Crystal and Magnetic Structure of Ba_2CaOsO_6

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Ba_2CaOsO_6 is an ordered double perovskite with Os^{6+} ($5d^2$, t_{2g}^2) on a FCC lattice. It is isostructural and isoelectronic with Ba_2YReO_6 based on Re^{5+} ($5d^2$, t_{2g}^2) which has been studied earlier by our group.[1] Magnetic properties are compared in Table 1. Note that the unit cell constants differ by less than 0.1% but the Curie–Weiss θ values differ by a factor of four.

Previous magnetic and heat capacity studies suggested that long range AF order occurs near 50 K for the Os phase, while the Re material shows a random frozen spin ground state. [2] Our goals were three-fold: (1) to refine the crystal structure (2) to check that Fm-3m symmetry is still found at 4 K and (3) to search for magnetic reflections indicative of long range order.

The results of the crystal structure refinement are shown in Fig. 1 and Table 2.

Comparison of high angle diffraction data between 280 K and 3.5 K showed no evidence of peak splitting or broadening, indicating that, within the instrumental resolution, there is no transition to lower symmetry at 3.5 K. Also, no magnetic reflections were observed even with very long counting times, 63 hr. We estimate from simulations and previous experience with C2 that the upper limit for an ordered moment on Os, assuming a Type I FCC magnetic structure as found for Ba_2YRuO_6, is ≈ 0.6 μ_B.

Subsequent μSR data collected in August 2013 indicate long range order at T_N = 50 K with an estimated ordered moment of ≈ 0.2 – 0.3 μ_B. A manuscript is in preparation.

References

[1] Aharen et al, Phys. Rev. B 81 (2010) 064436.
[2] K. Yamamura et al, J. Solid State Chem. 179 (2006) 605.

Table 1

Compound	a_0(Å)	C (emu-K/mole)	$\mu_{eff}(\mu_B)$	θ_C(K)
Ba_2YReO_6 [1,2]	8.3627(2)	0.466	1.93	-616(7)
Ba_2CaOsO_6	8.3635(1)	0.333	1.63	-149(1)

Table 2

		280 K		
	x	y	z	B_{iso} (Å^2)
Ba	0.25	0.25	0.25	0.587(52)
Ca	0.5	0.5	0.5	0.704(105)
Os	0	0	0	0.269(57)
O	0.2294(23)	0	0	0.966(50)
a_0	8.3619(6)			
	λ = 1.33 Å	λ = 2.37 Å	X-ray (λ = 1.54056 Å)	
χ^2	2.91	1.98	2.78	
R_p	3.56	3.69	13.8	
R_{wp}	4.72	5.07	17.7	
R_{exp}	2.77	3.6	10.61	
R_{Bragg}	3.69	2.20	15.2	
R_F	2.26	1.68	12.3	

Bond (Å)	
Ba-O	2.9613(2)
Ca-O	2.2619(17)
Os-O	1.9191(17)

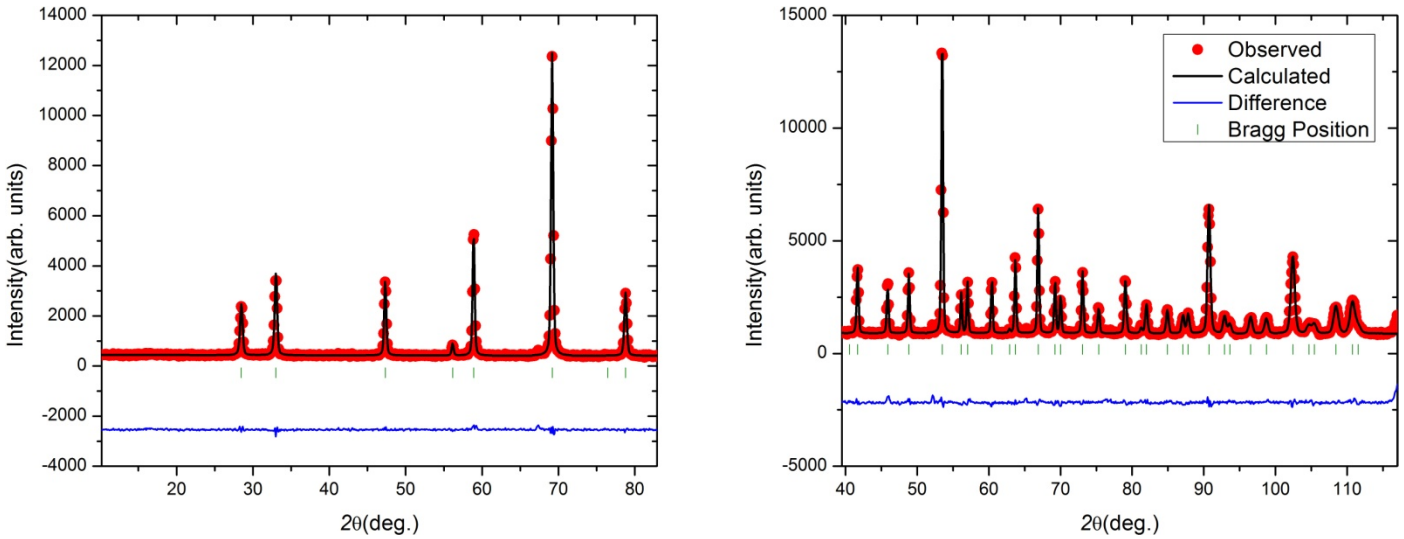

Figure 1 Room temperature powder neutron diffraction patterns of Ba_2CaOsO_6 at 280K, for λ = 2.3719 Å (left) and 1.3305 Å (right).