Supporting Information for:

The nature of halogen bonding of Cl$_2$ and Br$_2$ with water in solid clathrate hydrates

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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 Cl\textsubscript{2} guest positions from symmetry distinct positions from the X-ray diffraction data.

2) **Br2 TS-I Hydrate cages.rar**

   Cartesian coordinates for cages and Br\textsubscript{2} 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 $\sigma^*$ 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 $\sigma^*$ antibonding orbital on Cl$_2$ and the one ELPs on the water molecule closest to a guest atom.