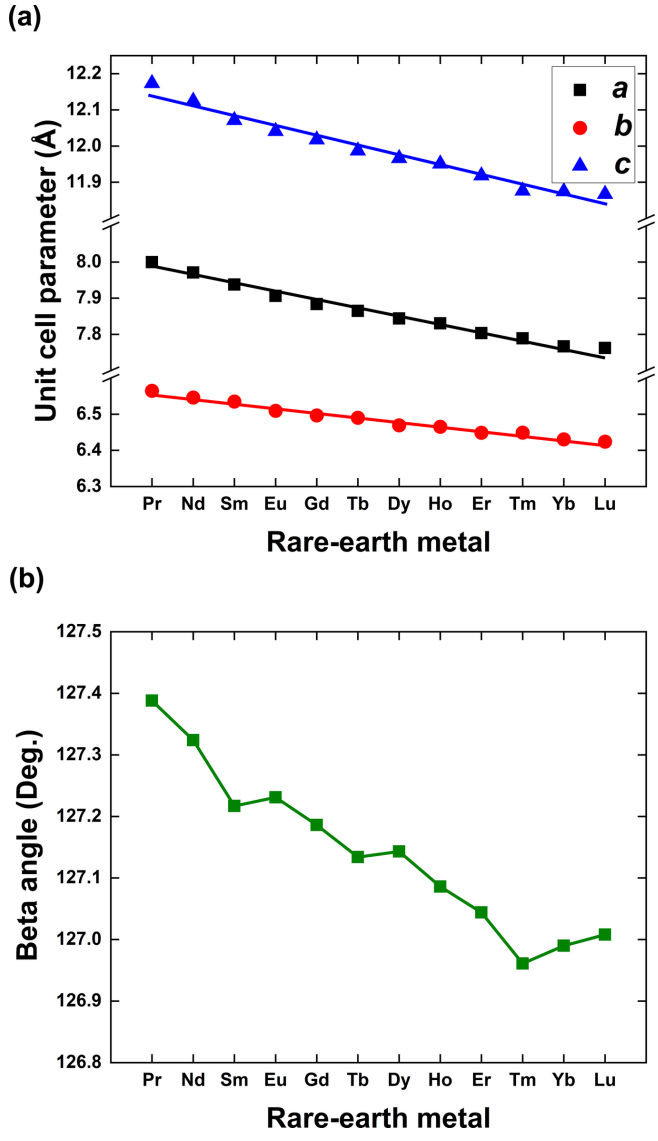


Figure 6
Variation of unit-cell parameters for $RECl_3{\cdot}6H_2O$ as determined from single-crystal X-ray diffraction experiments.

4. Refinement and Methodology

Crystal data are summarized in Table 18. SCXRD data were collected under a constant stream of cold nitrogen gas to protect the crystals from air and moisture and to control the measurement temperature. After the structures were solved, the *STRUCTURE TIDY* (Gelato & Parthé, 1987) program was used to standardize the atomic coordinates, and the unit cell was transformed to the conventional monoclinic space group $P2/c$ for the $RECl_2(H_2O)_6Cl$ series.

Acknowledgements

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Table 18
Experimental details.

For all structures: $Z = 2$. Experiments were carried out at 100 K with Ag $K\alpha$ radiation, $\lambda = 0.56086$ Å using a Bruker D8 Venture Duo. Absorption was corrected for by multi-scan methods (*SADABS*; Krause *et al.*, 2016). All H-atom parameters were refined.

	$[LaCl(H_2O)_7]Cl_2$	$[CeCl(H_2O)_7]Cl_2$	$[PrCl_2(H_2O)_6]Cl$
Crystal data			
M_r	371.37	372.58	355.36
Crystal system, space group	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$	Monoclinic, $P2/c$
a, b, c (Å)	7.9432 (5), 8.2316 (4), 9.2203 (5)	7.8995 (3), 8.2129 (3), 9.1961 (3)	7.9997 (3), 6.5647 (2), 12.1734 (4)
α, β, γ (°)	70.507 (2), 73.098 (2), 81.522 (2)	70.451 (1), 73.172 (1), 81.658 (1)	90, 127.388 (1), 90
V (Å^3)	542.92 (5)	537.39 (3)	507.95 (3)
μ (mm^{-1})	2.42	2.60	2.90
Crystal size (mm)	0.28 × 0.12 × 0.06	0.26 × 0.22 × 0.17	0.06 × 0.06 × 0.05
Data collection			
T_{min}, T_{max}	0.044, 0.064	0.214, 0.257	0.218, 0.257
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	43724, 3350, 3078	28063, 3304, 3239	15235, 1567, 1486
R_{int}	0.069	0.031	0.058
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.717	0.718	0.716
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.016, 0.032, 1.01	0.009, 0.019, 1.17	0.014, 0.027, 1.05
No. of reflections	3350	3304	1567
No. of parameters	157	157	71
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.40, −0.44	0.32, −0.30	0.38, −0.39

	$[NdCl_2(H_2O)_6]Cl$	$[SmCl_2(H_2O)_6]Cl$	$[EuCl_2(H_2O)_6]Cl$
Crystal data			
M_r	358.69	364.80	366.41
Crystal system, space group	Monoclinic, $P2/c$	Monoclinic, $P2/c$	Monoclinic, $P2/c$
a, b, c (Å)	7.9710 (3), 6.5460 (2), 12.1246 (5)	7.9375 (8), 6.5351 (7), 12.0713 (11)	7.9062 (2), 6.5092 (2), 12.0410 (4)
α, β, γ (°)	90, 127.324 (1), 90	90, 127.217 (2), 90	90, 127.231 (1), 90
V (Å^3)	503.09 (3)	498.65 (9)	493.38 (3)
μ (mm^{-1})	3.11	3.51	3.75
Crystal size (mm)	0.16 × 0.12 × 0.11	0.25 × 0.21 × 0.18	0.13 × 0.13 × 0.11
Data collection			
T_{min}, T_{max}	0.201, 0.257	0.204, 0.257	0.218, 0.257
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23233, 1559, 1536	27415, 1553, 1533	21905, 1529, 1504
R_{int}	0.036	0.046	0.038
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.716	0.717	0.716
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.007, 0.017, 1.11	0.010, 0.023, 1.19	0.007, 0.016, 1.13
No. of reflections	1559	1553	1529
No. of parameters	72	72	72
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.30	0.48, −0.85	0.29, −0.32

	$[GdCl_2(H_2O)_6]Cl$	$[TbCl_2(H_2O)_6]Cl$	$[DyCl_2(H_2O)_6]Cl$
Crystal data			
M_r	371.70	373.37	376.95
Crystal system, space group	Monoclinic, $P2/c$	Monoclinic, $P2/c$	Monoclinic, $P2/c$
a, b, c (Å)	7.8835 (3), 6.4964 (3), 12.0176 (4)	7.8646 (3), 6.4903 (3), 11.9871 (5)	7.8439 (3), 6.4693 (3), 11.9660 (5)
α, β, γ (°)	90, 127.186 (1), 90	90, 127.134 (1), 90	90, 127.143 (1), 90
V (Å^3)	490.33 (3)	487.79 (4)	484.02 (4)
μ (mm^{-1})	3.99	4.24	4.51
Crystal size (mm)	0.33 × 0.25 × 0.20	0.3 × 0.16 × 0.12	0.23 × 0.19 × 0.14
Data collection			
T_{min}, T_{max}	0.172, 0.257	0.223, 0.257	0.184, 0.257
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26021, 1532, 1520	11117, 1503, 1481	21844, 1501, 1485
R_{int}	0.037	0.024	0.037
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.718	0.716	0.718
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.009, 0.021, 1.23	0.009, 0.020, 1.10	0.008, 0.018, 1.19
No. of reflections	1532	1503	1501
No. of parameters	72	72	72
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.44, −0.38	0.36, −0.37	0.42, −0.48

	$[HoCl_2(H_2O)_6]Cl$	$[ErCl_2(H_2O)_6]Cl$	$[TmCl_2(H_2O)_6]Cl$
Crystal data			
M_r	379.38	381.71	383.38
Crystal system, space group	Monoclinic, *P*2/*c*	Monoclinic, *P*2/*c*	Monoclinic, *P*2/*c*
a, *b*, *c* (Å)	7.8303 (3), 6.4651 (2), 11.9509 (4)	7.8035 (2), 6.4488 (2), 11.9182 (4)	7.7889 (4), 6.4490 (3), 11.8760 (6)
α, β, γ (°)	90, 127.086 (1), 90	90, 127.044 (1), 90	90, 126.961 (1), 90
V (Å^3)	482.63 (3)	478.71 (3)	476.66 (4)
μ (mm^{-1})	4.77	5.07	5.37
Crystal size (mm)	0.14 × 0.10 × 0.07	0.23 × 0.22 × 0.17	0.17 × 0.11 × 0.10
Data collection			
T_{min}, T_{max}	0.222, 0.257	0.175, 0.257	0.207, 0.257
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10309, 1480, 1454	24599, 1481, 1479	16364, 1481, 1464
R_{int}	0.026	0.034	0.033
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.715	0.717	0.717
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.009, 0.020, 1.07	0.009, 0.020, 1.30	0.007, 0.016, 1.15
No. of reflections	1480	1481	1481
No. of parameters	72	72	72
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.31, −0.36	0.47, −0.88	0.39, −0.48

	$[YbCl_2(H_2O)_6]Cl$	$[LuCl_2(H_2O)_6]Cl$
Crystal data		
M_r	387.49	389.42
Crystal system, space group	Monoclinic, *P*2/*c*	Monoclinic, *P*2/*c*
a, *b*, *c* (Å)	7.7666 (2), 6.4305 (2), 11.8745 (3)	7.7621 (3), 6.4241 (3), 11.8671 (5)
α, β, γ (°)	90, 126.991 (1), 90	90, 127.008 (1), 90
V (Å^3)	473.69 (2)	472.54 (4)
μ (mm^{-1})	5.69	6.00
Crystal size (mm)	0.30 × 0.23 × 0.20	0.17 × 0.14 × 0.14
Data collection		
T_{min}, T_{max}	0.168, 0.257	0.201, 0.257
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19224, 1464, 1439	23799, 1464, 1436
R_{int}	0.035	0.041
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.717	0.718
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.008, 0.017, 1.19	0.009, 0.020, 1.28
No. of reflections	1464	1464
No. of parameters	72	72
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.62, −0.74	0.78, −0.82

Computer programs: *SAINT* (Bruker, 2016), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/1* (Sheldrick, 2015*b*), *CrystalMaker* (Palmer, 2014) and *publCIF* (Westrip, 2010).

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supporting information

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Comprehensive structural study of lanthanide(III) chloride hydrates: [*RE*Cl$_3$·*x*H$_2$O (*RE* = La–Nd, Sm–Lu; *x* = 6, 7)]

Thimira Kandabadage, Beau Legnon and Sviatoslav Baranets

Computing details

Di-μ-chlorido-bis[heptaaqualanthanum(III)] tetrachloride (La)

Crystal data

$[LaCl(H_2O)_7]Cl_2$
M_r = 371.37
Triclinic, $P\overline{1}$
a = 7.9432 (5) Å
b = 8.2316 (4) Å
c = 9.2203 (5) Å
α = 70.507 (2)°
β = 73.098 (2)°
γ = 81.522 (2)°
V = 542.92 (5) Å^3
Z = 2
$F(000)$ = 356
D_x = 2.272 Mg m^{-3}
Ag $K\alpha$ radiation, λ = 0.56086 Å
Cell parameters from 9869 reflections
θ = 2.4–23.7°
μ = 2.42 mm^{-1}
T = 100 K
Plate, colorless
0.28 × 0.12 × 0.06 mm

Data collection

Bruker D8 Venture Duo diffractometer
ω scans
Absorption correction: multi-scan SADABS-2016/2 (Bruker, 2016)
T_{min} = 0.044, T_{max} = 0.064
43724 measured reflections
3350 independent reflections
3078 reflections with $I > 2\sigma(I)$
R_{int} = 0.069
θ_{max} = 23.7°, θ_{min} = 2.1°
h = −11→11
k = −11→11
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.032
S = 1.01
3350 reflections
157 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0128P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}
Extinction correction: SHELXL-2018/1 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0070 (6)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
La1	0.21799 (2)	0.18615 (2)	0.32361 (2)	0.00928 (4)
Cl1	−0.14698 (6)	0.17974 (5)	0.51434 (5)	0.01189 (8)
Cl2	0.21093 (6)	0.77753 (5)	0.03491 (5)	0.01465 (8)
Cl3	0.34270 (6)	0.38778 (5)	0.71161 (5)	0.01506 (9)
O1	0.0304 (2)	0.42402 (17)	0.17472 (17)	0.0149 (3)
O2	0.07092 (19)	0.08113 (17)	0.16194 (16)	0.0148 (3)
O3	0.2234 (2)	0.46276 (18)	0.38494 (18)	0.0188 (3)
O4	0.2311 (2)	0.09299 (18)	0.61748 (16)	0.0153 (3)
O5	0.3868 (2)	0.35162 (17)	0.04773 (16)	0.0145 (3)
O6	0.5212 (2)	0.2280 (2)	0.34138 (17)	0.0173 (3)
O7	0.4532 (2)	−0.01065 (18)	0.19716 (17)	0.0164 (3)
H1A	−0.060 (4)	0.447 (3)	0.219 (3)	0.030 (7)*
H1B	0.077 (4)	0.509 (3)	0.119 (3)	0.028 (7)*
H2A	0.015 (4)	0.143 (3)	0.103 (3)	0.033 (7)*
H2B	0.116 (4)	0.003 (4)	0.131 (3)	0.035 (7)*
H3A	0.259 (4)	0.470 (4)	0.458 (3)	0.042 (8)*
H3B	0.199 (4)	0.553 (4)	0.330 (4)	0.051 (9)*
H4A	0.144 (4)	0.052 (3)	0.677 (3)	0.027 (7)*
H4B	0.261 (4)	0.171 (3)	0.644 (3)	0.030 (7)*
H5A	0.360 (4)	0.367 (4)	−0.033 (3)	0.038 (8)*
H5B	0.485 (4)	0.339 (4)	0.031 (4)	0.046 (9)*
H6A	0.549 (5)	0.312 (4)	0.344 (4)	0.059 (11)*
H6B	0.596 (4)	0.151 (4)	0.352 (3)	0.048 (9)*
H7A	0.535 (4)	0.031 (4)	0.131 (3)	0.036 (8)*
H7B	0.464 (5)	−0.115 (4)	0.228 (4)	0.057 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.00924 (5)	0.00899 (5)	0.00984 (5)	−0.00066 (3)	−0.00284 (3)	−0.00281 (3)
Cl1	0.0113 (2)	0.01008 (16)	0.01293 (17)	−0.00054 (14)	−0.00208 (15)	−0.00269 (14)
Cl2	0.0132 (2)	0.01316 (18)	0.01800 (19)	−0.00013 (15)	−0.00398 (16)	−0.00561 (15)
Cl3	0.0163 (2)	0.01438 (18)	0.01599 (19)	0.00004 (16)	−0.00586 (17)	−0.00548 (15)
O1	0.0113 (7)	0.0128 (6)	0.0165 (6)	−0.0003 (5)	−0.0020 (5)	−0.0007 (5)
O2	0.0168 (7)	0.0134 (6)	0.0173 (6)	0.0035 (5)	−0.0082 (6)	−0.0072 (5)
O3	0.0242 (8)	0.0134 (6)	0.0228 (7)	0.0012 (6)	−0.0101 (6)	−0.0083 (6)
O4	0.0155 (7)	0.0178 (6)	0.0135 (6)	−0.0060 (5)	−0.0035 (6)	−0.0041 (5)
O5	0.0128 (7)	0.0175 (6)	0.0122 (6)	−0.0009 (5)	−0.0036 (5)	−0.0028 (5)
O6	0.0130 (7)	0.0187 (7)	0.0231 (7)	−0.0009 (6)	−0.0062 (6)	−0.0086 (6)

