

Raman studies of A_2MWO_6 tungstate double perovskites

R. L. Andrews, A. M. Heyns and P. M. Woodward

Supporting Information

Table S1: Refined values of lattice parameters as taken from Rietveld refinements of X-ray powder diffraction data.

	Ba_2MgWO_6	Sr_2ZnWO_6	Ba_2CaWO_6	Ca_2MgWO_6	Sr_2CaWO_6	Ca_2CaWO_6
Space Group	Fm3m	$P2_1/n$	$I4/m$	$P2_1/n$	$P2_1/n$	$P2_1/n$
Tolerance Factor (τ)	1.038	0.976	0.972	0.926	0.917	0.867
a (Å)	8.0994(2)	5.6305(1)	5.9355(4)	5.4224(4)	5.7698(1)	5.5464(5)
b (Å)	-	5.6064(0)	-	5.5467(7)	5.8536(3)	5.8088(9)
c (Å)	-	7.9239(4)	8.3929(5)	7.7178(3)	8.1968(1)	8.0001(6)
β (deg)	-	89.9554(3)	-	90.0809(8)	90.0638(2)	89.7996(6)

Table S2: The frequencies of the oxygen symmetric stretching mode, ν_1 , and the oxygen bending mode, ν_5 , for 14 different A_2MWO_6 double perovskites.

	Tolerance factor	Symmetry	ν_1 (cm^{-1})	ν_5 (cm^{-1})	Reference
Ba_2NiWO_6	1.048	$Fm\bar{3}m$	816	434	[23]
Ba_2MgWO_6	1.038	$Fm\bar{3}m$	812	441	This study
Ba_2ZnWO_6	1.035	$Fm\bar{3}m$	822	431	[23]
Ba_2MnWO_6	1.014	$Fm\bar{3}m$	810	420	[28]
Ba_2CaWO_6	0.972	$I4/m$	834	410	This study
Sr_2MgWO_6	0.979	$I4/m$	857	450	[29]
Sr_2CoWO_6	0.979	$I4/m$ & $P2_1/n$	850	443	[24]
Sr_2ZnWO_6	0.977	$P2_1/n$	855	440*	This study
Sr_2MnWO_6	0.956	$P2_1/n$	830	444	[28]
Sr_2CdWO_6	0.930	$P2_1/n$	824	439 [†]	This study
Sr_2CaWO_6	0.917	$P2_1/n$	818	441 [†]	This study
Ca_2MgWO_6	0.926	$P2_1/n$	836	472	This study
Ca_2CoWO_6	0.926	$P2_1/n$	825	476	[24]
Ca_2CaWO_6	0.867	$P2_1/n$	811	459*	This study

*In these compounds two peaks of comparable intensity were assigned as originated from a ν_5 vibration. The value given in this table is the average of those two frequencies. [†]In these compounds two modes were assigned to a ν_5 vibration, but one of the two modes was much stronger than the other and is used here.

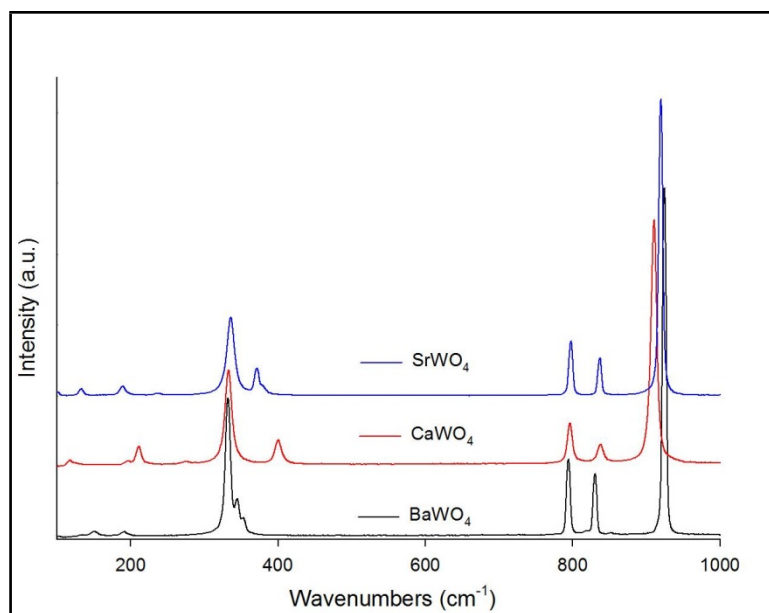


Figure S1: Raman Spectra of the scheelite phases BaWO₄, SrWO₄ and CaWO₄.