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Stabilities of Al or Ga atoms for encapsulation in silicon clathrates I HIDEKAZU TOMONO, KAZUO TSUMURAYA, Meiji University
— Clathrates are cagelike compounds and encapsulate endohedral atoms inside the cages of the host network. On the one hand, the clathrates with host atoms silicon, germanium, or tin have been synthesized only when group 1 alkali metal atoms or group 2 alkaline earth metal atoms coexist as electron donors or group 17 halogen atoms coexist as electron acceptors. On the other hand, the group 13 atoms such as Al, Ga, In atoms are substituted for the host frame atoms. There has been no explanation of the mechanism of the solution of these atoms into the frame or insoluble into the cages. We investigate this through calculating the enthalpies of solution of these atoms into silicon clathrate I by use of an *ab initio* method. We discuss the energies of solution of group 13 atoms into the cages with those into frame structure.

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