Electronic Supplementary Material (ESI) for RSC Advances.

Microhydration effects on the structures and electrophilic properties of cytidine

Peng Shao[a], Li-Ping Ding[b,*], Jiang-Tao Cai[a], Cheng Lu[c,*], Bo Liu[a,] and Chang-Bo Sun[a]

[a]*Department of Physics, Shaanxi University of Science & Technology, Xi'an 710021, China*

[b]*Department of Optoelectronic Science & Technology, College of Elecrical & Information Engineering, Shaanxi University of Science & Technology, Xi'an 710021, China*

[c]*Beijing Computational Science Research Center, Beijing, 100084, China*

Table S1. Relative energies (ΔE), vertical electron affinities (VEAs), vertical detachment energies (VDEs), hydration energies (E_{hyd}) and intermolecular contacts for the neutral and anionic monohydrated cytidine.

Structure	ΔE (eV)	VEA (eV)	E_{hyd} (kcal mol^{-1})	Intermolecular contacts
Cw-Na	0.00	-0.41	13.22	$N_3\cdots H_w-O_w\cdots H-N_4$
Cw-Nb	0.16	-0.57	9.43	$H_w-O_w\cdots H-O_{5'}$
Cw-Nc	0.18	-0.62	9.17	$O_{4'}-H_w\cdots O_w-H\cdots O_{5'}$
Cw-Nd	0.19	-0.46	8.98	$O_2\cdots H_w-O_w\cdots H-O_{2'}$
Cw-Ne	0.21	-0.77	8.52	$N_4-H\cdots O_w$
Structure	ΔE (eV)	VDE (eV)	E_{hyd} (kcal mol^{-1})	Intermolecular contacts
Cw-Aa	0.00	1.42	17.29	$N_3\cdots H_w-O_w\cdots H-N_4$
Cw-Ab	0.06	1.44	15.90	$O_2\cdots H_w-O_w-H_w\cdots N_3$
Cw-Ac	0.16	1.32	13.41	$O_{3'}\cdots H_w-O_w-H_w\cdots O_{4'}$
Cw-Ad	0.17	1.33	13.37	$O_2\cdots H_w-O_w-H_w\cdots O_{2'}$
Cw-Ae	0.22	1.39	12.16	$N_4\cdots H_w-O_w$

*Correspondence to: Li-Ping Ding, Shaanxi University of Science & Technology, Xi'an 710021, China.
E-mail address: scu_ding@163.com (Li-Ping Ding), lucheng@calypso.cn (Cheng Lu)

Fig. S1. Molecular structures for cytidine monohydrates (first line) and their anions (second line), with intermolecular distances in angstrom.

