

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

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Transition metal bis(arene) sandwich complexes may adopt eclipsed or staggered conformations due to the aromatic ring rotations about the metal-arene axis.<sup>a,b</sup> In this study, the group VI (Cr, Mo, and W) metal bis(toluene) complexes are synthesized in a laser-ablation molecular beam source, and their rotational conformers are identified by pulsed-field-ionization zero-electron-kinetic-energy (ZEKE) spectroscopy. For Cr-bis(toluene), the ZEKE spectrum shows three distinctive vibrationless (0-0) transitions between the ground electronic states of the neutral and ionic complexes at 42739(5), 42745(5), and 42805(5)  $\text{cm}^{-1}$ , corresponding to ionization energies of 180°, 60°/120°, and 0° rotamers. In addition, the spectrum exhibits metal-toluene bending (164, 180, 196, and 223  $\text{cm}^{-1}$ ) and stretching (278 and 291  $\text{cm}^{-1}$ ) frequencies of these rotamers. The ground electronic states of the 0° and 180° rotamers are  $^1A_1$  ( $C_{2v}$ ) and  $^1A_g$  ( $C_{2h}$ ) in the neutral form and  $^2A_1$  ( $C_{2v}$ ) and  $^2A_g$  ( $C_{2h}$ ) in the ionized form, respectively. For the 60° and 120° rotamers, the ground states of the neutral molecules are  $^1A$  ( $C_2$ ), and those of the corresponding ions are  $^2A$  ( $C_2$ ). Through the variation of the molecular beam conditions, the eclipsed conformer (0°) is determined to be more stable than the staggered ones (180°, 120°, and 60°). Similarly, multiple conformers are identified for the Mo and W complexes.

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<sup>a</sup>B.S. Sohnlein, S. Li, and D.S. Yang, *J. Chem. Phys.* 123, 214306 (2005); B.S. Sohnlein and D.S. Yang, *J. Chem. Phys.* 124, 134305 (2006)

<sup>b</sup>S.Y. Ketkov, H.L. Sezle, and F.G.N. Cloke, *Angew. Chem. Int. Ed.* 46, 7072 (2007) and references therein.