Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

$Sr_5Os_3O_{13}$: A Mixed Valent Osmium(V, VI) Layered Perovskite Variant Exhibiting Temperature Dependent Charge Distribution

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Table SI-1: Crystallographic data obtained from Rietveld structure refinements of RT PXRD of $Sr_5Os_3O_{13}$.

Temperature /K	295 (Cell 2)
Space group (no.), Z	*Pnma* (62), 4
Lattice parameters /Å	14.166007(92)
	11.015738(58)
	7.076877(44)
V /Å^3	1104.340(12)
ρ_{xray} /g×cm^3	7.317913(76)
Rp	0.0432
Rwp	0.0636
Rexp	0.0139
GOF	1.32

Table SI-2: Atomic coordinates and isotropic thermal displacement parameters from Rietveld structure refinements of RT PXRD of $Sr_5Os_3O_{13}$ (cell 2).

Site	*x*	*y*	*z*	*Occ*	*B*eq
Os1	0.00000	0.00000	0.00000	1	1.00(35)
Os2A	0.10836(17)	0.25000	0.34165(28)	1	1.00(64)
Os2B	-0.10915(17)	0.25000	-0.32241(30)	1	1.00(63)
Sr1	0.00000	0.00000	0.50000	1	1.20(55)
Sr2	0.22575(13)	0.00600(48)	0.16882(25)	1	1.20(45)
Sr3A	0.13647(32)	0.25000	-0.16512(67)	1	1.20(13)
Sr3B	-0.11346(33)	0.25000	0.17670(66)	1	1.20(13)
O1	-0.0119(25)	0.25000	0.4778(52)	1	1.80(52)
O2A	0.2170(19)	0.25000	0.1819(37)	1	1.80(77)
O2B	-0.2003(21)	0.25000	-0.1399(39)	1	1.80(87)
O3	0.12490(90)	-0.0130(25)	-0.1248(17)	1	1.80(39)
O4A	0.0505(14)	0.1220(21)	0.1689(28)	1	1.80(61)
O4B	-0.0403(14)	0.1280(22)	-0.1848(29)	1	1.80(61)
O5A	0.1520(14)	0.1239(18)	0.4930(27)	1	1.80(48)
O5B	-0.1678(14)	0.1236(19)	-0.4488(25)	1	1.80(53)

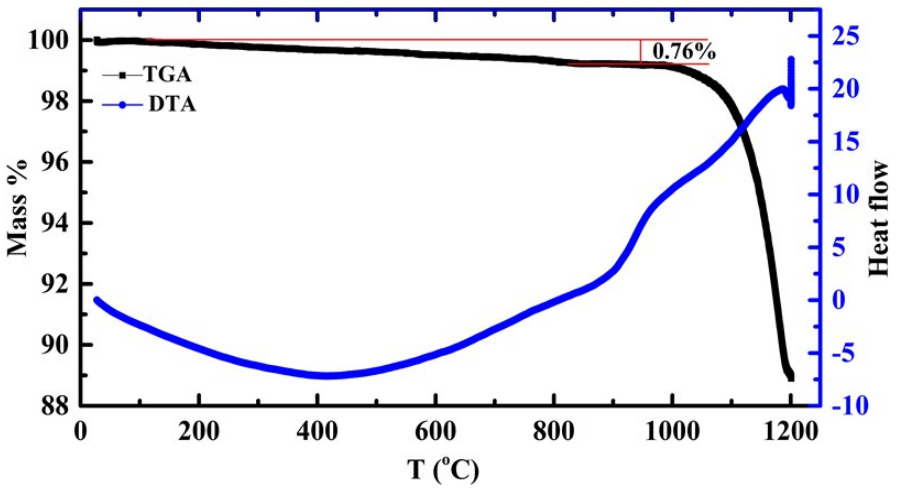

Figure SI-1: Thermogravimetric (TGA/DTA) analysis plot of $Sr_5Os_3O_{13}$.

Table SI-3a, b and c: Bond valence sum calculation for Os1, Os2A and Os2B for 50K, 100K and 500K data.

