

Supplementary Material

Stability and electronic, magnetic and optical properties of XScO₃ (X=Mo, W) perovskites

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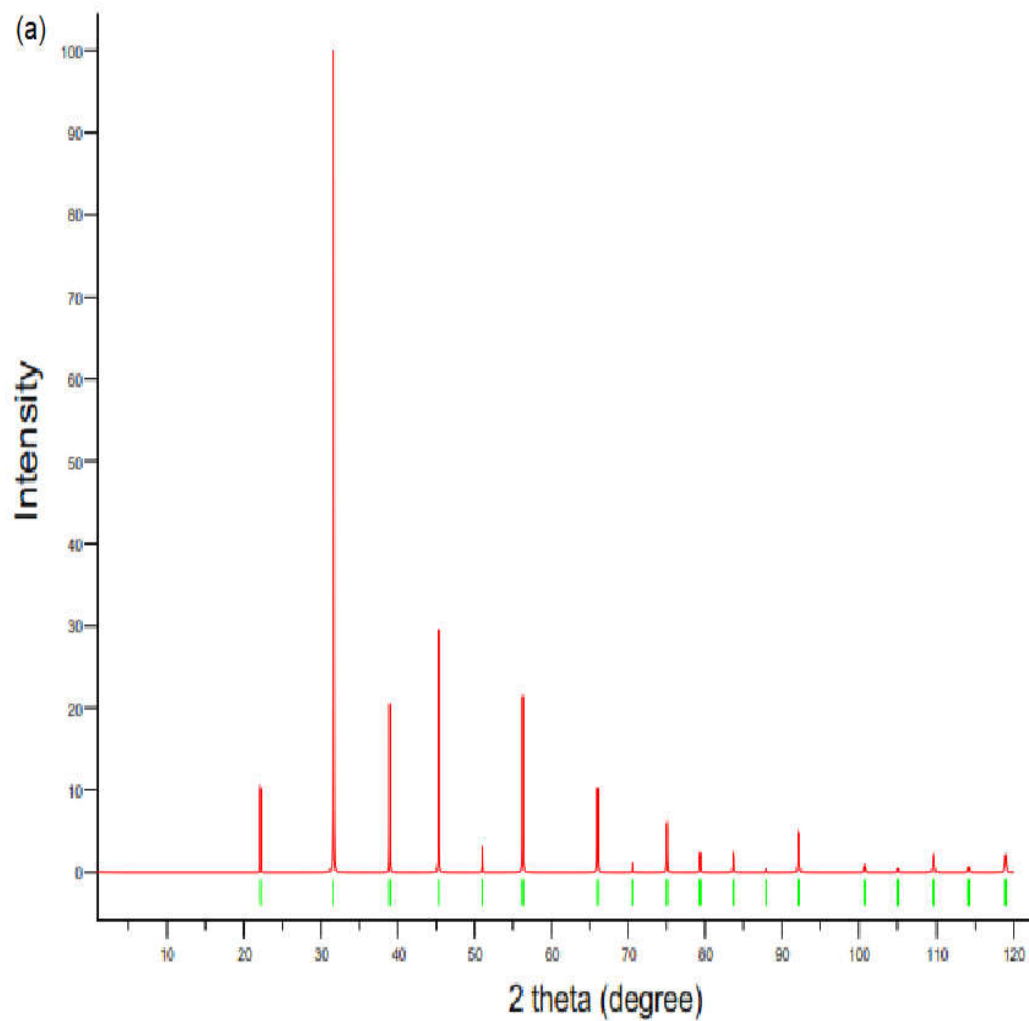
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Table S1 Phonon frequencies at Gamma for the relaxed structures of the perovskites MoScO₃ and WScO₃

