Structure-properties of Diethylmetallic Azides Clusters of Aluminum and Gallium by DFT

XIA Qi-ying[1,2]，MA Deng-xue[2]，YANG Ji-min[1]

（1. *School of Chemistry and Chemical Engineering*，*Linyi Normal University*，*Linyi* 276005，*China*；

2. *School of Chemical Engineering*，*Nanjing University of Science and Technology*，*Nanjing* 210094，*China*）

Abstract：$(Et_2MN_3)_n$（$n = 1$ to 3，M = Al，Ga）clusters were studied by DFT/B3LYP method with SDD basis set. The dimer$(Et_2MN_3)_2$ and trimer$(Et_2MN_3)_3$（M = Al，Ga）are found to exhibit four-membered M_2N_2 and six-membered M_3N_3 ring structure，respectively. Compared with the monomer，the order of the bond length changes for the dimer $(Et_2MN_3)_2$ and trimer$(Et_2MN_3)_3$（M = Al，Ga）is as follows：N_α—M > N_α—N_β > N_β—N_γ ≈ M—C. Binding energies of the dimer $(Et_2AlN_3)_2$ and trimer$(Et_2AlN_3)_3$ clusters are 35.44 and 45.61 kJ·mol^{-1} lower than that of $(Et_2GaN_3)_2$ and $(Et_2GaN_3)_3$ clusters，respectively. Thermodynamic properties show that the dimer is the main composition of the $(Et_2MN_3)_n$（$n = 1$ to 3，M = Al，Ga）clusters at 298.2 K. The dimerization and trimerization are very favorable thermodynamically below 500 K.

Key words：physical chemistry；$(Et_2MN_3)_n$（$n = 1$ to 3，M = Al，Ga）；density functional theory（DFT）；binding energy；thermodynamic property

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1　Introduction

Clusters containing group ⅢA elements such as the group ⅢA dialkyl azides compounds have been studied extensively due to their distinctive properties. They will ignite if exposed to air，and explode when heated，releasing lots of heats and nitrogen gas. These properties enable their new applications，such as the igniters for both solid and liquid propellants and autoignition compositions under oil well. Especially，Et_2AlN_3 compound can be used as low-temperature igniter since its melting point is as low as −403 K. These compounds are used as the azidating agents[1]. They can be used to generate thin films of MN（M = Al，Ga and In）in various chemical vapor deposition（CVD）systems[2-3].

Diethylaluminum azide and diethylgallium azide are important group ⅢA dialkyl azides. Roman and Infrared studies reported that the molecule consisted of trimer in solution（symmetric D_{3h}）[4]. ^{1}H NMR results showed that diethylaluminum azide was a trimer with stable six-membered ring structure in solution[5]. The trimer-monomer equilibrium of diethylaluminum azide in solution was determined using the cryoscopic method，^{1}H NMR and ^{27}Al NMR[6]. Obviously，relatively little structural information in the gas state is available for these compounds. Therefore，we describe DFT results for the clusters of $(Et_2MN_3)_n$（$n = 1$ to 3，M = Al，Ga）. The geometric structures，binding energies，and thermodynamic properties are presented. Comparisons are also made between the $(Et_2AlN_3)_n$ and $(Et_2GaN_3)_n$（$n = 2$ to 3）clusters，and the $(Et_2MN_3)_n$ and $(Me_2MN_3)_n$（$n = 2$ to 3，M = Al，Ga）clusters.

2　Methods

The geometries of$(Et_2MN_3)_n$ clusters（$n = 1$ to 3，M = Al，Ga）were fully optimized by DFT method at the B3LYP/SDD level. SDD basis set had been successfully applied to $(Me_2MN_3)_n$ clusters（$n = 1$ to 3，M = Al，Ga）[7-8]. The found stationary points were characterized by frequency analysis（only real frequencies）. All calculations were carried out with the Gaussian98 program[9].

