02

Interpretation of electronic spectra of a number of 5-substituted uracils in aqueous solution based on modeling of their H-complexes with water molecules and the orbital approach

© S.N. Tseplina, E.E. Tseplin ¶

Institute of Molecule and Crystal Physics, Ufa Federal Research Centre, Russian Academy of Sciences, Ufa, Russia

¶ e-mail: tzeplin@mail.ru

Received March 19, 2025
Revised June 30, 2025
Accepted July 17, 2025

Absorption spectra of 5-hydroxymethyluracil, uracil, 5-fluorouracil and 5-bromouracil in a neutral aqueous solution were obtained. The modeling of hydrogen complexes of molecules of the compounds under consideration with water molecules was carried out, and then the absorption spectra in aqueous solution were calculated using the TDDFT B3LYP/6-311+G(d,p) method in combination with the polarizable continuum model. The linear dependence of the energies of electronic transitions obtained from the absorption spectra on the values of the energy gap between the corresponding occupied and vacant molecular orbitals of the calculated hydrogen complexes is shown.

Keywords: absorption spectra, 5-hydroxymethyluracil, uracil, hydrogen complex, OMO-UMO energy gap, solvent effect.

DOI: 10.61011/EOS.2025.08.62019.7686-25

Introduction

Uracil and its 5-methyl substituted derivative (thymine) are nitrogenous bases of nucleic acids and have been actively studied. Other 5-substituted uracils also attract special attention, as they can integrate into the nucleic acid structure, causing damage and consequently altering their properties. For example, it was found that 5-halogenated uracils (5-fluorouracil and 5-bromouracil), when present in nucleic acid structure, can cause its destruction under radiation exposure, i.e., can act as radiosensitizers in cancer treatment [1,2]. Recently, another 5-substituted uracil — 5-hydroxymethyluracil (5hmU) — has been attracting increased attention, since it was initially discovered that its presence in gene structures correlates with chronic inflammatory diseases and cancer [3], and more recently it was found that 5hmU together with 5-hydroxymethylcytosine is a surrogate marker for myeloid malignant neoplasms [4]. It was previously established that 5hmU occurs as a base in the genomes of various organisms and that its amount in RNA structure affects its transcription rate [5]. Alongside this, it was found that DNA in which thymine is replaced by 5hmU becomes more flexible and hydrophilic [6].

While extensive work has been devoted to the excited states, electronic structures, and hydration shells of DNA and RNA bases [7–19] and continues actively [20,21], studies considering electronic transitions and solvation shells of 5hmU are scarce. In a recent study on spectroscopic properties of 5hmU [22], an absorption spectrum in dimethyl sulfide solution was presented, and calculations of electronic transitions for the gas phase and including the effect of dimethyl sulfide and methanol solvents were performed based on the polarizable continuum model.

One of the approaches describing the effect of polar solvent on absorption and luminescence spectra is the supermolecule method, where several solvent molecules from the primary solvation shell, forming hydrogen bonds with the dissolved molecule, are added to describe specific solvent effects. This hydrogen-bonded complex is then embedded in a dielectric continuum, modeling general solvent effects. Use of time-dependent density functional theory (TDDFT) combined with the polarizable continuum model in this approach showed good reproduction of absorption and luminescence spectra and their shifts in various polar solvents [9,12,13,23–27].

This approach was applied for absorption and luminescence spectral calculations of uracil and its substituted derivatives in aqueous solution in [9,12,13]. For modeling the hydrogen-bonded complex structure of uracil molecule, 4 water molecules were added. Construction of this complex was based on experimental results of the primary hydration shell of thymine [10] and NMR experimental data [7] on the structure of the primary solvation shell of uracil in water-DMSO solution, according to which no water molecule is bonded to the uracil C-H groups, while the carbonyl (C=O) and imino (N-H) groups form hydrogen bonds with water molecules. Molecular dynamics calculations of the uracil hydration shell [8,11] showed that the primary solvation shell consists of 9 water molecules, 6 of which form hydrogen bonds with uracil. Additionally, one hydrogen bond belongs to the amide H atom, but unlike shown in [12], each carbonyl oxygen atom forms

two hydrogen bonds. In [14], experimental refinement of [10] data showed that stable hydrogen-bonded thymine-water complexes form in the gas phase with 5 water molecules. Taking this into account, and the methylation fact of uracil, work [15] used 6 water molecules for constructing the uracil hydrogen complex. The constructed hydrogen complex of uracil corresponds to the structure obtained from molecular dynamics data [8,11]. Calculation of this 6-water-molecule uracil supermolecule showed the best reproduction of the experimental absorption band shift in aqueous solution compared to gas phase calculations in this approximation [27].

In the present work, the absorption spectrum of 5hmU in neutral aqueous solution was obtained, and calculations of its electronic spectrum in water were performed including formation of a hydrogen-bonded complex of 5hmU molecule with 7 water molecules from the primary hydration shell. Additionally, spectral data for 5hmU were compared with analogous data for uracil (U), 5-fluorouracil (5FU), and 5-bromouracil (5BrU).

