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Tricaesium tetrachloridozincate(II) chloride

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(n–Cl) = 0.001 Å
R factor = 0.010
wR factor = 0.035
Data-to-parameter ratio = 20.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The crystal structure of Cs_3ZnCl_5 is isotypic with Cs_3CoCl_5 and Cs_3NiCl_5. All atoms are located on crystallographic symmetry elements, Cs at $m2m$ and 422, Zn at $\overline{4}2m$, and Cl at $4/m$ and m.

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Comment

The structure of the title compound is isotypic with Cs_3CoCl_5 (Williams *et al.*, 1980) and Cs_3NiCl_5 (Sassmannshausen & Lutz, 1998). It is built up from $ZnCl_4^-$ tetrahedra, between which Cs^+ cations and Cl^- anions are located (Fig. 1). The structure can be considered to be composed of two types of layers lying parallel to (001) (Fig. 2). One type of layer (at $z = \frac{1}{4}$ and $\frac{3}{4}$) consists of isolated nearly regular $ZnCl_4^-$ tetrahedra, with Cs^+ cations lying between them. The Zn—Cl distance is 2.2584 (6) Å, which can be compared with the value of 2.253 Å reported for Cs_2ZnCl_4 (McGinnety, 1974). The second type of layer (at z = 0 and $\frac{1}{2}$) contains Cs^+ cations forming rectangles and trapezia (Fig. 2). The Cl^- anion (Cl1) is located in the centre of each rectangle in such a way that, when the structure is viewed along the c direction, Cl^- lies exactly above atom Cs2 in the neighbouring layer (Fig. 2).

Atoms Cs1 and Cs2 are coordinated by eight and ten Cl atoms, respectively. The Cs—Cl distances lie between 3.4236 (6) and 3.6367 (6) Å for Cs1, and between 3.6232 (7)

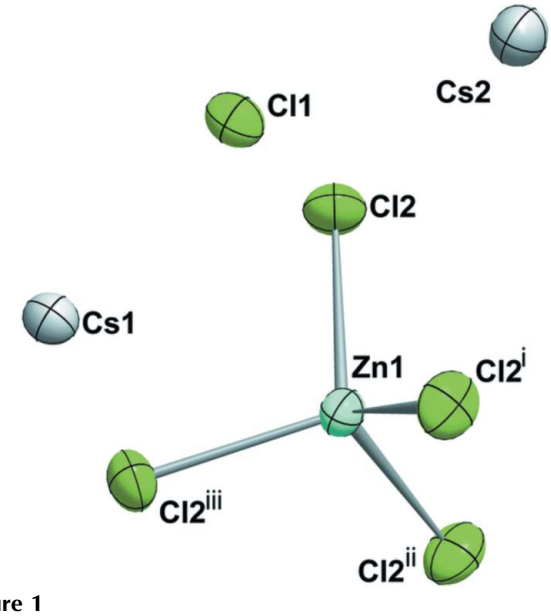

Figure 1
The asymmetric unit of Cs_3ZnCl_5, with additional Cl atoms to complete the coordination of Zn. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $x, -y, \frac{3}{2} - z$; (ii) $1 - x, y, \frac{3}{2} - z$; (iii) $1 - x, -y, z$]

and 3.8164 (6) Å for Cs2. The average distances of 3.503 and 3.778 Å for Cs1 and Cs2, respectively, are close to the corresponding values in the isotypic compound Cs_3CoCl_5 (3.502 and 3.726 Å; Williams *et al.*, 1980).

Experimental

Crystals of the title compound were obtained unintentionally in an experiment aimed at the preparation of a phosphate. Two solutions were combined, namely NaOH (2.5 mmol) and H_3PO_3 (2.5 mmol) in water (5 ml), and $ZnCO_3$ (2.5 mmol) and H_3PO_3 (1.5 mmol) in water (5 ml). The combined mixture was stirred for 8 h and the resulting solution was left to stand at room temperature for two weeks. Colourless lozenge-shaped crystals were deposited, which were filtered off and washed with a solution of ethanol–water (4:1 *v*/*v*). The chemical composition of the reported compound was confirmed by microprobe analysis.

Crystal data

Cs_3ZnCl_5
M_r = 641.4
Tetragonal, $I4/mcm$
a = 9.2421 (18) Å
c = 14.4928 (15) Å
V = 1237.9 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 11.69 mm^{-1}
T = 292 K
0.20 × 0.12 × 0.05 mm

Data collection

Oxford Diffraction XCalibur2 CCD area-detector diffractometer
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.103, T_{max} = 0.290
7208 measured reflections
374 independent reflections
349 reflections with $I > 3\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.010
$wR(F^2)$ = 0.035
S = 1.01
374 reflections
18 parameters
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *JANA2000* (Petříček *et al.*, 2000); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *JANA2000*.

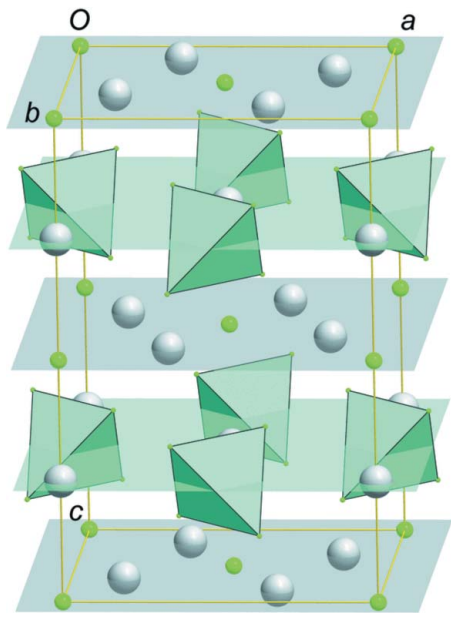

Figure 2
A view of the unit-cell contents of Cs_3ZnCl_5, with layers parallel to (001) highlighted. The $ZnCl_4^-$ anions are represented by tetrahedra.

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