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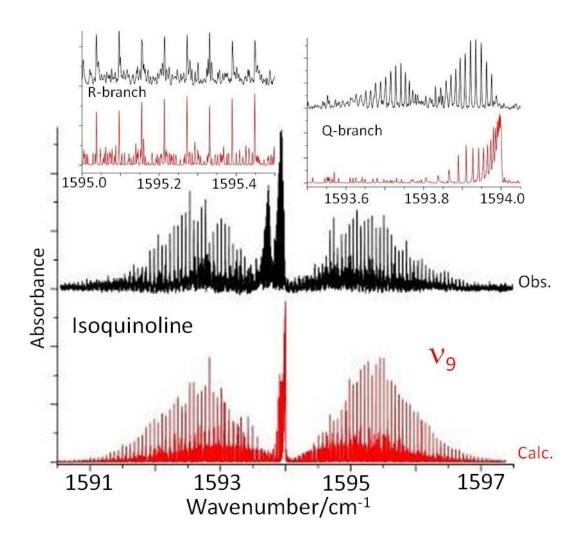


Fig. S1: Overall view of the  $\nu_9$  band of isoquinoline: in black, the SPIRALES spectrum; in red, the  $\nu_9$  band simulated at  $T_{rot} = 35(5)$  K using a Gaussian line shape of 0.0017 cm<sup>-1</sup> FWHM. Two insets display in the R-branch a good agreement between (obs-calc)  $\nu_9$  spectra, while the observed structured Q-branch split is not reproduced by the simulation.