Supplementary data for the article:

Veljković, D. Ž.; Medaković, V. B.; Andrić, J. M.; Zarić, S. D. C-H/O Interactions of Nucleic Bases with a Water Molecule: A Crystallographic and Quantum Chemical Study. *CrystEngComm* **2014**, *16* (43), 10089–10096. <u>https://doi.org/10.1039/c4ce00595c</u>

Supplementary Information

C-H/O interactions of nucleic bases with water molecule. Crystallographic and quantum chemical study.

Dušan Ž. Veljković, Vesna B. Medaković, Jelena M. Andrić, Snežana D. Zarić*

INFLUENCE OF COUNTER ANIONS/CATIONS COMPOSING OF THE UNIT CELL

In cases where nucleic bases are positively charged (nitrogen atoms are protonated), they form hydrogen bonds between N-H groups and counter anions. In that way, N-H groups are not available for interactions with water molecules and water molecules form C-H/O interaction.

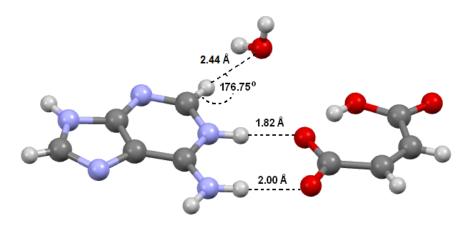


Fig. S1. View of RIGMIE crystal structure showing simultaneous interactions of positively charged nucleic basis with counter ion and with water molecule.

S. Sridhar and K. Ravikumar, *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, 2007, **63**, 0415-0418; CSD REFCODE: RIGMIE.