

Mass-analyzed threshold ionization spectroscopy of some sandwich molecules. (IAMS, Academia Sinica, Taiwan^a, G. A. Razuvaev Institute of Organometallic Chemistry, Russian Academy of Sciences^b) Sheng-Yuan Tzeng^a(flyswimcamel@hotmail.com), Pei-Ying Wu^a(d01223104@ntu.edu.tw), Sergey Yulievich Ketkov^b(sketkov@iomc.ras.ru), and Wen-Bih Tzeng^a(wbt@sinica.edu.tw)

We applied the photo ionization efficiency and mass-analyzed threshold ionization (MATI) techniques to record the cation spectra of (η^6 -benzene)(η^6 -biphenyl)chromium and bis(η^6 -biphenyl)chromium. The adiabatic ionization energies (IEs) of these two sandwich molecules are determined to be 43374 and $42874 \pm 10 \text{ cm}^{-1}$, respectively. The prominent features appeared at 63, 150, 209, and 270 cm^{-1} with respect to the 0^+ band in the MATI spectrum of (η^6 -benzene)(η^6 -biphenyl)chromium result from the ring bending vibrations of the cation. We also performed the density functional theory (DFT) calculations at the B3PW91/6-311++G(d,p) level to predict the optimized molecular structure, transition energy, and vibrational frequency for these species. These calculations underestimates the IEs of these species by no more than 2%. The 0^+ band in the MATI spectrum of bis(η^6 -biphenyl)chromium has a full width at half maximum of about 200 cm^{-1} , which is much broader than a typical value of $10\text{--}20 \text{ cm}^{-1}$. This broad spectral feature likely results from overlap of the 0^+ bands of six conformational isomer. Our DFT calculations support the present experimental findings.