Perovskite	MoScO ₃		WScO ₃	
	[cm-1]	[THz]	[cm-1]	[THz]
1	-245.02	-7.3456	-304.50	-9.1287
2	-245.02	-7.3456	-304.50	-9.1287
3	-245.02	-7.3456	-304.50	-9.1287
4	-239.36	-7.1760	-293.11	-8.7874
5	-239.36	-7.1760	-293.11	-8.7874
6	-239.36	-7.1760	-293.11	-8.7874
7	0	0	0	0
8	0	0	0	0
9	0	0	0	0
10	190.29	5.7048	170.34	5.1067
11	190.29	5.7048	170.34	5.1067
12	190.29	5.7048	170.34	5.1067
13	722.97	21.6741	744.35	22.3150
14	722.97	21.6741	744.35	22.3150
15	722.97	21.6741	744.35	22.3150

Simulated Powder diffraction patterns

The perovskite structures were simulated for X-ray diffraction (XRD) using Cu-K α radiation of wavelength $\lambda = 0.154059$ nm. The diffraction patterns for MoScO₃ and WScO₃ are shown in Figures S1(a) and (b) respectively.



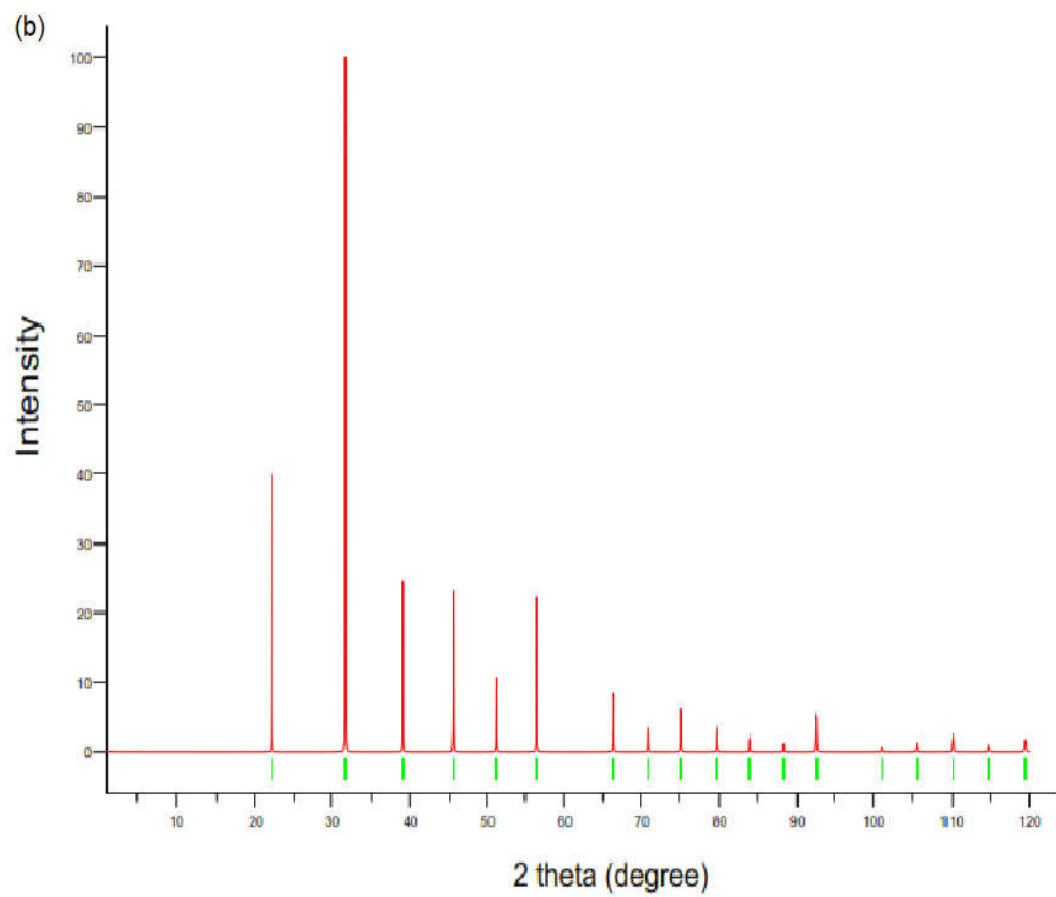


Figure S1 The powder XRD patterns for the perovskites (a) MoScO_3 and (b) WScO_3