

INTERMOLECULAR INTERACTION
INFLUENCE ON THE DIRECTION
OF OH-BOND IN H₂O MOLECULE

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S u m m a r y

Comparative study of the direction of the OH-bond in a molecule H₂O in the liquid and gas phases is carried out. A force constant matrix of a molecule H₂O in the liquid phase is also calculated. The vibrational spectroscopy inverse spectral problem is solved with this purpose. The 3N-matrix method is used where the frequencies of both eigen and noneigen normal vibrations are included into the evaluation procedure. It is found that the direction of the chemical bond O–H does not coincide with the direction of the straight line connecting the nuclei of the atoms O and H and that the deviation of the chemical bond is equal to 6° for a molecule H₂O in the liquid phase and 2° for a molecule H₂O in the gas phase. The possibility of 'mixing' of different types of eigen and noneigen normal vibrations of a molecule H₂O in the liquid phase is taken into account. "Mixing" of the forms of eigen and noneigen normal vibrations of a molecule H₂O increases the deviation angle up to 7.5°. Such a relatively big angle between OH-bonds (115°) can cause a more compact water molecule packing in comparison with ice. This may be the reason for increasing the volume of water at freezing.