ROTATIONAL CONFORMERS OF GROUP VI METAL (Cr, Mo, and W) BIS(MESITYLENE) SANDWICH COMPLEXES

SUDESH KUMARI, and DONG-SHENG YANG, *Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055.*

Group VI metal bis(mesitylene) sandwich complexes were produced by interactions between laser-vaporized metal atoms and mesitylene vapor in pulsed molecular beams, identified by photoionization time-of-flight mass spectrometry, and studied by pulsed-field-ionization zero-electron-kinetic-energy spectroscopy and density functional theory calculations. Although transition metal bis(arene) sandwiches may adopt eclipsed and staggered conformations, the group VI metal bis(mesitylene) complexes were determined to be in the eclipsed form. In this configuration, two rotational conformers, with methyl group dihedral angles of 0° and 60°, were identified for each complex. The adiabatic ionization energies of the 0° and 60° rotamers were measured to be 40557/40359, 42138/41697, and 41452/41000 cm^{-1} for the Cr, Mo, and W complexes, with the uncertainty of ∼5 cm^{-1}. The ground electronic states of the $0°(D_{3h})/60°(D_{3d})$ rotamers are $^1A_1'/^1A_{1g}$ in the neutral form and $^2A_1'/^2A_{1g}$ in the ionized form.