Theoretical spectroscopic parameters for the low-lying states of isotopic variants of HCO+ and HOC+

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The theoretical spectroscopic parameters are derived for all isotopologues of HCO$^+$ and HOC$^+$ involving H, D, $^{16}$O, $^{17}$O, $^{18}$O, $^{12}$C, and $^{13}$C by means of a two-step procedure. Full-dimensional rovibrotational calculations are first carried out to obtain numerically exact rovibrational energies for $J=0$-$15$ in both parities. Effective spectroscopic constants for the vibrational ground state, $\nu_1$, $\nu_2$, and $\nu_3$ are determined by fitting the calculated rovibrational energies to appropriate spectroscopic Hamiltonians. Combining our vibration-rotation corrections with the available experimental ground-state rotational constants, we also derive the new estimate for the equilibrium structure of HCO$^+$, $r_e(CH)=1.091981(7)$ Å, and for the equilibrium structure of HOC$^+$, $r_e(HO)=0.990482(7)$ Å. Regarding the spectroscopic parameters, our estimates are in excellent agreement with available experimental results for both HCO$^+$ and HOC$^+$: the agreement for the rotational constants $B$ is within 3 MHz, for the quartic centrifugal distortion constants $D$ within 1 kHz, and for the effective $\ell$-doubling constants $q$ within 2 MHz. We thus expect that our results can provide useful assistance in analyzing expected observations of the rare forms of HCO$^+$ and HOC$^+$ that are not yet experimentally known.

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Minimum energy path $V_{\text{MEP}}$ and effective bending potential $\Delta V_{\nu_1, \nu_3}$ for the (0,0), (1,0) and (2,0) stretching states along the Jacobi angle $\Theta$. The curves are shifted to coincide at $\Theta=0^\circ$ for HCO$^+$ and at $\Theta=180^\circ$ for HOC$^+$.