

# NMR CHEMICAL SHIFTS IN NUCLEOTIDES: INFLUENCE OF THE Mg (II) COORDINATION SITE

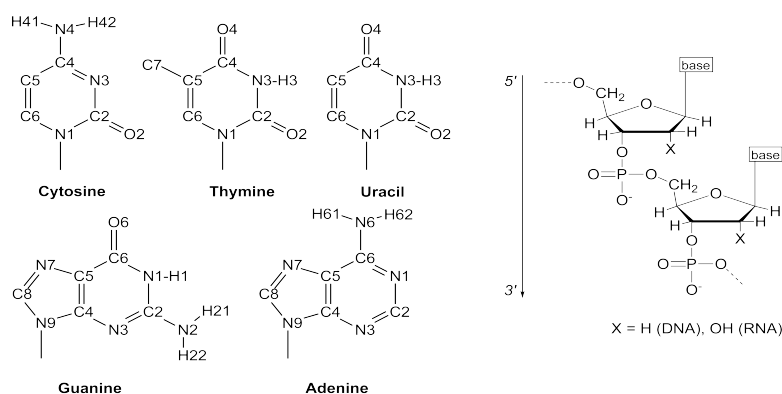
LI. Armangué<sup>1</sup>, C. Fonseca Guerra<sup>2</sup>, M. Swart<sup>1,3</sup>, M. Solà<sup>1</sup>, F.M. Bickelhaupt<sup>2</sup>

<sup>1</sup>Institut de Química Computacional & Dept. de Química, University of Girona, Campus Montilivi, Girona, 17071, SPAIN

<sup>2</sup>Dept. of Theoretical Chemistry & Amsterdam Center for Multiscale Modeling, VU University, De Boelelaan 1083, 1081 HV Amsterdam, THE NETHERLANDS

<sup>3</sup>Institució Catalana de Recerca i Estudis Avançats (ICREA), Pg. Lluís Companys 23, Barcelona, 08010, SPAIN

Magnesium is one of the most abundant metal-ions in biochemistry. It is an essential cofactor for various enzymatic reactions involving nucleotides. We have computationally explored if the coordination site of magnesium ions at nucleotides can be uniquely inferred from NMR chemical shifts, using DFT at the BP86 and SSB-D levels of theory. The latter functional has been proposed as a new all-round density functional [1,2] and was recently shown to perform excellently in computations of <sup>13</sup>C-NMR chemical shifts [3]. Our investigations focus on the situation in aqueous solution about which little is known, at variance with the more abundant X-ray crystal structures of DNA and RNA complexes with Mg<sup>2+</sup> [4, 5]. We used for our computations the Amsterdam Density Functional (ADF) program in combination with the conductor-like screening model (COSMO) for simulating bulk solvation in water. Our model systems comprise the nucleotides of all five nucleic acids occurring in DNA and RNA (see illustration). Mg<sup>2+</sup> ions have been coordinated to various sites at the phosphate group.



## References

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