Bond Flexing, Twisting, Anharmonicity and Responsivity for the IR-active modes of Benzene

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Abstract

In this investigation we have used NG-QTAIM to fully quantity the response to the four IR-active modes of all the bonding in benzene in terms of bond-flexing, bond-torsion and bond-anharmonicity that includes the tendencies towards IR-responsivity and IR-non-responsivity. Bond-anharmonicity is found to be lacking for the C-C bonds comprising the lowest frequency mode (721.57 cm-1) measured as the absence of bond critical point (BCP) sliding. Additionally, bond-flexing was absent for this mode harmonic-like variation of the profile of the variation of the wrapping (torsion) of the {p,p'} path-packet, referred to as the Precession K, along the conventional QTAIM bond-path, the remaining three IR-active mode possessed step-like variations in the K profiles. The presence of non-nuclear attractors was detected for the IR-active mode with frequency 1573.93 cm-1 with C-C K profiles that most closely resemble those of the relaxed benzene. We quantified the C-H bonds in terms of bond-flexing and bond-anharmonicity and IR-responsivity and IR-non-responsivity.

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