The Influence of Various Solvents on Energetic Property and Stability in C_5H_4 Divalent Five-Membered Ring: A DFT Studies

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ABSTRACT

By using density functional theory (DFT) in B3LYP/6-311++G(d, p) level of theory and conductor-like polarizable continuum modem (CPCM) we examined solvent effects on energy levels in C_5H_4 for both singlet and triplet states. For this purpose, different solvents, such as gaseous and aqueous solvents, Diethyl ether, Nitro methane, DMSO, Acetonitrile, Methanol, Ethanol, Acetone, Dichloroethane, THF, Aniline, Chlorobenzene, Chloroform, diethyl ether, dichloromethane, toluene, benzene, CCl_4, cyclohexane, and heptanes, were used Selectively. The findings suggest that selecting a different solvent changes level of energy, Electrophilicity, Chemical hardness, Chemical potential, and dipole moment for both singlet and triplet states, due to changes in aprotic or perotic properties of solvent. Based on the results, the most stable structure for C_5H_4 is achieved when the solvent used for both singlet and triplet state is in gaseous phase while the lowest stability is observed when an aqueous solvent is employed for both singlet and triplet states.

Key words: DFT; CPCM; Singlet–Triplet; Carbenes.

INTRODUCTION

Carbenes are compounds found in singlet or triplet forms, hence referred to as amphiprotic compounds [1]. Such compounds have been the subject of many theoretical and experimental studies and identified as intermediate products in many chemical reactions [2-16]. The compounds were first developed and identified in 1991. Two major types of carbenes are Silylene and Germylene. Silylenes are produced through different mechanisms such as thermal decomposition, photochemical mechanisms in silicon hydrates and Organosylanes. They are also key intermediates in CVD [8]. Cyclopentadienyldene, a five-membered ring carbene, is a cyclic conjugated compound found in interstellar medium. The stable state of the five-membered ring for the singlet structures Silylenes and Germylenes was first synthesized and identified by Denk *et al* and their properties were compared to those of other carbenes [9-11]. Spin multiplicity of Carbenes and the arrangements of spins are among determinant factors in Carbene reactivity and activity. The multiplicity plays a key

role in energy ratio of pi and sigma orbital in base, singlet, and triplet states. In addition, properties of singlet and triplet Carbenes can be examined in terms of electrons and spatial characteristics. Theoretical studies by E. Vessally *et al* and M.Z. Kassaee *et al* show that changing substituent plays a key role in reactivity and activity of carbenes in base state [12-16]. Research has indicated that type of solvent or substituent (electron donor/acceptor) influence energy level and stability of carbenes. This can be easily verified by examining perturbation orbital diagram. In fact, ó-electron-withdrawing substituents inductively stabilize the nonbonding orbital by increasing its S character. This increases Ã-pð gap, leading to formation of singlet state. In contrast, ó-electron-donating substituents induce a small ó-pð gap which favors the triplet state.

In cases of substituent change, mesomeric effects may influence stability of carbenes [12-16]. Electron-donating substituent increase chemical activity of these compounds and a substituent with lone electron pair adds to this effect. When ó orbital is not stabilized it has almost no charge, leading to increased ó-pð gap [14-17]. Solvent type is also effective in energy level for singlet and triplet C_5H_4. Different behaviors observed in singlet and triplet states can be attributed to protic or aprotic properties as well as solvent behavior in interaction with C_5H_4. The present study attempts to explore the effects on solvent type as well as changes in Chemical potential, Chemical hardness, Electrophilicity, and HOMO-LUMO gap.

Electrophilicity was first defined and examined by Parr *et al* [18]. This factor was successfully employed in explaining many systems and describing reactions through organic methods. In some reactions, this factor is regarded as a key player in reaction efficiency for Diels-Alder reactions. Electrophilicity stems from electron structure and is independent of interventions by nuclei. Domingo *et al* studied relationship between electron effects of substituents, electrophilicity, and Hammett constant for ethylene [18-34]. Electrophilicity, largest amount of charge transferred by electrons, chemical hardness, and chemical potential were calculated using Equations (1) to (6), where *I* denotes ionization potential and *A* is electron affinity.