For the following polymerization
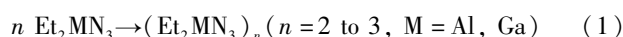
$$n\ Et_2MN_3 \rightarrow (Et_2MN_3)_n\ (n = 2\ to\ 3，M = Al，Ga)\quad（1）$$

the binding energy（ΔE）of complex is determined as

$$\Delta E = E_n - n E_1 \quad (n = 2 \text{ to } 3) \qquad (2)$$

where E_n and E_1 are the total energies of the clusters （Et_2MN_3）$_n$（$n = 2$ to 3；M = Al，Ga）and the isolated molecule Et_2MN_3（M = Al，Ga），respectively.

3 Results and Discussions

3.1 Structures of clusters

Figure 1 gives the structures of the Et_2MN_3 monomer and its clusters fully optimized at B3LYP/SDD level. The partial geometric parameters are summarized in Table 1. Et_2AlN_3，（Et_2AlN_3）$_2$，（Et_2AlN_3）$_3$，Et_2GaN_3，（Et_2GaN_3）$_2$ and（Et_2GaN_3）$_3$ are labeled as 1A，2A，3A，1B，2B and 3B in Fig 1，respectively（the H atoms of the dimer and trimer are omitted for clarity reasons）. For the trimer，we also present the Al_3N_3 and Ga_3N_3 cyclic core of the structures labeled as 3A′ and 3B′.（Et_2MN_3）$_2$ dimer and （Et_2MN_3）$_3$ trimer are formed by two and three Al or Ga atoms bridged by the α-nitrogen of the azide groups （connectivity：Et_2M—N_α—N_β—N_γ），respectively， which consists with the results studied by experimental method[2-6]. It has been previously established that in the dimers（H_2GaN_3）$_2$[10] and ［Cl_2InN_3（THF）$_2$］$_2$（THF = tetrahydrofuran）[11]，the trimers（Cl_2GaN_3）$_3$[12]， ［（CH_3）$BrGaN_3$］$_3$[13]，and（H_2GaN_3）$_3$[10]，cross-linking of the Ga or In atoms occurs via the α-nitrogen of the N_3 ligand. Our previously computational results also show that （H_2AlN_3）$_n$（$n = 2$ to 4）[14]，（H_2GaN_3）$_n$（$n = 2$ to 4）[15] and（Me_2AlN_3）$_n$（$n = 2$ to 3）[7-8] clusters are formed by Al or Ga atoms bridged by the α-nitrogen of the azide groups. On the other hand，the N_3In［（CH_2）$_3NMe_2$］$_2$ compound forms a polymeric structure in which cross-linking of the In atoms occurs via the γ-nitrogen of the N_3 ligand[16]. The（Et_2MN_3）$_2$ dimer did not be established for the Et_2MN_3 system（M = Al，Ga）before.

Computational results show a chair-like conformation （Al_3N_3 and Ga_3N_3 cyclic）of the trimer（Et_2MN_3）$_3$. The chair-like structure has been suggested for the （H_2AlN_3）$_3$[14]，（H_2GaN_3）$_3$[10,15] and（Cl_2GaN_3）$_3$[12] in gas phase. However，（Et_2GaN_3）$_3$ and（Et_2AlN_3）$_3$ in solution is a planar Ga—N and Al—N ring with D_{3h} symmetry[4].

