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## Structures and stability of $N_{13}^+$ and $N_{13}^-$ clusters

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**Abstract** The structures and stabilities of eleven  $N_{13}^+$  and  $N_{13}^-$  isomers have been investigated with second-order Møller–Plesset (MP2) and density functional theory (DFT) methods. Five  $N_{13}^+$  isomers and six  $N_{13}^-$  isomers are all reasonable local minima on their potential energy hypersurfaces. The most stable  $N_{13}^+$  cation is structure **C-2** with  $C_{2v}$  symmetry, which contains a pentazole ring and two  $N_4$  open chains. It is different from those of the  $N_7^+$  and  $N_9^+$  clusters, but similar to the  $N_{11}^+$  cluster. Meanwhile, the most stable  $N_{13}^-$  structure **A-2** is composed of a pentazole ring and a six-membered ring connected by two nitrogen atoms. It is not only different from those of the  $N_7^-$  and  $N_9^-$  clusters, but also from the  $N_{11}^-$  cluster. The decomposition pathways of structures **C-2** and **A-2** were investigated at the B3LYP/(aug)-cc-pVDZ level. From the barrier heights of the structures **C-2** and **A-2** decomposition processes, it is suggested that **C-2** is difficult to observe experimentally and **A-2** may be observed as a short-lived species.

**Keywords** Nitrogen cluster · Ab initio · DFT ·  $N_{13}^+$  ·  $N_{13}^-$

### Introduction

Homo-polynitrogen molecules are of general interest not only in forming potential high-energy density materials (HEDMs), but also in their intriguing molecular structures and properties. The nitrogen atom is isoelectronic with the CH group and many  $(CH)_n$  compounds have been synthesized. Numerous nitrogen clusters have been predicted theoretically, only a few have been synthesized. The azide ion  $N_3^-$  was first synthesized in 1890 [1]. However, after an entire century, in 1998 Christe and

coworkers [2] synthesized the salt  $[N_5^+][AsF_6^-]$  by reacting  $N_2F^+AsF_6^-$  with  $HN_3$  in anhydrous hydrogen fluoride at  $-78^\circ C$ . It is very surprising that the synthesized nitrogen clusters are ions containing odd-numbered nitrogen atoms rather than even-numbered nitrogen clusters.

Many of theoretical investigations on more odd-numbered nitrogen ionic clusters, such as  $N_3^+$ , [3, 4]  $N_5^+$ , [3, 5, 6, 7, 8]  $N_5^-$ , [3, 5, 9, 10]  $N_7^+$ , [3, 11]  $N_7^-$ , [3, 11, 12]  $N_9^+$ , [3, 13]  $N_9^-$ , [3, 13]  $N_{11}^-$ , [14]  $N_{11}^+$  [14] and  $N(N_3)_4^+$ , [12] have been performed. Christe et al. [5] found the novel  $N_5^+$  cation is an open-chain structure by means of NMR, IR and Raman data. The experimental results are consistent with their own CCSD(T)/6-311+G(2d) theoretical results. Wang et al. [5] found that the most stable  $N_5^-$  anion is a complex with a weak  $N_2...N_3^-$  bonding. Our calculations [11] suggested that the open chain  $N_7^+$  is the most stable species. For the  $N_7^-$  cluster, Michels et al. [12] demonstrated that the open chain structure  $N(N_3)_2^-$  is a genuine minimum on the potential energy surface at the HF/6-31G\* and MP2/6-31G\* levels. For the  $N_9^+$  and  $N_9^-$  clusters, we [13] reported that the most stable  $N_9^-$  cluster is an open-chain structure with  $C_{2v}$  symmetry; meanwhile only one stable structure of  $N_9^+$  cation with  $C_{2v}$  symmetry was found. Recently we [14] have reported that the ionic  $N_{11}^-$  was also an open-chain structure; while the most stable structure of the cation  $N_{11}^+$  is composed of a pentazole structure unit. Michels et al. [12] reported that the tetraazidammonium cation,  $N(N_3)_4^+$ , is a stable structure with  $D_{2d}$  symmetry. Based on this previous work on the  $N_{2n+1}$  ( $n \geq 6$ ) nitrogen clusters, generally, the most stable isomers for many odd-numbered ionic clusters are open chain structures. Is this conclusion applicable to the  $N_{13}$  ionic clusters? To answer this question, it is necessary to study the  $N_{13}$  ionic clusters further.

