

Supplementary Information

Probing the Vibrational Spectroscopy of the Deprotonated Thymine Radical by Photodetachment and State-Selective Autodetachment Photoelectron Spectroscopy via Dipole-Bound States

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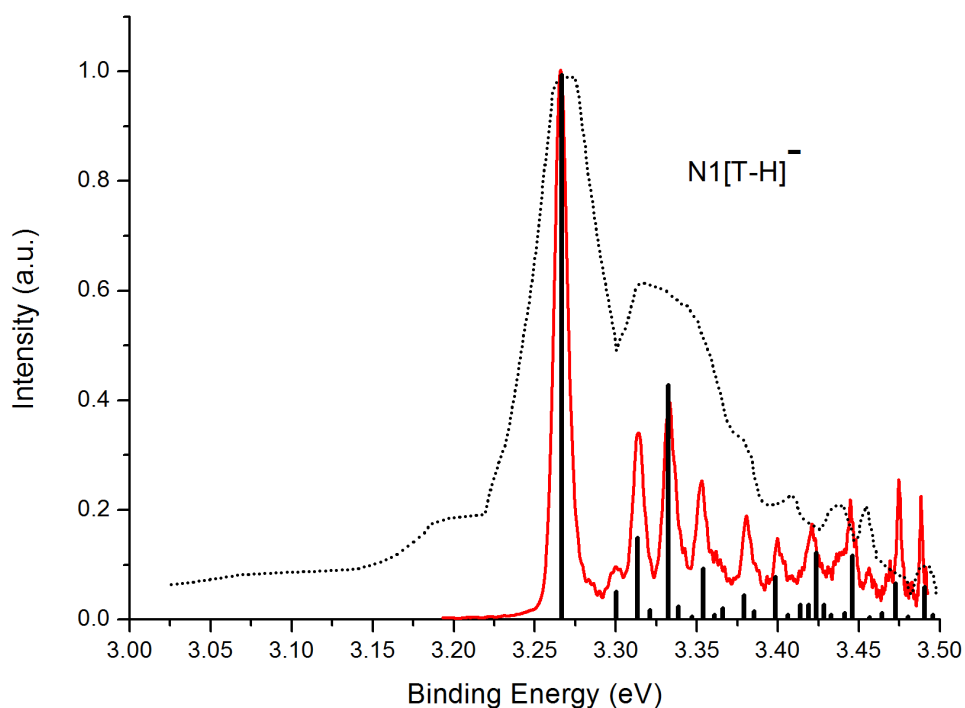


Figure S1. Comparison of the current 354.84 nm photoelectron spectrum (red) with the previous spectrum at the same wavelength (dotted line) and the previous Franck-Condon simulation (vertical bars) for the N1[T-H]⁻ isomer.²³

