International Journal of Science and Research (IJSR)
ISSN (Online): 2319-7064
Index Copernicus Value (2013): 6.14 | Impact Factor (2013): 4.438

# Global and Reactivity Descriptors Studies of Cyanuric Acid Tautomers in Different Solvents by using of Density Functional Theory (DFT)

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**Abstract:** ***Density functional theory method was used to study HOMO-LUMO energies and global reactivity descriptors of cyanuric acid tautomers at level of B3LYP theory and 6-311++G (d,p) basis set. The effects of solvents on the tautomeric structure properties were studied by means of the self-consistent reaction-field (SCRF) method based on PCM. CA8 tautomer in gas phase, CA5 tautomer in all solvents act as a hard acid because the higher the energy of the LUMO of an acid, the harder it is as an acid. The order of the stability of tautomers in gas phase: CA11 ≈ CA1> CA10 > CA3 > CA2 > CA6 > CA7 > CA4> CA5 > CA9 > CA8. According to electrophilicity index (ω), the tautomer CA8 is a good electrophile in gas phase and in solvents which is act as a good, more reactive, nucleophile.***

**Keywords:** Cyanuric acid tautomers, HOMO-LUMO energy gap, chemical hardness (η) and electrophilicity index (ω).

## 1. Introduction

Cyanuric acid ($C_3H_3N_3O_3$) existing in two tautomeric forms, one is enol form (2,4,6-trihydroxy-1,3,5- triazine) and another one is keto form (1,3,5-triazine-2,4,6- trione). Their derivatives are of great interest for the both in theoretical and practical applications and have been comprehensively applied in both everyday life and industries since late 1950s [1]. The isocyanuric acid functional derivatives differ with high thermal-physical and physical-mechanical parameters and are recommended as a modifier to create different composite materials to be applied [2–4]. Isocyanuric acid derivatives reveal fungicidal, bactericidal, flame retardants and other important properties [5] and exhibiting biological activity are used in pharmacology [6] and extensively applied, for instance, as dyestuffs, optical bleaches, surface active agents and pesticides [7,8].

The prediction of the reactivity of chemical species is one of the main purposes of theoretical chemistry and a lot of work has been done on this line. Density functional theory [9, 10] has been quite successful in providing theoretical background of popular qualitative chemical concepts. In this context, several reactivity descriptors have been proposed and used to analyze chemical reactivity and site selectivity. Hardness, global softness, electronegativity and polarizability are the global reactivity descriptors widely used to understand the global nature of molecules in terms of their stability and it is possible to gain knowledge about the reactivity of molecules.

## 2. Theoretical Background

### Global and local reactivity descriptors

From the Koopman's theorem, the ionization potential (IP) and electron affinity (EA) are the Eigen value of the HOMO and LUMO with change of sign [11]

$$IP \approx -E_{HOMO} \text{ and } EA \approx -E_{LUMO} \quad (1)$$

Several global chemical reactivity descriptors of molecules such as hardness (η), chemical potential (μ) , softness (S), electronegativity (χ) and electrophilicity index (ω) were calculated based on the density functional theory (DFT). The global hardness ( η ), and chemical potential (μ) [12-15] is defined as the second and first derivative of the energy (E), with respect to the number of electrons (N), at constant external potential, $v(\vec{r})$, captures the resistance of a chemical species to changing its electronic number

$$\eta = \frac{1}{2}\left(\frac{\partial^2 E}{\partial N^2}\right)_{V(\vec{r})} \text{ and } \mu = \left(\frac{\partial E}{\partial N}\right)_{V(\vec{r})} \quad (2)$$

In equation (2), E and $v(\vec{r})$ are electronic energy and external potential of an N-electron system respectively. Softness [16] is a property of molecules that measures the extent of chemical reactivity. It is the reciprocal of hardness and electronegativity has been defined as the negative of the electronic chemical potential in Mulliken sense.

$$S = \frac{1}{\eta} \text{ and } \chi = -\mu = \left(\frac{\partial E}{\partial N}\right)_{V(\vec{r})} \quad (3)$$

