

Laboratory studies on the infrared emission spectra of fullerene C₆₀ thin films

T. Wakabayashi,¹ H. Suzuki,¹ M. Hatanaka,² and T. Kodama³

¹*Department of Chemistry, Kindai University, Japan*

²*Department of Chemistry, Keio University, Japan*

³*Kanagawa Institute of Technology, Japan*

Fullerene C₆₀ has been detected in interstellar objects at late stages of the stellar evolution, such as post asymptotic giant branch (post-AGB) stars, protoplanetary nebulae (PPNe), planetary nebulae (PNe), reflection nebulae, and young stellar objects (YSOs) [1-3]. It is natural to consider that the relative intensity of multiple emission bands of a single molecular species in the infrared (IR) spectra can be exploited as a probe for vibrational temperature of an ensemble of the molecules. Concerning C₆₀, variations are observed for the relative intensity of bands for four IR-active vibrational modes of T_{1u} symmetry. The thermal emission mechanism [1] and the UV-induced fluorescent mechanism [2] are proposed. However, the observations do not simply follow either mechanism. There must be another factor to be taken into considerations.

We have conducted laboratory studies on the measurement of IR emission spectra of fullerene C₆₀ at elevated temperatures. Using a commercial FTIR spectrometer, power spectra of heated samples of a thin film of C₆₀ deposited on a KBr slab were recorded in a range of 300–400 K. Theoretical simulations were performed under the assumption of Boltzmann distributions of molecules in vibrationally excited states up to seven vibrational quanta. Figure 1 depicts an image of contribution of vibrationally excited molecules to the IR emission of bands for T_{1u} modes of C₆₀ at ambient temperature.

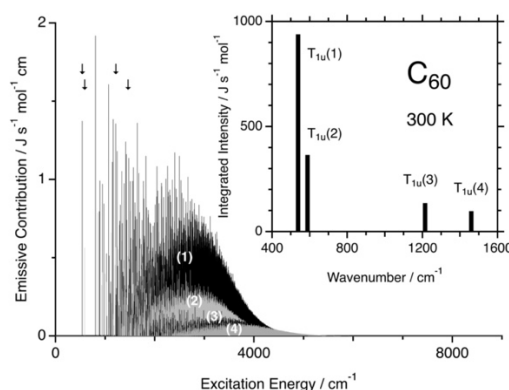


Figure 1: The simulated IR emission intensity of four vibrational T_{1u} modes of the fullerene C₆₀ molecule. Contributions from vibrationally excited states including 46 fundamentals and their overtones and combinations with excitations up to seven vibrational quanta are taken into considerations.

References

- [1] J. Cami, J. Bernard-Salas, E. Peeters, & S. E. Malek, 2010, *Science* 329, 1180.
- [2] K. Sellgren, M. W. Werner, J. G. Ingalls, J. D. T. Smith, T. M. Carleton, & C. Joblin, 2010, *ApJ*. 722, L54.
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