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Strain energies of cubane derivatives with different substituent groups

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Abstract

Homodesmotic reaction and isodesmotic reaction were designed for the computation of strain energies (SE) for a series of cubane derivatives. Total energies of the optimized geometric structures at the DFT-B3LYP/6-31G* level were used to derive the SE. The SE value of cubane is 169.13 kcal/mol for homodesmotic reaction, which is in good agreement with the experimental value. The variation of SE with respect to the number of substituents is similar for the homodesmotic reaction and isodesmotic reaction. The SE values of polynitrocubane and polydifluoroaminocubane increase slightly as up to four substituent groups being added to the cage skeleton. On contrary, the SE dramatically increases when the number of substituent groups *m* increases from 5 up to 8. For polynitratocubane, the SE decreases slightly at the beginning then increases as the number of group increases. For polyazidocubane, there are very small group effects on the SE. Among four types of substituent groups, the nitro group has greatest effect on the strain energy of caged cubane skeleton. The calculated SE value of octanitrocubane is 257.20 kcal/mol, while that of octaazidocubane is 166.48 kcal/mol via isodesmotic reaction. The azido group releases the strain energy of cubane skeleton when the number of azido groups is less than 7. The interactions among the substituted groups deviated from group additivity. The substituted groups withdraw electrons from the cubane, reducing the repulsion between C–C bonds and resulting the release the strain of the skeleton for isomers with fewer substituents. Group repulsions increase sharply with more and more nitro, nitrato and difluoroamino groups being attached to cubane, resulting large strains of the skeleton. The average negative charges of the substituted groups influence the strain energy of cubane derivatives.
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Keywords: Cubane derivatives; Strain energy; DFT-B3LYP; Homodesmotic reaction; Isodesmotic reaction

1. Introduction

Cubane (C_8H_8) and its derivatives have been the subject of numerous investigations ever since Eaton's synthesis of the parent compound in 1964 [1,2]. Cubane is one of such strained hydrocarbon system [3] having symmetric cubic cage with the mutually perpendicular C–C bonds. It has high positive heats of formation (HOFs), high density and better thermal stability, therefore cubane and its derivatives have significant potential for military and commercial applications as high energy density materials. Octanitrocubane (ONC) is potentially a very important high performance energetic compound, which was finally synthesized in 2000 after many years of effort [4].

Strain is an important concept in structural organic chemistry [5]. The concept of strain and strain energy (SE) provides a basis that helps to correlate structures, stabilities and reactivities of molecules. Strain energies can be defined as the difference between energies for a process that releases strain as determined by experiment and as obtained from a model that does not involve strain [6].

However, experimental data for the SE are available only for a small number of strained compounds, such as cyclopropane and cyclobutane. For large molecule, various conditions can yield great discrepancies. For example, the reported experimental values of SE for cubane are 157 kcal/mol, 161.2 kcal/mol and 162.7 kcal/mol, respectively [7–9]. The reported strain energy of cubane was derived from the enthalpies of formation of solid cubane and sublimation enthalpy of cubane [7]. But the sublimation enthalpy of cubane is suspect [10,11]. In Ref. [12], strain enthalpy of 162.8 ± 2.3 kcal/mol was calculated for cubane.

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Despite these differences in the numerical values used, the strain energies calculated still be significant.

This paper discussed the calculated SE using B3LYP [13,14] hybrid DFT method with 6-31G* basis set via homodesmotic reaction [15] and isodesmic reaction [16] for a series of (the number of substituent groups: $m = 1$–8) polynitrocubane, polydifluoroaminocubane, polyazidocubane and polynitratocubane. The effects of substituent groups on the SE of cubane cage skeleton were compared.

2. Computational methods

The DFT-B3LYP method [13,14] with 6-31G* basis set via homodesmotic reaction and isodesmotic reaction were used for the prediction of SE. The methods of homodesmotic reaction and isodesmotic reaction have been employed very successfully to calculate SE from total energies (E_0) and the zero-point energies (ZPE) obtained from ab initio calculations [6,17–21].