Using Koopmans theorem for closed-shell molecules, η, μ and χ can be redefined as:

$$\eta \approx \frac{1}{2}(IP - EA) \approx \frac{1}{2}(\varepsilon_{LUMO} - \varepsilon_{HOMO}) \quad (4)$$

$$\mu \approx \frac{1}{2}(IP + EA) \approx \frac{1}{2}(\varepsilon_{HOMO} - \varepsilon_{LUMO}) \quad (5)$$

$$\chi = \frac{I + A}{2} \quad (6)$$

The concept of electrophilicity viewed as a reactivity index was introduced by Parr et al.[12] It is based on a second order expansion of the electronic energy with respect to the charge transfer ΔN at fixed geometry. This index, which measures the stabilization in energy when the system acquires an additional electronic charge ΔN from the environment, is defined by the following simple and more

familiar form [17] in terms of the electronic chemical potential (μ) and the chemical hardness( η ). Electrophilicity is a useful structural depictor of reactivity and is frequently used in the analysis of the chemical reactivity of molecules.

$$\omega = \frac{\mu^2}{2\eta} \quad (7)$$

On the other hand, the maximum amount of electronic charge that an electrophile system may accept is given by [18]

$$\Delta N_{max} = -\frac{\mu}{\eta} \quad (8)$$

The maximum charge transfer $\Delta N_{max}$ towards the electrophile was evaluated using Eq. (8).Thus, while the quantity defined by Eq. (8) describes the propensity of the system to acquire additional electronic charge from the environment; the quantity defined in Eq. (7) describes the charge capacity of the molecule.

Very recently, Ayers and co-workers [19, 20] have proposed two new reactivity indices to quantify nucleophilic and electrophilic capabilities of a leaving group, nucleofugality ($\Delta E_n$) and electrofugality ($\Delta E_e$), defined as follows

$$\Delta E_n = EA + \omega = \frac{(\mu+\eta)^2}{2\eta} \quad (8)$$

$$\Delta E_e = IP + \omega = \frac{(\mu-\eta)^2}{2\eta} \quad (9)$$

## 3. Computational Methods

Molecular geometries of tautomeric forms of Cyanuric acid were fully optimized by using the Gaussian quantum chemistry software package Gaussian 09 w [21] at DFT/B3LYP level of theory, using the 6-311++G (d,p) basis set. Following the geometry optimizations, analytical frequency calculations were preceded following the standard procedures, to obtain the thermo chemical properties. In addition the effects of solvents on the tautomeric structure properties were studied by means of the self-consistent reaction-field (SCRF) method based on PCM developed by Tomasi and coworkers [22] , it is one of the most widely used approaches. In this model, a solute is considered inside a cavity and the solvent as a structure less medium characterized by some parameters such as its dielectric constant, molar volume and polarizability. This consideration can substantially improve the simulation results for the electronic or vibrational spectroscopy of real molecular systems [23,24].The solvents chose for this studies are polar protic solvents namely water (ε = 74.80) and ethanol (ε = 24.55) and polar aprotic solvents like tetrahydrofuran(THF) (ε = 7.50) and dimethylformamide (ε = 38.00).

We focus on the HOMO and LUMO energies in order to determine, the usefulness of global reactivity descriptors namely, Chemical hardness (η), chemical potential (μ), polarizability (α) electrophilicity index (ω), softness (S), nucleofugality, and electrofugality, values for the prediction of the reactivity of the cyanuric acid tautomers.

## 4. Results and Discussion

**Calculation of the HOMO, LUMO and band gaps energies**

Energies of HOMO and LUMO are popular quantum mechanical descriptors. The highest occupied molecular orbital (HOMO), it represents the distribution and energy of the least tightly held electrons in the molecule and the lowest unoccupied molecular orbital (LUMO) because it describes the easiest route to the addition of more electrons to the system. In fact, the energy of the HOMO is a good approximation to the lowest ionization potential of the molecule but the energy of the LUMO generally is a poor approximation to the molecule's electron affinity. A molecule whose HOMO is not doubly occupied or that does not have a large HOMO - LUMO energy gap is chemically reactive.

High value of HOMO energy is likely to indicate a tendency of the molecule to donate electrons to appropriate acceptor molecule of low empty molecular orbital energy. The lower values of LUMO energy show more probability to accept electrons. The concept of hard and soft nucleophiles and electrophiles has been also directly related to the relative energies of the HOMO and LUMO orbital's. Hard nucleophiles have a low energy HOMO, soft nucleopphiles have a high energy HOMO, hard electrophiles have a high energy LUMO and soft electrophiles have a low energy LUMO [25]. HOMO-LUMO gap is an important stability index [26]. Figure 1 shows that of Cyanuric acid the HOMO and LUMO diagrams of eleven structural isomers cyanuric acid tautomers at B3LYP/6-311++G(d,p) level in gas phase.