$$\mu = (\varepsilon_H + \varepsilon_L)/2 \qquad ...(1)$$

$$\eta = \varepsilon_L - \varepsilon_H \qquad ...(2)$$

$$\omega = \mu^2/2\eta = \chi^2/2\eta \qquad ....(3)$$

$$\chi = -\mu = -(\delta_E/\delta_N)_{V(r)} H \approx (I+A)/2H \approx -1/2 \ (\varepsilon_{HOMO} + \varepsilon_{LUMO}) \ ...(4)$$

$$\eta = (\delta_{2E}/\delta_{N2})_{V(r)} = (I-A)H \approx (\varepsilon_{LUMO} - \varepsilon_{HOMO}) \qquad ...(5)$$

$$\Delta N_{max} = -\mu/\eta \qquad ...(6)$$

Computational details

Density functional theory (DFT) calculations of C_5H_4 carbene structure in different solvent were conducted in which geometries, energies and Electrophilicity index values were obtained at the B3LYP/6-311++G(d, p) level of theory. The B3LYP method combines Becke's three-Parameter exchange (B3) function with the correlation function of Lee-Yong-Parr (LYP) [36]. To calculate solvation energies, a popular continuum model of solvation, the conductor-like polarizable continuum model (CPCM) have been used [37]. For this purpose "scrf=(cpcm,solvent= solvent name)" key-word used indicates that additional basis functions are to be added to the basis set specified in the route section. Value of energetic parameters are self consistent field calculation used closed-shell (RB3LYP) for the singlet state and unrestricted open-shell (UB3LYP) for the triplet state [38]. All calculations were conducted using *GAUSSIAN 98W* program package [39]. However, obtained parameters are calculated in gas phase condition, 298 K temperature and 1 atm pressure.

RESULTS AND DISCUSSION

We first obtained the optimized gaseous structure for C_5H_4 and identified its energetic parameters (Fig 1). Then, the results were compared to optimum parameters for the same structure in other solvents.

Energetic property

Energy levels in C_5H_4 were identified in the presence of different solvents. For this purpose, thermal energy, enthalpy, and Gibbs free energy were calculated. Since these parameters in

Table 1: Calculated zero point vibration energy (Kcal/mol), dipole moment (Debye), enthalpy (Kcal/mol), gibbs free energy (Kcal/mol), thermal energy (Kcal/mol), enthalpy gaps (Kcal/mol), gibbs free energy gaps (Kcal/mol) and thermal energy gaps (Kcal/mol) for the singlet and triplet states of divalent five-membered ring C_5H_4 in Water, DMSO, Nitro methane, Acetonitrile, Methanol, Ethanol and Acetone solvents by B3LYP/6-311++G (d, p) level of theory

Spin multiplicity	Solvent	ZPVE	Dipole moment	G	H	E	ΔG_{s-t}	ΔH_{s-t}	ΔE_{s-t}
Singlet	Water	40.93491	1.8085	-120969.6288	-120949.6568	-120950.2491	8.342612	7.996233	7.996232
	DMSO	40.94798	1.7981	-120969.5535	-120949.5877	-120950.1801	8.372732	8.020705	8.020705
	Nitro methane	40.95106	1.7888	-120969.5222	-120949.5589	-120950.1512	8.382772	8.028235	8.028235
	Acetonitrile	40.94612	1.7840	-120969.5253	-120949.5545	-120950.1468	8.374615	8.026980	8.027608
	Methanol	40.95157	1.7862	-120969.4989	-120949.5325	-120950.1249	8.385282	8.033883	8.034510
	Ethanol	40.95895	1.7669	-120969.4318	-120949.4616	-120950.0540	8.404107	8.057100	8.057100
	Acetone	40.96422	1.7635	-120969.3803	-120949.4102	-120950.0025	8.418540	8.072160	8.072160
Triplet	Water	41.22728	1.3668	-120977.9715	-120957.6530	-120958.2454			
	DMSO	41.23587	1.3613	-120977.9263	-120957.6084	-120958.2008			
	Nitro methane	41.23947	1.3582	-120977.9049	-120957.5871	-120958.1795			
	Acetonitrile	41.24039	1.3575	-120977.8999	-120957.5815	-120958.1745			
	Methanol	41.24229	1.3556	-120977.8842	-120957.5664	-120958.1594			
	Ethanol	41.25142	1.3490	-120977.8359	-120957.5187	-120958.1111			
	Acetone	41.25789	1.3444	-120977.7989	-120957.4823	-120958.0747			

Table 2: Calculated zero point vibration energy (Kcal/mol), dipole moment (Debye), enthalpy (Kcal/mol), gibbs free energy (Kcal/mol), thermal energy (Kcal/mol), enthalpy gaps (Kcal/mol), gibbs free energy gaps (Kcal/mol) and thermal energy gaps (Kcal/mol) for the singlet and triplet states of divalent five-membered ring C_5H_4 in THF, Aniline, Chloro benzene, Chloroform, Diethylether and Gas solvents by B3LYP/6-311++G (d, p) level of theory.

