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# Solvent effects on stability and $^{15}N$ NMR shielding of 5-methylcytosine tautomers: A theoretical approach

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ABSTRACT

The structure and energies of the tautomers of 5-methylcytosine in gas phase were predicted using Density Functional Theory (DFT) method. Solvent-induced effects on stability and $^{15}N$ NMR shielding on the most stable tautomers of 5-methylcytosine were calculated using DFT combined with the polarizable continuum model (PCM) and using the gauge-invariant atomic orbitals (GIAO). In a wide range of solvent dielectrics, the 1-H-oxo-amino form (T6) is predicted as the most stable tautomer and the total electronic energy values of the more stable tautomers in the liquid phase decrease with an increase in the dielectric constant. Direct and indirect solvent effects on $^{15}N$ NMR shielding of the pyrimidine ring of three dominant tautomers are also calculated. It has been shown that in trivalent nitrogens, the observed solvent-induced shielding variation is more strongly related to the intensity of the solvent reaction field rather than on the change of molecular geometry induced by the solvent.



## 1. Introduction

Most of the current investigations in quantum chemistry consist of the study of chemical processes in condensed phases. Thus, self-consistent reaction field (SCRF) models, which are based on a very simple but powerful approach to treat the solvent, allow a quantum mechanical description of the solute at a computational cost slightly higher than that required in gas phase calculations. However, some important electronic effects associated with specific solute–solvent interactions are neglected by these methods [1]. SCRF is based on Onsager reaction field theory of electrostatic solvation. In this model, the solvent is considered as a uniform dielectric with a given dielectric constant, $\varepsilon$. The solute is placed into a cavity within the solvent [2]. SCRF approaches differ in how they define the cavity and the reaction field. Tomasi's Polarized Continuum Model (PCM) [3] defines the cavity as a union of a series of interlocking atomic spheres. PCM is a method directed to study the electronic structure and properties of molecular systems in the presence of solvent effects. In this approach the solvent is represented as a continuous and homogeneous dielectric medium while the solute, which is assumed to occupy a cavity of suitable shape inside the continuum medium, is described at the chosen quantum mechanical level. The reaction potential of the medium polarized by the solute charge distribution is described with the aid of an apparent charge distribution spread on the cavity surface [14]. The effect of polarization of the solvent continuum is represented numerically [3]. In more detail, the solute wave function is determined by a nonlinear Schrödinger equation:

$$H_M\Psi = E\Psi \& H_M = H_M^0 + V_{MS}$$

where $H_M^0$ is the Hamiltonian of the isolated molecule and $V_{MS}$ is the solute–solvent interaction potential operator, in which a part, $V(\Psi)$, depends on the solute wave function [14]. It is this term which introduces the nonlinearity in the Hamiltonian.

Heterocyclic tautomerism has been studied extensively for the past two decades due to its biological importance and highly solvent-dependent nature [4]. The relative stability of tautomers of the nucleobases is important for the structure and functioning of DNA. The occurrence of certain tautomers has been suggested as a possible mechanism of spontaneous mutation [5]. Numerous calculations have been reported for the lowest energy tautomers of cytosine and its methyl derivatives, both as isolated molecules and interacting with water molecules [1,6–10].

Knowledge of the tautomerisation energies in a simple model for molecules such as cytosine or other pyrimidine bases can provide useful information on the intrinsic stability of various tautomers of molecules. In addition, knowing how these tautomerisation energies change in different environments can give an insight into the influence of solvent effects on molecular stability [8]. It has

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been shown that solute–solvent interactions can affect the relative stability of the tautomeric forms [4].

Heterocyclic tautomeric equilibria are highly sensitive to the environmental effects such as solvent polarity. For example, the equilibrium constant for the pyridone/hydroxy pyridine equilibrium has been shown to change by a factor 1000 on going from a polar to a non polar solvent [11]. It is very likely that the interpretation of data obtained in solution in terms of the relative stability of the tautomers in the gas phase will be erroneous. Therefore, the effect of the solvation and association of environmental effects is an essential prerequisite.

