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Intrinsic Dynamic Nature of Neutral Hydrogen Bonds Elucidated with QTAIM Dual Functional Analysis: Role of the Compliance Force Constants and QTAIM-DFA Parameters in Stability

The group of Professor Waro Nakanishi and Dr. Satoko Hayashi

Invited for this month's cover picture is Professor Satoko Hayashi's group from the Faculty of Systems Engineering at Wakayama University (Japan). The cover picture shows Japanese lanterns for the Bon festival dance dangling on two ropes, and several molecular graphs with contour maps for hydrogen bonds (HBs) emerging from the lanterns. The curves of the ropes may correspond to the ΔE (energy of formation) and C_{ij} (compliance constant) values for HBs, for which the product will be constant. Read the full text of their Full Paper at 10.1002/open.201800051.

What are the main challenges in the broad area of your research?

To improve the causality of experimental results, we have proposed a concept called "Keisan-sendo", which is a calculation-derived method to study the chemical sciences. In Keisan-sendo, the calculations are performed prior to the experimental process, and the theoretical conclusions are obtained independently. The experimental results are yielded from the corresponding experimental processes. The final conclusions are obtained by examining both the theoretical and the experimental data. Specifically, NMR parameters are analyzed based on the MO theory, the concept of the extended hypervalent interactions is proposed, and interactions are presented in a unified form, employing quantum theory of atoms-in-molecules dual functional analysis (QTAIM-DFA). Elucidation of the hydrogen bond (HB) nature in this work is based on this methodology.

What was the biggest surprise on the way to the results presented in this paper?

Recently, we proposed a highly reliable method to generate the perturbed structures for QTAIM-DFA, called CIV, which employs the coordinates corresponding to the compliance force constants, C_{ij} for internal vibrations. It is necessary to check the high applicability of CIV to a wide range of HBs to establish QTAIM-DFA on a firm basis. Using this methodology, the energies of the formation of neutral HBs from the components (ΔE) are demonstrated to be inversely proportional to C_{ij} for the HBs.

What advice can you give to students interested in your field or chemistry in general?

Taro, a member of our research group and the first author of this paper, is a second-year graduate student. He has worked diligently on this subject to reach the final conclusions. Taro's quiet dedication resulted in this achievement. Young researchers need to advance research of sublime projects, and sometimes they need to recognize the importance of believing in themselves and pushing forward.