Title:	Encapsulation of paramagnetic diatomic molecules B2, O2 and Ge2 inside C60
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Abstract:	Density functional theoretic (DFT) calculations have been carried out for B2@C60, O2@C60 and Ge2@C60 to study the influence of confinement on the relative stability between the singlet and the triplet states of paramagnetic diatomic molecules B2, O2 and Ge2. Although the energy gap between the respective singlet and triplet states of B2 and O2 remains unaltered on encapsulation inside the C60 cage, the relative stability of the singlet and triplet states of the complex Ge2@C60 varies with the orientation of Ge2 inside the cage. Unlike that of B2 and O2, the bond length of Ge2 is reduced significantly inside the cage.
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