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Cerium arsenate, $CeAsO_4$

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(As–O) = 0.007 Å
R factor = 0.031
wR factor = 0.082
Data-to-parameter ratio = 12.7

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

$CeAsO_4$ was synthesized by the high-temperature solid-state reaction between CeO_2, K_2CO_3 and $(NH_4)H_2AsO_4$. The compound is isostructural with compounds of the monazite structure type. The structure is built up from CeO_8 bis-disphenoids and AsO_4 tetrahedra, joined by corners and edges.

Comment

The crystal structure of cerium arsenate, $CeAsO_4$, is similar to that of the rare earth phosphates $A^{III}PO_4$, in which the atomic number of A^{III} is lower than 65 (Mooney, 1948; Niy *et al.*, 1995), *viz.* lanthanum orthovanadate $LaVO_4$ (Rice & Robinson, 1976) and cerium vanadate (Range *et al.*, 1990). The structure of these compounds has been reported in the non-conventional space group $P2_1/n$. The lanthanide phosphates have also been described in space group $P2_1/a$ (Jaulmes, 1972). The structure of $CeAsO_4$ is built up from chains of alternating edge-sharing AsO_4 tetrahedra and CeO_8 bis-disphenoids, extending parallel to the [001] direction and joined laterally by corner- and edge-sharing bis-disphenoids, which form 'zigzag'

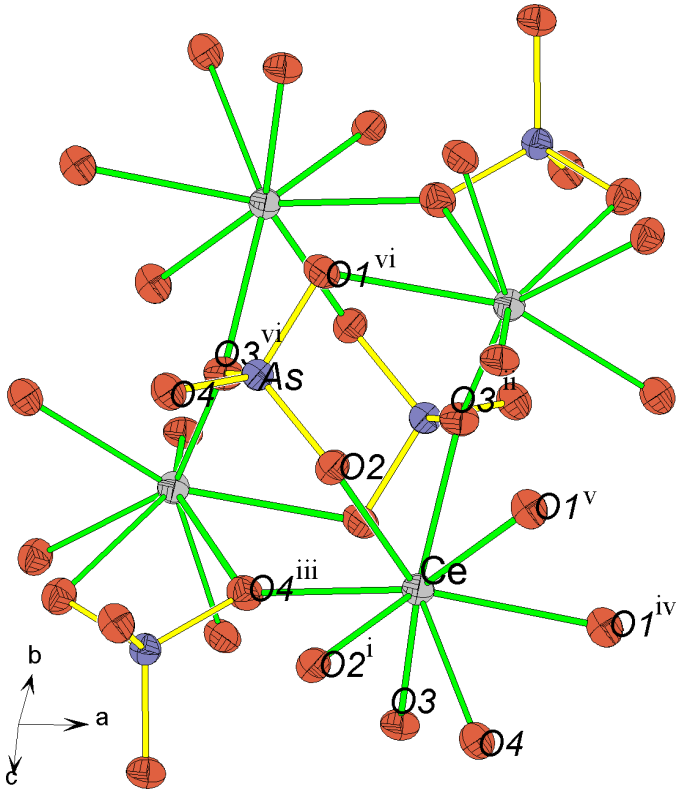

Figure 1
A view of a sheet in the structure of $CeAsO_4$, shown with 50% probability displacement ellipsoids.

chains parallel to the *a* axis. A projection of the structure, showing the displacement ellipsoids, is presented in Fig. 1.

Each CeO_8 bis-disphenoid is attached to seven AsO_4 tetrahedra and six other CeO_8 polyhedra. It shares one of its edges with a tetrahedron and two others with two CeO_8 polyhedra. It is, in addition, attached to the six tetrahedra and the remaining four CeO_8 polyhedra by sharing corners. The AsO_4 tetrahedron shares its four oxygen corners with seven different CeO_8 polyhedra, sharing an edge with one and a corner with the six others. In the present structure, the bis-disphenoid coordination polyhedron can be viewed as two interpenetrating tetrahedra, one elongated and the other compressed. The calculated valence is 2.955 for Ce (Brown & Altermatt, 1985). The AsO_4 tetrahedron is slightly distorted, due to the complex bond interaction occurring at each oxygen anion.

Experimental

Single crystals of $CeAsO_4$ were grown in a covered Pt crucible by melting a mixture of K_2CO_3, CeO_2 and $(NH_4)H_2AsO_4$ in a molar ratio of 1:4:3. The melt was heated at 1073 K for 36 h to ensure homogeneity. It was cooled to room temperature at a rate of 0.06 K min^{-1}. The product was washed with hot water. A clear colorless crystal was physically separated from the matrix for analysis.

Crystal data

$CeAsO_4$
M_r = 279.03
Monoclinic, $P2_1/n$
a = 6.975 (1) Å
b = 7.177 (1) Å
c = 6.759 (2) Å
β = 104.69 (1)°
V = 327.29 (12) Å^3
Z = 4
D_x = 5.663 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 2.8–28.0°
μ = 23.77 mm^{-1}
T = 293 (2) K
Parallelepiped, colorless
0.10 × 0.06 × 0.03 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.22, T_{max} = 0.53
1478 measured reflections
712 independent reflections
681 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 27.0°
$h = -8 \rightarrow 8$
$k = -9 \rightarrow 9$
$l = -8 \rightarrow 0$
2 standard reflections
frequency: 120 min
intensity decay: 0.4%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.082
S = 1.24
712 reflections
56 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0592P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.03
$\Delta\rho_{max}$ = 1.97 e Å^{-3}
$\Delta\rho_{min}$ = −3.18 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.46 (5)

Table 1
Selected geometric parameters (Å, °).

Ce—O2^{i}	2.460 (7)	Ce—O2	2.619 (7)
Ce—O3^{ii}	2.472 (7)	Ce—O1^{v}	2.636 (8)
Ce—O4^{iii}	2.476 (7)	As—O1^{vi}	1.683 (6)
Ce—O4	2.543 (7)	As—O4	1.685 (7)
Ce—O1^{iv}	2.551 (7)	As—O3^{vi}	1.692 (7)
Ce—O3	2.562 (6)	As—O2	1.699 (7)
O1^{vi}—As—O4	115.6 (4)	O1^{vi}—As—O2	106.7 (4)
O1^{vi}—As—O3^{vi}	103.3 (3)	O4—As—O2	99.7 (3)
O4—As—O3^{vi}	116.6 (3)	O3^{vi}—As—O2	115.0 (4)

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

Data collection: *CAD*-4 *EXPRESS* (Duisenberg, 1992; Macíček & Yordanov, 1992); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL*97.

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