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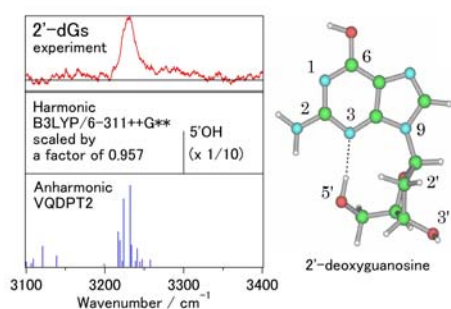
Conformational analysis of the guanine nucleosides based on *ab initio* anharmonic vibrational calculation*H. Asami*¹; *H. Saigusa*¹; *K. Yagi*²

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The guanine nucleosides consisting of the base moiety and sugar group can reveal various types of conformers and isomers in addition to the keto-enol tautomerization of guanine. Recently, we obtained IR spectra of guanosine (Gs) and 2'-deoxyguanosine (2'-dGs) in the gas phase and found that the transitions associated with the sugar group substantially differ for the two species [1]. Specifically, the IR spectrum of 2'-dGs reveals a broad transition at 3230cm⁻¹, which is assigned to the 5'-OH stretching vibration. The broadening is consistent with the occurrence of internal hydrogen bonding with the N3 atom of guanine. However, the frequency redshift of 21 cm⁻¹ with respect to that of Gs cannot be explained readily by the conventional harmonic frequency calculation.

More precise prediction of the vibrational frequencies for such hydrogen-bonded systems requires a quantum mechanical treatment of the vibrational motion as well as a reliable anharmonic potential energy surface (PES). Therefore, we have performed an anharmonic frequency calculation by using the second-order vibrational quasi-degenerate perturbation theory (VQDPT2) based on the vibrational self-consistent field zeroth-order Hamiltonian [2]. Then, a full 93 dimensional anharmonic PES has been derived from *ab initio* electronic structure theory using the multiresolution method [3]. The result shows that the broad IR transition can be explained satisfactorily by taking account of high-order anharmonic couplings. It is therefore suggested that rigorous treatment of the anharmonicity is needed in the structural assignment of flexible biomolecular systems.

[1] H. Asami, S. Urashima, and H. Saigusa, *Phys. Chem. Chem. Phys.* 2009, 11, 10466.[2] K. Yagi, S. Hirata, and K. Hirao, *Phys. Chem. Chem. Phys.* 2008, 10, 1781.[3] K. Yagi, S. Hirata, K. Hirao, *Theor. Chem. Acc.* 2007, 118, 681.

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