*Ab initio* calculation of nuclear magnetic shielding has become an indispensable aid in the investigation of molecular structure and accurate assignment of NMR spectra of compounds. Because most of the systems studied experimentally are in solution, the formulation of satisfactory theoretical models for solvated systems has been the object of continuously increasing interest [12].

In this study, the polarizable continuum model (PCM), without any explicit solvent molecules, and the gauge-invariant atomic orbital (GIAO) method are used to calculate solvent effects on relative stabilities and nitrogen NMR shielding on the pyrimidine ring of the most stable 5-methylcytosine tautomers (Fig. 1) in a wide range of solvents encompassing a broad spectrum of dielectric constant, $\varepsilon$. The diversity of nitrogen atoms in these molecules makes them good candidates for a preliminary investigation of the influence of solvent polarity on nuclear magnetic shielding. Direct and indirect contributions to the total solvation effect are also examined. Direct effects involve perturbation of the solvent on the electronic wave function of the solute held at fixed geometry; indirect effects are due to the relaxation of the solute geometry under the influence of the solvent [12].

In this research, we studied the energy and the shielding variation in terms of nonspecific solute–solvent interactions and do not include specific influences that may arise from hydrogen bonding, protonation, molecular association, ionic interactions, aromaticity of solvent, or any other through-space magnetic shielding effects.

## 2. Computational details

Geometry optimization and shielding calculations for all seven tautomers of 5-methylcytosine in the gas and solution phases were performed with Gaussian 03 [13]. Full optimization of geometries has been carried out at the B3LYP/6-31G* level. Nuclear magnetic resonance (NMR) calculations have been done with the B3LYP method and 6-311++G** basis set. Geometry optimizations were performed without any symmetry constraint.

Relative solvent effects on $^{15}$N NMR shielding of the pyrimidine rings were calculated using the corresponding nuclear shielding in cyclohexane as reference. Direct ($\Delta\sigma_{dir}$) and indirect ($\Delta\sigma_{ind}$) solvent effects are obtained with a slight modification of the method used by Cammi et al [14]. Instead of deriving $\Delta\sigma_{ind}$ from the difference of the PCM optimized shielding and the PCM shielding of the molecule held at the geometry optimized in vacuum, it is obtained from the shielding calculated in vacuum for a molecule that is geometry optimized in solution. Thus,

$$\Delta\sigma_{dir} = \sigma_{sol}(R_v) - \sigma_{cyc}(R_v)$$
$$\Delta\sigma_{ind} = \sigma_{vac}(R_s) - \sigma_{vac}(R_{cyc})$$

where $\sigma_{sol}(R_v)$ is the value of the nuclear shielding computed in solution but with the solute in the geometry optimized in vacuum, and $\sigma_{vac}(R_s)$ is the value of the nuclear shielding in vacuum but with the solute geometry optimized in solution. $\sigma_{cyc}(R_v)$ and $\sigma_{vac}(R_{cyc})$ are the corresponding parameters for calculations with cyclohexane.

## 3. Results and discussion

### 3.1. Gas phase

The energies and relative stabilities of 5-methylcytosine structures in the gas phase and in water are given in Table 1. The obtained relative stabilities at the DFT level revealed the 1-H-oxo-amino (T6) form to be at the lowest energy. Moreover the results indicate that a substantial amount of the 1-H-oxo-amino (T6), hydroxy-amino (T4), and oxo-imino (T7) can be present in the gas phase. This is in agreement with previous experimental studies [10].

