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Study of the Chelating Capacity of Nucleobase Analogs with Biological Interest: *Ab initio* Molecular Orbital Calculations and Single-Crystal X-ray Structural Study of 6-Amino-5-formyl-1,3-dimethyluracil-benzoylhydrazone

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Abstract *Ab initio* molecular orbital calculations at the RHF/6-31G* level using the GAUSSIAN94 program package have allowed us to simulate the molecular structures for different conformations of 6-amino-5-formyl-1,3-dimethyluracil-benzoylhydrazone. The contribution of the atomic orbitals of the potential donor atoms to the higher occupied molecular orbitals allows us to propose theoretical arguments to justify the different chelating behavior found for this compound in several metal complexes. Further, the molecular structure of 6-amino-5-formyl-1,3-dimethyluracil-benzoylhydrazone has been determined by single-crystal X-ray diffraction methods. The compound crystallizes in the monoclinic system (space group $P2_1/n$) with cell dimensions: $a = 12.111(5)$, $b = 5.743(5)$, $c = 22.636(5)$ Å, $\beta = 98.60(5)°$. The structure was solved from 1719 reflections with $I>2\sigma(I)$. The final R $[I>2\sigma(I)]$ was 0.0506 for 217 parameters. The azomethine double bond substituents are in the *E* conformation and the N51 atom is in the *cis* position with respect to the N6 atom, due to the formation of an intramolecular hydrogen bond N6-H···N51. The geometrical data are in good agreement with those calculated by means of *ab initio* methods.

Keywords *Ab initio*, Molecular structure, Uracil, Hydrazone

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Introduction

The biological activity of complexes derived from hydrazones has been widely studied and reported. These complexes are active in processes such as antibacterial, antitumoral, antiviral, antimalarial and antituberculosis effects.[1,2] In the title compound, we have tried to extend the potentially N,O-bidentate chelating capability of benzoylhydrazones with another metal binding site (N6 or O4) supplied by a 6-aminouracil moiety. This potential N,N,O- or O,N,O-tridentate character is very similar to that shown by several thiosemicarbazones with biological activity.[3] Moreover, the presence of the uracil ring may aid the resulting compounds to show a structural analogy with the ones present in biological systems. This feature may be useful for potential pharmacological applications due to the azomethinic bond which may be mainly hydrolysed in cancer cells, liberating the uracil derivative, which may act as either an alkylating agent or antimetabolite.

This paper has been focused from two different points of view. Firstly, the power of *ab initio* methods to simulate the structure of the title compound, hereafter denoted as H_2BEZDO, has been checked by comparing the optimized geometrical parameters with those obtained from single-crystal X-ray diffraction measurements. In addition to this, we have carried out *ab initio* theoretical calculations at the RHF level with different basis sets for different geometrical possibilities of this molecule in order to justify the different N,N,O [4] or O,N,O-tridentate [5] chelating behaviors found for this ligand in several metal complexes.

Crystallographic work

The Schiff base ligand was prepared as reported elsewhere.[4] Crystals suitable for X-ray diffraction were obtained from a recrystallization in ethanol, but in this case, the organic compound contains half a molecule of ethanol per formula unit. The presence of the organic solvent in the crystalline material was quantitatively corroborated from TG-EGA experiments (Shimadzu TGA-50H thermobalance provided with a FTIR Nicolet-510 apparatus).

