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Journal of Molecular Structure: THEOCHEM 811 (2007) 215–221

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Theoretical study of the acidity and basicity of uric acid and its interaction with water

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Received 18 January 2007; accepted 16 February 2007
Available online 22 February 2007

Abstract

The proton affinity (PA) of the O atoms and the deprotonation enthalpies (DPE) of the NH bonds of isolated uric acid are calculated using the density functional theory (B3LYP) combined with the 6-31++G(d,p) basis set. The optimized geometries, energies and harmonic vibrational frequencies of monohydrated uric acid are calculated at the same level of theory. The five stable complexes between uric acid and water are the ones in which the oxygen atom of water accepts the acidic NH proton while donating a proton to the carbonyl oxygens of uric acid. The binding energies of these complexes ranging from 24 to 37 kJ mol^{-1} are analysed in terms of PAs for O atoms and the acidity of the NH groups of isolated uric acid. A natural bond orbital analysis is performed to understand the nature of hydrogen bonding interaction in monohydrated uric acid and also to reveal the inter-relations between electronic structure and other properties.

Keywords: Uric acid; B3LYP/6-31++G(d,p) calculations; Proton affinity of O atoms; Deprotonation enthalpy of NH bonds; Interaction with water; Natural bond orbital analysis

1. Introduction

It has been discussed in several works that uric acid (UA) is a naturally occurring antioxidant [1–3]. Among purines and pyrimidines, UA shows the greatest susceptibility to ozone induced degradation [4]. UA is also known to protect unsaturated fatty acids from air oxidation [5,6] and DNA from damage in systems which generate superoxide and peroxy radicals [7].

The keto–enol tautomerism of UA (Fig. 1) has been the subject of several investigations. In the solid state, UA is characterized by a planar triketo structure [8]. Theoretical calculations have shown that the triketo form is the most stable tautomer in the gas phase [9–11]. UV–visible spectroscopy and semi-empirical calculations have shown that in acidic conditions, UA would exist in the keto form [12], whereas at basic conditions, it would exist as a mono-anion, deprotonated at the N3H site [12,13]. Similar conclusions have been obtained by ^{13}C NMR techniques, showing that the mono-anion obtained by deprotonation of the N3H site is the dominant form in basic aqueous solution [14].

It has been recently shown that the barrier height for keto–enol tautmerism is large for a simple intramolecular proton transfer. The inclusion of a water molecule in the proton transfer reaction path reduces the barrier height significantly. More specifically, the interaction with water at the N3H3 and O2 sites of UA has been shown to decrease the height of the barrier for the keto–enol tautomerism [11]. To the best of our knowledge, the interaction between UA and water at the other sites of UA has not been investigated and the interaction energies have not been reported so far.

In the present work, the interaction between UA and a water molecule is investigated for the all the possible binding sites. It is important to note that the 3 oxygen atoms

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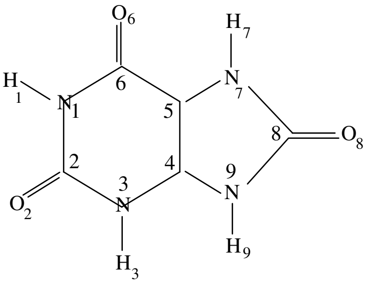
doi:10.1016/j.theochem.2007.02.021



Uric Acid

Fig. 1. Structure and atom labelling in uric acid.

and 4 NH bonds are available for hydrogen bonding formation. It can thus be anticipated that similarly to nucleobases such as uracil, cytosine or guanine, closed complexes between the carbonyl groups and the NH bonds will be formed, leading to five stable conformations. Studying all these complexes together at the same level of theory allows us to analyse their relative stability in terms of properties of the binding sites. As shown by experimental results [15] and MP2/B3LYP calculations [11] of the electron affinity, UA can be considered as a good electron donor.

