STRUCTURES AND SPECTROSCOPIC PROPERTIES CALCULATED FOR $C_6H_7^+$ AND ITS COMPLEXES WITH Ne, Ar, N_2, OR CO_2

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Explicitly correlated coupled cluster theory at the CCSD(T)-F12x (x = a, b) level[a] in conjunction with the double-hybrid density functional B2PLYP-D[b] has been employed in a study of the benzenium ion ($C_6H_7^+$) and its complexes with simple ligands (L = Ne, Ar, N_2, or CO_2).[c] The ground-state rotational constants of $C_6H_7^+$ are predicted to be A_0 = 5445 MHz, B_0 = 5313 MHz, and C_0 = 2731 MHz. For the complexes with L = Ne, Ar or N_2, the energetically most favourable structure is of π-bonded type, but for the most strongly bound complex $C_6H_7^+ \cdot CO_2$ a conformer with the CO_2 ligand lying in the ring-plane of the $C_6H_7^+$ moiety is slightly lower in energy.

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