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ORIGINAL PAPER

Charge transfer and first hyperpolarizability: cage-like radicals $C_{59}X$ and lithium encapsulated $Li@C_{59}X$ (X=B, N)

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Abstract Very recently, two new cage-like radicals ($C_{59}B$ and $C_{59}N$) formed by a boron or nitrogen atom substituting one carbon atom of C_{60} were synthesized and characterized. In order to explore the structure–property relationships of combination the cage-like radical and alkali metal, the endohedral $Li@C_{59}B$ and $Li@C_{59}N$ are designed by lithium (Li) atom encapsulated into the cage-like radicals $C_{59}B$ and $C_{59}N$. Further, the structures, natural bond orbital (NBO) charges, and nonlinear optical (NLO) responses of $C_{59}B$, $C_{59}N$, $Li@C_{59}B$, and $Li@C_{59}N$ were investigated by quantum chemical method. Three density functional methods (BHandHLYP, CAM-B3LYP, and M05-2X) were employed to estimate their first hyperpolarizabilities (β_{tot}) and obtained the same trend in the β_{tot} value. The β_{tot} values by BHandHLYP functional of the pure cage-like radicals $C_{59}B$ (1.30×10^3 au) and $C_{59}N$ (1.70×10^3 au) are close to each other. Interestingly, when one Li atom encapsulated into the electron-rich radical $C_{59}N$, the β_{tot} value of the $Li@C_{59}N$ increases to 2.46×10^3 au. However, when one Li atom encapsulated into the electron-deficient radical $C_{59}B$, the β_{tot} value of the $Li@C_{59}B$ sharply decreases to 1.54×10^2 au. The natural bond orbital analysis indicates that the encapsulated Li atom leads to an obvious charge transfer and valence electrons distribution plays a significant role in the β_{tot} value. Further, frontier molecular orbital explains that the interesting charge transfer between the encapsulated Li atom and cage-like radicals ($C_{59}B$ and $C_{59}N$) leads to differences in the β_{tot} value. It is our expectation that this work will provide useful information for the design of high-performance NLO materials.

Keywords Alkali metal · Cage-like radical · Charge transfer · First hyperpolarizability · NLO

Introduction

Nonlinear optical (NLO) materials have developed quickly in the past several decades, because of their wide applications in optoelectronics and photonics field [1–7]. Much effort has been devoted to find important factors to enhance the NLO response for designing some new high-performance NLO materials. These strategies include extending π-electron systems [2], twisting π-electron systems [8, 9], changing the relative position of donor and acceptor [10–12], increasing push–pull effects [5], doping alkali metal into organic compounds [13–18] etc. So far, alkali metal endohedral fullerenes show remarkable NLO response owing to extensive π-electron conjugation along with charge delocalization. Recently, workers have reported the NLO response of $Li@C_{60}Cl_8$ [19] and $Na@C_{60}C_{60}@F$ [20], which may be beneficial for further designing and synthesizing NLO molecular materials.

Research has made clear that all-carbon fullerene (C_{60}) strictly obey the isolated pentagon rule (IPR) [21], which avoids pentagon–pentagon contacts by surrounding each pentagon with five hexagons. So it is relatively stable and synthesizable. Recently, a large number of endohedral fullerenes have been reported, for example, C_{60} endohedral complexes with ions F^-, Na^+, Mg^{2+}, Al^{3+} [22], atom Li [23–25], and Gd [26], or molecules LiF [27, 28], and NH_4Cl [29] etc. In addition, the cage-like radicals ($C_{59}B$ and $C_{59}N$) have been achieved and reported, which have attracted wide attention in

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fullerene science [30–33]. An interesting question arises: how does the endohedral effect of cage-like radical fullerenes influence their nonlinear optical properties?

In order to answer this question, we have paid attention to the cage-like radicals ($C_{59}B$ and $C_{59}N$) and a new type of endohedral fullerene derivatives (Li@$C_{59}B$ and Li@$C_{59}N$) formed by encapsulating one Li atom into the cage-like radicals ($C_{59}B$ and $C_{59}N$). In the present work, the structures, natural bond orbital (NBO) charges, first hyperpolarizabilities, and frontier molecular orbitals of the four molecules are explored by using quantum chemical calculation. We hope the present work can provide new ideas for the design of new optical and photoelectric devices with high performances.

