SUPPORTING INFORMATION

Deciphering the Electronic Structure and Conformational Stability of 2-Pyridinecarboxaldehyde

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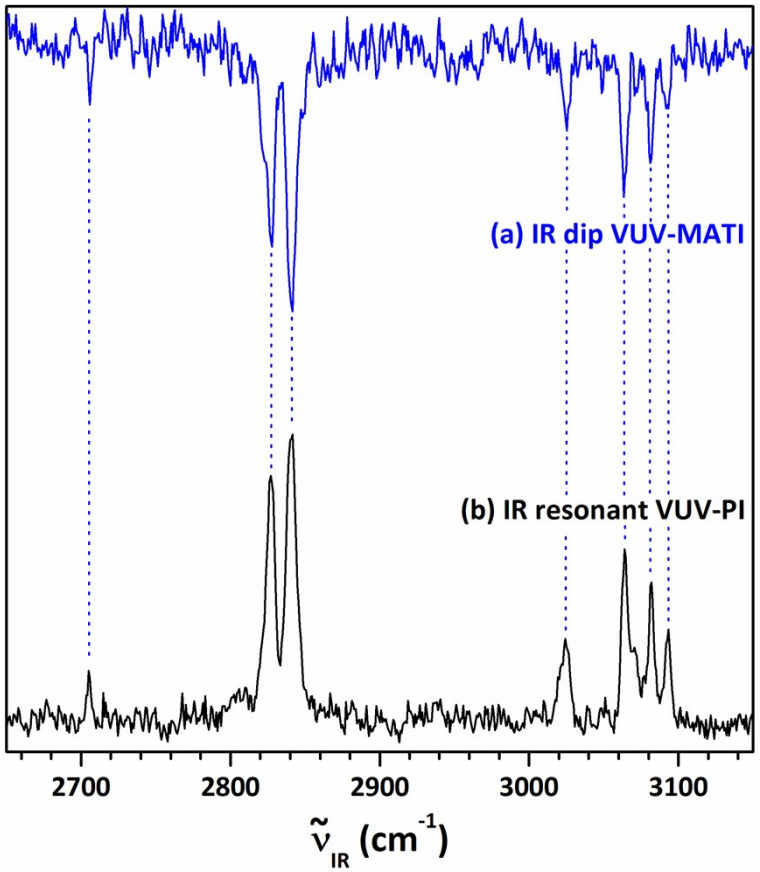

Figure S1 (a) IR dip VUV-MATI spectrum of 2-PCA, measured by monitoring the origin band in the VUV-MATI spectrum. (b) IR resonant VUV-PI spectrum recorded with VUV photon energy tuned to approximately 100 cm^{-1} below the adiabatic ionisation threshold of 2-PCA.

