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The structure and stability of $B_{36}N_{36}$ cages: a computational study

Abstract The structure and stability of 22 $B_{36}N_{36}$ cage molecules containing four-membered (F_4), five-membered (F_5), six-membered (F_6), eight-membered (F_8) and 12-membered (F_{12}) rings have been computed at the B3LYP/6-31G* level of density functional theory. The most stable structure (**1**) has T_d symmetry with six F_4 and 32 F_6 rings, following the isolated square rule, while the fullerene-like structures (12 F_5 and 26 F_6) and also structures with F_8 and F_{12} are much higher in energy.

Keywords DFT · Inorganic fullerene · Structure · Stability

Introduction

Stoichiometric boron nitrides $(BN)_n$, the isoelectronic analogues to carbon fullerenes, have been a subject of extensive and intensive investigations. In contrast to carbon fullerenes (C_{60} and C_{70}), there is no direct evidence for the most favored structures of BN analogues, despite advanced synthesis and characterization [1–11]. In contrast, recent advances and developments in theoretical methods and computer technology provide an alternative tool for elucidating the structure and stability of $(BN)_n$.

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While the stability of carbon fullerenes is governed by the isolated pentagon rule (IPR), i.e., the maximal and perfect separation of the strained pentagons, the stability of $(BN)_n$ can be estimated by the isolated square rule (ISR), i.e., the maximal and perfect separation of the strained squares. In 1993, Jensen and Toftlund [12] carried out ab initio calculations on two $B_{12}N_{12}$ clusters, and found that the isomer with squares and hexagons is more stable than that with pentagons and hexagons by 210 kcal mol^{-1}, while just the opposite energetic order is found for the corresponding C_{24} isomers by 22 kcal mol^{-1} at the MP2/DZP level of theory [12]. The enhanced stability of $B_{12}N_{12}$ is ascribed to the absence of the less favored B–B and N–N bonds generally. Also in 1993, Haiduc and co-authors [13] studied the structures and stability of a set of alternating boron–nitrogen cages $(BN)_n$ and pointed out the relationship between the number of the squares and hexagons. This relationship was further validated systematically by Sun et al. [14, 15] in 1995 on large cages (up to $B_{41}N_{41}$).

Further systematic study on the structure and stability of $(BN)_n$ (n = 10–30) composed entirely of squares and hexagons was carried out by Seifert et al. [16] in 1997 at the density-functional tight-binding level of theory (DFTB), and they found that the alternant structures $B_{12}N_{12}$, $B_{16}N_{16}$ and $B_{28}N_{28}$ are "magic" with anomalous stability, which correlates with their large HOMO–LUMO gaps.

However, the stability of the alternant $(BN)_n$ structures over the fullerene structures has been questioned by Rogers et al. [17] on the basis of systematic DFTB calculations on a wider range of cluster sizes (n = 10–35). They found that the most stable fullerene structures with three N–N and three B–B bonds are more stable than the corresponding most stable alternant isomers over the entire range of the cluster sizes. The origin for this energetic relationship has been ascribed to the competing forces of chemical (three B–B and N–N bonds) and steric (six squares) frustrations. They pointed that this relationship also exists for large clusters like $(BN)_{36}$ and $(BN)_{72}$. For example, the alternant isomer of $(BN)_{36}$ in T_d symmetry is higher in energy than the three most stable

fullerene-like (two oblates/ C_3, one prolate/ D_3) isomers by 140.8, 98.5 and 170.1 kcal mol^{-1}, respectively, and the alternant (BN)$_{72}$ in T symmetry is higher in energy than the most stable fullerene cage in C_3 symmetry by 161.0 kcal mol^{-1}, and the least stable fullerene cage in C_3 symmetry by 83.0 kcal mol^{-1}.

In contrast to the DFTB results by Rogers et al. [17] B3LYP density functional calculations on (BN)$_n$ (n = 12–14, 16, 24) [18–20] predicted that the alternant isomers are more stable than the fullerene isomers, e.g., 230 kcal mol^{-1} for (BN)$_{12}$ (210 kcal mol^{-1} at MP2/DZP) [12] 136 kcal mol^{-1} for (BN)$_{13}$, 160 kcal mol^{-1} for (BN)$_{14}$ and 200 kcal mol^{-1} for (BN)$_{16}$ and 149 kcal mol^{-1} for (BN)$_{24}$, respectively. It is notable that the energy span for the most stable (BN)$_n$ structure between DFTB and B3LYP is more than 300 kcal mol^{-1}, and therefore too large simply to be ascribed to the effects of insufficiency in methods or basis sets.