O7	0.0157 (8)	0.0126 (6)	0.0187 (7)	−0.0007 (5)	−0.0016 (6)	−0.0044 (5)

Geometric parameters (Å, º)

La1—Cl1^{i}	2.9376 (4)	O2—H2B	0.79 (3)
La1—Cl1	2.9187 (5)	O3—H3A	0.82 (3)
La1—O1	2.5443 (13)	O3—H3B	0.78 (3)
La1—O2	2.5504 (13)	O4—H4A	0.78 (3)
La1—O3	2.5315 (13)	O4—H4B	0.84 (3)
La1—O4	2.5873 (13)	O5—H5A	0.80 (3)
La1—O5	2.5233 (14)	O5—H5B	0.75 (3)
La1—O6	2.5413 (15)	O6—H6A	0.77 (3)
La1—O7	2.5643 (13)	O6—H6B	0.80 (3)
O1—H1A	0.75 (3)	O7—H7A	0.78 (3)
O1—H1B	0.79 (3)	O7—H7B	0.81 (3)
O2—H2A	0.80 (3)		
Cl1—La1—Cl1^{i}	73.941 (12)	O6—La1—O1	123.86 (5)
O1—La1—Cl1^{i}	128.72 (4)	O6—La1—O2	141.04 (4)
O1—La1—Cl1	69.96 (4)	O6—La1—O4	69.20 (5)
O1—La1—O2	67.52 (4)	O6—La1—O7	69.14 (5)
O1—La1—O4	130.45 (4)	O7—La1—Cl1^{i}	68.54 (4)
O1—La1—O7	124.76 (4)	O7—La1—Cl1	139.55 (4)
O2—La1—Cl1	79.41 (3)	O7—La1—O4	104.74 (4)
O2—La1—Cl1^{i}	71.07 (3)	La1—Cl1—La1^{i}	106.059 (12)
O2—La1—O4	135.97 (5)	La1—O1—H1A	119 (2)
O2—La1—O7	74.71 (4)	La1—O1—H1B	117 (2)
O3—La1—Cl1^{i}	140.68 (4)	H1A—O1—H1B	109 (3)
O3—La1—Cl1	84.97 (4)	La1—O2—H2A	124.0 (19)
O3—La1—O1	70.08 (5)	La1—O2—H2B	119 (2)
O3—La1—O2	137.58 (4)	H2A—O2—H2B	110 (2)
O3—La1—O4	74.18 (5)	La1—O3—H3A	125.3 (19)
O3—La1—O6	68.30 (5)	La1—O3—H3B	123 (2)
O3—La1—O7	134.49 (5)	H3A—O3—H3B	112 (3)
O4—La1—Cl1^{i}	68.28 (3)	La1—O4—H4A	112.1 (19)
O4—La1—Cl1	73.83 (4)	La1—O4—H4B	114.3 (17)
O5—La1—Cl1	136.61 (3)	H4A—O4—H4B	112 (2)
O5—La1—Cl1^{i}	133.83 (3)	La1—O5—H5A	126 (2)
O5—La1—O1	66.80 (5)	La1—O5—H5B	116 (2)
O5—La1—O2	81.23 (5)	H5A—O5—H5B	108 (3)
O5—La1—O3	83.78 (5)	La1—O6—H6A	124 (3)
O5—La1—O4	140.90 (5)	La1—O6—H6B	123 (2)
O5—La1—O6	72.77 (5)	H6A—O6—H6B	112 (3)
O5—La1—O7	68.91 (5)	La1—O7—H7A	119 (2)
O6—La1—Cl1	138.86 (3)	La1—O7—H7B	128 (2)
O6—La1—Cl1^{i}	107.32 (4)	H7A—O7—H7B	113 (3)

Symmetry code: (i) −*x*, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···Cl3^{ii}	0.75 (3)	2.48 (3)	3.1947 (15)	161 (3)
O1—H1*B*···Cl2	0.79 (3)	2.38 (3)	3.1365 (16)	161 (2)
O2—H2*A*···Cl2^{iii}	0.80 (3)	2.38 (3)	3.1378 (14)	157 (3)
O2—H2*B*···Cl2^{iv}	0.79 (3)	2.26 (3)	3.0382 (13)	172 (3)
O3—H3*A*···Cl3	0.82 (3)	2.47 (3)	3.2552 (15)	160 (3)
O3—H3*B*···Cl1^{ii}	0.78 (3)	2.92 (3)	3.2954 (13)	112 (2)
O3—H3*B*···Cl2	0.78 (3)	2.72 (3)	3.4160 (16)	150 (3)
O4—H4*A*···O2^{i}	0.78 (3)	2.08 (3)	2.859 (2)	174 (3)
O4—H4*B*···Cl3	0.84 (3)	2.31 (3)	3.1488 (15)	179 (2)
O5—H5*A*···Cl3^{v}	0.80 (3)	2.34 (3)	3.1308 (14)	167 (3)
O5—H5*B*···Cl2^{vi}	0.75 (3)	2.44 (3)	3.1690 (15)	163 (3)
O5—H5*B*···O5^{vi}	0.75 (3)	2.67 (3)	2.986 (3)	108 (2)
O6—H6*A*···Cl3^{vii}	0.77 (3)	2.57 (3)	3.3288 (16)	168 (3)
O6—H6*B*···Cl1^{viii}	0.80 (3)	2.93 (3)	3.3705 (14)	117 (2)
O6—H6*B*···O4^{ix}	0.80 (3)	2.24 (3)	3.038 (2)	169 (3)

Symmetry codes: (i) −*x*, −*y*, −*z*+1; (ii) −*x*, −*y*+1, −*z*+1; (iii) −*x*, −*y*+1, −*z*; (iv) *x*, *y*−1, *z*; (v) *x*, *y*, *z*−1; (vi) −*x*+1, −*y*+1, −*z*; (vii) −*x*+1, −*y*+1, −*z*+1; (viii) *x*+1, *y*, *z*; (ix) −*x*+1, −*y*, −*z*+1.

Di-*μ*-chlorido-bis[heptaaquacerium(III)] tetrachloride, (Ce)

Crystal data

$[CeCl(H_2O)_7]Cl_2$
M_r = 372.58
Triclinic, $P\overline{1}$
a = 7.8995 (3) Å
b = 8.2129 (3) Å
c = 9.1961 (3) Å
α = 70.451 (1)°
β = 73.172 (1)°
γ = 81.658 (1)°
V = 537.39 (3) Å^3
Z = 2
F(000) = 358
D_x = 2.303 Mg m^{-3}
Ag *Kα* radiation, *λ* = 0.56086 Å
Cell parameters from 9812 reflections
θ = 2.5–23.7°
μ = 2.60 mm^{-1}
T = 100 K
Plate, colorless
0.26 × 0.22 × 0.17 mm

Data collection

Bruker D8 Venture Duo diffractometer
ω scans
Absorption correction: multi-scan SADABS-2016/2 (Bruker, 2016)
T_{min} = 0.214, T_{max} = 0.257
28063 measured reflections
3304 independent reflections
3239 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 23.7°, θ_{min} = 1.9°
h = −11→11
k = −11→11
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.009
$wR(F^2)$ = 0.019
S = 1.17
3304 reflections
157 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0036P)^2 + 0.0733P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Extinction correction: SHELXL-2018/1 (Sheldrick 2015b), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0349 (8)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ce1	0.21779 (2)	0.18632 (2)	0.32382 (2)	0.00590 (2)
Cl1	−0.14612 (3)	0.17948 (3)	0.51435 (3)	0.00867 (4)
Cl2	0.21050 (3)	0.77796 (3)	0.03514 (3)	0.01125 (4)
Cl3	0.34287 (3)	0.38691 (3)	0.71200 (3)	0.01174 (4)
O1	0.03034 (11)	0.42224 (10)	0.17488 (9)	0.01184 (13)
O2	0.07253 (10)	0.08169 (10)	0.16291 (9)	0.01131 (13)
O3	0.22060 (11)	0.46047 (10)	0.38631 (10)	0.01504 (14)
O4	0.23110 (10)	0.09321 (10)	0.61518 (9)	0.01193 (13)
O5	0.38549 (10)	0.35125 (10)	0.04929 (8)	0.01117 (13)
O6	0.52006 (10)	0.22922 (11)	0.34141 (9)	0.01312 (14)
O7	0.45125 (10)	−0.00898 (10)	0.19850 (9)	0.01262 (14)
H1A	−0.062 (3)	0.449 (2)	0.218 (2)	0.034 (5)*
H1B	0.074 (2)	0.507 (2)	0.120 (2)	0.034 (5)*
H2A	0.122 (2)	0.003 (2)	0.132 (2)	0.034 (5)*
H2B	0.020 (2)	0.144 (2)	0.103 (2)	0.033 (4)*
H3A	0.251 (3)	0.468 (2)	0.458 (2)	0.042 (5)*
H3B	0.191 (3)	0.554 (3)	0.333 (2)	0.050 (6)*
H4A	0.142 (2)	0.055 (2)	0.6783 (19)	0.023 (4)*
H4B	0.255 (2)	0.162 (2)	0.6465 (19)	0.028 (4)*
H5A	0.353 (2)	0.362 (2)	−0.028 (2)	0.026 (4)*
H5B	0.487 (3)	0.348 (2)	0.027 (2)	0.034 (5)*
H6A	0.602 (3)	0.156 (2)	0.343 (2)	0.035 (5)*
H6B	0.553 (3)	0.312 (3)	0.347 (2)	0.044 (5)*
H7A	0.535 (2)	0.030 (2)	0.134 (2)	0.028 (4)*
H7B	0.472 (2)	−0.108 (3)	0.232 (2)	0.039 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ce1	0.00610 (3)	0.00554 (3)	0.00634 (3)	−0.00042 (2)	−0.00203 (2)	−0.00178 (2)
Cl1	0.00832 (9)	0.00669 (9)	0.00983 (9)	−0.00012 (7)	−0.00148 (7)	−0.00192 (7)
Cl2	0.01010 (10)	0.00970 (10)	0.01461 (10)	0.00029 (8)	−0.00330 (8)	−0.00484 (8)
Cl3	0.01327 (10)	0.01078 (10)	0.01287 (10)	0.00063 (8)	−0.00533 (8)	−0.00471 (8)
O1	0.0101 (3)	0.0093 (3)	0.0125 (3)	0.0001 (3)	−0.0021 (3)	0.0003 (3)
O2	0.0137 (3)	0.0101 (3)	0.0124 (3)	0.0033 (3)	−0.0068 (3)	−0.0051 (3)

O3	0.0198 (4)	0.0105 (3)	0.0190 (4)	0.0010 (3)	−0.0093 (3)	−0.0070 (3)
O4	0.0126 (3)	0.0141 (3)	0.0105 (3)	−0.0051 (3)	−0.0029 (3)	−0.0040 (3)
O5	0.0093 (3)	0.0133 (3)	0.0096 (3)	−0.0008 (3)	−0.0022 (3)	−0.0019 (3)
O6	0.0090 (3)	0.0151 (3)	0.0178 (3)	−0.0006 (3)	−0.0049 (3)	−0.0071 (3)
O7	0.0103 (3)	0.0086 (3)	0.0157 (3)	0.0003 (3)	0.0003 (3)	−0.0031 (3)

Geometric parameters (Å, º)

Ce1—Cl1^{i}	2.9282 (2)	O2—H2B	0.783 (19)
Ce1—Cl1	2.8986 (2)	O3—H3A	0.79 (2)
Ce1—O1	2.5276 (7)	O3—H3B	0.80 (2)
Ce1—O2	2.5229 (7)	O4—H4A	0.800 (17)
Ce1—O3	2.5076 (8)	O4—H4B	0.781 (18)
Ce1—O4	2.5580 (7)	O5—H5A	0.798 (17)
Ce1—O5	2.5018 (7)	O5—H5B	0.768 (19)
Ce1—O6	2.5214 (7)	O6—H6A	0.82 (2)
Ce1—O7	2.5397 (8)	O6—H6B	0.79 (2)
O1—H1A	0.762 (19)	O7—H7A	0.775 (18)
O1—H1B	0.77 (2)	O7—H7B	0.78 (2)
O2—H2A	0.797 (19)		

