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Dispersion-corrected first-principles calculation of terahertz vibration, and evidence for weak hydrogen bond formation[1] MASAE TAKAHASHI, YOICHI ISHIKAWA, Tohoku University, HIROMASA ITO, RIKEN — A weak hydrogen bond (WHB) such as CH–O is very important for the structure, function, and dynamics in a chemical and biological system WHB stretching vibration is in a terahertz (THz) frequency region Very recently, the reasonable performance of dispersion-corrected first-principles to WHB has been proven. In this lecture, we report dispersion-corrected first-principles calculation of the vibrational absorption of some organic crystals, and low-temperature THz spectral measurement, in order to clarify WHB stretching vibration. The THz frequency calculation of a WHB crystal has extremely improved by dispersion correction. Moreover, the discrepancy in frequency between an experiment and calculation and is 10 1/cm or less. Dispersion correction is especially effective for intermolecular mode. The very sharp peak appearing at 4 K is assigned to the intermolecular translational mode that corresponds to WHB stretching vibration. It is difficult to detect and control the WHB formation in a crystal because the binding energy is very small. With the help of the latest intense development of experimental and theoretical technique and its careful use, we reveal solid-state WHB stretching vibration as evidence for the WHB formation that differs in respective WHB networks

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