Methods

Absorption spectra of 5hmU (Aldrich, $\geq 97\,\%$), U (Aldrich, $\geq 99\,\%$), 5FU (Aldrich, $\geq 99\,\%$) and 5BrU (Aldrich, $\geq 98\,\%$) were recorded in neutral (pH 7.0) aqueous solution in a quartz cuvette with 2 mm optical path length on a ShimadzuUV-2401 spectrophotometer with scanning speed 210 nm/min and spectral gap width 1 nm.

Quantum-chemical calculations were carried out using density functional theory (DFT) with the B3LYP exchange-correlation functional [28,29] and the 6-311+G(d,p) basis set employing GAUSSIAN 09 software [30]. The influence of the aqueous solution was taken into account by constructing a hydrogen complex of U, 5FU and 5BrU molecules with 6 water molecules, and for the 5hmU molecule with 7 water molecules, which were placed in a water continuum modeled by the polarizable continuum theory (PCM) [31,32].

Stationary points on the potential energy surface were localized with full optimization of all geometric parameters and checked for the absence of imaginary frequencies. Electronic spectra calculations were done by TDDFT using B3LYP functional and the same basis set 6-311+G(d,p) for 60 excited singlet states. Chemcraft 1.7 [33] was used for visualizing geometry, molecular orbitals, and simulating computed electronic spectra. To simulate the calculated electronic spectra, Gaussian curves with a half-maximum width of 0.6 eV were used, which corresponds to the experimental half-maximum width of the first absorption band of uracil in water.

Results and discussion

Absorption spectra of U, 5hmU, 5FU, and 5BrU recorded in neutral aqueous solution are shown in Fig. 1, *a*. Calculated electronic spectra of the hydrogen-bonded complexes of these molecules with water molecules in aqueous continuum are shown in Fig. 1, *b*. Interpretation and characteristics of the absorption spectra are given in the table.

For constructing the hydrogen complex structures of U, 5FU, and 5BrU molecules (Fig. 2, *b*–*d*) the structure of the hydrogen complex proposed for the U molecule with 6 water molecules [15] was taken, which showed the best reproduction of the experimental absorption band shifts in this class of calculations [27]. The structure of this complex also corresponds to experimental data [7,14] and molecular dynamics data [8,11]. For 5-halogenated uracils, a similar hydrogen complex structure was used because the halogen atoms in these compounds do not form stable hydrogen bonds with water molecules, a result obtained in this work from calculations and previously shown by molecular dynamics [34]. Since the 5hmU molecule additionally contains a hydroxyl group that forms hydrogen bonds with water molecules, an additional seventh water molecule coordinated by a hydrogen bond to the oxygen atom of the hydroxyl group was added to its hydrogen complex (Fig. 2, *a*). Adding this water molecule bonded to the hydroxyl group is consistent with the fact that DNA containing 5hmU becomes more hydrophilic [6]. Only the diketo form of the studied compounds was considered when constructing hydrogen complexes and calculating electronic spectra in this work, since this form is the most stable in the ground electronic state for uracil and its 5-substituted derivatives [35–37].

The first absorption band of the studied compounds in aqueous solution, according to calculations, corresponds mainly to the electronic transition from the highest occupied molecular orbital (HOMO) $\pi_{(C=C)}$ to the lowest unoccupied molecular orbital (LUMO) $\pi^*_{(C=C)}$ in the first excited state S_{1A} (Fig. 3, table). Both orbitals have predominant electron density contribution on the $\pi - C = C$-bond. The excited state notation includes not only a digit subscript indicating the order of the excited state in that compound but also a letter subscript indicating the HOMO–LUMO transition responsible for that state. The letter is added because states arising from the same nature of electronic transition have different order numbers in different compounds of the series.

In the studied series U, 5hmU, 5FU, and 5BrU, a red shift of the first absorption band is observed: 4.80, 4.76, 4.67, and 4.50 eV (Fig. 1, *a*, table). A similar shift was noted in halogenated uracils [17] and in the series containing U, thymine, 5FU, and 5-chlorouracil [12]. Calculated electronic spectra of hydrogen complexes reproduce the observed bathochromic shift of the first band (Fig. 1, *b*, table).

Figure 3 shows changes of some higher HOMO and lower UMO energies in the studied compounds. It is seen that the energy gap between HOMO $\pi_{(C=C)}$ and LUMO $\pi^*_{(C=C)}$ decreases along the series, leading to a decrease in the electronic transition energy to state $S_{1A}$and corresponding observed red shift of the first absorption band.

Analysis of the HOMO-LUMO energy gap reduction in a similar series containing U, thymine, 5FU, and 5-