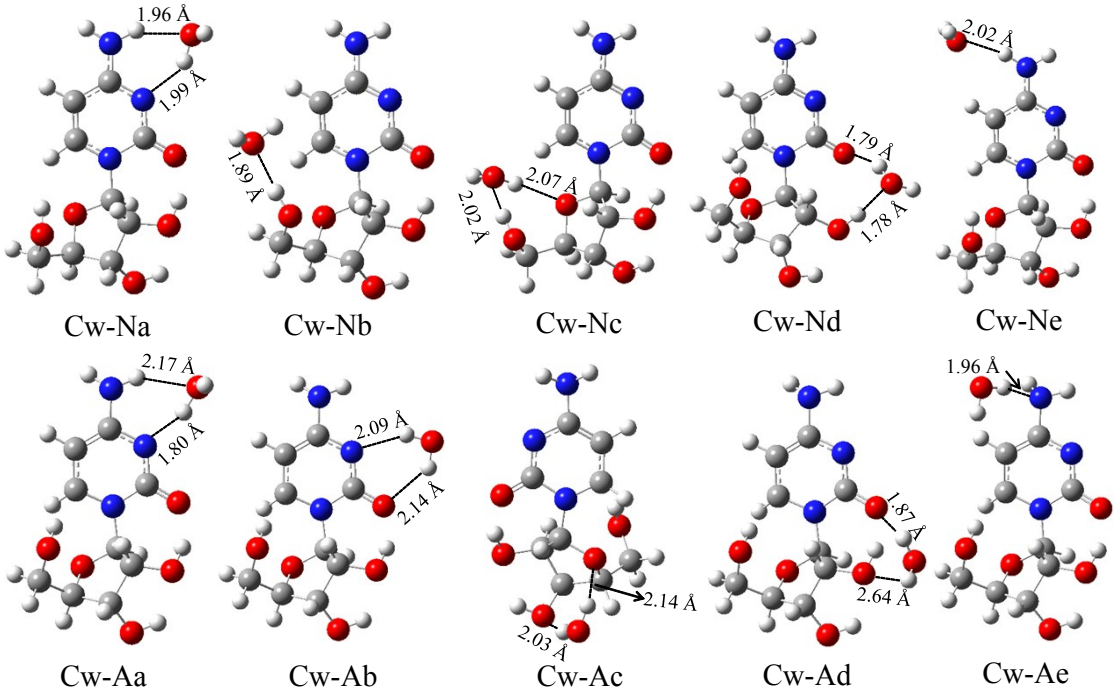


Fig.S2. The selected low-lying structures for cytidine dihydrates (first line) and their anions (second line). The blue, red, grey and white balls represent N, O, C and H atoms, respectively.

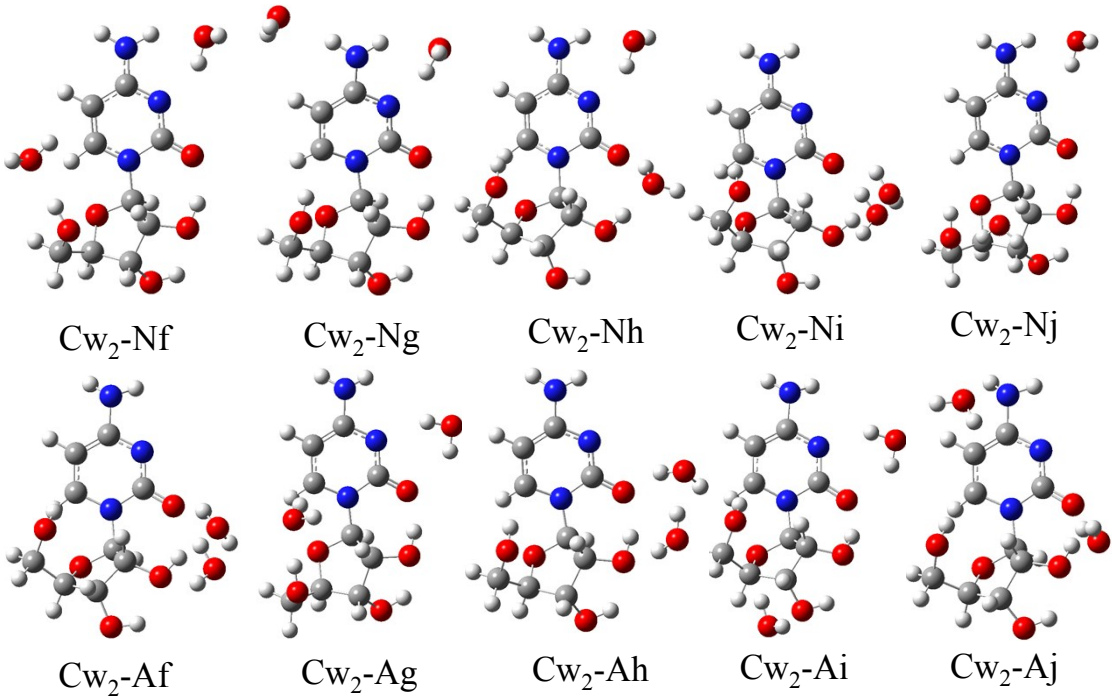


Fig.S3. The selected low-lying structures for cytidine trihydrates (first line) and their anions (second line). The blue, red, grey and white balls represent N, O, C and H atoms, respectively.