Computational details

The density functional theory (DFT) [34, 35] has been widely used to optimize the geometries of radicals and fullerene systems. In the present work, the optimized geometry structures of $C_{59}B$, $C_{59}N$, Li@$C_{59}B$, and Li@$C_{59}N$ with all real frequencies have been carried out using the B3LYP functional combined with the 6-31G* basis set. On the other hand, considering relatively good accuracy and moderate computational costs, we have optimized the geometric structures of $C_{59}B$ and Li@$C_{59}B$ using the M05-class functional (M05-2X). It was found that the structure parameters calculated by the B3LYP functional are close to that calculated by the M05-2X functional (for more details see Table 1). Besides, NBO charges were also calculated at the B3LYP/6–31+G* level of theory.

In this work, to correct the basis-set superposition error in the bond energy calculation, the counterpoise (CP) correction was used. The interaction energy (E_{int}) [36, 37] was calculated at the B3LYP/6-31G* level according to Eq. (1),

$$E_{\text{int}}(\text{AB}) = E(\text{AB})_{\text{AB}} - \left[E(\text{A})_{\text{AB}} + E(\text{B})_{\text{AB}}\right] \tag{1}$$

where E_{int} is the difference between the energies of the Li atom (A) and $C_{59}X$ (B) and the sum of the energies of the Li@$C_{59}X$(X=B, N) (AB).

Further, it is very necessary to choose a suitable method for evaluating their nonlinear optical properties. For a medium-size system, Champagne and Nakano pointed out that the BHandHLYP functional can reproduce the hyperpolarizability values provided by the more sophisticated single, double, and perturbative triple excitation coupled-cluster [CCSD(T)] method [38, 39]. In this work, the first hyperpolarizabilities were calculated at the BHandHLYP/6-31+G* level. In order to confirm the reliability and accuracy of this method, we also use the CAM-B3LYP [40] and M05-2X [41] methods to calculate the first hyperpolarizabilities. The results show that the β_{tot} values obtained by the CAM-B3LYP and M05-2X functionals are close to that obtained by the BHandHLYP functional. Therefore, the BHandHLYP functional is satisfactory for calculating the first hyperpolarizabilities of the four molecules.

The polarizability (α_0) is determined by:

$$\alpha_0 = \frac{1}{3}\left(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}\right) \tag{2}$$

The first hyperpolarizability (β_{tot}) is determined by:

$$\beta_{tot} = \left(\beta_x^2 + \beta_y^2 + \beta_z^2\right)^{1/2} \tag{3}$$

In which

$$\beta_i = \beta_{iii} + \beta_{ijj} + \beta_{ikk}(i, j, k = x, y, z) \tag{4}$$

All calculations were performed by using the Gaussian 09 program package [42].

Table 1 The corresponding bond length (Å), bond angle(°) of $C_{59}B$, Li@$C_{59}B$ by two methods

	B3LYP		M05-2X	
	$C_{59}B$	Li@$C_{59}B$	$C_{59}B$	Li@$C_{59}B$
B-C1	1.549	1.558	1.548	1.559
B-C2	1.525	1.505	1.527	1.449
B-C8	1.549	1.558	1.548	1.559
B-Li		2.221		2.189
C1–B–C2	118.6	117.0	118.7	117.0
C1–B–C8	106.3	104.4	106.3	104.1
C2–B–C8	118.6	116.8	118.7	116.9

Results and discussion

Optimized geometries and interaction energies (E_{int})

The optimized geometric structures of the four molecules at the B3LYP level are presented in Fig. 1. When a boron or nitrogen atom substitutes one carbon atom of the pristine buckminsterfullerene, $C_{60}(I_h)$ cage, the models of cage-like radicals ($C_{59}B$ and $C_{59}N$) are formed. Further, the structures of Li@$C_{59}B$ and Li@$C_{59}N$ are obtained by encapsulating a Li atom into the cage-like radicals ($C_{59}B$ and $C_{59}N$). The corresponding geometric parameters are given in Fig. 2. The C-B-C bond angle of the cage-like radical $C_{59}B$ are in the range of 106.3–118.6°, which is close to the C-N-C bond angle of the cage-like radical $C_{59}N$ (107.2–118.8°). Significantly, after encapsulating one Li atom, the C-N-C bond angles of Li@$\mathbf{C}_{59}N$

