

## Author's Accepted Manuscript

Octahedral and trigonal-prismatic coordination preferences in nb-, MO-, TA-, and W-based ABX<sub>2</sub> layered Oxides, oxynitrides, and Nitrides

Akira Miura, Kiyoharu Tadanaga, Eisuke Magome, Chikako Moriyoshi, Yoshihiro Kuroiwa, Takei Takahiro, Nobuhiro Kumada



PII: S0022-4596(15)30035-9  
DOI: <http://dx.doi.org/10.1016/j.jssc.2015.06.028>  
Reference: YJSSC18955

To appear in: *Journal of Solid State Chemistry*

Received date: 30 April 2015  
Revised date: 10 June 2015  
Accepted date: 11 June 2015

Cite this article as: Akira Miura, Kiyoharu Tadanaga, Eisuke Magome, Chikako Moriyoshi, Yoshihiro Kuroiwa, Takei Takahiro and Nobuhiro Kumada, Octahedral and trigonal-prismatic coordination preferences in nb-, MO-, TA-, and W-based ABX<sub>2</sub> layered Oxides, oxynitrides, and Nitrides, *Journal of Solid State Chemistry*, <http://dx.doi.org/10.1016/j.jssc.2015.06.028>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting galley proof before it is published in its final citable form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

1 *Manuscript Draft*

2

3 Title: Octahedral and Trigonal-Prismatic Coordination Preferences in Nb-, Mo-, Ta-, and W-based ABX<sub>2</sub>

4 Layered Oxides, Oxynitrides, and Nitrides

5 Type of Manuscript: Article

6 Authors: Akira Miura<sup>a\*</sup>, Kiyoharu Tadanaga<sup>a</sup>, Eisuke Magome<sup>b</sup>, Chikako Moriyoshi<sup>b</sup>, Yoshihiro Kuroiwa<sup>b</sup>,

7 Takei Takahiro<sup>c</sup>, and Nobuhiro Kumada<sup>c</sup>

8 Affiliations: a) Division of Materials Chemistry, Faculty of Engineering, Hokkaido University, Kita 13

9 Nishi8, Kita-ku, Sapporo 060-8628, Japan, b) Department of Physical Science, Hiroshima University, 1-3-1

10 Kagamiyama, Higashihiroshima, Hiroshima 739-8526, Japan, c) Center for Crystal Science and Technology,

11 University of Yamanashi, 7-32 Miyamae, Kofu 400-8511, Japan. Tel: +81-11-706-6578, E-mail:

12 amiura@eng.hokudai.ac.jp

13

---

14 **Abstract:** Crystallographic and electronic structures of Nb-, Mo-, Ta-, and W-based layered oxides,  
15 oxynitrides, and nitrides were analyzed to elucidate the structural relationship between layered oxides and  
16 nitrides consisting of octahedral and trigonal-prismatic layers. The electron density, as derived by  
17 synchrotron X-ray analysis of LiNbO<sub>2</sub> and Ta<sub>5-x</sub>(O,N)<sub>6</sub>, showed orbital overlaps between Nb–Nb and Ta–Ta  
18 metals in the trigonal layers. Computational calculations based on DFT exhibited that these overlaps  
19 stabilized these structures by lowering the hybridization states composed of the  $d_{xy}$ ,  $d_{x^2-y^2}$ , and  $d_{z^2}$   
20 orbitals below the Fermi level. The crystal structures and formation energies suggest that tuning the Fermi  
21 level through the substitutions and vacancies of the cation/anion sites determines the structural preferences  
22 of the coordination. The properties and syntheses of these compounds are briefly described. This study  
23 enhances the understanding of layered oxides, oxynitrides, and nitrides to further the development of new  
24 synthetic approaches, compounds, and applications.

---

25 **Keywords:** X-Ray diffraction, First-principles calculations, Maximum entropy method, Layered structure,  
26 Metal-metal bonding

Download English Version:

<https://daneshyari.com/en/article/7758626>

Download Persian Version:

<https://daneshyari.com/article/7758626>

[Daneshyari.com](https://daneshyari.com)