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The formation mechanism and the binding energy of the body-centred regular tetrahedral structure of He_5^{+*}

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We propose the formation mechanism of the body-centred regular tetrahedral structure of the He_5^+ cluster. The total energy curve for this structure has been calculated by using a modified arrangement channel quantum mechanics method. The result shows that a minimal energy of -13.9106 a.u. occurs at a separation of $1.14a_0$ between the nucleus at the centre and nuclei at the apexes. Therefore we obtain the binding energy of 0.5202 a.u. for this structure. This means that the He_5^+ cluster may be stable with a high binding energy in a body-centred regular tetrahedral structure.

Keywords: He_5^+ cluster, formation mechanism, binding energy
PACC: 3640, 3420

1. Introduction

In the past ten years, the formation and stability of helium cluster ions have been extensively studied. The structures of the helium cluster ion have been theoretically studied by Gianturco and de Lara-Castells.[1] They considered that the stable structures for this cluster may be formed in the forms shown in Fig.1. We see that the geometries of He_5^+ may be a linear core of He_3^+ or a core of He_2^+ with additional atoms approaching the ends or the centre of these cores. The core carries a positive charge and the additional atoms are mainly bounded by weak polarization forces. Because the polarization forces are very weak, the binding energies of the clusters formed in the above way are very small. We propose in this paper that the more strong binding structure for He_5^+ may be in a body-centred regular tetrahedral structure formed from the interaction of He^+ at the centre with four atoms at the apexes, as shown in Fig.2. In order to investigate the stability of this structure, the binding energy of the structure is calculated by using a modified arrangement channel quantum mechanics method.[2,3] This method is based on the arrangement channel quantum mechanics (ACQM) method provided by Levin *et al.*[4] Gou *et al*[2] have modified the ACQM method by giving the new channel-coupling matrix which includes the Coulomb interaction ignored by Levin *et al* and by choosing the channel physically not mathematically. This modified ACQM (MACQM) method has been used to calculate the structures and energies of H_n (n=3,5,7,9,13)[2,5–8] successfully.

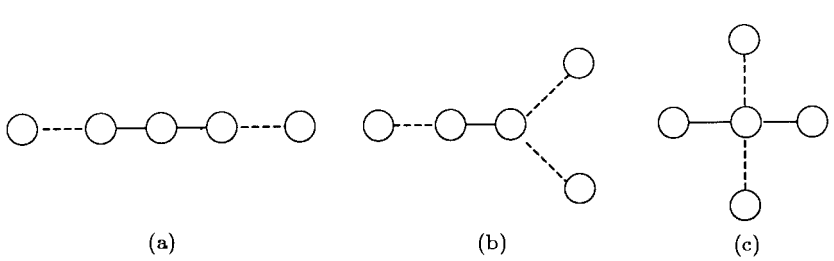


Fig.1. The possible stable structures for He_5^+.

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2.The formation mechanism

We think that the cluster He_5^+ can be formed in a body-centred regular tetrahedral structure by the interaction of He^+ at the centre E with four neighbouring helium atoms at the apexes A, B, C and D, as shown in Fig.2(a). The detailed formation mechanism is shown in Fig 2. There are five nuclei symbolized by A, B, C, D and E, and nine electrons symbolized by e_1, e_3, e_5, e_7, e_9 $\uparrow$, with positive spin $\downarrow$ and by e_2, e_4, e_6, e_8, with negative spin $\downarrow$. At the beginning, we suppose that the first helium atom is situated at the apex A with electrons e_1 $\uparrow$ and e_2 $\downarrow$, the second helium atom is situated at apex B with electrons e_3 $\uparrow$ and e_4 $\downarrow$, the third helium atom is situated at apex C with electrons e_5 $\uparrow$ and e_6 $\downarrow$, the fourth helium atom is situated at apex D with electrons e_7 $\uparrow$ and e_8 $\downarrow$, and the helium ion He^+ is situated at the centre E with electron e_9 $\uparrow$. The electrons e_i $\uparrow$ (i=1,3,5,7,9) are localized around the nuclei A, B, C, D and E respectively. At a certain moment, the electron e_2 of the helium atom He (e_1, e_2) at apex A may interact with the helium ion He^+ (e_9) at the centre E and form the bond AE [$He^+(e_1) + e_2$+$He^+(e_9)$] by the resonance of e_2 between He^+ (e_1) at A and He^+ (e_9) at E. In the meantime, all the electrons around the nuclei B, C and D are localized. In this way, the four bonds can be formed sequentially and instantaneously with equal opportunities, as shown in Fig.2. The resonance of these four bonds around the centre E makes He^+ at the centre and the four He atoms at the apexes bond together to form the body-centred regular tetrahedral structure of the He^+ cluster. Therefore, the cluster He_5^+ can be formed in the body-centred regular tetrahedral structure by the interaction of He^+ with four neighbouring He atoms according to the following four channels