(a) Os(1), Os(2A) +5 and Os(2B) +6, B= 0.485 for +5 & 0.375 for +6, Ro = 1.87 for +5 & 1.904 for +6, T = 50K

Os-O	Dist.(Ri)	M	R_0-R_i	(R_0-R_i)/ B	$exp^{(R0-Ri)/B}$	M* $exp^{(R0-Ri)/B}$	Valency
Os(1)-O(4A)	1.935	2	-0.065	-0.13402	0.87457	1.74914	4.96737
Os(1)-O(4B)	1.97	2	-0.1	-0.20619	0.81368	1.62736	
Os(1)-O3	1.981	2	-0.111	-0.22887	0.79544	1.59087	
Os(2A)-O5A	1.879	2	-0.009	-0.01856	0.98161	1.96323	
Os(2A)-O2A	1.897	1	-0.027	-0.05567	0.94585	0.94585	5.16756
Os(2A)-O1	1.984	1	-0.114	-0.23505	0.79053	0.79053	
Os(2A)-O4A	2.02	2	-0.15	-0.30928	0.73398	1.46795	
Os(2B)-O2B	1.842	1	0.062	0.16533	1.17979	1.17979	
Os(2B)-O5B	1.835	2	0.069	0.184	1.20202	2.40403	5.95035
Os(2B)-O1	1.961	1	-0.057	-0.152	0.85899	0.85899	
Os(2B)-O4B	2.01	2	-0.106	-0.28267	0.75377	1.50754	

(b) Os(1), Os(2A) +5 and Os(2B) +6; B= 0.485 for +5 & 0.375 for +6; Ro = 1.87 for +5 & 1.904 for +6; T = 100K

Os-O	Dist.(Ri)	M	R_0-R_i	(R_0-R_i)/ B	$exp^{(R0-Ri)/B}$	M* $exp^{(R0-Ri)/B}$	Valency
Os(1)-O(4A)	1.937	2	-0.067	-0.13814	0.87097	1.74195	4.96018
Os(1)-O(4B)	1.970	2	-0.1	-0.20619	0.81368	1.62736	
Os(1)-O3	1.981	2	-0.111	-0.22887	0.79544	1.59087	
Os(2A)-O5A	1.876	2	-0.006	-0.01237	0.98771	1.97541	
Os(2A)-O2A	1.891	1	-0.021	-0.0433	0.95763	0.95763	5.19782
Os(2A)-O1	1.982	1	-0.112	-0.23093	0.7938	0.7938	
Os(2A)-O4A	2.019	2	-0.149	-0.30722	0.73549	1.47098	
Os(2B)-O2B	1.845	1	0.059	0.15733	1.17039	1.17039	
Os(2B)-O5B	1.838	2	0.066	0.176	1.19244	2.38488	5.92008
Os(2B)-O1	1.960	1	-0.056	-0.14933	0.86128	0.86128	
Os(2B)-O4B	2.011	2	-0.107	-0.28533	0.75176	1.50353	

(c) Os(1) +5 and Os(2A) +6; B= 0.485 for +5 & 0.375 for +6; Ro = 1.87 for +5 & 1.904 for +6; T = 500K

Bond	Dist.(Ri)	M	R_0-R_i	(R_0-R_i)/ B	$exp^{(R0-Ri)/B}$	M* $exp^{(R0-Ri)/B}$	Valency
Os(1)-O(4A)	1.953	4	-0.083	-0.17113	0.84271	3.37083	4.97488
Os(1)-O3	1.977	2	-0.107	-0.22062	0.80202	1.60405	
Os(2A)-O5A	1.862	2	0.042	0.112	1.11851	2.23703	
Os(2A)-O2A	1.841	1	0.063	0.168	1.18294	1.18294	
Os(2A)-O1	1.957	1	-0.053	-0.14133	0.8682	0.8682	5.71742
Os(2A)-O4A	2.03	2	-0.126	-0.336	0.71462	1.42925	