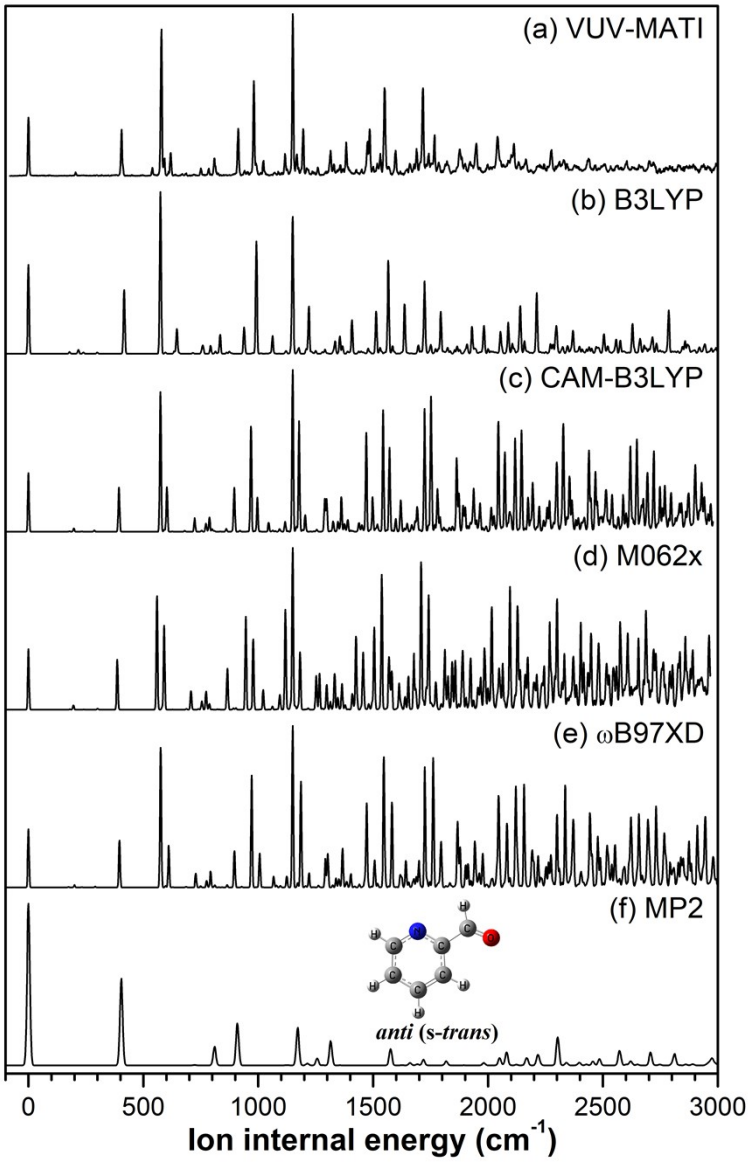

Figure S2 (a) VUV-MATI spectrum of 2-PCA. Simulated spectra based on FC factors and vibrational frequencies calculated for the optimised geometries (C_S symmetry) of the s-*trans* (*anti*) conformer of 2-PCA in the S_0 and D_0 states at the (b) B3LYP, (c) CAM-B3LYP, (d) M062X, (e) ωB97XD, and (f) MP2 levels with the cc-pVTZ basis set.