Spin multiplicity	Solvent	ZPVE	Dipole moment	G	H	E	$\Delta G_{s\text{-}t}$	$\Delta H_{s\text{-}t}$	$\Delta E_{s\text{-}t}$
Singlet	Dichloro ethane	41.00018	1.7048	-120969.0610	-120949.0920	-120949.6844	8.513292	8.168167	8.168167
	THF	41.02883	1.6611	-120968.8250	-120948.8624	-120949.4553	8.586710	8.236565	8.235937
	Aniline	41.03894	1.6480	-120968.7384	-120948.7770	-120949.3694	8.613065	8.262292	8.262920
	Chloro benzene	41.05506	1.6088	-120968.5408	-120948.5737	-120949.1661	8.662637	8.319395	8.319395
	Chloroform	41.07633	1.5809	-120968.3738	-120948.4099	-120949.0029	8.712837	8.367712	8.367085
	Diethyl ether	41.09534	1.5521	-120968.2050	-120948.2449	-120948.8373	8.764292	8.416030	8.416030
	Gas	41.53874	1.0374	-120964.0560	-120944.1147	-120944.7070	9.913300	9.570600	9.570700
Triplet	Dichloro ethane	41.29637	1.3151	-120977.5742	-120957.2602	-120957.8525			
	THF	41.32409	1.2943	-120977.4117	-120957.0989	-120957.6913			
	Aniline	41.33421	1.2868	-120977.3515	-120957.0393	-120957.6323			
	Chloro benzene	41.35905	1.2684	-120977.2034	-120956.8931	-120957.4855			
	Chloroform	41.37848	1.2541	-120977.0867	-120956.7776	-120957.3700			
	Diethyl ether	41.39809	1.2398	-120976.9693	-120956.6609	-120957.2533			
	Gas	41.86005	0.9311	-120973.9693	-120953.6853	-120954.2777			

Table 3: Calculated zero point vibration energy (Kcal/mol), dipole moment (Debye), enthalpy (Kcal/mol), gibbs free energy (Kcal/mol), thermal energy (Kcal/mol), enthalpy gaps (Kcal/mol), gibbs free energy gaps (Kcal/mol) and thermal energy gaps (Kcal/mol) for the singlet and triplet states of divalent five-membered ring C5H4 in Dichloro methane, Toluene, Benzene, CCl4, Cyclohexane and Heptane solvents by B3LYP/6-311++G (d, p) level of theory

Spin multiplicity	Solvent	ZPVE	Dipole moment	G	H	E	$\Delta G_{s\text{-}t}$	$\Delta H_{s\text{-}t}$	$\Delta E_{s\text{-}t}$
Singlet	Dichloro methane	41.01257	1.6869	-120968.9574	-120948.9941	-120949.5865	8.545922	8.195777	8.195777
	Toluene	41.21874	1.3805	-120967.0762	-120947.1236	-120947.7159	9.084317	8.736055	8.736682
	Benzene	41.23337	1.3645	-120966.9400	-120946.9824	-120947.5747	9.118830	8.776842	8.776842
	CCl4	41.23686	1.3613	-120966.9155	-120946.9604	-120947.5528	9.127615	8.783117	8.783117
	Cyclohexane	41.27353	1.3231	-120966.6470	-120946.6981	-120947.2905	9.211700	8.862810	8.862810
	Heptane	41.27487	1.3023	-120966.5177	-120946.5607	-120947.1537	9.234917	8.894185	8.894185
Triplet	Dichloro methane	41.30857	1.3058	-120977.5033	-120957.1899	-120957.7823			
	Toluene	41.52931	1.1467	-120976.1605	-120955.8596	-120956.4526			
	Benzene	41.54545	1.1356	-120976.0588	-120955.7592	-120956.3516			
	CCl4	41.54791	1.1339	-120976.0431	-120955.7435	-120956.3359			
	Cyclohexane	41.57699	1.1140	-120975.8587	-120955.5609	-120956.1533			
	Heptane	41.59369	1.1028	-120975.7526	-120955.4549	-120956.0479			

