

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

A tale of three double perovskites: Ba_2XOsO_6 ($\text{X}=\text{Na,Ca,Y}$)¹
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Davis — High valent Os based double perovskites are one center of current interest
because they display extreme interplay of large spin orbit coupling and strong elec-
tronic correlation. We present electronic and magnetic structures of three cubic Os
based double perovskites with Os^{+7} (d^1), Os^{+6} (d^2), Os^{+5} (d^3). For these first princi-
ples based calculation we used an onsite hybrid exchange only on Os(5d), as imple-
mented in Wien2k. While $\text{Ba}_2\text{NaOsO}_6$ is a ferromagnetic Mott insulator, the other
two show antiferromagnetic ordering. For comparison purposes we have investigated
only the ferromagnetic ordered phase of these three materials. A metal-insulator
transition by changing spin orbit coupling direction is found in all three materials,
however each double perovskite is metallic for different magnetic directions. Sur-
prises from looking at the radial charge densities will be discussed. We provide a
resolution to the riddle: why, despite d^1 configuration, does $\text{Ba}_2\text{NaOsO}_6$ remain
cubic. This material introduces a new class of $J= 3/2$ Mott insulator.

¹DOE Stockpile Stewardship Academic Alliance Program

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Date submitted: 13 Nov 2014

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