Electronic Supplementary Information for

Photoelectron Spectrum of the Pyridyl Radical

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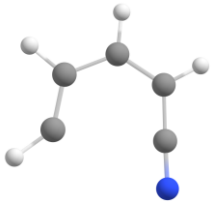
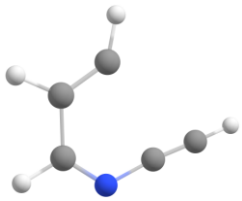
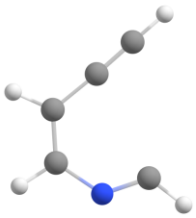
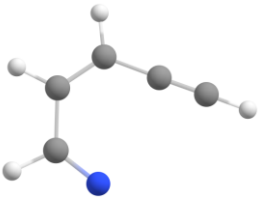
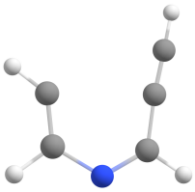
Table S1: Calculated ionisation energies for the open shell isomers suggested by Liu et al.[1]

	Open shell isomer	$IE_{calc.}$ (S_0^+)/ eV	$IE_{calc.}$ (T_1^+)/ eV
1		6.10	9.11 eV
2		4.42	8.47
3		no convergence	8.35
4		6.45	8.98
5		5.20	8.19

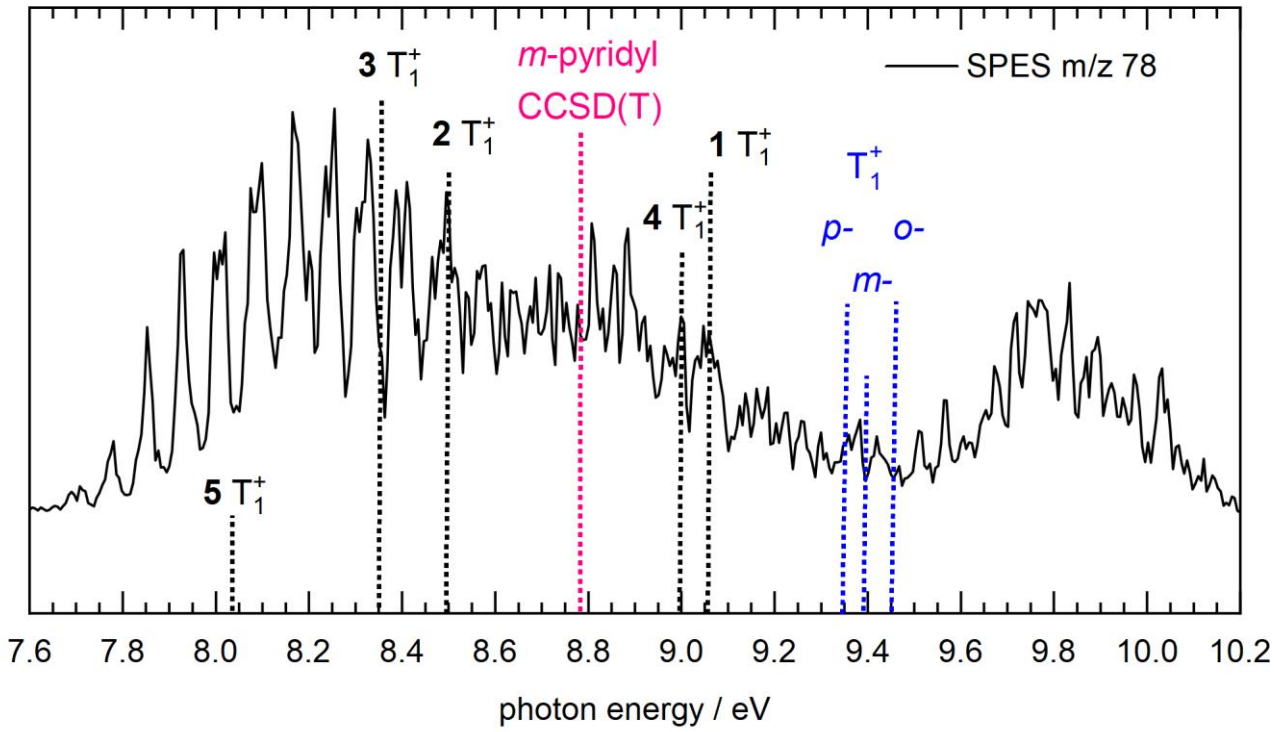


Fig. S1: SPES of m/z = 78 from 9.5 – 10.2 eV. The IE of m-pyridyl, computed by CCSD(T) is given as a purple line. For comparison the computed IEs for transitions into the triplet cation of the open-chain isomers are given as black lines. A second band starting at 9.6 eV is most likely due to transitions into the triplet states of the pyridyl cations. Due to the close-lying ionization energies, an identification of further isomers in addition to *o*- and *p*-pyridyl is not possible.

Notes and references

[1]: R. Liu, T. T.-S. Huang, J. Tittle and D. Xia, *J. Phys. Chem. A*,2000, **104**, 8368–8374.