J. Nanoanalysis., 6(2): 121-128, Spring 2019

ORIGINAL RESEARCH PAPER

A theoretical study of the influence of solvent polarity on the structure and spectral properties in the interaction of C_{20} and Si_2H_2

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Received: 2019-01-04 Accepted: 2019-03-05 Published: 2019-05-10

ABSTRACT

In this investigation, the interaction of C_{20} and Si_2H_2 molecules was explored in the M06-2X/6-311++G(d,p) level of theory in gas solution phases. The obtained interaction energy values with standard method were corrected by basis set superposition error (BSSE) during the geometry optimization for all molecules at the same level of theory. Also, the bonding interaction between the C_{20} and Si_2H_2 fragments was analyzed by means of the energy decomposition analysis (EDA). The results obtained from these calculations reveal interaction between C_{20} and Si_2H_2 increases in the presence of more polar solvents. There are good correlations between these parameters and dielectric constants of solvents. The wavenumbers of IR-active, symmetric and asymmetric stretching vibrations of Si-H groups and ^{29}Si NMR chemical shift values in different solvents were correlated with the Kirkwood–Bauer–Magat equation (KBM).

Keywords: *C_{20} cage, $C_{20}...Si_2H_2$ molecules, energy decomposition analysis (EDA), solvent effect, Kirkwood–Bauer–Magat equation (KBM)*

How to cite this article
Kazemi Z, Ghiasi R, Jamehbozorgi, S. A theoretical study of the influence of solvent polarity on the structure and spectral properties in the interaction of C_{20} and Si_2H_2. J. Nanoanalysis., 2019; 6(2): 121-128. DOI: 10.22034/JNA.2019.667135

INTRODUCTION

Many theoretical and experimental studies have been reported about the structure and properties of C_{20} molecule [1-6]. C_{20} molecule is potentially the smallest fullerene. The synthesis and characterization of this molecule have been performed in the gas phase [7]. The notable structure of C_{20} has been the question of numerous theoretical researches [8, 9]. Fullerenes are considered as promising candidates for basic elements in nanoscale devices, and several instances of fullerene-based devices have been already considered both experimentally and theoretically [10, 11]. Modification of C_{20} is a matter of common attention for experimentalists and theoreticians to seem into the structure as well as electronic properties. The structure and properties of fullerene C_{20} and its derivatives $C_{20}(C_2H_2)_n$ and $C_{20}(C_2H_4)_n$ (n=1–4) have been explored [11], and illustrated that the most stable fullerene C_{20} and its derivatives $C_{20}(C_2H_2)_n$ and $C_{20}(C_2H_4)_n$ (n=1–3) reveal significant aromaticity, while $C_{20}(C_2H_2)_4$ and $C_{20}(C_2H_4)_4$ have no spherical aromaticity. Furthermore, heteroatom impacts on structure, stability and aromaticity of X_nC_{20-n} fullerenes have been established [12]. The interaction of C_{20} with N_2X_2 (X=H, F, Cl, Br, Me) has been investigated theoretically [13]. Also, theoretical study of solvent effect on the interaction of C_{20} and N_2H_2 has been reported[14].

The synthesis and characterization of several homonuclear combinations –Si≡Si- have been investigated [15-17]. The large number of reviews

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published during the past decade reflects the progress in this field [18-20]. Their Lewis acidic character has been supported by the reactions of REER (E= Si, Ge, Sn) with R′NC: (R′ = But, Mesitylene, $SiMe_3$) [21-23]. Also, reactivity of a disilyne RSi≡SiR (R= $Si^iPr[CH(SiMe_3)_2]_2$) toward π-Bonds has been investigated[24].

Solvent exhibits significant role in physical and chemical processes. The presence of specific and non-specific interactions between the solvent and the solute molecules is responsible for the change in several properties such as molecular geometry, the electronic structure and dipole moment of the solute [14, 25-34].

Numerous experimental and theoretical investigations have been reported about adsorption of ethylene (C_2H_4) and acetylene (C_2H_2) at various surfaces [35-37]. Many investigations have been exploring the more reactivity of the π bond of the disilenes toward many reagents, rather than alkenes and alkynes. This increase reactivity attributed to the relatively small HOMO-LUMO gap and its biradical character [38]. For instance, smooth [2 + 2] cycloadditions of the π bond of disilenes toward alkenes and alkynes to give the disilacyclobutane and disilacyclobutene derivatives, respectively [39, 40]. Furthermore, there are much less reports about the π bond nature of disilynes with a silicon-silicon triple bond, which has two clear π bonds (π_{in} and π_{out}) [15, 41-43], although small number researches have reported about the reactivity of alkyne analogues [22, 44, 45]. An evaluation of the chemical behavior of heavier group 14 element alkyne analogues with that of alkynes has special attention [22, 46, 47].

