

Table S1 Adsorption energies ( $E_{ad}$ , in kJ/mol) of all complexes obtained at the CAM-B3LYP/6-31G\* level

	He	Ne	Ar	Kr
B1Rg	-6.6	-17.2	-7.1	-12.5
B2Rg	-1.9	-22.9	-3.1	-13.9
B1Rg-In	143.6	301.7	1049.7	1305.0

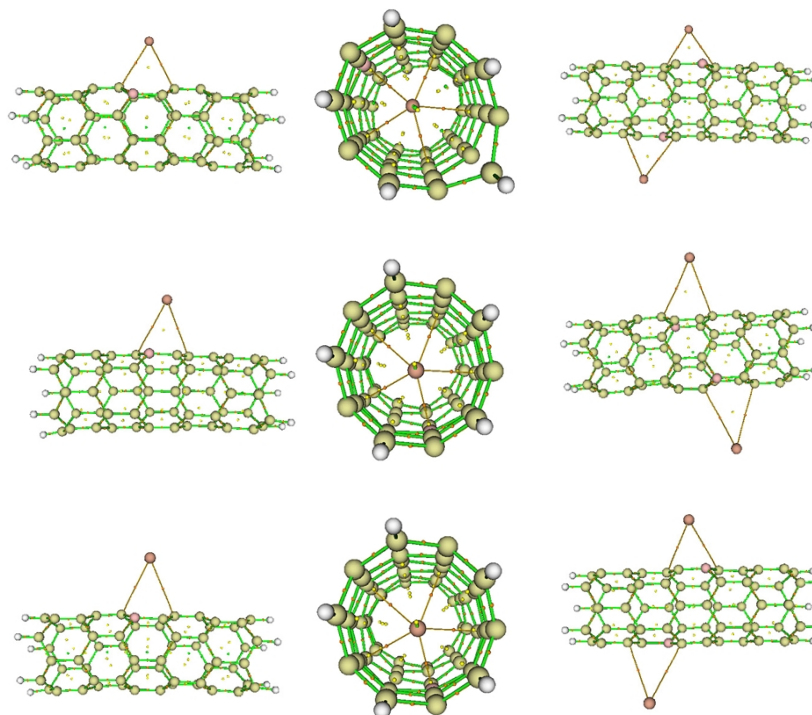
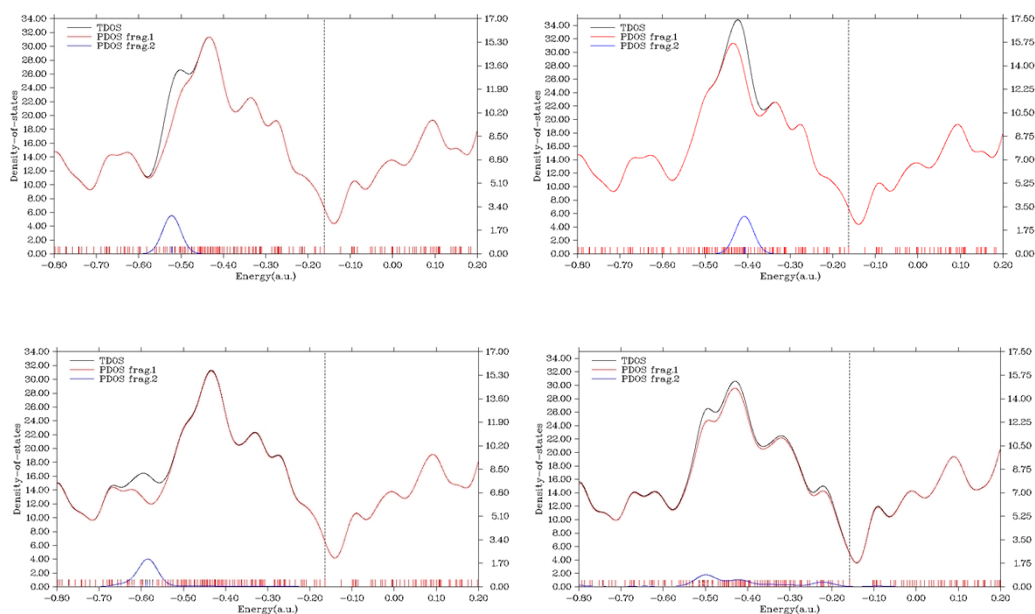


Figure S1 Interaction paths of complexes of Ne, Ar and Kr



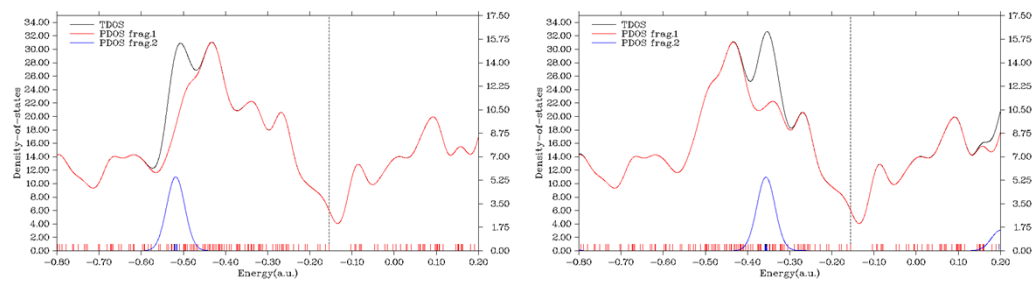


Figure S2 DOS of complexes of Ne and Ar