AN EXPERIMENTAL TEST OF QUANTUM CHEMICAL CALCULATIONS OF THE He-He VAN DER WAALS POTENTIAL

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The He dimer has a binding energy of about 10^{-3} K ($7{\cdot}10^{-3}$ cm^{-1}) and is therefore the most weakly bound of all naturally occuring diatomic molecules in the ground state. Since the atom has only two electrons in a closed shell the calculation of the interaction potential is, in principle, straight-forward using well established quantum chemical methods except that an extremely high precision is required to obtain the correct binding energy. Thus the dimer binding energy provides an exceedingly stringent test of quantum chemical algorithms. Recently Anderson[a] has used his "exact" Quantum Monte Carlo (QMC) method to calculate a few points on the potential curve with a relative precision of better than $2{\cdot}10^{-4}$. He finds excellent agreement with the latest MR-ACPF (averaged coupled pair functional) method calculations of Gdanitz[b].

Since the He dimer is not optically active, is present only in very low concentrations at 10^{-3} K temperatures and, moreover, very fragile it is not accessible using usual spectroscopic techniques. Recently our group has demonstrated that the huge size of the dimer ($<$R$>$ $\cong$ 50Å) can be measured by diffracting the dimers in a beam of atoms and clusters formed in a cryogenic nozzle expansion from a nanostructured transmission grating[c]. The relative diffraction intensities up to the 7^{th} order can be measured and provide information on the extent to which the effective slit width is reduced because of the finite extent of the dimer. Since the average size is inversely proportional to the sqrt of the binding energy, $<$R$>$ thus provides direct information on the binding energy. New improved experiments with better statistics evaluated with a better theory will be compared with the latest calculations of Gdanitz. The remaining errors in the experiment and the approximations in the theory will be discussed.

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[a] J.B. Anderson, *J. Chem. Phys.* 115, 4546 (2001) and private communications

[b] R.J. Gdanitz, *Mol. Phys.* 99, 923 (2001) and private communications

[c] R.E. Grisenti, W. Schöllkopf, J.P. Toennies, G.C. Hegerfeldt, T. Köhler and M. Stoll, *Phys. Rev. Lett.* 85, 2284 (2000)