Atomistic mechanisms of the tautomerization of the G·C base pairs through the proton transfer: quantum-chemical survey

Ol'ha O. Brovarets¹ · Alona Muradova² · Dmytro M. Hovorun¹,²

Received: 5 September 2021 / Accepted: 23 November 2021 / Published online: 2 December 2021
© The Author(s), under exclusive licence to Springer-Verlag GmbH Germany, part of Springer Nature 2021

Abstract
This study is devoted to the investigation of the G·C*O₂(WC)↔G*NH₃·C*(WC), G·C*O₂(WC)↔G*NH₃·C*(WC) and G·C*O₂(WC)↔G*NH₃·C(wWC) bas e tautomerization reactions occurring through the proton transfer, obtained at the MP2/6-311++G(2df,pd)//B3LYP/6-311++G(d,p) level of theory in gas phase under normal conditions (‘WC’ means base pair in Watson-Crick configuration, T=298.15 K). These reactions lead to the formation of the G*NH₃·C*(WC), G*NH₃·C*(WC) and G*NH₃·C(wWC) base pairs by the participation of the G*NH₃ base with NH₂ group. Gibbs free energies of activation for these reactions are 6.43, 11.00 and 1.63 kcal·mol⁻¹, respectively. All of these tautomerization reactions are dipole active. Finally, we believe that these non-dissociative processes, which are tightly connected with the tautomeric transformations of the G·C base pairs, play an outstanding role in supporting of the spatial structure of the DNA and RNA molecules with various functional purposes.

Keywords G·C base pair · Proton transfer · Tautomer · H-bond · Quantum-chemical calculations

Introduction
In recent years according to the analysis of the literature [1–7], the interest of researchers to the investigation of the prototropic tautomerism significantly increased. It is obviously connected with the fact that this research topic is multidisciplinary and covers wide areas of knowledge such as chemistry, biochemistry, structural and quantum biology, molecular and quantum pharmacology, condensed matter physics, crystal physics, electronic technologies, and biomolecular technologies [8–13].

It occurs as intensive accumulation of the data within the framework of the classical models, describing these processes [14–18], as well as successful searches of both novel atomistic mechanisms of the prototropic tautomerization of the molecular objects [19–22] and novel instruments for the penetration into the course of these processes.

Shortly saying, now the mechanisms of the tautomerization of the base pairs, which are accompanied by significant changing of their geometry [23–26], actively enter the arena. It is suggested that exactly these tautomeric transitions are not only responsible for the structural transitions in the nucleic acids, but also for the supporting of their unique spatial structures, having certain biological functions.

Aim of this work is to deepen the existing ideas about the quantum mechanisms of the tautomerization of the G·C pairs of nucleotide bases through the proton transfer along the intermolecular neighboring H-bonds as their intrinsic property. We have chosen for its successful realization biologically important G·C base pairs, which monomers are in the basic and rare tautomeric forms.

As a result of the provided quantum-chemical investigations for the first time the following regularities were revealed.

Tautomerizations of the G·C base pairs are controlled by the transition states, joined by the intermolecular H-bonds and covalent bridges.
In all cases without any exception, mechanisms of the tautomerization are step-by-step realized by the proton transfer.

**Computational methods**

**Density functional theory calculations of the geometry and vibrational frequencies**

Equilibrium geometries of the investigated G·C base pairs and transition states (TSs) of their tautomerizations and rotations, as well as their harmonic vibrational frequencies have been calculated using Gaussian’09 program package [27] at the B3LYP/6-311++G(d,p) level of theory [28–32], which approved itself successfully for the calculations of the similar systems and processes, and shown acceptable level of accuracy and adequacy of the obtained results [32, 33]. A scaling factor that is equal to 0.9668 has been applied in the present work for the correction of the frequencies for all complexes [21, 22, 34].