In the basis of the extensive attentions on the nature of alkene analogues of silicon, we are interested in the theoretical study of interaction fullerene C_{20} with Si_2H_2 in both gas and solution phases. Experimental study has not reported about the interaction between C_{20} and Si_2H_2, yet. Therefore, theoretical study and the effective factors of this interaction are attractive for us. The structure, frontier orbital analysis, selected IR-active vibration, thermochemical parameters and ^{29}Si NMR chemical shift of the $C_{20}…Si_2H_2$ have been explored. In addition, the influence of the solvent on the structural properties of $C_{20}…Si_2H_2$ molecule will be evaluated.

COMPUTATIONAL METHODS

All calculations were carried out with the Gaussian 09 suite program [48]. The calculations of systems contain C, Si and H described by the standard 6-311++G(d,p) basis set [49-52]. Geometry optimization was performed utilizing with the hybrid functional of Truhlar and Zhao (M06-2X) [53].

A vibration analysis was performed at each stationary point found, that confirm its identity as an energy minimum.

The interaction energy, I.E, can be evaluated from the difference between energy of the molecule and sum of the energies of the C_{20} and Si_2H_2:

$$I.E = E(C_{20}…Si_2H_2) - [E(C_{20}) + E(Si_2H_2)]$$

The calculated interaction energies have corrected for basis set superposition errors (BSSE), which were computed for all calculations using the counterpoise correction method of Boys and Bernardi [54]. This error is owing to the different number of basis functions included in the molecule and monomer calculations. Since the molecule employs a basis set larger than the one employed by monomers, in most cases this error models the molecule to be too attractive. As it has been studied before, when BSSE is corrected along the whole surface, important changes in the potential energy surface appear, not only in the energy, but also in the position of the minimum as well as its topology [55, 56].

We have studied the solvation effects by using self-consistent reaction field (SCRF) approach, in particular using the polarizable continuum model (PCM) [57].

The GaussSum 3.0 software package was used to evaluate the detailed analysis of the atomic orbitals contributions to the complex [58].

Chemical shift values are calculated using the Gauge independent atomic orbital (GIAO) method at the same method and basis sets of optimization [59].

The bonding interactions between the C_{20} and Si_2H_2 fragments have been analyzed by means of the energy decomposition analysis implemented in Multiwfn 3.3.5. package [60]. In this method, the instantaneous interaction energy (E_{int}) between the two fragments can be divided into three main components:

$$\Delta E_{int} = \Delta E_{polar} + \Delta E_{els} + \Delta E_{Ex}$$

E_{polar} is electron density polarization term (also called as induction term)

$$E_{polar} = E(SCF\ last) - E(SCF\ 1st)$$

E_{els} is electrostatic interaction term, and E_{Ex} is exchange repulsion term.

RESULTS AND DISCUSSION

Interaction energies

The computed interaction energies (I.E) for the C_{20}…Si_2H_2 molecule (Fig. 1) in the gas phase and various solvents have been gathered in Table 1. The comparison of interaction energy value in gas phase and solution phase show more interaction between C_{20} and Si_2H_2 in solution phase. It can be expected that interaction between C_{20} and Si_2H_2 increases in the presence of more polar solvents. There is a good linear correlation between interaction energy values and dielectric constants of solvents:

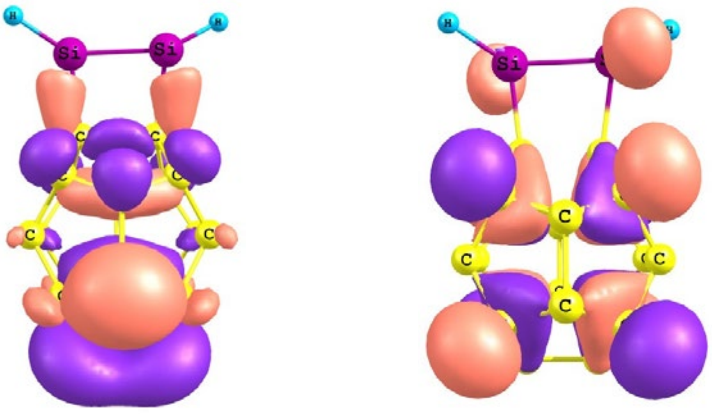
$$I.E = -0.039\,\varepsilon - 99.34; \qquad R^2 = 0.983$$

Where, ε is the dielectric constant of solvent. The interaction energy in gas phase was corrected by the BSSE. The uncorrected and corrected by BSSE of interaction energies is -98.78 kcal/mol and -96.45 kcal/mol, respectively.

