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# High precision calculation of structural properties of three-body molecular ions

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The investigation on high-precision calculations of molecular ions emerges as a captivating and fascinating domain of research. The meticulous exploration of molecular ions necessitates a comprehensive understanding of their structural, electronic and dynamic properties. In a molecular system, unlike in an atomic system, describing nuclear motion is significantly more complicated due to the constraints on its movement. Consequently, calculations beyond the Born-Oppenheimer approximation become exceedingly intricate. Apart from the approximation method, such as *coupled-cluster*, *density functional*, *perturbation* theory etc., the *Ritz variational* method turns out to be one of the most efficient methods to accurately determine structural properties of a three-body molecular system [1-4]. In this work, we have studied the structural properties of various symmetric and asymmetric molecular three-body systems, such as $H_2^+$, $D_2^+$, $T_2^+$, HD+, DT+ (and their muonic substitutions) *etc.*, using the trial wave function expanded in explicitly correlated *Hyllerass* type basis set of the form: $\Psi(r_1, r_2, r_{12}) = \left(1 + k\hat{P}_{12}\right) \sum_{i=1}^{N} C_i r_1^{l_i} r_2^{m_i} r_{12}^{n_i}\ exp(-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12})$, where $(r_1, r_2, r_{12})$ are the relative coordinates, $\hat{P}_{12}$ is the two-particle permutation operator, $(l_i, m_i, n_i)$ and $(\alpha_i, \beta_i, \gamma_i)$ are basis set parameters and non-linear exponents, $k = +1(-1)$ is for symmetric singlet (triplet) and $k = 0$ is for an asymmetric system. Further, we consider an additional large parameter M in the power of inter-nuclear distance $r_{12}$ to ensure that the factor $r_{12}^{n_i+M} exp(-\gamma_i r_{12})$ replicates the notion of Gaussian profile essential for capturing the localized nature of nuclear motion. The *stabilization method* [5] is utilized to accurately determine the energy eigenvalues and geometrical quantities (such as expectation values of inter-nuclear distance, nuclear-particle separation, corresponding angles, cusps *etc.*) of ground and some low-lying singly excited states, as well as continuum embedded *Feshbach* resonance states. Moreover, we have tried to expand the present explicitly correlated method to assess its viability in investigating *four-body* molecular systems, such as $Ps_2$ and $H_2$ molecules, which offer intriguing characteristics unique to such systems.

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