Title:	Noble gas hydrides in the triplet state: HNgCCO+ (Ng = He, Ne, Ar, Kr, and Xe)
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Abstract:	Motivated by the very recent investigations of neutral noble gas compounds in the open-shell configuration, we explored a new series of noble gas hydrides in the triplet state. The possible existence of noble gas-inserted ketenyl cations, HNgCCO+ (Ng = He, Ne, Ar, Kr, and Xe), in their triplet electronic state has been predicted by various ab initio quantum chemical techniques. Density functional theory (DFT), second-order Møller–Plesset perturbation theory (MP2), and coupled-cluster theory (CCSD(T)) based methods have been employed to investigate the structures, energetics, harmonic vibrational frequencies, and charge distribution analysis of these ions. The aforementioned ions have been found to be thermodynamically stable with respect to all plausible 2-body and 3-body dissociation channels, except the 2-body dissociation pathway leading to the formation of global minima products (Ng + HCCO+). Nevertheless, each of the predicted HNgCCO+ ions is connected to the global minima products through a transition state with a finite barrier height on the potential energy surface, which confirms the kinetic stability of the metastable species. Detailed analysis of the optimized structural parameters, energetics, and harmonic vibrational frequencies of the predicted species clearly indicated that a strong covalent bond exists between H and Ng atoms, while a comparatively weak interaction is found between Ng and C atoms. Moreover, charge distribution and atoms-in-molecules (AIM) analysis strongly concurred with the above inferences and also suggested that the predicted metastable ions should exist essentially in the form of [HNg]+[CCO] complex. These results ultimately indicate that these predicted species may be prepared and characterized by suitable experimental technique(s) under a cryogenic environment.
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