Cl1—Ce1—Cl1^{i}	73.953 (7)	O6—Ce1—O1	123.87 (3)
O1—Ce1—Cl1^{i}	128.491 (19)	O6—Ce1—O2	140.89 (3)
O1—Ce1—Cl1	70.026 (19)	O6—Ce1—O4	69.23 (2)
O1—Ce1—O4	130.70 (2)	O6—Ce1—O7	69.36 (3)
O1—Ce1—O7	124.61 (3)	O7—Ce1—Cl1^{i}	68.459 (19)
O2—Ce1—Cl1	79.796 (18)	O7—Ce1—Cl1	139.540 (18)
O2—Ce1—Cl1^{i}	70.981 (18)	O7—Ce1—O4	104.66 (3)
O2—Ce1—O1	67.44 (2)	Ce1—Cl1—Ce1^{i}	106.047 (7)
O2—Ce1—O4	135.98 (2)	Ce1—O1—H1A	120.9 (13)
O2—Ce1—O7	74.40 (3)	Ce1—O1—H1B	117.9 (13)
O3—Ce1—Cl1^{i}	140.40 (2)	H1A—O1—H1B	105.8 (18)
O3—Ce1—Cl1	84.317 (19)	Ce1—O2—H2A	117.0 (13)
O3—Ce1—O1	70.16 (3)	Ce1—O2—H2B	123.0 (12)
O3—Ce1—O2	137.56 (3)	H2A—O2—H2B	111.1 (17)
O3—Ce1—O4	74.09 (3)	Ce1—O3—H3A	125.9 (14)
O3—Ce1—O6	68.59 (3)	Ce1—O3—H3B	122.9 (14)
O3—Ce1—O7	135.12 (3)	H3A—O3—H3B	111.1 (19)
O4—Ce1—Cl1^{i}	68.263 (18)	Ce1—O4—H4A	114.1 (11)
O4—Ce1—Cl1	73.723 (18)	Ce1—O4—H4B	117.9 (12)
O5—Ce1—Cl1	136.599 (19)	H4A—O4—H4B	104.8 (15)
O5—Ce1—Cl1^{i}	133.776 (18)	Ce1—O5—H5A	122.1 (12)
O5—Ce1—O1	66.70 (3)	Ce1—O5—H5B	120.1 (13)
O5—Ce1—O2	81.00 (2)	H5A—O5—H5B	108.9 (17)
O5—Ce1—O3	84.25 (3)	Ce1—O6—H6A	124.5 (12)
O5—Ce1—O4	141.04 (3)	Ce1—O6—H6B	127.8 (15)
O5—Ce1—O6	72.84 (2)	H6A—O6—H6B	107.7 (18)
O5—Ce1—O7	69.00 (3)	Ce1—O7—H7A	119.7 (12)

O6—Ce1—Cl1	138.654 (18)	Ce1—O7—H7B	129.6 (14)
O6—Ce1—Cl1^{i}	107.53 (2)	H7A—O7—H7B	107.2 (18)

Symmetry code: (i) −*x*, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···Cl3^{ii}	0.762 (19)	2.458 (19)	3.1945 (8)	162.9 (18)
O1—H1*B*···Cl2	0.77 (2)	2.405 (19)	3.1380 (8)	160.6 (17)
O2—H2*A*···Cl2^{iii}	0.797 (19)	2.251 (19)	3.0368 (8)	168.6 (17)
O2—H2*B*···Cl2^{iv}	0.783 (19)	2.411 (19)	3.1383 (8)	155.0 (16)
O3—H3*A*···Cl3	0.79 (2)	2.50 (2)	3.2501 (9)	160.9 (18)
O3—H3*B*···Cl1^{ii}	0.80 (2)	2.91 (2)	3.3040 (8)	112.9 (16)
O3—H3*B*···Cl2	0.80 (2)	2.71 (2)	3.4188 (9)	147.3 (18)
O4—H4*A*···O2^{i}	0.800 (17)	2.068 (17)	2.8609 (11)	171.2 (16)
O4—H4*B*···Cl3	0.781 (18)	2.369 (18)	3.1466 (8)	173.7 (16)
O5—H5*A*···Cl3^{v}	0.798 (17)	2.354 (17)	3.1286 (8)	164.0 (16)
O5—H5*B*···Cl2^{vi}	0.768 (19)	2.446 (19)	3.1699 (8)	157.6 (17)
O5—H5*B*···O5^{vi}	0.768 (19)	2.601 (17)	2.9858 (15)	112.9 (15)
O6—H6*A*···Cl1^{vii}	0.82 (2)	2.936 (18)	3.3662 (8)	115.2 (14)
O6—H6*A*···O4^{viii}	0.82 (2)	2.25 (2)	3.0451 (11)	164.9 (17)
O6—H6*B*···Cl3^{ix}	0.79 (2)	2.55 (2)	3.3165 (8)	164.4 (18)

Symmetry codes: (i) −*x*, −*y*, −*z*+1; (ii) −*x*, −*y*+1, −*z*+1; (iii) *x*, *y*−1, *z*; (iv) −*x*, −*y*+1, −*z*; (v) *x*, *y*, *z*−1; (vi) −*x*+1, −*y*+1, −*z*; (vii) *x*+1, *y*, *z*; (viii) −*x*+1, −*y*, −*z*+1; (ix) −*x*+1, −*y*+1, −*z*+1.

Hexaaquadichloridoprotactinium(III) chloride (Pr)

Crystal data

$[PrCl_2(H_2O)_6]Cl$
M_r = 355.36
Monoclinic, *P*2/*c*
a = 7.9997 (3) Å
b = 6.5647 (2) Å
c = 12.1734 (4) Å
β = 127.388 (1)°
V = 507.95 (3) Å^3
Z = 2
F(000) = 340
D_x = 2.323 Mg m^{-3}
Ag *Kα* radiation, *λ* = 0.56086 Å
Cell parameters from 6065 reflections
θ = 2.5–23.7°
μ = 2.90 mm^{-1}
T = 100 K
Plate, green
0.06 × 0.06 × 0.05 mm

Data collection

Bruker D8 Venture Duo diffractometer
ω scans
Absorption correction: multi-scan SADABS-2016/2 (Bruker, 2016)
T_{min} = 0.218, T_{max} = 0.257
15235 measured reflections
1567 independent reflections
1486 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 23.7°, θ_{min} = 2.5°
h = −11→11
k = −9→9
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.014
$wR(F^2)$ = 0.027

S = 1.05	All H-atom parameters refined
1567 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0063P)^2]$
71 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: dual	$\Delta\rho_{max}$ = 0.38 e Å^{-3}
Hydrogen site location: difference Fourier map	$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Pr1	0.500000	0.14679 (2)	0.250000	0.00584 (3)
Cl1	0.29528 (6)	−0.17308 (5)	0.05469 (4)	0.01042 (7)
Cl2	0.000000	0.62270 (8)	0.250000	0.01100 (10)
O1	0.1632 (2)	0.29975 (19)	0.05765 (13)	0.0114 (2)
O2	0.2337 (2)	0.0446 (2)	0.28224 (14)	0.0120 (2)
O3	0.4395 (2)	0.42625 (18)	0.35562 (13)	0.0116 (2)
H1A	0.063 (4)	0.265 (4)	0.044 (3)	0.030 (7)*
H1B	0.132 (4)	0.327 (3)	−0.015 (3)	0.027 (7)*
H2A	0.251 (4)	0.083 (4)	0.348 (3)	0.032 (7)*
H2B	0.192 (4)	−0.065 (4)	0.268 (2)	0.025 (6)*
H3A	0.508 (4)	0.524 (4)	0.384 (2)	0.030 (7)*
H3B	0.323 (4)	0.454 (4)	0.328 (3)	0.027 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pr1	0.00553 (6)	0.00602 (5)	0.00598 (6)	0.000	0.00349 (5)	0.000
Cl1	0.00986 (19)	0.00979 (16)	0.01028 (17)	−0.00112 (13)	0.00542 (15)	−0.00229 (13)
Cl2	0.0102 (3)	0.0119 (2)	0.0114 (2)	0.000	0.0068 (2)	0.000
O1	0.0075 (6)	0.0150 (6)	0.0101 (6)	0.0006 (5)	0.0046 (5)	0.0029 (4)
O2	0.0139 (7)	0.0124 (6)	0.0140 (6)	−0.0029 (5)	0.0107 (6)	−0.0020 (5)
O3	0.0089 (6)	0.0101 (5)	0.0159 (6)	−0.0013 (5)	0.0076 (5)	−0.0040 (5)

Geometric parameters (Å, º)

Pr1—Cl1^{i}	2.8312 (4)	Pr1—O3^{i}	2.4513 (12)
Pr1—Cl1	2.8312 (4)	O1—H1A	0.75 (3)
Pr1—O1^{i}	2.4677 (13)	O1—H1B	0.78 (3)
Pr1—O1	2.4677 (13)	O2—H2A	0.76 (3)
Pr1—O2	2.4818 (13)	O2—H2B	0.77 (2)
Pr1—O2^{i}	2.4817 (13)	O3—H3A	0.78 (3)
Pr1—O3	2.4513 (12)	O3—H3B	0.80 (3)
Cl1—Pr1—Cl1^{i}	84.250 (16)	O3^{i}—Pr1—O1	69.35 (5)

O1—Pr1—Cl1^{i}	147.16 (3)	O3—Pr1—O1	75.14 (4)
O1^{i}—Pr1—Cl1	147.16 (3)	O3^{i}—Pr1—O1^{i}	75.14 (4)
O1^{i}—Pr1—Cl1^{i}	76.31 (3)	O3—Pr1—O1^{i}	69.35 (5)
O1—Pr1—Cl1	76.31 (3)	O3—Pr1—O2^{i}	138.35 (4)
O1^{i}—Pr1—O1	131.98 (6)	O3^{i}—Pr1—O2	138.35 (4)
O1—Pr1—O2^{i}	120.50 (4)	O3^{i}—Pr1—O2^{i}	69.97 (4)
O1—Pr1—O2	73.29 (4)	O3—Pr1—O2	69.97 (4)
O1^{i}—Pr1—O2^{i}	73.29 (4)	O3^{i}—Pr1—O3	83.09 (6)
O1^{i}—Pr1—O2	120.50 (4)	Pr1—O1—H1A	119 (2)
O2^{i}—Pr1—Cl1	77.35 (3)	Pr1—O1—H1B	125.5 (19)
O2—Pr1—Cl1^{i}	77.35 (3)	H1A—O1—H1B	105 (3)
O2^{i}—Pr1—Cl1^{i}	79.51 (3)	Pr1—O2—H2A	117 (2)
O2—Pr1—Cl1	79.51 (3)	Pr1—O2—H2B	121.3 (18)
O2^{i}—Pr1—O2	148.63 (6)	H2A—O2—H2B	108 (2)
O3—Pr1—Cl1	142.92 (3)	Pr1—O3—H3A	122.8 (18)
O3—Pr1—Cl1^{i}	108.20 (3)	Pr1—O3—H3B	120.2 (17)
O3^{i}—Pr1—Cl1	108.20 (3)	H3A—O3—H3B	109 (2)
O3^{i}—Pr1—Cl1^{i}	142.92 (3)		

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···Cl1^{ii}	0.75 (3)	2.42 (3)	3.1498 (14)	166 (3)
O1—H1*B*···Cl2^{iii}	0.78 (3)	2.40 (3)	3.1706 (13)	172 (2)
O2—H2*A*···Cl1^{iv}	0.76 (3)	2.40 (3)	3.1575 (13)	175 (2)
O2—H2*B*···Cl2^{v}	0.77 (2)	2.49 (2)	3.2291 (14)	163 (2)
O3—H3*A*···Cl1^{vi}	0.78 (3)	2.36 (3)	3.1303 (14)	174 (2)
O3—H3*B*···Cl2	0.80 (3)	2.41 (3)	3.1919 (14)	166 (2)

Symmetry codes: (ii) −*x*, −*y*, −*z*; (iii) −*x*, −*y*+1, −*z*; (iv) *x*, −*y*, *z*+1/2; (v) *x*, *y*−1, *z*; (vi) −*x*+1, *y*+1, −*z*+1/2.

Hexaaquadichloridoneodymium(III) chloride (Nd)

Crystal data

$[NdCl_2(H_2O)_6]Cl$	*F*(000) = 342
M_r = 358.69	D_x = 2.368 Mg m^{-3}
Monoclinic, *P*2/*c*	Ag *Kα* radiation, *λ* = 0.56086 Å
a = 7.9710 (3) Å	Cell parameters from 9892 reflections
b = 6.5460 (2) Å	*θ* = 2.5–23.7°
c = 12.1246 (5) Å	*μ* = 3.11 mm^{-1}
β = 127.324 (1)°	*T* = 100 K
V = 503.09 (3) Å^3	Plate, purple
Z = 2	0.16 × 0.12 × 0.11 mm

Data collection

Bruker D8 Venture Duo diffractometer	T_{min} = 0.201, T_{max} = 0.257
ω scans	23233 measured reflections
Absorption correction: multi-scan SADABS-2016/2 (Bruker, 2016)	1559 independent reflections
	1536 reflections with $I > 2\sigma(I)$
	R_{int} = 0.036

θ_{max} = 23.7°, θ_{min} = 2.5°
h = −11→11
k = −9→9
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.007
$wR(F^2)$ = 0.017
S = 1.11
1559 reflections
72 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0058P)^2 + 0.0784P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}
Extinction correction: SHELXL-2018/1 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0145 (7)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
Nd1	0.500000	0.14781 (2)	0.250000	0.00585 (3)
Cl1	0.29595 (3)	−0.17132 (3)	0.05545 (2)	0.01031 (4)
Cl2	0.000000	0.62320 (5)	0.250000	0.01090 (5)
O1	0.16396 (10)	0.30014 (11)	0.05851 (7)	0.01173 (12)
O2	0.23447 (10)	0.04554 (11)	0.28178 (8)	0.01176 (12)
O3	0.44019 (11)	0.42581 (11)	0.35561 (7)	0.01172 (12)
H1A	0.063 (2)	0.268 (3)	0.0458 (17)	0.031 (4)*
H1B	0.137 (2)	0.327 (2)	−0.0083 (18)	0.024 (4)*
H2A	0.246 (3)	0.083 (3)	0.3463 (18)	0.034 (4)*
H2B	0.187 (2)	−0.061 (3)	0.2652 (16)	0.028 (4)*
H3A	0.511 (2)	0.526 (3)	0.3820 (16)	0.029 (4)*
H3B	0.327 (3)	0.463 (2)	0.3272 (16)	0.028 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.00556 (3)	0.00614 (4)	0.00597 (4)	0.000	0.00356 (3)	0.000
Cl1	0.01013 (8)	0.00972 (9)	0.00982 (9)	−0.00096 (6)	0.00539 (7)	−0.00215 (7)
Cl2	0.01039 (12)	0.01175 (13)	0.01133 (13)	0.000	0.00699 (10)	0.000
O1	0.0084 (3)	0.0150 (3)	0.0102 (3)	0.0005 (2)	0.0048 (2)	0.0031 (2)
O2	0.0136 (3)	0.0115 (3)	0.0142 (3)	−0.0033 (2)	0.0105 (3)	−0.0026 (3)
O3	0.0102 (3)	0.0104 (3)	0.0154 (3)	−0.0013 (2)	0.0081 (2)	−0.0037 (2)

Geometric parameters (Å, º)

Nd1—Cl1	2.8145 (2)	Nd1—O3^{i}	2.4328 (7)
Nd1—Cl1^{i}	2.8145 (2)	O1—H1A	0.749 (16)

