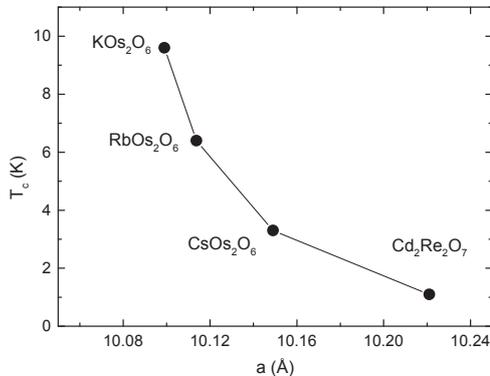


Single crystal growth and superconducting properties of RbOs_2O_6

Above: Critical temperature T_c as a function of lattice parameter a for superconducting pyrochlores

Superconducting β -pyrochlore oxide RbOs_2O_6 single crystals has been synthesized by encapsulation techniques (evacuated and sealed quartz ampoule). The ampoule was placed in the preheated furnace at 600 °C, kept for 1 h, cooled down to 400 °C at a rate of 5 °C/h, and finally cooled down to room temperature at a rate of 150 °C/h. As a result, RbOs_2O_6 octahedra shaped single crystals with a size up to 0.3 mm have been grown.

Bulk superconductivity with $T_c = 6.4$ K was observed in magnetisation and specific heat measurements. For members of β -pyrochlore AOs_2O_6 family ($A = \text{K, Rb, Cs}$) the transition temperature was found to decrease with increasing the ionic radius of A cation (9.6 K for KOs_2O_6 and 3.3 K for CsOs_2O_6) [1].

Band structure calculations for KOs_2O_6 show significant instability and anharmonicity of the K ions ("rattling") [2], which seems to be consistent with a rather high anisotropic displacement parameter derived for the K ions from our crystal structure studies [3].

Crystal structure of RbOs_2O_6

Detailed single crystal X-ray diffraction studies at room temperature show Bragg peaks that violate $Fd\bar{3}m$ symmetry, like for KOs_2O_6 [3]. With a comparative structure refinement the structure is identified as **non-centrosymmetric** ($F43m$). Compared to the ideal β -pyrochlore lattice ($Fd\bar{3}m$), both Os tetrahedral and O octahedral network exhibit breathing mode like volume changes accompanied by anisotropic character of the Rb channels.

The structure of β -pyrochlore RbOs_2O_6 has been solved from single crystal X-ray data measured at room temperature ($\text{SMART CCD, MoK}_{\alpha 1}$):

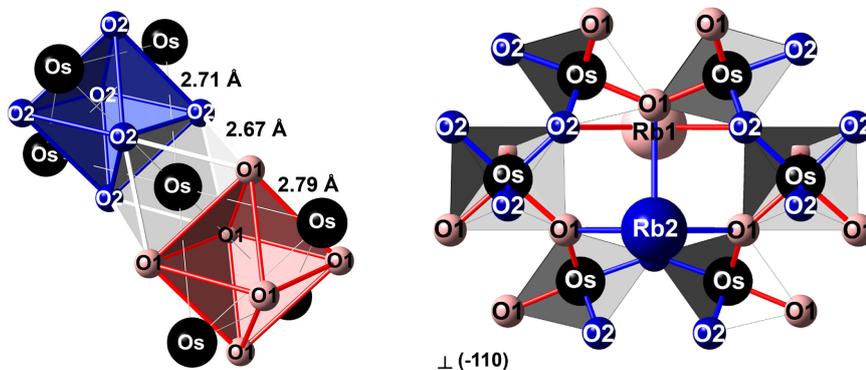
Below: Atomic coordinates and isotropic displacement parameters (U_{iso})

RbOs_2O_6						KOs_2O_6 [3]
	Site	x	y	z	U_{iso}	U_{iso}
Os	16e	0.8758(1)	x	x	0.0039(1)	0.0005(1)
Rb1	4c	1/4	1/4	1/4	0.0304(1)	0.063(5)
Rb2	4b	1/2	1/2	1/2	0.0375(1)	0.062(4)
O1	24f	0.1895(1)	0	0	0.0027(2)	0.005(1)
O2	24g	0.5551(2)	1/4	1/4	0.0190(3)	0.005(1)