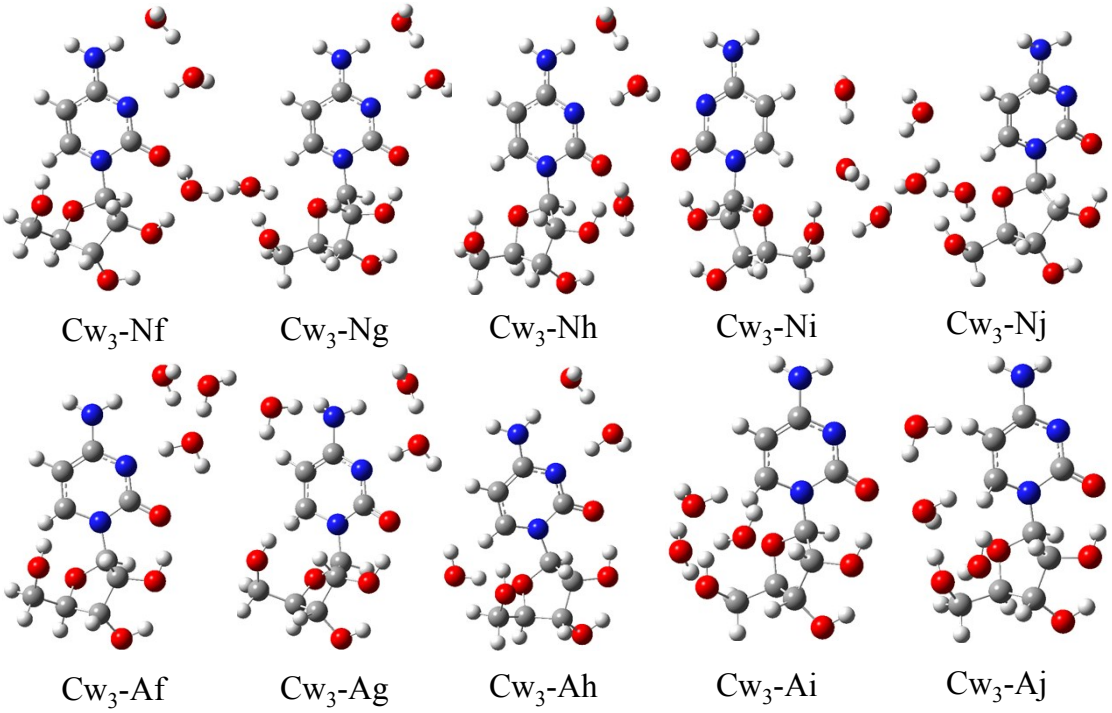


Fig.S4. The selected low-lying structures for cytidine tetrahydrates (first line) and their anions (second line). The blue, red, grey and white balls represent N, O, C and H atoms, respectively.