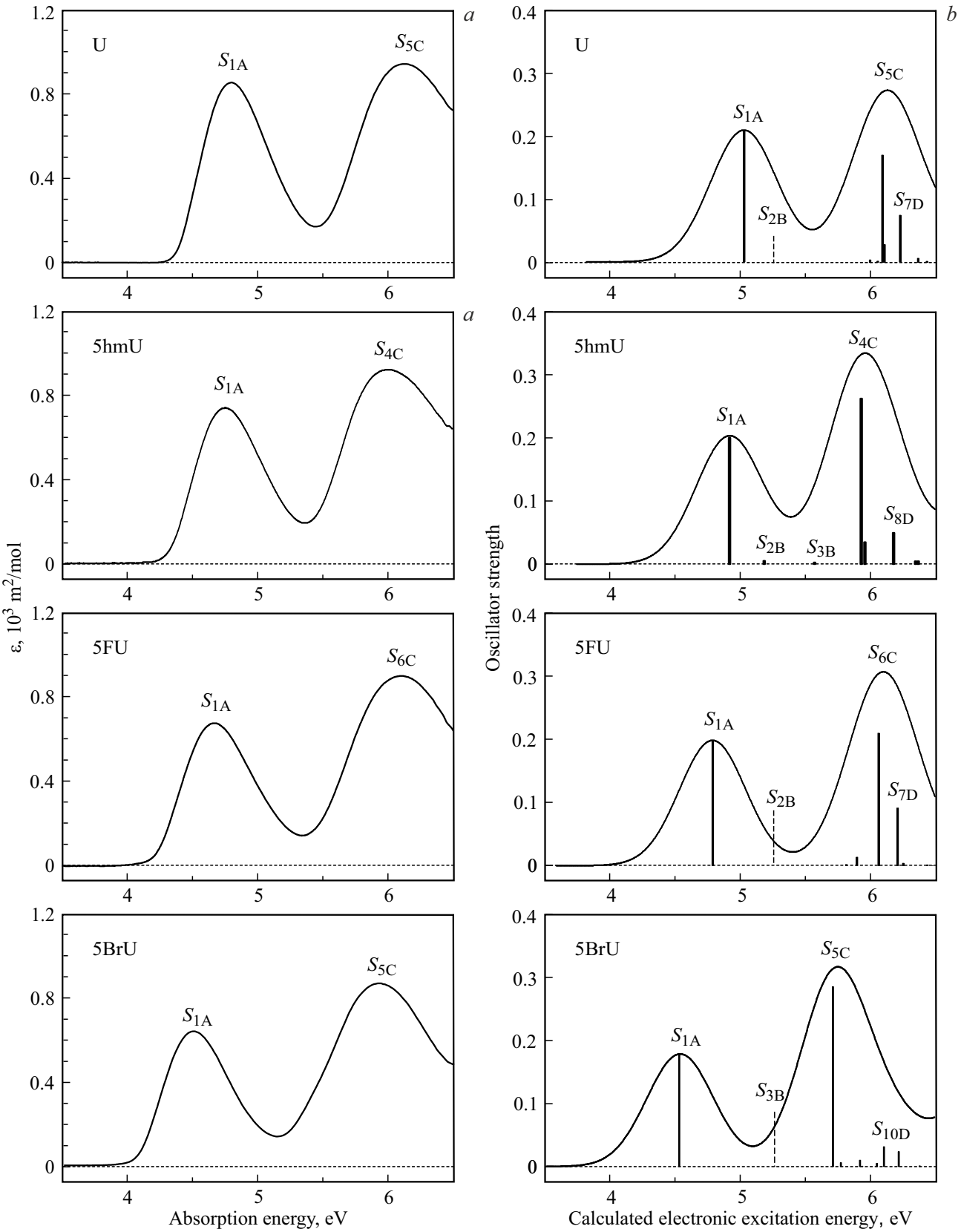

Figure 1. (*a*) Absorption spectra of U, 5hmU, 5FU, and 5BrU in neutral aqueous solution.(*b*) PCM TDDFT B3LYP/6-311+G(d,p) calculated electronic spectra of hydrogen complexes of the studied molecules with water molecules in the aqueous continuum.

Interpretation of absorption spectra of U, 5hmU, 5FU, and 5BrU in neutral aqueous solution based on PCM TDDFT B3LYP/6-311+G(d,p) calculations of hydrogen complexes with water molecules