The nature of the C…Si chemical bond in the C_{20}…Si_2H_2 molecule has been investigated using an energy decomposition analysis (EDA). These calculations show that the total interaction energy between C_{20} and Si_2H_2 is -98.78 kcal/mol. Also, EDA calculations reveal that the polarization energy (-198.62 kcal/mol) stabilized the C_{20}…Si_2H_2 adduct, whereas the sum of electrostatic and exchanging energy destabilized the adduct by 99.84 kcal/mol.

Solvation energies

The stabilization energies by solvents (solvation energy, E_{solv}) have been calculated (Table 1). These values are the relative energy of the title compound in a solvent to that in the gas phase. As we can see the solvation energies are dependent on the size of the dielectric constant of solvents, and these values decrease with the increase of dielectric constants of solvents. As a result, the stability of C_{20}…Si_2H_2 molecule increases in more polar solvents. This is because a dipole in the molecule will induce a dipole in the medium, and the electric field applied to the solute by the solvent (reaction) dipole will in turn interact with the molecular dipole to result in net stabilization. Hence, C_{20}…Si_2H_2 molecule has more stability in polar solvent rather than in



HOMO **LUMO**

Fig. 1. The plots of frontier orbitals of C_{20}…Si_2H_2 molecules.

Table 1. Dielectric constant of solvents, total energy (in a.u), interaction energy (in kcal/mol), solvation energy (in kcal/mol), dipole moment (in Debye) values of C_{20}…Si_2H_2 molecule in gas and solution phases in M06-2X/6-311++G(d,p) level of theory.

X	ε	$E(C_{20}… Si_2H_2)$	$E_{interaction}$	E_{solv}	μ_{tot}
gas	-	-1341.5288	-98.78	-	4.44
Chloroform	4.71	-1341.5324	-99.51	-2.25	6.31
chlorobenzene	5.70	-1341.5326	-99.58	-2.43	6.47
THF	7.58	-1341.5330	-99.65	-2.65	6.65
DiMethylDiSulfide	9.60	-1341.5333	-99.72	-2.82	6.80
DiChloroEthane	10.13	-1341.5333	-99.73	-2.85	6.83

the gas phase. There is a good correlation between dielectric constants and E_{solv}:

$$E_{solv} = -0.107\varepsilon - 1.789; R^2 = 0.979$$

Geometrical parameters

Selected geometrical parameters of $C_{20}\ldots Si_2H_2$ molecule are given in Table 2. These values show that Si-C and Si-Si distances increase in solution rather than to that in the gas phase. On the other hand, these values are dependent on the size of the dielectric constant of solvents, and these values increase with the increase of dielectric constants of solvents. There is a good correlation between these parameters and dielectric constants:

$$\mathrm{r(SiSi)} = 5 \times 10^{-5}\varepsilon + 2.132;\ R^2 = 0.988$$

$$\mathrm{r(SiC)} = 8 \times 10^{-5}\varepsilon + 1.914;\ R^2 = 0.979$$

Also, the comparison of interaction energy value in gas phase and solution phase and SiC distances show that SiC distance decrease with the decrease of interaction energies. There is a good correlation between interaction energy and SiC distances:

$$\mathrm{r(SiC)} = -379.0\ \mathrm{I.E} + 626.1;\ R^2 = 0.998$$

Dipole moments

The dipole moments of $C_{20}\ldots Si_2H_2$ molecule in gas phase and different solvents have been listed in Table 1. As seen in Table 1, these values increase in solution phase. In the solution phase, dipole moments increase with increasing of polarity of the solvents. Also, these values show a good relationship with interaction energy values:

$$\mu = -0.868\ E_{solv} + 4.355; \qquad R^2 = 1$$

Molecular orbital analysis

The energies of the frontier orbitals (HOMO, LUMO) along with the corresponding HOMO–LUMO energy gaps for of $C_{20}\ldots Si_2H_2$ molecule in gas phase and different solvents are given in Table 2.