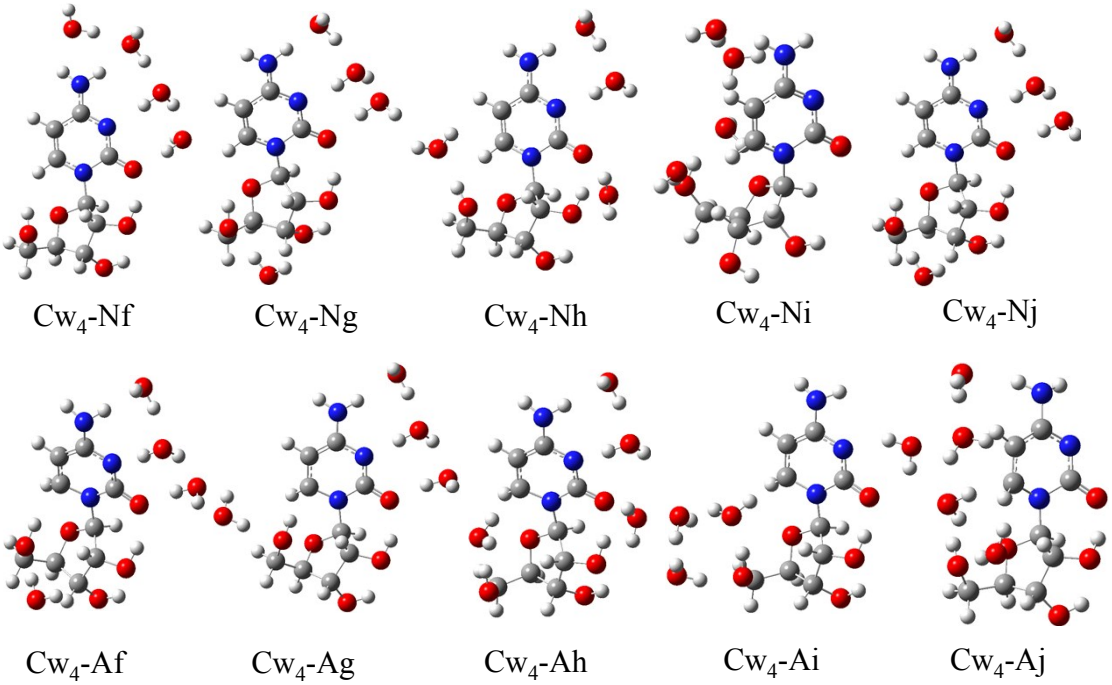


Fig. S5. Singly occupied molecular orbitals (SOMOs) for the anions of cytidine and its monohydrates.

