Crystal structure of europium arsenate, EuAsO$_4$

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Abstract

EuAsO$_4$, tetragonal, $I\bar{4}_{1}$/amd (no. 141), $a = 7.1617(2)$ Å, $c = 6.3750(2)$ Å, $V = 327.0$ Å$^3$, $Z = 4$, $R_g(F) = 0.015$, $wR_{	ext{ref}}(F^2) = 0.031$, $T = 296$ K.

Source of material

EuAsO$_4$ was prepared by heating the stoichiometric mixture of Eu$_2$O$_3$ (ChemPur, 99.9 %) and As$_2$O$_5$ (Alfa Aesar, 99.9 %) in corundum crucibles enclosed in evacuated quartz glass ampoules up to 823 K and annealed at this temperature for about two weeks [1]. Single crystals of EuAsO$_4$ were obtained by endothermic chemical transport reaction with TeCl$_4$ (Aldrich, 99 %) as transport agent [2]. The microcrystalline powder material (600 mg) was enclosed in an evacuated quartz glass tube together with the transport agent (100 mg) and then treated in the temperature range from 1348 K to 1243 K. The absence of impurities was confirmed by EDXS (Phillips XL 30, LaB$_6$ filament, Si (Li) detector, 25 kV).

Experimental details

Lattice parameters were determined by means of powder X-ray diffraction (Huber G670 camera, CoK$_\alpha$, $\lambda = 1.78897$ Å, LaB$_6$ ($a = 4.15692$ Å) as internal standard). The fitting of the peak profile and the refinement of the lattice parameters was carried out with the program WinCSD [3].

Discussion

EuAsO$_4$ crystallizes isomorphously to SmAsO$_4$ [4], DyAsO$_4$ [5], HoAsO$_4$ [2] and LuAsO$_4$ [6] in the xenotime structure type. The europium ion is surrounded by eight oxygen atoms. Six of them belong to different [AsO$_4$] tetrahedra. The [EuO$_6$] polyhedron (bisdisphenoid) can be considered as principal building unit of the structure. These condense by common edges and form interpenetrating chains parallel to [100] and [010]. The chains are interconnected via edge-linked tetrahedra in the direction of [001] forming a three-dimensional framework. Two of the coordinatizing [AsO$_4$] tetrahedra are connected to an isolated [EuO$_6$] polyhedron in equatorial position through common corners and two in axial position of the bisdisphenoid through common edges. These opposite edges are aligned parallel to [001]. The interatomic distances $d(\text{As}—\text{O}) = 1.638$ Å and $d(\text{Eu}—\text{O}) = 2.349 - 2.468$ Å correspond well with the data from related compounds HoAsO$_4$ ($d(\text{As}—\text{O}) = 1.684$ Å, $d(\text{Ho}—\text{O}) = 2.294 - 2.422$ Å [2]) and SmAsO$_4$ ($d(\text{As}—\text{O}) = 1.683$ Å, $d(\text{Sm}—\text{O}) = 2.359 - 2.480$ Å [4]).

Table 1. Data collection and handling.

| Crystal: | colorless prism, size 0.033 x 0.037 x 0.040 mm |
| Wavelength: | Ag K$_\alpha$ radiation (0.56088 Å) |
| $\mu$: | 15.403 cm$^{-1}$ |
| Diffractometer, scan mode: | Rigaku R-AXIS Spider, $\phi$-scan |
| $2\theta_{\text{max}}$: | 81.36° |
| $N(\text{hk}l)/\text{measured}, N(\text{hk}l)/\text{unique}$: | 4019, 590 |
| Criterion for $I_{\text{obs}} > 2\sigma(I_{\text{obs}})$: | $I_{\text{obs}} > 2\sigma(I_{\text{obs}})$, 511 |
| Programs: | WinCSD [3], SHELXS-97 [7], SHELX-97 [8], STRUCTURE TIDY [9], DIAMOND [10] |

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

<table>
<thead>
<tr>
<th>Atom</th>
<th>Site</th>
<th>$x$</th>
<th>$y$</th>
<th>$z$</th>
<th>$U_{11}$</th>
<th>$U_{22}$</th>
<th>$U_{33}$</th>
<th>$U_{12}$</th>
<th>$U_{13}$</th>
<th>$U_{23}$</th>
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<tbody>
<tr>
<td>Eu(1)</td>
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<td>0</td>
<td>44</td>
<td>$\frac{1}{2}$</td>
<td>0.00532(3)</td>
<td>$U_{11}$</td>
<td>0.00366(4)</td>
<td>0</td>
<td>0</td>
<td>0</td>
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<tr>
<td>As(1)</td>
<td>4b</td>
<td>0</td>
<td>44</td>
<td>$\frac{1}{2}$</td>
<td>0.00493(5)</td>
<td>$U_{11}$</td>
<td>0.00334(7)</td>
<td>0</td>
<td>0</td>
<td>0</td>
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<tr>
<td>O(1)</td>
<td>16k</td>
<td>0</td>
<td>0.0703(1)</td>
<td>0.2050(1)</td>
<td>0.0150(4)</td>
<td>0.0053(3)</td>
<td>0.0063(2)</td>
<td>0</td>
<td>0</td>
<td>$-0.0012(2)$</td>
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