

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<sup>a</sup> in conjunction with the double-hybrid density functional B2PLYP-D<sup>b</sup> 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  $CO_2$ ).<sup>c</sup> 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  $\pi$ -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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