The calculated HOMO and LUMO energy level, and HOMO-LUMO energy gap ($\Delta E_g$) are summarized in Table 1 in gas phase and different solvents. Results from the table 1, CA11 ≈ CA1 tautomers are stable in an absolute sense, having a large HOMO-LUMO gap comparing other tautomers in gas phase and different solvents. The order of the stability of tautomers in gas phase: CA11 ≈ CA1> CA10 > CA3 > CA2 > CA6 > CA7 > CA4> CA5 > CA9 > CA8. Therefore CA8 tautomer is least stable in gas phase. The order of stability is similar in all solvents, but CA4 tautomer is in ethanol different and the order are: CA11 > CA1 ≈ CA10 > CA3 > CA2 > CA9 > CA8 > CA6 > CA7 > CA4 > CA5. This trend is different from our previous studies of relative emerges of cyanuric acid tautomers [27]. CA8 tautomer in gas

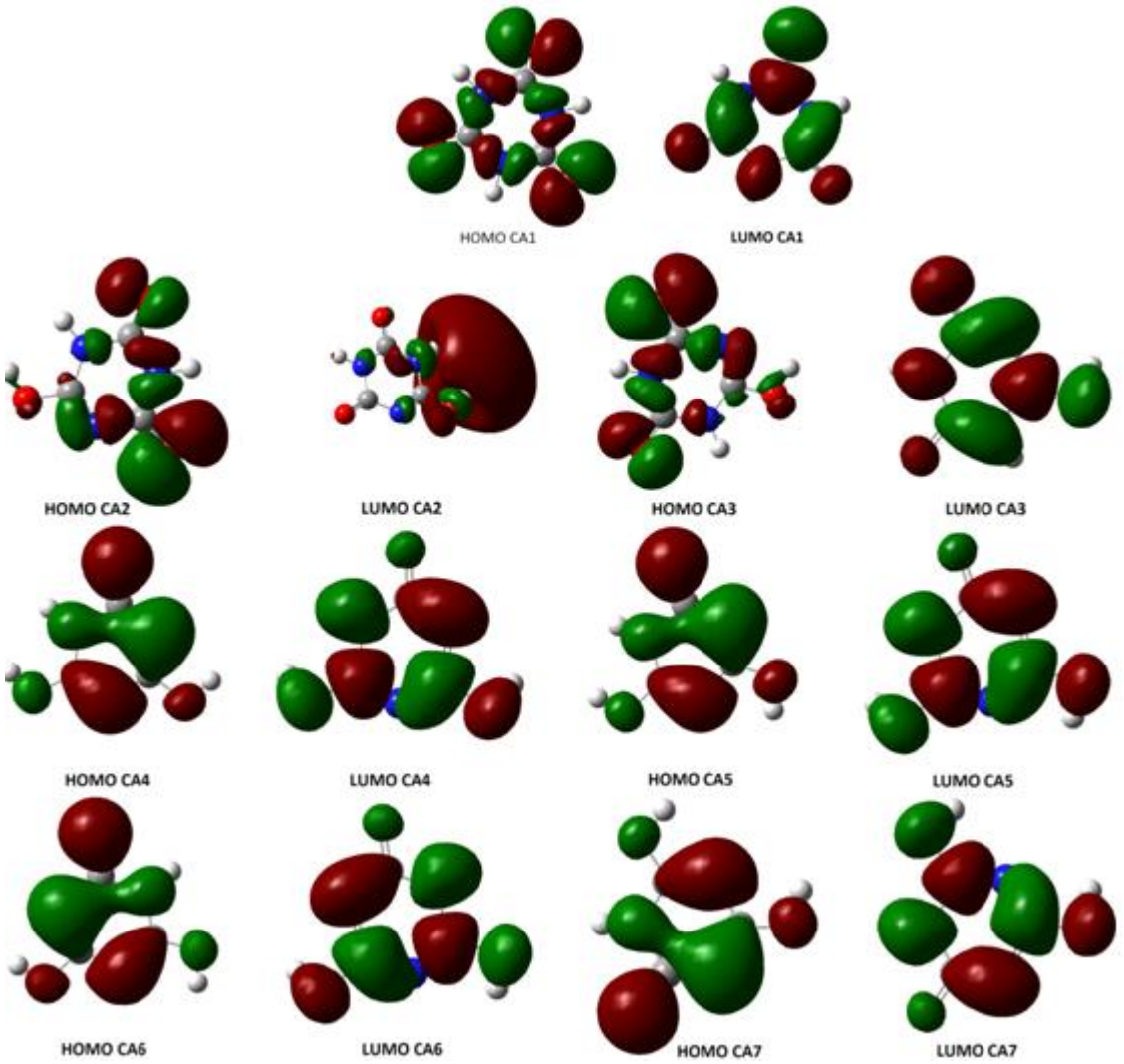


**Figure:** The HOMO and LUMO diagrams of cyanuric acid tautomers at B3LYP/6-311++G(d,p) level in gas phase.

**Table 1:** The theoretical electronic properties (HOMO, LUMO) and energy gap **(**Eg) and reactive descriptors ionization potential (IP), electron affinity (EA), electronegativity (χ), hardness (η), softness (s), chemical potential (μ), softness (S), electrophilicity index (ω), charge transfer ($\Delta N_{max}$), nucleofugality ($\Delta E_n$) and electrofugality ($\Delta E_e$) of cyanuric acid tautomers calculated by B3LYP/6-311++ G(d,p) in gas phase and different solvents