In the present work, we studied the equilibrium structures, energies, and vibrational frequencies of  $N_{13}^+$  and  $N_{13}^-$  clusters, and attempted to find the possible decomposition pathways of some isomers.

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## Computational method

Geometries were fully optimized using density-functional theory (DFT), and second-order Møller–Plesset perturbation theory (MP2) [15]. The core orbitals were kept frozen in the MP2 method. The DFT method used in the present work is the hybrid density functional B3LYP approach, i.e., Beck's three-parameter nonlocal functional with the nonlocal correlation functional of Lee, Yang, and Parr [16, 17]. For the cation  $N_{13}^+$ , the basis set is the correlation-consistent basis set of Dunning [18], specifically the polarized valence double-zeta (cc-pVDZ) set, as well as for the anion  $N_{13}^-$ , the basis set is augmented with diffuse functions (aug-cc-pVDZ). Vibrational frequencies computed at the same level have been used for the characterization of stationary points and zero-point energy (ZPE) correction. All the stationary points have been positively identified for minima (NIMAG=0) or transition states (NIMAG=1). Improved energies were obtained by B3LYP/(aug)-cc-pVTZ//B3LYP/(aug)-cc-pVDZ+ZPE-

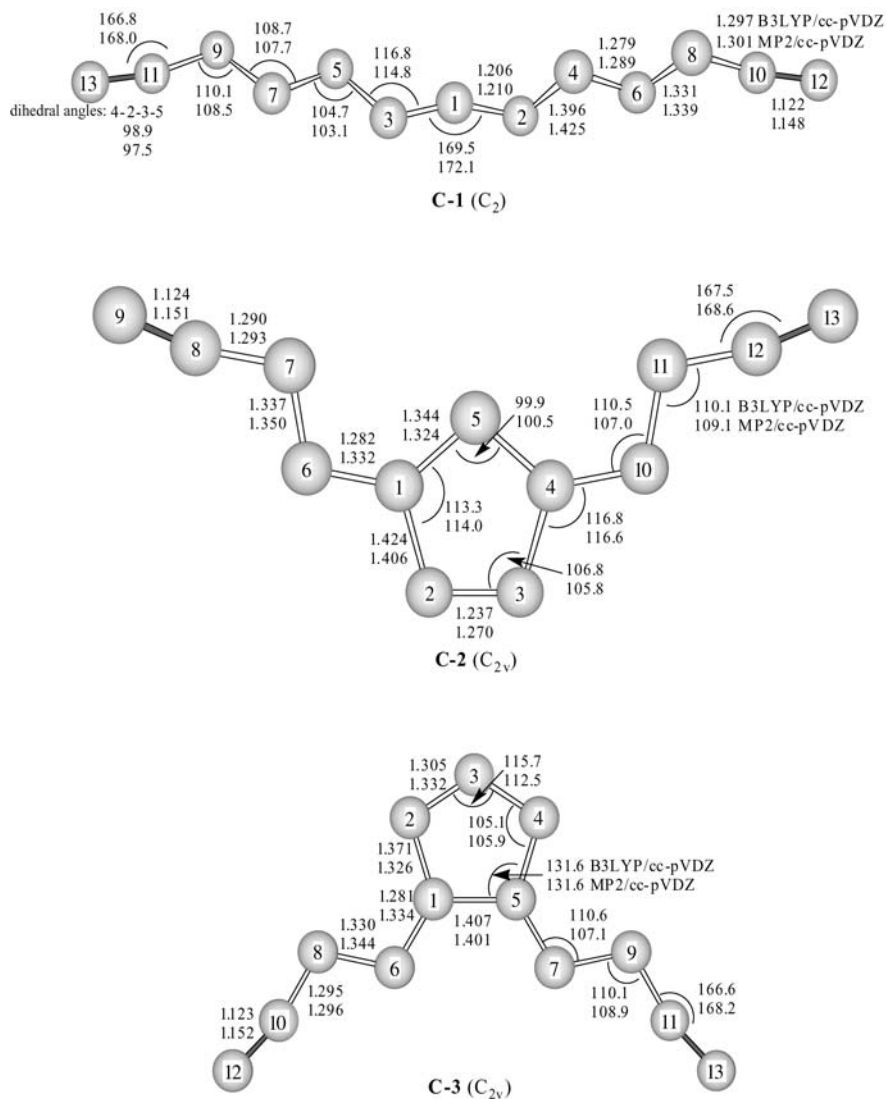
(B3LYP/(aug)-cc-pVDZ) single-point calculations. The minimum energy pathways connecting the reactants and products were confirmed using the intrinsic reaction coordinate (IRC) method with the Gonzalez–Schlegel second-order algorithm [19, 20].