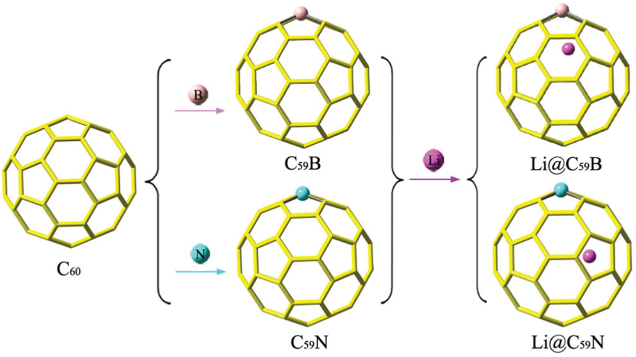

Fig. 1 The optimized structures of C_{60}, $C_{59}B$, $C_{59}N$, Li@$C_{59}B$, and Li@$C_{59}N$

Table 2 The natural bond orbitals (NBO) of important atoms and the interaction energies (E_{int} kcal mol^{-1}) of $C_{59}B$, $C_{59}N$, Li@$C_{59}B$, Li@$C_{59}N$

	$C_{59}B$	$C_{59}N$	Li@$C_{59}B$	Li@$C_{59}N$
q_B	0.702		0.527	
q_N		−0.362		−0.369
q_{C1}	−0.279	0.194	−0.269	0.223
q_{C2}	−0.250	0.200	−0.354	0.142
q_{C8}	−0.288	0.231	−0.287	0.237
q_{Li}			0.555	0.535
E_{int}			−35.21	−63.66

(106.8–118.5°) are slightly larger than that of the Li@$C_{59}B$ (104.4–117.0°). The bond lengths of the four molecules are clearly shown in Fig. 2. We can find that the C-B bond lengths of the $C_{59}B$ and Li@$C_{59}B$ are slightly larger than the C-N bond lengths of the $C_{59}N$ and Li@$C_{59}N$. In addition, the Li-N distance of Li@$C_{59}N$ is about 3.980 Å, which is larger than the Li-B distance of the Li@$C_{59}B$ (2.221 Å).

To further evaluate the stabilities of the two molecules (Li@$C_{59}B$ and Li@$C_{59}N$), we calculated the interaction energy (E_{int}) at the B3LYP/6-31G* level of theory with a counterpoise correction. The results are listed in Table 2, the E_{int} values of Li@$C_{59}B$ and Li@$C_{59}N$ are −35.21 kcal mol^{-1} and −63.66 kcal mol^{-1}. This shows that the encapsulating one Li atom and the cages have strong attraction in the two molecules. Furthermore, the E_{int} value of Li@$C_{59}N$ is larger than that of the Li@$C_{59}B$, which demonstrates that Li@$C_{59}N$ is more stable. Numerous studies illustrate that the DFT method often underestimates the diffusion interaction [43, 44], which means that the actual E_{int} values of the two molecules should be larger than the calculated values. Thus, the corresponding stability is also better than the calculated results.

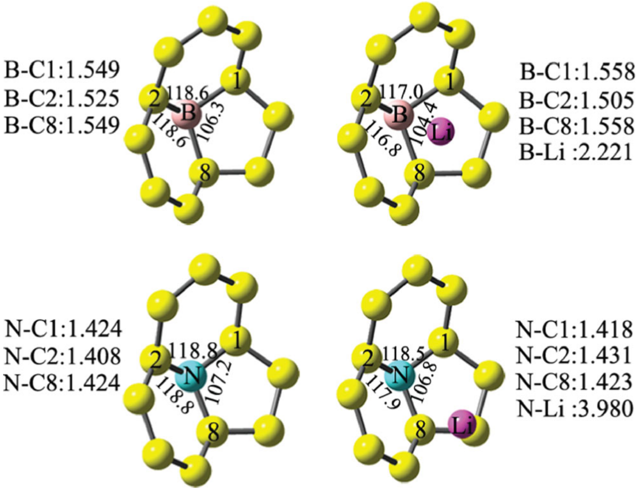

Fig. 2 The corresponding bond length (Å), bond angle(°) of $C_{59}B$, $C_{59}N$, Li@$C_{59}B$, Li@$C_{59}N$ at B3LYP/6-31G* level

