

NATURE OF THE FREQUENCY
SHIFT OF HYDROGEN VALENCE
VIBRATIONS IN WATER MOLECULES

I.V. Zhyganiuk, M.P. Malomuzh

I.I. Mechnikov National University of Odessa
(2, Dvoryanska Str., Odessa 65026, Ukraine;
e-mail: zhyganiuk@gmail.com)

S u m m a r y

The physical nature of the frequency shift of hydrogen valence vibrations in the water molecule due to its interaction with neighbor molecules has been studied. Electrostatic forces connected with multipole moments of molecules are supposed to give a dominating contribution to the intermolecular interaction. The frequency shift was calculated for the case when two neighbor molecules form a dimer. The obtained result is in qualitative agreement with the frequency shifts observed for water vapor, hexagonal ice, and liquid water, as well as for aqueous solutions of alcohols. This fact testifies to the electrostatic nature of H-bonds used to describe both the specific features of intermolecular interaction in water and the macroscopic properties of the latter.