## Abstract Submitted for the MAR08 Meeting of The American Physical Society

Pressure-Induced Intermetallic Valence Transition in BiNiO<sub>3</sub> MASAKI AZUMA, MASAHIKO TSUJIMOTO, SHINTARO ISHIWATA, SEIJI ISODA, YUICHI SHIMAKAWA, MIKIO TAKANO, Inst. Chem. Res., Kyoto Univ., SANDRA CARLSSON, JENNIFER RODGERS, J. PAUL ATTFIELD, CSEC Univ. Edinburgh, MATTHEW G. TUCKER, RAL ISIS — The valence state change of BiNiO<sub>3</sub> perovskite under pressure has been investigated by a powder neutron diffraction study and electronic state calculations. At ambient pressure, BiNiO<sub>3</sub> has the unusual charge distribution  $Bi_{0.5}^{3+}Bi_{0.5}^{5+}Ni^{2+}O_3$  with ordering of  $Bi^{3+}$ and Bi<sup>5+</sup> charges on the A sites of a highly distorted perovskite structure. High pressure neutron diffraction measurements and Bond valence sum calculations show that the pressure-induced melting of the charge disproportionated state leads to a simultaneous charge transfer from Ni to Bi, so that the high pressure phase is metallic  $Bi^{3+}Ni^{3+}O_3$ . This unprecedented charge transfer between A and B site cations coupled to electronic instabilities at both sites leads to a variety of ground states. and it is predicted that a Ni-charge disproportionated state should also be observable.

[1] M. Azuma et al., J. Am. Chem. Soc., 129, (2007) 14433.

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