In the homodesmotic reaction, not only is numbers of bonds of various types conserved but the valence environment around each atom is preserved as well. The advantage of using homodesmotic reaction is that cancellation of errors, associated with truncation of the basis set and incomplete electron correlation recovery, occurs to a large extent [18]. The homodesmotic reactions used to derive the SE of title compounds are as follows:

$$C_8H_8 + 12CH_3CH_3 \rightarrow 8(CH_3)_3CH \quad (1)$$

$$C_8H_{8-m}X_m + 12CH_3CH_3 \rightarrow (8-m)(CH_3)_3CH + m(CH_3)_3CX \quad (2)$$

where m is the number of substituent groups in cubane derivatives molecules $C_8H_{8-m}X_m$ (X = –NF_2, –NO_2, N_3 and –ONO_2). The change of energies, with correction of zero-point vibrational energy (ZPE), in this homodesmotic reaction is:

$$\Delta E_n = \Sigma E_{\text{product}} - \Sigma E_{\text{reactant}} + \Delta\text{ZPE} \quad (3)$$

We anticipate Eqs. (1) and (2) to be exothermic in the direction written, or $\Delta E_n < 0$. We wish to define SE as a positive quantity. Therefore, we relate SE with $-\Delta E_n$ for Eq. (1) and (2) [6]. We calculated the SE of cubane from the above procedure as a criterion. The predicted value is 169.13 kcal/mol that is close to the experimental value of 162.7 kcal/mol [8].

In addition, we calculate the strain energy of cubane derivatives via the experiment SE of cubane as a criterion. To be specific, we take cubane as a reference compound. The strain energy was computed according to the energy change of isodesmic reaction:

$$C_8H_8 + m(CH_3)_3CX \rightarrow C_8H_{8-m}X_m + m(CH_3)_3CH \quad (4)$$

where m is the number of substituent groups in cubane derivatives $C_8H_{8-m}X_m$ (X = –NF_2, –NO_2, N_3 and –ONO_2). C_8H_8 is cubane. From the isodesmic reaction (4), the relative SE of cubane derivatives can be calculated from the following equation:

$$\Delta E = \Sigma E_{\text{product}} - \Sigma E_{\text{reactant}} + \Delta\text{ZPE} \quad (5)$$

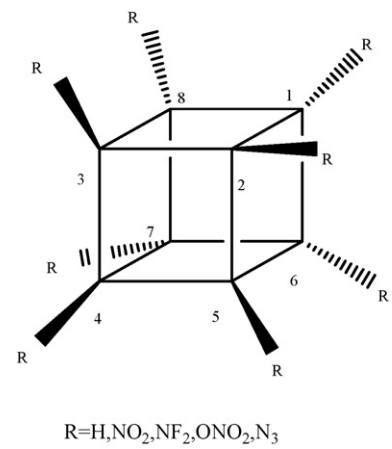

Fig. 1. Molecular framework and atomic numbering of cubane.

Table 1
Calculated total energy (E_0), zero-point energy (ZPE) of the reference compounds at the B3LYP/6-31G* level[a]

Compound	E_0	ZPE
Cubane	−309.460340	338.06
CH_3CH_3	−79.830417	193.61
$CH(CH_3)_3$	−158.458817	340.66
$C(CH_3)_3NF_2$	−412.157174	339.45
$C(CH_3)_3N_3$	−322.043940	348.61
$C(CH_3)_3NO_2$	−362.961526	348.01
$C(CH_3)_3ONO_2$	−438.139668	357.64

[a] E_0 is in a.u., ZPE is in kJ/mol. The scaling factor for ZPE is 0.98 [24].

The relative SE values of cubane derivatives plus the experimental SE value of cubane is the absolute values for the strain of cubane derivatives.

Computations were performed with the Gaussian 98 package [22] at the B3LYP method. The optimizations were performed without any symmetry restrictions using the default convergence criteria in the programs. All of the optimized structures were characterized to be true local energy minima on the potential energy surfaces without imaginary frequencies.

3. Results and discussion

Fig. 1 shows the molecular framework and atomic numbering of cubane. Table 1 lists the total energies and zero-point ener-

Table 2
Calculated and experimental strain energies (kcal/mol) of cubane

Method	SE
B3LYP/6-31G*[a]	169.13
MP2/6-31G(d,p)	165.4 (Ref. [11])
Exp.	157 (Ref. [7])
	161.2 (Ref. [9])
	162.7 (Ref. [8])

[a] This work.

