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Cohesion in clathrates I; covalencies and ionicity KAZUO TSUMURAYA, Meiji University, HARUKI EGUCHI, Ishikawajima Harima Heavy Industry (IHI), HIDEKAZU TOMONO, Meiji University — We present the roles of endohedral atoms in the cohesion of group 14 clathrates I. Taking a view that the clathrate I consists of a sheaf of one-dimensional connections of $Na@Si_{24}$ cages interleaved in three perpendicular directions, we calculate the electronic structures with an *ab initio* method and find that 30% of the $3s^1$ charge of each endohedral sodium atom transfers to the frame and the remaining charge forms a bonding state between the endohedral atoms: the roles of cohesion is the covalent bonds between the endohedral atoms in the cages and between the frame atoms, together with the ionic bond between the host and the endohedral atoms.

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