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Title:	Topological studies related to molecular systems formed during the Big Bang: H ₃ ⁺ as an example
Authors:	Mukherjee, B. (/jspui/browse?type=author&value=Mukherjee%2C+B.) Shamasundar, K.R. (/jspui/browse?type=author&value=Shamasundar%2C+K.R.) Adhikari, S. (/jspui/browse?type=author&value=Adhikari%2C+S.) Baer, M. (/jspui/browse?type=author&value=Baer%2C+M.)
Keywords:	Molecular systems Surrounding conical intersections Creation
Issue Date:	2019
Publisher:	Wiley Online Library
Citation:	International Journal of Quantum Chemistry, 119(16).
Abstract:	In the present article are analyzed the non-adiabatic coupling terms (NACT) for two molecular systems, namely H ₃ ⁺ and H ₃ . In contrast to previous occasions in which the NACTs are studied along (closed) circular contours usually surrounding conical intersections (ci), in the present article are studied distribution of the NACTs in (planar) configuration spaces (CS). The motivation for this study has to do with a novel idea being mentioned earlier (Molec. Phys., 116, 2435 [2018]; ArXiv:1801.00103) that NACTs are like a Glue (eventually) associated with the ability of creating molecules and/or protecting them from breaking up. It was found that the distributions of the NACTs due to the two molecules are similar as long as the attention is given to regions close to their equilateral cis, but then they behave significantly different in other regions. In case of H ₃ ⁺ , the NACTs are distributed rather uniformly whereas, in case of H ₃ they become spiky the closer they approach the diatom axis. The main conclusion of this study is that the glue which has its origin in the NACTs is most likely to be effective in case of H ₃ ⁺ that explains the creation and later survival of this molecule.
URI:	https://onlinelibrary.wiley.com/doi/full/10.1002/qua.25949 (https://onlinelibrary.wiley.com/doi/full/10.1002/qua.25949) http://hdl.handle.net/123456789/1902 (http://hdl.handle.net/123456789/1902)
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