themselves have no use in singlet and triplet states, the gaps for values of these parameters in the two states were obtained. The results for the three parameters followed a nearly similar trend. Tables 1 to 4 and figure 2 present the gap in Gibb free energy for different solvents based on compound stability. Compounds with lower energy levels are expected to be more stable in solvents. As seen here, the lowest energy level, and therefore highest stability for carbene, is observed in solvents like DMSO and water. However, in gaseous solvents or heptanes an increase is observed in Gibbs free energy gaps, resulting in relative instability of structure compared to what observed in aqueous solvents. A similar trend was observed for thermal energy gap and enthalpy gap (see Fig. 2, 3 and Table 4).

Dipole moment indices

Tables 1, 2, and 3 present dipole moment values. The results indicate different dipole moments for C_5H_4 in various solvents. However, in all solvents, dipole moment is greater for singlet state compared to triplet state. To further investigate dipole moments, relative dipole moments were compared for singlet and triplet states. The results found for singlet and triplet states show that replacing aqueous solvent with gaseous ones change dipole moment. For the singlet state, water produces the largest dipole moment while the smallest dipole moment is observed in gaseous solvent. It should be noted, however, that the results are confirmed by dipole moments obtained for the triplet state.

HOMO and LUMO parameters

The HOMO or LUMO levels can be used to determine such parameters as Chemical hardness, Chemical potential, Electrophilicity, and max amount of electronic charge transfer (λ_{max}), which can, in turn, be used to identify or predict chemical properties. We employed quantum mechanics and DFT methods to examine effects of

Table 4: Relative enthalpy gaps (Kcal/mol), relative Gibbs free energy gaps (Kcal/mol) and relative thermal energy gaps (Kcal/mol) for the singlet and triplet states of divalent five-membered ring C_5H_4 in different solvents

	Solvent	Relative parameters		
		ΔG_{s-t}	ΔH_{s-t}	ΔE_{s-t}
Singlet-Tripletgaps	Water	0.000000	0.000000	0.000000
	DMSO	0.030122	0.024475	0.024475
	Nitro methane	0.040162	0.032005	0.032005
	Acetonitrile	0.032005	0.030750	0.031378
	Methanol	0.042672	0.037653	0.038280
	Ethanol	0.061497	0.060870	0.060870
	Acetone	0.075930	0.075930	0.075930
	Dichloro ethane	0.170682	0.171937	0.171937
	THF	0.244100	0.240335	0.239707
	Aniline	0.270455	0.266062	0.266690
	Chloro benzene	0.320027	0.323165	0.323165
	Chloroform	0.370227	0.371482	0.370855
	Diethyl ether	0.421682	0.419800	0.419800
	Gas	1.570690	1.574370	1.574470
	Dichloro methane	0.203312	0.199547	0.199547
	Toluene	0.741707	0.739825	0.740452
	Benzene	0.776220	0.780612	0.780612
	CCl_4	0.785005	0.786887	0.786887
	Cyclohexane	0.869090	0.866580	0.866580
	Heptane	0.892307	0.897955	0.897955

different solvents on singlet and triplet C_5H_4 structures.

Chemical hardness

Chemical hardness values show that singlet C_5H_4 in Cyclohexane has the largest

Table 5: Calculated ε_{HOMO} and ε_{LUMO} (eV), chemical hardness (eV), chemical potential (eV), electrophilicity values (eV) and maximum amount of electronic charge transfer in atomic units, for the singlet and triplet states of divalent five-membered ring C5H4 in Water, DMSO, Nitro methane, Acetonitrile, Methanol, Ethanol and Acetone solvents by B3LYP/6-311++G (d, p) level of theory