### 3.2. Solvent effects on structure

1-H-oxo-amino form is predicted to be the most stable form in water (Table 1). Our calculation revealed that the hydroxy-amino form becomes considerably destabilized by solvation. Regular variations for energy changes versus dielectric constant were observed for stable tautomers (1-H-oxo-amino, 3-H-oxo-amino (T1), and oxo-imino) in solution phase (see Fig. 2 and Table 2). It is well observed that energy values decrease nonlinearly with increasing in the solvent dielectric constant. It is clear that an increase in dielectric constants increases the solute–solvent electrostatic interac-

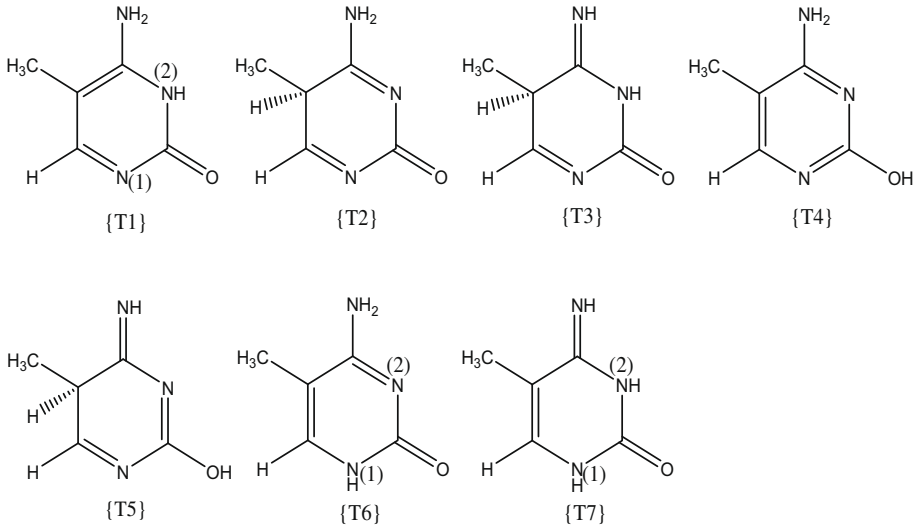


**Fig. 1.** Structures of 5-methylcytosine tautomers. The pyrimidine-type nitrogens in the stable tautomers are marked.

**Table 1**
Energies and relative stabilities of 5-methylcytosine tautomers.[a]

| | Gas phase ($\varepsilon = 1$) | | Water ($\varepsilon = 78.39$) | |
|---|---|---|---|---|
| | *E* | *R.E* | *E* | *R.E* |
| T1 | −434.2351629 | 6.8509 | −434.2717602 | 3.9167 |
| T2 | −434.2102683 | 22.4725 | −434.2673922 | 6.6576 |
| T3 | −434.2163962 | 18.6272 | −434.2425963 | 22.2173 |
| T4 | −434.2447220 | 0.8525 | −434.2673921 | 6.6577 |
| T5 | −434.1940410 | 32.6553 | −434.2179422 | 37.6880 |
| T6 | −434.2460806 | 0.0000 | −434.2780019 | 0.0000 |
| T7 | −434.2432367 | 1.7845 | −434.2710719 | 4.3486 |

[a] *E*, absolute energy (in Hartree); *R.E*, relative energy (in kcal/mol).