In addition to this controversy in the stability of (BN)$_n$ clusters, Pokropivny et al. [21] reported a B$_{24}$N$_{24}$ structure with 12 squares, eight hexagons and six octagons in O symmetry to be the lowest of any other near spherical molecules. They also reported that the most stable B$_{60}$N$_{60}$ cage has I_h symmetry with 30 squares, 20 hexagons and 12 decagons. Recently, Wu et al. [19, 20] found that the most stable (BN)$_{24}$ isomer has a structure containing two octagons, 16 hexagons and eight squares in S_8 symmetry, and is computed more stable than the structure by Pokropivny et al. [21] by 60.4 kcal mol^{-1}, but only 2.8 kcal mol^{-1} more stable than the alternant structure in S_4 symmetry.

In this paper, we present a B3LYP/6-31G* DFT investigation on the structure and stability of the (BN)$_{36}$ monomer cages. The isomers consist of four-membered (F_4), five-membered (F_5), six-membered (F_6), eight-membered (F_8) and 12-membered (F_{12}) rings. The most stable (BN)$_{36}$ is the T_d symmetrical structure with six isolated squares, while the fullerene-like structures (12 F_5 and 26 F_6) and structures with F_8 and F_{12} are much higher in energy.

Computational method

All structures were optimized at the B3LYP/6-31G* density functional level of theory with the Gaussian 98 program [22–25]. Benchmark calculations on B$_{12}$N$_{12}$ cages showed that the B3LYP results have the same trend as those of HF and MP2 calculations, and B3LYP/6-311 + G* gives both qualitative and quantitative agreement with B3LYP/6-31G*, and therefore the basis set effect is negligible.

Results and discussion

Design principle

To construct (BN)$_{36}$ cages, it is necessary to gain insight into the relationship between four-membered (F_4), five-

membered (F_5), six-membered (F_6), eight-membered (F_8), and 12-membered (F_{12}) -rings in polyhedrons. For cages consisting of F_4 and F_6, the number of F_4 is always equal to six ($F_4 = 6$), whereas the number of F_6 is $n - 4$ ($F_6 = n - 4$). For example, (BN)$_{36}$ have six F_4 and 32 F_6. This relationship has been used in the literature not only for (BN)$_n$ clusters but also for other systems [26, 27]. On the basis of the constructed structures, the stability of (BN)$_{36}$ isomers depends on the distance of the six F_4, that is, the larger the distance, the more stable the system, and molecule with maximal distance of the six F_4 should be the most stable structure, in line with the pentagon rule in fullerene chemistry [28]. On this basis, the number of stable isomers is rather limited, and this will facilitate the computations. However, it is also expected that large cages with well-separated F_4 can have several isomers very close in energy with reduced torsion strain, and the potential energy surfaces become flat rather than deep. Therefore, the best way for the (BN)$_n$ structures is to start with the configuration having the largest distances of the six F_4 and then to adjust their relative positions.

Structure

Isomers **1**–**9** in Fig. 1 are isomers with six F_4 and 32 F_6, and they have one hundred and eight (108) B–N bonds, but without direct B–B and N–N connections. They differ from the location or separation of the F_4 and F_6. On the basis of the Aufbau principle discussed above, structure **1** with the greatest separation (four B–N bonds in zigzag form) and perfect distribution of the six F_4 in T_d symmetry should be the most stable isomer. It is also the structure first reported by Sun et al. [14, 15].

Structure **2** has C_3 symmetry with the C_3 axis through the two F_6 in opposite location. Each F_6 along the C_3 axis is connected symmetrically with three F_4 via B–N or N–B bond. There are two types of F_4 separation, one is at the end of the tube by four B–N bonds and the second is between the two ends by three B–N bonds. Structure **3** has S_6 symmetry in a discus form, and the location of the six F_4 is like in case of **2**. The separation between F_4 is three B–N bonds. Structure **4** has C_2 symmetry and the C_2 axis goes through the centers of two F_4, which are located at the ends of an ellipsoid form. The other four F_4 are located in the middle of the ellipsoid form. The separation between F_4 is three B–N bonds.

Structure **5** has C_{3h} symmetry in a triangle form, and the six F_4 are divided into three groups. Each group is located at the corner of the triangle and the F_4 separation within the corner is two B–N bonds, while four B–N bonds between two corners. Structure **6** is C_1 symmetrical and the separation of the six F_4 has three B–N bonds.

