SHAPE OF THE LOCAL-VIBRATION BAND OF ADSORBED HYDROGEN-BONDED MOLECULAR COMPLEXES

V. E. KLYMENKO, I. V. KUZMENKO, and V. M. ROZENBAUM, *Institute of Surface Chemistry of National Academy of Sciences of Ukraine, Generala Naumova str. 17, Kiev-164, 03164 Ukraine..*

The temperature dependence of spectral bands of local vibrations is caused by the anharmonic coupling of these vibrations with the low-frequency vibrational modes [a]. This dependence is well described by the dephasing model, which gives a number of exact solutions [b] and takes into account the degeneration of low-frequency vibrations [c]. The possibilities of the dephasing model were most completely used for studying hydrogen bonds, which are characterized by the low-frequency libration modes and substantial anharmonicity [d]. The linear hydrogen-bonded complexes have the axial symmetry, which causes the double degeneration of antisymmetric and symmetric libration modes. In many cases, frequencies of these librations are close, so that one can assume that the libration modes are fourfold degenerate, this degeneration being removed upon adsorption of the molecular complexes. In this presentation, we consider a change in the shape of the vibrational band of the hydrogen atom caused by the interaction of such molecular complexes with a surface. The surface effect is taken into account by introducing the parameter of removal of the degeneration of low-frequency libration modes. As a coupling of the complex with the surface increases, the width of the spectral band and shift of its maximum decrease, and their ratio increases from 1.38 to 2.45.

---

[a] A. A. Maradudin, Theoretical and experimental aspects of the effects of point defects and disorder on the vibrations of crystalls, (Academic Press, New York, 1966).

[b] D. C. Langreth and M. Persson, Phys. Rev. B 43, 1353 (1991).

[c] V. M. Rozenbaum, Phys. Lett. A 165, 275 (1992).

[d] A. V. Iogansen and M. Sh. Rozenberg, Zh. Strukt. Khim. 30, 92 (1989).