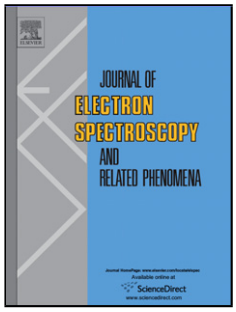

Title: X-Ray Spectroscopic Characterization of BaO, $Ba(OH)_2$, $BaCO_3$, and $Ba(NO_3)_2$

Authors: Osman Karslıoğlu, Lena Trotochau, Ioannis Zegkinoglo, Hendrik Bluhm

PII: S0368-2048(18)30006-9
DOI: https://doi.org/10.1016/j.elspec.2018.03.008
Reference: ELSPEC 46750

To appear in: *Journal of Electron Spectroscopy and Related Phenomena*

Received date: 24-2-2018
Accepted date: 22-3-2018

Please cite this article as: Karslıoğlu O, Trotochau L, Zegkinoglo I, Bluhm H, X-Ray Spectroscopic Characterization of BaO, $Ba(OH)_2$, $BaCO_3$, and $Ba(NO_3)_2$, *Journal of Electron Spectroscopy and Related Phenomena* (2010), https://doi.org/10.1016/j.elspec.2018.03.008

X-Ray Spectroscopic Characterization of BaO, $Ba(OH)_2$, $BaCO_3$, and $Ba(NO_3)_2$

Osman Karslıoğlu,[1] Lena Trotochaud,[1] Ioannis Zegkinoglou,[1,†] and Hendrik Bluhm[1,2,*]

[1] Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720 USA
[2] Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720 USA
† Present address: Department of Physics, Ruhr University Bochum, 44780 Bochum, Germany
* Corresponding author (hbluhm@lbl.gov)

ABSTRACT

Simple inorganic barium compounds are difficult to study spectroscopically in the surface sensitive soft X-ray regime due to significant surface contamination that can dominate the spectra. Here we present a near-edge X-ray absorption (NEXAFS) and X-ray photoelectron spectroscopic (XPS) study of four barium compounds: BaO, $Ba(OH)_2$, $BaCO_3$, and $Ba(NO_3)_2$. Using an ambient-pressure XPS instrument we prepared thin film samples in situ, which provided a high degree of control over the surface chemistry and significantly reduced the amount of contamination. The O K-edge spectrum for BaO presented here is in excellent agreement with the latest calculations in the literature, and indicates that experimental spectra in the literature for this compound may have suffered from carbonate contamination.

Keywords: NEXAFS; APXPS; barium oxide; barium hydroxide; barium carbonate; barium nitrate

1 Introduction

Barium is a constituent of many compounds used in technological applications such as NO_x traps for automotive exhaust abatement systems **(Takahashi et al. 1996)**, UHV getters **(Cooper 1929, Lederer 1934)**, solid oxide fuel cell electrodes **(Yang et al. 2011, Li et al. 2012)**, second-harmonic generation crystals in non-linear optics **(Miller et al. 1963)**, and high-temperature superconductors **(Wu et al. 1987)**.

NO_X traps are part of the abatement technology called "NO_X storage and reduction" (NSR), which is used in combination with lean-burn engines, i.e. engines where the O_2 content is higher than stoichiometric, such as diesel and some gasoline engines. In this technology, $BaO/BaCO_3$ is used as a NO_x (NO and NO_2) trap by forming $Ba(NO_3)_2$ to store the NO_x which is formed during the combustion process. $Ba(NO_3)_2$ is then decomposed during a relatively short period where NO_x is released and reacted with hydrocarbons on precious-metal catalysts to regenerate the storage material.