Structures, electrophilic properties and hydrogen bonds of cytidine, uridine, and their radical anions: microhydration effects

Supplementary Information

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FIG. S1 The selected low-lying structures for cytidine monohydrates (first line) and their anions (second line), with relative energies (eV) compared with lowest-energy structure and intermolecular distances (Å). The blue, red, grey and white balls represent N, O, C and H atoms, respectively.
**FIG. S2** The selected low-lying structures for uridine monohydrates (first line) and their anions (second line), with relative energies (eV) compared with lowest-energy structure and intermolecular distances (Å). The blue, red, grey and white balls represent N, O, C and H atoms, respectively.
**FIG. S3** Singly occupied molecular orbitals (SOMOs) for the low-lying anionic structures of cytidine monohydrates (first line) and uridine monohydrates (second line).
FIG. S4 Plots of the reduced density gradient (RDG) versus the electron density multiplied by the sign of the second Hessian eigenvalue (Sign(λ₂ρ)) for structure CW-Na.