| Tautomers | Gas | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | HOMO | LUMO | $\Delta E_g$ | I | A | χ | η | S | μ | ω | $\Delta N_{max}$ | $\Delta E_n$ | $\Delta E_e$ |
| CA1 | -8.3242 | -1.1021 | 7.2221 | 8.3228 | 1.1029 | 4.7128 | 3.6099 | 0.2770 | -4.7128 | 3.0764 | 1.3055 | 1.9735 | 11.3991 |
| CA2 | -8.0738 | -1.5184 | 6.5554 | 8.0749 | 1.5182 | 4.7965 | 3.2784 | 0.3050 | -4.7965 | 3.5089 | 1.4631 | 1.9907 | 11.5837 |
| CA3 | -8.0874 | -1.4694 | 6.6180 | 8.0860 | 1.4703 | 4.7782 | 3.3079 | 0.3023 | -4.7782 | 3.4510 | 1.4445 | 1.9807 | 11.5370 |
| CA4 | -7.8262 | -1.6354 | 6.1907 | 7.8248 | 1.6365 | 4.7307 | 3.0941 | 0.3232 | -4.7307 | 3.6164 | 1.5289 | 1.9799 | 11.4412 |
| CA5 | -7.7990 | -1.6218 | 6.1771 | 7.7990 | 1.6207 | 4.7099 | 3.0891 | 0.3237 | -4.7099 | 3.5905 | 1.5247 | 1.9697 | 11.3894 |
| CA6 | -7.8235 | -1.5647 | 6.2588 | 7.8235 | 1.5658 | 4.6946 | 3.1288 | 0.3196 | -4.6946 | 3.5220 | 1.5004 | 1.9562 | 11.3454 |
| CA7 | -7.8017 | -1.5565 | 6.2452 | 7.8022 | 1.5571 | 4.6796 | 3.1226 | 0.3202 | -4.6796 | 3.5066 | 1.4986 | 1.9495 | 11.3088 |
| CA8 | -7.5704 | -1.8069 | 5.7635 | 7.5696 | 1.8055 | 4.6875 | 2.8820 | 0.3470 | -4.6875 | 3.8121 | 1.6265 | 2.0066 | 11.3816 |
| CA9 | -7.4670 | -1.5456 | 5.9213 | 7.4659 | 1.5443 | 4.5051 | 2.9608 | 0.3377 | -4.5051 | 3.4274 | 1.5216 | 1.8831 | 10.8933 |
| CA10 | -8.2561 | -1.1456 | 7.1105 | 8.2561 | 1.1467 | 4.7014 | 3.5547 | 0.2813 | -4.7014 | 3.1090 | 1.3226 | 1.9623 | 11.3651 |
| CA11 | -8.3976 | -1.1048 | 7.2928 | 8.3982 | 1.1056 | 4.7519 | 3.6463 | 0.2743 | -4.7519 | 3.0964 | 1.3032 | 1.9908 | 11.4946 |
| **THF** | | | | | | | | | | | | | |
| CA1 | -8.2126 | -0.9470 | 7.2656 | 8.2123 | 0.9475 | 4.5799 | 3.6324 | 0.2753 | -4.5799 | 2.8873 | 1.2609 | 1.9398 | 11.0996 |
| CA2 | -8.1554 | -1.4014 | 6.7540 | 8.1565 | 1.4022 | 4.7794 | 3.3771 | 0.2961 | -4.7794 | 3.3819 | 1.4152 | 1.9797 | 11.5384 |
| CA3 | -8.1636 | -1.3633 | 6.8003 | 8.1628 | 1.3622 | 4.7625 | 3.4003 | 0.2941 | -4.7625 | 3.3352 | 1.4006 | 1.9730 | 11.4980 |
| CA4 | -7.8479 | -1.5239 | 6.3241 | 7.8466 | 1.5236 | 4.6851 | 3.1615 | 0.3163 | -4.6851 | 3.4715 | 1.4819 | 1.9479 | 11.3181 |
| CA5 | -7.8289 | -1.5212 | 6.3077 | 7.8297 | 1.5206 | 4.6752 | 3.1546 | 0.3170 | -4.6752 | 3.4644 | 1.4820 | 1.9438 | 11.2941 |
| CA6 | -7.8588 | -1.4858 | 6.3731 | 7.8596 | 1.4863 | 4.6730 | 3.1867 | 0.3138 | -4.6730 | 3.4263 | 1.4664 | 1.9400 | 11.2859 |
| CA7 | -7.8425 | -1.4858 | 6.3567 | 7.8422 | 1.4860 | 4.6641 | 3.1781 | 0.3147 | -4.6641 | 3.4225 | 1.4676 | 1.9365 | 11.2647 |
