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Spectroscopy and Quantum Mechanics of the Helium Dimer (He_2^+), Neon Dimer (Ne_2^+), Argon Dimer (Ar_2^+), Krypton Dimer (Kr_2^+), Xenon Dimer (Xe_2^+), Radon Dimer (Rn_2^+) and Ununoctium Dimer (Uuo_2^+) Molecular Cations

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Some of the simplest of all molecules are the Helium dimer, Neon dimer, Argon dimer, Krypton dimer, Xenon dimer, Radon dimer and Ununoctium dimer molecular cations, He_2^+, Ne_2^+, Ar_2^+, Kr_2^+, Xe_2^+, Rn_2^+ and Uuo_2^+. Because of their simplicity and importance, these molecular cations have received considerable attention from experimentalists as well as theoreticians [1-11]. The exact solution of the electronic Schrödinger equation for these cations plays an important role in investigating the molecular structure of more complex systems.

In this editorial, some of approximation as well as exact solutions of the Schrödinger equation for these cations have been studied and one the exact solutions have been considered in details. By making use of the perturbation theory, cosmological perturbation theory and also homotopy perturbation method with the help of the linear extrapolation techniques, we have presented a simpler novel method to obtain the numerical exact solution. The Mathematica 10 programs have been used to solve the related equations, numerically. Potential energy curves have been plotted versus internuclear distance for the ground and some of the electronic excited states (Figure 1). The electronic distribution functions' plots have been also investigated.

On the other hand, the Gaussian 09 is useful for theoretical, mathematical, physical, organic, inorganic, applied, quantum, spectroscopic and computational chemists and also experimental section that is not carry out. Gaussian 09 is an electronic structure program. Moreover, Gaussian 09 is used by chemists, chemical engineers, materials engineers, biochemists, physicists and others for research in established and emerging areas of chemical interests. This program does many computations on molecular structures and thermodynamic parameters and properties which some of them need to high computation power and also take more computers resources and some of them crash due to lack of resources, too. Therefore, to run such calculations for solving Schrödinger equation for these cations, we need to computation power of super computers such as IBM power, Sun Cray super computers and so on. But as getting access to such systems are limited and they are also too expensive, we can get such power by making a cluster of PCs. In this editorial, we also would like to discuss about parallel processing basics and running Gaussian 09 in parallel. However, measurement of uncertainty possesses an important role in theoretical, mathematical, computational, numerical, quantum and spectroscopic methods. The uncertainty is amount of probability error. Also, the uncertainty should be determined in an observation and then a probability way should be considered for uncertainty determining. In this editorial, the uncertainty for solving Schrödinger equation for these cations has also been identified and it has been described. Furthermore, because of identification and formation of new molecules such as Helium dimer (He_2^+), Neon dimer (Ne_2^+), Argon dimer (Ar_2^+), Krypton dimer (Kr_2^+), Xenon dimer (Xe_2^+), Radon dimer (Rn_2^+) and Ununoctium dimer (Uuo_2^+) molecular cations, theoretical, mathematical, physical, quantum and computational chemistry and also molecular spectroscopy gaining increasing importance in recent decades. In addition, these cations for the sake of their small atoms and need to identify and separations gains increasing importance. In this editorial, the molecular structure and thermodynamic parameters and properties of these cations have also been investigated and calculated (Figures 2 and 3).