Compared with the monomer，the bond lengths N_α—Al in the dimer and trimer structures increase by 20.5 and 21.9 ~ 22.2 pm，respectively. For the bond lengths N_α—Ga， the corresponding values are 20.2 and 21.4 ~ 21.7 pm. That is to say，the bond lengths N_α—Al and N_α—Ga increase as the clusters processing. This trend holds true for the changes of the N_α—N_β bond lengths as the（Et_2AlN_3）$_n$ and（Et_2GaN_3）$_n$（$n = 2$ to 3）cluster size enlarged. However-er，the trends disagree with those obtained for the N_β—N_γ bond lengths in the（Et_2AlN_3）$_n$ and（Et_2GaN_3）$_n$（$n = 2$ to 3）clusters. The Al—C bond lengths increase by 1.0 and 0.3 ~ 1.1 pm for the dimer and trimer respectively. As for the Ga—C bond lengths，the values are 0.3 ~ 1.3 pm and 0.0 ~ 1.7 pm. Note that the N_α—Ga bond length is always longer compared with N_α—Al. This fact reflects the weaker bonding in the case of Ga，which has also been found for the（Me_2AlN_3）$_n$（$n = 2$ to 3）clusters[7]. The bond length changes for the（Et_2AlN_3）$_n$ and（Et_2GaN_3）$_n$ （$n = 2$ to 3）clusters in the following orders：N_α—Al > N_α—N_β > N_β—N_γ ≈ Al—C，N_α—Ga > N_α—N_β > N_β—N_γ ≈ Ga—C. It holds true for the（Me_2AlN_3）$_n$（$n = 2$ to 3）clusters[7]. The increasing N_α—N_β，Al—C and Ga—C bond lengths show it could easily eliminate N_2 （N_β—N_γ）and —CH_2CH_3 groups to yield AlN and GaN ma-terials. For the（Et_2AlN_3）$_n$（$n = 1$ to 3），the N_α—N_β—N_γ bond angles are about 180.0° for all the structures，which is typical of those reported for the crystalline group ⅢA covalent azides. The average bond angles N_β—N_α—Al are ca. 129.7° and 117.1° in the structures 2A and 3A， respectively. The average bond angles N_α—Al—N_α are ca. 79.4° and 97.5° in the corresponding structures. The average bond angles Al-N_α-Al are about 100.6° and 125.3°. The above reported values of geometrical parame-ters are similar to those of the（Me_2AlN_3）$_n$（$n = 1$ to 3） clusters[7]，which shows that —CH_3 and —CH_2CH_3 groups have a little effect on the geometrical parameters of the basic building block. As for the（Et_2GaN_3）$_n$（$n = 1$ to 3），N_α—N_β—N_γ bond angles are about 180.0° for all the structures except for the monomer 1B. The average bond angles N_β—N_α—Ga，N_α—Ga—N_α and Ga—N_α—Ga are about 129.2°，78.3° and 101.7° in the dimer， respectively. As for the trimer，the average bond angles N_β—N_α—Ga，N_α—Ga—N_α and Ga—N_α—Ga are about 16.4°，95.7° and 126.3°，respectively.
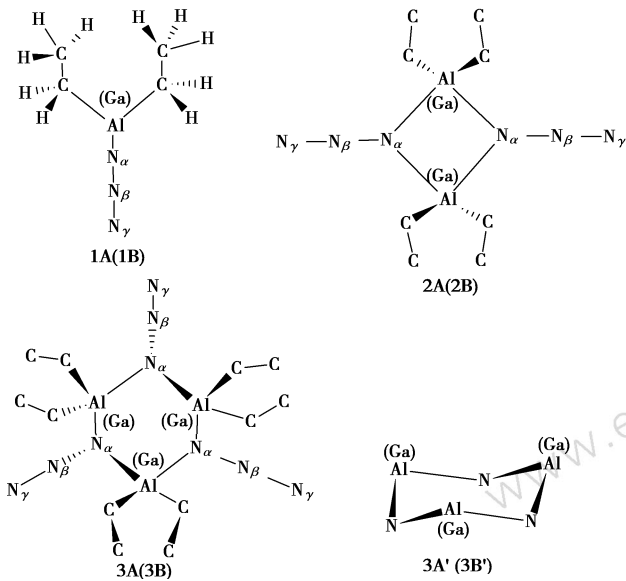
Fig. 1　Minima of $(Et_2MN_3)_n$ $(n = 1$ to 3, $M = Al$, $Ga)$
at the B3LYP/SDD level