Throughout this paper, bond lengths are given in ångströms, bond angles in degrees, total energies in Hartrees, relative energy and the zero-point vibrational energies in kcal mol<sup>-1</sup>. The B3LYP optimized geometry and the B3LYP/(aug)-cc-pVTZ energies have been used to discuss the structures and the energies for the  $N_{13}$  ionic clusters, respectively. All calculations in this study were carried out with the Gaussian 98 quantum chemistry package [21].

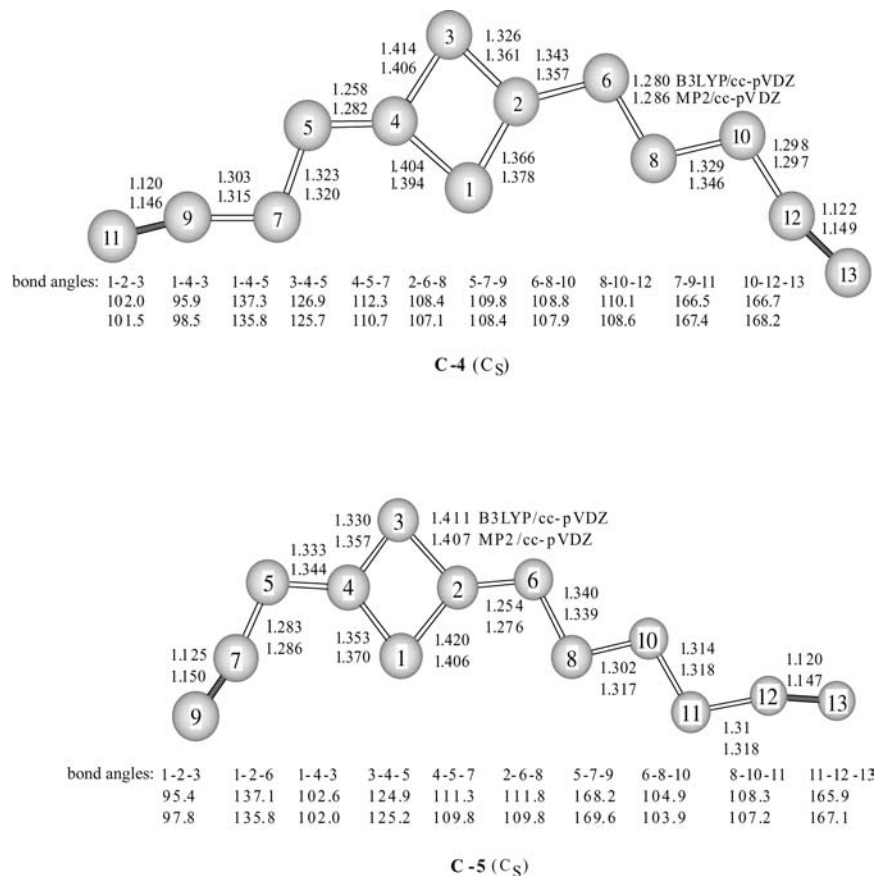
## Results and discussion

Optimized structures as well as their geometric parameters of  $N_{13}^+$  and  $N_{13}^-$  clusters are illustrated in Figs. 1, 2, 3

**Fig. 1** Optimized geometrical parameters of  $N_{13}^+$  isomers C-1, C-2, and C-3



**Fig. 2** Optimized geometrical parameters of  $N_{13}^+$  isomers **C-4** and **C-5**



**Table 1** Total energies  $E$  (in Hartrees) and zero point energies ZPE (in kcal mol<sup>-1</sup>) for the isomers of  $N_{13}^+$  and  $N_{13}^-$  clusters