We have confirmed local minima and transition states, localized by Synchronous Transit-guided Quasi-Newton method [35], on the potential energy landscape by the absence or presence, respectively, of one imaginary frequency in the vibrational spectra of the complexes.

All reaction pathways have been reliably confirmed by providing intrinsic reaction coordinate (IRC) calculations [35] from each TS in the forward and reverse directions at the B3LYP/6-311++G(d,p) level of theory.

All calculations have been performed in the continuum with ε=1 that adequately reflects the processes occurring in real biological systems without deprivation of the structurally functional properties of the bases in the composition of the DNA or RNA molecules and satisfactorily models the substantially hydrophobic recognition pocket of the DNA-polymerase machinery as a part of the replisome [36, 37].

**Single point energy calculations**

We continued geometry optimizations with electronic energy calculations as single point calculations at the MP2/6-311++G(2df,pd) level of theory [38, 39].

The Gibbs free energy $G$ for all structures was obtained in the following way:

$$G = E_{el} + E_{corr},$$  \hspace{1cm} (1)

where $E_{el}$ is the electronic energy and $E_{corr}$ - the thermal correction.

**QTAIM analysis**

Bader’s quantum theory of atoms in molecules (QTAIM) [40] was applied to analyze the electron density distribution, using program package AIMAll [41].

The presence of the bond critical point (BCP), namely, the so-called (3,-1) BCP, and a bond path between donor and acceptor of the H-bond or van der Waals contact, as well as the positive value of the Laplacian at this BCP ($\Delta \rho > 0$), were considered as criteria for the formation of the H-bond or van der Waals contact, respectively [42–45]. Wave functions were obtained at the B3LYP/6-311++G(d,p) level of theory, used for geometry optimization.

The atomic numbering scheme for the bases is conventional and rare tautomeric forms of the G and C bases are marked by an asterisk (*) [4].

**Obtained results and their discussion**

In this work investigated tautomerization pathways of the G·C base pairs are presented on Figure 1, and their discussion is outlined below.

It is interesting to note that G·C*O2(WC) base pair tautomerizes (Fig. 1a) through the double proton transfer along the N1H…N3 and O2H…N2 H-bonds and via the TSG·C*O2(WC) $\leftrightarrow$ G*NH3·C*t(WC), which is stabilized by the participation of the two intermolecular (C)N4H…O6(G) and (C)O2H…N2(G) H-bonds, and (G)N1-H-N3(C) covalent bridge. Eventually, this reaction leads to the formation of the G*NH3·C*t(WC) base pair, stabilized by three intermolecular N4H…O6, N3H…N1, and N2H…O2 H-bonds. Exactly the proton transfer along the lower O2H…N2 H-bond leads to the formation of the NH3 group at the G base.

Formed G*NH3·C*t(WC) base pair can transform via the mutual rotation (Fig. 1b) of the bases around the middle N3H…N1 H-bond, leading to the new reverse G*NH3·C*s(rWC) base pair, stabilized by the N3H…O6, N4H…N1, and N2H…N4 H-bonds. Transition state of this interconversion TSG*NH3·C*s(rWC) $\leftrightarrow$ G*NH3·C*t(rWC) is joined by three N4H…N1, N3H…N1, and N2H…N4 H-bonds and single N2…N3 van der Waals contact.

Another G·C*O2(WC) $\leftrightarrow$ G*NH3·C*s(WC) tautomerization reaction (Fig. 1c) occurs via the transfer of the proton, localized at the N1 nitrogen atom of the G base, to the N3 nitrogen atom of the C*O2 base and of the proton, localized at the O2 oxygen atom of the C*O2 base, to the N2 atom of the NH3 amino group of the G base and finally leads to the G*NH3·C*s(WC) base pair by the participation of the G*NH3 base with NH3 group. Transition state
a) $G·C^*O_2(WC) \leftrightarrow G^*_{NH3}·C^*(WC)$