| CA8 | -7.7690 | -1.0830 | 6.6860 | 7.7701 | 1.0828 | 4.4264 | 3.3437 | 0.2991 | -4.4264 | 2.9299 | 1.3238 | 1.8472 | 10.7000 |
| CA9 | -7.7772 | -1.0585 | 6.7186 | 7.7775 | 1.0594 | 4.4184 | 3.3590 | 0.2977 | -4.4184 | 2.9059 | 1.3154 | 1.8466 | 10.6834 |
| CA10 | -8.3813 | -1.1211 | 7.2602 | 8.3821 | 1.1211 | 4.7516 | 3.6305 | 0.2754 | -4.7516 | 3.1095 | 1.3088 | 1.9884 | 11.4916 |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| CA11 | -8.4031 | -1.1048 | 7.2983 | 8.4031 | 1.1056 | 4.7543 | 3.6487 | 0.2741 | -4.7543 | 3.0975 | 1.3030 | 1.9919 | 11.5006 |
| **Ethanol** | | | | | | | | | | | | | |
| CA1 | -8.1963 | -0.9225 | 7.2738 | 8.1968 | 0.9225 | 4.5596 | 3.6372 | 0.2749 | -4.5596 | 2.8580 | 1.2536 | 1.9356 | 11.0548 |
| CA2 | -8.1690 | -1.3878 | 6.7812 | 8.1701 | 1.3881 | 4.7791 | 3.3910 | 0.2949 | -4.7791 | 3.3677 | 1.4093 | 1.9796 | 11.5378 |
| CA3 | -8.1826 | -1.3443 | 6.8384 | 8.1832 | 1.3448 | 4.7640 | 3.4192 | 0.2925 | -4.7640 | 3.3189 | 1.3933 | 1.9741 | 11.5021 |
| CA4 | -8.2207 | -1.5075 | 6.7132 | 8.2197 | 1.5075 | 4.8636 | 3.3561 | 0.2980 | -4.8636 | 3.5242 | 1.4492 | 2.0166 | 11.7438 |
| CA5 | -7.8398 | -1.5075 | 6.3322 | 7.8406 | 1.5075 | 4.6741 | 3.1665 | 0.3158 | -4.6741 | 3.4497 | 1.4761 | 1.9421 | 11.2903 |
| CA6 | -7.8697 | -1.4749 | 6.3948 | 7.8683 | 1.4738 | 4.6711 | 3.1973 | 0.3128 | -4.6711 | 3.4121 | 1.4610 | 1.9383 | 11.2805 |
| CA7 | -7.8561 | -1.4776 | 6.3785 | 7.8556 | 1.4771 | 4.6663 | 3.1892 | 0.3136 | -4.6663 | 3.4137 | 1.4631 | 1.9367 | 11.2693 |
| CA8 | -7.8507 | -1.0912 | 6.7595 | 7.8496 | 1.0901 | 4.4698 | 3.3797 | 0.2959 | -4.4698 | 2.9558 | 1.3225 | 1.8657 | 10.8054 |
| CA9 | -7.8534 | -1.0749 | 6.7785 | 7.8528 | 1.0741 | 4.4634 | 3.3894 | 0.2950 | -4.4634 | 2.9389 | 1.3169 | 1.8649 | 10.7918 |
| CA10 | -8.3949 | -1.1184 | 7.2765 | 8.3941 | 1.1184 | 4.7562 | 3.6378 | 0.2749 | -4.7562 | 3.1093 | 1.3074 | 1.9908 | 11.5033 |
| CA11 | -8.4085 | -1.1102 | 7.2983 | 8.4080 | 1.1094 | 4.7587 | 3.6493 | 0.2740 | -4.7587 | 3.1027 | 1.3040 | 1.9933 | 11.5107 |
| **DMF** | | | | | | | | | | | | | |
| CA1 | -8.1935 | -0.9170 | 7.2765 | 8.1933 | 0.9165 | 4.5549 | 3.6384 | 0.2748 | -4.5549 | 2.8511 | 1.2519 | 1.9346 | 11.0444 |
| CA2 | -8.1690 | -1.3851 | 6.7840 | 8.1677 | 1.3851 | 4.7764 | 3.3913 | 0.2949 | -4.7764 | 3.3636 | 1.4084 | 1.9785 | 11.5313 |
| CA3 | -8.1881 | -1.3416 | 6.8465 | 8.1873 | 1.3410 | 4.7641 | 3.4231 | 0.2921 | -4.7641 | 3.3152 | 1.3917 | 1.9742 | 11.5025 |
