

Supplementary Materials for

Giant spin-induced electric polarization in absence of orbital order in (Bi_{0.5}Ag_{0.5})Mn₇O₁₂

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Table I Bond lengths and angles of Mn-O polyhedron in $\text{CaMn}_7\text{O}_{12}$ [1] and $(\text{Bi}_{0.5}\text{Ag}_{0.5})\text{Mn}_7\text{O}_{12}$.

$\text{CaMn}_7\text{O}_{12}$		$(\text{Bi}_{0.5}\text{Ag}_{0.5})\text{Mn}_7\text{O}_{12}$	
Mn-O bond length	$\angle \text{O-Mn-O}$	Mn-O bond length	$\angle \text{O-Mn-O}$
Square planar Mn1O_4			
1.905($\times 2$) (Å)	86.1°	1.903(3)($\times 2$)	89.1(1)°
1.910($\times 2$) (Å)		1.908(3)($\times 2$)	
octahedral Mn2O_6			
1.890($\times 2$)	88.2°	1.900(3)($\times 2$)	86.0(1)°
2.035($\times 2$)	88.4°	2.043(4)($\times 2$)	86.4(1)°
2.039($\times 2$)	89.0°	2.055(4)($\times 2$)	86.8(1)°
Octahedral Mn3O_6			
1.908($\times 6$)	89.9°	1.925(3)($\times 6$)	88.6(1)°

References

- [1] V. Pierre and C. Karin, CaMn₇O₁₂ Crystal Structure: Datasheet from "PAULING FILE Multinaries Edition – 2022" in SpringerMaterials, Springer-Verlag Berlin Heidelberg & Material Phases Data System (MPDS), Switzerland & National Institute for Materials Science (NIMS), Japan.
(https://materials.springer.com/isp/crystallographic/docs/sd_1243921)