Title:	Theoretical studies of host - Guest interaction in gas hydrates
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Abstract:	Ab initio calculations and atoms-in-molecules (AIM) analysis have been used to investigate the host - guest interaction in dodecahedral water cages using a variety of guest species that include monatomic (He, Ne, Ar, Kr, and Xe), diatomic (CO, H2, N2, O2, and NO), triatomic (CO2, NO2, and O 3) and polyatomic (CH4 and NH3) molecules. Geometry optimization for the guest species, host cage, and their complexes was carried out using the second order Müller - Plesset perturbation method with the 6-31G ** basis set. Single point energy calculations using the same method but different basis sets (6-31++G **, 6-311++G **, aug-cc-pVDZ, and aug-cc-pVTZ) were carried out for the MP2/6-31G ** optimized geometries. The interaction energy between the guest species and the host cage has been obtained in the complete basis set limit by basis set extrapolation. (Figure presented) © 2011 American Chemical Society
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