In recent years, the intrinsic proton donor and proton acceptor abilities of nucleobases have been discussed in several works [16–29]. In our previous works on the interaction between nucleobases and water, we have established a correlation between the hydrogen bond strength and the proton affinities (PA) of the proton acceptor site and the deprotonation enthalpies (DPE) of the proton donor [18]. In the present work, the same parameters are discussed for UA and its different complexes with water. It must be noticed that owing to the low solubility of uric acid in organic solvents, no data on its complexing ability have been reported in solution. The complexes between phenols derivatives and 1,3,7,9-tetramethyluric acid have been studied by IR spectroscopy and the thermodynamic constants indicate that the complexes are stronger than those involving 1,3-dimethyluracil or caffeine [30].

This work is arranged as follows. In the first part, the PAs of the O atoms and the DPEs of the NH bonds of isolated UA are reported. The second part deals with the optimized geometries of the water complexes, their energies and some relevant vibrational frequencies. Results from NBO analysis are presented in the last part of the work.

2. Computational methods

The geometries of isolated UA and their corresponding water complexes were fully optimized without symmetry restriction by the density functional theory using B3LYP exchange correlation functional [31,32] and the 6-31++G(d,p) basis functions. The binding energies with water were corrected for the zero-point vibrational energies (ZPE) and the basis set superposition errors (BSSE). The BSSE was computed by the counterpoise method [33]. The proton affinities and deprotonation enthalpies were computed at 298 K using the same level of theory. As demonstrated in other works [34,35] the B3LYP/6-31++G(d,p) computational level provides results comparable with the MP2 and experimental results as far as protonation and deprotonation enthalpies and hydrogen bond energies are concerned.

Charge on individual atoms and population of molecular orbitals were obtained by using the natural bond orbital (NBO) population scheme [36]. The GAUSSIAN 98 program was used for all the calculations reported in the present work [37].

3. Results and discussion

3.1. Proton affinities and deprotonation enthalpies of UA

Geometry optimization without any symmetry restriction shows that isolated uric acid is planar; the values of all the dihedral angles involving the atoms in the six-ring and in the five-ring, and the HNCO dihedral angles show that the deviation from planarity is less than 0.3°. The binding energies of UA with a guest molecule should be closely related to the basicity/acidity of the groups involved in the interaction. Therefore, we have in a first step calculated these parameters for the isolated UA.

The proton affinities (PA) of the oxygen atoms and the deprotonation enthalpies (DPE) of the NH bonds of UA are indicated in Table 1. The PA of the oxygen atoms and the DPE of the NH bonds of uracil (UR) calculated at the same computational level [17] are also given in the table for useful comparison with UA data. These results show that the PAs of the O atoms of UA are slightly smaller (by 2–8 kJ mol^{-1}) than the PAs for the corresponding O atoms in UR. In both molecules, the O6 atom is characterized by the largest basicity.

The calculated DPE values given in Table 1 show that the N3H3 and N9H9 bonds are much more acidic than the other two NH bonds. Our calculated DPE for the

Table 1
The B3LYP/6-31++G(d,p) proton affinities (PA) of the oxygen atoms and deprotonation enthalpies (DPE) of the NH bonds (kJ mol^{-1}) in uric acid at 298 K[a]

Uric acid			
PA		DPE	
O6 (C5 side)	851.4 (858.9)	N1H1	1411.4 (1446.7)
O6 (N1 side)	852.1 (847.0)	N3H3	1329.1 (1390.5)
O2 (N1 side)	814.9 (819.2)	N9H9	1333.5
O2 (N3 side)	806.7 (813.4)	N7H7	1404.7
O8 (N9 side)	832.2		
O8 (N9 side)	827.1		

The PA and DPE values for uracil are given in parentheses for comparison.

[a] Ref. [17], to have a valuable comparison, the atom labelling in uracil is the same as in uric acid; the N3H3 bond is vicinal to the C4H4 bond and the C5=O5 bond is vicinal to the C5H5 bond.