Isomers	B3LYP/(aug)-cc-pVDZ <sup>a</sup>		MP2/(aug)-cc-pVDZ	B3LYP/(aug)-cc-pVTZ	
	$E$	ZPE	$E$	$E$	
$N_{13}^+$	<b>C-1</b> ( <sup>1</sup> A <sub>1</sub> ,C <sub>2v</sub> )	-711.127051	34.8	-709.243278	-711.3160397
	<b>C-2</b> ( <sup>1</sup> A <sub>1</sub> ,C <sub>2v</sub> )	-711.1451065	37.2	-709.2854725	-711.3302928
	<b>C-3</b> ( <sup>1</sup> A <sub>1</sub> ,C <sub>2v</sub> )	-711.1196974	36.4	-709.2544724	-711.3042034
	<b>C-4</b> ( <sup>1</sup> A',C <sub>s</sub> )	-711.0818578	36.4	-709.2175471	-711.2687005
	<b>C-5</b> ( <sup>1</sup> A',C <sub>s</sub> )	-711.0712604	36.2	-709.204178	-711.2585166
$N_{13}^-$	<b>A-1</b> ( <sup>1</sup> A <sub>1</sub> ,C <sub>2v</sub> )	-711.6112085	34.7	-709.8021604	-711.7610278
	<b>A-2</b> (C <sub>1</sub> )	-711.6168377	37.2	-709.8253269	-711.7758962
	<b>A-3</b> (C <sub>1</sub> )	-711.5797232	35.5	-709.7745421	-711.7240838
	<b>A-4</b> ( <sup>1</sup> A <sub>1</sub> ,C <sub>2v</sub> )	-711.5648324	35.9	-709.7762732	-711.7144707
	<b>A-5</b> ( <sup>1</sup> A <sub>1</sub> ,C <sub>2v</sub> )	-711.5524752	35.5	-709.7659663	-711.7024254
	<b>A-6</b> ( <sup>1</sup> A <sub>1</sub> ,C <sub>2v</sub> )	-711.3650785	32.9	-709.6158951	-711.5063242

<sup>a</sup> The basis sets for  $N_{13}^+$  and  $N_{13}^-$  clusters are cc-pVDZ and aug-cc-pVDZ, respectively

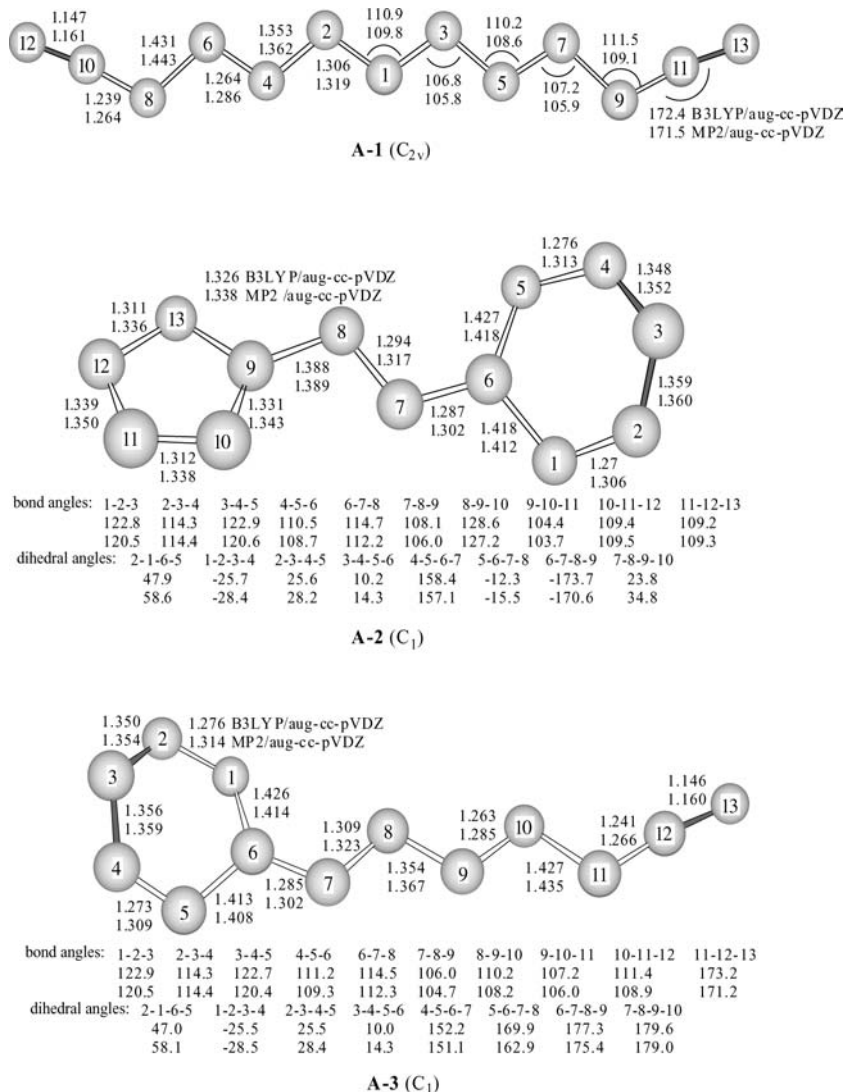
and 4. Their total energies, zero point energies (ZPE) and the relative energies corrected by ZPE are listed in Tables 1 and 2. All the eleven isomers of  $N_{13}$  ionic clusters are minima on their potential energy hypersurfaces at the B3LYP/(aug)-cc-pVDZ level of theory.