| CA4 | -7.8588 | -1.5048 | 6.3540 | 7.8575 | 1.5043 | 4.6809 | 3.1766 | 0.3148 | -4.6809 | 3.4488 | 1.4736 | 1.9445 | 11.3062 |
| CA5 | -7.8425 | -1.5048 | 6.3377 | 7.8428 | 1.5051 | 4.6739 | 3.1688 | 0.3156 | -4.6739 | 3.4470 | 1.4750 | 1.9419 | 11.2897 |
| CA6 | -7.8697 | -1.4722 | 6.3975 | 7.8703 | 1.4711 | 4.6707 | 3.1996 | 0.3125 | -4.6707 | 3.4091 | 1.4598 | 1.9380 | 11.2793 |
| CA7 | -7.8588 | -1.4749 | 6.3839 | 7.8583 | 1.4754 | 4.6669 | 3.1914 | 0.3133 | -4.6669 | 3.4122 | 1.4623 | 1.9368 | 11.2705 |
| CA8 | -7.8670 | -1.0912 | 6.7758 | 7.8681 | 1.0917 | 4.4799 | 3.3882 | 0.2951 | -4.4799 | 2.9617 | 1.3222 | 1.8700 | 10.8298 |
| CA9 | -7.8697 | -1.0776 | 6.7921 | 7.8700 | 1.0773 | 4.4737 | 3.3963 | 0.2944 | -4.4737 | 2.9464 | 1.3172 | 1.8690 | 10.8163 |
| CA10 | -8.3949 | -1.1184 | 7.2765 | 8.3952 | 1.1179 | 4.7565 | 3.6387 | 0.2748 | -4.7565 | 3.1089 | 1.3072 | 1.9910 | 11.5041 |
| CA11 | -8.4085 | -1.1102 | 7.2983 | 8.4088 | 1.1100 | 4.7594 | 3.6494 | 0.2740 | -4.7594 | 3.1035 | 1.3042 | 1.9935 | 11.5123 |
| **Water** | | | | | | | | | | | | | |
| CA1 | -8.1908 | -0.9116 | 7.2792 | 8.1900 | 0.9121 | 4.5511 | 3.6389 | 0.2748 | -4.5511 | 2.8459 | 1.2507 | 1.9338 | 11.0359 |
| CA2 | -8.1690 | -1.3878 | 6.7812 | 8.1696 | 1.3881 | 4.7788 | 3.3908 | 0.2949 | -4.7788 | 3.3676 | 1.4094 | 1.9795 | 11.5372 |
| CA3 | -8.1881 | -1.3388 | 6.8493 | 8.1892 | 1.3394 | 4.7643 | 3.4249 | 0.2920 | -4.7643 | 3.3137 | 1.3911 | 1.9743 | 11.5029 |
| CA4 | -7.8588 | -1.5021 | 6.3567 | 7.8583 | 1.5026 | 4.6805 | 3.1778 | 0.3147 | -4.6805 | 3.4468 | 1.4729 | 1.9442 | 11.3051 |
| CA5 | -7.8452 | -1.5048 | 6.3404 | 7.8439 | 1.5040 | 4.6739 | 3.1699 | 0.3155 | -4.6739 | 3.4458 | 1.4745 | 1.9418 | 11.2896 |
| CA6 | -7.8724 | -1.4694 | 6.4030 | 7.8713 | 1.4697 | 4.6705 | 3.2008 | 0.3124 | -4.6705 | 3.4076 | 1.4592 | 1.9378 | 11.2789 |
| CA7 | -7.8588 | -1.4749 | 6.3839 | 7.8599 | 1.4746 | 4.6673 | 3.1926 | 0.3132 | -4.6673 | 3.4115 | 1.4619 | 1.9369 | 11.2714 |
| CA8 | -7.8779 | -1.0939 | 6.7840 | 7.8765 | 1.0928 | 4.4847 | 3.3918 | 0.2948 | -4.4847 | 2.9648 | 1.3222 | 1.8720 | 10.8413 |
| CA9 | -7.8779 | -1.0803 | 6.7976 | 7.8781 | 1.0800 | 4.4791 | 3.3991 | 0.2942 | -4.4791 | 2.9512 | 1.3177 | 1.8711 | 10.8293 |
| CA10 | -8.3949 | -1.1184 | 7.2765 | 8.3957 | 1.1176 | 4.7567 | 3.6391 | 0.2748 | -4.7567 | 3.1087 | 1.3071 | 1.9911 | 11.5045 |
| CA11 | -8.4058 | -1.1075 | 7.2983 | 8.4069 | 1.1086 | 4.7577 | 3.6491 | 0.2740 | -4.7577 | 3.1016 | 1.3038 | 1.9930 | 11.5085 |