Table 1　Geometries of Et_2MN_3 monomer and its clusters ($M = Al$, Ga)

		1A(1B)	2A(2B)	3A(3B)
bond length /Å	N_β—N_γ	1.178(1.179)[1]	1.168(1.174)	1.165(1.171)
			1.168(1.174)	1.164(1.170)
				1.164(1.170)
	N_α—N_β	1.222(1.240)	1.252(1.250)	1.267(1.263)
			1.252(1.250)	1.268(1.263)
				1.268(1.263)
	Al—N_α (Ga—N_α)	1.800(1.907)	2.005(2.109)	2.021(2.124)
			2.005(2.109)	2.022(2.122)
			2.005(2.109)	2.020(2.122)
			2.005(2.109)	2.021(2.122)
				2.021(2.122)
				2.019(2.121)
	Al—C (Ga—C)	1.973(1.999)	1.980(2.002)	1.976(1.999)
		1.972(1.989)	1.980(2.002)	1.984(2.005)
			1.980(2.002)	1.976(1.998)
			1.980(2.002)	1.985(2.005)
				1.976(1.998)
				1.984(2.006)
bond angle /(°)	N_α—N_β—N_γ	179.7(175.5)	180.0(179.7)	179.3(179.5)
			180.0(179.7)	179.3(179.3)
				179.4(179.5)
	N_β—N_α—Al (N_β—N_α—Ga)	177.9(139.1)	129.4(128.7)	117.2(116.4)
			130.0(129.7)	117.2(116.5)
			130.0(129.7)	117.3(116.4)
			129.4(128.7)	117.0(116.5)
				116.9(116.3)
				117.2(116.4)
	N_α—Al—N_α (N_α—Ga—N_α)		79.4(78.3)	97.4(96.1)
			79.4(78.3)	97.6(95.5)
				97.5(95.6)
	Al—N_α—Al (Ga—N_α—Ga)		100.6(101.7)	125.2(126.3)
			100.6(101.7)	125.2(126.2)
				125.5(126.3)

Note：1) Data in parentheses are the geometric parameters of $(Et_2GaN_3)_n$ $(n = 1$ to $3)$.

3.2　Total Energies and Binding Energies

　　Table 2 reports the total energies, zero point energies(ZPE), and ZPE corrections for the binding energies of the $(Et_2MN_3)_n$ $(n = 2$ to 3, $M = Al$, $Ga)$ clusters. The proportions of ZPE corrections to their binding energies ΔE_{ZPEC} are 2.80%, 4.40%, 2.54% and 4.24% for 2A, 3A, 2B and 3B, respectively, which indicates the ZPE corrections for the binding energies are small, and the proportions are similar for the two dimers and two trimers, respectively. After the corrections of the ZPE, the binding energies are −171.37, −252.68, −135.93 and −207.07 kJ·mol^{-1} for 2A, 3A, 2B and 3B, respectively. The binding energies of the $(Et_2AlN_3)_n$ $(n = 2$ to $3)$ clusters are lower than those of the corresponding $(Et_2GaN_3)_n$ $(n = 2$ to $3)$ clusters. It is also found that the binding energies of the dimer $(Et_2MN_3)_2$ are very close to those of the dimer $(Me_2MN_3)_2$ $(M = Al, Ga)$[7], which hold true for the trimer.

