

Supporting Information for:

**The nature of halogen bonding of Cl₂ and Br₂ with water in solid
clathrate hydrates**

Hana Dureckova,^a Tom K. Woo,^a Konstantin A. Udachin, John A. Ripmeester,^{b,c} and Saman
Alavi,^{a,b,c}

^a *Department of Chemistry, University of Ottawa, Ottawa, Ontario K1N 6N5 Canada*

^b *National Research Council Canada, 100 Sussex Drive, Ottawa, Ontario K1A 0R6 Canada*

^c *Department of Chemical and Biological Engineering, University of British Columbia,
Vancouver, British Columbia V6T 1Z3 Canada*

Three zip files with Cartesian coordinates of clathrate hydrate cages with guests are included.

These are:

1) **Cl₂ CS-I Hydrate cages.rar**

Cartesian coordinates for cages and Cl₂ guest positions from symmetry distinct positions from the X-ray diffraction data.

2) **Br₂ TS-I Hydrate cages.rar**

Cartesian coordinates for cages and Br₂ guest positions from symmetry distinct positions from the X-ray diffraction data.

3) **Cages for NBO analysis.rar**

Cartesian coordinates for cages and guest positions from ab initio optimization of the guests in the cages.

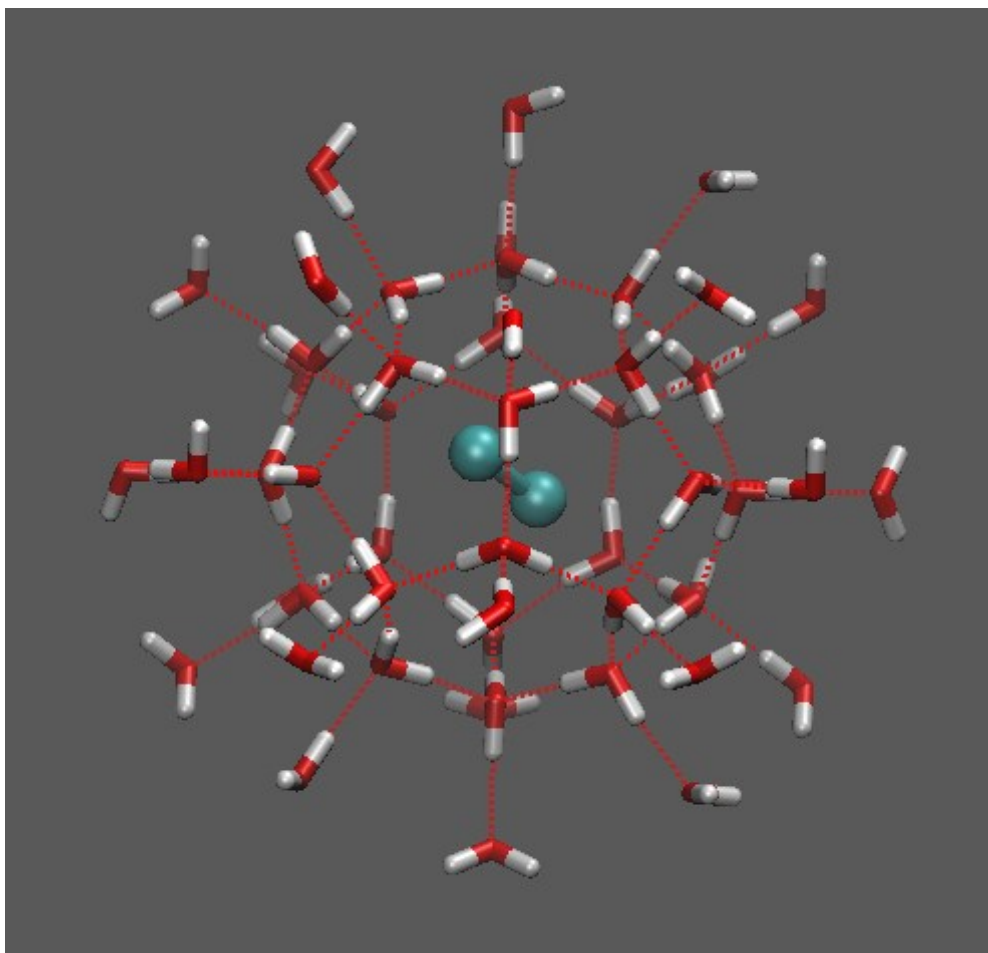


Figure S1. The configuration of the D cage with 20 shell water molecules extracted from the CS-I clathrate hydrate crystal structure with proton positions assigned to satisfy the ice rules.

