The Chalcogen bond: Can it be Formed by Oxygen?

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Supplementary information

Table S1: Reported van der Waals radii of atoms used in this study (values in Å) for the assignment of intermoelcular interactions between bonded atomic basins.

Atom	Bondi	Alvarez	Interaction	vdW(O)+vdW(X)(Alvarez)
H	1.20	1.20	O···H	2.70
C	1.70	1.77	O···C	3.27
N	1.55	1.66	O···N	3.16
O	1.52	1.50	O···O	3.00
F	1.47	1.46	O···F	2.96
S	1.80	1.89	O···S	3.39
Cl	1.75	1.82	O···Cl	3.32
Br	1.83	1.86	O···Br	3.36

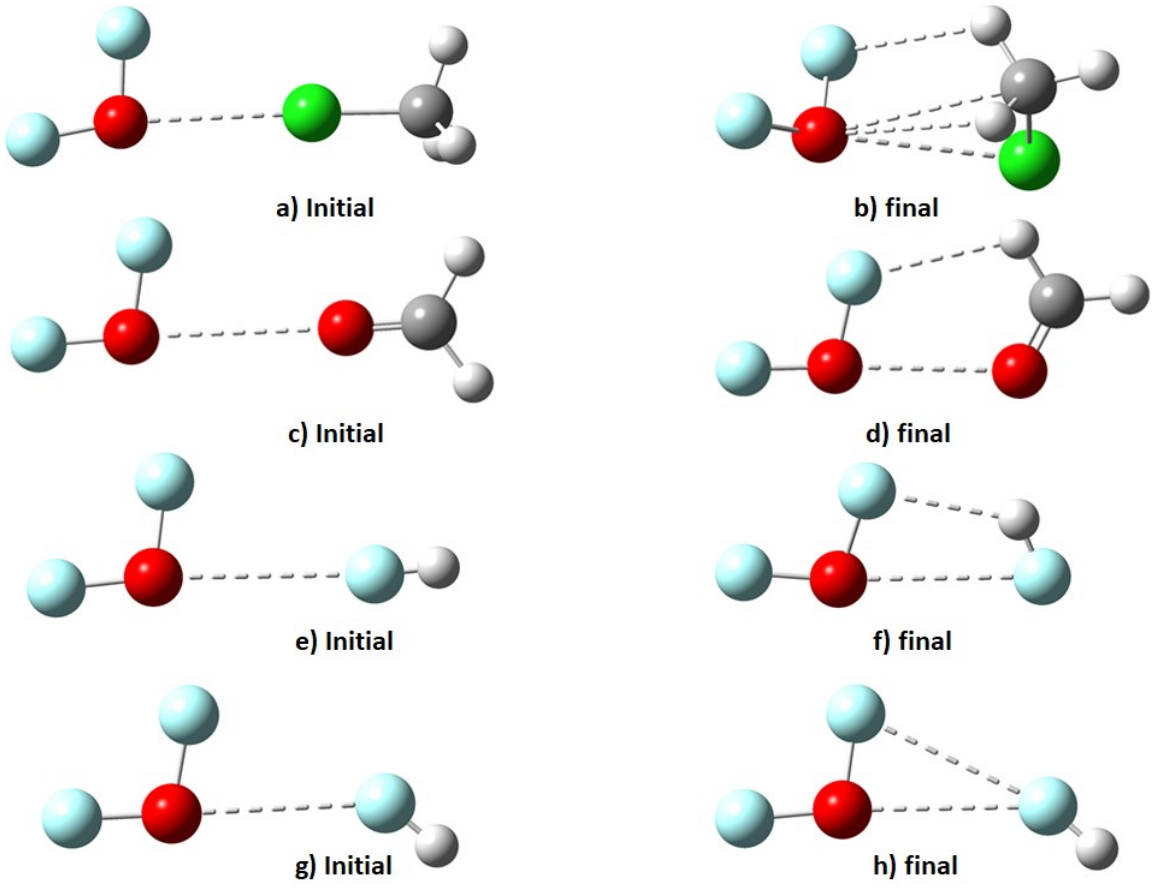

Figure S1. Examples showing the initial and final (M06-2X/aug-cc-pVTZ energy-minimized) geometries of some selected OF_2 binary complexes of a-b) CH_3Cl, c-d) H_2CO, e-f) HF and g-h) HF. Both M06-2X and MP2 methods produced similar complex geometries. Figure 4 shows the details of the M06-2X/aug-cc-pVTZ energy-minimized geometries of all the complexes