Table 3
Calculated total energy (E_0), zero-point energy (ZPE) of the title compounds at the B3LYP/6-31G* level[a]

Serial no.	Compound	NF_2		N_3		NO_2		ONO_2	
		E_0	ZPE	E_0	ZPE	E_0	ZPE	E_0	ZPE
1	1-	−563.160985	335.91	−473.050113	345.25	−513.964247	351.61	−589.147207	361.55
2	1,2-	−816.853905	333.57	−636.637383	352.15	−718.459180	357.93	−868.827925	377.32
3	1,3-	−816.858084	333.32	−636.638048	352.09	−718.462487	357.56	−868.830557	377.40
4	1,4-	−816.858942	333.20	−636.638506	359.37	−718.463245	357.39	−868.831596	377.29
5	1,3,5-	−1070.552260	330.40	−800.223647	358.19	−922.955702	362.89	−1148.511131	392.58
6	1,3,5,7-	−1324.243760	327.39	−963.807887	364.41	−1127.444015	367.68	−1428.183795	406.29
7	1,2,3,5,7-	−1577.923880	324.61	−1127.392017	371.09	−1331.920186	372.48	−1707.852460	420.98
8	Hexa-	−1831.601880	321.28	−1290.975690	378.00	−1536.395700	377.21	−1987.570047	417.75
9	Hepta-	−2085.278240	318.24	−1454.557834	384.45	−1740.866150	381.71	−2267.182094	448.49
10	Octa-	−2338.952770	315.52	−1618.139420	390.91	−1945.335589	385.97	−2546.834883	461.16

[a] E_0 is in a.u., ZPE is in kJ/mol. The scaling factor for ZPE is 0.98 [24]. 1- and 1,2- denote 1-substituted isomer and 1,2-di-substituted isomer, respectively

gies at the B3LYP/6-31G* level for seven reference compounds being enlisted in the homodesmotic reactions (1) and (2). Table 2 reports the calculated and experimental SE values of cubane. The homodesmotic reaction (1) is designed for cubane and the calculated value would be compared with the data of previous studies [7–9,18] in order to verify that computational results at the B3LYP/6-31G* level via the homodesmotic process are reliable for the calculated SE values of cubane derivatives. Through the homodesmotic reaction (1) at the B3LYP/6-31G* level, the SE value of cubane is 169.13 kcal/mol. The calculated value is in agreement with 162.7 kcal/mol from Ref. [8] and 162.8 ± 2.3 kcal/mol from Ref. [12]. It is also close to the calculated value of 165.4 kcal/mol at MP2/6-311G(d,p) level [18]. Table 3 lists the total energies and ZPE at the B3LYP/6-31G* level for polynitrocubane, polydifluoroaminocubane, polyazidocubane and polynitratocubane compounds. The total energies of 1,2-, 1,3- and 1,4-isomers shown in Table 3 are close to each other. The total energy of 1,2-isomer is slightly larger, while the total energy of 1,4-isomer is slightly smaller among three di-substituted isomers. It is the positional effects that make the repulsion energy smaller as the distance between the groups increasing. Therefore the total energy is small when the substitutent groups are kept away from each other. The values of SE for the title compounds, obtained from B3LYP method through using homodesmotic reactions (1) and (2), were listed in Table 4.

Table 4
Calculated strain energies (SE) (kcal/mol) of the title compounds at the B3LYP/6-31G* level via homodesmotic reactions[a]

Serial no.	Compound	NF_2	NO_2	N_3	ONO_2
1	1-	167.92	166.90	166.40	163.80
2	1,2-	171.61	172.03	165.31	164.18
3	1,3-	169.07	170.04	164.90	162.51
4	1,4-	168.53	169.61	162.87	161.88
5	1,3,5-	172.08	176.48	165.05	163.11
6	1,3,5,7-	176.81	186.13	166.02	169.03
7	1,2,3,5,7-	188.63	203.40	166.95	177.23
8	Hexa-	201.91	221.09	168.11	192.25
9	Hepta-	216.16	242.01	170.34	198.89
10	Octa-	231.47	263.63	172.92	217.53

[a] 1- and 1,2- denote 1-substituted isomer and 1,2-di-substituted isomer, respectively.