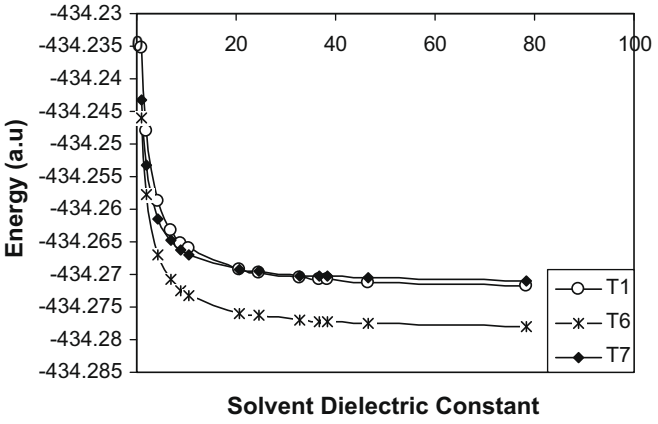


**Fig. 2.** Variation of energy with $\varepsilon$ for T1, T6, and T7.

**Table 2**
Absolute energies (a.u) of T1, T6, and T7 tautomers in different solvents.

| Solvent | Dielectric constant ($\varepsilon$) | T1 | T6 | T7 |
|---|---|---|---|---|
| Cyclohexane | 2.023 | −434.2479904 | −434.2576344 | −434.2532991 |
| Ether | 4.335 | −434.2586930 | −434.2669727 | −434.2614328 |
| Aniline | 6.890 | −434.2632154 | −434.2708357 | −434.2648041 |
| Dichloromethane | 8.930 | −434.2651575 | −434.2724811 | −434.2662408 |
| Dichloroethane | 10.36 | −434.2661049 | −434.2732769 | −434.2669386 |
| Acetone | 20.70 | −434.2692449 | −434.2759125 | −434.2692400 |
| Ethanol | 24.55 | −434.2697653 | −434.2763461 | −434.2696202 |
| Methanol | 32.63 | −434.2704719 | −434.2769332 | −434.2701351 |
| Acetonitrile | 36.64 | −434.2707097 | −434.2771306 | −434.2703081 |
| Nitromethane | 38.20 | −434.2707890 | −434.2771964 | −434.2703662 |
| Dimethylsulfoxide | 46.70 | −434.2711299 | −434.2774802 | −434.2706146 |
| Water | 78.39 | −434.2717602 | −434.2780019 | −434.2710719 |

tions, increases the dipole moment of solute (see Fig. 3 and Table 3), and finally increases the stability of solute.

### 3.3. Solvent effects on NMR spectra

The variations of nuclear magnetic shielding of the pyrimidine ring with the solvent dielectric constant for 1-H-oxo-amino, 3-H-oxo-amino, and oxo-imino tautomers were calculated. Calculated PCM–GIAO shielding data for the T1, T6, and T7 tautomers in a range of solvents available in Gaussian 03 are given in Tables 4–6, respectively. The shielding effect of $N_1$ in 3-H-oxo-amino form and $N_2$ in 1-H-oxo-amino form increases with the increasing the polarity of the solvent used.

The opposite effect is observed for $N_2$ in 3-H-oxo-amino form, $N_1$ in 1-H-oxo-amino form and $N_1$ and $N_2$ in oxo-imino form. In other words, as the dielectric constant of the solvent increases, trivalent and tetravalent nitrogens are shielded and deshielded,