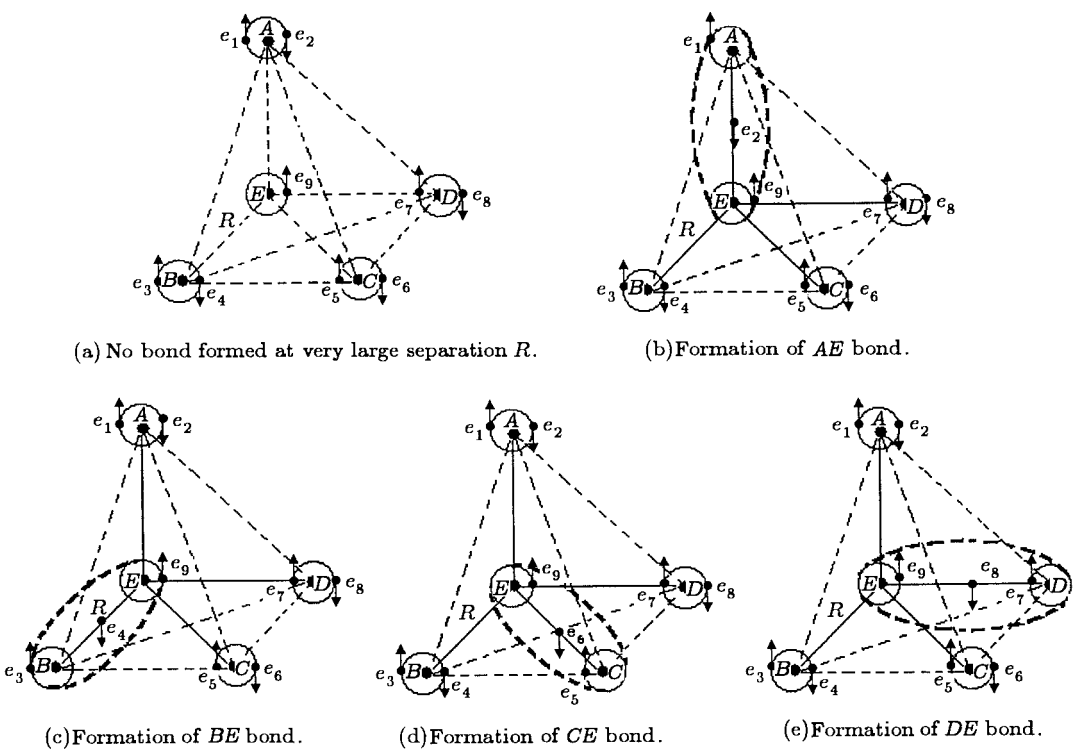


Fig.2. Formation of the instantaneous single electron bonds in the body-centred regular tetrahedral structure of the He_5^+ cluster.

$$\mathrm{He}(e_1,e_2)+\mathrm{He}(e_3,e_4)+\mathrm{He}(e_5,e_6)+\mathrm{He}(e_7,e_8)+\mathrm{He}^+(e_9)\rightarrow$$