It can be seen from Table 4 that the values of SE obtained from B3LYP method relate to the number of nitro, difluoroamino, azido and nitrato groups. The SE values for mono-substituent nitro, difluoroamino, azido and nitrato compounds and cubane itself are 167.92 kcal/mol, 166.90 kcal/mol, 166.40 kcal/mol, 163.80 kcal/mol and 169.13 kcal/mol, respectively. Therefore, the SE is somewhat released for mono-substituted isomers as compared to cubane itself. When the number of substituent groups (m) is 2, the SE values of 1,2-bis-difluoroaminocubane and 1,2-di-nitrocubane are 171.61 kcal/mol and 172.03 kcal/mol, respectively, which are larger than the calculated SE value of cubane. For the derivatives with two substituent groups ($m = 2$), the SE is affected by the position of substituents. Usually, for isomers with the same m, the shorter the distance between the substituent groups is, the stronger the repulsive energy is, and the larger the SE is. As for three di-substituted isomers, the SE values of 1,2-isomers are slightly larger, while SE values of the 1,4-isomer are smaller than those of 1,2- and 1,3-isomers. It is indicated that the value of SE is small when the substituent groups are kept away from each other. For polynitrocubane and ploydifluoroaminocubane, variations of SE with the number of substituent groups show that the SE increases with each additional substituent group being introduced to the cubane cage skeleton. For polynitratocubane, the SE decreases very slightly at the beginning but then increases gradually as the number of substituent groups increases. For polyazidocubane, there are only slight group effects on the SE. It is interesting to note that all the SE values for polyazidocubane, range from 166.40 to 168.11 kcal/mol, are smaller than that of cubane as $m \leq 6$. It shows that the azido group releases the SE of polyazidocubane as compared to cubane when the number of substituted groups is within 6. When m is 7 and 8, the SE values are 170.34 and 172.92 kcal/mol, respectively, which are larger than that of cubane. The SE values of polynitratocubane are larger than that of cubane when m is larger than 4. When the number of substituent groups is 8, the cubane derivatives have the largest SE values, which are 231.47 kcal/mol, 263.63 kcal/mol and 217.53 kcal/mol for octadifluoroaminocubane, octanitrocubane and octanitratocubane, respectively. However, octanitrocubane is still stable, which may be due to its symmetric structure.

Table 5
Calculated strain energies (SE) (kcal/mol) of the title compounds at the B3LYP/6-31G* level via isodesmotic reactions[a]

Serial no.	Compound	NF_2	NO_2	N_3	ONO_2
1	1	161.49 (−1.21)	160.47 (−2.23)	159.97 (−2.73)	157.37 (−5.33)
2	1,2-	165.17 (2.47)	165.60 (2.90)	158.87 (−3.83)	157.74 (−4.96)
3	1,3-	162.64 (−0.06)	163.61 (0.91)	158.47 (−4.23)	156.07 (−6.63)
4	1,4-	162.10 (−0.60)	163.17 (0.47)	156.44 (−6.26)	155.45 (−7.25)
5	1,3,5-	165.64 (2.94)	170.05 (7.35)	158.61 (−4.09)	156.68 (−6.02)
6	1,3,5,7-	170.38 (7.68)	179.70 (17.00)	159.58 (−3.12)	162.60 (−0.10)
7	1,2,3,5,7-	182.20 (19.50)	196.96 (34.26)	160.51 (−2.19)	170.79 (8.09)
8	Hexa-	195.48 (32.78)	214.66 (51.96)	161.67 (−1.03)	181.73 (19.03)
9	Hepta-	209.72 (47.02)	235.58 (72.88)	163.90 (1.20)	192.46 (29.76)
10	Octa-	225.04 (62.34)	257.20 (94.50)	166.48 (3.78)	211.10 (48.40)

[a] 1- and 1,2- denote 1-substituted isomer and 1,2-di-substituted isomer, respectively. Data in the parentheses were calculated by $C_8H_8 + m(CH_3)_3CX \rightarrow C_8H_{8-m}X_m + m(CH_3)_3CH$. Data outside parentheses were the data in the parentheses plus the experimental SE value of cubane, which is 162.7 kcal/mol.

Another reason is that the electrostatic repulsion between nitro groups are reduced by the charge redistribution within the nitro groups [23]. Therefore, the octasubstituted compounds are stability. As concerning the SE of cubane cage skeleton, nitro group has the largest effect compared to nitro, difluoroamino and nitrato groups.

Table 5 lists the SE values of cubane derivatives via isodesmotic reactions. These data are smaller than the corresponding data in Table 4 because the reference compounds are different. The difference of data between Table 4 and Table 5 is 6.44 kcal/mol. The variation of SE with respect to the number of substituents is similar for data in Tables 4 and 5. The data in Table 5 are believed to be more reliable than those in Table 4 since the formers are based on the experimental SE value of cubane. Strain energy of cubane derivatives, obtained from isodesmotic reaction (4), with respect to the number of substituted groups was shown in Fig. 2. As can be seen from Fig. 2, the SE dramatically increases for NF_2, NO_2 and ONO_2 substituted derivatives as the series number ≥7 (or $m \geq 5$). In contrast, there is only slight group effect on the SE values for polyazidocubanes.

