

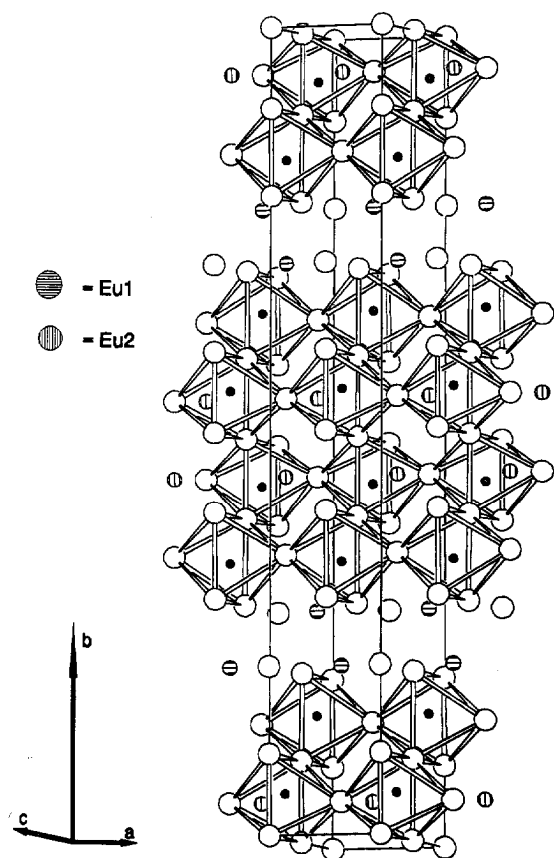
Crystal structures of dieuropium(II) ditantalum heptoxide, $\text{Eu}_2\text{Ta}_2\text{O}_7$ and europium(II) ditantalum hexoxide, EuTa_2O_6

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1. Structure of dieuropium(II) ditantalum heptoxide, $\text{Eu}_2\text{Ta}_2\text{O}_7$



Source of material: Single crystals are obtained from Ta, Eu_2O_3 and GeO_2 (molar ratio 2:1:2), using NaCl as a flux, in a sealed tantalum container at 1273 K (see ref. 1). A powder product is also obtained from Eu_2O_3 , Ta_2O_5 and NaCl (molar ratio 1:1:1) under the same conditions.

During attempts to prepare EuGeO_3 in a sealed tantalum container, $\text{Eu}_2\text{Ta}_2\text{O}_7$ was obtained previously as deep red single crystals. They grow from the container wall. $\text{Eu}_2\text{Ta}_2\text{O}_7$, like the isotopic $\text{Sr}_2\text{Ta}_2\text{O}_7$ (see ref. 2), contains quadruple layers of vertex connected octahedra with Eu^{2+} in between the $[\text{Ta}_2\text{O}_7]$ building blocks.

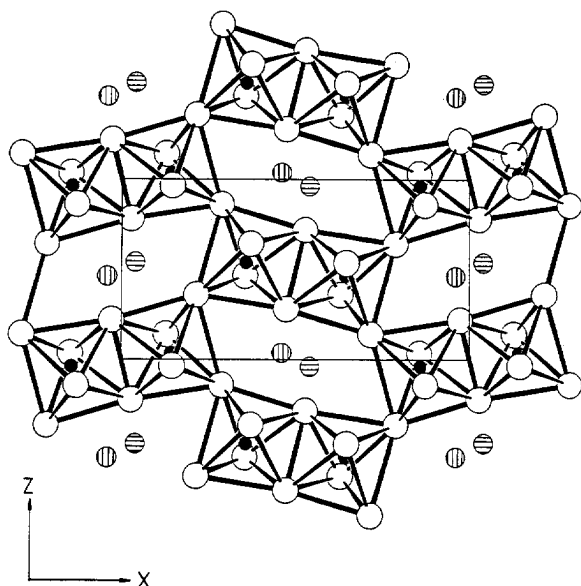
$\text{Eu}_2\text{O}_7\text{Ta}_2$, orthorhombic, $Cmcm$ (No. 63), $a = 3.9542(5) \text{ \AA}$, $b = 27.142(5) \text{ \AA}$, $c = 5.692(1) \text{ \AA}$, $V = 610.9 \text{ \AA}^3$, $Z = 4$, $R(F) = 0.047$, $R_w(F^2) = 0.097$.

