RESEARCH ARTICLE

Quantum chemical study of the adsorption of phosgene on $Al_{12}N_{12}$ nano-cluster

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ABSTRACT

This study investigated the adsorption of phosgene gas on $Al_{12}N_{12}$ nanocluster with using CAM-B3LYP functional. Six possible isomers of the interaction between $Al_{12}N_{12}$ nanocluster, and phosgene were considered. The interactions between nanocluster and phosgene were examined through energy decomposition analysis (EDA). Charge transfer between fragments were illustrated with ,electrophilicity-based charge transfer (ECT). Thermodynamics parameters of the interaction between of nanocluster and phosgene gas were calculated. The temperature and pressure effects on the thermodynamic parameters were illustrated.

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INTRODUCTION

Phosgene ($COCl_2$) and its derivatives are one of the main classes of air pollutants. In the natural world, it is employed in pesticides, dyes and pharmaceutical process. Phosgene was first used in World War I as a chemical weapon. The mortal dose for a human being is 2 ppm [1]. Furthermore, it is employed in the industrial synthesis many organic compounds, such as isocyanates, polyurethane, poly carbamates, and other materials [2]. Monitoring and controlling the amount of pollutants is main issue for our safety and health for modern society [3-5] . Many considerations have been focused on the progress of suitable gas-sensitive materials for hazardous chemical vapor detection. Air pollution is an alteration in the physical, chemical and biological properties of air that causes effects on human health and the surroundings [6]. Research shows that using nanostructures, due to enhancing ecological pollution, the prevalence of war diseases for preparation of gas sensor is considered [7].

Attentions to the nanostructures such as fullerene hollow nanocages of elements other than carbon have increased due to their exclusive electronic and optical properties [8-11]. Group III-V nitrides are between most favorable nanocages [12, 13]. In this family, useful applications have reported for AlN nanoclusters. These nanoclusters have revealed thermodynamic stability, and high thermal conductivity and low electron affinity [14]. The investigation of aluminum nitride nanoclusters (n=2-41) explored that $Al_{12}N_{12}$ nanocluster is energetically the most stable one, and can be reflected as an appropriated nanocluster [15]. $Al_{12}N_{12}$ nanocluster has been shown interesting applications in gas sensing and hydrogen storage [16]. Various computational investigations have been reported about adsorption of different molecules on the AlN nanocluster [17-23].

This theoretical study examined the interaction

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between $Al_{12}N_{12}$ nanocluster with phosgene. This work was done employing quantum chemical calculations, in which it is indeed an advantage of performing such calculations to provide insightful information at the lowest atomic scales especially for investigating the complicated nanostructures [24-28]. Variations in the structural parameters, frontier orbital energies and electron transfer between fragments were illustrated. Thermodynamics of this interaction were investigated and the temperature and pressure effects on the thermodynamic parameters were illustrated.

COMPUTATIONAL METHODS

Optimization and vibrational analysis were done with Gaussian 09 software package [29]. The standard 6-311G(d,p) basis set [30-33] _ ENREF_13 ENREF_14were considered for the elements, respectively. The geometries of the compound were optimized by the CAM-B3LYP functional. This functional is Handy and coworkers' long range corrected version of B3LYP using the Coulomb-attenuating method [34]. The identities of the optimized structures as an energy minimum were confirmed by vibrational analysis.

Energy decomposition analysis (EDA) was studied for illustration of the bonding interactions between the $Al_{12}N_{12}$ and phosgene [35-37]. The interaction energy (DE_{int}) between the two fragments was evaluated as $DE_{polar} + DE_{els} + DE_{Ex}$. Where DE_{polar}, DE_{els} and DE_{Ex} are the electron density polarization term (the induction term), the electrostatic interaction and the exchange repulsion terms, respectively. EDA calculations were performed on the optimized geometry with the used level of theory for optimization using Multiwfn 3.7 software package [38, 39]. The percentage contributions of atomic orbitals in the frontier orbitals were calculated using GaussSum 3.0 software package [40].