Natural bond orbital (NBO) analysis

The NBO charges were calculated at the B3LYP/6-31+G* level and the results are shown in Table 2. As we know, the $C_{60}(I_h)$ has no charge transfer due to its centrosymmetric structure. However, for the cage-like radicals $C_{59}B$, the charge of B atom is 0.702 and the negative charge mainly distributes three carbon atoms (C1, C2, C8) directly connected to the boron atom. Similarly, the charge of N atom is −0.362 and the positive charge mainly distributes three carbon atoms (C1, C2, C8) directly connected to the nitrogen atom in the cage-like radicals $C_{59}N$. Further, encapsulating one Li atom into the cage-like radicals ($C_{59}B$ and $C_{59}N$), the charges of Li atom of Li@$C_{59}B$/Li@$C_{59}N$ are 0.555/0.535, which indicates that the degree of ionization of lithium atom is almost equal in the two cages. Compared to the molecules without one Li doping, the charge of B atom becomes 0.527 in the Li@$C_{59}B$, while for Li@$C_{59}N$, the charge of N atom (−0.369) is almost no change. The results show that the transferred electron of the Li atom partially distributes to the boron atom in the Li@$C_{59}B$. For the Li@$C_{59}N$, the transferred electron of the Li atom almost distributes to the carbon fragments. According to the above analysis, the encapsulated Li atom is an important factor causing the variation in charge transfer.

Furthermore, how does electron distribution influence the nonlinear optical properties? For the pure cage-like radicals $C_{59}B$ and $C_{59}N$, the singlet electrons mainly distribute to three carbon atoms (C1, C2, C8) directly connected to the boron or nitrogen atom. The β_{tot} values of the pure cage-like radicals $C_{59}B$ (1.30×10^3 au) and $C_{59}N$ (1.70×10^3 au) are close to each other. When one Li atom encapsulated into the cage-like radicals ($C_{59}B$ and $C_{59}N$), the valence electrons of the Li atom almost distribute to the cage-like radical. The β_{tot} value of Li@ $C_{59}N$ increases to 2.46×10^3 au. However, the β_{tot} value of Li@$C_{59}B$ sharply decreases to 1.54×10^2 au.

Linear and nonlinear optical property

The polarizabilities (α_0) and the first hyperpolarizabilities (β_{tot}) of the four molecules ($C_{59}B$, $C_{59}N$, Li@$C_{59}B$, and Li@$C_{59}N$) were calculated by BHandHLYP, CAM-B3LYP, and M05-2X functionals and the results are listed in Table 3. It is clear that each method obtained the close α_0 values. In addition, the α_0 values of $C_{59}B$ (5.40×10^2–5.44×10^2 au), $C_{59}N$ (5.45×10^2–5.41×10^2 au), Li@$C_{59}B$ (5.35×10^2–5.41×10^2 au), and Li@$C_{59}N$ (5.62×10^2–5.68×10^2au) are very close, which shows that the encapsulated Li atom has little effect on the polarizabilities.

According to Table 3 and Fig. 3, different methods obtained the same trend in the β_{tot} value, so we chose the results of the BHandHLYP for further discussion. The first hyperpolarizabilities of the cage-like radicals $C_{59}B$ and $C_{59}N$ are 1.30×10^3 and 1.70×10^3 au, respectively. At the same time, the β_{tot} values of the pure cage-like radicals $C_{59}B$ (1.30×10^3 au) and $C_{59}N$ (1.70×10^3 au) are close to each other. Further, when one Li atom encapsulated into electron-rich radical $C_{59}N$, the β_{tot} value of Li@$C_{59}N$ increases to 2.46×10^3 au. However, when one Li atom encapsulated into electron-deficient radical $C_{59}B$, the β_{tot} value of Li@$C_{59}B$ sharply decreases to 1.54×10^2 au. The results show that the encapsulated Li atom influences the static first hyperpolarizabilities sensitively.

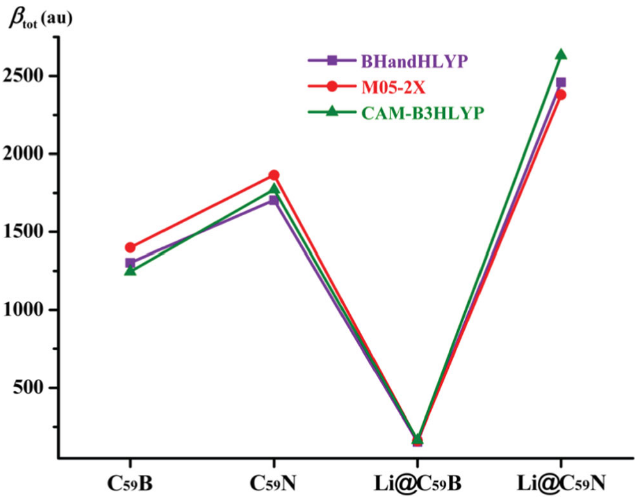

Fig. 3 The β_{tot} values of $C_{59}B$, $C_{59}N$, Li@$C_{59}B$, and Li@$C_{59}N$ by three methods