Table 1. Parameters used for the X-ray data collection

Crystal:	dark red, lath shaped, size 0.05 x 0.05 x 0.05 mm
Wavelength:	$\text{Mo K}\alpha$ radiation (0.71073 $\text{\AA}$)
μ :	559.40 cm^{-1}
Diffractometer:	Siemens Stoe AED2
Scan mode:	$\omega/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	66.04°
$N(hkl)_{\text{unique}}$:	702
Criterion for I_0 :	$I_0 > 2 \sigma(I_0)$
$N(\text{param})_{\text{refined}}$:	41
Program:	SHELXL-93

Table 2. Final atomic coordinates and displacement parameters (in $\text{\AA}^2$)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Eu(1)	4c	0	0.28809(7)	1/4	0.0086(6)	0.0212(9)	0.0214(8)	0	0	0
Eu(2)	4c	0	0.44698(7)	3/4	0.0115(6)	0.0135(6)	0.0142(6)	0	0	0
Ta(1)	4c	1/2	0.33996(5)	3/4	0.0066(5)	0.0094(5)	0.0106(6)	0	0	0
Ta(2)	4c	1/2	0.44464(5)	1/4	0.0069(5)	0.0101(5)	0.0089(5)	0	0	0
O(1)	8f	1/2	0.2920(6)	0.514(3)	0.021(8)	0.017(7)	0.023(9)	0	0	-0.017(8)
O(2)	4c	0	0.349(1)	3/4	0.01(1)	0.02(1)	0.07(3)	0	0	0
O(3)	8f	1/2	0.3997(6)	0.505(4)	0.023(9)	0.018(8)	0.02(1)	0	0	0.004(8)
O(4)	4c	0	0.455(1)	1/4	0.000(8)	0.03(2)	0.04(2)	0	0	0
O(5)	4a	1/2	1/2	1/2	0.05(2)	0.01(1)	0.01(1)	0	0	0.003(9)

2. Structure of europium(II) ditantalum hexoxide, EuTa₂O₆

Source of material: Only a few single crystals are obtained from a melt of Eu and S (molar ratio 2:3), using CsCl as a flux, in a sealed tantalum container at 973 K. The main product was EuS (see ref. 3).

During attempts to prepare Eu₂S₃ in sealed tantalum containers, EuTa₂O₆ was obtained as black single crystals. They grow from the container wall. EuTa₂O₆ contains double octahedra [Ta₂O₁₀] like the isotypic CaTa₂O₆ (see ref. 4). The [Ta₂O₁₀] groups are linked via all terminal oxygen atoms to form a network structure.

Table 3. Parameters used for the X-ray data collection

Crystal:	black, irregular shape
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	592.77 cm ⁻¹
Diffractometer:	Siemens Stoe AED2
Scan mode:	$\omega/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	65.14°
$N(hkl)_{\text{unique}}$:	919
Criterion for I_0 :	$I_0 > 2 \sigma(I_0)$
$N(\text{param})_{\text{refined}}$:	46
Program:	SHELXL-93

EuO₆Ta₂, orthorhombic, *Pnma* (No. 62), $a = 11.02(1)$ Å, $b = 7.640(7)$ Å, $c = 5.610(4)$ Å, $V = 472.3$ Å³, $Z = 4$, $R(F) = 0.048$, $R_w(F^2) = 0.124$.

Table 4. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Eu	4c	0.0402(1)	1/4	0.5387(2)	0.0140(5)	0.0087(4)	0.0136(4)	0	0.0010(4)	0
Ta	8d	0.14237(6)	0.99594(7)	0.0377(1)	0.0082(3)	0.0080(3)	0.0119(3)	0.0000(2)	0.0002(2)	0.0000(2)
O(1)	8d	0.974(1)	0.035(1)	0.221(2)	0.016(5)	0.008(4)	0.016(5)	0.000(4)	0.002(4)	-0.002(3)
O(2)	8d	0.214(1)	0.048(1)	0.361(2)	0.010(4)	0.008(4)	0.016(5)	-0.001(4)	0.002(4)	-0.004(4)
O(3)	4c	0.144(2)	1/4	0.967(3)	0.03(1)	0.007(6)	0.016(7)	0	0.004(6)	0
O(4)	4c	0.372(2)	1/4	0.643(3)	0.019(8)	0.002(5)	0.017(8)	0	0.000(6)	0

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