Inclusion of solvation effects leads also to changes on the molecular orbital energies (Table 2). In solution, HOMO and LUMO are destabilized, with respect to the corresponding values in a vacuum. A good relationship exists between frontier orbitals energies and polarity of solvents:

$$E(\mathrm{HOMO}) = -5 \times 10^{-5}\ \varepsilon - 0.248; \qquad R^2 = 0.988$$
$$E(\mathrm{LUMO}) = 5 \times 10^{-5}\ \varepsilon - 0.088; \qquad R^2 = 0.972$$

Also, HOMO-LUMO gap of $C_{20}\ldots Si_2H_2$ molecule in solution phase is more than that of gas phase. A good relationship exists between HOMO-LUMO gap and polarity of solvents:

$$\mathrm{Gap} = 0.002\varepsilon + 4.352; \qquad R^2 = 0.981$$

The variations in this property may be illustrated by considering the fact that neutral or charged species enhance their effective radii in solution phase. This signifies that the electrostatic potential q/r will forever diminish from gas phase to solution phase. As a result, solvated species will reduce their effective hardness and subsequently, and become softer in the solution phase [61].

The frontier orbitals distribution of $C_{20}\ldots Si_2H_2$ molecule is plotted in Fig. 1. Fig. 1 presents the HOMO and LUMO are distributed mainly on C_{20}. Percentage composition in terms of the defined groups of frontier orbitals illustrates the largest contributions of HOMO and LUMO arise from cage (97.0% and 89.0%, respectively).

Thermodynamic parameters

Absolute free energy and enthalpy values of studding $C_{20}\ldots Si_2H_2$ molecule are reported in Table 3. The solvation free energy and enthalpy values are computed via the following equation:

$$\Delta X_{solvation} = X_{solv} - X_{gas};\ X = G, H$$

Table 3 reports that the amount of ΔG_{solv} and

Table 2. Si-Si, Si-c bond lengths (in Å), frontier orbital energies (in a.u), HOMO-LUMO- gap (in eV), values of $C_{20}\ldots Si_2H_2$ molecule in gas and solution phases in M06-2X/6-311++G(d,p) level of theory.

X	r(Si-Si)	r(Si-C)	E(HOMO)	E(LUMO)	Gap
gas	2.1321	1.9127	-0.2488	-0.0908	4.300
Chloroform	2.1328	1.9147	-0.2485	-0.0881	4.365
chlorobenzene	2.1329	1.9149	-0.2486	-0.0880	4.370
THF	2.1330	1.9150	-0.2487	-0.0879	4.376
DiMethylDiSulfide	2.1331	1.9152	-0.2488	-0.0878	4.381
DiChloroEthane	2.1331	1.9152	-0.2488	-0.0878	4.381

ΔH_{solv} of $C_{20}...Si_2H_2$ molecule decrease with heightening the dielectric constant. There is a good relationship between ΔG_{solv} and ΔH_{solv} with dielectric constant values:

ΔG_{solv} = -0.109 ε - 1.795; $R^2 = 0.979$

ΔH_{solv} = -0.108 ε- 1.805; $R^2 = 0.979$

There is a good relationship between ΔG_{solv} and dipole moment values:

$\mu = -1.17\ \Delta G_{solv} + 5.117$; $R^2 = 1$

Consequently, more polar solvents, the increase in dipole moment of $C_{20}...Si_2H_2$ molecule influences its interaction with the solvent.

Vibrational analysis

Table 4 reports the wavenumbers of IR-active, symmetric and asymmetric stretching vibrations of Si-H groups of $C_{20}...Si_2H_2$ molecules in gas and solution phases. It can be seen that these values are greater in solution phase rather than gas phase. On the other hand, υ(SiH) values have increased with increasing of dielectric constant of solvents.

The first theoretical treatment of the solvent-induced stretching frequency shifts was given by Kirkwood–Bauer–Magat equation (KBM) and is shown through the following equation[62]:

$$\frac{(\nu_{gas} - \nu_{solution})}{\nu_{gas}} = \frac{\Delta\nu}{\nu_{gas}} = \frac{C(\varepsilon - 1)}{(2\varepsilon + 1)}$$

Where υ_{gas} is the vibrational frequency of a solute in the gas phase, $\upsilon_{solution}$ is the frequency of a solute in the solvent, ε is the dielectric constant of the solvent and C is a constant depending on the dimensions and electrical properties of the vibrating solute dipole.