A tabular colourless crystal with dimensions 0.34 x 0.16 x 0.08 mm^3 was mounted on a Stoe Ipds diffractometer (T=293(2) K) with graphite-monochromatized MoKα radiation (λ=0.71073 Å). The unit cell was determined from 25 random reflections (7≤θ≤15°). The intensities were collected using the ω-scan mode, in the range 1.80°<θ<24.09°. A total of 9386 reflections were measured with -13≤*h*≤13, -6≤*k*≤6, -25≤*l*≤26. They were averaged to 2434 independent ones (R_{int}=0.0375), 1719 with I>2σ(I) retained for structure solution and refinement. Data were corrected by Lorentz and polarization but not for absorption. Crystal data: CCDC 119504, $C_{15}H_{15}N_5O_{3.5}$, M = 321.32, monoclinic, space group P2$_1$/n, *a* = 12.111(5), *b* = 5.743(5), *c* = 22.636(5) Å, β = 98.60(5)°, V
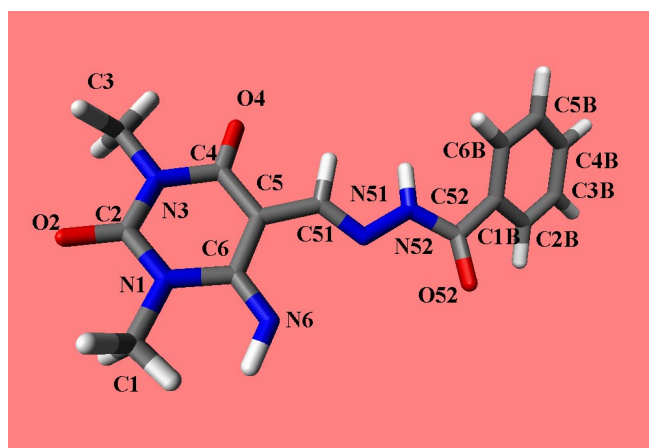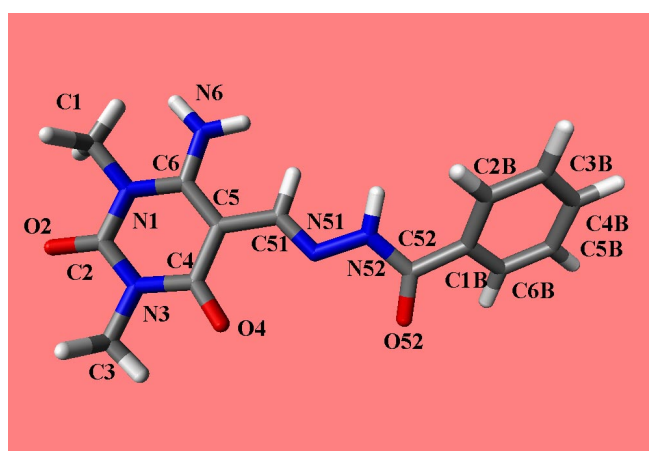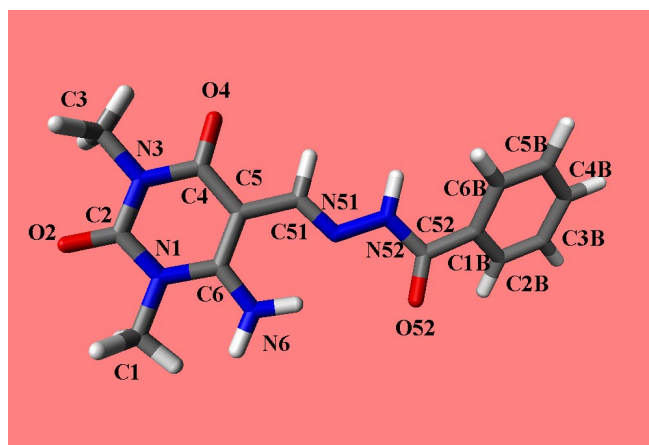
Figure 1 *Optimized structures (6-31G*) on which* ab initio *calculations have been performed.* Top: neutral *native* conformation; middle: neutral *contrary* conformation; bottom: *N6-deprotonated* native *monoanion*

= 1557(2) Å^3, Z = 4, D_c = 1.371 Mg·m^{-3}, absorption coefficient 0.101 mm^{-1}, $F(000)$ = 672.

Structure solution and refinement

The structure was solved by direct methods using the MULTAN system, locating most of the non-H atoms. The remaining non-H atoms were revealed from a subsequent Fourier synthesis. The refinement was carried out anisotropically on F^2. All H atoms were placed in geometrically calculated positions with isotropic displacement parameters related to those of the parent atom using riding models. The Fourier map shows the presence of half a disordered molecule of ethanol per formula unit, related to the other half through an inversion center. Therefore we treated it as a carbon atom with occupation factor 1 and an oxygen atom with occupation factor ½, the temperature factors found in both atoms being very large because of the high disorder. All calculations and drawings were performed using the SHELXL93 and PLATON99 systems. The weighting scheme was w^{-1} = $\sigma^2(F_o)$ + (0.1060P)^2, where P=Å (F$_o^2$ +2F$_c^2$). The final R indices [I>2σ(I)] were R = 0.0506 and wR^2 = 0.1452 for 217 parameters, g.o.f. = 1.154; max. and min. Δρ were +0.502 and -0.205 e·Å^{-3}.

