Supporting Online Material for: ‘Electronic spectra of gas-phase polycyclic aromatic nitrogen heterocycle cations: isoquinoline$^+$ and quinoline$^+$’ by V. Dryza, J. Sanelli, E.G. Robertson and E.J. Bieske


References

Figure 1.  Electron promotions and molecular orbitals involved in the optical absorptions of naphthalene\(^+\), isoquinoline\(^+\), and quinoline\(^+\). Note the double excitation character for the \(D_3\leftarrow D_0\) transition of naphthalene\(^+\) and the \(D_4\leftarrow D_0\) transitions of isoquinoline\(^+\) and quinoline\(^+\).
Figure 2. Simulated stick spectra for the $D_2\leftarrow D_0$ band system of naphthalene (top), and $D_3\leftarrow D_0$ band systems of isoquinoline$^+$ (middle), and quinoline$^+$ (bottom). Simulated spectra were generated as described in Section 2.2 in the article. Convoluted simulated spectra and experimental spectra, along with the FC active modes, are depicted in Figure 3.
Figure 3. $D_2 \rightarrow D_0$ band system of naphthalene (top), and $D_3 \rightarrow D_0$ band systems of isoquinoline$^+$ (middle), and quinoline$^+$ (bottom). Simulated spectra were generated as described in Section 2.2 in the article. The calculated bands are represented as Gaussians with full width half maximum of 80 cm$^{-1}$. For each molecule, the simulated spectrum (red trace) is shown below the experimental spectrum (blue trace). Main Franck-Condon active vibrational modes are depicted at right. Stick spectra for the three species are shown in Figure 2.