Structure **7** has C_2 symmetry in a rhomboidal form, and the C_2 axis goes through the centers of two F_4 located at the *trans* positions. The other four F_4 are divided into two groups and they are also located at the *trans* position, and the two F_4 within a group are separated by one B–N bond. The next one is by four B–N
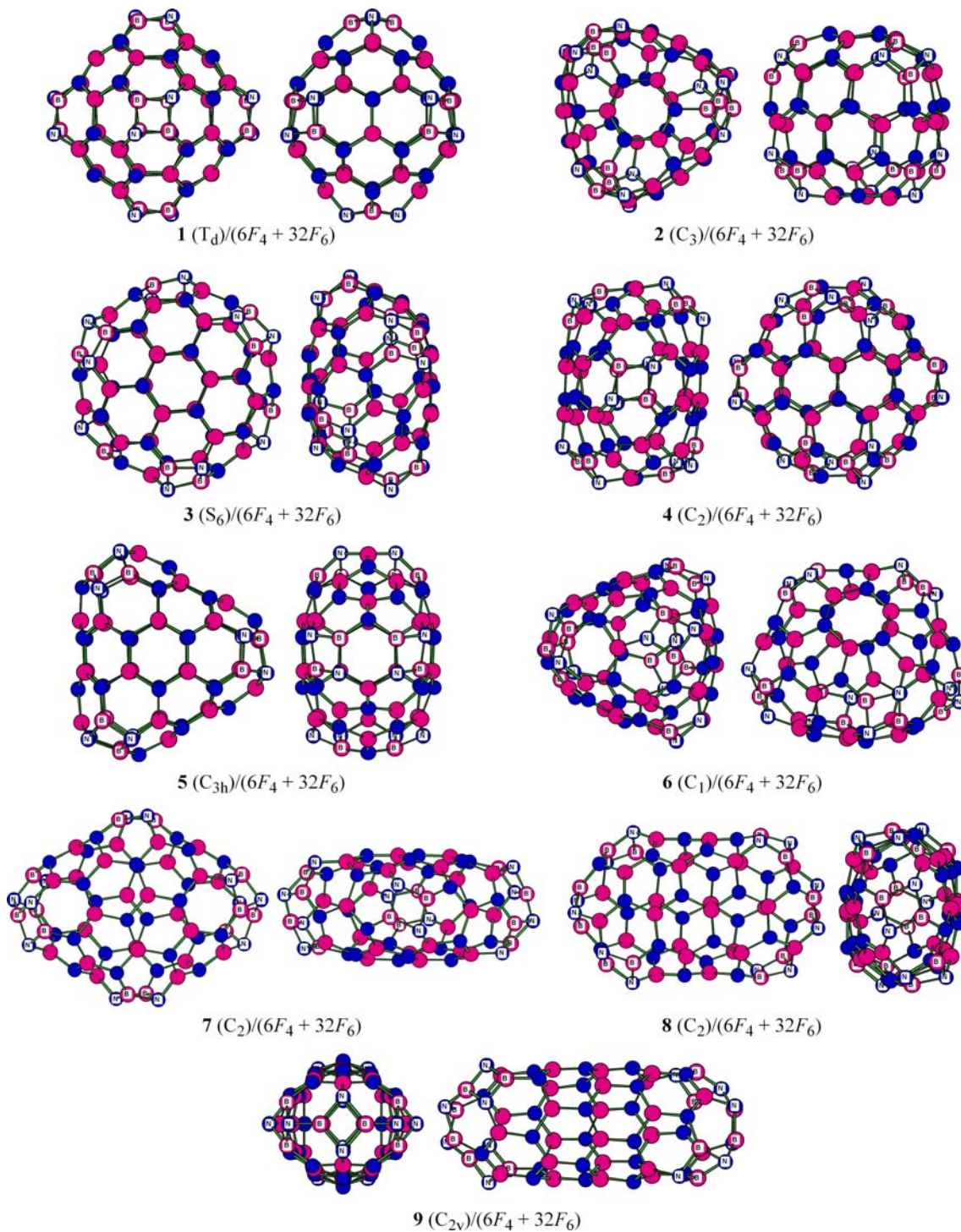
Fig. 1 B3LYP/6-31G* optimized $B_{36}N_{36}$ structures with only F_4 and F_6 (**1–9**)

bonds. Structure **8** has C_2 symmetry in a flat tube form, and the six F_4 are divided into two groups and located at the ends of the tube. The F_4 separation at the tube end is one B–N bond, while four B–N bonds between the ends. Structure **9** has C_{2v} symmetry in a tube form; the conformation is similar to that of structure **8**, one can consider that structure **8** can be deduced by rotation the two F_4 along the C_2 axis from **9**.