### $N_{13}^+$ isomers

From Table 2, the energetic stability ordering of the five  $N_{13}^+$  isomers is **C-2**>**C-1**>**C-3**>**C-4**>**C-5**. As shown in Fig. 1, the most stable structure **C-2** with  $C_{2v}$  symmetry is

composed of a five-membered ring and two  $N_4$  open chains in *int* position. It is energetically lower than structure **C-1** by 6.3 kcal mol<sup>-1</sup>. The bond lengths of the pentazole ring are close to the aromatic N–N bond length (1.35 Å) [9]. To analyze the aromaticity of the pentazole ring further, we have calculated the NICS(1.0) value [22], by placing a ghost atom 1.0 Å above the geometric center of the pentazole ring. The NICS(1.0) value for **C-2** is -11.0, comparable to the value for benzene (-10.0) [23], indicating that the pentazole ring is aromatic. It is similar to the most stable structure of  $N_{11}^+$ , [14] which contains a pentazole ring and two  $N_3$  open chains. **C-3**, containing a

**Fig. 3** Optimized geometrical parameters of  $N_{13}^-$  isomers **A-1**, **A-2**, and **A-3**



**Table 2** Relative energies (in kcal mol<sup>-1</sup>) for the isomers of  $N_{13}^+$  and  $N_{13}^-$  clusters

Isomers		B3LYP/(aug)-cc-pVDZ <sup>a</sup>	MP2/(aug)-cc-pVDZ <sup>a</sup>	B3LYP/(aug)-cc-pVTZ+ZPE <sup>b</sup>
$N_{13}^+$	<b>C-1</b> ( <sup>1</sup> A <sub>1</sub> ,C <sub>2v</sub> )	0.0	0.0	0.0
	<b>C-2</b> ( <sup>1</sup> A <sub>1</sub> ,C <sub>2v</sub> )	-9.0	-26.5	-6.3
	<b>C-3</b> ( <sup>1</sup> A',C <sub>s</sub> )	6.2	-7.0	9.4
	<b>C-4</b> ( <sup>1</sup> A',C <sub>s</sub> )	29.9	16.1	31.5
	<b>C-5</b> ( <sup>1</sup> A',C <sub>s</sub> )	36.4	24.5	37.7
$N_{13}^-$	<b>A-1</b> ( <sup>1</sup> A <sub>1</sub> ,C <sub>2v</sub> )	0.0	0.0	0.0
	<b>A-2</b> (C <sub>1</sub> )	-1.0	-14.5	-6.8
	<b>A-3</b> (C <sub>1</sub> )	20.5	17.3	24.0
	<b>A-4</b> ( <sup>1</sup> A <sub>1</sub> ,C <sub>2v</sub> )	30.3	16.2	30.4
	<b>A-5</b> ( <sup>1</sup> A <sub>1</sub> ,C <sub>2v</sub> )	37.7	22.7	37.6
	<b>A-6</b> ( <sup>1</sup> A <sub>1</sub> ,C <sub>2v</sub> )	152.6	116.9	158.0

