B.5.6. Weakly Bound Triatomic Molecules and Diatomic Molecular Anions--*Yong Li, Jianmin Yuan and C.D. Lin*

In recent years helium dimers and trimers have attracted a lot of attention from theorists [1]. Both have already been identified in the laboratories [2,3]. These species have binding energies of the order of mK, and the second state of the helium trimer has been shown to exhibit properties resembling that of an Efimov state [1]. These molecules are characterized by their large size. Since the binding energies are very small, they are not easily detected except in the very low temperature environment. Such environments are provided in the intersteller medium, in a supersonic jet and in laser-cooled atom traps.

Our goal in this project is to identify other molecular species that have binding energies of the same order, i.e. of the order of degrees Kelvin or less. The calculations are carried out with the hope helping experimentalists searching for these exotic species in the future.

The calculations were carried out using the hyperspherical approach. For the triatomic molecules, we include only the pair interactions and treat the molecule as a three-atom system. From the lowest J=0 adiabatic potential curve we calculated the binding energies of the states supported by the lowest potential curve. The pair interaction potential is adopted from what is available in the literature. The hyperspherical potential curves depend sensitively on the masses of the particles in the system.

We have found that the binding energies of He-He-Li and He-He-Na are of the order of fractions of one degree Kelvin (Publication #97). We have also examined the triatomic atoms and anions like He-He-H, He-He-H^- and He-H-H. The binding energies are very sensitive to the isotopes (Publication #104). Since it may be easier to identify weakly bound molecules if they are charged we have used the standard Born-Oppenheimer approximation to investigate the He_2^-, $HeNe^-$ and $HeAr^-$ ions. The excited states of these ions have been calculated as well (Publication #105).

The calculated J=0 binding energies of some of these molecules are given below:

Binding Energies		Ref.
$^{4}He^{4}He^{4}He$	106.0 mK	[1]
$^{4}He^{4}He^{3}He$	10.2mK	[1]
$^{4}He^{4}He^{6}Li$	31.4mK	#97
$^{4}He^{4}He^{7}Li$	45.7mK	#97
$^{4}He^{4}He^{23}Na$	103.1mK	#97
$^{4}He^{4}He^{1}H^{-}$	1.71 K, 0.787 K, 5.33 mK	#104
$^{4}He\ ^{1}H^{-}$	1.37 K(J=0); 0.556 K (J=1)	#105
$^{4}He^{4}He^{-}$	No bound states	#105
$^{40}Ar^{1}H^{-}$	1295K, 948.9K, 659.2K, … (J=0)	#105
$^{4}He^{4}He^{1}H$	no bound states	#104
$^{4}He^{1}H^{1}H$	68.2 mK	#104

Binding energies of other isotopes are to be found in the references quoted.

References

1. B.D. Esry, C.D. Lin and C.H. Greene, Phys. Rev. A 54, 394 (1996) and references therein.
2. F. Luo *et al.*, J. Chem. Phys. 104, 1151 (1996).
3. W. Schollkopf and J.P. Toennis, Science 266, 1345 (1994).