phase, CA5 tautomer is in all solvents act as a hard acid because the higher the energy of the LUMO of an acid, the harder it is as an acid.

The global and chemical reactivity descriptors, hardness (η), chemical potential (μ), softness (S), electronegativity (χ) and electrophilicity index (ω) were calculated from HOMO and LUMO energies and incorporated in Table 1. Figures 2, 3 and 4 shows represent the variation of hardness (η), electrophilicity index (ω) and potential (μ) of cyanuric acid tautomers in gas phase and in different solvents.

**Chemical hardness (η)**

Chemical hardness is a useful concept for understanding the behaviour of chemical systems. It is measures the resistance to change in the electron distribution in a collection of nuclei and electrons. Chemical hardness was calculated by using of equation (4) and is presented in table 1. The chemical hardness (η) of cyanuric acid tautomers was show similar trend to the $\Delta E_g$ , because of the chemical hardness (η) is equal to the energy gap difference between the LUMO and HOMO orbitals [$\eta = (\varepsilon_{LUMO} - \varepsilon_{HOMO})$]. The Fig.2 represents the solvent effect of the chemical hardness of cyanuric acid tautomers in different solvents.

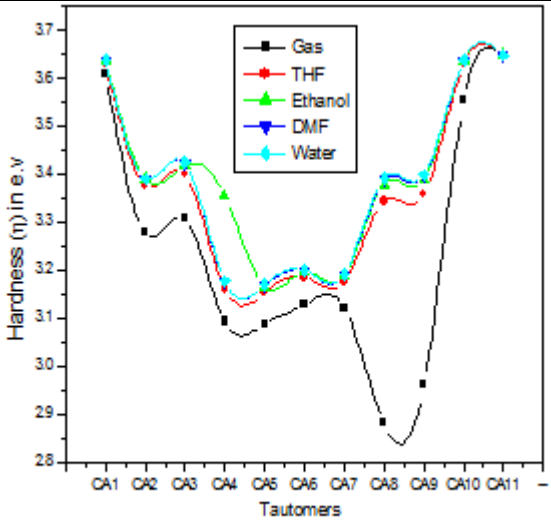


Fig.2: Chemical hardness (η) Vs tautomers of cyanuric acid at B3LYP/6-311++G(d,p) level in gas phase and different solvents.

