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赤外分光によるベンゼン二量体エキシマー状態の構造研究

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A structural study on the excimer state of an isolated benzene dimer using infrared spectroscopy in the skeletal vibration region

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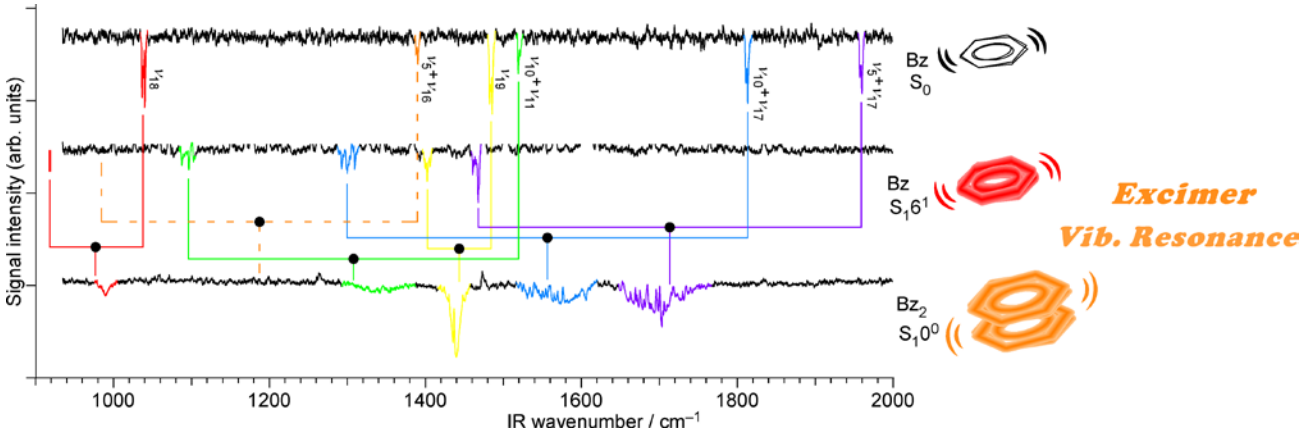

ベンゼン二量体は芳香族分子間の相互作用を考える上で重要な系であり、発光材料などの機能分子の形成機構の基礎的理解に不可欠である。本研究では、ベンゼン二量体の励起状態が形成するエキシマー状態の赤外分光を初めて行った。これまでエキシマー状態では電子状態が共鳴状態にあることが知られていたが、振動状態についても共鳴状態にあることを初めて明らかにした。

Vibrational structure and geometry of the excimer (EXC) state of the isolated benzene dimer, where the electronic excitation is equally shared between the two benzene (Bz) units, was studied by IR spectroscopy. Each band position locates nearly at the average of the corresponding vibrations in the electronic ground and excited states of the Bz monomer. This frequency averaging is explained by an excitation exchange model that takes into account vibrational excitations. This model clarifies that Franck–Condon factors between the S_1–S_0 transition of the monomer govern not only the magnitude of the EXC interaction, but also the configuration of vibrational states.