$$\left\{\begin{array}{l} AE[\mathrm{He}^+(e_1)+e_2+\mathrm{He}^+(e_9)]+\mathrm{He}(e_3,e_4)+\mathrm{He}(e_5,e_6)+\mathrm{He}(e_7,e_8) \\ BE[\mathrm{He}^+(e_3)+e_4+\mathrm{He}^+(e_9)]+\mathrm{He}(e_1,e_2)+\mathrm{He}(e_5,e_6)+\mathrm{He}(e_7,e_8) \\ CE[\mathrm{He}^+(e_5)+e_6+\mathrm{He}^+(e_9)]+\mathrm{He}(e_1,e_2)+\mathrm{He}(e_3,e_4)+\mathrm{He}(e_7,e_8) \\ DE[\mathrm{He}^+(e_7)+e_8+\mathrm{He}^+(e_9)]+\mathrm{He}(e_1,e_2)+\mathrm{He}(e_3,e_4)+\mathrm{He}(e_5,e_6) \end{array}\right\}\rightarrow \mathrm{He}_5^+.$$

3. The method for calculation of total energy

According to the MACQM method,[2] the four channels shown in Fig.2 are selected for the calculation of the total energy of the system. The wavefunction for the bond AE in the first channel is formulated from the linear combination of the wavefunction $A(1,2)$ for the helium atom at A multiplying the wavefunction $E(9)$ for the helium ion at E and the wavefunction $A(1)$ for the helium ion at A multiplying the wavefunction $E(2,9)$ for the helium atom at E. The total wavefunction for the whole system with the first channel is

$$N_1[A(1,2)E(9)+A(1)E(2,9)]B(3,4)C(5,6)D(7,8).$$

In the same way, we may write down the other channel wavefunctions. The four channel wavefunctions are

$$\left.\begin{aligned}
\Psi_1 &= N_1[A(1,2)E(9)+A(1)E(2,9)]B(3,4)C(5,6)D(7,8)\\
\Psi_2 &= N_2[A(3,4)E(9)+B(3)E(4,9)]A(1,2)C(5,6)D(7,8)\\
\Psi_3 &= N_3[A(5,6)E(9)+C(5)E(6,9)]A(1,2)B(3,4)D(7,8)\\
\Psi_4 &= N_4[A(7,8)E(9)+D(7)E(8,9)]A(1,2)B(3,4)C(5,6)
\end{aligned}\right\}, \tag{1}$$

where N_i (i=1,2,3,4) are normalization factors, $A(1)$, $B(3)$, $C(5)$, $D(7)$ and $E(9)$ are the ground-state wavefunctions of hydrogen-like helium ions, and $A(1,2)$, $B(3,4)$, $C(5,6)$, $D(7,8)$ and $E(i,9)$ (i=2,4,6,8) are the ground-state wavefunctions of the helium atoms. They have the forms of

$$A(1,2)=\frac{\mu^3}{\pi}\exp[-\mu(r_{A_1}+r_{A_2})],$$

$$A(1)=\left(\frac{\mu'^3}{\pi}\right)^{1/2}\exp(-\mu' r_{A_1}),$$

where μ=1.6875 is the effective nuclear charge for electrons of He determined by variation method, and μ'=2.0 is the nuclear charge for the He^+ electron. The expressions in the brackets of Eq.(1) denote the wavefunctions of He_2^+.

Under the Born–Oppenheimer approximation, the Hamiltonian of the system is

$$\hat{H}=-\frac{1}{2}\sum_{i=1}^{9}\nabla_i^2-\sum_{\gamma=A}^{E}\sum_{i=1}^{9}\frac{Z}{r_{\gamma i}}+\sum_{i=1}^{9}\sum_{j>i}^{9}\frac{1}{r_{ij}}+\frac{1}{2}\sum_{u=A}^{E}\sum_{\nu\neq u}^{E}\frac{Z^2}{R_{u\nu}}. \tag{2}$$