NH bonds are in good agreement with the relative stabilities of the anions given in [11,12]. The order of stability of the mono-anions calculated by the MNDO or AMI methods [12] and by the B3LYP functional using the 6-311++G(d,p) basis set [11] is indeed $UAN3^- > UAN9^- > UAN7^- > UAN1^-$. In contrast with the PAs, the DPEs for the NH bonds of UA and UR appear to be markedly different. For example, the DPE of the N1H1 bond of UA is ca. 36 kJ mol^{-1} lower than that of uracil and the difference is still larger for the DPE of the N3H3 bond which is ca 62 kJ mol^{-1} lower in UA [17]. It is also interesting to note that in 5-F uracil, the DPE of the N1H1 bond is about the same as in UA (1414.7 kJ mol^{-1}) but that the DPE of the N3H3 bond (1359.2 kJ mol^{-1}) is ca 30 kJ mol^{-1} larger that in UA [26]. A possible explanation of the large acidity of both the N3H3 and N9H9 bonds of UA is an electrostatic proximity effect arising from the repulsion between the two adjacent NH bonds. This interpretation agrees with the fact that the most stable protonated tautomers of triazoles and tetrazoles possess non-adjacent NH bonds in their structures [38].

3.2. Optimized geometries and hydrogen bond energies in monohydrated UA

The optimized structures of the A, B, C, D and E complexes between UA and water are illustrated in Fig. 2. As for the nucleobases–water interaction, the five stable closed complexes are the ones in which the oxygen atom of water accepts the acidic NH proton while donating a proton to the carbonyl oxygen of UA. The pseudo six-rings formed in this way are planar or nearly so, the largest OH···O=C dihedral angle of $-5.5°$ being predicted for the B complex.

