STRUCTURES AND SPECTROSCOPIC PROPERTIES CALCULATED FOR C$_6$H$_7^+$ 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$_6$H$_7^+$) and its complexes with simple ligands (L = Ne, Ar, N$_2$, or CO$_2$).$^c$ The ground-state rotational constants of C$_6$H$_7^+$ 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 $\pi$-bonded type, but for the most strongly bound complex C$_6$H$_7^+$ · CO$_2$ a conformer with the CO$_2$ ligand lying in the ring-plane of the C$_6$H$_7^+$ moiety is slightly lower in energy.

$^c$P. Botschwina and R. Oswald, J. Phys. Chem. A 115, 13664 (2011);