Structures **10–12** in Fig. 2 are the corresponding fullerene-like forms with pentagons ($F_5 = 12$) and hexagons ($F_6 = 26$) and have three B–B and N–N bonds. They are also the most stable structures reported by Rogers et al. [17]. The 12 F_5 form six isolated pentagon pairs (IPP), the first three IPP differ from their locations. There are two individual IPP, one with the B–B annelation and another one with the N–N annelation.
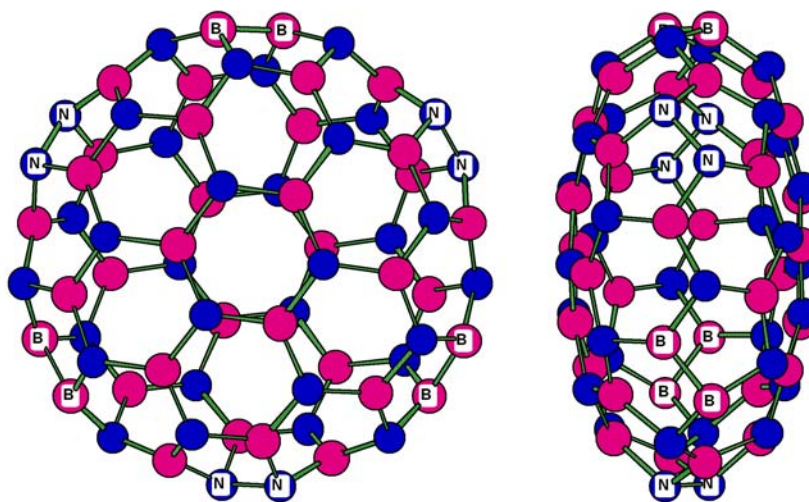
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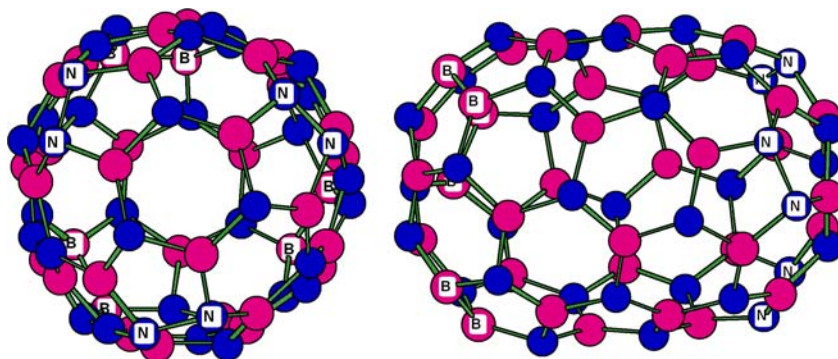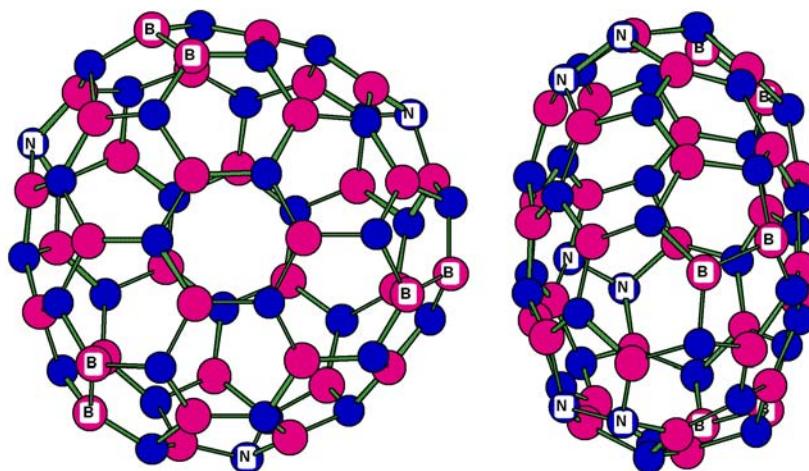
10 (C_3)/($12F_5 + 26F_6$)

11 (C_3)/($12F_5 + 26F_6$)

12 (D_3)/($12F_5 + 26F_6$)

Structure **10** has C_3 symmetry in a tube form, and the three IPP with B–B annelation are at one end, and the other three IPP with N–N annelation are at another end. The IPP are separated by three B–N bonds. Structure **11** also has C_3 symmetry in discus form, and the separation of the IPP is one B–N bond. Structure **12** has D_3 sym-

metry in a discus form, and the shared B–B and N–N bonds locate at the periphery and the IPP has a separation of one B–N bond.