Computational details

Theoretical calculations were carried out on 6-amino-1,3-dimethyl-5-formyluracil-benzoylhydrazone molecule (H$_2$BEZDO) both in neutral *native* and *contrary* conformations, and on the anion *native* conformation as well (fig. 1), by using *ab-initio* methods with the GAUSSIAN94 program package. In a first step, the calculation consisted on the optimization of the geometries of these species in the isolated approach in order to test the reliability of the procedure on comparing the theoretical results with the XRD ones. In this paper, we compare the experimental and calculated geometries of the cited molecule only in the neutral *native* conformation because it is the only one that exists in a pure form, the other two species -neutral *contrary* and anion *native* conformations- being only in coordinated form.

Geometry optimizations were accomplished with the RHF approach using different basis sets (STO-3G, 4-31G, 6-31G and 6-31G*), as implemented in the GAUSSIAN94 suite.[6,7] This program was run on a HP-XClass computer until the default convergence criteria were satisfied. The starting point of the optimization procedure was different in each case. For the neutral *native* conformation, the semiempirical (AM1) optimized geometry was used. For the *contrary* conformation, the same parameters as in the above case were used but some dihedral angles were modified to obtain the *cis*-conformation between the atoms C4 and N51 (see below). For the anion *native* conformation, the initial geometrical parameters were those from RHF/6-31G* calculation on the neutral *na-*

tive conformation, with hydrogen H61 removed and the residual charge on this species set to –1.

To save computational time, we used an iterative method to optimize the geometry of the neutral *native* conformation, where the geometrical parameters obtained at the STO-3G level were used as input in the RHF/4-31G calculations and so on until the RHF/6-31G* one. The same procedure was followed to optimize the geometry of the *contrary* conformation, but in this conformation, the dihedral angles C6-C5-C51-H51 and C4-C5-C51-H51 were constrained to 0 and 180° respectively, in order to preclude the uracil moiety turning around the bond C5-C51 during the optimization, to get the *native* form. In this way, a RHF/6-31G calculation of the vibrational frequencies for the *contrary* conformation revealed that such conformation is a saddle point of first order. Finally, the optimization of the geometry of the *native* conformation anion was carried out at the RHF/6-31G* level without restrictions.

Likewise, the residual charges of the atoms were obtained by Mulliken's population analysis, as well as the contributions of atomic orbitals of each atom to the border molecular orbitals from LUMO to HOMO-7 in the neutral conformations and from LUMO to HOMO-8 in the anion.

Results and discussion

In figure 2, a view of the XRD molecular structure is depicted; in the tables 1 and 2, the positional parameters and bond lengths, angles and torsions between non-H atoms are given.

The geometry of the uracil ring is very similar to the one found in several 6-amino-1,3-dimethyluracil derivatives.[8-13] The C2=O2 group distance (1.212 Å) is a little shorter than the C4=O4 one (1.240 Å), and the C6-N6 bond distance (1.320 Å) is shorter than the expected value for such a single bond, due to the delocalization of the N6 electronic pair in the π system of the uracil ring, which lends imine character rather than a true primary amino group. Both uracil and phenyl rings are virtually planar, with average torsion angles of 3.1 and 0.8°, respectively. They are angled to each other by 38.2°. In the uracil ring, the largest deviations from the mean-endocyclic-plane of exocyclic atoms are C51 (0.132 Å) and O4 (0.120 Å). The chain between the two rings (C51-N51-N52-C52) is also nearly plane, forming angles of 8.9 and 33.0° with the uracil and phenyl rings, respectively. The O52 is displaced out of this chain (0.106 Å). The planarity of the chain indicates the N52 lone pair is delocalized with the C51=N51 and C52=O52 double bonds. Making the N51-N52 (1.390 Å) and N52-C52 (1.335 Å) bond distances shorter than the expected values for the corresponding single bonds. Likewise, the azomethine double bond substituents are in the *E* conformation. The N51 atom is in the *cis* position with respect to the N6 atom because of the formation of an intramolecular hydrogen bond N6-H···N51 (N6···N51, 2.701 Å; N6-H···N51, 132°), which explains the appearance of two sig-