RESULTS AND DISCUSSION

Energetic aspects

The various isomers of the adsorption of $COCl_2$ gas on the $Al_{12}N_{12}$ nanocluster are presented in Fig. 1. The absolute energy and relative energy values of these isomers are calculated at the CAM-B3LYP/6-311G(d,p) level of theory (Table 1). It can found, **E**-isomer is a most stable isomer.

Stability of $Al_{12}N_{12}…COCl_2$ isomers are evaluated by cohesive energy (E_{coh})

$$E_{coh} = E_{Al12N12…COCl2} - (12\ E_{Al} + 12\ E_N + E_C + E_O + 2\ E_{Cl})$$

Where, $E_{Al12N12…COCl2}$ is energy of complex, E_{Al}, E_N, E_C, E_O and E_{Cl} are energy of aluminum, nitrogen, carbon, oxygen and chlorine atoms, respectively. The calculated E_{coh} values show that **E**-isomer is most stable isomers (Table 1). It can be found, pure $Al_{12}N_{12}$ nanocluster (E_{coh} = -279.75 eV) is more stable than metal doped $Al_{12}N_{12}$ nanocluster.

Energy decomposition analysis (EDA)

Energy decomposition analysis (EDA) was used to clarify the nature of the Al…Cl chemical bond in the **E**-isomer of $Al_{12}N_{12}…COCl_2$ molecule. The EDA calculation results of **E**-isomer show that the interaction energy between $Al_{12}N_{12}$ and $COCl_2$ are calculated as -183.46558 kcal/mol. Moreover, while the polarization energies equal to -457.81 kcal/mol stabilized $Al_{12}N_{12}…$ $COCl_2$ complex, the sum of the electrostatic and exchanging energies destabilized the $Al_{12}N_{12}…$ $COCl_2$ complex by 274.30 kcal/mol in **E**-isomer.

Bond distances

The most important bond distance between atoms in the different isomers of $Al_{12}N_{12}…COCl_2$ molecule are shown in Fig. 1. It can be observed, the shortest distances values between Al and Cl atoms in the **E**-isomer of $Al_{12}N_{12}…COCl_2$ molecule is 2.131 Å. On the other hand, the shortest distances values between N and Cl atom is 1.785 Å.

Thermodynamic parameters

Free energy enthalpy and entropy change values (DG, DH and DS, respectively) of $Al_{12}N_{12}…COCl_2$ complex formation are calculated in the basis of the following reactions:

$$Al_{12}N_{12} + COCl_2 \rightarrow Al_{12}N_{12}…COCl_2;\ D X = X(Al_{12}N_{12}…COCl_2) - X(Al_{12}N_{12}) - X(COCl_2);\ X=G, H, S$$

The calculated DG, DH and DS values of this reaction in the 298 K and 1atm pressure are -26.40 kcal/mol, -31.35 kcal/mol and -16.59 cal/mol.K, respectively. The negative DG and DH values of the **E**-isomer of $Al_{12}N_{12}…COCl_2$ complex formation reveals that this reaction is spontaneous and exothermic, respectively. The negative DS values of these reactions are logical. Because, formation of the one molecule after interaction between two

