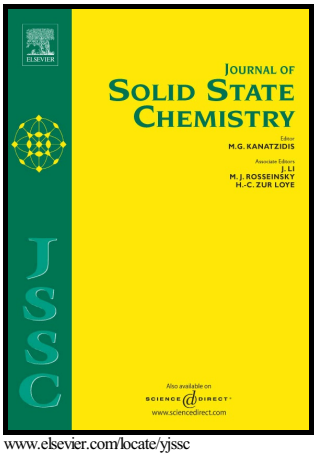

www.elsevier.com/locate/yjssc

Type I antiferromagnetic order in Ba_2LuReO_6: Exploring the role of structural distortions in double perovskites containing $5d^2$ ions

Jie Xiong, Jiaqiang Yan, Adam A. Aczel, Patrick M. Woodward

PII: S0022-4596(17)30486-3
DOI: http://dx.doi.org/10.1016/j.jssc.2017.11.040
Reference: YJSSC20040

To appear in: *Journal of Solid State Chemistry*

Received date: 28 July 2017
Revised date: 28 November 2017
Accepted date: 29 November 2017

Cite this article as: Jie Xiong, Jiaqiang Yan, Adam A. Aczel and Patrick M. Woodward, Type I antiferromagnetic order in Ba_2LuReO_6: Exploring the role o structural distortions in double perovskites containing $5d^2$ ions, *Journal of Soli State Chemistry,* http://dx.doi.org/10.1016/j.jssc.2017.11.040

Type I antiferromagnetic order in Ba_2LuReO_6: Exploring the role of structural distortions in double perovskites containing $5d^2$ ions

Jie Xiong,[1] Jiaqiang Yan,[2,3] Adam A. Aczel,[4] Patrick M. Woodward[1*]

[1] Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio 43210-1185, USA

[2] Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

[3] Department of Materials Science and Engineering, The University of Tennessee, Knoxville, TN 37996, USA

[4] Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

[*]**Corresponding Author.** woodward@chemistry.ohio-state.edu

Abstract

The structural, electrical, and magnetic properties of the double perovskite Ba_2LuReO_6 have been examined. It is an insulator whose temperature dependent conductivity is consistent with variable range hopping electrical transport. A transition to an antiferromagnet state with type I order occurs below T_N = 31 K. High resolution time-of-flight neutron powder diffraction measurements show that it retains the cubic double perovskite structure down to 10 K. High intensity, low resolution neutron powder diffraction measurements confirm the antiferromagnetic order and indicate that cubic symmetry is still observed at 1.5 K. The small ordered moment of $0.34(4)\mu_B$ per Re is comparable to estimates of moments on $5d^2$ ions in other antiferromagnetically ordered cubic double perovskites. Comparisons with related double perovskites containing $5d^2$ ions, such as Os^{6+} and Re^{5+}, reveal that subtle changes in structure or