Table 2　Energies of the Et_2MN_3 monomer and its clusters ($M = Al$, Ga)　kJ·mol^{-1}

structure	E	ΔE	ZPE	ΔE_{ZPEC}
1A	−1483583.37		377.24	
2A	−2967342.90	−176.16	759.47	−171.37
3A	−4451013.92	−263.81	1143.31	−252.68
1B	−852464.18		374.90	
2B	−1705067.74	−139.38	753.39	−135.93
3B	−2557608.39	−215.85	1133.85	−207.07

3.3　Thermodynamic property

　　On the basis of vibrational analysis and statistical thermodynamic, the standard thermodynamic functions, heat capacities ($C_{P,m}^0$), entropies (S_m^0) and enthalpies (H_m^0), were obtained and listed in Table 3. The magnitudes of heat capacities (C_P^0) for the clusters with the same number of molecules(n) are approximately at the same temperature, and larger than $n \times C_P^0(1A)$ or $n \times C_P^0(1B)$ by 11.12~15.63, 14.11~15.19, 23.28~33.83 and 27.83~33.16 J·mol^{-1}·K^{-1} for $n = 2$ and 3 respectively. In the course of $1 \rightarrow 2 \sim 3(1A \rightarrow 2A \sim 3A$ or $1B \rightarrow 2B \sim 3B)$, the entropy decreases at any temperature from 200.0 to 700.0K due to the decrease of probability. The gradient of ΔS to temperature decreases as temperature increases. The polymerization is an exothermic process since the polymeriza-

tion causes the decrease of enthalpy. ΔH_T increases slightly as temperature increases, indicating that the polymerization weakens as temperature increases. The dimerization and trimerization enthalpies in the $(Et_2MN_3)_n$ (n = 2 to 3, M = Al, Ga) clusters are close to those obtained in the $(Me_2MN_3)_n$ clusters[7]. From the equation of $\Delta G = \Delta H - T\Delta S$, the values of ΔG at different temperatures could be obtained. On going from $1 \rightarrow 2 \sim 3$, the value of ΔG_T is negative with the temperature ranging from 298.2 K to 500.0 K, which show that the polymeri-

zation can occur spontaneously. The value of ΔG_T increases as temperature increases, indicating that the spontaneity decreases as temperature increases. The absolute values of ΔG_T for the dimer and trimer at 298.2 K are large, which show that there is no monomer existing. The proportions for 2A : 3A and 2B : 3B are equal to 2450600000 : 1 and 41188000 : 1 at 298.2 K, which reveal that the diethylaluminum and diethylgallium azides systems both consist of the dimer. This holds true for dimethylaluminum and dimethylgallium azides clusters[7].

Table 3　Thermodynamic properties of Et$_2$MN$_3$(M = Al, Ga) monomer and its clusters at different temperatures

structure	T/K	$C_P^0/\text{J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$	$S_T^0/\text{J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$	$H_T^0/\text{kJ} \cdot \text{mol}^{-1}$	$\Delta S_T^{1)}/\text{J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$	$\Delta H_T^{2)}/\text{kJ} \cdot \text{mol}^{-1}$	$\Delta G_T^{3)}/\text{kJ} \cdot \text{mol}^{-1}$
1A	298.2	169.83	475.05	33.78			
	500.0	233.54	578.60	74.76			
	700.0	279.92	664.96	126.36			
2A	298.2	350.78	746.36	66.58	− 203.74	− 172.35	− 111.59
	500.0	482.62	960.53	151.35	− 196.67	− 169.54	− 71.21
	700.0	575.47	1138.58	257.71	− 191.34	− 166.38	− 32.44
3A	298.2	532.77	950.04	98.55	− 475.11	− 255.47	− 113.79
	500.0	732.27	1275.16	227.23	− 460.64	− 249.73	− 19.41
	700.0	873.59	1545.33	388.61	− 449.55	− 243.15	71.54
1B	298.2	172.54	473.31	34.31			
	500.0	235.35	578.02	75.74			
	700.0	281.18	664.90	127.64			
2B	298.2	359.19	785.65	70.01	− 160.97	− 134.54	− 86.54
	500.0	486.49	1002.89	155.94	− 153.15	− 131.47	− 54.90
	700.0	577.55	1181.92	262.87	− 147.88	− 128.34	− 24.82
3B	298.2	545.45	1018.92	104.07	− 401.01	− 205.93	− 86.35
	500.0	738.12	1348.69	234.50	− 385.37	− 199.79	− 7.11
	700.0	876.70	1620.34	396.75	− 374.36	− 193.24	68.81