Spin multiplicity	Solvent	ε_{HOMO}	ε_{LUMO}	μ	η	ω	ΔN_{max}
Singlet	Water	-0.23621	-0.11984	-0.178025	0.116370	0.136172	1.529819
	DMSO	-0.23620	-0.11975	-0.177975	0.116450	0.136003	1.528338
	Nitro methane	-0.23616	-0.11964	-0.177900	0.116520	0.135806	1.526777
	Acetonitrile	-0.23613	-0.11974	-0.177935	0.116390	0.136011	1.528783
	Methanol	-0.23617	-0.11978	-0.177975	0.116390	0.136073	1.529126
	Ethanol	-0.23611	-0.11961	-0.177860	0.116500	0.135769	1.526695
	Acetone	-0.23612	-0.11977	-0.177945	0.116350	0.136074	1.529394
Triplet	Water	-0.23879	0.00239	-0.118200	0.241180	0.028964	0.490090
	DMSO	-0.23876	0.00234	-0.118210	0.241100	0.028978	0.490294
	Nitro methane	-0.23878	0.00232	-0.118230	0.241100	0.028988	0.490377
	Acetonitrile	-0.23878	0.00232	-0.118230	0.241100	0.028988	0.490377
	Methanol	-0.23878	0.00231	-0.118235	0.241090	0.028992	0.490419
	Ethanol	-0.23878	0.00226	-0.118260	0.241040	0.029010	0.490624
	Acetone	-0.23877	0.00222	-0.118275	0.240990	0.029023	0.490788

Table 6: Calculated ε_{HOMO} and ε_{LUMO} (eV), chemical hardness (eV), chemical potential (eV), electrophilicity values (eV) and maximum amount of electronic charge transfer in atomic units, for the singlet and triplet states of divalent five-membered ring C5H4 in THF, Aniline, Chloro benzene, Chloroform, Diethylether and Gas solvents by B3LYP/6-311++G (d, p) level of theory

Spin multiplicity	Solvent	ε_{HOMO}	ε_{LUMO}	μ	η	ω	ΔN_{max}
Singlet	Dichloro ethane	-0.23607	-0.11964	-0.177855	0.116430	0.135843	1.527570
	THF	-0.23605	-0.11955	-0.177800	0.116500	0.135677	1.526180
	Aniline	-0.23602	-0.11950	-0.177760	0.116520	0.135593	1.525575
	Chloro benzene	-0.23594	-0.11948	-0.177710	0.116460	0.135586	1.525932
	Chloroform	-0.23594	-0.11939	-0.177665	0.116550	0.135413	1.524367
	Diethyl ether	-0.23590	-0.11934	-0.177620	0.116560	0.135333	1.523850
	Gas	-0.23592	-0.11942	-0.177670	0.116500	0.135479	1.525064
Triplet	Dichloro ethane	-0.23879	0.00199	-0.118400	0.240780	0.029110	0.491735
	THF	-0.23880	0.00182	-0.118490	0.240620	0.029174	0.492436
	Aniline	-0.23880	0.00175	-0.118525	0.240550	0.029200	0.492725
	Chloro benzene	-0.23881	0.00159	-0.118610	0.240400	0.029260	0.493386
	Chloroform	-0.23883	0.00146	-0.118685	0.240290	0.029310	0.493924
	Diethyl ether	-0.23884	0.00132	-0.118760	0.240160	0.029363	0.494504
	Gas	-0.23956	-0.00296	-0.121260	0.236600	0.031073	0.512511

Table 7. Calculated ε_{HOMO} and ε_{LUMO} (eV), chemical hardness (eV), chemical potential (eV), electrophilicity values (eV) and maximum amount of electronic charge transfer in atomic units, for the singlet and triplet states of divalent five-membered ring C_5H_4 in Dichloro methane, Toluene, Benzene, CCl$_4$, Cyclohexane and Heptane solvents by B3LYP/6-311++G (d, p) level of theory

Spin multiplicity	Solvent	ε_{HOMO}	ε_{LUMO}	μ	η	ω	ΔN_{max}
Singlet	Dichloro methane	-0.23608	-0.11962	-0.177850	0.116460	0.135800	1.527134
	Toluene	-0.23575	-0.11911	-0.177430	0.116640	0.134951	1.521176
	Benzene	-0.23579	-0.11913	-0.177460	0.116660	0.134973	1.521173
	CCl4	-0.23575	-0.11918	-0.177465	0.116570	0.135085	1.522390
	Cyclohexane	-0.23573	-0.11902	-0.177375	0.116710	0.134786	1.519793
	Heptane	-0.23563	-0.11912	-0.177375	0.116510	0.135017	1.522402
Triplet	Dichloro methane	-0.23880	0.00192	-0.118440	0.240720	0.029137	0.492024
	Toluene	-0.23896	0.00032	-0.119320	0.239280	0.029750	0.498663
	Benzene	-0.23898	0.00019	-0.119395	0.239170	0.029801	0.499206
	CCl4	-0.23898	0.00017	-0.119405	0.239150	0.029808	0.499289
	Cyclohexane	-0.23902	-0.00008	-0.119550	0.238940	0.029907	0.500335
	Heptane	-0.23904	-0.00023	-0.119635	0.238810	0.029966	0.500963

