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Abstract:	Ab initio calculations using Hartree-Fock (HF) and second order Møller-Plesset perturbation (MP2) theoretic methods using the 6-31G basis set have been used to study the interaction between H+, H-, He, Li+ and H2 with C60 fullerene. The barrier for penetration of the guest species through the center of the hexagon of the cage is reported. There is a substantial change in the HOMO-LUMO energy gap for the endohedral complex of C60 fullerene when the proton or hydride ion is encapsulated. The calculated HOMO-LUMO energy gap for the endohedral complex is correlated with the orbital energy of the guest species. The interaction of the guest species with the host is examined by a critical point analysis using Bader's theory of atoms in molecules. The effect of the guest species on the electrostatic potential inside and outside of the C60 cage is also discussed.
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