HIGH VIBRATIONAL STATE ENERGY REDISTRIBUTION IN PARTIALLY DEUTERATED CYCLOPENTENES

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Experimental investigations of high vibrational states in medium-size molecules show clear evidence of large intramolecular redistribution of the vibrational energy (IVR). In particular, the CH bond stretching vibration energy rapidly relaxes in combination states involving deformations of the angles adjacent to the initially excited CH bond[a,b].

In this contribution, the overtone spectra (Δv=1 to 6) of cyclopentene 3,3,4,4-d_4 and cyclopentene 1,2,3,3,4,4,5-d_7 are analyzed with a model formulated in curvilinear internal coordinates including also the coupling between the ring-puckering motion and the vibrations.

In the dihydrogenated compound, the analysis of the spectra indicates a progressive localization of the CH stretching vibrations with increasing energy. At high energy (from Δv=4 to 6),the spectra of the two compounds evidence different IVR for CHD or CH_2 groups.

[a] S. Rodin-Bercion, D. Cavagnat, L. Lespade and P. Maraval, J.Phys.Chem.,99, 3005 (1995)

[b] L. Lespade, S. Rodin-Bercion and D. Cavagnat, J.Phys.Chem., 101, 2568 (1997)