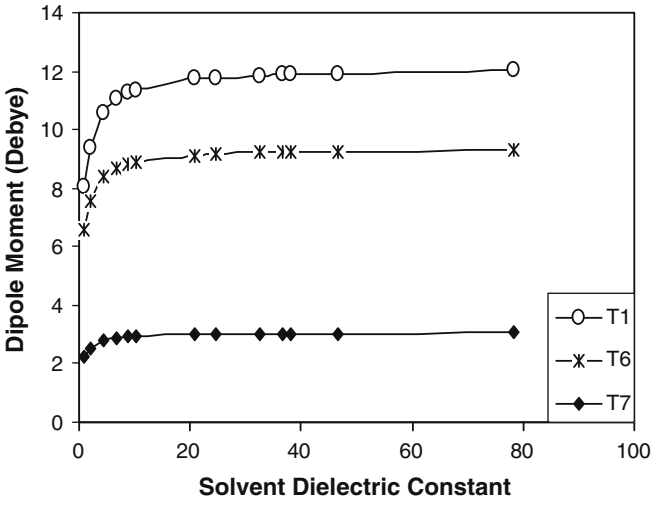


**Fig. 3.** Variation of dipole moment with $\varepsilon$ for T1, T6, and T7.

**Table 3**
Variation of dipole moment (Debye) with $\varepsilon$ for T1, T6, and T7.

| Solvent | Dielectric constant ($\varepsilon$) | T1 | T6 | T7 |
|---|---|---|---|---|
| Vacuum | 1.000 | 8.0180 | 6.5536 | 2.2350 |
| Cyclohexane | 2.023 | 9.3805 | 7.5648 | 2.5301 |
| Ether | 4.335 | 10.5487 | 8.3694 | 2.7668 |
| Aniline | 6.890 | 11.0541 | 8.6933 | 2.8685 |
| Dichloromethane | 8.930 | 11.2638 | 8.8342 | 2.9124 |
| Dichloroethane | 10.36 | 11.3681 | 8.8902 | 2.9327 |
| Acetone | 20.70 | 11.7328 | 9.1348 | 3.0019 |
| Ethanol | 24.55 | 11.7756 | 9.1642 | 3.0127 |
| Methanol | 32.63 | 11.8602 | 9.2125 | 3.0255 |
| Acetonitrile | 36.64 | 11.8798 | 9.2258 | 3.0292 |
| Nitromethane | 38.20 | 11.8863 | 9.2303 | 3.0351 |
| Dimethylsulfoxide | 46.70 | 11.9143 | 9.2641 | 3.0405 |
| Water | 78.39 | 12.0092 | 9.3146 | 3.0583 |

**Table 4**
GIAO nitrogen NMR shielding (ppm) of pyrimidine heterocycle for T1.

| Solvent | Dielectric constant ($\varepsilon$) | N(1) (ppm) | N(2) (ppm) |
|---|---|---|---|
| Vacuum | 1.000 | −38.9812 | 98.1047 |
| Cyclohexane | 2.023 | −24.8260 | 96.4470 |
| Ether | 4.335 | −13.1486 | 95.1580 |
| Aniline | 6.890 | −8.1970 | 94.6895 |
| Dichloromethane | 8.930 | −6.2767 | 94.4111 |
| Dichloroethane | 10.36 | −5.2564 | 94.3157 |
| Acetone | 20.70 | −1.6900 | 94.1059 |
| Ethanol | 24.55 | −1.2152 | 94.0140 |
| Methanol | 32.63 | −0.5117 | 93.9233 |
| Acetonitrile | 36.64 | −0.2933 | 93.8817 |
| Nitromethane | 38.20 | −0.2255 | 93.8679 |
| Dimethylsulfoxide | 46.70 | 0.0874 | 93.8063 |
| Water | 78.39 | 0.9000 | 93.8343 |

respectively. We attributed these trends to the delocalization of the lone pair electrons of tetravalent nitrogens into the Π-electron system of the aromatic ring, as influenced by either solvent polarity or some forms of specific solvent-to-solute interaction.

As mentioned earlier, the total solvation effect consists of two distinct contributions: $\Delta\sigma_{dir}$ and $\Delta\sigma_{ind}$. The former contribution is directly related to the intensity of the solvent reaction field used in the PCM calculation, whereas the latter is due to the relaxation of the molecular geometry of the solute brought about by the solvent. Tables 7–9 list $\Delta\sigma_{dir}$ and $\Delta\sigma_{ind}$ calculated for the T1, T6, and T7 tautomers, respectively. The presented results show that $\Delta\sigma_{dir}$

**Table 5**
GIAO nitrogen NMR shielding (ppm) of pyrimidine heterocycle for T6.

| Solvent | Dielectric constant ($\varepsilon$) | N(1) (ppm) | N(2) (ppm) |
|---|---|---|---|
| Vacuum | 1.000 | 93.0462 | 3.7153 |
| Cyclohexane | 2.023 | 92.4357 | 11.0832 |
| Ether | 4.335 | 91.9207 | 16.8697 |
| Aniline | 6.890 | 91.5245 | 19.0836 |
| Dichloromethane | 8.930 | 91.3447 | 20.0152 |
| Dichloroethane | 10.36 | 91.2292 | 20.5140 |
| Acetone | 20.70 | 91.1670 | 22.5471 |
| Ethanol | 24.55 | 91.0969 | 22.8235 |
| Methanol | 32.63 | 90.9966 | 23.1219 |
| Acetonitrile | 36.64 | 90.9662 | 23.2461 |
| Nitromethane | 38.20 | 91.0148 | 23.2436 |
| Dimethylsulfoxide | 46.70 | 90.9674 | 23.4256 |
| Water | 78.39 | 90.9820 | 23.9680 |

