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Combination of Electronic Structure Calculations and Rovibrational Spectroscopic Constants for Enhancement of Lennard-Jones Potential in the Description of Molecules Involving Gas-Nobles

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Abstract: The properties of noble gases are of great interest for the development of Modeling techniques and as standard values for experimental studies. The diatomic molecules of noble gases in their fundamental electronic states represent ideal prototypes of van der Waals type molecules, their spectroscopic and thermodynamic properties have been extensively studied both theoretically [1, 2] and experimentally [3,4]. These molecules are of special interest in the field of metrology [1]. Since to determine the properties of thermophysical fluid, it is necessary to know the potential energy curve between two noble gas atoms. In this work, we first determined the electronic energies for the ground state via the coupled[5] cluster method - CCSD(t) for the following molecular systems: He-He, He-Ne, He-Ar, He-Kr, He-Xe, Ne- Ar, Ne-Kr, Ne-Xe, Ar-Ar, Ar-Kr, Ar-Xe, Kr-Kr, Kr-Xe and Xe-Xe. These energies were calculated for three different basis sets; aug-cc-pVTZ, aug-cc-pVQZ and aug-cc-pV5Z. These energies were then carefully adjusted using the analytical form named Improved Lenard Jones (ILJ) in order to obtain the additional parameter beta of each molecular system. This parameter accounts for the hardness/softness of the two involved partners. In particular, we can observe that the aug-cc-pV5Z basis set with the corrected BSSE [6] provided (for all studied systems) beta parameter values very close to 9 (Experimental value). The quality of the ILJ analytical form (using the adjusted parameter beta) was tested tthrough the rovibrational spectroscopic constant calculations. The ILJ obtained results agree very well with the experimental data [4] and theoretical [7] results available for in the literature.

Key-words: Gas nobles, Electronic energies, Improved Lennard Jones and Rovibrational spectroscopic constants .

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