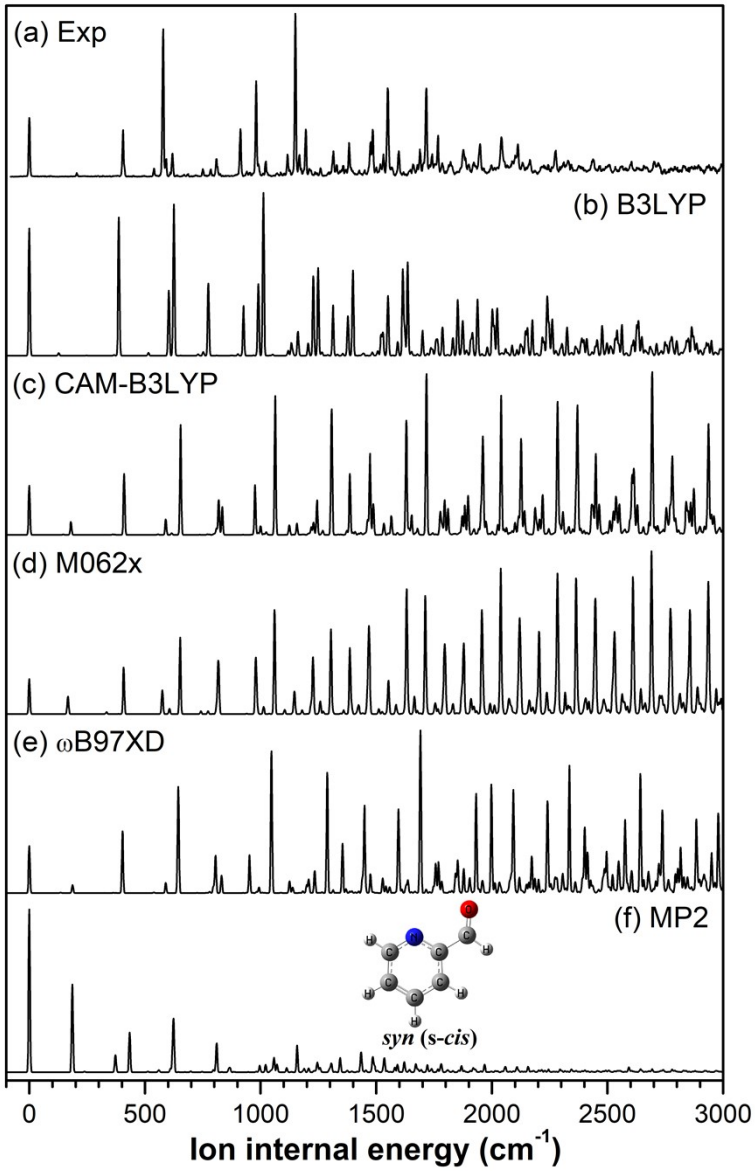

Figure S3 (a) VUV-MATI spectrum of 2-PCA. Simulated spectra based on FC factors and vibrational frequencies calculated for the optimised geometries (C_S symmetry) of the s-*cis* (*syn*) conformer of 2-PCA in the S_0 and D_0 states at the (b) B3LYP, (c) CAM-B3LYP, (d) M062X, (e) ωB97XD, and (f) MP2 levels with the cc-pVTZ basis set.

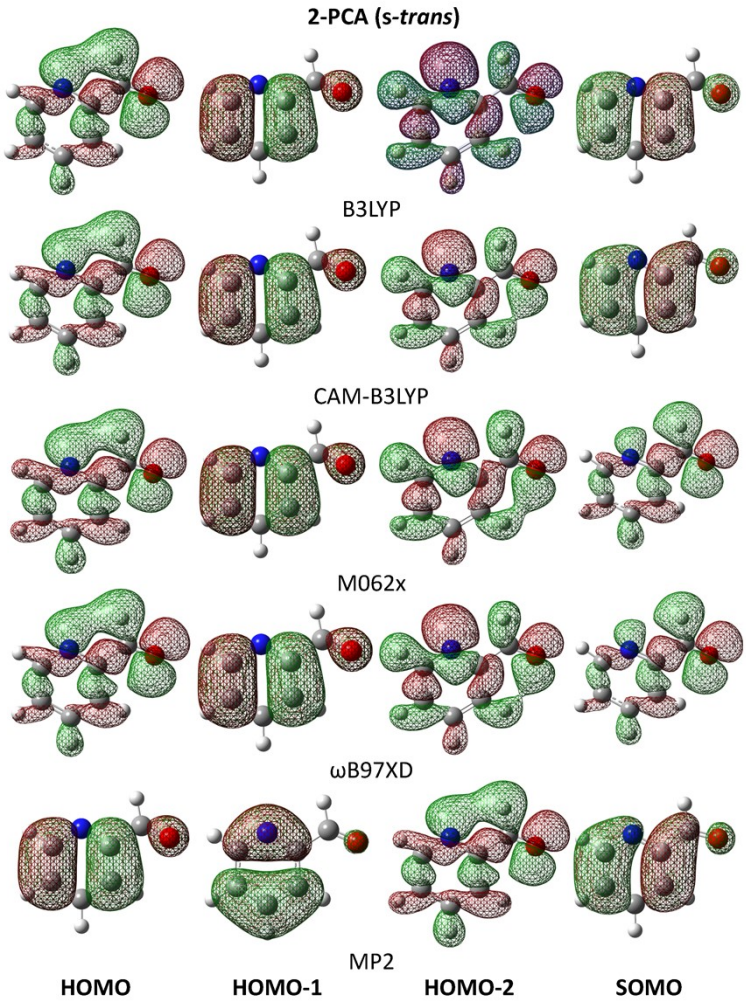

Figure S4 Three outermost valence orbitals and SOMOs of the s-*trans* conformer of 2-PCA optimised at the (a) B3LYP, (b) CAM-B3LYP, (c) M062X, (d) ωB97XD, and (e) MP2 levels with the cc-pVTZ basis set. All MOs were analysed using NBO calculations.