

## Accepted Manuscript

A comprehensive study of magnetic exchanges in the layered oxychalcogenides  $\text{Sr}_3\text{Fe}_2\text{O}_5\text{Cu}_2\text{Q}_2$  ( $Q = \text{S}, \text{Se}$ )

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PII: S0304-8853(17)30719-9

DOI: <http://dx.doi.org/10.1016/j.jmmm.2017.07.026>

Reference: MAGMA 62957

To appear in: *Journal of Magnetism and Magnetic Materials*

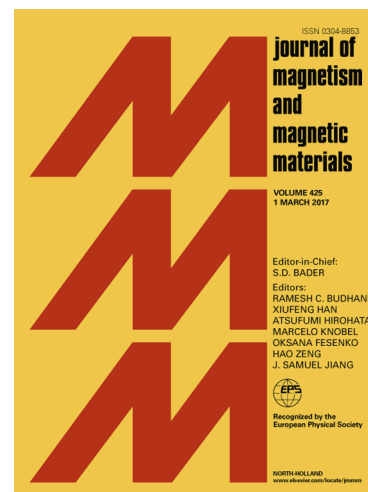
Received Date: 24 February 2017

Revised Date: 21 May 2017

Accepted Date: 6 July 2017

Please cite this article as: M. Lü, O. Mentré, E.E. Gordon, M-H. Whangbo, A. Wattiaux, M. Duttine, N. Tiercelin, H. Kabbour, A comprehensive study of magnetic exchanges in the layered oxychalcogenides  $\text{Sr}_3\text{Fe}_2\text{O}_5\text{Cu}_2\text{Q}_2$  ( $Q = \text{S}, \text{Se}$ ), *Journal of Magnetism and Magnetic Materials* (2017), doi: <http://dx.doi.org/10.1016/j.jmmm.2017.07.026>

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# A comprehensive study of magnetic exchanges in the layered oxychalcogenides $\text{Sr}_3\text{Fe}_2\text{O}_5\text{Cu}_2\text{Q}_2$ ( $\text{Q} = \text{S}, \text{Se}$ )

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## Abstract

The layered oxysulfide  $\text{Sr}_3\text{Fe}_2\text{O}_5\text{Cu}_2\text{S}_2$  was prepared, and its crystal structure and magnetic properties were characterized by synchrotron x-ray diffraction (XRD), powder neutron diffraction (PND), Mössbauer spectroscopy measurements and by density functional theory (DFT) calculations. In addition, the spin exchange interactions leading to the ordered magnetic structure of  $\text{Sr}_3\text{Fe}_2\text{O}_5\text{Cu}_2\text{S}_2$  were compared with those of its selenium analogue  $\text{Sr}_3\text{Fe}_2\text{O}_5\text{Cu}_2\text{Se}_2$ . The oxysulfide  $\text{Sr}_3\text{Fe}_2\text{O}_5\text{Cu}_2\text{S}_2$  adopts a G-type antiferromagnetic (AFM) structure at a

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