Table 8: Relatives chemical hardness, chemical potential, electrophilicity values and maximum amount of electronic charge transfer in atomic units for the singlet state of divalent five-membered ring C_5H_4 in different solvents

Spin multiplicity	Solvent	μ_{rel}	η_{rel}	ω_{rel}	$\Delta N_{max(rel)}$	Dipole moment $_{(rel)}$
Singlet state	Water	0.000000	0.000020	0.001386	0.010026	0.7711
	DMSO	0.000050	0.000100	0.001217	0.008545	0.7607
	Nitro methane	0.000125	0.000170	0.001020	0.006984	0.7514
	Acetonitrile	0.000090	0.000040	0.001225	0.008990	0.7466
	Methanol	0.000050	0.000040	0.001287	0.009333	0.7488
	Ethanol	0.000165	0.000150	0.000983	0.006902	0.7295
	Acetone	0.000080	0.000000	0.001288	0.009601	0.7261
	Dichloro ethane	0.000170	0.000080	0.001057	0.007777	0.6674
	THF	0.000225	0.000150	0.000891	0.006387	0.6237
	Aniline	0.000265	0.000170	0.000807	0.005782	0.6106
	Chloro benzene	0.000315	0.000110	0.000800	0.006139	0.5714
	Chloroform	0.000360	0.000200	0.000627	0.004574	0.5435
	Diethyl ether	0.000405	0.000210	0.000547	0.004057	0.5147
	Gas	0.000355	0.000150	0.000693	0.005271	0.0000
	Dichloro methane	0.000175	0.000110	0.001014	0.007341	0.6495
	Toluene	0.000595	0.000290	0.000165	0.001383	0.3431
	Benzene	0.000565	0.000310	0.000187	0.001380	0.3271
	CCl$_4$	0.000560	0.000220	0.000299	0.002597	0.3239
	Cyclohexane	0.000650	0.000360	0.000000	0.000000	0.2857
	Heptane	0.000650	0.000160	0.000231	0.002609	0.2649

chemical hardness while the smallest chemical hardness was observed in acetone. Values found for triplet C_5H_4 indicate the lowest and highest Chemical hardness in gaseous and aqueous solvents, respectively (Tables 5, 6, 7, 8 and 9). The difference between singlet and triplet states is attributable to differences in interaction between carbene and solvent.

Chemical potential

Chemical potential values show that singlet C_5H_4 reaches its highest Chemical potential when solved in Ceptane or Cyclohexane while the lowest potential is observed in C_5H_4 solved in water. For the triplet state, the largest and the smallest chemical potentials were found for aqueous and gaseous solvents, respectively. This indicates totally different chemical potentials for singlet and triplet states (Tables 5, 6, 7, 8 and 9).

Electrophilicity indices

Electrophilicity may be associated with

reaction stability. In addition, solvents influence HOMU or LUMO levels in carbenes, and therefore, are expected to change Electrophilicity as well. Our findings, however, indicate that singlet C_5H4 reaches the highest level of Electrophilicity when solved in Water, DMSO, or Nitromethane while the lowest level of Electrophilicity is observed in Heptane. When water is used as solvent, greater level of interactions occurs between solvent and carbene and as we shift toward such solvents as DSMO, Electrophilicity is reduced in singlet carbenes. The results for triplet state is, however, completely different. Aqueous solvent results in the lowest level of Electrophilicity while the highest level is achieved through gaseous solvent (see Fig. 4 and 5). This can be due to adverse effects of aqueous solvent compared to gaseous solvents

Maximum amount of electronic charge

As mentioned earlier, the largest electron charge received by a system can be calculated using λ_{max}. The results indicate the largest "N_{max} for