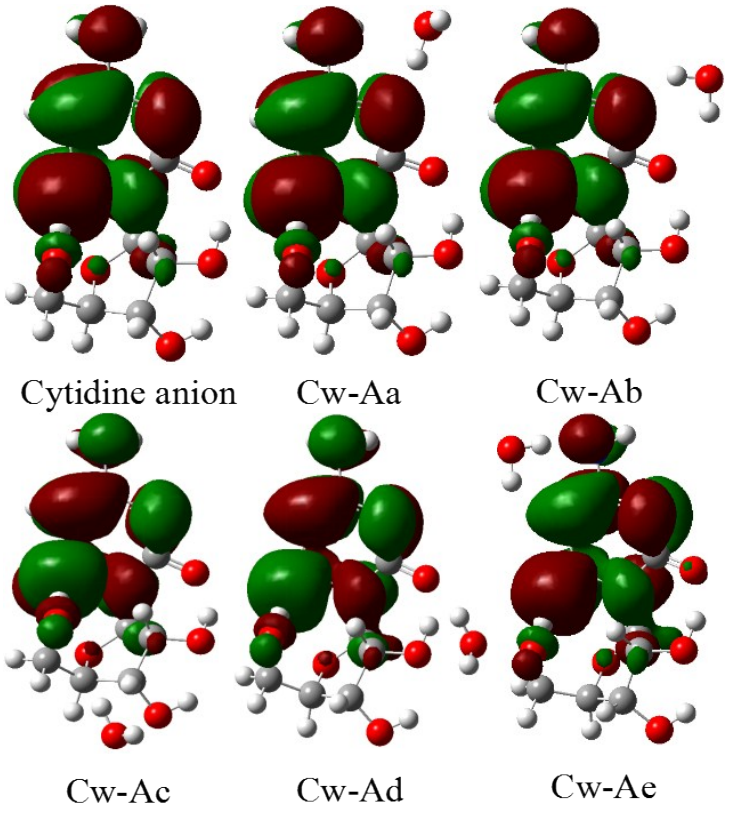
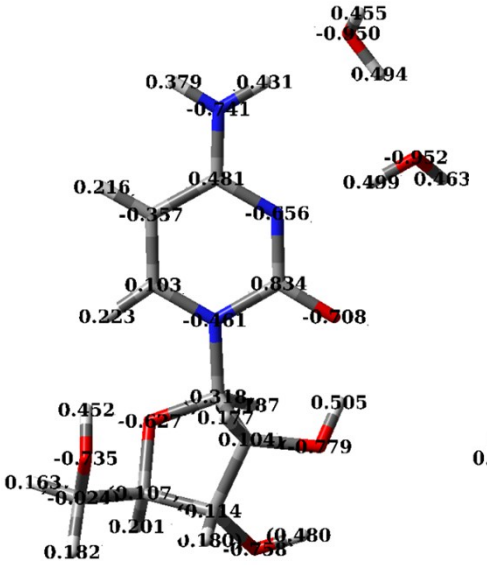
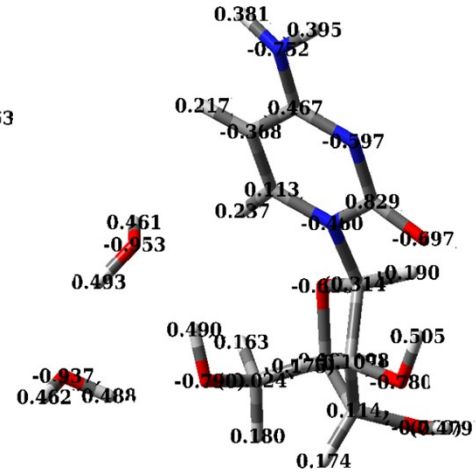