	S	OMO-UMO	E^{exp}, eV (nm)	ε, 10^3 m^2/mol	E^{calc}, eV	f
U	S_{1A}	$\pi_{(C=C)} \rightarrow \pi^*_{(C=C)}$	**4.80 (258.5)** (258.4)[a] (259)[b] (259)[c] (259.5)[d]	**0.86** 0.81[a] 0.81[b] 0.91[c] 0.82[d]	5.03	0.2091
	S_{2B}	$n_{O2}(a') \rightarrow \pi^*_{(C=C)}$			5.26	0.0003
	S_{5C}	$\pi_{(C=C)} \rightarrow \pi^*_{(C=O1)}$	**6.12 (202.5)** (202.4)[a] (202)[b] (202.5)[d]	0.95 0.90[a] 0.88[b] 0.92[d]	6.09	0.1695
	S_{7D}	$n_{N2}(a'') \rightarrow \pi^*_{(C=C)}$			6.23	0.0740
5hmU	S_{1A}	$\pi_{(C=C)} \rightarrow \pi^*_{(C=C)}$	**4.76 (260.5)**	**0.75**	4.92	0.2008
	S_{2E}	$n_{O3}(a') \rightarrow \pi^*_{(C=C)}$			5.19	0.0053
	S_{3B}	$n_{O2}(a') \rightarrow \pi^*_{(C=C)}$			5.57	0.0027
	S_{4C}	$\pi_{(C=C)} \rightarrow \pi^*_{(C=O1)}$	**6.00 (206.6)**	**0.93**	5.93	0.2633
	S_{8D}	$n_{N2}(a'') \rightarrow \pi^*_{(C=C)}$			6.18	0.0495
5FU	S_{1A}	$\pi_{(C=C)} \rightarrow \pi^*_{(C=C)}$	**4.67 (265.7)** (265.3)[a] (266)[c]	0.68 0.70[a] 0.61[c]	4.80	0.1987
	S_{2B}	$n_{O2}(a') \rightarrow \pi^*_{(C=C)}$			5.27	0.0001
	S_{6C}	$\pi_{(C=C)} \rightarrow \pi^*_{(C=O1)}$	**6.10 (203.2)** (203.3)[a]	**0.90** 0.92[a]	6.07	0.2101
	S_{7D}	$n_{N2}(a'') \rightarrow \pi^*_{(C=C)}$			6.21	0.0913
5BrU	S_{1A}	$\pi_{(C=C)} \rightarrow \pi^*_{(C=C)}$	**4.50 (275.5)** (277.3)[a]	**0.64** 0.70[a]	4.54	0.1784
	S_{3B}	$n_{O2}(a') \rightarrow \pi^*_{(C=C)}$			5.23	0.0001
	S_{5C}	$\pi_{(C=C)} \rightarrow \pi^*_{(C=O1)}$	**5.95 (208.5)** (211.3)[a]	**0.87** 1.00[a]	5.72	0.2855
	S_{10D}	$n_{N2}(a'') \rightarrow \pi^*_{(C=C)}$			6.12	0.0314

Note: Data taken from works: [a][17], [b][18], [c][12], d[19]. S — excited singlet state numbers, subscript digit indicates the excited state order, subscript letter indicates the nature of electronic transition; OMO-UMO — molecular orbital pair contributing most to excited state; E^{calc} and E^{exp} — calculated and experimental vertical electronic transition energies in water; f — oscillator strength; ε —molar absorption coefficient.

chlorouracil from the orbital viewpoint was presented in [12]. Destabilization of HOMO is explained by increased electron density on the substituent, contributing an antibonding effect to HOMO. This effect is due to interaction of the HOMO of 5-substituted uracil with lower-lying orbitals — the nonbonding pairs of the substituent. For 5hmU, the energy of this OMO $n_{O3}(a')$ is shown in Fig. 3. LUMO stabilization in this series is explained in [12] by the increased electronegativity of the substituent.

The second weak electronic transition $n\pi^*$ to the excited state labeled here as S_B occurs mainly from the nonbonding orbital of the second oxygen atom (see atom numbering in Fig. 2, *a*) $n_{O2}(a')$ to LUMO $\pi^*_{(C=C)}$ (Fig. 3, table). In 5hmU, an additional higher HOMO appears compared to U — the lone pair of the oxygen atom of the hydroxyl group $n_{O3}(a')$, which interacts with HOMOs $\pi_{(C=C)}$ and $n_{O2}(a')$ causing destabilization of the first and stabilization of the second. This interaction, as mentioned above, results in the observed bathochromic shift of the first band in 5hmU spectrum relative to U. On the other hand, as shown by calculations, the second excited state in 5hmU becomes S_E ($n_{O3}(a') \rightarrow \pi^*_{(C=C)}$) not S_B ($n_{O2}(a') \rightarrow \pi^*_{(C=C)}$) as in U. The transition to state S_B shifts to higher energy (Fig. 1, *b*, table).