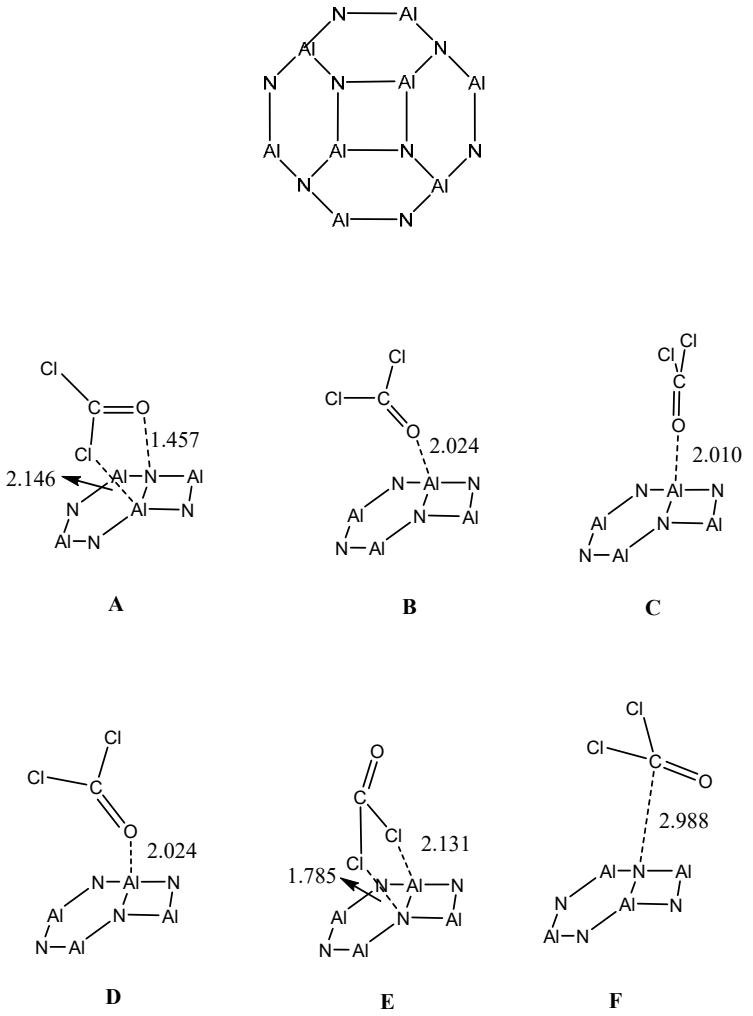

Fig. 1. Front view of the $Al_{12}N_{12}$ nanocluster, the various isomers of the adsorption of $COCl_2$ gas on the $Al_{12}N_{12}$ nanocage, and the most important bond distance between atoms (in Å) .

Table 1. Total energy (E, a.u), relative energy (ΔE, kcal/mol), and cohesive energy (ΔE_{coh}, eV) values of the possible isomers of the $Al_{12}N_{12}$…phosgene molecule at the CAM-B3LYP/6-311G(d,p) level of theory.

Isomer	E	ΔE	ΔE_{coh}
A	-4600.9724	39.41	-165.96
B	-4601.0093	16.27	-166.96
C	-4601.0066	17.93	-166.89
D	-4601.0093	16.27	-166.96
E	-4601.0352	0.00	-167.67
F	-4600.9942	25.76	-166.55

molecules decrease entropy of reaction.

Formation constant values (K) of the $Al_{12}N_{12}$… $COCl_2$ complex is calculated by the following formula:

$$\Delta G = -nRT \ln K$$

The calculated K value is 2.32 ´ 10^{19}.

The effect of pressure on the thermodynamic properties is explored. The temperature and pressure-dependent behaviors of this reaction are investigated in a wide range of conditions (T = 100–1000 K and P = 0.1–1000 atm (Tables 2 and 3).

During the adsorption process, the enhancement

Table 2. Temperature dependence of thermodynamics parameters of the formation E-isomer of $Al_{12}N_{12}$…phosgene molecule at the CAM-B3LYP/6-311G(d,p) level of theory.