Table 1 *Atomic coordinates (× 10⁴) and equivalent isotropic displacement parameters (× 10³ Å²) for non-hydrogen atoms, with esd's in parentheses*

	x/a	*y/b*	*z/c*	U_{eq} [a]
N1	-1252(1)	11402(4)	1583.5(8)	40.4(5)
C2	-501(2)	12894(5)	1373(1)	42.9(6)
N3	613(2)	12370(4)	1528.4(9)	43.8(6)
C4	1014(2)	10435(5)	1859(1)	40.5(6)
C5	211(2)	9021(5)	2089(1)	37.8(6)
C6	-926(2)	9491(5)	1930(1)	36.4(6)
C1	-2439(2)	11940(6)	1408(1)	57.0(8)
O2	-822(2)	14554(4)	1063.9(9)	60.4(6)
C3	1423(2)	13925(6)	1305(1)	62.3(8)
O4	2032(1)	10034(4)	1933.3(9)	57.4(6)
N6	-1700(1)	8151(4)	2107.0(9)	46.8(6)
C51	636(2)	7176(5)	2486(1)	41.0(6)
N51	15(2)	5721(4)	2713.7(9)	43.8(6)
N52	591(2)	4178(4)	3121.6(9)	44.0(6)
C52	24(2)	2673(5)	3411(1)	42.2(6)
O52	-989(1)	2377(4)	3283(1)	65.0(6)
C1B	679(2)	1352(5)	3914(1)	39.7(6)
C2B	266(2)	-768(5)	4073(1)	56.7(8)
C3B	788(3)	-1931(7)	4573(2)	73(1)
C4B	1707(3)	-992(7)	4916.0(1)	70(1)
C5B	2125(2)	1060(7)	4759(1)	61.6(9)
C6B	1621(2)	2254(5)	4260(1)	47.1(7)
C22 [b]	-64(5)	8948(8)	167(2)	109(2)
O33 [b,c]	-776(6)	8921(10)	476(3)	106(2)

[a] U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor
*[b] From the disordered ethanol*
[c] Refined with occupation 1/2

nals for the hydrogens of 6-amino group in the ^{1}H-NMR spectrum.

Despite the fact that the theoretical calculations only account for the intramolecular interactions while the experimental XRD data include both intra and intermolecular ones, the comparison between the experimental X-ray diffraction geometry of the neutral *native* conformation and that obtained from RHF/6-31G* calculation (see table 1) is highly satisfactory. The average values of the absolute deviations between the calculated and experimental geometrical parameters are 0.01(1) Å (bond lengths), 0.7(7)° (bond angles) and 3(3)° (bond torsions). In this way, two examples may be quoted to emphasize the quality of the optimized *native* structure: (a) the geometrical data of the intramolecular N6-H···N51 bond (N6···N51, 2.713 Å; N6-H···N51, 128°) and (b) the dihedral angle between the mean square planes passing through the endocyclic atoms of the uracil and the benzene rings (34.9°). Despite the fact that both geometrical fea-

Figure 2 *Molecular structure of 6-amino-1,3-dimethyl-5-formyluracil-benzoylhydrazone, showing the atom labeling scheme (ellipsoids at 50% probability). The disordered ethanol molecule is omitted for clarity*
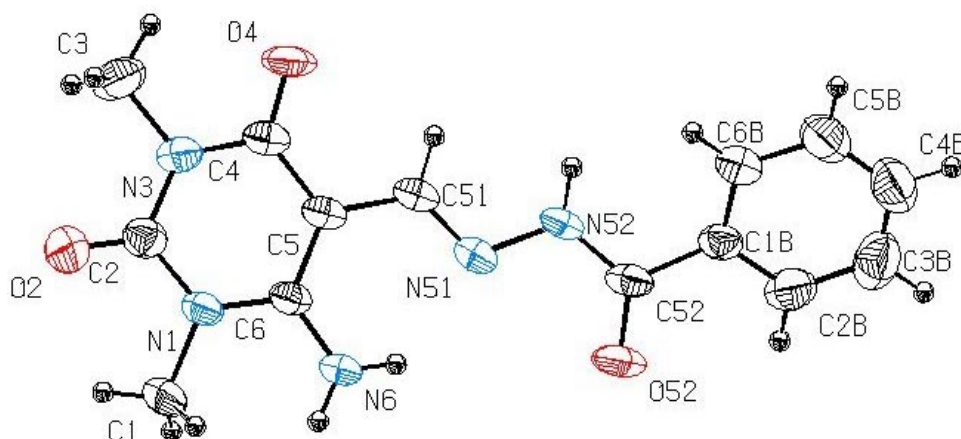
Table 2 *Interatomic distances (Å), angles (°) and torsions (°) for non-hydrogen atoms from (1) XRD data and (2) native conformation with RHF/6-31G* calculation*