{Proton transfer along the N1H…N3 and O2H…N2 H-bonds}

$G·C^*O_2(WC)$

$(\Delta G=0.00 / \Delta E=0.00 / \mu=9.98)$

$TS_{G·C^*O_2(WC)\rightarrow G^*_{NH3}·C^*(WC)}$

$(\nu_i=71.4.6 i \text{ cm}^{-1})$

$(\Delta G=6.43 / \Delta E=8.45 / \mu=10.75)$

$G^*_{NH3}·C^*(WC)$

$(\Delta G=5.17 / \Delta E=4.78/ \mu=11.51)$

b) $G^*_{NH3}·C^*\rightarrow G^*_{NH3}·C^*(tWC)$

{Rotation around the middle (C)N3H…N1(G) H-bond}

$G^*_{NH3}·C^*(WC)$

$(\Delta G=0.00 / \Delta E=0.00 / \mu=11.51)$

$TS_{G^*_{NH3}·C^*(WC)\rightarrow G^*_{NH3}·C^*(tWC)}$

$(\nu_i=64.5 i \text{ cm}^{-1})$

$(\Delta G=16.00 / \Delta E=16.73 / \mu=12.04)$

c) $G·C^*O_2(WC) \leftrightarrow G^*_{NH3}·C^*(WC)$

{Proton transfer along the N1H…N3 and O2H…N2 H-bonds}

$G·C^*O_2(WC)$

$(\Delta G=0.00 / \Delta E=0.00 / \mu=7.91)$

$TS_{G·C^*O_2(WC)\rightarrow G^*_{NH3}·C^*(WC)}$

$(\nu_i=1112.0 i \text{ cm}^{-1})$

$(\Delta G=11.00 / \Delta E=14.41 / \mu=9.47)$

$G^*_{NH3}·C^*(WC)$

$(\Delta G=12.66 / \Delta E=12.99 / \mu=10.91)$

Fig. 1. Tautomeric and conformational transformations of the G-C base pairs through the proton transfer and mutual rotations of the bases, obtained at the MP2/6-311++G(2df,pd)//B3LYP/6-311++G(d,p) level of theory in gas phase under normal conditions ('WC' means base pair in Watson-Crick configuration; $\Delta G$ – relative Gibbs free energy ($T=298.15$ K), kcal·mol$^{-1}$; $\Delta E$ – electronic energy, kcal·mol$^{-1}$; $\nu_i$ – imaginary frequency at the TS; $\mu$ – dipole moment of the complex, D). Intermolecular A-H…B H-bonds and A…B van der Waals contacts are designated by the dotted lines, their lengths H…B and A…B are presented in Angstroms. Symbol "↓" means displacement of the base on the right down relatively the base on the left.
d) \( G_{\text{NH3}}^* \cdot C^*(\text{WC}) \leftrightarrow G \cdot C(\text{rw}_{\text{WC}}) \)
{Rotation around the middle (C)N3H…N1(G) H-bond}

\[
G_{\text{NH3}}^* \cdot C^*(\text{WC}) \\
(\Delta G=0.00/ \Delta E=0.00/ \mu=10.91)
\]

\[
T_{\text{SG}} G_{\text{NH3}}^* \cdot C^*(\text{WC}) \leftrightarrow G \cdot C(\text{rw}_{\text{WC}}) \\
(\Delta G=97.0 i \text{ cm}^{-1})
\]

\[
G \cdot C(\text{rw}_{\text{WC}}) \\
(\Delta G=-31.67/ \Delta E=-30.18/ \mu=8.57)
\]

e) \( G^* \cdot C^* \text{O}_2(\text{WC}) \leftrightarrow G_{\text{NH3}}^* \cdot C(\text{w}_{\text{WC}}) \)
{Proton transfer along the upper O6H…N4 and lower O2H…N2 H-bonds}

\[
G^* \cdot C^* \text{O}_2(\text{WC}) \\
(\Delta G=0.00/ \Delta E=0.00/ \mu=6.91)
\]

\[
T_{\text{SG}} G^* \cdot C^* \text{O}_2(\text{WC}) \leftrightarrow G_{\text{NH3}}^* \cdot C(\text{w}_{\text{WC}}) \\
(\Delta G=732.7 i \text{ cm}^{-1})
\]

\[
G_{\text{NH3}}^* \cdot C(\text{w}_{\text{WC}}) \\
(\Delta G=-3.36/ \Delta E=-3.02/ \mu=8.54)
\]

