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Charge asymmetry of the first excited rotational states of diatomic molecules using explicitly correlated all-particle Gaussian functions NIKITA KIRNOSOV, KEEPER SHARKEY, LUDWIK ADAMOWICZ, The University of Arizona — Highly accurate interparticle distances and correlation functions of the HD^+ cation in its first rotationaly excited state found in the non-Born-Oppenheimer approach are reported. To describe each state, 8000 explicitly correlated Gaussian functions were used. After careful optimization of the linear and nonlinear parameters, the correlation function, expectation values for interparticle distances, and nuclear correlation functions were computed. The results allow to us explicate the charge asymmetry dependence on the vibrational excitation and the effects of the rotational excitation.

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