Table 9: Relative chemical hardness, chemical potential, electrophilicity values and maximum amount of electronic charge transfer in atomic units for the triplet state of divalent five-membered ring C_5H_4 in different solvents

Spin multiplicity	Solvent	μ_{rel}	η_{rel}	ω_{rel}	$\Delta N_{max(rel)}$	Dipole moment $_{(rel)}$
Triplet state	Water	0.003060	0.004580	0.000000	0.000000	0.4357
	DMSO	0.003050	0.004500	0.000014	0.000204	0.4302
	Nitro methane	0.003030	0.004500	0.000024	0.000287	0.4271
	Acetonitrile	0.003030	0.004500	0.000024	0.000287	0.4264
	Methanol	0.003025	0.004490	0.000028	0.000329	0.4245
	Ethanol	0.003000	0.004440	0.000046	0.000534	0.4179
	Acetone	0.002985	0.004390	0.000059	0.000698	0.4133
	Dichloro ethane	0.002860	0.004180	0.000146	0.001645	0.3840
	THF	0.002770	0.004020	0.000210	0.002346	0.3632
	Aniline	0.002735	0.003950	0.000236	0.002635	0.3557
	Chloro benzene	0.002650	0.003800	0.000296	0.003296	0.3373
	Chloroform	0.002575	0.003690	0.000346	0.003834	0.3230
	Diethyl ether	0.002500	0.003560	0.000399	0.004414	0.3087
	Gas	0.000000	0.000000	0.002109	0.022421	0.0000
	Dichloro methane	0.002820	0.004120	0.000173	0.001934	0.3747
	Toluene	0.001940	0.002680	0.000786	0.008573	0.2156
	Benzene	0.001865	0.002570	0.000837	0.009116	0.2045
	CCl4	0.001855	0.002550	0.000844	0.009199	0.2028
	Cyclohexane	0.001710	0.002340	0.000943	0.010245	0.1829
	Heptane	0.001625	0.002210	0.001002	0.010873	0.1717

Fig. 1: Various show of C$_5$H$_4$ carbene with a five membered ring conformation
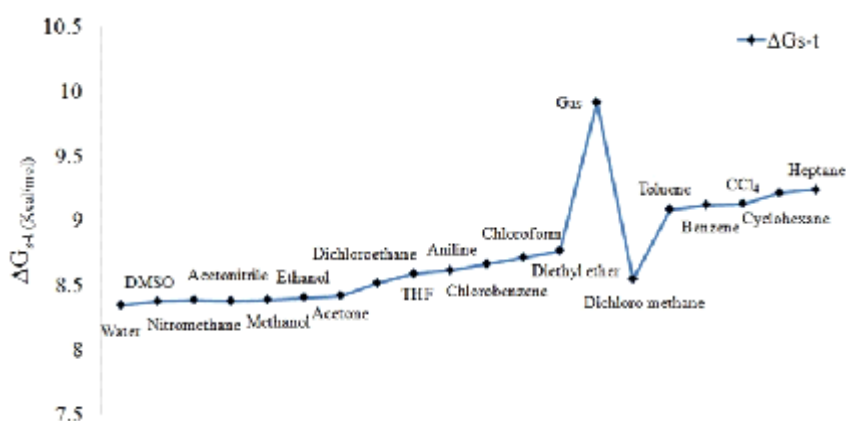

Fig. 2: Compared obtained results for gibbs free energy gaps, thermal energy gaps and enthalpy energy gaps of five membered ring (C$_5$H$_4$) carbenes structure in various solvents
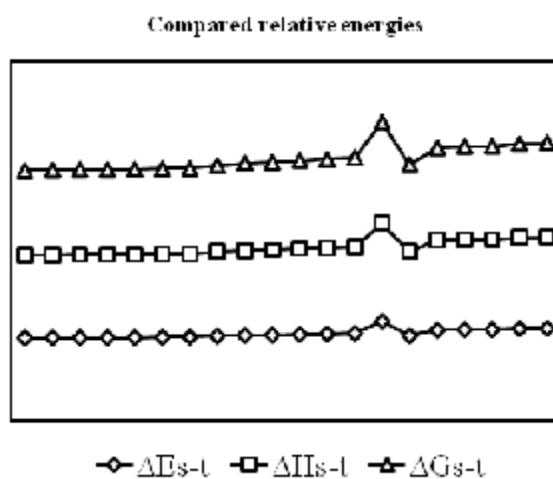

