

“Covalent Magnetism” and Invar-like Behavior within Ternary Nitrides: An *ab initio* Study

Samir F. Matar^a, Abdesalem Houari^b, Mohamed A. Belkhir^b, and Mirvat Zakhour^c

^a Institut de Chimie de la Matière Condensée de Bordeaux-CNRS, Université Bordeaux 1, Pessac, France

^b Laboratoire de Physique Théorique, Département de Physique, Université de Bejaia, Route de Targua-Ouzemour, 06000 Bejaia, Algeria

^c Laboratoire de Chimie Physique des Matériaux. Faculté des Sciences II, Université Libanaise-Fanar and Faculté des Sciences et de Génie Informatique, Université “Saint-Esprit” de Kaslik-Jounieh, Lebanon

Reprint requests to S. F. Matar. E-mail: s.matar@u-bordeaux1.fr

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Dedicated to Dr. Bernard Chevalier on the occasion of his 60th birthday

Magnetic properties and bonding analyses of perovskite structure-derived $T\text{Fe}_3\text{N}$ ($T = \text{Ru}, \text{Os}$) nitrides have been investigated within density functional theory using both pseudo potential and all electron methods. At equilibrium, spin degenerate non-magnetic (NM) and ferromagnetic (FM) calculations of energy *versus* volume show that the ground state of the two compounds is ferromagnetic. Magnetic moments of Ru/Os and Fe, respectively, being situated at two different crystallographic sites are studied over a wide range of the cubic lattice parameter. The volume expansion indicates that iron atoms show itinerant magnetism while Ru and Os exhibit a localized behavior. Important magnetovolume effects are observed, with saturation of the magnetic moment reached in RuFe_3N but not in OsFe_3N . The electronic structure is visualized for the different binding characters Fe–N *versus* Ru/Os–N with the help of electron localization plots. The density of states of the ferromagnetic ground state is interpreted on the basis of a covalent magnetic model which goes beyond the Stoner rigid band model. An Invar-like behavior is predicted for the two nitrides.

Key words: Ternary Iron Nitrides, Magnetic Properties, Magnetovolume Effects,
Invar-like Behavior, Covalent Magnetism