View metadata, citation and similar papers at core.ac.uk

brought to you by CORE

provided by Illinois Digital Environment for Access to Learning and Scholarship Repository

ELECTRONIC AND VIBRATIONAL STRUCTURE OF BUCKY BOWL

MASAAKI BABA, AYUMI KANAOKA, *Division of Chemistry, Graduate School of Science, Kyoto University, Kyoto, Japan*; MASATOSHI MISONO, *Applied Physics, Fukuoka University, Fukuoka, Japan*; HIDEHIRO SAKURAI, *Division of Applied Chemistry, Graduate School of Engineering, Osaka University, Suita, Japan*; MASASHI TSUGE, *Institute of Low Temperature Science, Hokkaido University, Sapporo, JAPAN*; PAVITHRAA SUNDARARAJAN, *Department of Applied Chemistry, National Chiao Tung University, Hsinchu, Taiwan*; YUAN-PERN LEE, *Department of Applied Chemistry, National Chiao Tung University, Hsinchu, Taiwan*.

Bucky bowl is the molecule of nonplanar polycyclic aromatic hydrocarbons. We analyzed the vibronic sructure in the $S_1 \leftarrow S_0$ fluorescence excitation spectra of jet-cooled sumanene and corannulene. The spectrum is congested with a large number of vibronic bands, which are mostly assigned to out-of-plane vibrational modes. The S_1 state of corannulene is identified to $^1E_2$ by the normal mode analysis, which is consistent with the result of SAC-CI calculation. The excitation energy of $^1A_2$ state was lower than that of the $^1E_2$ state by the TD-DFT method. The isolated corannulene molecule is considered to be a normal pentagon with considerable out-of-plane distortion (C_{5v}).

We observed the IR spectrum of corannulene in solid $para$-H_2, which also indicates that the moelcule has a structure with five-fold symmetry in the S_0 state. We found the IR bands originated from protonated corannulene molecules, which are produced by the chemical reaction with a proton.

[1] P. Sundararajan, M. Tsuge, M. Baba, and Y.-P. Lee, ACS Earth Space Chem. **2**, 1001 (2018)

[2] S. Kunishige, M. Baba, H. Sakurai, et al., J. Chem. Phys. **139**, 044313 (2013)