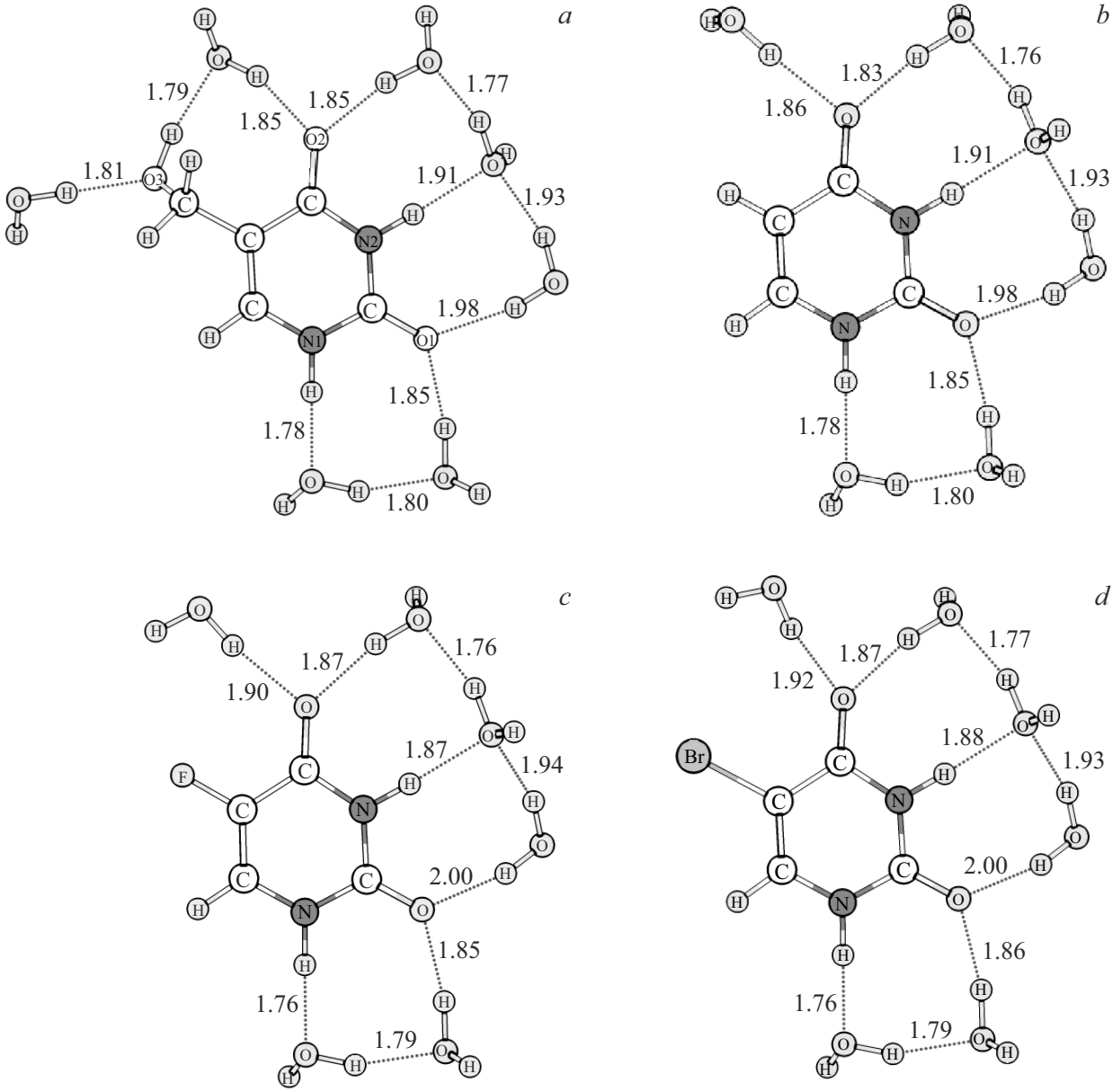

Figure 2. Optimized geometric structures of hydrogen-bonded complexes of (*a*) 5hmU, (*b*) U, (*c*) 5FU, and (*d*) 5BrU with water molecules. Fig. 2, *a* shows numbering of oxygen and nitrogen atoms in the studied molecules. Numbers next to dashed lines denoting hydrogen bonds are the calculated hydrogen bond lengths in angstroms.

The second absorption band in the studied compounds mainly arises from two intense electronic transitions to states S_C ($\pi_{(C=C)} \rightarrow \pi^*_{(C=O1)}$) and S_D ($n_{N2}(a'') \rightarrow \pi^*_{(C=C)}$). The first is more intense and largely determines the maximum position of the second band (Fig. 1, *b*). This transition occurs predominantly from HOMO $\pi_{(C=C)}$ to π-UMO of the C=O1-bond ($\pi^*_{(C=O1)}$). In 5hmU, a bathochromic shift of this band from 6.12 to 6.00 eV is observed (Fig. 1), caused by a decrease in the energy gap between HOMO $\pi_{(C=C)}$ and UMO $\pi^*_{(C=O1)}$ due to destabilization of $\pi_{(C=C)}$ through interaction with HOMO $n_{O3}(a')$ and stabilization of UMO $\pi^*_{(C=O1)}$ by the inductive effect of the hydroxymethyl group (Fig. 3). In 5FU absorption, this band shifts toward higher energy to 6.10 eV (compared to 5hmU), while in 5BrU it shifts back red to 5.95 eV (Fig. 1, table).

Calculated hydrogen complexes reproduce the experimental shifts of the second absorption band in the compound series studied (Fig. 1, *b*). These band shifts correspond to changes in the energy gap $\pi_{(C=C)} \rightarrow \pi^*_{(C=O1)}$ across the series: increased in 5FU and decreased in 5BrU compared to 5hmU (Fig. 3), corresponding to hypsochromic shift in 5FU absorption and bathochromic shift in 5BrU.