	(1)	(2)		(1)	(2)
N1-C1	1.465(3)	1.461	C5B-C6B-C1B	120.2(3)	120.3
N1-C2	1.384(3)	1.393	C4B-C5B-C6B	120.7(3)	120.0
O2-C2	1.212(3)	1.198	C6B-C1B-C2B	118.8(2)	119.4
N3-C2	1.376(3)	1.364	C3B-C2B-C1B	119.9(3)	120.3
N3-C3	1.471(3)	1.465	C5B-C4B-C3B	120.0(3)	119.9
N3-C4	1.386(3)	1.395	C4B-C3B-C2B	120.5(3)	120.1
O4-C4	1.240(3)	1.205	C6-N1-C2-N3	0.0(3)	0.0
C5-C4	1.425(4)	1.439	C6-N1-C2-O2	179.4(3)	180.0
C5-C6	1.397(3)	1.381	C1-N1-C2-N3	178.9(3)	180.0
N6-C6	1.320(3)	1.330	C1-N1-C2-O2	0.3(3)	0.0
C6-N1	1.373(3)	1.374	C2-N1-C6-C5	0.8(3)	0.0
C5-C51	1.434(4)	1.453	C2-N1-C6-N6	179.5(3)	180.0
N51-C51	1.283(3)	1.260	C1-N1-C6-C5	180.0(3)	179.7
N51-N52	1.390(3)	1.364	C1-N1-C6-N6	0.4(3)	0.0
N52-C52	1.335(3)	1.364	N1-C2-N3-C4	2.2(3)	0.0
O52-C52	1.230(3)	1.197	N1-C2-N3-C3	179.5(2)	180.0
C52-C1B	1.493(4)	1.501	O2-C2-N3-C4	177.0(3)	180.0
C1B-C2B	1.384(4)	1.391	O2-C2-N3-C3	0.3(2)	0.0
C2B-C3B	1.383(5)	1.382	C2-N3-C4-C5	5.3(3)	0.0
C4B-C3B	1.369(5)	1.388	C2-N3-C4-O4	174.4(3)	180.0
C5B-C4B	1.350(5)	1.385	C3-N3-C4-C5	177.5(3)	180.0
C6B-C5B	1.383(4)	1.385	C3-N3-C4-O4	2.8(3)	0.0
C6B-C1B	1.384(4)	1.389	N3-C4-C5-C6	6.1(3)	0.0
N1-C6-C5	119.4(2)	120.2	N3-C4-C5-C51	173.1(3)	179.7
C6-N1-C2	122.9(2)	122.5	O4-C4-C5-C6	173.6(3)	180.0
C6-N1-C1	120.7(2)	120.5	O4-C4-C5-C51	7.2(2)	0.0
C2-N1-C1	116.4(2)	117.0	C4-C5-C6-N1	4.1(3)	0.0
N6-C6-N1	118.9(2)	117.2	C4-C5-C6-N6	176.3(3)	180.0
O2-C2-N1	121.0(2)	120.5	C51-C5-C6-N1	175.1(3)	179.7
N3-C2-N1	116.6(2)	116.6	C51-C5-C6-N6	4.5(3)	0.0
O2-C2-N3	122.4(2)	123.0	C4-C5-C51-N51	177.9(3)	179.2
O4-C4-N3	118.9(2)	119.0	C6-C5-C51-N51	3.0(3)	1.1
O4-C4-C5	124.2(2)	124.4	C5-C51-N51-N52	175.5(3)	180.0
N3-C4-C5	116.9(2)	116.6	C51-N51-N52-C52	176.3(3)	171.6
N6-C6-C5	121.8(2)	122.5	N51-N52-C52-O52	9.3(3)	2.2
C2-N3-C4	124.3(2)	124.6	N51-N52-C52-C1B	169.9(2)	177.7
C2-N3-C3	117.3(2)	118.8	N52-C52-C1B-C2B	155.6(3)	152.4
C4-N3-C3	118.3(2)	116.6	N52-C52-C1B-C6B	30.5(3)	28.9
C6-C5-C4	119.7(2)	119.5	O52-C52-C1B-C2B	25.2(3)	27.5
C6-C5-C51	123.5(2)	123.8	O52-C52-C1B-C6B	148.7(3)	151.2
C4-C5-C51	116.7(2)	116.7	C52-C1B-C2B-C3B	173.6(3)	180.0
C51-N51-N52	114.6(2)	118.3	C6B-C1B-C2B-C3B	0.5(3)	1.3
C52-N52-N51	119.7(2)	118.8	C52-C1B-C6B-C5B	173.1(3)	179.5
N51-C51-C5	123.8(2)	123.1	C2B-C1B-C6B-C5B	0.8(2)	0.8
O52-C52-N52	122.8(2)	123.2	C1B-C2B-C3B-C4B	0.5(3)	0.8
O52-C52-C1B	120.4(2)	122.0	C2B-C3B-C4B-C5B	1.5(3)	0.0
N52-C52-C1B	116.7(2)	114.8	C3B-C4B-C5B-C6B	1.3(3)	0.7
C6B-C1B-C52	122.7(3)	123.1	C4B-C5B-C6B-C1B	0.0(3)	0.3
C2B-C1B-C52	118.3(2)	117.4			