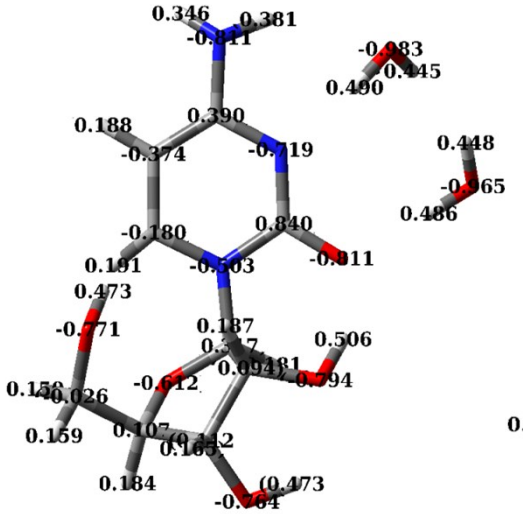
Fig. S6. Charge distributions in the first two lowest energy structures of cytidine dihydrates and their anions.



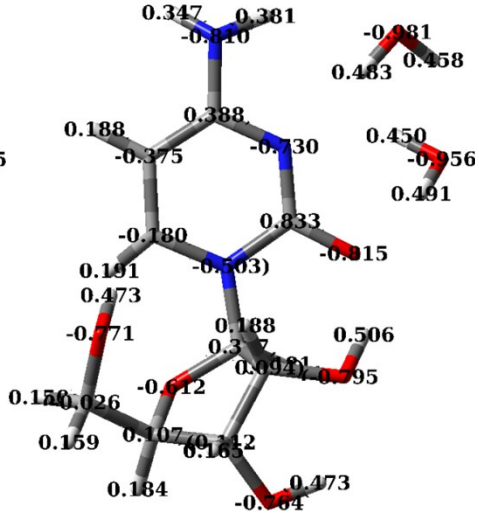
Cw_2-Na



Cw_2-Nb

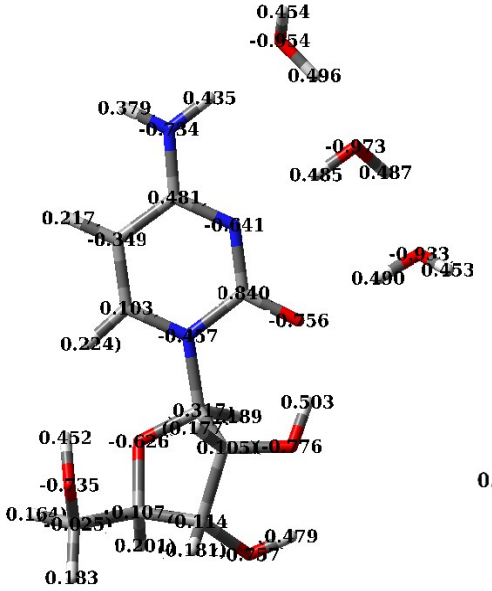


Cw_2-Aa

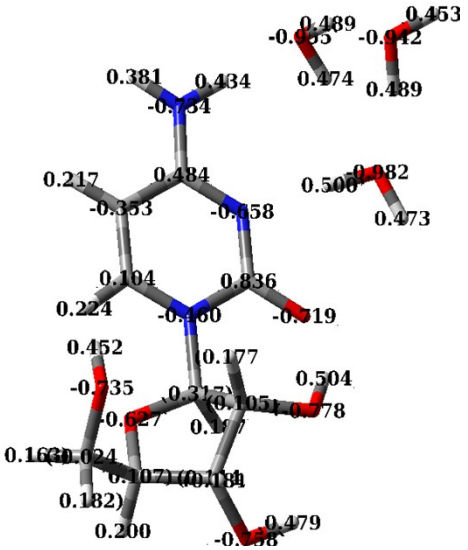


Cw_2-Ab

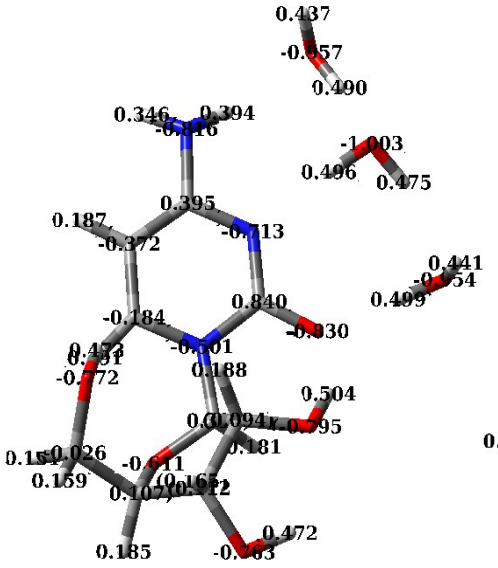
Fig. S7. Charge distributions in the first two lowest energy structures of cytidine trihydrates and their anions.