Inspired by the recent work by Pokropivny et al. [21] and Wu et al. [19, 20] that eight-membered rings can stabilize the cage structures, we carried out a set of $B_{36}N_{36}$ isomers containing several F_8. Structures **13–20** in Fig. 3 are isomers with F_4, F_6 and F_8. Structure **13** has seven F_4, thirty F_6 and one F_8, and is C_2 symmetrical. The C_2 axis goes through the centers of the F_8 and one F_4. Structure **14** is C_{4h} symmetrical and has a tube form with eight F_4, 28 F_6 and two F_8. The two F_8 are located at the ends of the tube. This is in agreement with the tube form of $B_{24}N_{24}$ structure [29]. As structure **14**, structure **15** has also eight F_4, 28 F_6 and two F_8, but in a drum form in C_4 symmetry.

Structure **16** has D_2 symmetry with ten F_4, 24 F_6 and four F_8 in a form of packed luggage with two diagonal belts. The belt around the periphery has eight F_4 and eight F_6 in an alternating order, while the orthogonal belt has four F_4 and four F_8 in an alternating arrangement. Structure **17** has D_2 symmetry, and ten F_4, 24 F_6

and four F_8. The four F_8 are divided into two groups, one group has two-isolated F_8 without F_4 annelations, while another group has two F_8 and each of them is annelated with four F_4.

Structure **18** has S_4 symmetry containing 12 F_4, 20 F_6 and six F_8. There are two F_8 in annelation with four F_4, and four F_8 in annelation with two F_4. There are two F_4 bridging two F_8. Structure **19** has C_4 symmetry and 12 F_4, 20 F_6 and six F_8. There are two F_6 in annelation with four F_4 and four F_8 in annelation with two F_4, and four F_4 bridging two F_8. Structure **20** is C_2 symmetrical and has 12 F_4, 20 F_6 and six F_8. Each F_8 is in annelation with two F_4.

In addition, we have also investigated two structures with 12-membered rings as shown in Fig. 4. The first one is structure **21**, which has 12 F_4, 24 F_6 and two F_{12}, and is therefore S_{12} symmetrical. Each F_{12} are fused by six F_4 and six F_6 alternately. The next example is structure **22**, which is D_6 symmetrical and has 18 F_4, 12 F_6, six F_8 and two F_{12} in a cogwheel form. The C_6 axis goes through the centers of the two F_{12}. The periphery has a belt from six F_4 and six F_8, and they are connected alternatively.

Fig. 3 B3LYP/6-31G* optimized $B_{36}N_{36}$ structures with F_4, F_6 and F_8 (**13–20**)
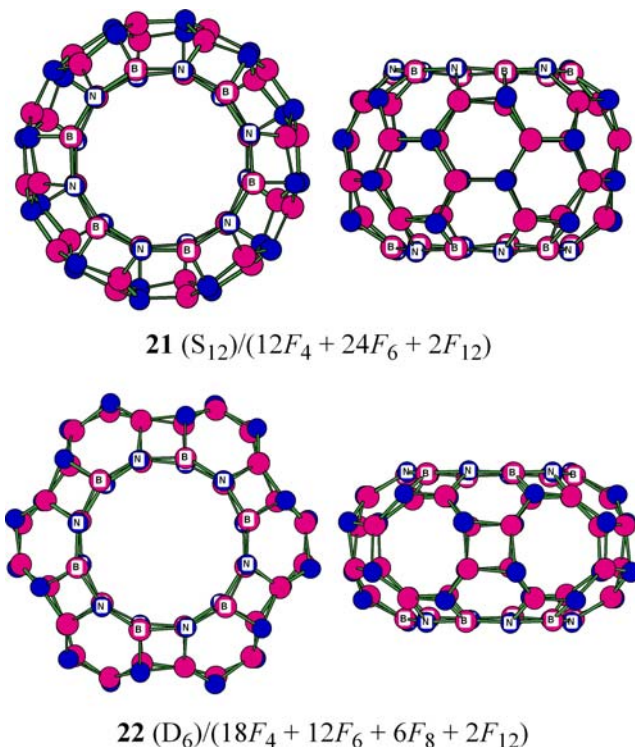
21 (S_{12})/($12F_4 + 24F_6 + 2F_{12}$)