Nd1—O1^{i}	2.4532 (7)	O1—H1B	0.722 (17)
Nd1—O1	2.4532 (7)	O2—H2A	0.770 (18)
Nd1—O2^{i}	2.4629 (6)	O2—H2B	0.760 (17)
Nd1—O2	2.4629 (6)	O3—H3A	0.793 (16)
Nd1—O3	2.4328 (7)	O3—H3B	0.782 (16)
Cl1^{i}—Nd1—Cl1	84.154 (9)	O3^{i}—Nd1—O1	69.38 (2)
O1—Nd1—Cl1	76.348 (18)	O3—Nd1—O1	75.17 (2)
O1^{i}—Nd1—Cl1^{i}	76.348 (18)	O3^{i}—Nd1—O1^{i}	75.17 (2)
O1^{i}—Nd1—Cl1	147.078 (18)	O3—Nd1—O1^{i}	69.38 (2)
O1—Nd1—Cl1^{i}	147.077 (18)	O3—Nd1—O2	70.11 (2)
O1^{i}—Nd1—O1	132.04 (3)	O3^{i}—Nd1—O2^{i}	70.11 (2)
O1—Nd1—O2	73.13 (2)	O3^{i}—Nd1—O2	138.33 (2)
O1—Nd1—O2^{i}	120.74 (2)	O3—Nd1—O2^{i}	138.33 (2)
O1^{i}—Nd1—O2	120.74 (2)	O3^{i}—Nd1—O3	83.16 (3)
O1^{i}—Nd1—O2^{i}	73.13 (2)	Nd1—O1—H1A	119.8 (13)
O2—Nd1—Cl1^{i}	77.397 (17)	Nd1—O1—H1B	125.2 (12)
O2^{i}—Nd1—Cl1	77.398 (17)	H1A—O1—H1B	106.3 (16)
O2—Nd1—Cl1	79.318 (18)	Nd1—O2—H2A	119.3 (12)
O2^{i}—Nd1—Cl1^{i}	79.318 (18)	Nd1—O2—H2B	123.0 (12)
O2—Nd1—O2^{i}	148.45 (3)	H2A—O2—H2B	107.0 (16)
O3—Nd1—Cl1^{i}	108.189 (17)	Nd1—O3—H3A	120.5 (11)
O3—Nd1—Cl1	142.963 (17)	Nd1—O3—H3B	122.7 (11)
O3^{i}—Nd1—Cl1^{i}	142.964 (17)	H3A—O3—H3B	105.9 (15)
O3^{i}—Nd1—Cl1	108.190 (17)		

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···Cl1^{ii}	0.749 (16)	2.418 (16)	3.1491 (7)	165.6 (16)
O1—H1*B*···Cl2^{iii}	0.722 (17)	2.451 (18)	3.1661 (8)	170.8 (15)
O2—H2*A*···Cl1^{iv}	0.770 (18)	2.387 (18)	3.1552 (8)	175.3 (17)
O2—H2*B*···Cl2^{v}	0.760 (17)	2.490 (17)	3.2267 (8)	164.0 (15)
O3—H3*A*···Cl1^{vi}	0.793 (16)	2.337 (17)	3.1290 (7)	176.1 (15)
O3—H3*B*···Cl2	0.782 (16)	2.413 (16)	3.1894 (7)	172.0 (15)

Symmetry codes: (ii) −*x*, −*y*, −*z*; (iii) −*x*, −*y*+1, −*z*; (iv) *x*, −*y*, *z*+1/2; (v) *x*, *y*−1, *z*; (vi) −*x*+1, *y*+1, −*z*+1/2.

Hexaaquadichloridosamarium(III) chloride (Sm)

Crystal data

$[SmCl_2(H_2O)_6]Cl$	V = 498.65 (9) Å^3
M_r = 364.80	Z = 2
Monoclinic, $P2/c$	$F(000)$ = 346
a = 7.9375 (8) Å	D_x = 2.430 Mg m^{-3}
b = 6.5351 (7) Å	Ag $K\alpha$ radiation, λ = 0.56086 Å
c = 12.0713 (11) Å	Cell parameters from 9537 reflections
β = 127.217 (2)°	θ = 3.0–23.7°

μ = 3.51 mm^{-1}
T = 100 K

Plate, yellow
0.25 × 0.21 × 0.18 mm

Data collection

Bruker D8 Venture Duo diffractometer
ω scans
Absorption correction: multi-scan SADABS-2016/2 (Bruker, 2016)
T_{min} = 0.204, T_{max} = 0.257
27415 measured reflections

1553 independent reflections
1533 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 23.7°, θ_{min} = 2.5°
h = −11→11
k = −9→9
l = −17→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.010
$wR(F^2)$ = 0.023
S = 1.19
1553 reflections
72 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: difference Fourier map

All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0104P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.85 e Å^{-3}
Extinction correction: SHELXL-2018/1 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0299 (11)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Sm1	0.500000	0.14983 (2)	0.250000	0.00823 (4)
Cl1	0.29725 (4)	−0.16793 (4)	0.05721 (3)	0.01414 (5)
Cl2	0.000000	0.62416 (6)	0.250000	0.01522 (7)
O1	0.16623 (14)	0.30030 (14)	0.06034 (9)	0.01545 (15)
O2	0.23649 (13)	0.04788 (14)	0.28158 (9)	0.01546 (15)
O3	0.44104 (14)	0.42539 (13)	0.35504 (9)	0.01546 (15)
H1A	0.072 (3)	0.272 (3)	0.048 (2)	0.030 (5)*
H1B	0.135 (4)	0.333 (3)	−0.013 (3)	0.039 (6)*
H2A	0.250 (3)	0.085 (3)	0.351 (2)	0.028 (4)*
H2B	0.187 (3)	−0.062 (3)	0.2644 (18)	0.024 (4)*
H3A	0.510 (3)	0.525 (3)	0.381 (2)	0.041 (5)*
H3B	0.324 (3)	0.457 (3)	0.3251 (18)	0.029 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sm1	0.00783 (5)	0.00820 (5)	0.00880 (4)	0.000	0.00510 (3)	0.000
Cl1	0.01386 (12)	0.01289 (12)	0.01390 (11)	−0.00140 (8)	0.00746 (10)	−0.00317 (8)
Cl2	0.01447 (16)	0.01628 (16)	0.01618 (16)	0.000	0.00993 (14)	0.000

O1	0.0105 (4)	0.0191 (4)	0.0140 (4)	0.0011 (3)	0.0059 (3)	0.0040 (3)
O2	0.0174 (4)	0.0152 (4)	0.0192 (4)	−0.0043 (3)	0.0139 (3)	−0.0029 (3)
O3	0.0141 (4)	0.0131 (4)	0.0204 (4)	−0.0018 (3)	0.0111 (3)	−0.0052 (3)

Geometric parameters (Å, º)

Sm1—Cl1	2.7906 (3)	Sm1—O3	2.4057 (8)
Sm1—Cl1^{i}	2.7906 (3)	O1—H1A	0.693 (19)
Sm1—O1^{i}	2.4269 (8)	O1—H1B	0.79 (3)
Sm1—O1	2.4269 (8)	O2—H2A	0.81 (2)
Sm1—O2	2.4349 (8)	O2—H2B	0.78 (2)
Sm1—O2^{i}	2.4349 (8)	O3—H3A	0.78 (2)
Sm1—O3^{i}	2.4057 (8)	O3—H3B	0.794 (19)
Cl1^{i}—Sm1—Cl1	83.829 (14)	O3—Sm1—O1	75.20 (3)
O1—Sm1—Cl1	76.40 (2)	O3^{i}—Sm1—O1	69.44 (3)
O1^{i}—Sm1—Cl1^{i}	76.40 (2)	O3—Sm1—O1^{i}	69.44 (3)
O1^{i}—Sm1—Cl1	146.94 (2)	O3^{i}—Sm1—O1^{i}	75.20 (3)
O1—Sm1—Cl1^{i}	146.94 (2)	O3^{i}—Sm1—O2^{i}	70.30 (3)
O1^{i}—Sm1—O1	132.20 (4)	O3—Sm1—O2	70.30 (3)
O1—Sm1—O2^{i}	120.94 (3)	O3—Sm1—O2^{i}	138.31 (3)
O1—Sm1—O2	73.00 (3)	O3^{i}—Sm1—O2	138.31 (3)
O1^{i}—Sm1—O2^{i}	73.00 (3)	O3—Sm1—O3^{i}	83.07 (4)
O1^{i}—Sm1—O2	120.94 (3)	Sm1—O1—H1A	120.8 (17)
O2^{i}—Sm1—Cl1^{i}	79.06 (2)	Sm1—O1—H1B	126.5 (17)
O2—Sm1—Cl1	79.06 (2)	H1A—O1—H1B	105 (2)
O2^{i}—Sm1—Cl1	77.44 (2)	Sm1—O2—H2A	119.3 (13)
O2—Sm1—Cl1^{i}	77.44 (2)	Sm1—O2—H2B	123.1 (13)
O2^{i}—Sm1—O2	148.24 (4)	H2A—O2—H2B	106.3 (18)
O3^{i}—Sm1—Cl1^{i}	143.00 (2)	Sm1—O3—H3A	121.5 (16)
O3^{i}—Sm1—Cl1	108.38 (2)	Sm1—O3—H3B	120.0 (13)
O3—Sm1—Cl1^{i}	108.38 (2)	H3A—O3—H3B	108 (2)
O3—Sm1—Cl1	143.00 (2)		

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···Cl1^{ii}	0.693 (19)	2.484 (19)	3.1594 (10)	165 (2)
O1—H1*B*···Cl2^{iii}	0.79 (3)	2.39 (3)	3.1685 (9)	169.2 (19)
O2—H2*A*···Cl1^{iv}	0.81 (2)	2.35 (2)	3.1586 (9)	175.9 (18)
O2—H2*B*···Cl2^{v}	0.78 (2)	2.48 (2)	3.2358 (10)	163.6 (17)
O3—H3*A*···Cl1^{vi}	0.78 (2)	2.36 (2)	3.1367 (10)	176 (2)
O3—H3*B*···Cl2	0.794 (19)	2.41 (2)	3.1908 (9)	167.7 (18)

Symmetry codes: (ii) −*x*, −*y*, −*z*; (iii) −*x*, −*y*+1, −*z*; (iv) *x*, −*y*, *z*+1/2; (v) *x*, *y*−1, *z*; (vi) −*x*+1, *y*+1, −*z*+1/2.

Hexaaquadichloridoeuropium(III) chloride (Eu)

Crystal data

$[EuCl_2(H_2O)_6]Cl$
M_r = 366.41
Monoclinic, $P2/c$
a = 7.9062 (2) Å
b = 6.5092 (2) Å
c = 12.0410 (4) Å
β = 127.231 (1)°
V = 493.38 (3) Å^3
Z = 2
$F(000)$ = 348
D_x = 2.466 Mg m^{-3}
Ag $K\alpha$ radiation, λ = 0.56086 Å
Cell parameters from 9987 reflections
θ = 2.5–23.7°
μ = 3.75 mm^{-1}
T = 100 K
Plate, colorless
0.13 × 0.13 × 0.11 mm

Data collection

Bruker D8 Venture Duo diffractometer
ω scans
Absorption correction: multi-scan SADABS-2016/2 (Bruker, 2016)
T_{min} = 0.218, T_{max} = 0.257
21905 measured reflections
1529 independent reflections
1504 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 23.7°, θ_{min} = 2.5°
h = −11→11
k = −9→9
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.007
$wR(F^2)$ = 0.016
S = 1.13
1529 reflections
72 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0058P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Extinction correction: SHELXL-2018/1 (Sheldrick 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0155 (6)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Eu1	0.500000	0.15065 (2)	0.250000	0.00549 (3)
Cl1	0.29777 (3)	−0.16684 (3)	0.05730 (2)	0.00967 (4)
Cl2	0.000000	0.62348 (4)	0.250000	0.01034 (6)
O1	0.16667 (11)	0.30060 (11)	0.06078 (8)	0.01088 (13)
O2	0.23665 (11)	0.04821 (11)	0.28100 (8)	0.01108 (13)
O3	0.44219 (11)	0.42430 (10)	0.35568 (8)	0.01082 (13)
H1A	0.062 (2)	0.268 (2)	0.0449 (17)	0.029 (4)*
H1B	0.134 (3)	0.332 (2)	−0.011 (2)	0.028 (4)*
H2A	0.250 (2)	0.085 (2)	0.3479 (17)	0.024 (4)*
H2B	0.193 (2)	−0.060 (2)	0.2653 (16)	0.026 (4)*

H3A	0.513 (2)	0.523 (2)	0.3791 (16)	0.030 (4)*
H3B	0.334 (2)	0.458 (2)	0.3268 (16)	0.025 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Eu1	0.00511 (3)	0.00572 (3)	0.00569 (4)	0.000	0.00329 (3)	0.000
Cl1	0.00927 (9)	0.00919 (9)	0.00941 (10)	−0.00089 (7)	0.00505 (8)	−0.00199 (7)
Cl2	0.00946 (13)	0.01139 (13)	0.01076 (14)	0.000	0.00643 (12)	0.000
O1	0.0075 (3)	0.0138 (3)	0.0098 (3)	0.0005 (2)	0.0044 (3)	0.0026 (3)
O2	0.0130 (3)	0.0106 (3)	0.0135 (3)	−0.0026 (2)	0.0101 (3)	−0.0020 (3)
O3	0.0083 (3)	0.0095 (3)	0.0147 (4)	−0.0013 (2)	0.0071 (3)	−0.0039 (3)

Geometric parameters (Å, º)

