Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Vibrational Signatures of Watson-Crick Base Pairing in Adenine-Thymine mimics

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Electronic Supplementary Information

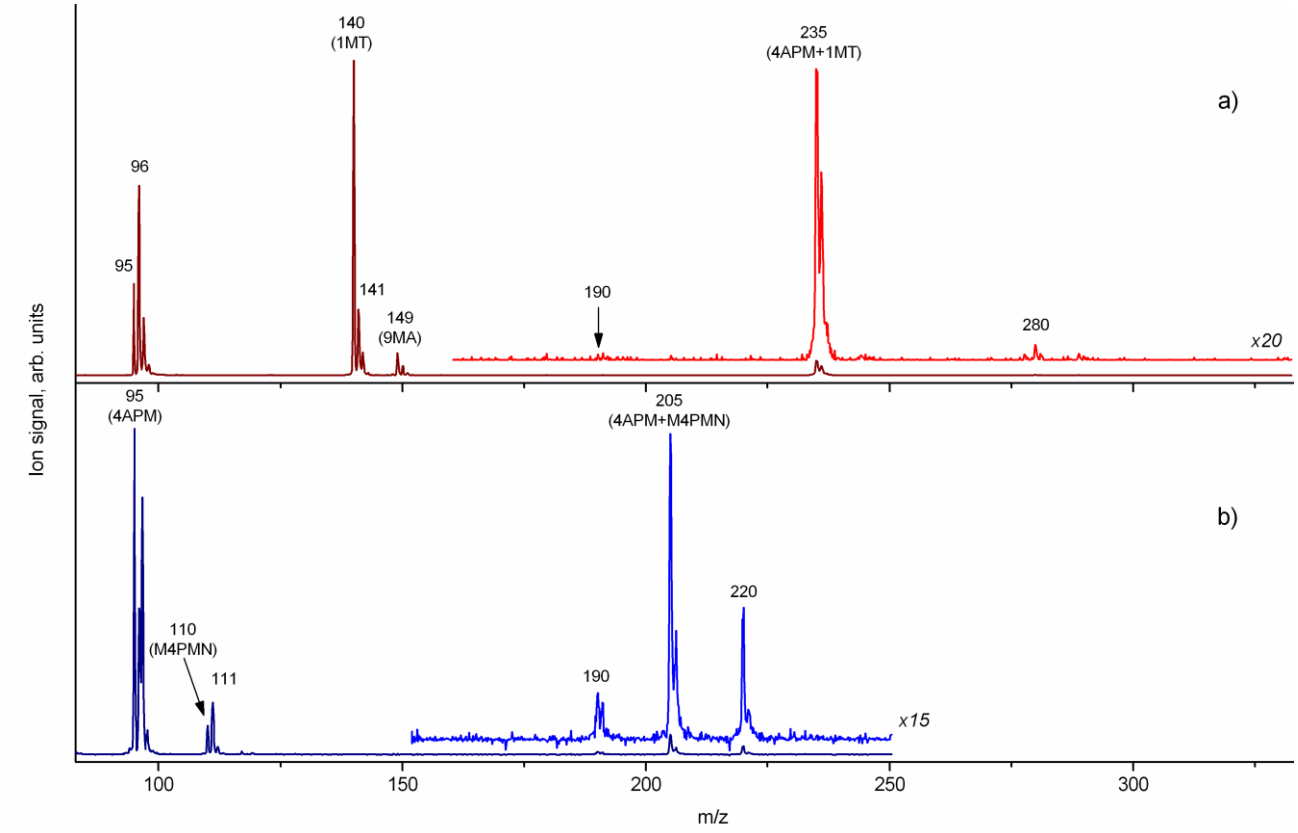
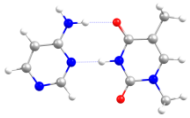
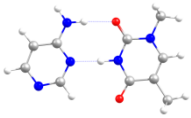
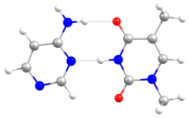
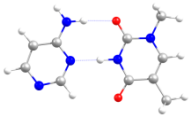


Figure S1. Time-of-flight fsMPI mass spectra of the 4APM-1MT (a) and 4APM-M4PMN (b) systems. 9MA (m/z=149) indicates 9-methyladenine impurity.

Table T1. Calculated structures and relative energies of different conformers of the 4APM–1MT heterodimer at the B3LYP/aug-cc-pVDZ and MO6-2X/aug-cc-pVDZ levels of theory [a]

	B3LYP/aug-cc-pVDZ		M06-2X/aug-cc-pVDZ	
	WC	rWC	WC	rWC
				
ΔE	-13.0	-12.3	-14.8	-14.4
ΔE_B	-11.8	-11.1	-13.7	-13.2
ΔE_0	-10.4	-9.9	-12.8	-12.0
H···N	1.835	1.834	1.780	1.777
∠NH···N	178.2	178.6	179.9	179.8
H···O	1.884	1.920	1.918	1.943
∠NH···O	176.5	175.8	175.7	175.1

All energies are in kcal/mol, distances are in Å, and angles are in degrees(°). ΔE and ΔE_B represents the supermolecular interaction energy without and with basis set superposition error (BSSE) correction. ΔE_0 represents the zero point vibrational energy (ZPVE) corrected ΔE_B.