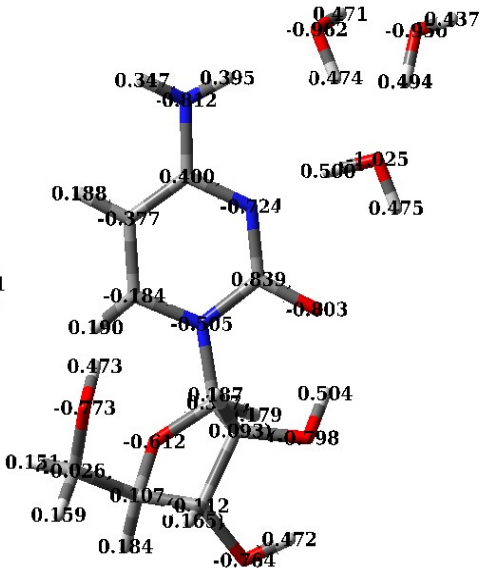
Cw_3-Na



Cw_3-Nb

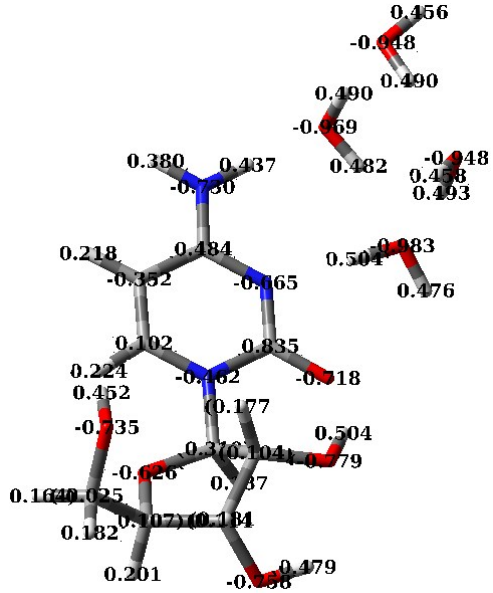


Cw_3-Aa

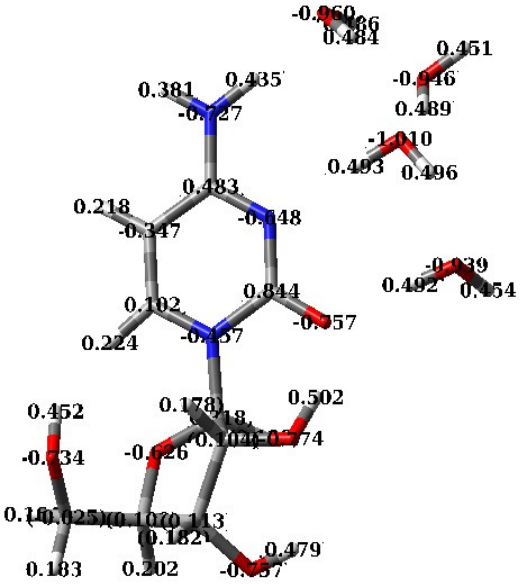


Cw_3-Ab

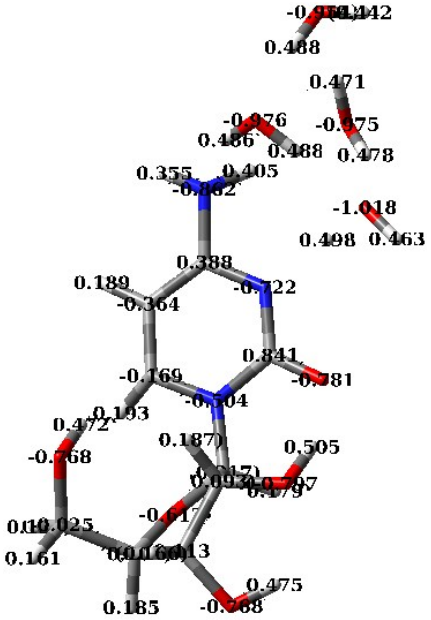
Fig. S8. Charge distributions in the first two lowest energy structures of cytidine tetrahydrates and their anions.



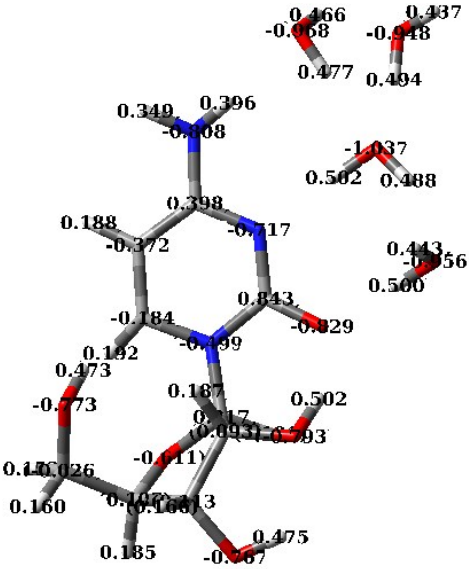
Cw_4-Na



Cw_4-Nb



Cw_4-Aa



Cw_4-Ab

Fig. S9. Charge distributions in neutral and anionic cytidine and their lowest energy monohydrates.