The following two-level expression is employed to further understand the origin of the β_{tot} values [45, 46].

$$\beta_{tot} \propto \frac{\Delta\mu \cdot f_0}{\Delta E^3} \tag{5}$$

The β_{tot} value is proportional to the difference between the dipole moments of the ground state and the crucial excited state ($\Delta\mu$), the oscillator strength (f_0), and the inverse of the third power of the transition energy (ΔE). According to the

Table 3 The polarizability (α_0, au) and the first hyperpolarizability (β_{tot}, au) with BHandHLYP, CAM-B3LYP, and M05-2X methods, the difference of dipole moments ($\Delta\mu$, au) between the ground and excited state, the oscillator strength f_0, the transition energies (ΔE, eV), and the $(f_0\cdot\Delta\mu)/\Delta E^3$ (au) values at the B3LYP/6-31G(d) level

		$C_{59}B$	$C_{59}N$	Li@$C_{59}B$	Li@$C_{59}N$
BHandHLYP	α_0	5.44×10^2	5.44×10^2	5.41×10^2	5.68×10^2
	β_x	1.75×10^2	-2.84×10^2	1.43×10^2	4.86×10^2
	β_y	1.29×10^3	−39.53	18.74	1.09×10^3
	β_z	0.54	1.68×10^3	−52.43	2.15×10^3
	β_{tot}	1.30×10^3	1.70×10^3	1.54×10^2	2.46×10^3
M05-2X	α_0	5.40×10^2	5.41×10^2	5.35×10^2	5.62×10^2
	β_x	1.96×10^2	-3.44×10^2	1.51×10^2	4.57×10^2
	β_y	1.39×10^3	−43.03	28.03	1.15×10^3
	β_z	0.31	1.83×10^3	−45.28	2.03×10^3
	β_{tot}	1.40×10^3	1.87×10^3	1.60×10^2	2.38×10^3
CAM-B3HLYP	α_0	5.44×10^2	5.45×10^2	5.41×10^2	5.67×10^2
	β_x	1.81×10^2	-3.13×10^2	1.57×10^2	5.27×10^2
	β_y	1.23×10^3	−40.66	16.68	1.22×10^3
	β_z	0.30	1.74×10^3	−45.27	2.27×10^3
	β_{tot}	1.25×10^3	1.77×10^3	1.65×10^2	2.63×10^3
	f_0	0.0084	0.0136	0.0118	0.0357
B3LYP	ΔE	1.7294	1.7252	2.9530	1.5815
	$\Delta\mu$	0.58	0.48	0.34	0.56
	$(f_0\cdot\Delta\mu)/\Delta E^3$	19.07	25.59	3.50	1.03×10^2

two-level model expression, the transition energy is the main factor in the first hyperpolarizability. The f_0, ΔE, and $\Delta\mu$ for the four molecules are obtained by B3LYP/6-31G* level of theory. Firstly, as shown in Table 3 and Fig. 4, the β_{tot} value of the cage-like radical $C_{59}B$ (1.30×10^3 au) is close to the β_{tot} value of the cage-like radical $C_{59}N$ (1.70×10^3 au), the ΔE values of the two molecules are nearly 1.73 eV. Secondly, the β_{tot} value of Li@$C_{59}N$ (2.46×10^3 au) is obviously larger than that of the Li@$C_{59}B$ (1.54×10^2 au), which is inverse to the ΔE values (1.5815 eV for Li@$C_{59}N<2.9530$ eV for Li@$C_{59}B$). Furthermore, the $(f_0\cdot\Delta\mu)/\Delta E^3$ values of four molecules are shown in Table 3. As one can see, the order of the $(f_0\cdot\Delta\mu)/\Delta E^3$ values is Li@$C_{59}N$ (1.03×10^2)>$C_{59}N$ (25.59)≈ $C_{59}B$ (19.07)>Li@$C_{59}B$ (3.50 au). The calculated results show that the interesting encapsulated Li atom effect on the first hyperpolarizability is well explained by the three main factors ΔE, f_0 and $\Delta\mu$.