Fig. 1 (continued)

\( T_{\text{SG}} G^* \cdot C^* \text{O}_2(\text{WC}) \leftrightarrow G_{\text{NH3}}^* \cdot C(\text{w}_{\text{WC}}) \) of this reaction is characterized by the (G)O6…N4(C) van der Waals contact and two (G) N1-H-N3(C) and (G)N2-H-O2(C) covalent bridges.

Formed \( G_{\text{NH3}}^* \cdot C^*(\text{WC}) \) base pair can transform (Fig. 1d) by the mutual rotation of the bases around the middle N3H…N1 H-bond into the reverse G-C(\text{rw}_{\text{WC}}) base pair. Transition state \( T_{\text{SG}} G_{\text{NH3}}^* \cdot C^*(\text{WC}) \leftrightarrow G \cdot C(\text{rw}_{\text{WC}}) \) of this reaction is joined by three intermolecular N3H…N1, N2H…N4, and N2H…O2 H-bonds, and N2…N3 van der Waals contact. Finally, this \( G_{\text{NH3}}^* \cdot C^*(\text{WC}) \leftrightarrow G \cdot C(\text{rw}_{\text{WC}}) \) reaction leads to the G-C(\text{rw}_{\text{WC}}) base pair.

The most interesting case represents the \( G^* \cdot C^* \text{O}_2(\text{WC}) \leftrightarrow G_{\text{NH3}}^* \cdot C(\text{w}_{\text{WC}}) \) transformation (Fig. 1e), since proton transfer within the \( G^* \cdot C^* \text{O}_2(\text{WC}) \) base pair leads not only to the changing of its tautomeric status, but also to its geometrical rearrangement. \( G^* \cdot C^* \text{O}_2(\text{WC}) \) base pair tautomerizes through the proton transfer along the upper O6H…N4 and lower O2H…N2 H-bonds from the O6 atom of the G* base to the N4 atom of the C*O2 base and from the O2 atom of the C*O2 base to the N2 atom of the G* base, respectively, via the \( T_{\text{SG}} G^* \cdot C^* \text{O}_2(\text{WC}) \leftrightarrow G_{\text{NH3}}^* \cdot C(\text{w}_{\text{WC}}) \). Finally, the C base shifts down accordingly the \( G_{\text{NH3}}^* \cdot C(\text{w}_{\text{WC}}) \) base pair by the participation of the \( G_{\text{NH3}}^* \) base with NH3 group.

Activation Gibbs free energies for the considered tautomerization reactions varies in the range
1.63–11.00 kcal·mol⁻¹, reaching maximum value for the G·C*O₂(WC)↔G*NH₃·C*(WC) reaction, while minimum - for the G*·C*O₂(WC)↔G*NH₃·C*(WC)₁ reaction.

Altogether four G·C base pairs were revealed, involving G*NH₃ base with NH₃ group - G*NH₃·C*(rWC), G*NH₃·C*(tWC), G*NH₃·C*(s(WC)), and G*NH₃·C*(wWC) (Fig. 1).

Considered G·C base pairs form the following order in terms of their relative Gibbs free ΔG and electronic ΔE energies (in kcal·mol⁻¹): G·C(rwWC) (0.00 and 0.00) < G*NH₃·C(wWC)₁ (16.08 and 14.54) < G·C*O₂(WC) (19.43 and 17.53) < G*·C*O₂(WC) (19.44 and 17.56) < G*NH₃·C*(tWC) (24.60 and 22.32) < G*NH₃·C*(WC) (31.67 and 30.17) < G*NH₃·C*(rWC) (32.97 and 31.80).