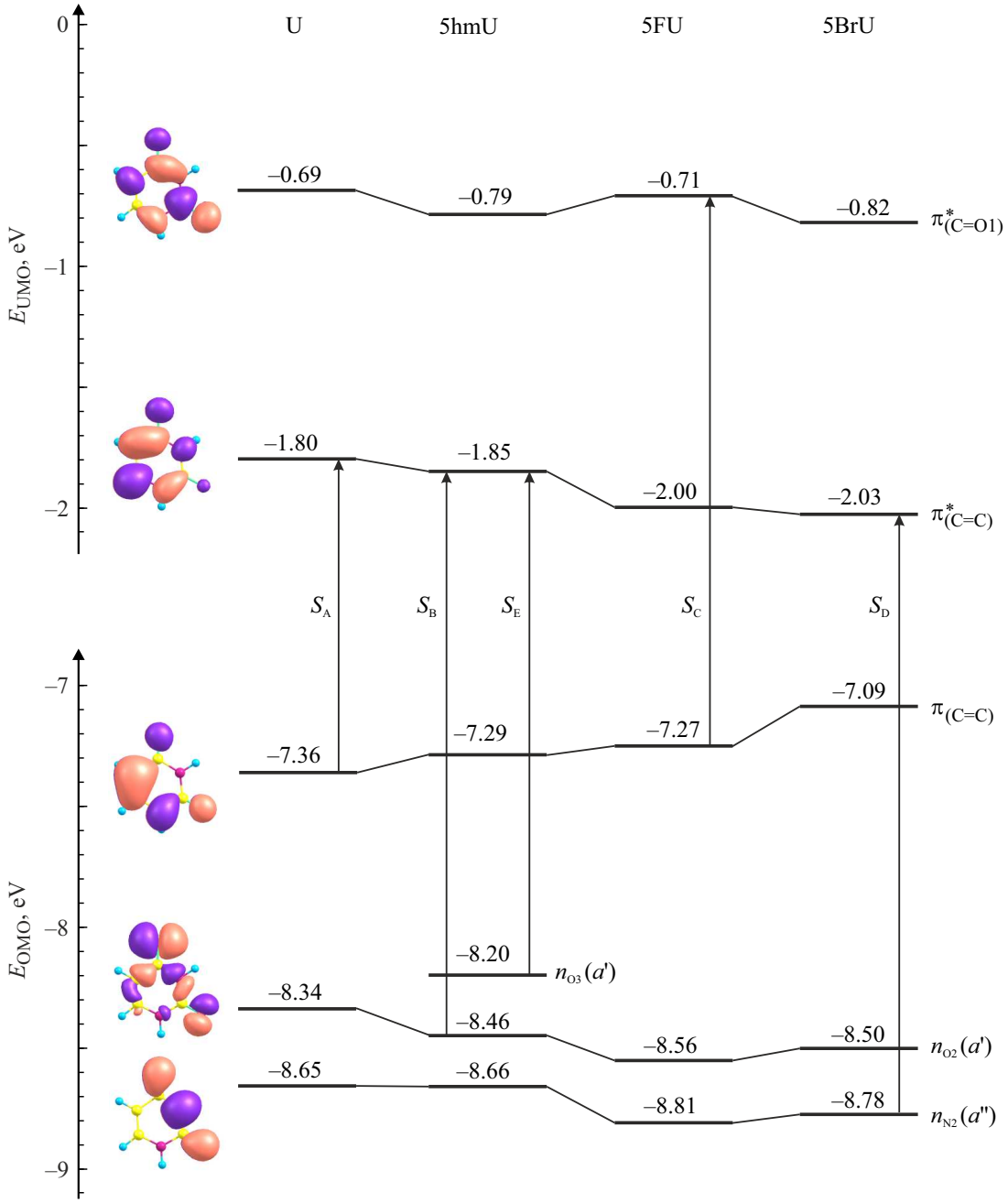

Figure 3. Energies of some higher OMOs (E_{OMO}) and lower UMOs (E_{UMO}) from B3LYP/6-311+G(d,p) calculations of hydrated hydrogen complexes of U, 5hmU, 5FU, and 5BrU molecules. Vertical arrows indicate OMO-UMO pairs predominantly responsible for transitions to excited singlet states (S_A, S_B et. c.). Molecular orbital depiction is for U molecule in gas phase.

In the single-pole approximation (assuming $i \rightarrow a$ transition does not mix with others), the singlet transition energy in TDDFT is given by [38,39]

$$E(S)^{SPA} = \varepsilon_a - \varepsilon_i + \int\int \varphi_i^*(\vec{r})\varphi_a(\vec{r}) \times \left[\frac{2}{|\vec{r}-\vec{r}'|} + (f_{XC}^{\uparrow\uparrow} - f_{XC}^{\uparrow\downarrow})\right]\varphi_i(\vec{r}')\varphi_a^*(\vec{r}')d\vec{r}'d\vec{r}, \quad (1)$$

where ε_a and ε_i — are energies of UMO and OMO, φ is one-electron wave function, $f_{XC}^{\uparrow\uparrow}$ and $f_{XC}^{\uparrow\downarrow}$ are exchange and correlation integral kernels, and $f_H = \frac{1}{|\vec{r}-\vec{r}'|}$ is the Coulomb integral kernel.

If changes in these integrals are small across the compound series compared to the energy gap magnitude, a correlation occurs between the singlet transition energy and the OMO–UMO gap that predominantly contributes to this transition. According to (1), these integrals will be similar if corresponding one-electron wave functions

(MOs) are similar across the series. This condition is satisfied here for the considered π-MOs in the compounds U, 5hmU, 5FU, and 5BrU. Pearson correlation coefficient for the first band energy and the HOMO–LUMO gap $\pi_{(C=C)}$ $\pi^*_{(C=C)}$ in this series is $R = 0.9857$ with root mean square deviation $SD = 0.044$ eV, and for the second band energy and corresponding gap $\pi_{(C=C)} \rightarrow \pi^*_{(C=O1)}$ $R = 0.9246$ and $SD = 0.079$ eV. One cause for the lower correlation coefficient for the second band is that the band maximum energy may differ somewhat from that of the considered electronic transition maximum, as the second band is formed by two intense electronic transitions. This applies especially to U and 5FU, where calculated intensities of the second transition to excited state S_D are only about twice smaller than for S_C state (Fig. 1, *b*).