It can be observed that solvent-induced stretching vibrational frequency shifts on the base of KBM equation, have a good linear relationship:

For symmetric stretching of Si-H bonds:

$$\frac{\Delta\nu}{\nu_{gas}} = \frac{0.014(\varepsilon - 1)}{(2\varepsilon + 1)};\ R^2 = 0.999$$

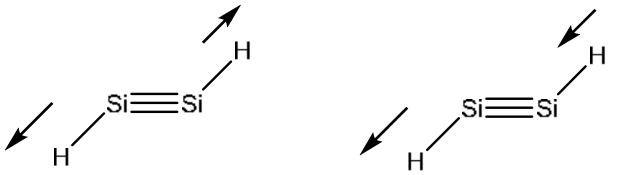
and for, asymmetric stretching of Si-H bonds:

$$\frac{\Delta\nu}{\nu_{gas}} = \frac{0.014(\varepsilon - 1)}{(2\varepsilon + 1)} + 0.002;\ R^2 = 0.999$$

Table 3. Thermochemical parameters of interaction between C_{20} and Si_2H_2 molecule in gas and solution phases M06-2X/6-311++G(d,p) level of theory.

X	G(a.u)	H(a.u)	S(cal/mol.K)	ΔG_{solv}(kcal/mol)	ΔH_{solv}(kcal/mol)	ΔS_{solv}(cal/mol.K)
gas	-1341.4298	-1341.3813	102.126	-	-	-
Chloroform	-1341.4335	-1341.3849	102.101	-2.27	-2.27	-25.00
chlorobenzene	-1341.4337	-1341.3852	102.103	-2.45	-2.46	-23.00
THF	-1341.4341	-1341.3856	102.105	-2.67	-2.67	-21.00
DiMethylDiSulfide	-1341.4344	-1341.3859	102.108	-2.84	-2.85	-18.00
DiChloroEthane	-1341.4344	-1341.3859	102.108	-2.88	-2.88	-18.00

Table 4. The wave-numbers of IR-active symmetric and asymmetric stretching vibrations of Si-H (in cm^{-1}) and ^{29}Si NMR chemical shifts (in ppm, respect to TMS) of $C_{20}...Si_2H_2$ molecule in gas and solution phases in M06-2X/6-311++G(d,p) level of theory.



X	υ_{asym}	υ_{sym}	$\delta(^{29}Si)$
gas	2266.02	2272.53	157.64
Chloroform	2276.32	2283.06	150.77
chlorobenzene	2277.04	2283.82	150.78
THF	2277.89	2284.70	150.80
DiMethylDiSulfide	2278.55	2285.40	150.83
DiChloroEthane	2278.67	2285.52	150.83

KBM equation only takes into account the solvent dielectric constants. The frequency shifts depend on the solvent dielectric constant.

^{29}Si NMR spectra

^{29}Si NMR spectral data of $C_{20}\cdots Si_2H_2$ are gathered in Table 4. In the $C_{20}\cdots Si_2H_2$ molecule, chemical shift of Si in gas phase is equal to 157.64 ppm. In various solvents, the chemical shift value of Si is decreased. These values are increased by increasing the solvent polarity.

The dependency of values of chemical shifts on dielectric constant of solvents has been investigated, and there are good relationships between these shifts values and dielectric constant:

$$\delta(^{29}\mathrm{Si}) = 0.011\,\varepsilon + 150.7; \qquad R^2 = 0.998$$

Dependency of the chemical shift values of Si atom in the $C_{20}\cdots Si_2H_2$ versus $(\varepsilon - 1)/(2\varepsilon + 1)$ of KBM equation exhibits a linear relationship between these chemical shift values and KBM parameters. These equations are as follows:

$$\delta(^{29}\mathrm{Si}) = -0.005(\varepsilon-1)/(2\varepsilon+1) + 0.045; \qquad R^2 = 0.976$$

CONCLUSION

Theoretical investigation of the interaction of C_{20} and Si_2H_2 molecules at the M06-2X/6-311++G(d,p) level of theory in gas solution phases shows that the interaction energy values increase from vacuum to different solvents and interaction between C_{20} and Si_2H_2 increases with increasing of dielectric constant of solvents. Solvation energy values indicate the increasing of stability of title complex in more polar solvents. The energy decomposition analysis (EDA) explored the significant interaction between C_{20} and Si_2H_2 in $C_{20} \cdots Si_2H_2$ molecule (I.E=-98.78 kcal/mol). On the other hand, the polarization energy stabilized adduct, although the sum of electrostatic and exchanging energy destabilized the $C_{20} \cdots Si_2H_2$ molecule. Also, our calculations showed the good relationship between chemical shift values of ^{29}Si NMR, IR-active symmetric and asymmetric stretching vibrations of Si-H groups and KBM solvent parameters.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this manuscript.

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