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Formation Mechanism and Binding Energy for Regular Tetrahedral Structure of Li_4

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Abstract: The formation mechanism for the regular tetrahedral structure of Li_4 cluster is proposed. The curve of the total energy versus the separation R between the two nuclei has been calculated by using the method of Gou's modified arrangement channel quantum mechanics (MACQM). The result shows that the curve has a minimal energy of -29.8279 a.u. at $R=14.50a_0$. When R approaches infinity the total energy of four lithium atoms has the value of -29.7121 a.u. So the binding energy of Li_4 with respect to four lithium atoms is the difference of 0.1158 a.u. for the above two energy values. Therefore the binding energy per atom for Li_4 is 0.029 a.u., or 0.7878 eV, which is greater than the binding energy per atom of 0.453 eV for Li_2, the binding energy per atom of 0.494 eV for Li_3 and the binding energy per atom of 0.632 eV for Li_5 calculated previously by us. This means that the Li_4 cluster may be formed stably in a regular tetrahedral structure of side length $R=14.50a_0$ with a greater binding energy.

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Key words: Li_4 cluster, formation mechanism, binding energy

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