tures involve long-distance interactions, they are in good agreement with the experimental XRD data. Thus, it may be concluded that the theoretical method employed successfully simulates the experimental data.

In order to assess the chelating capabilities of the ligand in its different forms, we have analyzed both the residual charges on the heteroatoms and the atomic orbital coefficients of the LCAOs which define the molecular orbitals. The residual charges on the heteroatoms are negative in all cases (see table 3). This fact, together with the steric hindrances of the substituents, suggest that the *contrary* conformation of H_2BEZDO should coordinate to the metal ion through the atoms O4, N51 and O52, while the *native* conformation, both neutral or anion, could do so through the atoms N6, N51 and O52.

The main contributions of atomic orbitals in the selected molecular orbitals are given in the table 4. As known, the most influential molecular orbitals in the metal-ligand bond are the highest occupied with σ-symmetry. Because of the non-planarity of our molecular species, the σ- or π-character of the M.O. has been assigned depending on the contribution of each type of atomic orbital, (s, p_x, p_y, p_z), to the molecular orbital. Thus, when the highest contribution corresponds to the s, p_x or p_y atomic orbitals, then the molecular orbital will be classified as σ, and if the p_z A.O. is dominant, the M.O will be π.

Table 3 *Residual charges (e.u.) in the heteroatoms (6-31G* basis set)*

Heteroatom	Neutral		N6-monoanion
	native	*contrary*	*native*
N1	-0.856	-0.853	-0.831
O2	-0.625	-0.626	-0.688
N3	-0.848	-0.845	-0.836
O4	-0.640	-0.562	-0.721
N51	-0.371	-0.189	-0.285
N52	-0.648	-0.667	-0.660
O52	-0.597	-0.560	-0.617
N6	-0.984	-0.931	-0.747

These results show that the atom N6 does not contribute to the orbitals σ-HOMO-6 and σ-HOMO-5 neither in the neutral *native* conformation nor in the *contrary* one. Additionally, some contributions of the atoms O52, O4 and N51 are found in the same orbitals for the *contrary* conformation. This explains the O4,N51,O52-tridente behavior observed in some metal complexes with neutral H_2BEZDO.[5] Also, these data clearly indicate that this ligand cannot act as a

Table 4 *Contributions of atomic orbitals of heteroatoms to selected MOs (6-31G*) for the forms studied*