The data in the parentheses of Table 5 were calculated by using the isodesmotic reaction of $C_8H_8 + m(CH_3)_3CX \rightarrow C_8H_{8-m}X_m + m(CH_3)_3CH$, that is, these

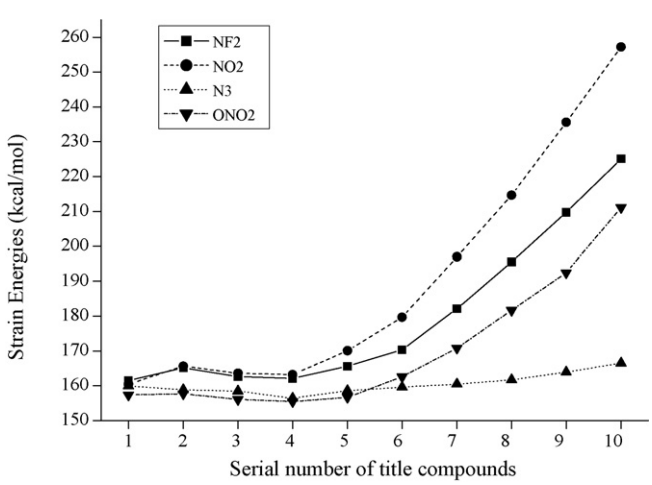

Fig. 2. Strain energy of cubane derivatives with different substituent groups.

are relative SE. An absolute value of SE could then be obtained by adding the SE of cubane to the data in the parentheses of Table 5. For polysubstituted cubane, the group interactions include those of ortho-, meta- and para-groups. As m is 8 for Eq. (4), the destabilization energy of octadifluoroaminocubane from the isodesmic reaction was calculated to be 62.34 kcal/mol. The energy change contains twelve 1,2-interactions, twelve 1,3-interactions and four 1,4-interactions for octasubstituted species. In octadifluoroaminocubane, twelve 1,2-interactions, twelve 1,3-interactions and four 1,4-interactions between difluoroamino groups would be expected to give a destabilization energy of $12 \times 2.47 + 12 \times (-0.06) + 4 \times (-0.60) = 26.52$ kcal/mol. However, the actual destabilization energy, computed for formation of octadifluoroaminocubane, is larger than the estimated values by 35.82 kcal/mol. For octanitrocubane, octazidocubane and octanitratocubane, the destabilization energies are calculated to be 47.60 kcal/mol, −121.76 kcal/mol and −168.08 kcal/mol, respectively. The differences between the estimated and actual values are 46.90 kcal/mol, 125.54 kcal/mol and 216.48 kcal/mol, respectively. Formation of hepta- from cubane plus 7 molecules of $(CH_3)_3CX$ (X = –NF_2, –NO_2, N_3 and –ONO_2) introduces nine 1,2-interactions, nine 1,3-interactions and three 1,4-interactions between substituted groups. The destabilization energies are expected to be 19.89 kcal/mol, 35.70 kcal/mol, −91.32 kcal/mol and −126.06 kcal/mol for heptadifluoroaminocubane, heptanitrocubane, heptazidocubane and heptanitratocubane, respectively. The differences between the expected destabilization energies and those directly computed are 27.13 kcal/mol, 37.18 kcal/mol, 92.52 kcal/mol, 155.82 kcal/mol, respectively. The differences between the destabilization energies that are expected on the basis of the dinitrocubane results and those directly computed is much larger for octa- and hepta-isomers then those with fewer substituents. This demonstrates that the interactions of the substituted group deviate from group additivity.

Table 6shows the average Mulliken charges on NF_2, NO_2, N_3 and ONO_2 groups for cubane derivatives at the B3LYP/6-31G* level. These four groups are of high electronegativity, therefore as the H atom on cubane skeleton was substituted by NF_2, NO_2, N_3 and ONO_2 groups, the density of electron on

Table 6
Average Mulliken charges on NF_2, NO_2, N_3 and ONO_2 groups for cubane derivatives at the B3LYP/6-31G* level[a]

Serial no.	Compound	NF_2	NO_2	N_3	ONO_2
1	1	−0.3482	−0.4096	−0.2934	−0.4088
2	1,2-	−0.3353	−0.3795	−0.2838	−0.3941
3	1,3-	−0.3317	−0.3851	−0.2817	−0.3937
4	1,4-	−0.3343	−0.3895	−0.2827	−0.3956
5	1,3,5-	−0.3167	−0.3625	−0.2715	−0.3809
6	1,3,5,7-	−0.3029	−0.3412	−0.2624	−0.3690
7	1,2,3,5,7-	−0.2939	−0.3191	−0.2584	−0.3621
8	Hexa-	−0.2867	−0.3022	−0.2561	−0.3606
9	Hepta-	−0.2789	−0.2847	−0.2546	−0.3578
10	Octa-	−0.2729	−0.2716	−0.2546	−0.3506

[a] 1- and 1,2- denote 1-substituted isomer and 1,2-di-substituted isomer, respectively.