Eu1—Cl1	2.7788 (2)	Eu1—O3	2.3884 (7)
Eu1—Cl1^{i}	2.7788 (2)	O1—H1A	0.760 (15)
Eu1—O1^{i}	2.4131 (7)	O1—H1B	0.766 (19)
Eu1—O1	2.4131 (7)	O2—H2A	0.784 (16)
Eu1—O2	2.4206 (7)	O2—H2B	0.759 (16)
Eu1—O2^{i}	2.4206 (7)	O3—H3A	0.783 (16)
Eu1—O3^{i}	2.3884 (7)	O3—H3B	0.737 (15)
Cl1^{i}—Eu1—Cl1	83.904 (10)	O3—Eu1—O1	75.50 (3)
O1—Eu1—Cl1	76.376 (18)	O3^{i}—Eu1—O1	69.33 (2)
O1^{i}—Eu1—Cl1^{i}	76.376 (18)	O3—Eu1—O1^{i}	69.33 (2)
O1^{i}—Eu1—Cl1	146.839 (18)	O3^{i}—Eu1—O1^{i}	75.50 (3)
O1—Eu1—Cl1^{i}	146.840 (18)	O3^{i}—Eu1—O2^{i}	70.34 (2)
O1^{i}—Eu1—O1	132.29 (3)	O3—Eu1—O2	70.34 (2)
O1—Eu1—O2^{i}	121.05 (3)	O3—Eu1—O2^{i}	138.36 (2)
O1—Eu1—O2	72.97 (3)	O3^{i}—Eu1—O2	138.36 (2)
O1^{i}—Eu1—O2^{i}	72.97 (3)	O3—Eu1—O3^{i}	83.55 (3)
O1^{i}—Eu1—O2	121.05 (3)	Eu1—O1—H1A	121.7 (12)
O2^{i}—Eu1—Cl1^{i}	79.036 (19)	Eu1—O1—H1B	127.1 (12)
O2—Eu1—Cl1	79.037 (19)	H1A—O1—H1B	102.6 (16)
O2^{i}—Eu1—Cl1	77.317 (17)	Eu1—O2—H2A	118.7 (11)
O2—Eu1—Cl1^{i}	77.317 (17)	Eu1—O2—H2B	121.7 (11)
O2^{i}—Eu1—O2	148.02 (3)	H2A—O2—H2B	107.3 (15)
O3^{i}—Eu1—Cl1^{i}	143.185 (18)	Eu1—O3—H3A	118.5 (11)
O3^{i}—Eu1—Cl1	107.979 (18)	Eu1—O3—H3B	120.7 (12)
O3—Eu1—Cl1^{i}	107.980 (18)	H3A—O3—H3B	107.7 (15)
O3—Eu1—Cl1	143.185 (18)		

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···Cl1^{ii}	0.760 (15)	2.407 (15)	3.1537 (7)	167.5 (16)

O1—H1*B*···Cl2^{iii}	0.766 (19)	2.407 (19)	3.1649 (8)	170.6 (14)
O2—H2*A*···Cl1^{iv}	0.784 (16)	2.373 (17)	3.1549 (8)	175.1 (14)
O2—H2*B*···Cl2^{v}	0.759 (16)	2.500 (15)	3.2308 (7)	162.1 (14)
O3—H3*A*···Cl1^{vi}	0.783 (16)	2.349 (16)	3.1307 (7)	175.7 (14)
O3—H3*B*···Cl2	0.737 (15)	2.455 (15)	3.1842 (7)	170.3 (15)

Symmetry codes: (ii) −*x*, −*y*, −*z*; (iii) −*x*, −*y*+1, −*z*; (iv) *x*, −*y*, *z*+1/2; (v) *x*, *y*−1, *z*; (vi) −*x*+1, *y*+1, −*z*+1/2.

Hexaaquadichloridogadolinium(III) chloride (Gd)

Crystal data

$[GdCl_2(H_2O)_6]Cl$
M_r = 371.70
Monoclinic, *P*2/*c*
a = 7.8835 (3) Å
b = 6.4964 (3) Å
c = 12.0176 (4) Å
β = 127.186 (1)°
V = 490.33 (3) Å^3
Z = 2
F(000) = 350
D_x = 2.518 Mg m^{-3}
Ag *Kα* radiation, *λ* = 0.56086 Å
Cell parameters from 9213 reflections
θ = 2.5–23.8°
μ = 3.99 mm^{-1}
T = 100 K
Plate, colorless
0.33 × 0.25 × 0.20 mm

Data collection

Bruker D8 Venture Duo diffractometer
ω scans
Absorption correction: multi-scan SADABS-2016/2 (Bruker, 2016)
T_{min} = 0.172, T_{max} = 0.257
26021 measured reflections
1532 independent reflections
1520 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 23.8°, θ_{min} = 2.5°
h = −11→11
k = −9→9
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.009
$wR(F^2)$ = 0.021
S = 1.23
1532 reflections
72 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0082P)^2 + 0.0734P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}
Extinction correction: SHELXL-2018/1 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0279 (9)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Gd1	0.500000	0.15160 (2)	0.250000	0.00581 (3)
Cl1	0.29831 (4)	−0.16561 (4)	0.05775 (3)	0.01005 (5)
Cl2	0.000000	0.62367 (6)	0.250000	0.01075 (7)

O1	0.16722 (14)	0.30084 (14)	0.06138 (9)	0.01150 (15)
O2	0.23723 (13)	0.04881 (14)	0.28098 (9)	0.01135 (15)
O3	0.44242 (14)	0.42417 (13)	0.35554 (9)	0.01117 (15)
H1A	0.060 (3)	0.266 (3)	0.047 (2)	0.028 (5)*
H1B	0.139 (3)	0.329 (3)	−0.008 (2)	0.023 (5)*
H2A	0.254 (3)	0.086 (3)	0.350 (2)	0.029 (5)*
H2B	0.189 (3)	−0.068 (3)	0.264 (2)	0.030 (5)*
H3A	0.513 (4)	0.532 (3)	0.381 (2)	0.037 (5)*
H3B	0.325 (3)	0.458 (3)	0.326 (2)	0.027 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Gd1	0.00572 (4)	0.00572 (4)	0.00615 (4)	0.000	0.00367 (3)	0.000
Cl1	0.00989 (11)	0.00916 (11)	0.00986 (11)	−0.00088 (8)	0.00532 (10)	−0.00202 (8)
Cl2	0.01014 (16)	0.01129 (16)	0.01144 (16)	0.000	0.00685 (14)	0.000
O1	0.0083 (4)	0.0145 (4)	0.0100 (4)	0.0004 (3)	0.0046 (3)	0.0025 (3)
O2	0.0127 (4)	0.0110 (4)	0.0138 (4)	−0.0024 (3)	0.0098 (3)	−0.0017 (3)
O3	0.0100 (4)	0.0088 (4)	0.0151 (4)	−0.0010 (3)	0.0078 (3)	−0.0032 (3)

Geometric parameters (Å, º)

Gd1—Cl1^{i}	2.7699 (3)	Gd1—O3^{i}	2.3762 (8)
Gd1—Cl1	2.7699 (3)	O1—H1A	0.79 (2)
Gd1—O1	2.4026 (9)	O1—H1B	0.75 (2)
Gd1—O1^{i}	2.4026 (9)	O2—H2A	0.80 (2)
Gd1—O2^{i}	2.4101 (8)	O2—H2B	0.82 (2)
Gd1—O2	2.4101 (8)	O3—H3A	0.83 (2)
Gd1—O3	2.3762 (8)	O3—H3B	0.79 (2)
Cl1—Gd1—Cl1^{i}	83.855 (12)	O3^{i}—Gd1—O1^{i}	75.58 (3)
O1^{i}—Gd1—Cl1^{i}	76.37 (2)	O3—Gd1—O1^{i}	69.37 (3)
O1—Gd1—Cl1	76.37 (2)	O3^{i}—Gd1—O1	69.37 (3)
O1—Gd1—Cl1^{i}	146.74 (2)	O3—Gd1—O1	75.58 (3)
O1^{i}—Gd1—Cl1	146.74 (2)	O3—Gd1—O2	70.41 (3)
O1—Gd1—O1^{i}	132.40 (4)	O3^{i}—Gd1—O2^{i}	70.41 (3)
O1^{i}—Gd1—O2	121.09 (3)	O3^{i}—Gd1—O2	138.44 (3)
O1^{i}—Gd1—O2^{i}	72.98 (3)	O3—Gd1—O2^{i}	138.44 (3)
O1—Gd1—O2	72.97 (3)	O3^{i}—Gd1—O3	83.65 (4)
O1—Gd1—O2^{i}	121.09 (3)	Gd1—O1—H1A	120.3 (15)
O2—Gd1—Cl1	78.99 (2)	Gd1—O1—H1B	125.0 (15)
O2^{i}—Gd1—Cl1^{i}	78.99 (2)	H1A—O1—H1B	106 (2)
O2—Gd1—Cl1^{i}	77.21 (2)	Gd1—O2—H2A	117.6 (15)
O2^{i}—Gd1—Cl1	77.21 (2)	Gd1—O2—H2B	121.9 (14)
O2—Gd1—O2^{i}	147.83 (4)	H2A—O2—H2B	108 (2)
O3—Gd1—Cl1	143.24 (2)	Gd1—O3—H3A	121.6 (14)
O3—Gd1—Cl1^{i}	107.92 (2)	Gd1—O3—H3B	121.0 (14)

O3^{i}—Gd1—Cl1	107.92 (2)	H3A—O3—H3B	106 (2)
O3^{i}—Gd1—Cl1^{i}	143.24 (2)		

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···Cl1^{ii}	0.79 (2)	2.39 (2)	3.1527 (9)	165 (2)
O1—H1*B*···Cl2^{iii}	0.75 (2)	2.43 (2)	3.1651 (9)	170.1 (19)
O2—H2*A*···Cl1^{iv}	0.80 (2)	2.36 (2)	3.1519 (9)	175 (2)
O2—H2*B*···Cl2^{v}	0.82 (2)	2.44 (2)	3.2284 (9)	161.7 (18)
O3—H3*A*···Cl1^{vi}	0.83 (2)	2.30 (2)	3.1290 (9)	178 (2)
O3—H3*B*···Cl2	0.79 (2)	2.40 (2)	3.1790 (9)	169.1 (19)

Symmetry codes: (ii) −*x*, −*y*, −*z*; (iii) −*x*, −*y*+1, −*z*; (iv) *x*, −*y*, *z*+1/2; (v) *x*, *y*−1, *z*; (vi) −*x*+1, *y*+1, −*z*+1/2.

Hexaaquadichloridoterbium(III) chloride (Tb)

Crystal data

$[TbCl_2(H_2O)_6]Cl$
M_r = 373.37
Monoclinic, *P*2/*c*
a = 7.8646 (3) Å
b = 6.4903 (3) Å
c = 11.9871 (5) Å
β = 127.134 (1)°
V = 487.79 (4) Å^3
Z = 2
F(000) = 352
D_x = 2.542 Mg m^{-3}
Ag *Kα* radiation, *λ* = 0.56086 Å
Cell parameters from 9445 reflections
θ = 2.5–23.7°
μ = 4.24 mm^{-1}
T = 100 K
Plate, colorless
0.3 × 0.16 × 0.12 mm

Data collection

Bruker D8 Venture Duo diffractometer
ω scans
Absorption correction: multi-scan SADABS-2016/2 (Bruker, 2016)
T_{min} = 0.223, T_{max} = 0.257
11117 measured reflections
1503 independent reflections
1481 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 23.7°, θ_{min} = 2.5°
h = −10→11
k = −9→9
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.009
$wR(F^2)$ = 0.020
S = 1.10
1503 reflections
72 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.008P)^2 + 0.0701P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}
Extinction correction: SHELXL-2018/1 (Sheldrick 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0117 (6)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Tb1	0.500000	0.15305 (2)	0.250000	0.00536 (3)
Cl1	0.29840 (4)	−0.16404 (4)	0.05842 (3)	0.00937 (5)
Cl2	0.000000	0.62554 (6)	0.250000	0.01012 (7)
O1	0.16832 (14)	0.30085 (14)	0.06248 (10)	0.01064 (16)
O2	0.23848 (14)	0.05048 (15)	0.28092 (10)	0.01085 (16)
O3	0.44279 (14)	0.42471 (14)	0.35533 (9)	0.01056 (16)
H1A	0.065 (3)	0.265 (3)	0.049 (2)	0.026 (5)*
H1B	0.139 (3)	0.325 (3)	−0.011 (2)	0.028 (5)*
H2A	0.257 (3)	0.088 (3)	0.353 (2)	0.030 (5)*
H2B	0.194 (3)	−0.058 (3)	0.262 (2)	0.026 (5)*
H3A	0.519 (3)	0.525 (3)	0.383 (2)	0.028 (5)*
H3B	0.327 (3)	0.453 (3)	0.326 (2)	0.033 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Tb1	0.00486 (4)	0.00550 (4)	0.00570 (4)	0.000	0.00318 (3)	0.000
Cl1	0.00902 (11)	0.00878 (12)	0.00908 (11)	−0.00078 (8)	0.00481 (10)	−0.00186 (9)
Cl2	0.00953 (16)	0.01080 (17)	0.01046 (17)	0.000	0.00626 (14)	0.000
O1	0.0076 (4)	0.0132 (4)	0.0094 (4)	0.0004 (3)	0.0043 (3)	0.0024 (3)
O2	0.0123 (4)	0.0102 (4)	0.0132 (4)	−0.0030 (3)	0.0094 (3)	−0.0027 (3)
O3	0.0089 (4)	0.0088 (4)	0.0145 (4)	−0.0011 (3)	0.0073 (3)	−0.0035 (3)

Geometric parameters (Å, º)

Tb1—Cl1^{i}	2.7617 (3)	Tb1—O3	2.3646 (9)
Tb1—Cl1	2.7617 (3)	O1—H1A	0.77 (2)
Tb1—O1	2.3870 (9)	O1—H1B	0.77 (2)
Tb1—O1^{i}	2.3870 (9)	O2—H2A	0.82 (2)
Tb1—O2^{i}	2.3940 (9)	O2—H2B	0.76 (2)
Tb1—O2	2.3940 (9)	O3—H3A	0.81 (2)
Tb1—O3^{i}	2.3646 (9)	O3—H3B	0.77 (2)
Cl1—Tb1—Cl1^{i}	83.649 (12)	O3—Tb1—O1^{i}	69.48 (3)
O1^{i}—Tb1—Cl1^{i}	76.35 (2)	O3^{i}—Tb1—O1^{i}	75.59 (3)
O1—Tb1—Cl1	76.35 (2)	O3—Tb1—O1	75.59 (3)
O1—Tb1—Cl1^{i}	146.61 (2)	O3^{i}—Tb1—O1	69.49 (3)
O1^{i}—Tb1—Cl1	146.61 (2)	O3^{i}—Tb1—O2	138.44 (3)
O1—Tb1—O1^{i}	132.61 (4)	O3—Tb1—O2^{i}	138.44 (3)

O1^{i}—Tb1—O2	121.23 (3)	O3—Tb1—O2	70.52 (3)
O1^{i}—Tb1—O2^{i}	72.84 (3)	O3^{i}—Tb1—O2^{i}	70.52 (3)
O1—Tb1—O2	72.84 (3)	O3—Tb1—O3^{i}	83.57 (5)
O1—Tb1—O2^{i}	121.24 (3)	Tb1—O1—H1A	119.7 (16)
O2—Tb1—Cl1	78.81 (2)	Tb1—O1—H1B	124.1 (16)
O2^{i}—Tb1—Cl1^{i}	78.81 (2)	H1A—O1—H1B	106 (2)
O2—Tb1—Cl1^{i}	77.27 (2)	Tb1—O2—H2A	117.3 (14)
O2^{i}—Tb1—Cl1	77.27 (2)	Tb1—O2—H2B	119.8 (15)
O2—Tb1—O2^{i}	147.71 (5)	H2A—O2—H2B	110 (2)
O3^{i}—Tb1—Cl1	108.08 (2)	Tb1—O3—H3A	119.5 (14)
O3^{i}—Tb1—Cl1^{i}	143.22 (2)	Tb1—O3—H3B	118.8 (16)
O3—Tb1—Cl1	143.22 (2)	H3A—O3—H3B	112 (2)
O3—Tb1—Cl1^{i}	108.08 (2)		

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···Cl1^{ii}	0.77 (2)	2.41 (2)	3.1527 (9)	164 (2)
O1—H1*B*···Cl2^{iii}	0.77 (2)	2.40 (2)	3.1661 (10)	172 (2)
O2—H2*A*···Cl1^{iv}	0.82 (2)	2.33 (2)	3.1524 (10)	175 (2)
O2—H2*B*···Cl2^{v}	0.76 (2)	2.51 (2)	3.2283 (10)	158.8 (19)
O3—H3*A*···Cl1^{vi}	0.81 (2)	2.33 (2)	3.1297 (10)	173.2 (19)
O3—H3*B*···Cl2	0.77 (2)	2.43 (2)	3.1798 (9)	166 (2)

Symmetry codes: (ii) −*x*, −*y*, −*z*; (iii) −*x*, −*y*+1, −*z*; (iv) *x*, −*y*, *z*+1/2; (v) *x*, *y*−1, *z*; (vi) −*x*+1, *y*+1, −*z*+1/2.

