Title:	Improved Estimates of Host-Guest Interaction Energies for Endohedral Fullerenes Containing Rare Gas Atoms, Small Molecules, and Cations
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Abstract:	Endohedral fullerenes have evinced much interest from the fundamental and applications points of view. However, given the nature of the weak interaction between the guest species and the host cage in these confined systems, the interaction energy values obtained using various theoretical methods, and different basis sets vary over a wide range. For example, the reported interaction energy for the HF@C60 system ranges from −2.5 kcal/mol to −14.9 kcal/mol. In the present manuscript, we report reliable interaction energy values for different endohedral fullerenes (He@C60, Ne@C60, Ar@C60, Kr@C60, H2@C60, HF@C60, H2O@C60, NH3@C60, CH4@C60, Li+@C60, Na+@C60, and K+@C60) obtained using the domain-based local pair natural orbital coupled-cluster singles, doubles, and perturbative triples (DLPNO-CCSD(T)) method and the def2-TZVP basis set. We believe that these energy values could be considered as benchmark values, and the performance of other quantum chemical methods could be assessed accordingly. Local energy decomposition analysis within the DLPNO-CCSD(T) framework is used to estimate the electrostatic, exchange, and dispersion components of the interaction energy for some of the endohedral fullerenes.
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