**Table 6**
GIAO nitrogen NMR shielding (ppm) of pyrimidine heterocycle for T7.

| Solvent | Dielectric constant ($\varepsilon$) | N(1) (ppm) | N(2) (ppm) |
|---|---|---|---|
| Vacuum | 1.000 | 118.3405 | 93.4679 |
| Cyclohexane | 2.023 | 115.7566 | 92.5412 |
| Ether | 4.335 | 113.3933 | 91.5030 |
| Aniline | 6.890 | 112.4113 | 91.0820 |
| Dichloromethane | 8.930 | 111.9736 | 90.8914 |
| Dichloroethane | 10.36 | 111.7658 | 90.8076 |
| Acetone | 20.70 | 111.0460 | 90.4905 |
| Ethanol | 24.55 | 110.9370 | 90.4523 |
| Methanol | 32.63 | 110.7972 | 90.4112 |
| Acetonitrile | 36.64 | 110.7528 | 90.4049 |
| Nitromethane | 38.20 | 110.7044 | 90.3469 |
| Dimethylsulfoxide | 46.70 | 110.6402 | 90.3374 |
| Water | 78.39 | 110.4848 | 90.2566 |

**Table 7**
Value of $\Delta\sigma_{dir}$ and $\Delta\sigma_{ind}$ calculated for T1.

| Solvent | Dielectric constant ($\varepsilon$) | $\Delta\sigma_{dir}$ (ppm) | | $\Delta\sigma_{ind}$ (ppm) | |
|---|---|---|---|---|---|
| | | N(1) | N(2) | N(1) | N(2) |
| Cyclohexane | 2.023 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| Ether | 4.335 | 9.8361 | −2.2235 | 0.7612 | 0.4910 |
| Aniline | 6.890 | 13.8147 | −3.1800 | 1.1107 | 0.7003 |
| Dichloromethane | 8.930 | 15.4931 | −3.5935 | 1.0293 | 0.7025 |
| Dichloroethane | 10.36 | 16.3045 | −3.7956 | 1.0962 | 0.7403 |
| Acetone | 20.70 | 18.9645 | −4.4680 | 1.4938 | 0.9347 |
| Ethanol | 24.55 | 19.4014 | −4.5799 | 1.4913 | 0.9339 |
| Methanol | 32.63 | 19.9916 | −4.7317 | 1.4289 | 0.9221 |
| Acetonitrile | 36.64 | 20.1900 | −4.7829 | 1.4327 | 0.9221 |
| Nitromethane | 38.20 | 20.2562 | −4.8000 | 1.4265 | 0.9221 |
| Dimethylsulfoxide | 46.70 | 20.5405 | −4.8736 | 1.4293 | 0.9200 |
| Water | 78.39 | 21.0629 | −5.0092 | 1.5378 | 0.9901 |

