Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Cadmium(II) metaarsenate(V), $CdAs_2O_6$

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(As–O) = 0.001 Å
R factor = 0.018
wR factor = 0.042
Data-to-parameter ratio = 20.0

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

Received 6 February 2001
Accepted 28 February 2001
Online 9 March 2001

$CdAs_2O_6$ is isotypic with other metaarsenates MAs_2O_6 (M = Ca, Mn, Ni, Co, Hg, Pb) and adopts the $PbSb_2O_6$ structure type. The Cd and As atoms are situated on positions with site symmetry ($\bar{3}m$) and (32), respectively. They are coordinated octahedrally by O atoms with distances d(Cd—O) = 2.302 (2) Å and d(As—O) = 1.826 (1) Å.

Comment

Like other metaarsenates $M^{II}As_2O_6$ reported by Magnéli (1941) [structure refinements: M = Ca, Pb (Losilla *et al.*, 1995); Mn, Ni, Co (Nakua & Greedan, 1995); Hg (Weil, 2000; Mormann & Jeitschko, 2000], $CdAs_2O_6$ crystallizes in the $PbSb_2O_6$ structure type (Wells, 1984), which is based on a hexagonal array of O atoms. Layers of octahedral interstices alternate along the c axis of which two-thirds are filled by As atoms and one-third by M atoms. The AsO_6 octahedra are connected by edge sharing to form honeycomb sheets with the composition $[As_2O_6]^{2-}$ (Fig. 1). The M atoms are situated below and above the vacant sites of the $[As_2O_6]^{2-}$ layers, which leads to isolated MO_6 octahedra with site symmetry ($\bar{3}m$) for the M atoms. The As atoms have site symmetry (32) (Fig. 2). The resulting distances of d(Cd—O) = 2.302 (2) Å and d(As—O) = 1.826 (1) Å compare well with d(Cd—O) = 2.31 Å and d(As—O) = 1.82 Å calculated from the radii for six-coordinated Cd and As and three-coordinated O given by Shannon (1976).

Experimental

Single crystals of $CdAs_2O_6$ were prepared by chemical transport reaction of microcrystalline material in sealed and evacuated silica ampoules using $PtCl_2$ as transport agent (993 K → 953 K, 14 d). Microcrystalline $CdAs_2O_6$ was synthesized by solid-state reaction of the binary oxides in closed silica ampoules at 953 K for 5 d.

Crystal data

As_2CdO_6
M_r = 358.24
Trigonal, $P\bar{3}1m$
a = 4.8269 (10) Å
c = 4.8660 (10) Å
V = 98.18 (4) Å^3
Z = 1
D_x = 6.059 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 9.4–17.7°
μ = 22.22 mm^{-1}
T = 293 (2) K
Prismatic, brown
0.33 × 0.31 × 0.22 mm

Data collection

Siemens–Stoe AED-2 diffractometer
$\omega/2\theta$ scans
Absorption correction: numerical (*HABITUS*; Herrendorf, 1993); see below
T_{min} = 0.019, T_{max} = 0.129
2446 measured reflections
240 independent reflections
240 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 40.0°
$h = -8 \rightarrow 8$
$k = -8 \rightarrow 8$
$l = -8 \rightarrow 8$
3 standard reflections
frequency: 120 min
intensity decay: none

 DOI: 101107/S1600536801003865

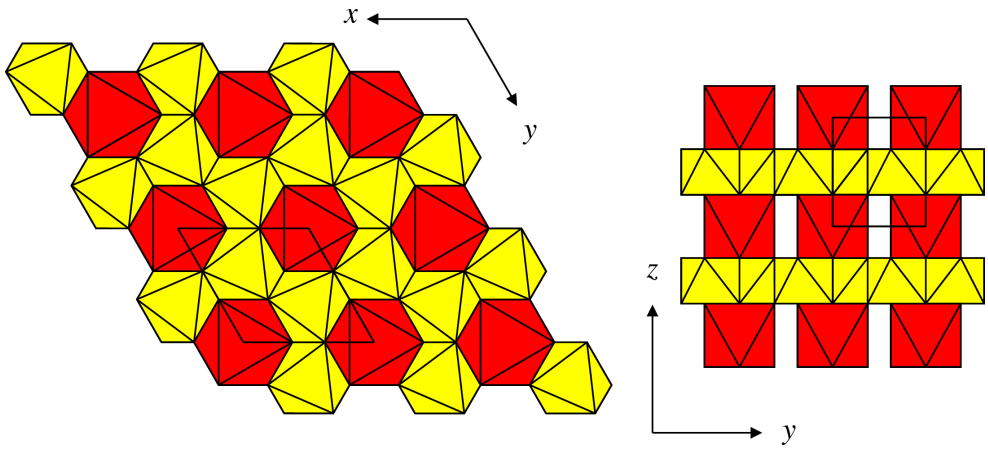

Figure 1
Projection of the structure along [001] (left) and [100] (right). CdO_6 octahedra are red and AsO_6 octahedra are yellow.

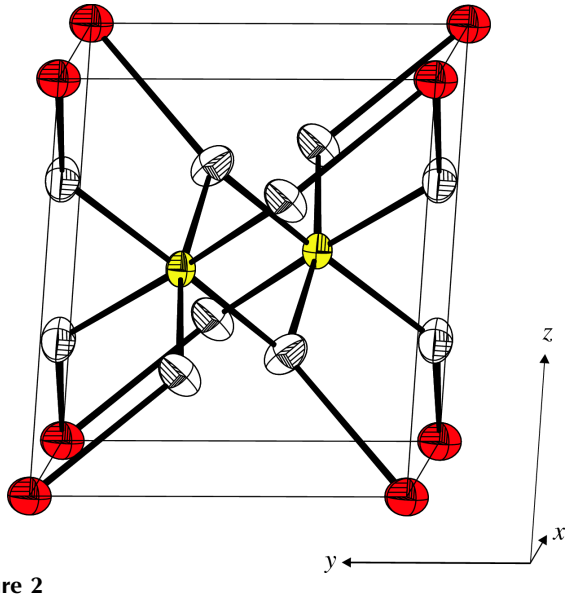

Figure 2
The unit cell with anisotropic displacement ellipsoids at the 90% probability level; Cd atoms are red and As atoms are yellow.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.018$
$wR(F^2) = 0.042$
$S = 1.23$
240 reflections
12 parameters

$w = 1/[\sigma^2(F_o^2) + (0.0116P)^2 + 0.3303P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.27$ e Å^{-3}
$\Delta\rho_{min} = -0.88$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.267 (15)

Table 1
Selected geometric parameters (Å).

Cd1—O1^{i}	2.3019 (17)	As1—O1^{ii}	1.8256 (11)

Symmetry codes: (i) $x-y-1, x-1, -z$; (ii) $-y, x-y, z$.

The crystal shape was optimized by minimizing the internal R value of ψ scan data for ten selected reflections using the program *HABITUS* (Herrendorf, 1993). The habit so derived was used for the numerical absorption correction.

Data collection: *STADI*4 (Stoe & Cie, 1995); cell refinement: *STADI*4; data reduction: *STADI*4; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ATOMS* (Dowty, 1995); software used to prepare material for publication: *SHELXL*97.

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