Conclusion

Absorption spectra in neutral aqueous solution of 5hmU as well as U, 5FU, and 5BrU have been obtained. The hydrogen complex structures of these molecules with water were modeled, consisting of 7 water molecules for 5hmU and 6 water molecules for U, 5FU, and 5BrU. The resulting 5hmU hydrogen complex structure corresponds to the fact that DNA containing 5hmU instead of thymine becomes more hydrophilic.

It was shown that electronic spectra calculations of modeled hydrogen complexes by TDDFT B3LYP/6-311+G(d,p) with PCM well reproduce their absorption spectra in neutral aqueous solution and the experimentally observed band shifts in the studied compound series. A linear dependence was found in the series between electronic transition energies obtained from absorption spectra and the energy gaps between the corresponding occupied and unoccupied molecular orbitals calculated for the hydrogen complexes. For the energy of the first absorption band and the energy gap between the HOMO $\pi_{(C=C)}$ and the LUMO $\pi^*_{(C=C)}$ the Pearson linear correlation coefficient is $R = 0.9857$ with a root mean square deviation of $SD = 0.044$ eV. For the energy of the second absorption band and the corresponding energy gap, the correlation coefficient is $\pi_{(C=C)} \rightarrow \pi^*_{(C=O1)}$ $R = 0.9246$ with a root mean square deviation of $SD = 0.079$ eV.

Acknowledgments

This work was carried out using the facilities of the „Spectrum“ Regional Center for Collective Use of the Ufa Federal Research Center of RAS. The authors also thank the „Chemistry“ Center for Collective Use at Ufa Institute of Chemistry of RAS for providing access to the supercomputer used for quantum-chemical calculations.

Funding

The work was performed within the state assignment of the Ministry of Science and Higher Education of the Russian Federation No. 125020601570-5.

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] T.S. Lawrence, M.A. Davis, J. Maybaum, P.L. Stetson, W.D. Ensminger. Radiat. Res., **123** (2), 192 (1990). DOI: 10.2307/3577544
[2] P.W. McLaughlin, W.R. Mancini, P.L. Stetson, H.S. Greenberg, N. Nguyen, H. Seabury, D.B Heidorn, T.S. Lawrence. Int. J. Radiat. Oncol. Biol. Phys., **26** (4), 637 (1993). DOI: 10.1016/0360-3016(93)90281-Y
[3] N.E. Geacintov, S. Broyde. *The chemical biology of DNA damage* (Wiley VCH, Weinheim, 2010), p. 7–12. DOI: 10.1002/9783527630110
[4] D. Gackowski, M. Gawronski, C. Kerr, T. Radivoyevitch, E. Zarakowska, M. Starczak, A. Abakir, A. Ruzov, J.P. Maciejewski, R. Olinski. Haematologica, **105** (5), e213 (2020). DOI: 10.3324/haematol.2019.224030
[5] M. Janoušková, Z. Vaníková, F. Nici, S. Boháčová, D. Vítovská, H. Šanderová, M. Hocek, L. Krásný. Chem. Commun., **53** (99), 13253 (2017). DOI: 10.1039/C7CC08053K
[6] S. Carson, J. Wilson, A. Aksimentiev, P.R. Weigele, M. Wanunu. Nucleic Acids Res., **44** (5), 2085 (2016). DOI: 10.1093/nar/gkv1199
[7] M. Chahinian, H.B. Seba, B. Ancian. Chem. Phys. Lett., **285** (5–6), 337 (1998). DOI: 10.1016/S0009-2614(98)00109-2
[8] M.-P. Gaigeot, M. Sprik. J. Phys. Chem. B, **107** (38), 10344 (2003). DOI: 10.1021/jp034788u
[9] R. Improta, V. Barone. J. Am. Chem. Soc., **126** (44), 14320 (2004). DOI: 10.1021/ja0460561
[10] Y. He, C. Wu, W. Kong. J. Phys. Chem. A, **108** (6), 943 (2004). DOI: 10.1021/jp036553o
[11] M.-P. Gaigeot, M. Sprik. J. Phys. Chem. B, **108** (22), 7458 (2004). DOI: 10.1021/jp049940m
[12] T. Gustavsson, A. Banyasz, E. Lazzarotto, D. Markovitsi, G. Scalmani, M.J. Frisch, V. Barone, R. Improta. J. Am. Chem. Soc., **128** (2), 607 (2006). DOI: 10.1021/ja056181s
[13] T. Gustavsson, N. Sarkar, E. Lazzarotto, D. Markovitsi, V. Barone, R. Improta. J. Phys. Chem. B, **110** (26), 12843 (2006). DOI: 10.1021/jp062266j
[14] M. Busker, M. Nispel, T. Haber, K. Kleinermanns, M. Etinski, T. Fleig. ChemPhysChem, **9** (11), 1570 (2008). DOI: 10.1002/cphc.200800111
[15] M. Etinski, C.M. Marian. Phys. Chem. Chem. Phys., **12** (19), 4915 (2010). DOI: 10.1039/B925677F
[16] S.N. Tseplina, E.E. Tseplin. the Lowest High Energy Chem., **55** (1), 96 (2021). DOI: 10.1134/S0018143921010136.
[17] W.Z. Lohmann. Naturforsch. C, **29** (9–10), 493 (1974). DOI: 10.1515/znc-1974-9-1007
[18] L.B. Clark, I. Tinoco. J. Am. Chem. Soc., **87** (1), 11 (1965). DOI: 10.1021/ja01079a003

