Supplementary Material (ESI) for Faraday Discussions
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The effect of microhydration on ionization energies of thymine: Supplementary Materials.

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I. VIES VERSUS CHARGE TRANSFER

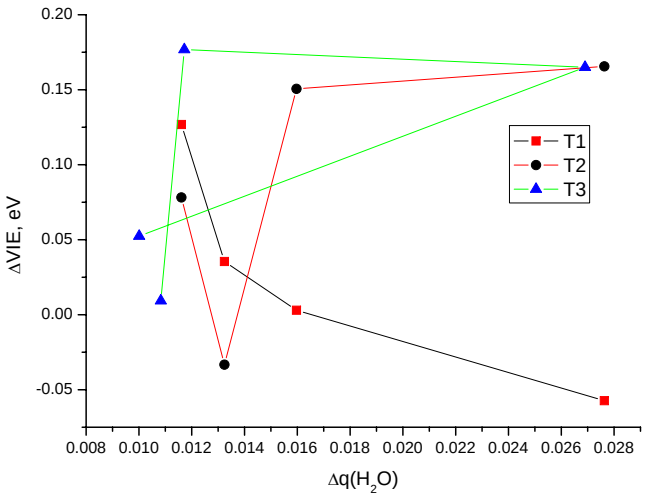

FIG. 1: VIEs versus the degree of charge transfer to water in different ionized states of the three thymine monohydrates.

II. CHARGE DISTRIBUTION OBTAINED BY NBO ANALYSIS

The following files contain NBO charges computed using EOM-IP-CCSD/6-31+G(d) densities for T1, T2, and T3, respectively: t1_charges.txt, t2_charges.txt, t3_charges.txt

III. EQUILIBRIUM STRUCTURES OF NEUTRAL AND IONIZED THYMINE-WATER CLUSTERS

Cartesian geometries of otpimized structures are given in geometry.txt.

IV. VIBRATIONAL FREQUENCIES AND FRANCK-CONDON FACTORS

Vibrational frequencies for thymine in the geometry of T1 and T2 clusters can be found in the following files:

T1 neutral: t1_neutral_without_H2O_vibrations.txt
T1 inonised state: t1_is_without_H2O_vibrations.txt

T2 neutral: t2_neutral_without_H2O_vibrations.txt
T2 inonised state: t2_is_without_H2O_vibrations.txt

Franck-Condom factors and intensities, calculated by ezSpectrum for thymine moiety can be found in the following files:

T1: t1_ezSpectrum_out.txt

T2: t2_ezSpectrum_out.txt

Calculated intensities for water motion and overall clusters are in the file

FCF_overall.txt

These intensities fitted with Gaussians with 0.05 eV width are in the file:

FCFs_overall_fitted.txt