**Electrophilicity index (ω)**

The electrophilicity index has been used as structural depictor for the analysis of the chemical reactivity of molecules [26-28]. It measures the propensity of a species them to accept electrons. A good, more reactive, nucleophile is characterized by a lower value of **(ω)**, in opposite a good electrophile is characterized by a high value of (ω). The electrophilicity index values were calculated by equation (6)

and are presented in table 1. The effect of solvents on electrophilicity index of cyanuric acid tautomers are shown in Fig.3. The tautomer CA8 is a good electrophile in gas phase and in solvents which is act as a good, more reactive, nucleophile. CA1 and CA9 tautomers have lower values in all solvent phase, so that tautomers are good nucleophiles.

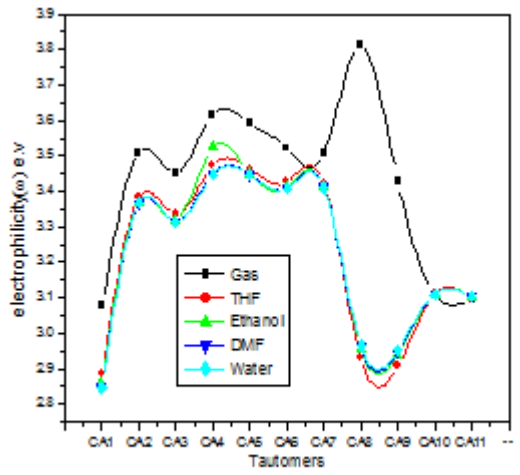


Fig.3: electrophilicity index (ω) Vs tautomers of cyanuric acid at B3LYP/6-311++G(d,p) level in gas phase and different solvents.

**Chemical potential (μ)**

Physically, chemical potential (μ) describes the escaping tendency of electrons from an equilibrium system. The values of μ were calculated by equation (5) and for all compounds are presented in Table 1. The greater the electronic chemical potential, the less stable or more reactive is the compound. From the Fig 3. The tautomers of CA9 is less stable and more reactive in the gas phase and CA8 and CA9 tautomers are less stable and more reactive in the all solvents. The CA4 tautomer is shows in different trend in ethanol solvent.

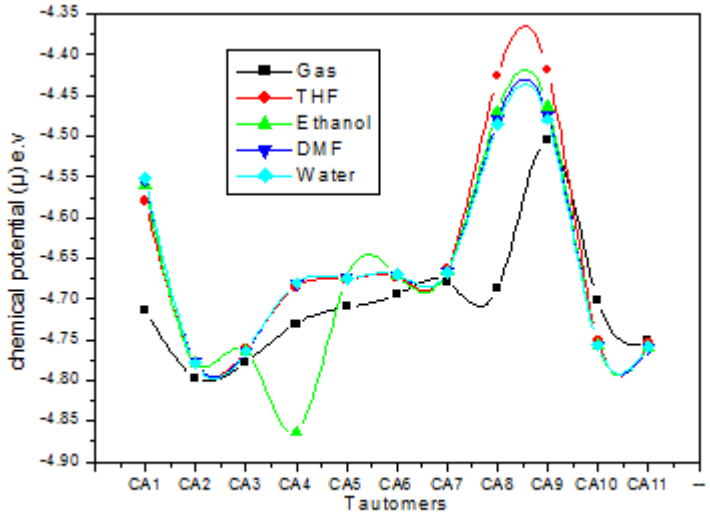


Fig.4: chemical potential (μ) Vs tautomers of cyanuric acid at B3LYP/6-311++G(d,p) level in gas phase and different solvents.

## 5. Conclusion

The HOMO and LUMO energies in order to determine, the usefulness of global reactivity descriptors namely, the electrophilicity, Chemical hardness (η), chemical potential (μ), polarizability (α) electrophilicity index (ω), softness (S), nucleofugality, and electrofugality, values for the prediction of the reactivity of the cyanuric acid tautomers.Solvents effect on the molecules are studied by using four solvents namely: THF, ethanol, DMF and water. The order of the stability of tautomers in gas phase: CA11 ≈ CA1> CA10 > CA3 > CA2 > CA6 > CA7 > CA4> CA5 > CA9 > CA8. Therefore CA8 tautomer is least stable in gas phase. The order of stability is similar in all solvents, but CA4 tautomer is in ethanol different and the order are: CA11 > CA1 ≈ CA10 > CA3 > CA2 > CA9 > CA8 > CA6 > CA7 > CA4 > CA5. From electrophilicity index (ω), results the tautomer CA8 is a good electrophile in gas phase and in solvents which is act as a good, more reactive, nucleophile. CA1 and CA9 tautomers have lower values in all solvent phase.

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