C atom decreases and thus alleviated some repulsion between C–C bonds. As m is 1, the loss of negative charge from C atom reduces the repulsion between C–C bonds. So, the SE values of mono-isomers are smaller than that of cubane. As the number of substituted groups increases, the charge redistribution brings on the average negative charges on each substituted groups decreasing. On the other hand, however, the total number of group interactions increases sharply with increasing number of nitrato, nitro and difluoroamino groups. The net effect of these contradictory factors is that the total repulsion among the substituted groups increases as the groups increase. As can be seen from Fig. 3, the average negative charges are in the order of nitrato > nitro > difluoroamino > azido. The average negative charges of nitro derivatives decrease sharply when m increases from 3 up to 8. Although the negative charges on nitrato groups are large, the negative charges distribute among three oxygen atoms, and the NO_2 moieties of $–ONO_2$ are far apart from each other for polynitratocubanes than the nitro group for polynitrocubanes, resulting less repulsion among nitrato groups. As for polyazidocubanes, the smallest negative charges as well as the linear structure of azido groups result in small group repulsions. Therefore the SE value of polyazidocubane has slight changes with the number of substituents. For polynitro and polydifluoroamino derivatives, the negative charges of nitro groups is larger than those of the latter, and the distances among the nitro groups in the former is smaller than those in the latter due to the radii of oxygen atom being larger than that of fluorine. Consequently, repulsions among nitro groups are larger than those among difluoroamino groups. Therefore the SE value of polynitrocubane dramatically increases from 5 up to 8. As a whole, on one hand, these four types of substituent groups withdraw electrons from the cubane, reducing the repulsion between C–C bonds and resulting the release the strain of the skeleton. On the other hand, group repulsions increase sharply with more and more substituents being attached to cubane, resulting large strains of the skeleton.

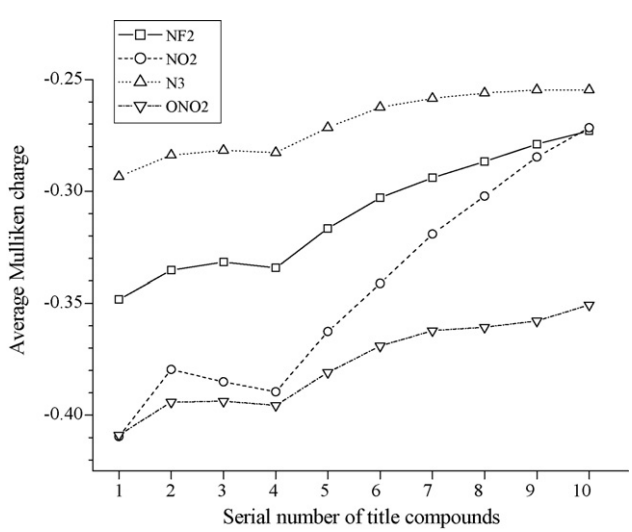

Fig. 3. Average Mulliken charge of four substituted groups on cubane derivatives.

4. Conclusion

(1) The SE values of polynitrocubane and polydifluoroamino increase slightly as the number of substituent groups (m) increases from 1 to 4, while the SE dramatically increases when m increase from 5 to 8. For polynitratocubane, the SE decreases slightly at the beginning then increases as the number of group increases. For polyazidocubane, there are only slight group effects on the SE.
(2) For isomers, the position of the substituent groups affects the SE of cubane derivatives. When the distance between the substituent groups is far away from each other, the SE values of cubane derivatives decrease.
(3) The SE of nitro derivatives increases more than those of difluoroamino and nitrato isomers, while the SE of polyazidocubanes decreases as $m \leq 6$ but increase slightly as m is up to 7.
(4) The SE values are different via homodesmotic reaction and isodesmic reaction because the criteria for the SE are different for these reactions. However, variations of the SE values with respect to the substituents are similar.
(5) The interactions of substituted groups deviate from group additivity, and the average charge on the substituted group influences the strain energy of cubane derivatives.

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