T(K)	ΔG(kcal.mol^{-1})	ΔH(kcal/mol^{-1})	ΔS (cal.mol^{-1}.K^{-1})	K
100	-30.48	-33.16	-26.76	4.11×10^{66}
200	-28.19	-32.17	-19.91	6.38×10^{30}
300	-26.38	-31.35	-16.54	1.66×10^{19}
400	-24.84	-30.67	-14.58	3.71×10^{13}
500	-23.45	-30.08	-13.27	1.78×10^{10}
600	-22.51	-29.56	-12.31	1.58×10^{8}
700	-20.98	-29.08	-11.56	3.55×10^{6}
800	-19.85	-28.62	-10.96	2.65×10^{5}
900	-18.79	-28.18	-10.44	3.64×10^{4}
1000	-17.76	-27.75	-9.99	7.63×10^{3}

Table 3. Pressure dependence of thermodynamics parameters of the formation E-isomer of $Al_{12}N_{12}$…phosgene molecule at the CAM-B3LYP/6-311G(d,p) level of theory.

P	ΔG(kcal.mol^{-1})	ΔH(kcal/mol^{-1})	ΔS (cal.mol^{-1}.K^{-1})
0.1	-25.04	-31.35	-21.17
1	-26.40	-31.35	-16.59
10	-27.77	-31.35	-12.02
100	-29.13	-31.35	-7.44
1000	-30.50	-31.35	-2.86

of DG, DH and DS are observed distinctly along with the increasing of the temperature. Therefore, the adsorption occurs easily under lower temperature. There are good linear correlations between of DG and DH with temperature:

$DG = 0.0137\ T - 30.838; \quad R^2 = 0.9855$

$DH = 0.0058\ T - 33.245; \quad R^2 = 0.9794$

But, there is not good linear correlations between DS values and temperature:

$DS = 0.0155\ T - 23.136 \quad R^2 = 0.796$

The temperature dependency of DS values is fitted by a quadratic equation:

$DS = -3' 10^{-5}\ T^2 + 0.0459\ T - 29.214; \ R^2 = 0.9585$

During the adsorption process, the decreasing of DG values is observed distinctly along with the increasing of the pressure. Therefore, the adsorption occurs easily under higher pressure. There are good linear correlations between of DG with the logarithm of pressure:

$DG = -1.3642 \log (P) - 26.404; \quad R^2 = 1$

The variation of DS during the adsorption increases distinctly along with the enhancement of pressure. There are good linear correlations between of DS with logarithm of pressure:

$DS = 4.5757 \log (P) - 16.59; \quad R^2 = 1$

Molecular orbital analysis

The frontier orbitals energy, the corresponding HOMO–LUMO energy gaps, hardness, chemical potential values of $Al_{12}N_{12}$… $COCl_2$, $Al_{12}N_{12}$ and $COCl_2$ molecules are given in Table 4. Plots of frontier orbitals of **E**-isomer of $Al_{12}N_{12}$…phosgene molecule are presented in Fig. 2. Comparison of the frontier orbitals energy values in the **E**-isomer of $Al_{12}N_{12}$… $COCl_2$ with $Al_{12}N_{12}$ nanocluster shows $COCl_2$ adsorption meaningfully destabilizes and stabilizes the HOMO and LUMO levels of $Al_{12}N_{12}$ nanocluster, respectively. However, it seems that the $COCl_2$ share electron with the LUMO level because of its strong stabilization. On the other hand, comparison of the HOMO-LUMO gap value in the **E**-isomer of $Al_{12}N_{12}$… $COCl_2$ with $Al_{12}N_{12}$ nanocluster indicates $COCl_2$ adsorption meaningfully increases this value. Therefore, we believe that the $Al_{12}N_{12}$ may be a suitable nanoscale carrier for $COCl_2$ gas.