Notably, that difference in Gibbs free and electronic energies between the classical G·C(WC) and reverse G·C(rwWC) base pairs consists 11.53 and 13.09 kcal·mol⁻¹, respectively, while the G·C*O₂(WC) and G*·C*O₂(WC) base pairs are iso-energetical (19.43 and 19.44 kcal·mol⁻¹, respectively).

**Conclusions**

This paper reports for the first time novel tautomORIZATION mechanisms for the G·C base pairs, leading to the base pairs by the participation of the G*NH₃ base with NH₃ group - G*NH₃·C*(tWC), G*NH₃·C*(s(WC)), and G*NH₃·C*(wWC). Gibbs free energies of activation for these reactions are 6.43, 11.00, and 1.63 kcal·mol⁻¹, respectively, obtained at the MP2/6-311++G(2df,pd)//B3LYP/6-311++G(d,p) level of theory in gas phase under normal conditions (T=298.15 K).

In all cases without any exception tautomeric transitions are dipole active (μ=6.91–11.51 D) with minimum realized at the starting G·C*O₂(WC) (9.98 D), G·C*O₂(WC) (7.91 D), and G*·C*O₂(WC) (6.91 D) base pairs.

**Authors' contributions** OB—idea formulation, setting of the task, calculation of the data, building of the graphs, data extrapolation, preparing, and proofreading of the draft of the manuscript. AM—idea formulation, calculation of the data, preparing, and proofreading of the draft of the manuscript. DH—idea formulation, preparing, and proofreading of the draft of the manuscript. All authors contributed to the article and approved the submitted version.