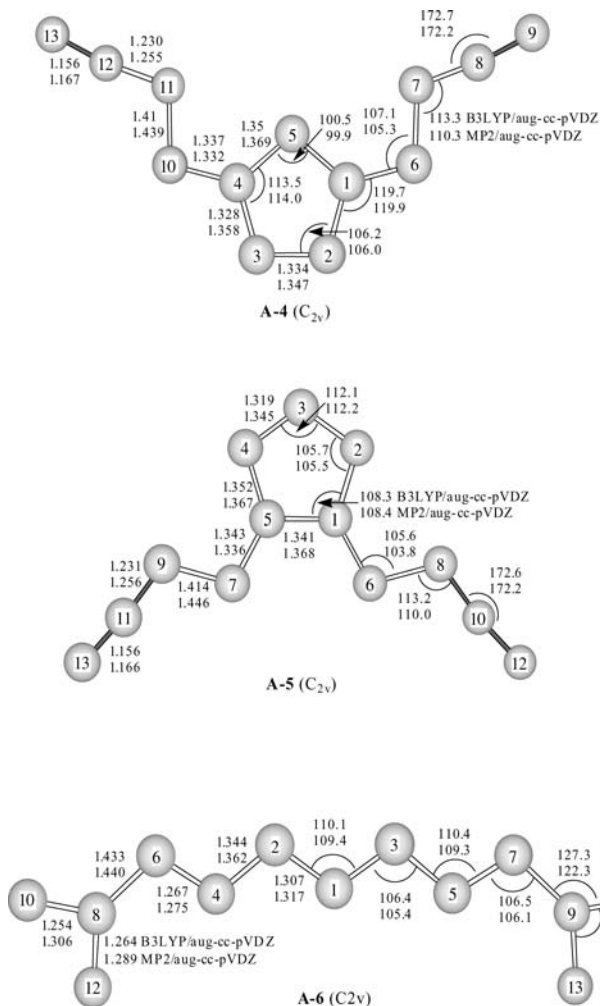
<sup>a</sup> The basis sets for  $N_{13}^+$  and  $N_{13}^-$  clusters are cc-pVDZ and aug-cc-pVDZ, respectively

<sup>b</sup> Relative energies at the B3LYP/(aug)-cc-pVTZ//B3LYP/(aug)-cc-pVDZ +ZPE(B3LYP/(aug)-cc-pVDZ) level

pentazole ring and two open chains  $N_4$  in *para* position, has  $C_{2v}$  symmetry and the <sup>1</sup>A<sub>1</sub> electronic state. It lies energetically higher than **C-1** by 9.4 kcal mol<sup>-1</sup>. The NICS(1.0) value for **C-3** is -9.7. It is more negative than that for **C-2**, suggesting that **C-2** should be more aromatic than **C-3**, in agreement with their relative stabilities.

Different from isomers of  $N_7^+$  and  $N_9^+$  clusters, **C-1** is the third lowest structure in energy among the five  $N_{13}^+$  isomers. It has  $C_2$  symmetry and the <sup>1</sup>A electronic state.

**C-4** ( $C_{2v}$ ), containing a four-membered ring and two open  $N_4$  chains in adjoining positions, is higher in energy than **C-1** by 31.5 kcal mol<sup>-1</sup>. Structure **C-5** ( $C_s$ ) contains a

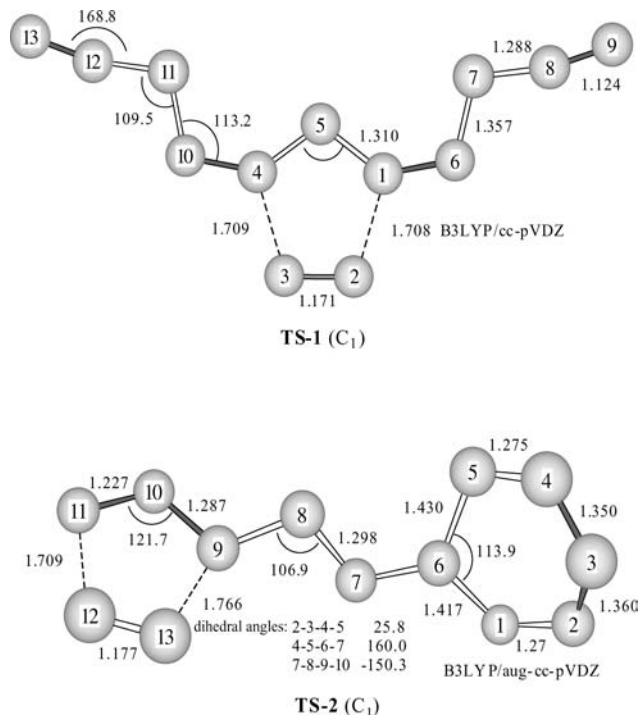


**Fig. 4** Optimized geometrical parameters of  $N_{13}^-$  isomers **A-4**, **A-5**, and **A-6**

four-membered ring and two open  $N_4$  and  $N_5$  chains, and it is the least stable of the five  $N_{13}^+$  isomers, which is energetically higher by about  $37.7 \text{ kcal mol}^{-1}$  than structure **C-1**. Due to their instability, no further discussion is given for these isomers in the present work. We also studied the structures containing six-membered ring, but none of them were found to be stable.