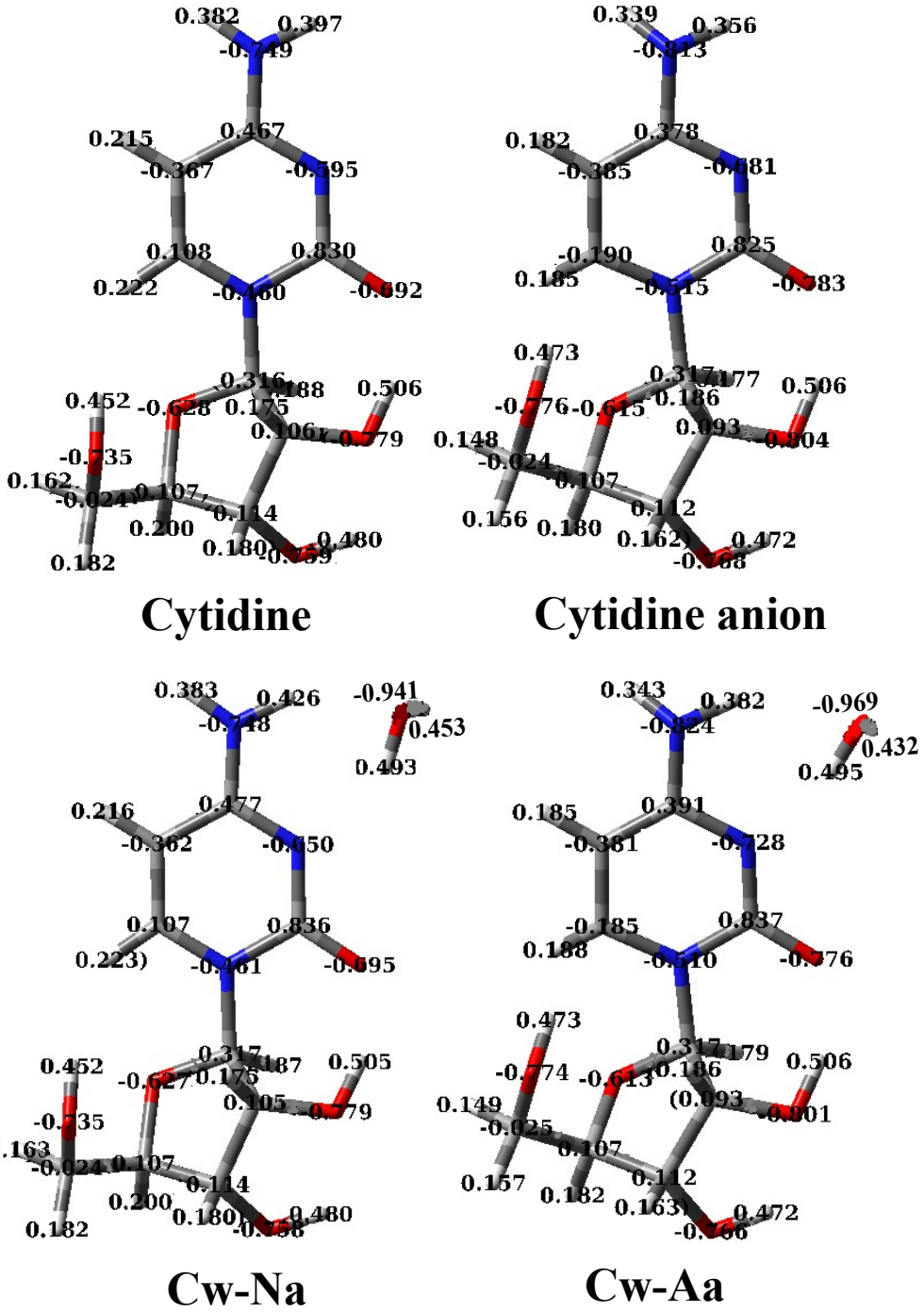


Fig. S10. The transition processes for one isomer to another for the Cw_2-Na isomer.