

Molecular Recognition Analyzed by Observing Intramolecular Interconversion with EPR Spectroscopy

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Molecular recognition between Rebek's cleft **R** and 4-(2-benzimidazolyl)-aminomethyl-2,6-di-*tert*-butyl-phenol (**Bi**) is investigated by means of EPR spectroscopy. Their specific intermolecular interactions are distinguished from non-specific interactions represented by mere protonation on addition of benzoic acid. Both interactions are related to intramolecular interconversions at the C_α-atom of **Bi**^{*}, where a two-jump mechanism is found for free and protonated **Bi**^{*} and a two-site exchange for the complexed ligand. While NMR spectroscopy indicates the existence of 1:1 and 1:2 receptor-substrate complexes, the faster time scale of EPR spectroscopy allows to identify one 1:2 as well as three 1:1 associates and to elucidate their formation conditions. Based upon the corresponding hf parameters, binding modes and sites are proposed for the key-in-the-lock system.

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