22 (D_6)/($18F_4 + 12F_6 + 6F_8 + 2F_{12}$)
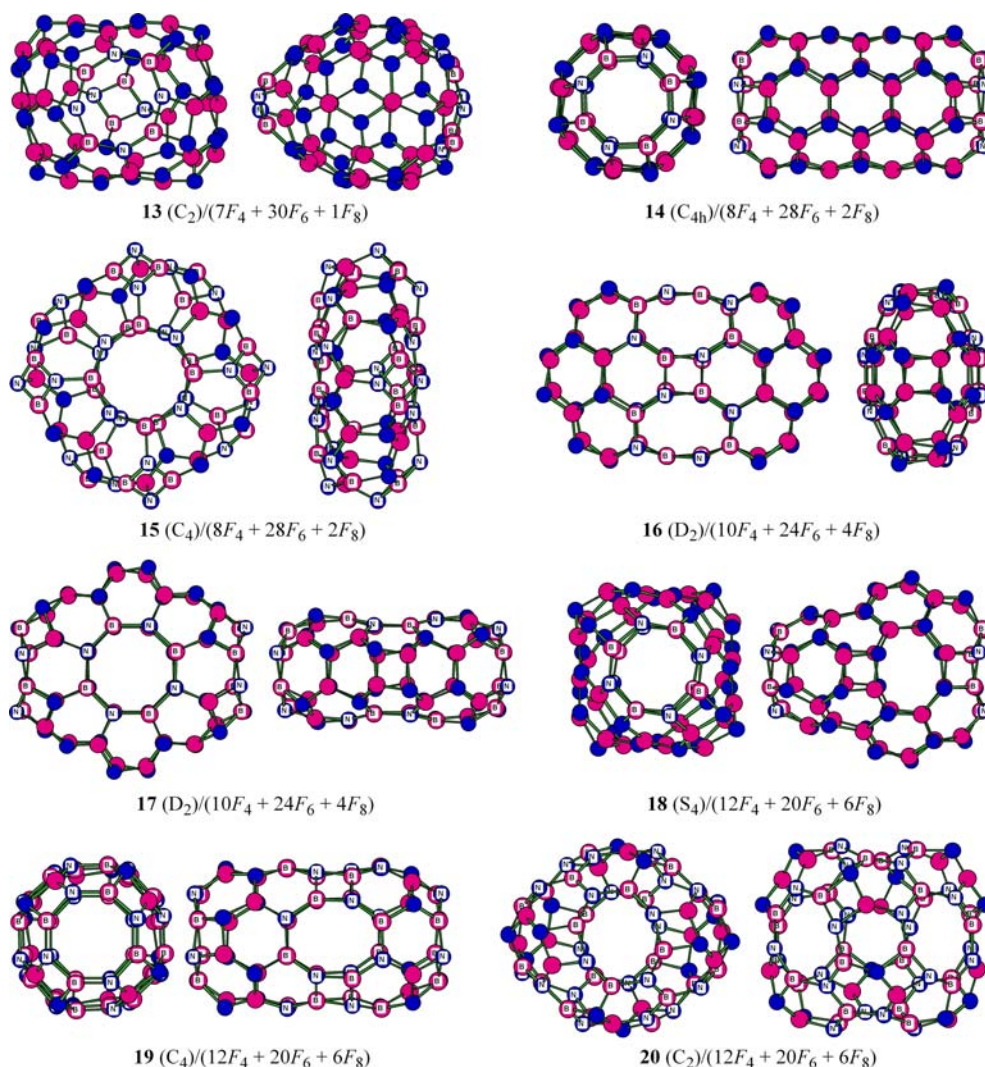
Fig. 4 B3LYP/6-31G* optimized $B_{36}N_{36}$ structures with F_4, F_6, F_8 and F_{12} (**21–22**)

Stability

Table 1 summarizes the B3LYP/6-31G* total electronic energies, the gap between frontier orbitals (HOMO–LUMO) and the relative energies. On the basis of the Aufbau principle, structure **1** with the maximal and perfect separation of the six F_4 should be the most stable isomer and this is verified by the relative energies in Table 1.