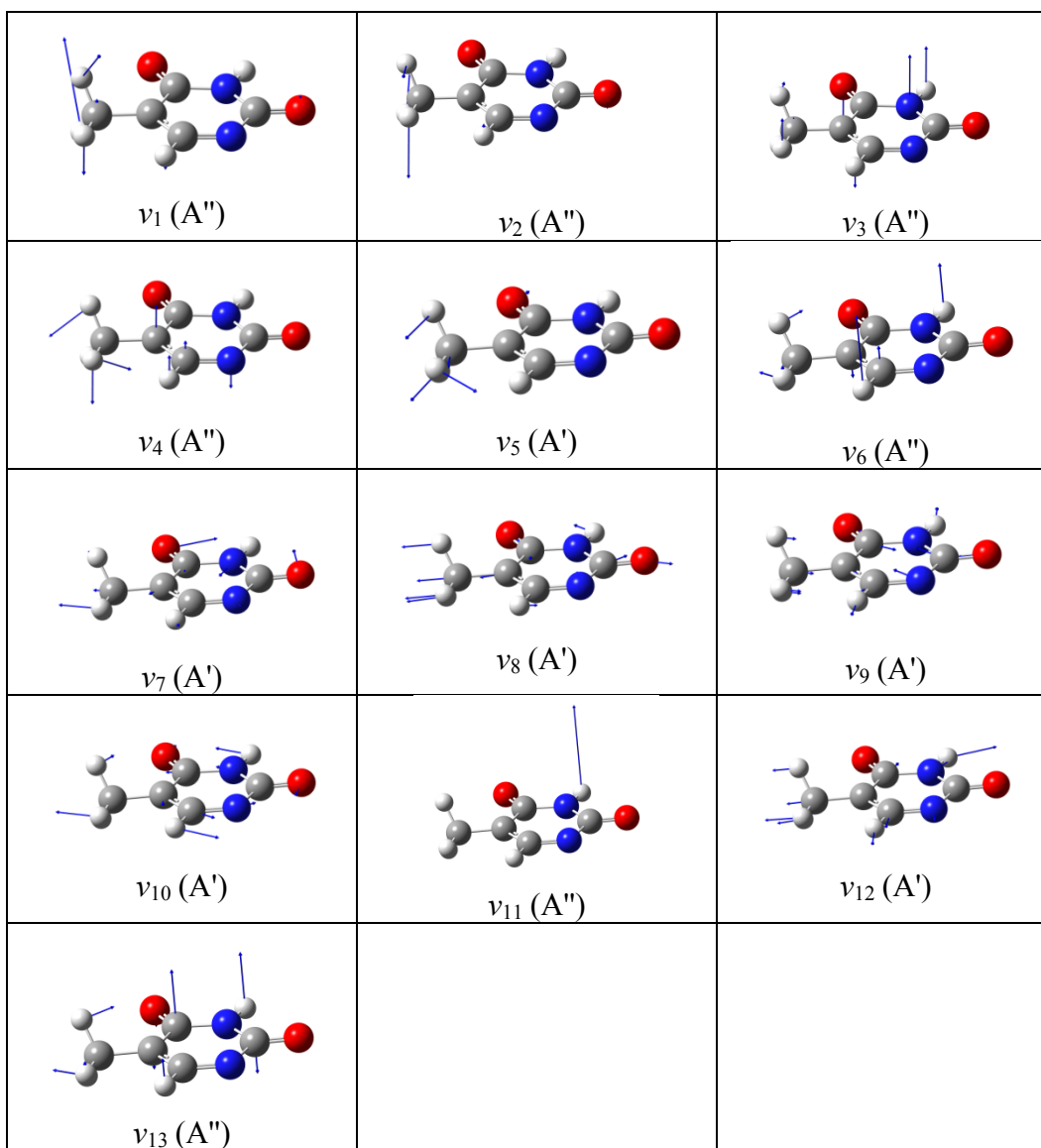


Figure S2. The thirteen lowest frequency normal modes of $N1[T-H]^\bullet$. The arrows indicate the displacement vectors. See Table S1 and Table 2 for their calculated frequencies.

Table S1 The complete list of the symmetries and vibrational frequencies of the N1[T-H]• radical calculated with the B3LYP/6-311++G(d, p) method.

Mode	Symmetry	Theoretical (cm ⁻¹)
ν_1	A''	70
ν_2	A''	93
ν_3	A''	135
ν_4	A''	262
ν_5	A'	285
ν_6	A''	388
ν_7	A'	397
ν_8	A'	450
ν_9	A'	555
ν_{10}	A'	608
ν_{11}	A''	670
ν_{12}	A'	720
ν_{13}	A''	727
ν_{14}	A''	751
ν_{15}	A'	795
ν_{16}	A'	918
ν_{17}	A''	941
ν_{18}	A'	998
ν_{19}	A''	1019
ν_{20}	A'	1179
ν_{21}	A'	1223
ν_{22}	A'	1300
ν_{23}	A'	1342
ν_{24}	A'	1402
ν_{25}	A'	1413
ν_{26}	A'	1423
ν_{27}	A''	1453
ν_{28}	A'	1484
ν_{29}	A'	1488
ν_{30}	A'	1708
ν_{31}	A'	1720
ν_{32}	A'	3021
ν_{33}	A''	3063
ν_{34}	A'	3121
ν_{35}	A'	3127
ν_{36}	A'	3581