	MO [a]	%p_z	E(eV)	N1	N3	N6	N51	N52	O2	O4	O52
						Contributions to LCAO [b] (%)					
Native	HOMO-6	2.9	-11.711	0.012	0.066	0.009	0.006	0.078	0.053	**0.280**	**0.273**
	HOMO-5	1.0	-11.417	0.004	0.058	0.004	**0.126**	0.075	0.021	**0.213**	**0.259**
	HOMO-4	92.1	-11.045	0.039	**0.538**	0.021	0.000	0.003	**0.110**	**0.166**	0.002
	HOMO-3	93.6	-10.672	0.020	0.000	0.070	0.039	**0.355**	0.004	0.069	**0.161**
	HOMO	96.3	-8.095	0.056	0.010	0.076	**0.177**	**0.147**	0.020	0.059	0.025
	LUMO	79.2	2.736	0.005	0.001	0.018	0.037	0.015	0.005	0.000	0.070
Contrary	HOMO-6	2.3	-11.385	0.001	0.012	0.001	0.019	**0.156**	0.008	0.057	**0.487**
	HOMO-5	16.8	-11.073	0.050	**0.134**	0.004	**0.183**	0.054	0.056	**0.280**	0.056
	HOMO-4	71.1	-10.395	0.001	**0.379**	0.025	0.052	0.061	**0.117**	**0.144**	0.047
	HOMO-3	91.7	-10.679	0.091	**0.109**	0.018	0.019	**0.228**	0.001	**0.167**	**0.108**
	HOMO	93.9	-8.190	0.082	0.003	0.065	**0.148**	**0.167**	0.021	0.038	0.031
	LUMO	71.6	2.775	0.014	0.005	0.037	0.070	0.005	0.008	0.001	0.059
Anion	HOMO-8	2.5	-8.283	0.009	0.014	0.045	0.019	**0.111**	0.002	0.077	**0.465**
	HOMO-6	2.0	-7.398	0.009	**0.103**	0.030	**0.111**	0.023	0.064	**0.415**	0.018
	HOMO-3	25.4	-6.955	0.067	0.003	**0.216**	**0.137**	0.023	0.015	0.005	0.044
	HOMO-2	38.3	-6.914	0.092	0.010	**0.183**	**0.124**	0.034	0.015	0.018	0.015
	HOMO-1	93.6	-6.206	**0.190**	0.027	**0.248**	0.071	**0.165**	0.024	0.000	0.049
	HOMO	96.3	-3.458	0.001	0.028	**0.130**	**0.189**	0.078	0.006	0.090	0.023
	LUMO	70.6	5.495	0.000	0.000	0.001	0.003	0.026	0.000	0.001	0.044

[a] The orbital labeled HOMO-1 is the MO which lies inmediately below the HOMO; that labeled HOMO-2 lies inmediately below and so on

[b] The contribution of one atom is calculated as the sum of the squared coefficients of that atom AOs in the LCAO that defines the MO; those higher than 0.1 are bold faced

N6,N51,O52-tridentate ligand in the neutral *native* form, although the three donor atoms exhibit negative charge.

However, in the anion *native* conformation, there are contributions of the atomic orbitals of the atoms N6 and N51 to the molecular orbital σ-HOMO-3 and contributions of the atoms N51 and O52 to the orbitals σ-HOMO-6 and σ-HOMO-8. Thus, it may be concluded that the deprotonation of the 6-amino group is essential for the involvement of the N6 in the coordination to the metal.[4] In this way, the structures of the related [Zn(HAMNU)$_2$(H$_2$O)$_2$] [14] and [Cu(DANU)$_2$(H$_2$O)$_2$] [15] complexes (where HAMNU$^-$ and DANU$^-$ are the 6-amino-3-methyl-5-nitrosouracilato and 6-amino-1,3-dimethyl-5-nitrosouracilato monoanions) offer two good explanatory examples of this fact. Thus, in the first compound, the deprotonation of the uracil ligand takes place on the N1-H group and the coordination to the metal occurs through the N5 and O4 atoms. In the second example, the uracil ligand has both endocyclic nitrogen atoms blocked by a methyl group; for this reason, the deprotonation must be through the 6-amino group, the void remaining position on N6 being occupied by the metal which is chelated by the N6 and N5 atoms.

With regard to the π-bonding capabilities, the studied species should not behave as π-acceptors. However, the neutral molecule, in both conformations, could be a π-donor through the atoms N51 (HOMO) and O52 and O4 (HOMO-3 and HOMO-4). Also, the anion itself could be π-donor through the atoms N6 (HOMO, HOMO-1 and HOMO-2) and N51 (HOMO).

Supplementary material available The corresponding CIF file (CCDC 119504) and 3D MOL2 files for the structures studied and the printout (6 pages) with geometrical parameters, charges, coordinates and atomic orbital contributions to molecular orbitals (LUMO to HOMO-8) for the 6-31G* optimized structures are available.

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