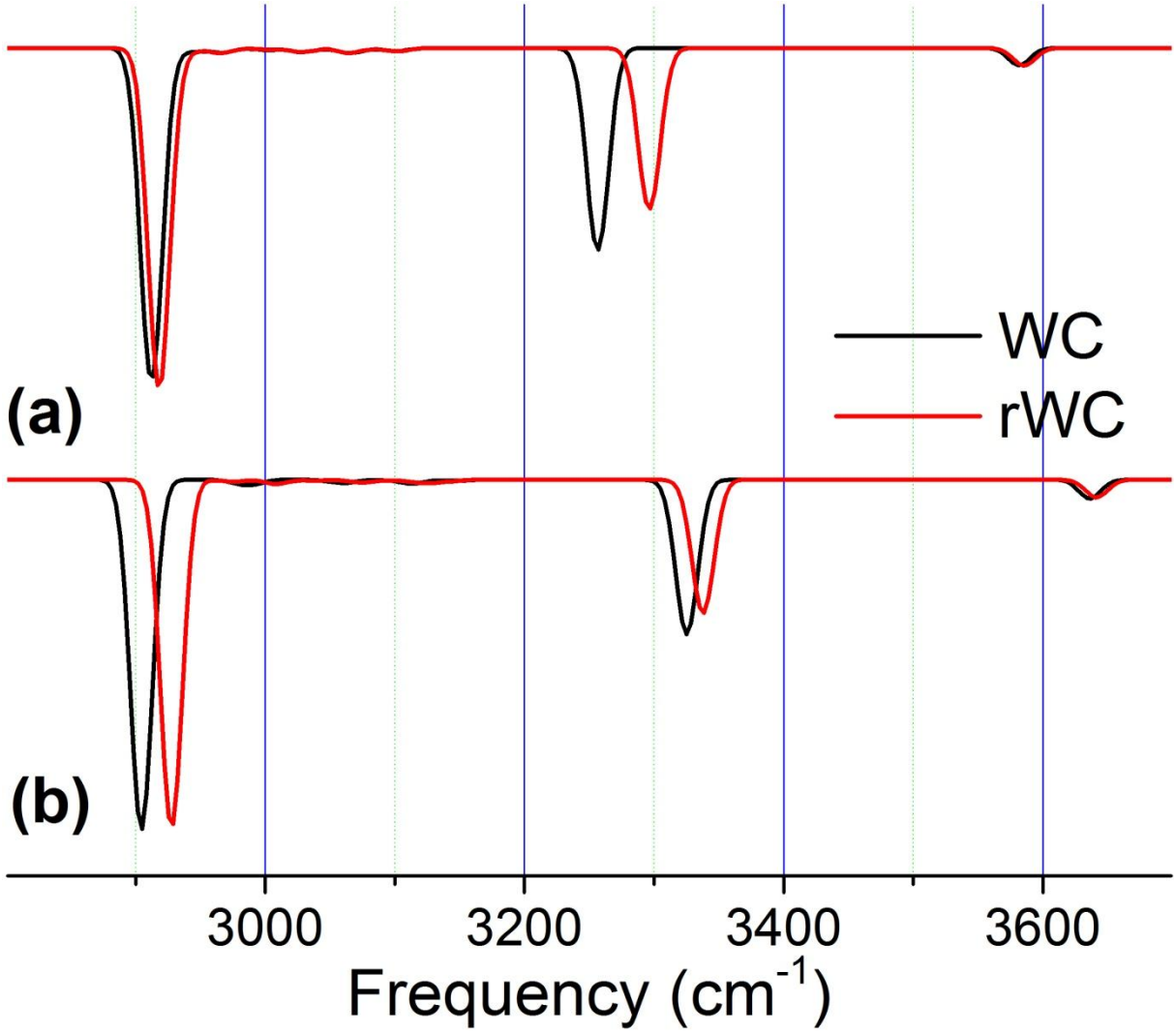


Figure S2. Calculated harmonic vibrational frequencies of different conformers of the 4APM–1MT heterodimer at the (a) B3LYP/aug-cc-pVDZ and (b) MO6-2X/aug-cc-pVDZ levels of theory. The B3LYP frequencies have been scaled by a factor of 0.9704[1], and the M06-2X frequencies by a factor of 0.9721[2].

REFERENCES

1. http://cccbdb.nist.gov/vibscalejust.asp

2. Y. Zhao, and D. G. Truhlar, *Theoretical Chemistry Accounts*, 2008, **120**, 215-241.