Hexaaquadichloridodysprosium(III) chloride (Dy)

Crystal data

$[DyCl_2(H_2O)_6]Cl$
M_r = 376.95
Monoclinic, *P*2/*c*
a = 7.8439 (3) Å
b = 6.4693 (3) Å
c = 11.9660 (5) Å
β = 127.143 (1)°
V = 484.02 (4) Å^3
Z = 2
F(000) = 354
D_x = 2.586 Mg m^{-3}
Ag *Kα* radiation, *λ* = 0.56086 Å
Cell parameters from 9894 reflections
θ = 2.7–23.7°
μ = 4.51 mm^{-1}
T = 100 K
Plate, yellow
0.23 × 0.19 × 0.14 mm

Data collection

Bruker D8 Venture Duo diffractometer
ω scans
Absorption correction: multi-scan SADABS-2016/2 (Bruker, 2016)
T_{min} = 0.184, T_{max} = 0.257
21844 measured reflections
1501 independent reflections
1485 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 23.8°, θ_{min} = 2.5°
h = −11→11
k = −9→9
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.008$
$wR(F^2) = 0.018$
$S = 1.19$
1501 reflections
72 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.006P)^2 + 0.0553P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.48$ e Å^{-3}
Extinction correction: SHELXL-2018/1 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0098 (6)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Dy1	0.500000	0.15396 (2)	0.250000	0.00517 (3)
Cl1	0.29906 (4)	−0.16263 (3)	0.05869 (3)	0.00928 (5)
Cl2	0.000000	0.62489 (5)	0.250000	0.00990 (6)
O1	0.16915 (13)	0.30103 (12)	0.06305 (8)	0.01025 (14)
O2	0.23924 (13)	0.05125 (12)	0.28056 (9)	0.01049 (14)
O3	0.44370 (14)	0.42381 (12)	0.35560 (8)	0.01037 (14)
H1A	0.065 (3)	0.264 (3)	0.046 (2)	0.027 (4)*
H1B	0.133 (3)	0.330 (2)	−0.011 (2)	0.030 (5)*
H2A	0.253 (3)	0.086 (3)	0.349 (2)	0.034 (5)*
H2B	0.195 (3)	−0.050 (3)	0.2644 (19)	0.026 (5)*
H3A	0.513 (3)	0.525 (3)	0.3771 (18)	0.028 (4)*
H3B	0.332 (3)	0.453 (3)	0.326 (2)	0.033 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Dy1	0.00492 (4)	0.00544 (4)	0.00538 (4)	0.000	0.00322 (3)	0.000
Cl1	0.00897 (11)	0.00907 (10)	0.00889 (10)	−0.00078 (7)	0.00491 (9)	−0.00194 (7)
Cl2	0.00935 (15)	0.01086 (13)	0.01022 (15)	0.000	0.00630 (13)	0.000
O1	0.0068 (3)	0.0132 (3)	0.0090 (3)	0.0003 (3)	0.0038 (3)	0.0022 (3)
O2	0.0121 (4)	0.0100 (3)	0.0127 (4)	−0.0028 (3)	0.0093 (3)	−0.0018 (3)
O3	0.0084 (4)	0.0097 (3)	0.0137 (3)	−0.0014 (3)	0.0070 (3)	−0.0033 (3)

Geometric parameters (Å, º)

Dy1—Cl1^{i}	2.7500 (2)	Dy1—O3^{i}	2.3480 (8)
Dy1—Cl1	2.7500 (2)	O1—H1A	0.755 (19)
Dy1—O1	2.3735 (8)	O1—H1B	0.78 (2)
Dy1—O1^{i}	2.3735 (8)	O2—H2A	0.79 (2)

Dy1—O2^{i}	2.3796 (8)	O2—H2B	0.712 (19)
Dy1—O2	2.3795 (8)	O3—H3A	0.787 (19)
Dy1—O3	2.3480 (8)	O3—H3B	0.75 (2)
Cl1—Dy1—Cl1^{i}	83.719 (11)	O3^{i}—Dy1—O1^{i}	75.83 (3)
O1^{i}—Dy1—Cl1^{i}	76.29 (2)	O3—Dy1—O1^{i}	69.43 (3)
O1—Dy1—Cl1	76.29 (2)	O3^{i}—Dy1—O1	69.43 (3)
O1—Dy1—Cl1^{i}	146.52 (2)	O3—Dy1—O1	75.83 (3)
O1^{i}—Dy1—Cl1	146.52 (2)	O3—Dy1—O2	70.52 (3)
O1—Dy1—O1^{i}	132.73 (4)	O3^{i}—Dy1—O2^{i}	70.52 (3)
O1^{i}—Dy1—O2	121.28 (3)	O3^{i}—Dy1—O2	138.48 (3)
O1^{i}—Dy1—O2^{i}	72.82 (3)	O3—Dy1—O2^{i}	138.48 (3)
O1—Dy1—O2	72.82 (3)	O3^{i}—Dy1—O3	83.94 (4)
O1—Dy1—O2^{i}	121.28 (3)	Dy1—O1—H1A	121.1 (14)
O2—Dy1—Cl1	78.83 (2)	Dy1—O1—H1B	127.6 (15)
O2^{i}—Dy1—Cl1^{i}	78.82 (2)	H1A—O1—H1B	101 (2)
O2—Dy1—Cl1^{i}	77.17 (2)	Dy1—O2—H2A	119.3 (15)
O2^{i}—Dy1—Cl1	77.17 (2)	Dy1—O2—H2B	122.6 (15)
O2—Dy1—O2^{i}	147.57 (4)	H2A—O2—H2B	106 (2)
O3—Dy1—Cl1	143.34 (2)	Dy1—O3—H3A	118.6 (13)
O3—Dy1—Cl1^{i}	107.77 (2)	Dy1—O3—H3B	118.8 (15)
O3^{i}—Dy1—Cl1	107.77 (2)	H3A—O3—H3B	109.0 (19)
O3^{i}—Dy1—Cl1^{i}	143.34 (2)		

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···Cl1^{ii}	0.755 (19)	2.413 (19)	3.1545 (9)	167.6 (19)
O1—H1*B*···Cl2^{iii}	0.78 (2)	2.39 (2)	3.1655 (8)	172.6 (16)
O2—H2*A*···Cl1^{iv}	0.79 (2)	2.37 (2)	3.1511 (9)	175.7 (19)
O2—H2*B*···Cl2^{v}	0.712 (19)	2.544 (19)	3.2303 (8)	162.7 (19)
O3—H3*A*···Cl1^{vi}	0.787 (19)	2.342 (19)	3.1276 (8)	176.2 (18)
O3—H3*B*···Cl2	0.75 (2)	2.44 (2)	3.1766 (8)	167.1 (19)

Symmetry codes: (ii) −*x*, −*y*, −*z*; (iii) −*x*, −*y*+1, −*z*; (iv) *x*, −*y*, *z*+1/2; (v) *x*, *y*−1, *z*; (vi) −*x*+1, *y*+1, −*z*+1/2.

Hexaaquadichloridoholmium(III) chloride (Ho)

Crystal data

$[HoCl_2(H_2O)_6]Cl$
M_r = 379.38
Monoclinic, *P*2/*c*
a = 7.8303 (3) Å
b = 6.4651 (2) Å
c = 11.9509 (4) Å
β = 127.086 (1)°
V = 482.63 (3) Å^3
Z = 2

F(000) = 356
D_x = 2.611 Mg m^{-3}
Ag *Kα* radiation, *λ* = 0.56086 Å
Cell parameters from 7807 reflections
θ = 2.5–23.7°
μ = 4.77 mm^{-1}
T = 100 K
Plate, yellow
0.14 × 0.10 × 0.07 mm

Data collection

Bruker D8 Venture Duo diffractometer
ω scans
Absorption correction: multi-scan SADABS-2016/2 (Bruker, 2016)
T_{min} = 0.222, T_{max} = 0.257
10309 measured reflections
1480 independent reflections
1454 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 23.7°, θ_{min} = 2.5°
h = −11→11
k = −9→9
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.009
$wR(F^2)$ = 0.020
S = 1.07
1480 reflections
72 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0056P)^2 + 0.0614P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Extinction correction: SHELXL-2018/1 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0063 (5)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Ho1	0.500000	0.15471 (2)	0.250000	0.00548 (3)
Cl1	0.29952 (5)	−0.16158 (4)	0.05941 (3)	0.00938 (5)
Cl2	0.000000	0.62505 (6)	0.250000	0.01026 (8)
O1	0.17011 (16)	0.30132 (14)	0.06373 (10)	0.01068 (17)
O2	0.24000 (16)	0.05173 (14)	0.28059 (10)	0.01065 (17)
O3	0.44395 (16)	0.42345 (14)	0.35534 (10)	0.01033 (17)
H1A	0.063 (3)	0.262 (3)	0.047 (2)	0.027 (5)*
H1B	0.140 (4)	0.330 (3)	−0.008 (3)	0.030 (6)*
H2A	0.253 (4)	0.091 (3)	0.348 (2)	0.029 (6)*
H2B	0.188 (3)	−0.059 (3)	0.260 (2)	0.026 (5)*
H3A	0.518 (4)	0.522 (3)	0.384 (2)	0.035 (6)*
H3B	0.322 (4)	0.459 (3)	0.325 (2)	0.029 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ho1	0.00520 (4)	0.00572 (4)	0.00561 (4)	0.000	0.00329 (3)	0.000
Cl1	0.00892 (13)	0.00922 (11)	0.00888 (12)	−0.00084 (9)	0.00478 (11)	−0.00183 (9)
Cl2	0.00948 (18)	0.01124 (17)	0.01035 (18)	0.000	0.00613 (16)	0.000
O1	0.0081 (4)	0.0135 (4)	0.0091 (4)	0.0002 (3)	0.0045 (4)	0.0023 (3)
O2	0.0122 (4)	0.0098 (4)	0.0130 (4)	−0.0027 (3)	0.0092 (4)	−0.0023 (3)

O3	0.0085 (4)	0.0092 (4)	0.0135 (4)	−0.0011 (3)	0.0067 (4)	−0.0027 (3)

Geometric parameters (Å, º)

Ho1—Cl1^{i}	2.7425 (3)	Ho1—O3^{i}	2.3372 (9)
Ho1—Cl1	2.7425 (3)	O1—H1A	0.78 (2)
Ho1—O1	2.3646 (10)	O1—H1B	0.76 (2)
Ho1—O1^{i}	2.3646 (10)	O2—H2A	0.79 (2)
Ho1—O2^{i}	2.3706 (9)	O2—H2B	0.79 (2)
Ho1—O2	2.3705 (9)	O3—H3A	0.79 (2)
Ho1—O3	2.3372 (9)	O3—H3B	0.82 (2)
Cl1—Ho1—Cl1^{i}	83.578 (12)	O3^{i}—Ho1—O1^{i}	75.86 (3)
O1^{i}—Ho1—Cl1^{i}	76.33 (2)	O3—Ho1—O1^{i}	69.40 (3)
O1—Ho1—Cl1	76.33 (2)	O3^{i}—Ho1—O1	69.41 (3)
O1—Ho1—Cl1^{i}	146.51 (3)	O3—Ho1—O1	75.86 (3)
O1^{i}—Ho1—Cl1	146.51 (3)	O3—Ho1—O2	70.61 (3)
O1—Ho1—O1^{i}	132.74 (5)	O3^{i}—Ho1—O2^{i}	70.61 (3)
O1^{i}—Ho1—O2	121.30 (3)	O3^{i}—Ho1—O2	138.55 (3)
O1^{i}—Ho1—O2^{i}	72.88 (3)	O3—Ho1—O2^{i}	138.55 (3)
O1—Ho1—O2	72.88 (3)	O3^{i}—Ho1—O3	83.96 (5)
O1—Ho1—O2^{i}	121.31 (3)	Ho1—O1—H1A	120.3 (16)
O2—Ho1—Cl1	78.70 (2)	Ho1—O1—H1B	125.2 (17)
O2^{i}—Ho1—Cl1^{i}	78.70 (2)	H1A—O1—H1B	104 (2)
O2—Ho1—Cl1^{i}	77.13 (2)	Ho1—O2—H2A	118.2 (16)
O2^{i}—Ho1—Cl1	77.13 (2)	Ho1—O2—H2B	122.9 (15)
O2—Ho1—O2^{i}	147.38 (5)	H2A—O2—H2B	109 (2)
O3—Ho1—Cl1	143.35 (3)	Ho1—O3—H3A	120.6 (16)
O3—Ho1—Cl1^{i}	107.83 (2)	Ho1—O3—H3B	121.1 (14)
O3^{i}—Ho1—Cl1	107.83 (2)	H3A—O3—H3B	109 (2)
O3^{i}—Ho1—Cl1^{i}	143.35 (3)		

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···Cl1^{ii}	0.78 (2)	2.40 (2)	3.1589 (11)	166 (2)
O1—H1*B*···Cl2^{iii}	0.76 (2)	2.41 (2)	3.1678 (10)	170 (2)
O2—H2*A*···Cl1^{iv}	0.79 (2)	2.37 (2)	3.1546 (10)	172 (2)
O2—H2*B*···Cl2^{v}	0.79 (2)	2.48 (2)	3.2320 (10)	161.6 (19)
O3—H3*A*···Cl1^{vi}	0.79 (2)	2.35 (2)	3.1309 (10)	172 (2)
O3—H3*B*···Cl2	0.82 (2)	2.36 (2)	3.1765 (10)	168.9 (19)

Symmetry codes: (ii) −*x*, −*y*, −*z*; (iii) −*x*, −*y*+1, −*z*; (iv) *x*, −*y*, *z*+1/2; (v) *x*, *y*−1, *z*; (vi) −*x*+1, *y*+1, −*z*+1/2.