**Availability of data and material** Not applicable.

**Code availability** Gaussian’09 program package – gaussian.com; AIM-All program package – http://aim.tkgristmill.com/.

**Declarations**

**Conflict of interest** The authors declare no competing interests.

**References**

1. Brovarets’ OO, Hovorun DM (2018) Renaissance of the tautomeric hypothesis of the spontaneous point mutations In: DNA: New ideas and computational approaches. Mitochondrial DNA – New Insights / Ed. by Herve Seligmann, London, United Kingdom, IntechOpen. ISBN 978-953-51-6167-7
2. Brovarets’ OO, Hovorun DM (2014) Why the tautomerization of the G·C Watson-Crick base pair via the DPT does not cause point mutations during DNA replication? QM and QTAIM comprehensive analysis. J Biomol Struct Dyn 32:1474–1499
3. Florian J, Leszcynski J (1996) Spontaneous DNA mutations induced by proton transfer in the guanine-cytosine base pairs: An energetic perspective. J Am Chem Soc 118:3010–3017
4. Brovarets’ OO, Hovorun DM (2010) How stable are mutagenic tautomers of the DNA bases? Biopol Cell 26:72–76
5. Brovarets’ OO, Hovorun DM (2020) A new era of the prototropic tautomerism of the quercetin molecule: A QM/QTAIM computational advances. J Biomol Struct Dyn 38:4774–4800
6. Brovarets’ OO, Pérez-Sánchez HE, Hovorun DM (2016) Structural grounds for the 2-aminopurine mutagenicity: A novel insight into the old problem of the replication errors. RSC Adv 6:99546–99557
7. Brovarets’ OO, Voiteshenko IS, Pérez-Sánchez H, Hovorun DM (2017) A QM/QTAIM research under the magnifying glass of the DPT tautomerisation of the wobble mispairs involving 2-aminopurine. New J Chem 41:7232–7243
8. Pospisil P, Ballmer P, Scapozza L, Folkers G (2003) Tautomerism in computer-aided drug design. J Rec Sign Trans 23:361–371
9. Dhaked DK, Ilenfeldt W-D, Patel H, Delannee V, Nicklaus MC (2020) Toward a comprehensive treatment of tautomerism in chemoinformatics including in InChi V2. J Chem Inf Model 60:1253–1275
10. Doboz R, Kolehmainen E, Valkonen A, Osmiawaloski B, Gawnick R (2007) Tautomeric preferences of phthalones and related compounds. Tetrathedron 63:9172–9178
11. Larina LI (2018) Tautomeric structure and reaction of azoles: Nuclear Magnetic Resonance spectroscopy. Adv Heterochem 124:123–321
12. Brovarets’ OO, Voiteshenko IS, Hovorun DM (2018) Physicochemical profiles of the wobbleWatson-Crick G*·2AP(w)↔G·2AP(WC) and A·2AP(w)↔A*·2AP(WC) tautomerisations: A QM/QTAIM comprehensive survey. Phys Chem Chem Phys 20:623–636
13. Gad SF, El-Demerdash SH, El-Mehasseb IM, El-Nahas AM (2019) Structure, stability and conversions of tautomers and rotamers of azulene-based uracil analogue. J Mol Struct 1182:271–282
14. Löwdin P-O (1963) Proton tunneling in DNA and its biological implications. Rev Mod Phys 35:724–732
15. Löwdin P-O (1966) Quantum genetics and the aperiodic solid: Some aspects on the biological problems of heredity, mutations, aging, and tumors in view of the quantum theory of the DNA molecule. In: Löwdin P-O (ed) Advances in Quantum Chemistry. Academic Press, New York, NY, London, pp 213–360
16. Polo DS, Mendieta-Moreno J, Trabada DG, Mendieta J, Ortega J (2019) Proton transfer in guanine-cytosine base pairs in B-DNA. J Chem Theor Comput 15:6984–6991
17. Slocombe L, Al-Khalili JS, Sacchi M (2021) Quantum and classical effects in DNA point mutations: Watson-Crick tautomerism in AT and GC base pairs. Phys Chem Chem Phys 23:4141–4150
18. Ceron-Carrasco JP, Requena A, Zuniga J, Michaux C, Perpete EA, Jaccquemin D (2009) Intermolecular proton transfer in microhydrated guanine-cytosine base pairs: A new mechanism for spontaneous mutation in DNA. J Phys Chem A 113:10549–10556
19. Brovarets’ OO, Hovorun DM (2015) New structural hypostases of the A-T and G-C Watson-Crick DNA base pairs caused by their mutagenic tautomerisation in a wobblar manner: A QM/QTAIM prediction. RSC Adv 5:99594–99605
20. Brovarets’ OO, Oliynyk TA, Hovorun DM (2019) Novel tautomerisation mechanisms of the biologically important conformers of the reverse Löwdin, Hoogsteen, and reverse Hoogsteen G*-C* DNA base pairs via proton transfer: A quantum-mechanical survey. Front Chem 7:597
21. Brovarets’ OO, Muradova A, Hovorun DM (2020) A quantum-mechanical looking behind the scene of the classical G-C nucleobase pairs tautomerization. Front Chem 8:574454