Note: 1) $\Delta S_T = (S_T^0)_i - n(S_T^0)_{1A(B)}$, 2) $\Delta H_T = (H_T^0 + E(HF) + ZPE)_i - n(H_T^0 + E(HF) + ZPE)_{1A(B)}$, 3) $\Delta G_T = \Delta H_T - T\Delta S_T$ (i = 2A, 3A, 2B and 3B with n = 2, 3, 2, 3 respectively), and a scale factor of 0.96 for frequencies is imposed.

4　Conclusions

　　DFT/B3LYP method with SDD basis set was used to calculate structures and properties of Et$_2$MN$_3$ (M = Al, Ga) systems consisting of up to three molecules predicts that $(Et_2MN_3)_n$ (n = 2 to 3, M = Al, Ga) all possess cyclic-like structures. Compared with the monomer, the structure changes are great. The proportions of ZPE corrections to their binding energies ΔE_{ZPEC} are less than 4.50%. The binding energies of − 171.37 and − 252.68 kJ · mol^{-1} for the $(Et_2AlN_3)_{n(n}$ = 2 to 3) clusters are lower than those of the corresponding $(Et_2GaN_3)_n$ clusters (− 135.93 and − 207.07 kJ · mol^{-1}). Thermodynamic properties show that the polymerization can occur sponta-

neously at 298.2 K, and dimer is the main component of the diethylaluminum and diethylgallium azides systems.

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叠氮二乙基铝和镓多聚体结构和性质的密度泛函理论研究

夏其英[1,2]，马登学[2]，杨吉民[1]

(1. 临沂师范学院化学化工学院，山东 临沂 276005；
2. 南京理工大学化工学院，江苏 南京 210094)

摘要： 采用 DFT-B3LYP/SDD 方法系统研究了 $(Et_2MN_3)_n$ ($n = 1 - 3$, M = Al, Ga) 体系。二聚体 $(Et_2MN_3)_2$ 和三聚体 $(Et_2MN_3)_3$ (M = Al, Ga) 分别拥有四元环 M_2N_2 和六元环 M_3N_3 结构。与单体相比，二聚体 $(Et_2MN_3)_2$ 和三聚体 $(Et_2MN_3)_3$ (M = Al, Ga) 的键长变化次序均为 $N_\alpha—M > N_\alpha—N_\beta > N_\beta—N_\gamma \approx M—C$。二聚体 $(Et_2AlN_3)_2$ 的结合能比 $(Et_2GaN_3)_2$ 低 35.44 kJ·mol^{-1}，而三聚体 $(Et_2AlN_3)_3$ 的结合能比 $(Et_2GaN_3)_3$ 低 45.61 kJ·mol^{-1}。热力学性质表明叠氮二乙基铝和镓体系在 298.2 K 温度下均以二聚体为主。在低于 500 K 的温度下，二聚化和三聚化反应在热力学上是有利的。

关键词： 物理化学；$(Et_2MN_3)_n$ ($n = 1 - 3$, M = Al, Ga)；密度泛函理论(DFT)；结合能；热力学性质

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《含能材料》进入 Elsevier 重要数据库 SCOPUS

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　　Scopus(www.scopus.com) 于 2004 年 11 月正式推出，是目前全球规模最大的文摘和引文数据库。Scopus 涵盖了由 4000 多家出版商出版发行的科技、医学和社会科学方面的 15,100 多种期刊。相对于其他单一的文摘索引数据库而言，Scopus 的内容更加全面，学科更加广泛，特别是在获取欧洲及亚太地区的文献方面，用户可检索出更多的文献数量，通过 Scopus，用户可以检索到 1966 年以来的 3000 多万条摘要和题录信息，以及 1996 年以来所引用的参考文献。数据每日更新。