The Hamiltonian $H^{(1)}$ and the interaction potential $V^{(1)}$ for the first channel are

$$\begin{aligned}\hat{H}^{(1)}=&-\frac{1}{2}\sum_{i=1}^{9}\nabla_i^2-Z\left(\frac{1}{r_{A_1}}+\frac{1}{r_{A_2}}+\frac{1}{r_{A_9}}+\frac{1}{r_{E_1}}+\frac{1}{r_{E_2}}\right.\\&\left.+\frac{1}{r_{E_9}}+\frac{1}{r_{B_3}}+\frac{1}{r_{B_4}}+\frac{1}{r_{C_5}}+\frac{1}{r_{C_6}}+\frac{1}{r_{D_7}}+\frac{1}{r_{D_8}}\right)\\&+\frac{1}{r_{12}}+\frac{1}{r_{19}}+\frac{1}{r_{29}}+\frac{1}{r_{34}}+\frac{1}{r_{56}}+\frac{1}{r_{78}}+\frac{Z^2}{R_{AE}},\end{aligned}$$

$$\hat{V}^{(1)}=\hat{H}-\hat{H}^{(1)}. \tag{3}$$

We can write down $\hat{H}^{(i)}$ and $\hat{V}^{(i)}$ for other channels in the same way.

Then we can write down the total wavefunction for the whole system of the four channels as

$$\Psi=\sum_{i=1}^{4}C_i\psi_i, \tag{4}$$

where C_i is the expanding coefficient, and the Hamiltonian of the system can be expressed as

$$\hat{H}=\hat{H}^{(i)}+\hat{V}^{(i)}\quad(i=1,2,3,4). \tag{5}$$

So the Schrödinger equation for the whole system

$$\hat{H}\,\Psi=E\,\Psi \tag{6}$$

becomes

$$\sum_{i=1}^{4}[E-\hat{H}^{(i)}-\hat{V}^{(i)}]C_i\psi_i=0. \tag{7}$$

Using the procedures of the MACQM method as in Ref.[2] to solve Eq.(7), the energy curve for the He_5^+ cluster can be obtained.

4. Results

The result of the present calculation of the total energy curve is shown in Fig.3, where R is the distance from the central nucleus to the peripheral nuclei. The curve has a minimal energy of −13.9106 a.u. when R

is 1.14 a_0, where a_0 is the radius of the first Bohr orbit. This minimal energy is lower than the minimal total energies (the lowest is -13.8310 a.u.) of the three structures shown in Fig.1. calculated by Gianturco and de Lara-Castells.[1] When R approaches ∞, the He_5^+ cluster discussed dissociates into the noninteracting system ($He^+ + He + He + He + He$), and the present curve has a total energy of -13.3904 a.u. when R approaches ∞. Hence the binding energy of the structure of the He_5^+ discussed is 0.5202 a.u. This energy is much greater than the dissociation energies of the He_5^+ studied in Ref.[1]. So we conclude that the He_5^+ cluster may exist in a stable state with a stronger binding energy in the body-centred regular tetrahedral structure.

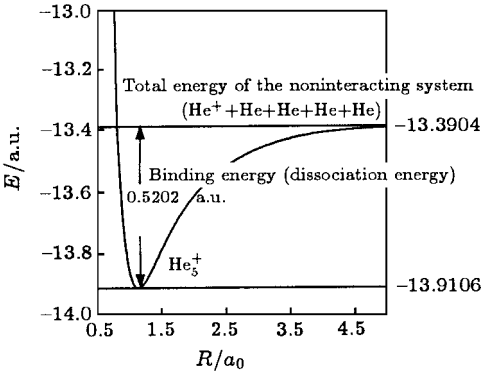


Fig.3. Variation of the total energy curve of He_5^+ with the distance R from the central nucleus to the peripheral nuclei.

References

[1] Gianturco F A and de Lara-Castells M P 1996 *Int. J. Quantum Chem.* **60** 593

[2] Gou Q Q, Zhang X Z and Liu J C 1989*Chin. J. At. Mol. Phys.* **6** 995

[3] Li P, Yin H, Gou Q Q and Miao J W 1999 *Commun. Theor. Phys.* **32** 467

[4] Levin F S and Kruger H 1977 *Phys. Rev.* A **15** 2147

[5] Gou Q Q, Zhou Q N and Liu J C 1988 *Chin. J. At. Mol. Phys.* **5** 781

[6] Li P, Yang S Q and Gou Q Q 1994 *Chin. J. At. Mol. Phys.* **11** 58

[7] Gou Q Q, Zhang X Z and Liu J C 1989 *Chin. J. At. Mol. Phys.* **6** 1053

[8] Gou Q Q, Yang S Q and Li P 1993 *Chin. J. At. Mol. Phys.* **10** 2676