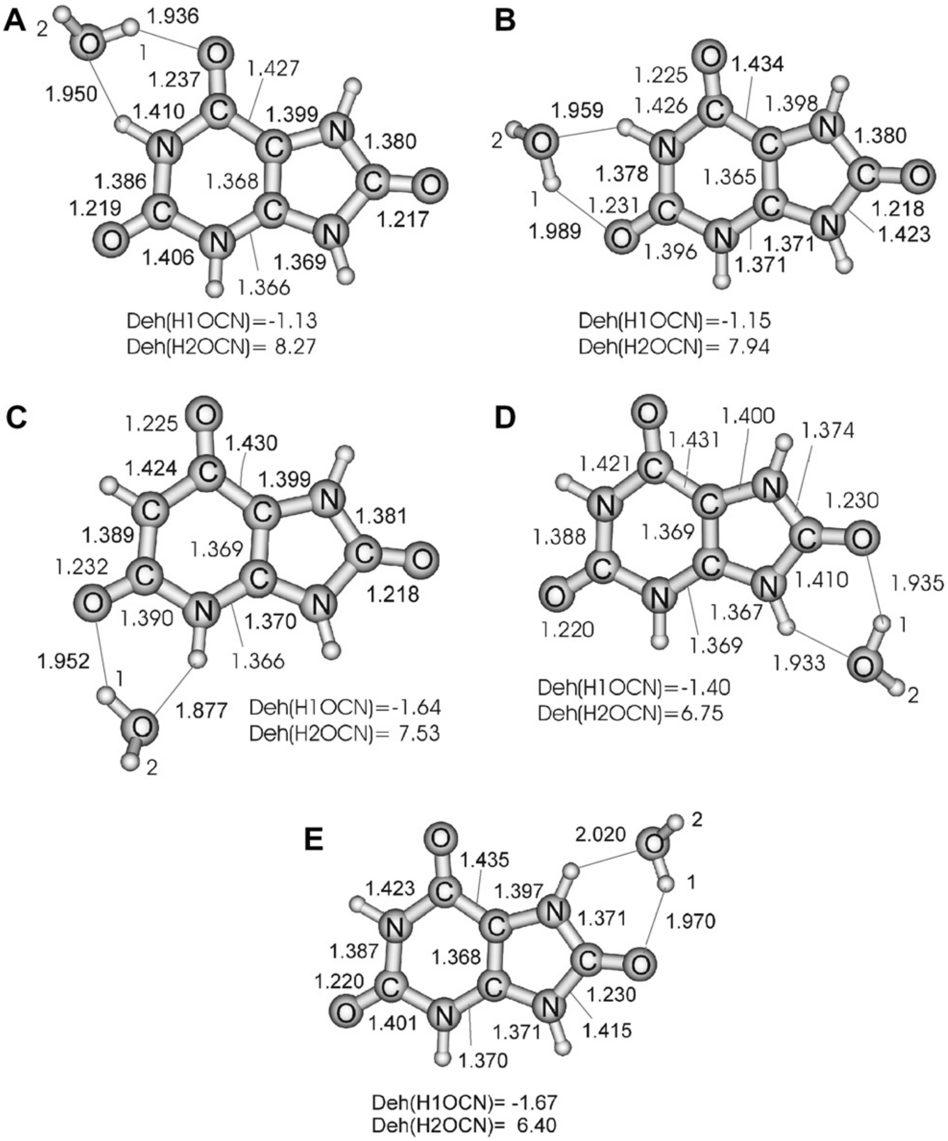


Fig. 2. B3LYP/6-31++G(d,p) optimized geometry of the A, B, C, D and E complexes between uric acid and a water molecule. Deh indicates the dihedral angles.

Table 2 reports some relevant geometrical parameters, like distances and angles, for isolated UR and the five monohydrated complexes. Our results show that the NH bond involved in the interaction is elongated between values ranging from 0.0107 (E) to 0.0153 Å (C); this largest elongation corresponds to the smallest NH···O intermolecular distance of 1.878 Å. Complex formation also results in an elongation of the OH bond of water by 0.0100 (B)–0.0147 Å (D); again in this case, the largest elongation parallels the shortest OH···O intermolecular distance of 1.934 Å. Interaction with water also results in a small elongation of the C═O bond ranging from 0.0120 to 0.0135 Å. There are also small variations of the distances in the six- or five-membered -ring of UA. More specifically, the CN bonds taking part in the formation of the closed structure are shortened. In complex A, as for example, the N1C6 distance equal to 1.421 Å in isolated UA is shortened by 0.011 Å in complex A.

Table 3
The B3LYP/6-31++G(d,p) calculated hydrogen bonding energies (kJ mol^{-1}) including ZPE and BSSE corrections for the five structures of the UA–water complexes

Complex	$-E_{HB}$	$-E_{HB}$ (ZPE)	$-E_{HB}$ (ZPE + BSSE)
A (N1H1, O6)	39.5	30.7	27.1
B (N1H1, O2)	36.9	28.2	24.5
C (N3H3, O2)	50.1	40.2	36.3
D (N9H9, O8)	50.6	40.6	37.0
E (N7H7, O8)	40.1	30.8	27.4

The binding energies of UA with a water molecule are reported in Table 3. The binding energies vary in between 24.5 and 37 kJ mol^{-1}. The C and D complexes are predicted to be the most stable ones. Interestingly, in these complexes, the NH bonds involved in the interaction are characterized by the largest acidity. A very rough correlation is obtained between the binding energies and the DPE values but no correlation between these energies and the PA values. This suggests that the acidity of the proton donor is a more important factor in determining the hydrogen bond energies than the basicity of the proton acceptor. This has been demonstrated for the classical nucleobases (uracil, thymine, cytosine and guanine) complexed with a water molecule [20] or with hydrogen peroxide [39]. In complexes between methane derivatives and their homoconjugated anions where $(CH\cdots C)^-$ hydrogen bonds are formed, the predominance of the proton donor in determining the binding energies has been recently demonstrated [40]. Several fittings were tried and the best fitting is obtained by the following equation where DPE and PA are weighted with respective factors of 1.5 and −0.5:

$$-E_{HB} = 4970\ \mathrm{e}^{-0.0032(1.5\mathrm{DPE}-0.5\mathrm{PA})} \qquad r = 0.997 \qquad (1)$$

This correlation is illustrated in Fig. 3.