22. Brovarets’ OO, Muradova A, Hovorun DM (2021) Novel mechanisms of the conformational transformations of the biologically important G-C nucleobase pairs in Watson-Crick, Hoogsteen and wobble configurations via the mutual rotations of the bases around the intermolecular H-bonds: A QM/QTAIM study. RSC Adv 11:25700–25730
23. Brovarets’ OO, Hovorun DM (2015) Tautomeric transition between wobble A-C DNA base mispair and Watson-Crick-like A-C* mismatch: Microstructural mechanism and biological significance. Phys Chem Chem Phys 17:15103–15110
24. Brovarets’ OO, Hovorun DM (2016) By how many tautomerisation routes the Watson–Crick-like A*C* DNA base mispair is linked with the wobble mismatches? A QM/QTAIM vision from a biological point of view. Struct Chem 27:119–131
25. Brovarets’ OO, Hovorun DM (2020) Quantum dancing of the wobble G-T(U/5BrU) nucleobase pairs and its biological roles. Chem Phys 1:100006
26. Brovarets’ OO, Hovorun DM (2015) Novel physico-chemical mechanism of the mutagenic tautomerisation of the Watson–Crick-like A-G and C-T DNA base mispairs: A quantum-chemical picture. RSC Adv 5:66318–66333
27. Frisch MJ, Trucks, GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, … Pople JA (2010) GAUSSIAN 09 (Revision B.01). Wallingford CT, Gaussian Inc
28. Parr RG, Yang W (1989) Density-functional theory of atoms and molecules. Oxford University Press, Oxford
29. Lee C, Yang W, Parr RG (1988) Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. Phys Rev B 37:785–789
30. Hariraran PC, Pople JA (1973) The influence of polarization functions on molecular orbital hydrogenation energies. Theor Chim Acta 28:213–222
31. Krishnan R, Binkley JS, Seeger R, Pople JA (1980) Self-consistent molecular orbital methods. XX. A basis set for correlated wave functions. J Chem Phys 72:650–654
32. Matta CF (2010) How dependent are molecular and atomic properties on the electronic structure method? Comparison of Hartree-Fock, DFT, and MP2 on a biologically relevant set of molecules. J Comput Chem 31:1297–1311
33. Brovarets’ OO, Zhurakivsky RO, Hovorun DM (2015) DPT tautomerisation of the wobble guanine-thymine DNA base mispair is not mutagenic: QM and QTAIM arguments. J Biomol Struct Dyn 33:674–689
34. Brovarets OO, Hovorun DM (2021) Does the G-G*syn DNA mismatch containing canonical and rare tautomers of the guanine tautomerise through the DPT? A QM/QTAIM microstructural study. Mol Phys 112:3033–3046
35. Peng C, Ayala PY, Schlegel HB, Frisch MJ (1996) Using redundant internal coordinates to optimize equilibrium geometries and transition states. J Comput Chem 17:49–56
36. Garcia-Morenos BE, Dwyer JJ, Gittis AG, Lattman EE, Spencer DS, Stites WE (1997) Experimental measurement of the effective dielectric in the hydrophobic core of a protein. Biophys Chem 64:211–224
37. Bayley ST (1951) The dielectric properties of various solid crystalline proteins, amino acids and peptides. Trans Faraday Soc 47:509–517
38. Frisch MJ, Head-Gordon M, Pople JA (1990) Semi-direct algorithms for the MP2 energy and gradient. Chem Phys Lett 166:281–289
39. Kendall RA, Dunning Jr TH, Harrison RJ (1992) Electron affinities of the first-row atoms revisited. Systematic basis sets and wave functions. J Chem Phys 96:6796–6806
40. Bader RFW (1990) Atoms in molecules: A quantum theory. Oxford University Press, Oxford
41. Keith, T.A. (2010). AIMAll (Version 10.07.01). Retrieved from aim.tgristmill.com.
42. Matta CF, Hernández-Trujillo J (2003) Bonding in polycyclic aromatic hydrocarbons in terms of the electron density and of electron delocalization. J Phys Chem A 107:7496–7504
43. Matta CF, Castillo N, Boyd RJ (2006) Atomic contributions to bond dissociation energies in aliphatic hydrocarbons. J Chem Phys 125(20):204103
44. Cukrowski I, Matta CF (2010) Hydrogen–hydrogen bonding: A stabilizing interaction in strained chelating rings of metal complexes in aqueous phase. Chem Phys Lett 499:66–69
45. Lecomte C, Espinosa E, Marta CF, Castillo N, Boyd RJ (2003) Bonding in polycyclic aromatic hydrocarbons in terms of the electron density and of electron delocalization. J Phys Chem A 107:7496–7504
Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.