Among the alternant structures **1–9**, **1** is the most stable isomer and the other structures are higher in energy. Interestingly, the difference in relative energy depends on the separation of the F_4 location. However, it is notable that structures **2–5** are only higher in energy by less than 10 kcal mol^{-1}. This indicates the reduced torsion strain in these large cage structures, and it is therefore expected that several isomers might co-exist for larger cages, in which the energetic factor of F_4 in well-located separation does not play the dominant role.

In contrast to the fully alternating isomers **1–9**, the fullerene-like structures (**10–12**) with three N–N and three B–B with 12 F_5 forming 26 F_6 = 26 are higher in energy by about 127–195 kcal mol^{-1}. This energetic order is in sharp contrast to that found by Rogers et al. [17] using the DFTB method, which predicts that the fullerene-like structures (**10–12**) are more stable than **1**. Although we do not have any explanation for this difference, it seems that the alternant structures are more stable than the fullerene-like isomers.

Structures **13–20** are isomers containing eight-membered rings (F_8). The relative energies in Table 1 indicate that the introduction of F_8 does not stabilize the cage structure to such an extent to be more stable than the most stable alternant isomer **1**, e.g., 13 (with one F_8) as the most stable structures containing F_8 is 38.9 kcal mol^{-1} less stable than 1. Furthermore, the energetic difference among **13–20** does not depend on the number of F_8. For example, both **14** and **15** have two F_8, but **14** is more stable than **15** by 414.2 kcal mol^{-1}. Structures **16** and **17** with four F_8, as well as structure **18–20** with six F_8 are higher in energy than **13** with one F_8 and **1** without F_8.

However, there is obvious evidence for the stability depending on the proximity of F_4 and F_8. For example, the two F_8 in **15** are not fused with F_4, but the more stable isomer **14** with the same ring combination as **15** has two F_8 fused with eight F_4. Even isomer **13** with one F_8 fused with four F_4 is more stable than **15** by 305.3 kcal mol^{-1}. The same trend is also found for isomers **16** and **17** having the same ring combination; e.g., **16** with four fused F_4 and F_8 is more stable than **17** without such connection by 192.3 kcal mol^{-1}.

In addition to structures with F_8, we have also computed two structures (21 and 22) with two F_{12}, and they are much higher in energy than 1 and also other alternant isomers (2–9). Therefore, introduction of F_{12}, as F_8, also cannot stabilize the large cages.

At this stage, one might ask the question about the competing effect between the chemical (N–N, B–B bonds) and steric (squares) frustration in determining the stable $(BN)_n$ structures. To evaluate the chemical and steric contributions, we have chosen the inorganic boron–nitride model molecules containing F_4 and F_6,

Table 1 The B3LYP/6-31G* total electronic (E_{tot}, au), relative energies (E_{rel}, kcal mol^{-1}) and the HOMO–LUMO gap (E_{Gap}, eV) as well as the dipole moment (μ, Debye) of $(BN)_{36}$ isomers

Isomer	E_{tot}	E_{Gap}	μ	E_{rel}
1 (T_d)	−2869.43680	5.22	0.00	0.0
2 (C_3)	−2869.42917	6.69	0.61	4.8
3 (S_6)	−2869.42670	6.60	0.31	6.3
4 (C_2)	−2869.42576	6.76	0.00	6.9
5 (C_{3h})	−2869.42136	6.33	0.00	9.7
6 (C_1)	−2869.41936	6.45	1.58	10.9
7 (C_2)	−2869.34421	6.26	0.36	58.1
8 (C_2)	−2869.31454	6.54	1.02	76.7
9 (C_{2v})	−2869.21833	5.59	1.09	137.1
10 (C_3)	−2869.23431	4.78	1.65	127.1
11 (C_3)	−2869.19567	4.97	1.47	151.3
12 (D_3)	−2869.12563	0.00	4.90	195.3
13 (C_2)	−2869.37475	0.12	6.28	38.9
14 (C_{4h})	−2869.38905	0.00	6.30	30.0
15 (C_4)	−2868.72896	1.89	6.42	444.2
16 (D_2)	−2869.06847	0.00	6.05	231.1
17 (D_2)	−2868.76210	0.00	6.00	423.4
18 (S_4)	−2869.16018	0.00	6.19	173.6
19 (C_4)	−2869.18865	0.13	6.05	155.7
20 (C_2)	−2869.10484	0.12	6.09	208.3
21 (S_{12})	−2869.13573	0.00	6.14	188.9
22 (D_6)	−2868.91236	0.00	6.01	329.1