Interestingly, the predominance of the proton donor in determining the hydrogen bond energies established by a statistical analysis is in good agreement with the present data [41]. It must be pointed, however, that the coefficients

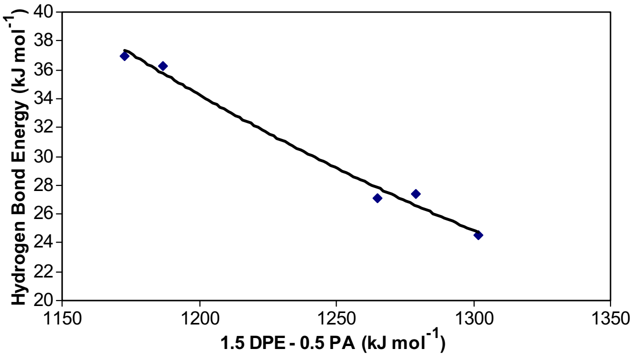


Fig. 3. E_{HB} as a function of (1.5 DPE–0.5 PA) (kJ mol^{-1}).

Table 2
Important bond lengths (R in Å) and bond angles (degrees) in the A, B, C, D and E complexes between UA and water

R	Isolated UA or H_2O	A	B	C	D	E
N1H1	1.0139	1.0267	1.0265	1.0139	1.0138	1.0139
N3H3	1.0105	1.0107	1.0105	1.0258	1.0107	1.0104
N7H7	1.0087	1.0085	1.0087	1.0085	1.0088	1.0194
N9H9	1.0090	1.0091	1.0090	1.0092	1.0220	1.0090
OH[a]	0.9652	0.9775	0.9752	0.9787	0.9799	0.9770
OH_2		0.9641	0.9642	0.9643	0.9640	0.9639
H3···H9	2.832	2.839	2.843	2.832	2.863	2.832

R/angle[b]	A	B	C	D	E
Intermolecular parameters					
C═O···H	1.941	1.988	1.954	1.934	1.968
NH···O	1.949	1.959	1.878	1.932	2.018
<OH···O	142.6	139.5	141.3	144.2	142.9
$<NH\cdots O_w$	143.6	144.2	144.9	135.9	132.1
H3···H9[c]	2.839	2.843	2.843	2.863	2.832
$<O_wH_1OC$	−4.6	−5.5	−1.3	−1.3	−3.9

[a] Bonded OH group of water.

[b] o_w indicate oxygen atom of water.

[c] Distance between the non-bonded H3 and H9 atoms.

of DPE and PA are different for positively and negatively charged hydrogen bond systems [40]. For the complexes involving classical nucleobases and a water molecule, the coefficients of DPE and PA are equal to 1.5 and 1, respectively [20]. Thus, the coefficients of PA and DPE in Eq. (1) are not universal and depend on the systems. As discussed in a previous work [27], these coefficients may be influenced by geometrical factors (intermolecular angles or deviation from planarity). More specifically, the correlation established for classical nucleobases predicts larger binding energies for the C and D complexes. This may be partially accounted for by the fact that the five-ring structure imposes another geometry for the hydrogen bond; in isolated UA, the H9···O8 distance of 2.670 Å is markedly longer than the H1···O6 distance of 2.5 Å.

Further, the repulsion between the two NH bonds may be somewhat smaller in the monohydrates. Indeed, our calculations predict a small increase by 2.5° of the C4N9H9 angle and a small increase of the H3···H9 distance of 0.031 Å on going from the free UA molecule (2.832 Å) to the D complex (2.863 Å).