Hexaaquadichloridoerbium(III) chloride (Er)

Crystal data

$[ErCl_2(H_2O)_6]Cl$
M_r = 381.71
Monoclinic, $P2/c$
a = 7.8035 (2) Å
b = 6.4488 (2) Å
c = 11.9182 (4) Å
β = 127.044 (1)°
V = 478.71 (3) Å^3
Z = 2
$F(000)$ = 358
D_x = 2.648 Mg m^{-3}
Ag $K\alpha$ radiation, λ = 0.56086 Å
Cell parameters from 9658 reflections
θ = 2.5–23.7°
μ = 5.07 mm^{-1}
T = 100 K
Plate, pink
0.23 × 0.22 × 0.17 mm

Data collection

Bruker D8 Venture Duo diffractometer
ω scans
Absorption correction: multi-scan SADABS-2016/2 (Bruker, 2016)
T_{min} = 0.175, T_{max} = 0.257
24599 measured reflections
1481 independent reflections
1479 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 23.7°, θ_{min} = 2.5°
h = −11→10
k = −9→9
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.009
$wR(F^2)$ = 0.020
S = 1.30
1481 reflections
72 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0069P)^2 + 0.1191P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.88 e Å^{-3}
Extinction correction: SHELXL-2018/1 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0321 (9)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Er1	0.500000	0.15555 (2)	0.250000	0.00519 (3)
Cl1	0.29999 (4)	−0.16033 (4)	0.05990 (3)	0.00919 (5)
Cl2	0.000000	0.62527 (6)	0.250000	0.00995 (7)
O1	0.17058 (14)	0.30150 (14)	0.06411 (10)	0.01031 (15)
O2	0.24065 (14)	0.05247 (15)	0.28058 (10)	0.01036 (15)
O3	0.44402 (15)	0.42330 (14)	0.35511 (10)	0.01044 (15)
H1A	0.062 (4)	0.263 (4)	0.048 (2)	0.029 (5)*
H1B	0.141 (4)	0.332 (3)	−0.007 (3)	0.029 (6)*
H2A	0.259 (4)	0.083 (4)	0.348 (2)	0.027 (5)*

H2B	0.193 (3)	−0.061 (4)	0.263 (2)	0.024 (5)*
H3A	0.518 (4)	0.519 (4)	0.380 (2)	0.029 (5)*
H3B	0.327 (4)	0.455 (4)	0.323 (2)	0.030 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Er1	0.00491 (4)	0.00568 (4)	0.00476 (4)	0.000	0.00279 (3)	0.000
Cl1	0.00883 (11)	0.00906 (12)	0.00820 (12)	−0.00080 (8)	0.00435 (10)	−0.00190 (8)
Cl2	0.00931 (15)	0.01105 (16)	0.00951 (16)	0.000	0.00568 (14)	0.000
O1	0.0075 (4)	0.0128 (4)	0.0083 (4)	0.0003 (3)	0.0036 (3)	0.0022 (3)
O2	0.0119 (4)	0.0105 (4)	0.0110 (4)	−0.0024 (3)	0.0081 (3)	−0.0017 (3)
O3	0.0087 (4)	0.0091 (4)	0.0130 (4)	−0.0011 (3)	0.0063 (3)	−0.0033 (3)

Geometric parameters (Å, º)

Er1—Cl1	2.7309 (3)	Er1—O3^{i}	2.3239 (9)
Er1—Cl1^{i}	2.7309 (3)	O1—H1A	0.78 (2)
Er1—O1	2.3538 (9)	O1—H1B	0.76 (3)
Er1—O1^{i}	2.3538 (9)	O2—H2A	0.76 (2)
Er1—O2^{i}	2.3579 (9)	O2—H2B	0.79 (2)
Er1—O2	2.3578 (9)	O3—H3A	0.77 (2)
Er1—O3	2.3239 (9)	O3—H3B	0.78 (2)
Cl1^{i}—Er1—Cl1	83.525 (12)	O3^{i}—Er1—O1^{i}	75.93 (3)
O1^{i}—Er1—Cl1	146.45 (2)	O3—Er1—O1^{i}	69.45 (3)
O1—Er1—Cl1^{i}	146.45 (2)	O3^{i}—Er1—O1	69.45 (3)
O1—Er1—Cl1	76.30 (2)	O3—Er1—O1	75.93 (3)
O1^{i}—Er1—Cl1^{i}	76.30 (2)	O3—Er1—O2	70.65 (3)
O1—Er1—O1^{i}	132.86 (5)	O3^{i}—Er1—O2^{i}	70.65 (3)
O1^{i}—Er1—O2	121.31 (3)	O3^{i}—Er1—O2	138.62 (3)
O1^{i}—Er1—O2^{i}	72.89 (3)	O3—Er1—O2^{i}	138.62 (3)
O1—Er1—O2	72.89 (3)	O3^{i}—Er1—O3	84.03 (5)
O1—Er1—O2^{i}	121.31 (3)	Er1—O1—H1A	120.7 (17)
O2—Er1—Cl1^{i}	77.07 (2)	Er1—O1—H1B	125.5 (19)
O2^{i}—Er1—Cl1	77.07 (2)	H1A—O1—H1B	104 (2)
O2—Er1—Cl1	78.64 (2)	Er1—O2—H2A	117.7 (17)
O2^{i}—Er1—Cl1^{i}	78.64 (2)	Er1—O2—H2B	122.2 (15)
O2—Er1—O2^{i}	147.25 (5)	H2A—O2—H2B	106 (2)
O3—Er1—Cl1^{i}	107.82 (2)	Er1—O3—H3A	117.0 (17)
O3—Er1—Cl1	143.35 (2)	Er1—O3—H3B	118.2 (17)
O3^{i}—Er1—Cl1^{i}	143.35 (2)	H3A—O3—H3B	112 (2)
O3^{i}—Er1—Cl1	107.82 (2)		

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···Cl1^{ii}	0.78 (2)	2.39 (2)	3.1557 (10)	166 (2)
O1—H1*B*···Cl2^{iii}	0.76 (3)	2.41 (3)	3.1632 (10)	170 (2)
O2—H2*A*···Cl1^{iv}	0.76 (2)	2.39 (2)	3.1502 (10)	176 (2)
O2—H2*B*···Cl2^{v}	0.79 (2)	2.47 (2)	3.2287 (10)	161 (2)
O3—H3*A*···Cl1^{vi}	0.77 (2)	2.36 (2)	3.1286 (10)	172 (2)
O3—H3*B*···Cl2	0.78 (2)	2.41 (2)	3.1689 (9)	167 (2)

Symmetry codes: (ii) −*x*, −*y*, −*z*; (iii) −*x*, −*y*+1, −*z*; (iv) *x*, −*y*, *z*+1/2; (v) *x*, *y*−1, *z*; (vi) −*x*+1, *y*+1, −*z*+1/2.

Hexaaquadichloridotantalum(III) chloride (Tm)

Crystal data

$[TmCl_2(H_2O)_6]Cl$
M_r = 383.38
Monoclinic, *P*2/*c*
a = 7.7889 (4) Å
b = 6.4490 (3) Å
c = 11.8760 (6) Å
β = 126.961 (1)°
V = 476.66 (4) Å^3
Z = 2
F(000) = 360
D_x = 2.671 Mg m^{-3}
Ag *Kα* radiation, *λ* = 0.56086 Å
Cell parameters from 9923 reflections
θ = 2.6–23.7°
μ = 5.37 mm^{-1}
T = 100 K
Plate, colorless
0.17 × 0.11 × 0.10 mm

Data collection

Bruker D8 Venture Duo diffractometer
ω scans
Absorption correction: multi-scan SADABS-2016/2 (Bruker, 2016)
T_{min} = 0.207, T_{max} = 0.257
16364 measured reflections
1481 independent reflections
1464 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 23.7°, θ_{min} = 2.5°
h = −11→11
k = −9→9
l = −17→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.007
$wR(F^2)$ = 0.016
S = 1.15
1481 reflections
72 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + 0.0685P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}
Extinction correction: SHELXL-2018/1 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0056 (5)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Tm1	0.500000	0.15657 (2)	0.250000	0.00505 (3)
Cl1	0.30008 (4)	−0.15947 (3)	0.06069 (2)	0.00896 (4)
Cl2	0.000000	0.62678 (5)	0.250000	0.00941 (6)
O1	0.17163 (12)	0.30137 (11)	0.06506 (8)	0.00987 (13)
O2	0.24195 (12)	0.05360 (12)	0.28076 (8)	0.00989 (13)
O3	0.44427 (13)	0.42399 (11)	0.35464 (8)	0.01000 (13)
H1A	0.072 (3)	0.261 (3)	0.050 (2)	0.032 (5)*
H1B	0.140 (3)	0.331 (2)	−0.012 (2)	0.020 (4)*
H2A	0.252 (3)	0.089 (3)	0.347 (2)	0.033 (5)*
H2B	0.197 (3)	−0.052 (3)	0.2624 (18)	0.019 (4)*
H3A	0.518 (3)	0.523 (3)	0.3800 (19)	0.028 (4)*
H3B	0.332 (3)	0.458 (3)	0.3247 (19)	0.023 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Tm1	0.00468 (3)	0.00528 (3)	0.00526 (3)	0.000	0.00302 (2)	0.000
Cl1	0.00875 (9)	0.00886 (9)	0.00844 (9)	−0.00085 (7)	0.00472 (8)	−0.00185 (7)
Cl2	0.00877 (13)	0.01055 (13)	0.00955 (13)	0.000	0.00584 (12)	0.000
O1	0.0068 (3)	0.0126 (3)	0.0084 (3)	0.0002 (2)	0.0037 (3)	0.0021 (2)
O2	0.0117 (3)	0.0094 (3)	0.0117 (3)	−0.0028 (3)	0.0087 (3)	−0.0021 (3)
O3	0.0085 (3)	0.0087 (3)	0.0134 (3)	−0.0013 (3)	0.0069 (3)	−0.0033 (2)

Geometric parameters (Å, º)

Tm1—Cl1	2.7246 (2)	Tm1—O3^{i}	2.3142 (7)
Tm1—Cl1^{i}	2.7246 (2)	O1—H1A	0.73 (2)
Tm1—O1^{i}	2.3414 (7)	O1—H1B	0.81 (2)
Tm1—O1	2.3414 (7)	O2—H2A	0.78 (2)
Tm1—O2^{i}	2.3446 (8)	O2—H2B	0.737 (18)
Tm1—O2	2.3446 (8)	O3—H3A	0.789 (19)
Tm1—O3	2.3142 (7)	O3—H3B	0.75 (2)
Cl1^{i}—Tm1—Cl1	83.158 (10)	O3^{i}—Tm1—O1	69.57 (3)
O1—Tm1—Cl1	76.368 (19)	O3—Tm1—O1	75.80 (3)
O1^{i}—Tm1—Cl1^{i}	76.368 (19)	O3^{i}—Tm1—O1^{i}	75.80 (3)
O1^{i}—Tm1—Cl1	146.34 (2)	O3—Tm1—O1^{i}	69.57 (3)
O1—Tm1—Cl1^{i}	146.34 (2)	O3—Tm1—O2	70.87 (3)
O1^{i}—Tm1—O1	132.99 (4)	O3^{i}—Tm1—O2^{i}	70.87 (3)
O1—Tm1—O2	72.77 (3)	O3^{i}—Tm1—O2	138.58 (3)
O1—Tm1—O2^{i}	121.47 (3)	O3—Tm1—O2^{i}	138.58 (3)
O1^{i}—Tm1—O2	121.47 (3)	O3^{i}—Tm1—O3	83.65 (4)
O1^{i}—Tm1—O2^{i}	72.77 (3)	Tm1—O1—H1A	118.9 (16)
O2—Tm1—Cl1^{i}	77.157 (19)	Tm1—O1—H1B	124.8 (13)
O2^{i}—Tm1—Cl1	77.156 (19)	H1A—O1—H1B	105 (2)

O2—Tm1—Cl1	78.38 (2)	Tm1—O2—H2A	120.0 (15)
O2^{i}—Tm1—Cl1^{i}	78.38 (2)	Tm1—O2—H2B	120.9 (14)
O2—Tm1—O2^{i}	147.09 (4)	H2A—O2—H2B	108 (2)
O3—Tm1—Cl1^{i}	108.24 (2)	Tm1—O3—H3A	118.8 (14)
O3—Tm1—Cl1	143.31 (2)	Tm1—O3—H3B	120.2 (13)
O3^{i}—Tm1—Cl1^{i}	143.31 (2)	H3A—O3—H3B	108.5 (19)
O3^{i}—Tm1—Cl1	108.24 (2)		

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···Cl1^{ii}	0.73 (2)	2.44 (2)	3.1573 (8)	165 (2)
O1—H1*B*···Cl2^{iii}	0.81 (2)	2.36 (2)	3.1602 (8)	169.7 (16)
O2—H2*A*···Cl1^{iv}	0.78 (2)	2.38 (2)	3.1485 (8)	173.4 (19)
O2—H2*B*···Cl2^{v}	0.737 (18)	2.528 (18)	3.2301 (8)	159.7 (18)
O3—H3*A*···Cl1^{vi}	0.789 (19)	2.343 (19)	3.1280 (8)	173.4 (18)
O3—H3*B*···Cl2	0.75 (2)	2.43 (2)	3.1714 (8)	169.4 (17)

Symmetry codes: (ii) −*x*, −*y*, −*z*; (iii) −*x*, −*y*+1, −*z*; (iv) *x*, −*y*, *z*+1/2; (v) *x*, *y*−1, *z*; (vi) −*x*+1, *y*+1, −*z*+1/2.