and these model systems can isomerize to the corresponding systems containing F_5 and F_6 with one B–B bond and one N–N bond. The isomerization energy of these models can reveal the difference between the steric frustration of one F_4 and one F_6 and the chemical frustration of two F_5. As shown in Fig. 5, the isomerizaton energy for the pentalene-type molecule (b) is 76.9 kcal mol^{-1}, and that of the s-indacene-type molecule (d) is 73.6 kcal mol^{-1} (both planar b and d are used for the energetic evaluation, because the non-planar b and d with pyramidal nitrogen centers at the N–B bond are only less than 1.5 kcal mol^{-1} more stable than the planar forms at the same level of theory). These energetic data indicate that the chemical frustration is less favored than the steric frustration and provide additional evidence for the enhanced stability of the alternant structure. It is to be expected that large systems, in which all the 12 F_5 are "isolated" and do not perturb to each other, are still higher in energy than the alternant isomers with six isolated F_6. On the basis of this analysis, it can be concluded that the discrepancy between DFT and DFTB might be a problem of insufficient DFTB parameters, which should be improved further. On the other hand, there is no direct relationship between dipole moment and the stability, and most of the isomers do not have or have only very small dipole moments because of their high symmetries. Thus, dipole moments do not determine the relative stability.

Apart from this energetic difference, the stability of the alternant can be governed by the stabilizing charge effects of the electropositive charged boron atoms and the electronegative charged nitrogen atoms despite the large strain in F_4. In contrast, B–B and N–N bonds have destabilizing rather than stabilizing effects. This is shown in Fig. 6 by the computed natural charges for A and B from a Natural Bond Orbital Analysis [30, 31]. Similar results are also found for C and D.
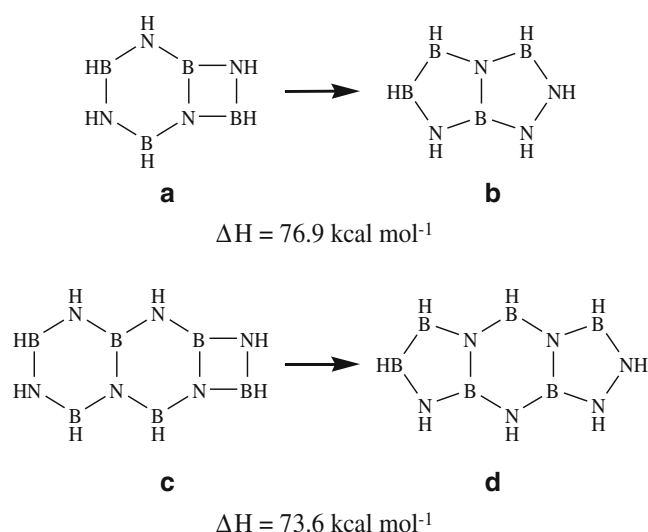

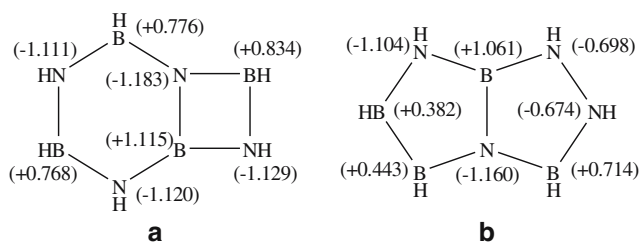**Fig. 5** Isomerization energy from F_4 and F_6 structure into two F_5 structure

Fig. 6 Computed natural charges at boron and nitrogen centers

Conclusion

The relationship between structure and stability of $(BN)_{36}$ cages structures has been computed at the B3LYP/6-31G* level of theory. The most stable isomer (**1**) is that with 32 hexagons (F_6) and six squares (F_4), and the six F_4 have their maximal separations. Other alterant structures are higher in energy. In contrast to the findings by Rogers et al., structure (**1**) is more stable than the fullerene-like isomers with three B–B and three N–N bonds. The origin of the enhanced stability of the alternant structure is the strong electrostatic interaction between boron and nitrogen in the alternating way, and this stabilizing contribution suppresses the strain (or steric) effects by the squares. Structures with large-sized rings (F_8 and F_{12}) are also higher in energy than the alternant structure.

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