Supporting information

High-Pressure Synthesis of 5*d* Cubic Perovskite $BaOsO_3$ at 17 GPa: Ferromagnetic Evolution over 3*d* to 5*d* Series

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Table 1S. Comparison of the lattice and structural parameters of the perovskite oxides.

	$CaOsO_3$	$CaRuO_3$ [1]	$CaFeO_3$ [2]	$SrOsO_3$	$SrRuO_3$ [3]
Space group	*P n m a*	*P n m a*	*P n m a*	*P n m a*	*P n m a*
a (Å)	5.57439(3)	5.5224	5.3501	5.55925(1)	5.5304
b (Å)	7.77067(4)	7.6626	7.5367	7.88779(2)	7.8446
c (Å)	5.44525(3)	5.3599	5.3236	5.59802(1)	5.5670
d_{cal} (g/cm^3)	7.836	5.54	4.45	8.817	6.51
Tr–O1 (Å)	2.003(1) ×2	1.985	1.918	1.9875(9)	1.983
Tr–O2 (Å)	1.978(4) ×2	1.993	1.922	1.9803(9)	1.981
Tr–O2 (Å)	2.037(4) ×2	1.993	1.925	1.9811(9)	1.988
Tr–O1–*Tr* (°)	151.7(1) ×2	149.6	158.4	165.7(1)	162.8
Tr–O2–*Tr* (°)	152.0(2) ×4	149.7	157.5	169.5(2)	162.8
BVS at A-site	1.90 (^{VIII})	2.18 (^{VIII})	2.00 (^{VIII})	2.09 (^{xII})	2.32 (^{xII})
BVS at B-site	3.55	3.93	4.09	3.77	4.00
Tolerance factor *t*	0.95	0.96	0.98	0.99	0.99
ϕ_{O2} (°)	9.6	10.6	8.4	1.7	5.9
φ_{O2}, φ_{O1}, $\phi_{lattice}$ (°)	14.6, 13.6, 14.5	15.6, 14.7, 16.2	10.8, 10.7, 6.3	7.1, 7.1, 8.2	8.9, 8.6, 7.9

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[3] Acta Crystallogr., Sect. C 1989, 45, 365.