Molecular IR Emission Spectra of Solid C_{60} and C_{70} Fullerenes

Wakabayashi, T.,[1]* Mukai, Y.,[1] Wakebe, K.,[1] Hatanaka, M.,[2] Kodama, T.[3]

[1] wakaba@chem.kindai.ac.jp, Kindai University, Higashi-Osaka 577-8502, Japan
[2] Department of Chemistry, Keio University, Yokohama 223-8522, Japan
[3] Kanagawa Institute of Technology, Atsugi 243-0292, Japan

Cosmic abundance of fullerene molecules has been a focus in astrophysics and interstellar chemistry, since the detection of the infrared (IR) emission bands of C_{60} and C_{70} in the planetary nebula.[1] Concerning IR absorption spectra, vibrational fingerprints of C_{60} in solid pH_2 were understood by the presence of a number of isotopomers, $^{13}C_x{}^{12}C_{60-x}$ (x = 0−3), and discussed along the Einstein's B coefficient.[2] For the estimation of molecular abundance in space, vibrational temperature is crucial, because the IR emission requires population of molecules in their vibrationally excited states.

We measured IR emission spectra of a thin plate of solid C_{60} in the laboratory for the study of temperature dependence of the intensity ratio of the four IR-active vibrational T_{1u} modes of the icosahedral molecule in a range of 300−370 K.[3] Figure 1 shows typical IR emission spectra of C_{60} and C_{70} at 353 K (80°C). The four IR emission bands of C_{60} easily saturate to the blackbody contour and numerous combination bands and overtones are intensified in-between. The same characteristics apply to the observed IR emission spectra of C_{70}. A relatively simple model based on Boltzmann distribution for the v = 1 level of normal modes in the individual molecule is compatible with the observed intensity ratios of the four IR emission bands of C_{60}. Figure 2 depicts simulated temperature dependence of the IR emission intensity for the T_{1u} modes of C_{60}.

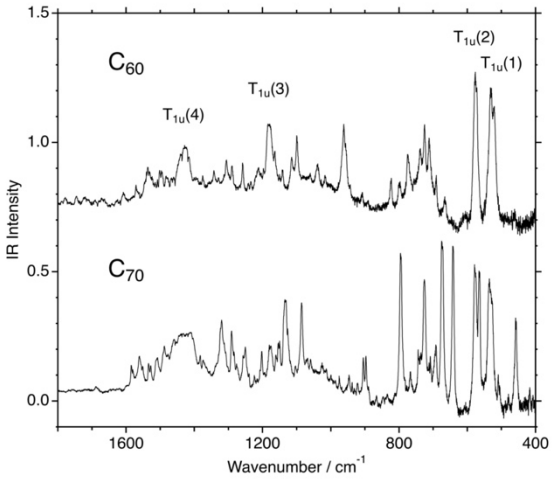

Fig. 1. IR emission spectra of thin plates of C_{60} and C_{70} fullerenes at elevated temperature of 353 K.

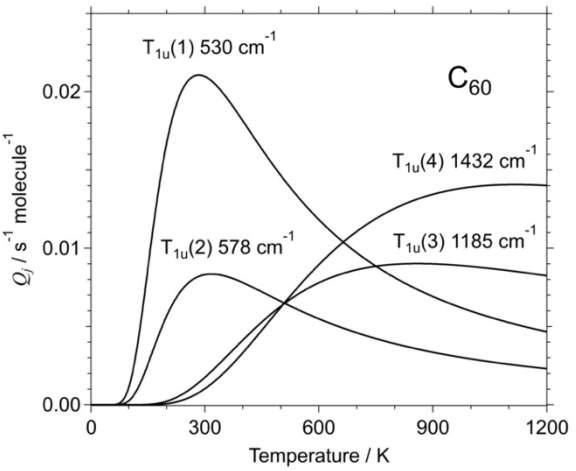

Fig. 2. Simulated temperature dependence of the IR emission intensities for the T_{1u} modes of C_{60}.

[1] Cami, J.; Bernard-Salas, J.; Peebles, E.; Malek, S. E. Detection of C_{60} and C_{70} in a young planetary nebula. *Science*, **2010**, *329*, 1180.
[2] Wakabayashi, T.; Momose, T.; Fajardo, M. E. Matrix isolation spectroscopy and spectral simulations of isotopically substituted C_{60} molecules. *J. Chem. Phys.* **2019**, *151*, 234301.
[3] This work is supported by Grant-in-Aid for Scientific Research, 20K05438, from The Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan.