EXCITED-STATE DYNAMICS IN THE S_1 STATE OF DIBENZOFURAN

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Dibenzofuran is a prototypical molecule of toxic dioxins and it is of great importance to investigate the excited-state dynamics. We have analyzed the vibronic structure of the $S_1\ ^1A_1 \leftarrow S_0$ transition of jet-cooled dibenzofuran. Several vibronic bands are stronger than the 0_0^0 band. These bands are found to be the A-type transition [a] and the intensity arises from vibronic coupling with the $S_2\ ^1B_2$ state.
We have observed rotationally resolved ultrahigh-resolution spectra of prominent vibronic bands and the changes with the magnetic field. We analyzed each rotational line and determined the rotational constants. It has been shown that the intramolecular vibrational redistribution (IVR) takes place remarkably in the high vibrational levels, but intersystem crossing (ISC) is not efficient in the isolated dibenzofuran molecule.

[a] M. Baba, M. Yamawaki, A. Doi, Y. Tatamitani, S. Kasahara, and H. Katô, Symposium on Molecular Spectroscopy, Ohio State University, Columbus 2005, TG04.