### $N_{13}^-$ isomers

Different from the open chain structures being the most stable isomers for  $N_7^-$ ,  $N_9^-$ , and  $N_{11}^-$  anion clusters, the open chain structure **A-1** with  $C_{2v}$  symmetry is not the most stable isomer for  $N_{13}^-$  anionic cluster. However, structure **A-2** composed of a pentazole ring and a six-membered ring is the most stable of the six  $N_{13}^-$  isomers. It is energetically lower than **A-1** by  $6.8 \text{ kcal mol}^{-1}$ . All bond lengths of the pentazole ring unit lie within the range from  $1.311$  to  $1.339 \text{ \AA}$ . Most of them are close to the aromatic N–N bond length ( $1.35 \text{ \AA}$ ). [9] The NICS(1.0) value for **A-2** is  $-12.1$ , suggesting that the pentazole ring is aromatic. The bond lengths of the six-



**Fig. 5** Optimized geometrical parameters of **TS-1** and **TS-2**

membered ring are slightly longer than those of the pentazole ring. The optimized geometries show that the pentazole ring is close to a planar structure and the six-membered ring favors the boat conformation. **A-1** is the second lowest-energy structure among the six  $N_{13}^-$  isomers. It has  $C_{2v}$  symmetry and the  $^1A_1$  electronic state. **A-3** ( $C_1$ ) contains a six-membered ring and an open  $N_7$  chain, and it is energetically higher than structure **A-1** by  $24.0 \text{ kcal mol}^{-1}$ . **A-4**, containing a pentazole ring and two open chains  $N_4$  in *int* position, has  $C_{2v}$  symmetry and the  $^1A_1$  electronic state, and it is energetically higher than structure **A-1** by  $30.4 \text{ kcal mol}^{-1}$ . **A-5** ( $C_{2v}$ ) contains a pentazole ring and two open  $N_4$  chains in adjoining position. **A-6** ( $C_{2v}$ ) is the least stable species among the six  $N_{13}^-$  isomers which is energetically higher than **A-1** by  $158.0 \text{ kcal mol}^{-1}$ . Due to the instability of above  $N_{13}^-$  isomers, there will be no further discussion of them.

### Transition states and decomposition pathways

Although the above eleven isomers are thermodynamically stable, the metastability and whether they can be synthesized and stored depend on the activation energy of reaction. Therefore, it is necessary to investigate the decomposition pathways. Since the most stable isomers always draw one's attention, we shall examine the decomposition reaction of the most stable structures **C-2** and **A-2**.

For **C-2**, we have located a transition state (**TS-1**) for decomposition to  $N_{11}^+ + N_2$  at the B3LYP/cc-pVDZ level. Calculation of the harmonic vibrational frequencies confirmed that it is a transition state, with an imaginary frequency of  $383i \text{ cm}^{-1}$ . As shown in Fig. 5, during the formation of **TS-1**, with symmetry changing from  $C_{2v}$  of **C-2**

**Table 3** Total energies  $E$  (in Hartrees), zero point energies ZPE (in kcal mol<sup>-1</sup>) and relative energies (in kcal mol<sup>-1</sup>) for the species involved in **C-2** and **A-2** decomposition systems