3.3. *Vibrational frequencies of the NH and OH groups*

Our calculated vibrational frequencies and infrared intensities of modes involving the NH groups (stretching and out-of-plane deformation) and the stretching vibration of the bonded OH group of water are reported in Table 4. These modes are almost decoupled from the other vibrations in the complexes. This is not the case for the three νC=O vibrations which are predicted between 1772 and 1837 cm^{-1} in isolated UA. These νC=O modes are coupled with the in-plane deformation vibrations of the vicinal NH groups. This coupling increases in the complexes, the νC=O vibration being shifted to lower frequencies and the in plane deformation of the NH groups to higher frequencies.

The $\Delta\nu$(NH) values range from 176 cm^{-1} (E) to 273 cm^{-1} (C). We note also a great increase of the infrared intensity that increases by a factor of ca. 6 in the C complex. The out-of-plane deformation vibration (γNH) appears also to be very sensitive to the interaction with water, the blue shift of this mode being more than 300 cm^{-1} in complex C. The $\Delta\nu$(OH) values of the bonded OH group of water are comprised between 133 cm^{-1} (B) and 217 cm^{-1} (D). Complex formation also results in a large infrared intensity increase of this mode. The largest $\Delta\nu$(NH) shift is observed for UA (C) and the largest $\Delta\nu$(OH) shift is predicted for UA (D).

It is interesting to compare the present data with those reported previously for the uracil [17]. The frequency shifts of the ν(NH) and ν(OH) vibrations and the elongations of the corresponding bonds in the UA–water and in the UR–water complexes are reported in Table 5. The $\Delta\nu$(NH) values are found to be greater for the UA–water complexes, whereas the $\Delta\nu$(OH) values are larger for the UR–water complexes. This agrees well with the fact that the NH bonds in UA are more acidic than UR and on the other

Table 4
Vibrational frequencies (cm^{-1}) of the stretching ν(NH) and νOH modes and out-of-plane bending (γNH) modes and infrared intensities (km mol^{-1}) [in parentheses] in isolated UA and Water and in their A, B, C, D, and E complexes

Isolated UA or H_2O	UA + H_2O complexes					Assignment
	A	B	C	D	E	
3684 (118)	3686 (116)	3683 (125)	3687 (117)	3683 (115)	3508 (332)	ν N7H
3672 (114)	3673 (112)	3674 (73)	3672 (122)	3452 (442)	3673 (105)	ν N9H
3647 (106)	3646 (100)	3648 (111)	3374 (616)	3646 (122)	3648 (100)	ν N3H
3611 (92)	3388 (474)	3394 (497)	3610 (173)	3612 (86)	3611 (90)	ν N1H
612 (8)	825 (135)	826 (134)	718 (13)[a]	651 (60)	613 (18)	γ N1H1
486 (236)	486 (248)	487 (231)	474 (156)	480 (128)	679[b] (129)	γ N7H7
423 (4)	431 (1)	426 (6)	762 (122)	441 (4)	444 (119)	γ N3H
392 (16)	397 (16)	387 (19)	411 (8)	722 (213)	404 (10)	γ N9H
3929 (54)	3897 (110)	3900 (110)	3894 (107)	3897 (107)	3901 (99)	ν^{as}OH
3806 (5)	3628 (398)	3673 (261)	3614 (250)	3589 (446)	3638 (325)	ν^{s} OH

[a] Coupled with the ν(N1C2) vibration.

[b] Two predominant modes at 679 and 744 cm^{-1}.