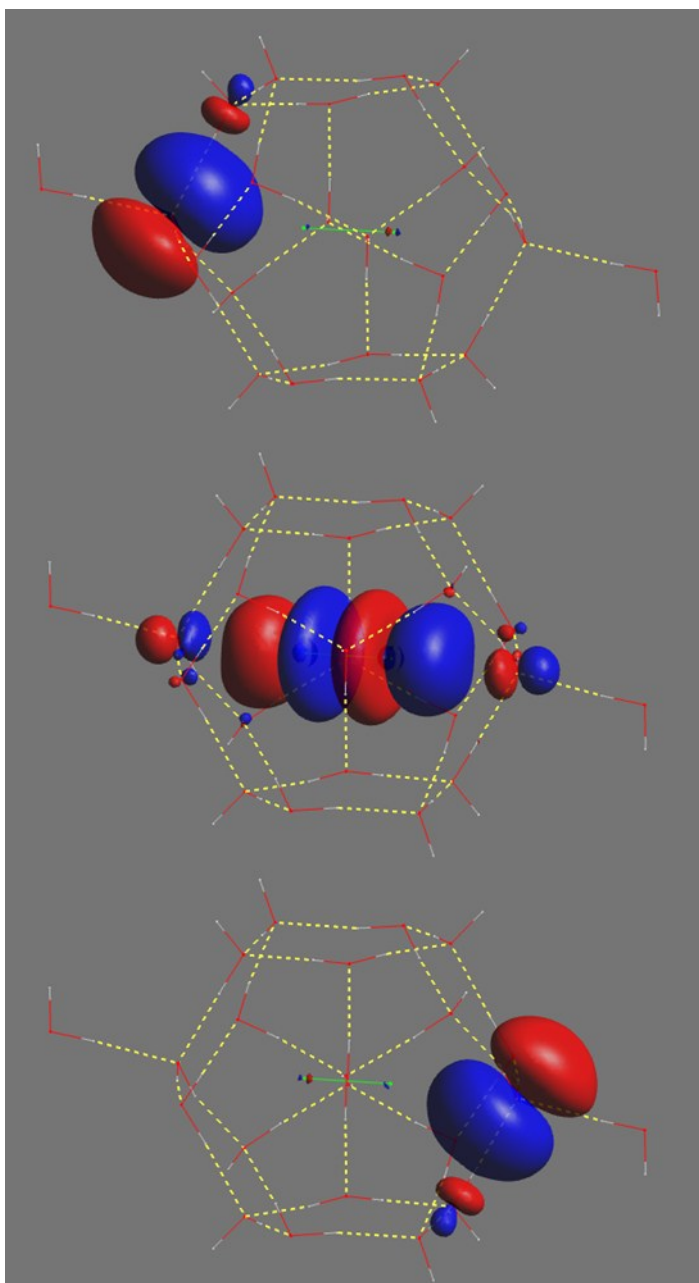


Figure S2. An alternative representation of the σ^* antibonding orbital on Cl_2 and the two ILPs on the water molecule closest to the guest atoms.

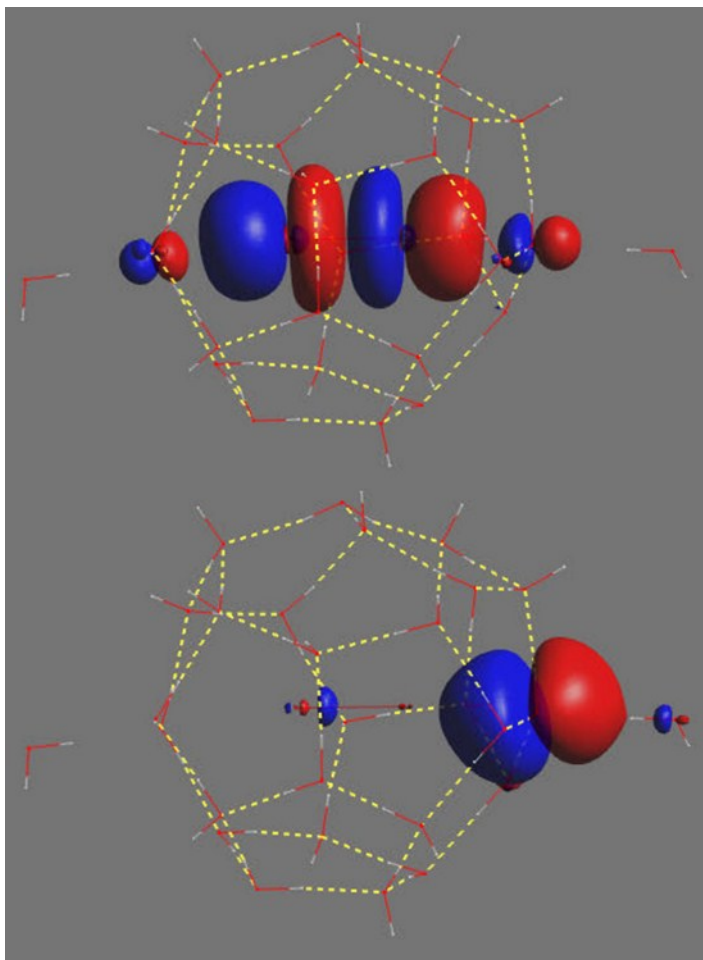


Figure S3. An alternative representation of the σ^* antibonding orbital on Cl_2 and the one ELPs on the water molecule closest to a guest atom.