Halogen Bonding and Cooperative Effects in Chlorine Clathrate: Ab Initio Periodic Study Supporting Information

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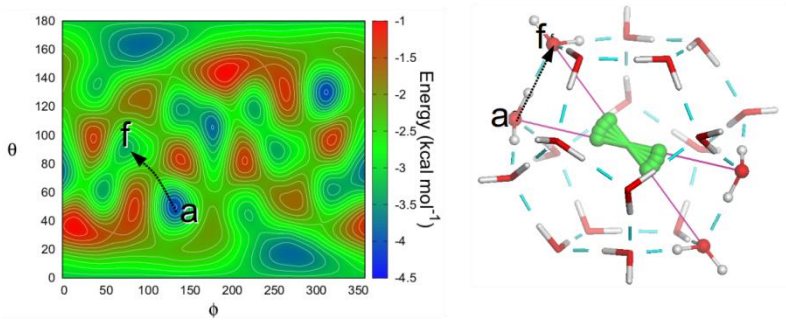

Figure S 1. Minimum energy path trough the stationary points a-f shown in the PES (left) and in the atomic structure(right) for $Cl_2@5^{12}$. The water molecules out of the cage are not shown for simplicity.

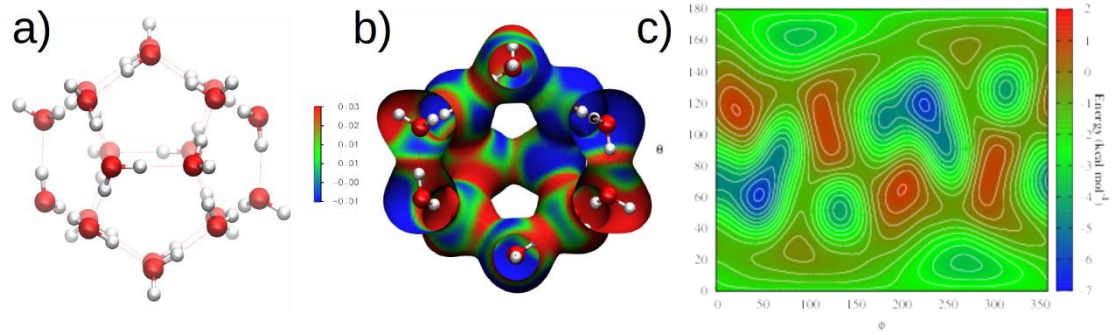

Figure S 2. Atomic structure, electrostatic potential and PES of the 5^{12} cage extracted from the crystal.

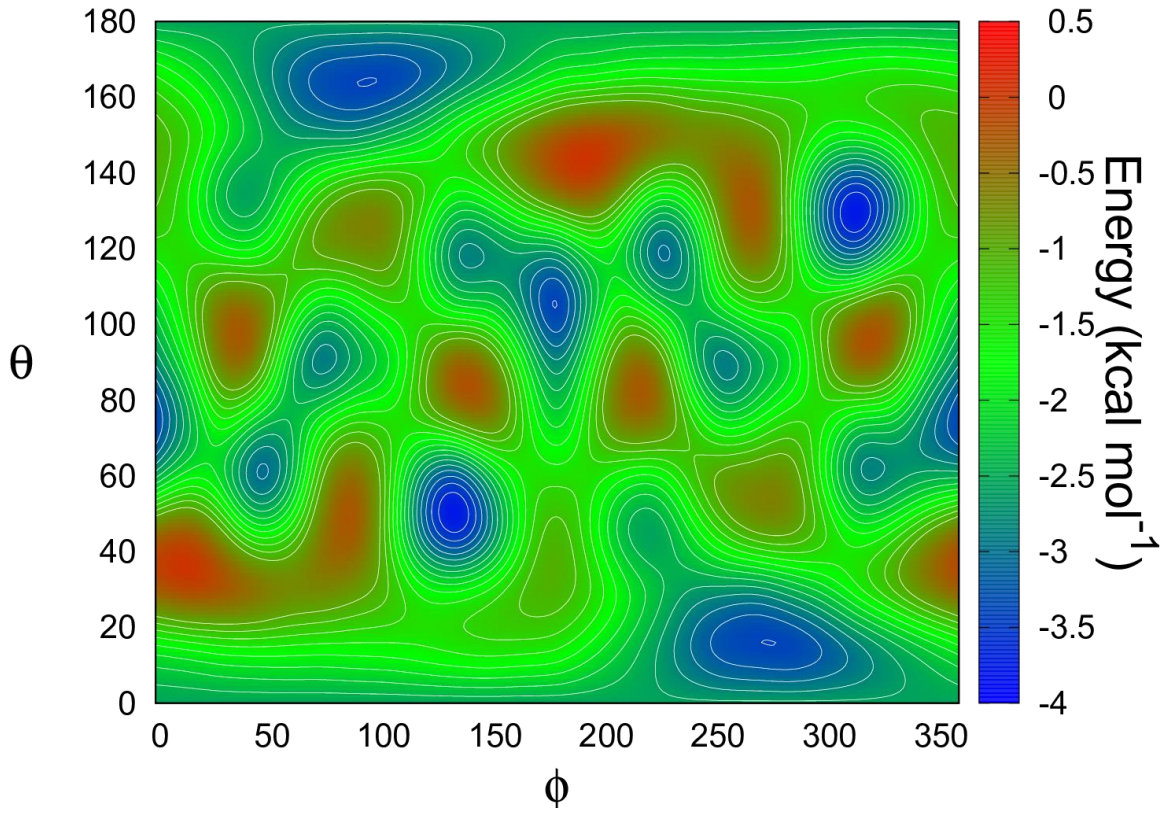

Figure S 3 Angular dependence of the PES for $Cl_2@5^{12}$ with the Cl-Cl distance = 2.105 Å