Table 5
Comparison of the frequency shifts (cm^{-1}) and the elongation of the NH and OH bonds (Å) between UA and uracil complexes (values in parentheses)[a] with a water molecule

Assignment	A	B	C	D	E
$\Delta\nu$ (NH)	223 (208)	217 (193)	273 (224)	220	176
Δr (NH)	0.0128 (0.0121)	0.0126 (0.0115)	0.0153 (0.0128)	0.0130	0.0107
$\Delta\nu$ (OH)	178 (192)	133 (150)	192 (193)	217	168
Δr (OH)	0.0123 (0.0130)	0.0100 (0.0108)	0.0135 (0.0134)	0.0147	0.0118

[a] From Ref. [18], the A, B and C complexes are formed at the same site as in UA, the two C atoms forming the double bond being in 4 and 5 positions.

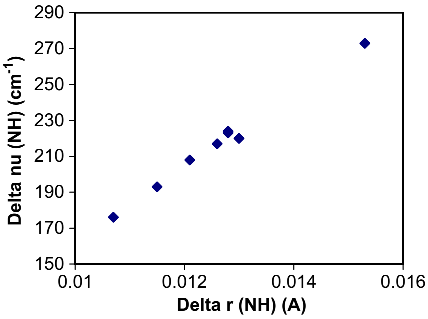


Fig. 4. $\Delta\nu$(NH) (cm^{-1}) as a function of Δr (NH) (Å) for UA and uracil complexed with water.

hand, O atoms in UR are more basic than in UA. Figs. 4 and 5 where the frequency shifts have been plotted as a function of the elongation of the corresponding bonds show that the points relative to the UA and UR complexes are situated on the same straight line. We have obtained the following correlations:

$$\Delta\nu(\mathrm{NH})\ (\mathrm{cm}^{-1}) = -47 + 20.9 \times 10^3 \Delta r(\mathrm{NH})\ (\text{Å}), \quad r = 0.992 \qquad (2)$$

$$\Delta\nu(\mathrm{OH})\ (\mathrm{cm}^{-1}) = -38 + 17.4 \times 10^3 \Delta r(\mathrm{OH})\ (\text{Å}), \quad r = 0.995 \qquad (3)$$

3.4. NBO charges on the N, O and H atoms and $\sigma^*(NH)$ and $\sigma^*(OH)$ population

Our NBO results show that the charge transfer resulting from the interaction with water is very weak. A charge transfer of 0.006 e takes place from the water molecule to UA in complex C, from UA to water (0.004 e) in complex E and it is negligible in the other cases. Thus, the H-bonding interaction is predominantly through electrostatic forces. Nevertheless, the molecular orbital population analysis reveals some interesting features that we feel worthy to be mentioned here.

The charges on the atoms involved in hydrogen bond formation and the population of the antibonding σ^*(NH) and σ^*(OH) orbitals are indicated in Table 6. Inspection of the data reveals that complex formation results in an increase of the positive charge on the H atom of the NH bond involved in the interaction. The charge on the N atom remains almost constant, the excess charge being delocalized in the vicinal CN bond. In contrast, in all the complexes, there is an increase of the polarity of the OH bond. The largest polarity increase is observed for the most stable C and D complexes where the H atom looses 0.032 and 0.031 e and the O atoms gains 0.043 and 0.049 e, respectively. The σ^*(NH) population does not change much while going from the isolated UA to the water complex except for the most stable complex C. For this complex the σ^*(NH) population increases from 0.0118 in isolated UA to 0.0417 e in the complex. It is also worth mentioning here that the increase of the σ^*(OH) population is the largest for the C and D complexes, being respectively equal to 0.0239 and 0.0260 e for these two complexes and between 0.0194 and 0.0234 e for the other ones.