[19] D. Voet, W.B. Gratzer, R.A. Cox, P. Doty. Biopolymers, **1** (3), 193 (1963). DOI: 10.1002/bip.360010302
[20] Y. Miura, Y. Yamamoto, S. Karashima, N. Orimo, A. Hara, K. Fukuoka, T. Ishiyama, T. Suzuki. J. Am. Chem. Soc., **145** (6), 3369 (2023). DOI: 10.1021/jacs.2c09803
[21] C.S. Anstöter, M. DelloStritto, M.L. Klein, S. Matsika. J. Phys. Chem. A, **125** (32), 6995 (2021). DOI: 10.1021/acs.jpca.1c05288
[22] M. Kumar, G. Jaiswar, M. Afzal, M. Muddassir, A. Alarifi, A. Fatima, N. Siddiqui, R. Ayub, N.A.Y. Abduh, W.S. Saeed, S. Javed. Molecules, **28** (5), 2116 (2023). DOI: 10.3390/molecules28052116
[23] S.N. Tseplina, E.E. Tseplin. Opt. Spectrosc., **129** (7), 737 (2021). DOI: 10.1134/S0030400X21050179.
[24] S.N. Tseplina, E.E. Tseplin. High Energy Chem., **58** (4), 369 (2024). DOI: 10.1134/S001814392470036X
[25] E.E. Tseplin, S.N. Tseplina, O.G. Khvostenko. Opt. Spectrosc., **125** (4), 506 (2018). DOI: 10.1134/S0030400X18100260.
[26] E.E. Tseplin, S.N. Tseplina. Chem. Phys. Lett., **716**, 142 (2019). DOI: 10.1016/j.cplett.2018.12.038
[27] R. Improta, F. Santoro, L. Blancafort. Chem. Rev., **116** (6), 3540 (2016). DOI: 10.1021/acs.chemrev.5b00444
[28] A.D. Becke. J. Chem. Phys., **98** (7), 5648 (1993). DOI: 10.1063/1.464913
[29] C. Lee, W. Yang, R.G. Parr. Phys. Rev. B, **37** (2), 785 (1988). DOI: 10.1103/PhysRevB.37.785
[30] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Cuseria, M.A. Robb, J.R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G.A. Petersson, H. Nakatsuji, M.Caricato, X. Li, H.P. Hratchian, A.F. Izmaylov, J. Bloino, G. Zheng, J.L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J.A. Montgomery, J.E. Peralta, F. Ogliaro, M. Bearpark, J.J. Heyd, E. Brothers, K.N. Kudin, V.N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J.C. Burant, S.S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J.M. Millam, M. Klene, J.E. Knox, J.B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, R.L. Martin, K. Morokuma, V.G. Zakrzewski, G.A. Voth, P. Salvador, J.J. Dannenberg, S. Dapprich, A.D. Daniels, O. Farkas, J.B. Foresman, J.V. Ortiz, J. Cioslowski, D.J. Fox. Gaussian 09, Revision C.1, Gaussian, Inc., Wallingford CT, 2009.
[31] J. Tomasi, B. Mennucci, R. Cammi. Chem. Rev., **105** (8), 2999 (2005). DOI: 10.1021/cr9904009
[32] S. Miertus, E. Scrocco, J. Tomasi. Chem. Phys., **55** (1), 117 (1981). DOI: 10.1016/0301-0104(81)85090-2
[33] G.A. Zhurko, D.A. Zhurko. Chemcraft, version 1.7 [Electronic source] URL: https://www.chemcraftprog.com
[34] S. Hamad, C. Moon, C.R.A. Catlow, A.T. Hulme, S.L. Price. J. Phys. Chem. B, **110** (7), 3323 (2006). DOI: 10.1021/jp055982e
[35] C.M. Marian, F. Schneider, M. Kleinschmidt, J. Tatchen. Eur. Phys. J. D, **20**, 357 (2002). DOI: 10.1140/epjd/e2002-00158-3
[36] D.A. Estrin, L. Paglieri, G.J. Corongiu. Phys. Chem., **98** (22), 5653 (1994). DOI: 10.1021/j100073a014
[37] N. Markova, V. Enchev, I. Timtcheva. J. Phys. Chem. A, **109** (9), 1981 (2005). DOI: 10.1021/jp046132m
[38] M.E. Casida, M. Huix-Rotllant. Annu. Rev. Phys. Chem., **63**, 287 (2012). DOI: 10.1146/annurev-physchem-032511-143803
[39] M.A.L. Marques, E.K.U. Gross. Annu. Rev. Phys. Chem., **55**, 427 (2004). DOI: 10.1146/annurev.physchem.55.091602.094449

Translated by J.Savelyeva