$a = 10.124(1)$ Å
 $F43m$ (No. 216)
 249 unique reflections
 16 parameters
 $R_1 = 0.021$
 $wR = 0.039$
 $R_{int} = 0.030$
 $S^{int} = 1.437$

Below: Anisotropic displacement parameters (ADP)

RbOs_2O_6							
	Site	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Os	16e	0.0039(1)	0.0039(1)	0.0039(1)	0.0006(1)	-0.0006(1)	0.0006(1)
Rb1	4c	0.0304(1)	0.0304(1)	0.0304(1)	0	0	0
Rb2	4b	0.0375(1)	0.0375(1)	0.0375(1)	0	0	0
O1	24f	0.0000(4)	0.0041(2)	0.0041(2)	0.0006(4)	0	0
O2	24g	0.0266(6)	0.0152(3)	0.0152(3)	0.0131(4)	0	0



Above: Structural details of β -pyrochlore RbOs_2O_6 at room temperature with $F43m$ space group symmetry showing: (left) the O-O interatomic distances in the octahedral network: the length $\text{O1-O1} = 2.79$ Å is longer and the length $\text{O2-O2} = 2.71$ Å is shorter than the distance $\text{O-O} = 2.74$ Å calculated for the ideal β -pyrochlore structure ($Fd\bar{3}m$); (right) the anisotropic nature of the Rb channels. Interatomic distances $\text{O2-Rb1} = 3.14$ Å and $\text{O1-Rb2} = 3.09$ Å are longer and shorter, respectively, compared to the ideal β -pyrochlore structure calculated with $Fd\bar{3}m$ symmetry ($\text{O-Rb} = 3.13$ Å). Shown is the structure projected along the $[-110]$ direction.

Comparison to KOs_2O_6

Below: Selected interatomic distances (Å) (KOs_2O_6 [3]); Δ : length difference (Å): maximal - minimal length (example: [length: K1-O2] - [length: K2-O1] = 0.082 Å).

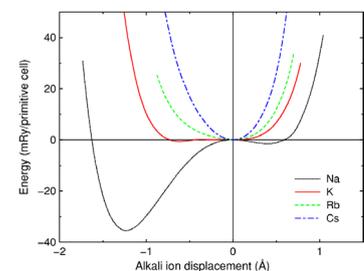
	RbOs_2O_6	Δ	KOs_2O_6	Δ
Os-O1	1.932	0.035	1.920	0.014
Os-O2	1.897		1.906	
Os-Os	3.561	0.037	3.548	0.044
Os-Os	3.598		3.592	
A1-O2	3.144	0.055	3.141	0.082
A2-O1	3.089		3.059	
A-A	4.384	-	4.372	-
O1-O2	2.665	-	2.653	-
O1-O1	2.790	0.078	2.819	0.124
O2-O2	2.713		2.695	

→ Only the O octahedral network length changes ($\Delta\text{Os-O}$) are stronger for RbOs_2O_6 than for KOs_2O_6 .

→ Os tetrahedral network length changes ($\Delta\text{Os-Os}$) and the anisotropic character ($\Delta\text{Rb-O}$) of the alkali ion channels are weaker for RbOs_2O_6 .

→ $U_{iso, \text{Rb}} / U_{iso, \text{K}} \approx 0.5$

→ Less alkali ion "rattling" in RbOs_2O_6



Above: Energy surface for a displacement Δ of alkali ions along $[111]$ direction (band structure calculations) [2].

References

- [1] S.M. Kazakov, N.D. Zhigadlo, M. Brühwiler, B. Batlogg, J. Karpinski, cond-mat/0403588 (2004).
- [2] J. Kuneš, T. Jeong and W.E. Pickett, Phys. Rev. B 70, 174510 (2004).
- [3] G. Schuck, S. M. Kazakov, K. Rogacki, N. D. Zhigadlo and J. Karpinski, cond-mat/0601465 (2006).