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The Editor, Journal of Molecular Spectroscopy

Dear Michael Heaven, PhD,

Dear Jun. Prof. Daniel Obenchain, PhD,

Dear Prof. Garry Grubbs II, PhD,

Please find enclosed the manuscript: “Toward Less Ambigous Vibrational Spectroscopic Notations for Hydrogen-Bonded Water and Methanol Clusters”. We kindly ask you to consider it as a paper for your special issue *Contributions of Bachelor and Master Student Research to Spectroscopy.*

Considering vibrational notations, normal modes with delocalized character are difficult to denote, representing these normal modes by contributions of internal coordinates provides an alternative route to derive notations. However, defining internal coordinate sets for this analysis in the first place becomes challenging as molecules get larger and topologically more complex, leading to a combinatorial explosion of possible definitions. In our recent work we proposed a systematic approach, which utilizes symmetry and topology, to considerable reduce the space of definable internal coordinate set. This algorithm selects an optimal coordinate set which has the highest separability in terms of the harmonic potential energy.

In this work, we have implemented an automatic detection and generation of internal coordinates along hydrogen bond axes. Using the enhanced "Nomodeco" toolkit, we apply this approach to various hydrogen-bonded clusters. Our analysis demonstrates how representing normal modes through internal coordinate contributions offers an alternative strategy for the precise annotation of vibrational motions. We discuss how this normal mode decomposition scheme aids in the clear identification of principal motion patterns and propose strategies for accurately assigning vibrational notations in these hydrogen-bonded systems. We believe this manuscript will be of significant interest to the broad readership of the *Journal of Molecular Spectroscopy*, and we respectfully submit it for consideration within the scope of the special issue.

We suggest the following reviewers:

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We are very much looking forward to hearing from you,

Sincerely yours,

Klaus Liedl