	Isomers	B3LYP/(aug)-cc-pVDZ <sup>a</sup>			B3LYP/(aug)-cc-pVTZ	
		$E$	ZPE	$E_{\text{rel}}$	$E$	$E_{\text{rel}}^{\text{b}}$
$\text{N}_{13}^+$	<b>C-2</b> ( <sup>1</sup> A <sub>1</sub> ,C <sub>2v</sub> )	-711.127051	34.8	0.0	-711.3302928	0.0
	<b>TS-1</b> (C <sub>1</sub> )	-711.1451065	37.2	4.1	-711.3210566	8.2
	$\text{N}_{11}^+(\text{C}_{2v})+\text{N}_2$	-711.1196974	36.4	-67.7	-711.3993605	-41.7
$\text{N}_{13}^-$	<b>A-2</b> (C <sub>1</sub> )	-711.6168377	37.2	0.0	-711.7758962	0.0
	<b>TS-2</b> (C <sub>1</sub> )	-711.5948992	34.8	11.4	-711.7222462	31.3
	$\text{N}_{11}^-(\text{C}_1)+\text{N}_2$	-711.6505872	33.0	-21.2	-711.7985483	-18.4

<sup>a</sup> The basis sets for  $\text{N}_{13}^+$  and  $\text{N}_{13}^-$  clusters are cc-pVDZ and aug-cc-pVDZ, respectively

<sup>b</sup> Relative energies at the B3LYP/(aug)-cc-pVTZ//B3LYP/(aug)-cc-pVDZ +ZPE(B3LYP/(aug)-cc-pVDZ) level

to C<sub>1</sub> of **TS-1**, the bond lengths of N1–N2 and N3–N4 increase to 1.708 and 1.709 Å. While the other bond lengths and bond angles changed slightly, suggesting that the interactions of N1 and N2 as well as N3 and N4 are weakened. Thus, the bond N1–N2 and N3–N4 would break easily, and **C-2** would dissociate into two species:  $\text{N}_{11}^++\text{N}_2$ . As show in Table 3, the decomposition barrier height of structure **C-2** is only 8.2 kcal mol<sup>-1</sup>. It is so low that it is rather doubtful if this isomer can ever be observed experimentally.

We found a transition state (**TS-2**) for  $\text{N}_{13}^- \rightarrow \text{N}_{11}^- + \text{N}_2$  at the B3LYP/cc-pVDZ level. During the process of **A-2** decomposing into  $\text{N}_{11}^- + \text{N}_2$ , the bond lengths of N11–N12 and N9–N13 increase to 1.709 and 1.766 Å, the other bond lengths and bond angles change slightly. This suggests that the decomposition mechanism of **A-2** is the cleavage of N9–N13 and N11–N12, and then nitrogen molecule is eliminated from the pentazole ring of the **A-2** isomer. IRC calculations confirmed that **TS-2** connects **A-2** on the reactant side to  $\text{N}_{11}^- + \text{N}_2$  on the product side. Table 3 shows that the dissociation barrier height for the  $\text{N}_2$  fission reaction of **A-2** is 31.3 kcal mol<sup>-1</sup>. Such a value suggests that it is possible to observe this isomer only as a short-lived species.

## Summary

We have reported geometries, energies, harmonic vibrational frequencies and bonding for five  $\text{N}_{13}^+$  isomers and six  $\text{N}_{13}^-$  isomers using ab initio and DFT methods. It is interesting that the most stable isomer for the  $\text{N}_{13}^+$  cluster presented here is the structure **C-2** (C<sub>2v</sub>) composed of a cyclic N<sub>5</sub> and two N<sub>4</sub> open chains. It is similar to the  $\text{N}_{11}^+$  cluster containing the pentazole structure, but different from the odd-numbered nitrogen cations (N<sub>5</sub><sup>+</sup> and N<sub>9</sub><sup>+</sup> clusters) with open-chain structures. In addition, the most stable species of the  $\text{N}_{13}^-$  cluster is structure **A-2** composed of a six-membered ring and a pentazole ring, which is different from those of N<sub>7</sub><sup>-</sup>, N<sub>9</sub><sup>-</sup>, and  $\text{N}_{11}^-$  clusters. The decomposition pathways of isomers **C-2** and **A-2** were studied at the B3LYP/(aug)-cc-pVDZ level. The barrier height of the decomposition process is 8.2 kcal mol<sup>-1</sup> for  $\text{N}_{13}^+(\text{C}_1) \rightarrow \text{N}_{11}^+(\text{C}_{2v}) + \text{N}_2$ , suggesting that **C-2** is difficult to be observed experimentally. And the barrier heights is

31.3 kcal mol<sup>-1</sup> for  $\text{N}_{13}^-(\text{C}_1) \rightarrow \text{N}_{11}^-(\text{C}_{2v}) + \text{N}_2$ , indicating that **A-2** might be observed as a short-lived species.

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