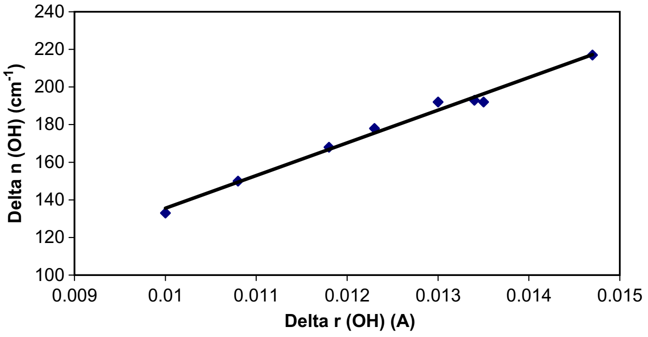


Fig. 5. $\Delta\nu$(OH) (cm^{-1}) as a function of Δr(OH) (Å) for UA and uracil complexed with water.

Table 6
NBO charges on the N, H and O atoms and occupation of the σ^* antibonding orbitals (e) in the isolated UA, H_2O and the five complexes (A, B, C, D and E) between them

Atom/ orbital	NBO charges					
	UA/ H_2O	A	B	C	D	E
N1	−0.678	−0.679	−0.679	−0.670	−0.678	−0.678
H1	0.465	0.488	0.487	0.464	0.464	0.464
N3	−0.639	−0.637	−0.633	−0.641	−0.637	−0.637
H3	0.461	0.460	0.460	0.483	0.463	0.463
N9	−0.639	−0.639	−0.640	−0.636	−0.636	−0.631
H9	0.459	0.460	0.459	0.461	0.485	0.459
N7	−0.619	−0.620	−0.619	−0.621	−0.609	−0.613
H7	0.471	0.470	0.471	0.470	0.471	0.495
O_w	−0.976	−1.013	−1.009	−1.019	−1.025	−1.018
H_1	0.488	0.514	0.514	0.520	0.519	0.514
σ^* population						
N1H1	0.0118	0.0357	0.0352	0.0121	0.0118	0.0118
N3H3	0.0118	0.0121	0.0121	0.0417	0.0117	0.0117
N9H9	0.0120	0.0121	0.0119	0.0121	0.0351	0.0122
N7H7	0.0110	0.0109	0.0110	0.011	0.011	0.0280
O_wH_1	0.000	0.0234	0.0194	0.0239	0.0260	0.0222

For both the bonded NH and OH groups, the frequency shifts of the stretching vibration are linearly related to the increase in occupation of the corresponding antibonding σ^* orbital:

$$\Delta\nu(\mathrm{NH})\ (\mathrm{cm}^{-1}) = 45.7 + 7.5 \times 10^3 \Delta\sigma^*(\mathrm{NH})\ (\mathrm{e}), \quad r = 0.9958 \qquad (4)$$

$$\Delta\nu(\mathrm{OH})\ (\mathrm{cm}^{-1}) = -110 + 12.6 \times 10^3 \Delta\sigma^*(\mathrm{OH})\ (\mathrm{e}), \quad r = 0.9947 \qquad (5)$$

4. Summary and conclusions

The PAs for the oxygen atoms and DPEs for the NH bonds have been calculated for uric acid. The basicity of the O atoms of UA is not much different from uracil but the acidities of the NH bonds are found to be much larger in uric acid. The five stable complexes between uric acid and water are found in which the oxygen atom of water accepts the acidic NH proton while donating a proton to the carbonyl oxygens of UA. The binding energies of these complexes range between 24 and 37 kJ mol^{-1}. These energies are mainly determined by the acidity of the NH groups, but the role of PA is also important. A natural bond orbital analysis shows that complex formation results in an increase of the polarity of the bonded OH group of water along with an increase of the population of the σ^*(OH) and σ^*(NH) antibonding orbitals. Good correlations have been observed between the frequency shifts of the NH and OH bonds involved in UA–water and UR–water complex formation and the change in the corresponding antibonding orbitals populations. The frequency shifts of the NH and OH bonds involved in UA–water complex formation are also found to correlate well with the change in the corresponding bond lengths, Δr (NH) and Δr (OH), respectively.

Acknowledgement

A.K.C. thanks DST, India for financial support through a project (SR/S1/PC-13/2005).

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