Electronic Supporting Information for

The First X-Ray Structure of a Silver–Nucleotide Complex: Interaction of Ion Ag(I) with Cytidine-5'-Monophosphate

Angel Terrón,[a]* *Lorenç Tomàs,*[a] *Antonio Bauzá,*[a] *Angel García-Raso,*[a] *Juan J. Fiol,*[a] *Elies Molins*[b] *and Antonio Frontera*[a,]*

[a]Departament de Química, Universitat de les Illes Balears, Ctra. de Valldemossa km 7.5, 07122 Palma de Mallorca, Spain. E-mail: toni.frontera@uib.es
[b]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus de la Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain

Table of contents:

1. Table S1

Table 1. Crystal data and structure refinement for **1**.

Identification code	1
Empirical formula	C9 H15 Ag N3 O9 P
Formula weight	448.08
Temperature	294(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P 21 21 21
Unit cell dimensions	a = 4.8225(14) Å
	b = 15.9142(19) Å
	c = 18.336(3) Å
	α = β = γ = 90°
Volume	1407.2(5) $Å^3$
Z	4
Density (calculated)	2.115 Mg/m^3
Absorption coefficient	1.602 mm^{-1}
F(000)	896
Crystal size	0.39 x 0.21 x 0.09 mm^3
Theta range for data collection	1.694 to 25.003°.
Index ranges	$-5 \leq h \leq 5$, $0 \leq k \leq 18$, $0 \leq l \leq 21$
Reflections collected	2634
Independent reflections	2475 [R(int) = 0.0411]
Completeness to theta = 25.003°	99.8 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2475 / 0 / 268
Goodness-of-fit on F^2	1.113
Final R indices [I>2sigma(I)]	R1 = 0.0338, wR2 = 0.0812
R indices (all data)	R1 = 0.0418, wR2 = 0.0851
Absolute structure parameter	0.00(3)
Largest diff. peak and hole	0.643 and -0.480 $e.Å^{-3}$

2. Experimental details

Analysis and physical measurements

Elemental microanalysis was carried using a Carlo Erba model 1108 microanalyzer. IR spectra (KBr) pellets were measured in a Bruker IFS 66 spectrometer.

Synthesis of the compound Ag(HCMP)·H_2O , H_2CMP: cytosine-5'-monophosphate

1 mmol de H_2CMP was dissolved in 10 ml water *MiliQ*, and mixed with a solution of 1 mmol $AgNO_3$ in 10 ml water *MiliQ* in the absence of light. The mixed was refluxed under stirring during two hours. The resultant solution was filtered with a paper filter. The remaining clear solution was left to cool and concentrate by evaporation preventing always the presence of light. The final pH of the solution was 3. One month later delicate crystalline needles appeared in the solution. The crystals were selected and dried in air and were adequate for X- Ray studies.

Elemental analysis of Ag(HCMP)·H_2O

Calculated as $C_9H_{15}AgN_3O_9P$: 24,13 (calc), **24.34** (exp); H: 3.37 (calc), **3.33** (exp); N: 9.38 (calc), **9.24** (exp). *IR:* 522m, 598w, 711w, 757w, 795m, 8744w, 971m, 993m, 1037s, 1058s, 1075m, 1110s, 1171m, 1215m, 1248w, 1287m 1404s, 1448s, 1486s, 1528m, 1614s, 1638s, 2342w, 2360w, 2789m, 2891m, 2965m, 3217s, 3396s.

The solid is soluble neither in organic solvents nor water, therefore no NMR data is provided.

X-ray data collection details

A suitable flat prismatic colorless crystal (dimensions 0.33 x 0.21 x 0.09 mm^3) of **1** was selected for X-ray single crystal diffraction experiments and mounted at the tip of a glass fiber on an Enraf-Nonius CAD4 diffractometer, with Mo-Kα radiation (λ=0.71073 Å) using a graphite crystal monochromator. After the random search of 25 reflections, the indexation procedure gives rise to the cell parameters, listed in Table S1. The data collection was done using ω-2ϑ scans. All structural resolution procedures were made using the WinGX package.[1] Solving for structure factor phases was performed by SIR2002[2] and the full-matrix refinement, by SHELXL97.[3]

3. Theoretical methods

The energies of all complexes included in this study were computed using the M06-2X/def2-TZVP level of theory by means of the program TURBOMOLE version 7.0.[4] We have used the crystallographic coordinates for the theoretical analysis of the noncovalent interactions present in the solid state. The interaction energies were calculated with correction for the basis set superposition error (BSSE) by using the Boys–Bernardi counterpoise technique.[5] The Bader's "Atoms in molecules" theory has been used to study the interactions discussed herein by means of the AIMall calculation package.[6] The MEPS calculations have been performed at the ab-initio/DFT-D level by means of the SPARTAN software.[7]

---

[1] 1. L. J. Farrugia, *J. Appl. Crystallogr*. 1999, **32**, 837–838.
[2] M. C. Burla, M. Camalli, B. Carrozzini, G. L. Cascarano, C. Giacovazzo, G. Polidori and R. Spagna, *J. Appl. Crystallogr*., 2003, **36**, 1103.
[3] G. M. Sheldrick, *Acta Crystallogr*., 2008, **A64**, 112.
[4] R. Ahlrichs, M. Bär, M. Hacer, H. Horn and C. Kömel, *Chem. Phys. Lett.*, 1989, **162**, 165.
[5] S. B. Boys and F. Bernardi, *Mol. Phys.*, 1970, **19**, 553.
[6] AIMAll (Version 13.05.06), Todd A. Keith, TK Gristmill Software, Overland Park KS, USA, 2013.
[7] Spartan '10, Wavefunction Inc. Irvine, CA. www.wavefun.com.