Supplementary Material for

Structure and IR Spectra of 3(5)-Aminopyrazoles and UV-Induced Tautomerization in Argon Matrix

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INDEX

Table S1 – TD-DFT(B3LYP)/6-311++G(d,p) calculated transition energies (to the 6 lowest singlet excited states) of the 3AP tautomer and oscillator strengths.

State	Symmetry	Energy/ nm	Oscillator Strength	Approximate description
S_1	A	257.5	0.0050	HOMO → LUMO
S_2	A	250.2	0.0003	HOMO → LUMO +1
S_3	A	223.6	0.0354	HOMO → LUMO +2
S_4	A	222.0	0.0147	HOMO → LUMO +3
S_5	A	214.3	0.0048	HOMO –1 → LUMO
S_6	A	207.7	0.0024	HOMO → LUMO +4

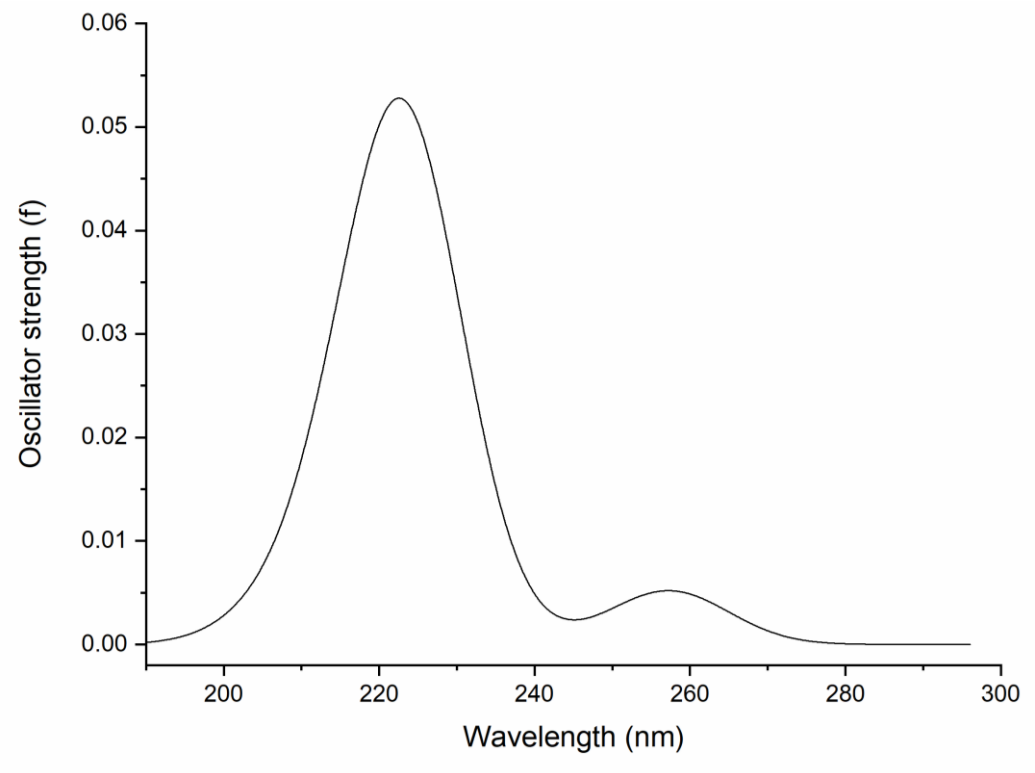

Figure S1. Simulated UV spectrum of the 3AP tautomer obtained from the TD-DFT(B3LYP)/6-311++G(d,p) calculations. A band width at half-height of 17.9 nm was used to simulate the spectrum.