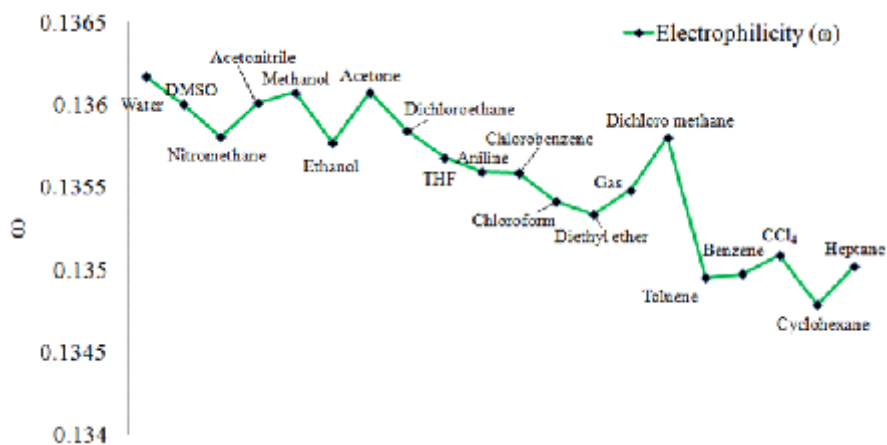**Fig. 3: Show comparison Gibbs free energy gaps (Kcal/mol) in various solvents**

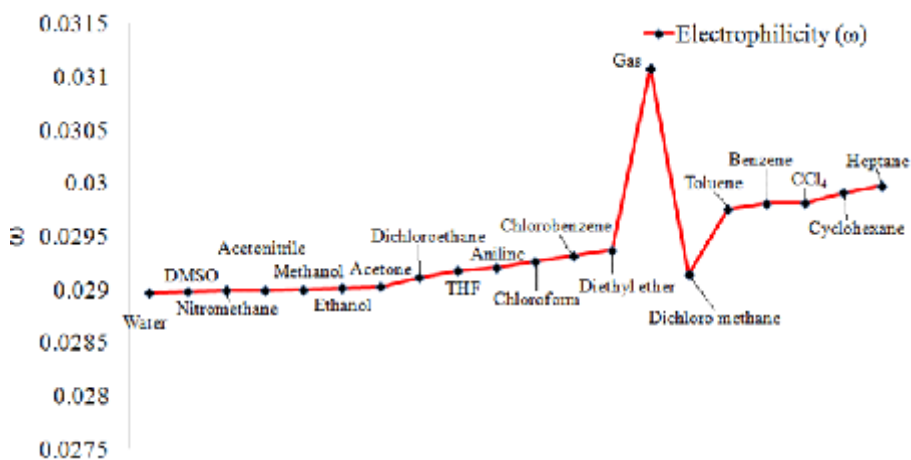**Fig. 4: Show comparison Electrophilicity in singlet state for various solvents**

Fig. 5: Show comparison Electrophilicity in triplet state for various solvents

aqueous solvent while the smallest λ_{max} was found for C_5H_4 solved in Cylcohexane. The results are totally different for triplet state where the largest λ_{max} is found for gaseous phase and the smallest λ_{max} is found when calculations are carried out for aqueous phase. All results confirm various effects of solvent on HOMO-LUMO level and dependent variables.

CONCLUSION

Quantum mechanics computations using B3LYP/6-311G (d, p) were carried out for singlet and triplet C_5H_4 through CPCM. The findings can be summarized as follows:

´   Examination of parameters revealed that energy levels and dipole moment for singlet and triplet Carbenes vary depending on type of solvent and its protic or aprotic properties. Solvent ability in engaging to structure of the compound can influence energy levels as well as HOMO or LUMO levels.

´   Aqueous solvent reduces energy level while increasing dipole moment. The opposite effect was observed for gaseous solvent.

´   Investigation of HOMO or LUMO levels showed that each solvent has different impacts on this parameter, resulting in different values for Chemical potential, Chemical hardness, Electrophilicity, and I_{max}.

´   For singlet state, the largest and smallest

Electrophilicities were observed for water and Cyclohexane, respectively while in triplet state, the lowest level of Electrophilicity was found for aqueous solvent and the highest level was observed for gaseous solvent.

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