2005 Vol.44 No.3 pp.525-528 DOI:

Formation Mechanism and Binding Energy for Equilateral Triangle Structure of Li_3 Cluster

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(Received: 2004-12-30; Revised:)

Abstract: The formation mechanism for the equilateral triangle structure of Li_3 cluster is proposed. The curve of the total energy versus the interatomic distance for this structure has been calculated by using the method of Gou's Modified Arrangement Channel Quantum Mechanics. The result shows that the curve has a minimal energy of -22.33860 a.u. at $R=5.82a_0$. The total energy of Li_3 when R approaches ∞ has the value of -22.28409 a.u. This is also the total energy of three lithium atoms dissociated from Li_3. The difference value of 0.054508 a.u. for the above two energy values is the dissociation energy of Li_3 cluster, which is also its binding energy. Therefore the binding energy per lithium atom for Li_3 is 0.018169 a.u.=0.494 eV, which is greater than the binding energy of 0.453 eV per atom for Li_2 calculated in a previous work. This means that the Li_3 cluster may be formed in the equilateral triangle structure of side length $R=5.82a_0$ stably with a stronger binding from the symmetrical interaction among the three lithium atoms.

PACS: 36.40.-c
Key words: Li_3 cluster, binding energy, equilateral triangle structure

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