Hexaaquadichloridoytterbium(III) chloride (Yb)

Crystal data

$[YbCl_2(H_2O)_6]Cl$
M_r = 387.49
Monoclinic, *P*2/*c*
a = 7.7666 (2) Å
b = 6.4305 (2) Å
c = 11.8745 (3) Å
β = 126.991 (1)°
V = 473.69 (2) Å^3
Z = 2
F(000) = 362
D_x = 2.717 Mg m^{-3}
Ag *Kα* radiation, *λ* = 0.56086 Å
Cell parameters from 9892 reflections
θ = 3.0–23.7°
μ = 5.69 mm^{-1}
T = 100 K
Plate, colorless
0.30 × 0.23 × 0.20 mm

Data collection

Bruker D8 Venture Duo diffractometer
ω scans
Absorption correction: multi-scan SADABS-2016/2 (Bruker, 2016)
T_{min} = 0.168, T_{max} = 0.257
19224 measured reflections
1464 independent reflections
1439 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 23.7°, θ_{min} = 2.5°
h = −11→11
k = −9→9
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.008
$wR(F^2)$ = 0.017
S = 1.19
1464 reflections
72 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0064P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.74 e Å^{-3}

Extinction correction: SHELXL-2018/1 (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0290 (7)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Yb1	0.500000	0.15772 (2)	0.250000	0.00506 (3)
Cl1	0.30072 (4)	−0.15810 (3)	0.06078 (3)	0.00886 (5)
Cl2	0.000000	0.62670 (5)	0.250000	0.00966 (7)
O1	0.17225 (14)	0.30159 (13)	0.06541 (9)	0.01013 (15)
O2	0.24258 (13)	0.05444 (13)	0.28053 (9)	0.00973 (15)
O3	0.44456 (14)	0.42323 (12)	0.35473 (9)	0.01004 (15)
H1A	0.069 (3)	0.261 (3)	0.047 (2)	0.030 (5)*
H1B	0.148 (3)	0.330 (3)	−0.003 (2)	0.025 (5)*
H2A	0.257 (3)	0.085 (3)	0.344 (2)	0.028 (5)*
H2B	0.193 (3)	−0.059 (3)	0.2600 (19)	0.022 (4)*
H3A	0.509 (3)	0.516 (3)	0.3768 (19)	0.025 (5)*
H3B	0.318 (3)	0.461 (3)	0.321 (2)	0.026 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Yb1	0.00471 (4)	0.00511 (4)	0.00532 (4)	0.000	0.00301 (3)	0.000
Cl1	0.00835 (11)	0.00860 (10)	0.00832 (12)	−0.00077 (8)	0.00433 (10)	−0.00180 (8)
Cl2	0.00878 (15)	0.01064 (14)	0.00987 (17)	0.000	0.00577 (14)	0.000
O1	0.0073 (4)	0.0127 (3)	0.0087 (4)	0.0002 (3)	0.0040 (3)	0.0025 (3)
O2	0.0110 (4)	0.0096 (3)	0.0111 (4)	−0.0024 (3)	0.0079 (3)	−0.0020 (3)
O3	0.0084 (3)	0.0081 (3)	0.0137 (4)	−0.0015 (3)	0.0066 (3)	−0.0030 (3)

Geometric parameters (Å, º)

Yb1—Cl1	2.7173 (3)	Yb1—H2A	2.74 (2)
Yb1—Cl1^{i}	2.7173 (3)	Yb1—H3A	2.729 (18)
Yb1—O1	2.3293 (8)	O1—H1A	0.74 (2)
Yb1—O1^{i}	2.3293 (8)	O1—H1B	0.74 (2)
Yb1—O2^{i}	2.3329 (8)	O2—H2A	0.72 (2)
Yb1—O2	2.3328 (8)	O2—H2B	0.795 (19)
Yb1—O3^{i}	2.3003 (8)	O3—H3A	0.720 (19)
Yb1—O3	2.3003 (8)	O3—H3B	0.84 (2)
Cl1^{i}—Yb1—Cl1	83.270 (11)	O3^{i}—Yb1—Cl1	107.85 (2)

Cl1^{i}—Yb1—H2A	74.1 (4)	O3^{i}—Yb1—Cl1^{i}	143.42 (2)
Cl1—Yb1—H2A	91.1 (4)	O3—Yb1—Cl1^{i}	107.85 (2)
Cl1—Yb1—H3A	154.1 (4)	O3—Yb1—Cl1	143.42 (2)
Cl1^{i}—Yb1—H3A	111.2 (4)	O3^{i}—Yb1—O1^{i}	76.11 (3)
O1^{i}—Yb1—Cl1^{i}	76.26 (2)	O3—Yb1—O1^{i}	69.54 (3)
O1—Yb1—Cl1^{i}	146.22 (2)	O3^{i}—Yb1—O1	69.55 (3)
O1^{i}—Yb1—Cl1	146.22 (2)	O3—Yb1—O1	76.11 (3)
O1—Yb1—Cl1	76.26 (2)	O3—Yb1—O2^{i}	138.77 (3)
O1—Yb1—O1^{i}	133.20 (4)	O3—Yb1—O2	70.77 (3)
O1—Yb1—O2^{i}	121.35 (3)	O3^{i}—Yb1—O2^{i}	70.77 (3)
O1—Yb1—O2	72.89 (3)	O3^{i}—Yb1—O2	138.77 (3)
O1^{i}—Yb1—O2	121.35 (3)	O3—Yb1—O3^{i}	84.16 (4)
O1^{i}—Yb1—O2^{i}	72.89 (3)	O3—Yb1—H2A	60.6 (4)
O1^{i}—Yb1—H2A	108.3 (4)	O3^{i}—Yb1—H2A	138.0 (4)
O1—Yb1—H2A	79.7 (4)	O3—Yb1—H3A	13.3 (4)
O1—Yb1—H3A	80.5 (4)	O3^{i}—Yb1—H3A	73.8 (4)
O1^{i}—Yb1—H3A	59.6 (4)	H2A—Yb1—H3A	73.5 (6)
O2^{i}—Yb1—Cl1^{i}	78.50 (2)	Yb1—O1—H1A	120.9 (16)
O2—Yb1—Cl1	78.50 (2)	Yb1—O1—H1B	122.8 (16)
O2—Yb1—Cl1^{i}	76.92 (2)	H1A—O1—H1B	105 (2)
O2^{i}—Yb1—Cl1	76.92 (2)	Yb1—O2—H2A	118.2 (16)
O2—Yb1—O2^{i}	146.92 (4)	Yb1—O2—H2B	121.4 (12)
O2^{i}—Yb1—H2A	151.2 (4)	H2A—O2—H2B	108 (2)
O2—Yb1—H2A	13.3 (4)	Yb1—O3—H3A	119.6 (14)
O2—Yb1—H3A	84.0 (4)	Yb1—O3—H3B	120.0 (13)
O2^{i}—Yb1—H3A	125.8 (4)	H3A—O3—H3B	107.0 (18)

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···Cl1^{ii}	0.74 (2)	2.43 (2)	3.1570 (9)	168 (2)
O1—H1*B*···Cl2^{iii}	0.74 (2)	2.44 (2)	3.1623 (9)	167 (2)
O2—H2*A*···Cl1^{iv}	0.72 (2)	2.44 (2)	3.1486 (9)	175 (2)
O2—H2*B*···Cl2^{v}	0.795 (19)	2.472 (19)	3.2287 (9)	159.5 (16)
O3—H3*A*···Cl1^{vi}	0.720 (19)	2.409 (19)	3.1273 (9)	175.4 (19)
O3—H3*B*···Cl2	0.84 (2)	2.33 (2)	3.1643 (8)	168.8 (17)

Symmetry codes: (ii) −*x*, −*y*, −*z*; (iii) −*x*, −*y*+1, −*z*; (iv) *x*, −*y*, *z*+1/2; (v) *x*, *y*−1, *z*; (vi) −*x*+1, *y*+1, −*z*+1/2.

Hexaaquadichloridolutetium(III) chloride (Lu)

Crystal data

$[LuCl_2(H_2O)_6]Cl$
M_r = 389.42
Monoclinic, *P*2/*c*
a = 7.7621 (3) Å
b = 6.4241 (3) Å
c = 11.8671 (5) Å
β = 127.008 (1)°
V = 472.54 (4) Å^3
Z = 2
F(000) = 364
D_x = 2.737 Mg m^{-3}
Ag *Kα* radiation, *λ* = 0.56086 Å
Cell parameters from 9948 reflections
θ = 2.5–23.7°

μ = 6.00 mm^{-1}
T = 100 K

Plate, colorless
0.17 × 0.14 × 0.14 mm

Data collection

Bruker D8 Venture Duo diffractometer
ω scans
Absorption correction: multi-scan SADABS-2016/2 (Bruker, 2016)
T_{min} = 0.201, T_{max} = 0.257
23799 measured reflections

1464 independent reflections
1436 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 23.7°, θ_{min} = 2.5°
h = −11→11
k = −9→9
l = −16→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.009
$wR(F^2)$ = 0.020
S = 1.28
1464 reflections
72 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: difference Fourier map

All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + 0.3367P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.82 e Å^{-3}
Extinction correction: SHELXL-2018/1 (Sheldrick 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0094 (5)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Lu1	0.500000	0.15824 (2)	0.250000	0.00529 (4)
Cl1	0.30110 (5)	−0.15719 (6)	0.06103 (4)	0.00912 (6)
Cl2	0.000000	0.62590 (8)	0.250000	0.00994 (9)
O1	0.17244 (18)	0.30166 (18)	0.06562 (12)	0.0104 (2)
O2	0.24293 (19)	0.05447 (19)	0.28021 (12)	0.0101 (2)
O3	0.4452 (2)	0.42271 (19)	0.35486 (12)	0.0102 (2)
H1A	0.070 (4)	0.258 (4)	0.052 (3)	0.027 (7)*
H1B	0.142 (4)	0.328 (4)	−0.007 (3)	0.022 (6)*
H2A	0.255 (4)	0.086 (4)	0.344 (3)	0.028 (7)*
H2B	0.193 (4)	−0.064 (5)	0.261 (3)	0.033 (7)*
H3A	0.517 (5)	0.523 (5)	0.378 (3)	0.037 (8)*
H3B	0.328 (4)	0.454 (4)	0.322 (3)	0.026 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Lu1	0.00480 (5)	0.00564 (5)	0.00535 (4)	0.000	0.00301 (3)	0.000
Cl1	0.00841 (14)	0.00916 (14)	0.00864 (14)	−0.00059 (12)	0.00451 (12)	−0.00171 (12)
Cl2	0.0089 (2)	0.0111 (2)	0.0103 (2)	0.000	0.00602 (18)	0.000

O1	0.0070 (5)	0.0131 (5)	0.0093 (5)	−0.0002 (4)	0.0039 (4)	0.0021 (4)
O2	0.0110 (5)	0.0107 (5)	0.0115 (5)	−0.0028 (4)	0.0083 (4)	−0.0020 (4)
O3	0.0076 (5)	0.0097 (5)	0.0130 (5)	−0.0010 (4)	0.0061 (4)	−0.0028 (4)

Geometric parameters (Å, º)

Lu1—Cl1^{i}	2.7113 (4)	Lu1—O3^{i}	2.2917 (12)
Lu1—Cl1	2.7113 (4)	O1—H1A	0.77 (3)
Lu1—O1^{i}	2.3246 (11)	O1—H1B	0.76 (3)
Lu1—O1	2.3246 (11)	O2—H2A	0.73 (3)
Lu1—O2^{i}	2.3272 (12)	O2—H2B	0.82 (3)
Lu1—O2	2.3272 (12)	O3—H3A	0.79 (3)
Lu1—O3	2.2917 (12)	O3—H3B	0.77 (3)
Cl1—Lu1—Cl1^{i}	83.270 (15)	O3^{i}—Lu1—O1	69.54 (4)
O1—Lu1—Cl1^{i}	146.14 (3)	O3—Lu1—O1	76.23 (4)
O1^{i}—Lu1—Cl1	146.14 (3)	O3^{i}—Lu1—O1^{i}	76.23 (4)
O1^{i}—Lu1—Cl1^{i}	76.23 (3)	O3—Lu1—O1^{i}	69.53 (4)
O1—Lu1—Cl1	76.23 (3)	O3—Lu1—O2	70.87 (4)
O1^{i}—Lu1—O1	133.30 (6)	O3^{i}—Lu1—O2^{i}	70.87 (4)
O1—Lu1—O2	72.85 (4)	O3^{i}—Lu1—O2	138.80 (4)
O1—Lu1—O2^{i}	121.47 (4)	O3—Lu1—O2^{i}	138.80 (4)
O1^{i}—Lu1—O2	121.47 (4)	O3^{i}—Lu1—O3	84.31 (6)
O1^{i}—Lu1—O2^{i}	72.85 (4)	Lu1—O1—H1A	118 (2)
O2—Lu1—Cl1	78.41 (3)	Lu1—O1—H1B	125.0 (19)
O2^{i}—Lu1—Cl1^{i}	78.41 (3)	H1A—O1—H1B	106 (3)
O2—Lu1—Cl1^{i}	76.86 (3)	Lu1—O2—H2A	119 (2)
O2^{i}—Lu1—Cl1	76.86 (3)	Lu1—O2—H2B	121.7 (19)
O2—Lu1—O2^{i}	146.71 (6)	H2A—O2—H2B	107 (3)
O3—Lu1—Cl1	143.49 (3)	Lu1—O3—H3A	118 (2)
O3—Lu1—Cl1^{i}	107.72 (3)	Lu1—O3—H3B	117.7 (19)
O3^{i}—Lu1—Cl1	107.72 (3)	H3A—O3—H3B	109 (3)
O3^{i}—Lu1—Cl1^{i}	143.49 (3)		

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···Cl1^{ii}	0.77 (3)	2.42 (3)	3.1591 (13)	163 (3)
O1—H1*B*···Cl2^{iii}	0.76 (3)	2.40 (3)	3.1625 (12)	171 (2)
O2—H2*A*···Cl1^{iv}	0.73 (3)	2.42 (3)	3.1517 (13)	175 (3)
O2—H2*B*···Cl2^{v}	0.82 (3)	2.45 (3)	3.2327 (13)	160 (3)
O3—H3*A*···Cl1^{vi}	0.79 (3)	2.34 (3)	3.1290 (13)	174 (3)
O3—H3*B*···Cl2	0.77 (3)	2.41 (3)	3.1653 (12)	167 (3)

Symmetry codes: (ii) −*x*, −*y*, −*z*; (iii) −*x*, −*y*+1, −*z*; (iv) *x*, −*y*, *z*+1/2; (v) *x*, *y*−1, *z*; (vi) −*x*+1, *y*+1, −*z*+1/2.