



	<b>Experiment title:</b> XAS characterizations of AlIV(OH) modified SBA15 and their use as an anchor site for the immobilization of W-type organometallic complexes	<b>Experiment number:</b> 30-02-1121
<b>Beamline:</b> 30B	<b>Date of experiment:</b> from: 27 April 2017 / 02 May 2017	<b>Date of report:</b>  <i>Received at ESRF:</i>
<b>Shifts:</b> 18	<b>Local contact(s):</b> Aguilar-Tapia, A	
<b>Names and affiliations of applicants</b> (* indicates experimentalists): Saidi, A; <sup>1</sup> Werghi, B; <sup>1</sup> Almaksoud, W <sup>1</sup> ; Guan, E; <sup>2</sup> Tao, M; <sup>2</sup> Aguilar-Tapia, A; <sup>1</sup> Ould-Chikh, S.; <sup>1</sup> Basset, J.-M.; <sup>1</sup> Gates, B.; <sup>2</sup>		
<sup>1</sup> KAUST Catalysis Center (KCC), King Abdullah University of Science and Technology, Thuwal, Saudi Arabia		
<sup>2</sup> Department of Chemical Engineering, University of California, Davis, CA 95616, USA		

The X-ray absorption spectroscopy (XAS) experiments were carried out at the CRG-FAME beamline (BM30B), at European Synchrotron Radiation Facility (ESRF) at Grenoble, France. The mass of each sample was calculated to yield optimal absorption measurements at the W L<sub>3</sub>-edge (giving a total X-ray absorbance of approximately 2.0 calculated at an energy 50 eV greater than the absorption edge), on the basis of the metal content and the XAS cell dimensions. Since there were some additional spare beam time, we have taken the opportunity to measure several samples related to the latter topic involving other grafted metals: Hf/Ta L<sub>III</sub>-edge and Zr K-edge. Samples were sealed into the XAS cells in an Ar-filled glovebox with < 1 ppm moisture and < 1 ppm O<sub>2</sub>, and brought to the beamline without air and moisture exposure.

Spectra were collected in transmission mode with the respective metal foil simultaneously scanned to calibrate the energy shift. XAS spectra were recorded using a cryogenic XAS cell, under vacuum and liquid nitrogen temperature or a custom-designed XAS cell at room temperature, under ambient Ar atmosphere. The figure below show samples measured at W

L<sub>3</sub>-edge. The spectra are in general of good quality and will allow us to conduct at least a proper first shell analysis by EXAFS (work still ongoing at the time of writing).

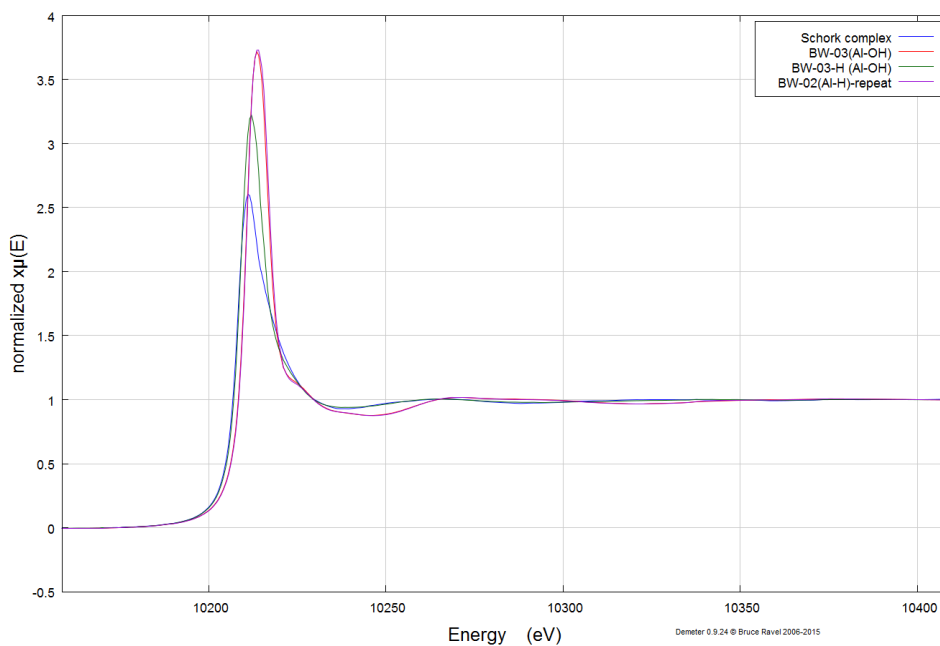


Figure 1: Selected XANES spectra of W based organometallic complexes grafted on Al single site isolated on silica surface.

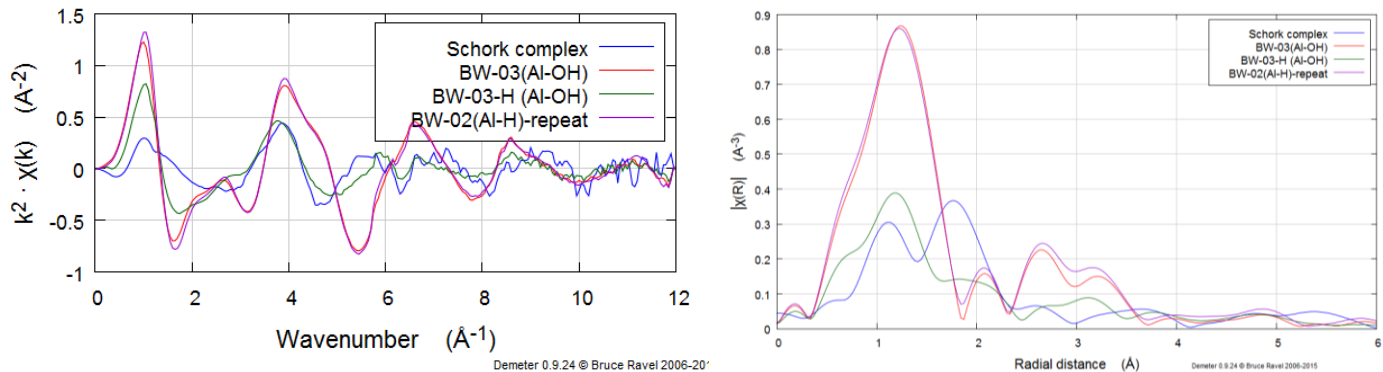


Figure 2: Selected  $k^2$ -weighted EXAFS and FT-EXAFS spectra of W based organometallic complexes grafted on Al single site isolated on silica surface.