**Table 8**
Value of $\Delta\sigma_{dir}$ and $\Delta\sigma_{ind}$ calculated for T6.

| Solvent | Dielectric constant ($\varepsilon$) | $\Delta\sigma_{dir}$ (ppm) | | $\Delta\sigma_{ind}$ (ppm) | |
|---|---|---|---|---|---|
| | | N(1) | N(2) | N(1) | N(2) |
| Cyclohexane | 2.023 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| Ether | 4.335 | −1.4446 | 5.6867 | 0.6572 | −0.5665 |
| Aniline | 6.890 | −2.0989 | 7.9842 | 0.7716 | −1.0180 |
| Dichloromethane | 8.930 | −2.3873 | 8.9536 | 0.8057 | −1.2557 |
| Dichloroethane | 10.36 | −2.5293 | 9.4223 | 0.8119 | −1.2606 |
| Acetone | 20.70 | −3.0072 | 10.9599 | 1.0457 | −1.1172 |
| Ethanol | 24.55 | −3.0875 | 11.2125 | 1.0448 | −1.1160 |
| Methanol | 32.63 | −3.1967 | 11.5539 | 1.0232 | −1.2381 |
| Acetonitrile | 36.64 | −3.2336 | 11.6687 | 1.0250 | −1.2386 |
| Nitromethane | 38.20 | −3.2460 | 11.7070 | 1.0628 | −1.3486 |
| Dimethylsulfoxide | 46.70 | −3.2991 | 11.8715 | 1.0608 | −1.3471 |
| Water | 78.39 | −3.3974 | 12.1738 | 1.1211 | −1.1689 |

**Table 9**
Value of $\Delta\sigma_{dir}$ and $\Delta\sigma_{ind}$ calculated for T7.

| Solvent | Dielectric constant ($\varepsilon$) | $\Delta\sigma_{dir}$ (ppm) | | $\Delta\sigma_{ind}$ (ppm) | |
|---|---|---|---|---|---|
| | | N(1) | N(2) | N(1) | N(2) |
| Cyclohexane | 2.023 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| Ether | 4.335 | −1.9189 | −0.3477 | −0.5007 | −0.8449 |
| Aniline | 6.890 | −2.7405 | −0.5133 | −0.6859 | −1.1920 |
| Dichloromethane | 8.930 | −3.0948 | −0.5880 | −0.7811 | −1.3535 |
| Dichloroethane | 10.36 | −3.2678 | −0.6252 | −0.8211 | −1.4211 |
| Acetone | 20.70 | −3.8424 | −0.7521 | −0.9872 | −1.6928 |
| Ethanol | 24.55 | −3.9378 | −0.7737 | −1.0024 | −1.7207 |
| Methanol | 32.63 | −4.0673 | −0.8032 | −1.0148 | −1.7444 |
| Acetonitrile | 36.64 | −4.1109 | −0.8132 | −1.0157 | −1.7434 |
| Nitromethane | 38.20 | −4.1255 | −0.8166 | −1.0538 | −1.8111 |
| Dimethylsulfoxide | 46.70 | −4.1882 | −0.8310 | −1.0558 | −1.8101 |
| Water | 78.39 | −4.3038 | −0.8579 | −1.1001 | −1.8886 |

decreased for tetravalent nitrogens in the pyrimidine ring with solvent dielectric constant and opposite effect occurred for trivalent nitrogens. On the other hand, in tetravalent nitrogens, $\Delta\sigma_{ind}$ is very effective on chemical shielding as compared with $\Delta\sigma_{dir}$, but in trivalent nitrogens, $\Delta\sigma_{ind}$ is less effective on chemical shielding in comparison with $\Delta\sigma_{dir}$.

## 4. Conclusion

This work is a brief assessment of the reliability of the polarizable continuum model in describing the influence of solvent on relative stability and $^{15}N$ NMR shielding for three dominant tautomers of 5-methylcytosine. The presented results show that PCM, in its simplest application, is able to reproduce the key aspects of solvent effect: its magnitude and sign. The approach used, however, does not take into account the consequences of specific solute–solvent interactions. B3LYP level of theory combined with 6-31G(d) basis set predicted that the total electronic energy values of the most stable tautomers in liquid phase decrease with increase in dielectric constant. Direct and indirect analysis of contributions to the total solvent effect shows that in trivalent nitrogens, the intensity of the reaction field determines shielding variation more than solute geometry does. This can serve as an important consideration when doing a large number of calculations to investigate solvent effects on nuclear magnetic shielding.

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