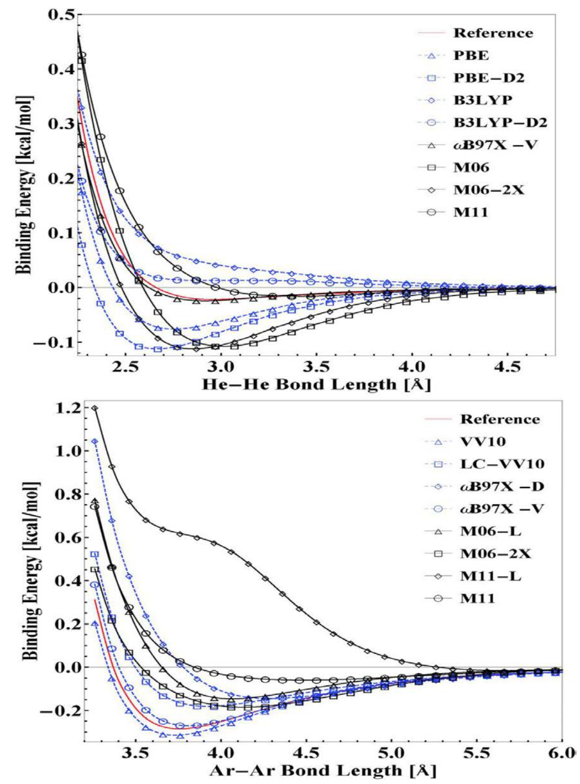

Figure 1: Binding energy curves versus internuclear distance for the ground and some of the electronic excited states of Helium dimer (He^{2+}) (left illustration) and Argon dimer (Ar^{2+}) (right illustration) molecular cations.

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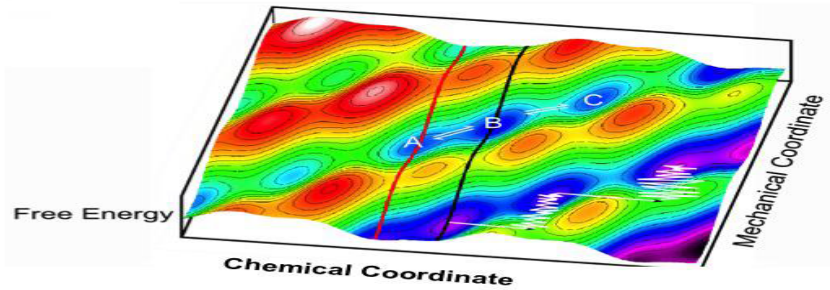

Figure 2: Simulation of free energy, chemical coordinate and mechanical coordinate of Ununoctium dimer (Uuo_2^+) molecular cation.

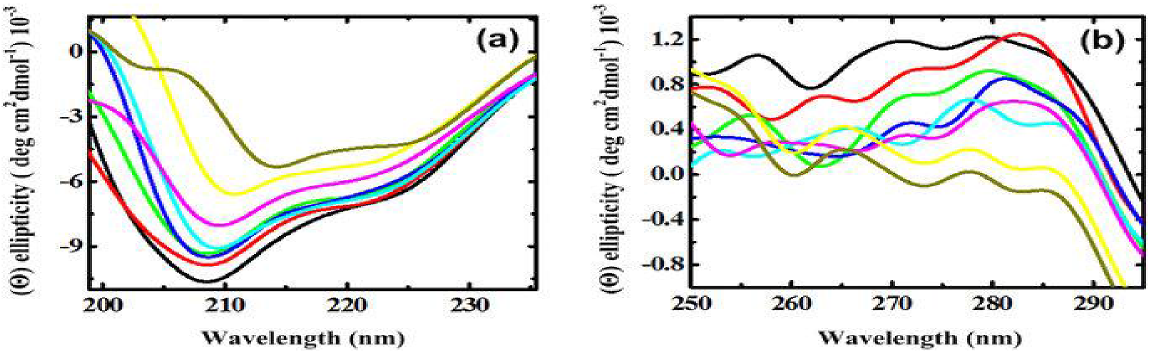

Figure 3: Elipticity of (a) Hydrogen (H_2) (dark–blue curve), Helium (He_2) (brown curve), Neon (Ne_2) (red curve), Argon (Ar_2) (yellow curve), Krypton (Kr_2) (black curve), Xenon (Xe_2) (light–blue curve), Radon (Rn_2) (pink curve) and Ununoctium (Uuo_2) (green curve) gas dimers and (b) Hydrogen dimer (H_2^+) (dark–blue curve), Helium dimer (He_2^+) (brown curve), Neon dimer (Ne_2^+) (red curve), Argon dimer (Ar_2^+) (yellow curve), Krypton dimer (Kr_2^+) (black curve), Xenon dimer (Xe_2^+) (light–blue curve), Radon dimer (Rn_2^+) (pink curve) and Ununoctium dimer (Uuo_2^+) (green curve) molecular cations.

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