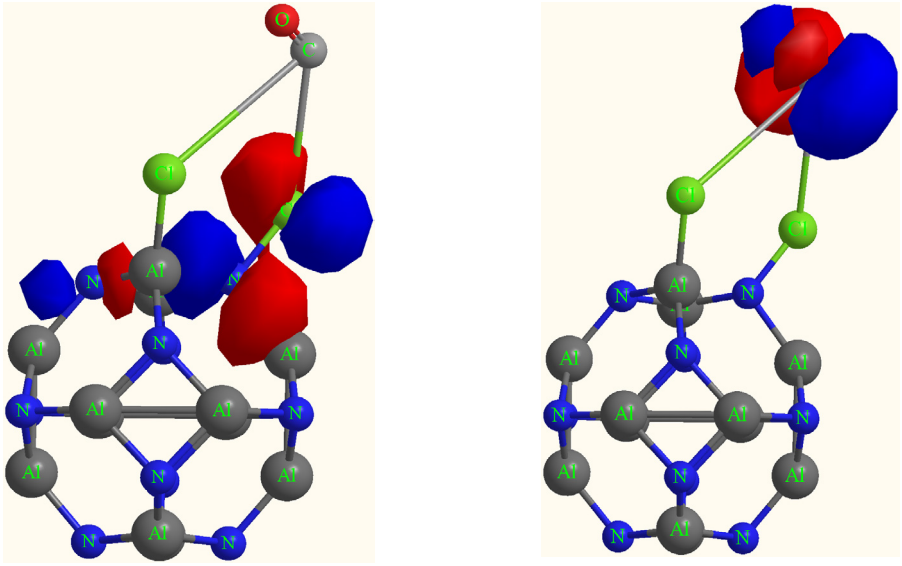

Fig. 2. Plots of frontier orbitals of E-isomer of $Al_{12}N_{12}$…phosgene molecule.

Table 4. Frontier orbital energy, hardness (η), chemical potential (μ) values (in eV) of the E-isomer of $Al_{12}N_{12}$…phosgene molecule at the CAM-B3LYP/6-311G(d,p) level of theory.

Molecule	E(HOMO)	E(LUMO)	Gap	η	μ
$Al_{12}N_{12}$	-7.15	-3.01	4.14	2.07	-5.08
$COCl_2$	-10.74	-0.41	10.33	5.16	-5.57
$Al_{12}N_{12}$… $COCl_2$	-7.91	-1.65	6.26	3.13	-4.78

Electrophilicity-based charge transfer (ECT)

Now, electrophilicity-based charge transfer (ECT) of **E**-isomer of $Al_{12}N_{12}$… $COCl_2$ molecule is calculated. ECT is defined as the difference between DN_{max} values of interacting molecules [41]:

$$ECT = DN_{max}(COCl_2) - DN_{max}(Al_{12}N_{12})$$

In this equation DN_{max} is defined as:

$$(\Delta N_{max})_i = \frac{\mu_i}{\eta_i}$$

η and μ are global hardness and chemical potential. They are defined as global reactivity descriptors [42-45] and determined on the basis of Koopman's theorem [46]. This value for $Al_{12}N_{12}$, $COCl_2$ and **E**-isomer of $Al_{12}N_{12}$… $COCl_2$ are calculated by the following equations:

$$\eta = \frac{E(LUMO) - E(HOMO)}{2}$$

$$\mu = \frac{E(HOMO) + E(LUMO)}{2}$$

The calculated DN_{max} value is 1.37. The positive value of ECT reveals charge flow from $Al_{12}N_{12}$ to $COCl_2$.

CONCLUSION

Computational investigation of the adsorption behavior of phosgene on $Al_{12}N_{12}$ nanocluster revealed **E**-isomer was a most stable isomer in between the studied isomers. The calculated E_{coh} values showed that **E**-isomer was most stable isomers. The larger HOMO-LUMO gap value in the **E**-isomer of $Al_{12}N_{12}$… $COCl_2$ rather than $Al_{12}N_{12}$ nanocluster showed that $COCl_2$ adsorption

meaningfully increases this value. Therefore, we believe that the $Al_{12}N_{12}$ may be a suitable nanoscale carrier for $COCl_2$ gas. The positive value of ECT revealed charge flow from $Al_{12}N_{12}$ to $COCl_2$ gas. Thermodynamics analysis showed easy adsorption under lower temperature and higher pressure.

CONFLICT OF INTEREST

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

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