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New Types of Explicitly Correlated Gaussian Functions for Non-Born-Oppenheimer Molecular? Calculations. MARTIN FORMANEK, KEITH JONES, University of Arizona, SERGIY BUBIN, Nazarbayev University, LUDWIK ADAMOWICZ, University of Arizona — In this work we explore the possibility of using a new functional form of Explicitly Correlated Gaussian-type functions (ECGs) for performing non-Born-Oppenheimer calculations of diatomic molecular systems. Namely we focus our attention on ECGs with pre-exponential factors in the form of sin/cos functions of the square of the internuclear distance (sin/cos-ECGs). These ECGs can be generated as linear combinations of ECGs with complex exponential parameters (complex-ECGs) The complex-ECGs were previously used to calculate energy levels of He atom [1] and with the sin/cos-ECGs the vibrational energy levels for the H_2 molecule described by an effective Morse potential were calculated [2]. The focus of this study is ab-initio description of a real diatomic molecule, namely HD^+, within the framework where the BO approximation is not assumed using these basis sets. The aim is to compare their accuracy and efficiency with ECGs with pre-exponential factors in the form of even powers of the internuclear distance and to assess their potential usefulness in non-BO calculations of molecules with more than two nuclei. [1] S. Bubin and L. Adamowicz, J. Chem. Phys. 124, 224317 (2006) [2] M. Formanek, K.L. Sharkey, N. Kirnosov and L. Adamowicz, J. Chem. Phys. 141, 154103 (2014)

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