Theoretical calculation of rovibronic energy levels and anharmonic resonances in the ground X $^2\Pi$ state of HCP^+ and DCP^+

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The spin–rovibronic levels of the HCP^+ radical cation and its deuteriated isotopomer in the ground X $^2\Pi$ state have been studied using high-level *ab initio* methods followed by variational calculations on the computed potential energy surfaces. All experimental levels are reproduced within 8 cm^{-1} and predictions of the rovibronic levels ($K \leq 3$) for energies up to 4500 cm^{-1} for HCP^+ and 4000 cm^{-1} for DCP^+ are provided. Anharmonic resonances are analyzed in detail and found to be more complex than previously thought.

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https://www.rsc.org/