Frontier molecular orbital analysis

Furthermore, the molecular orbitals of the considered transitions are shown in Fig. 5. Firstly, compared with the pure cage-like radicals $C_{59}B$ and Li@$C_{59}B$, the considered transition of radical $C_{59}B$ is the SOMO→LUMO and the considered transition of Li@$C_{59}B$ is HOMO→LUMO+3. For the pure cage-like radicals $C_{59}B$, the electron density of SOMO almost distributes to the $C_{59}B$ cage atoms excluding the boron atom. At the same time, the electron density mainly covers the boron atom and the neighboring carbon atoms in LUMO. On the contrary, for the Li@$C_{59}B$, the electron density of HOMO mainly covers the boron atom and the neighboring carbon atom. At the same time, the electron density almost distributes to the $C_{59}B$ cage atoms excluding the boron atom in LUMO+3. Secondly, compared with the pure cage-like radical $C_{59}N$ and Li@$C_{59}N$, the considered transition of the cage-like radicals $C_{59}N$ is the SOMO→LUMO+3 transition and the considered transition of Li@$C_{59}N$ is HOMO→LUMO+2 transition. For the pure cage-like radicals $C_{59}N$, the electron density of SOMO mainly covers the nitrogen atom and the neighboring carbon atom, at the same time, the electron density almost distributes to the $C_{59}N$ cage atoms excluding the nitrogen atom in LOMO+3. However, for the Li@$C_{59}N$, the electron density of HOMO almost distributes to the $C_{59}N$ cage atoms and the electron density mainly covers the carbon atoms which are distant from the nitrogen atom in LUMO+2. As mentioned above, the interesting charge transfer between the encapsulated Li atom and cage-like radicals ($C_{59}B$ and $C_{59}N$) explain that the first hyperpolarizabilities show differences.

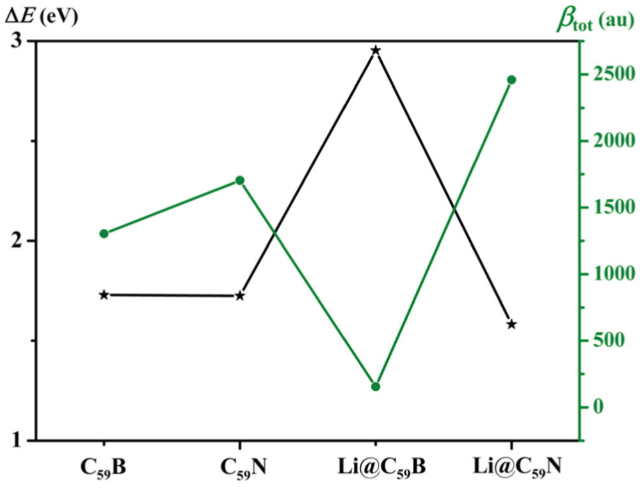

Fig. 4 The relationship between first hyperpolarizabilities (β_{tot}) and the transition energy (ΔE) of $C_{59}B$, $C_{59}N$, Li@$C_{59}B$, and Li@$C_{59}N$

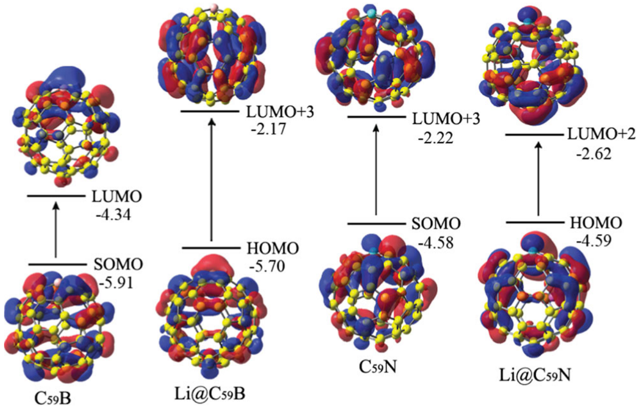

Fig. 5 The considered transitions and corresponding orbital energy (eV) for the four molecules

Conclusions

In the present paper, we focus on exploring the structures, stabilities, NBO charges, frontier molecular orbitals, linear, and nonlinear optical properties of the four molecules. The above investigations show that the E_{int} values of Li@$C_{59}B$ and Li@$C_{59}N$ are negative, which shows that the encapsulating one Li atom and cages have strong attraction in the two molecules. The natural bond orbital analysis indicates that the encapsulated Li atom leads to an obvious charge transfer and the valence electrons distribution plays a significant role in the β_{tot} value. Furthermore, frontier molecular orbital confirms that differences of the β_{tot} values can mainly be attributed to charge transfer between the encapsulated Li atom and cage-like radicals ($C_{59}B$ and $C_{59}N$). We used three DFT methods (BHandHLYP, CAM-B3LYP, and M05-2X) to calculate their first hyperpolarizabilities, and the three methods obtained the same order of the β_{tot} value. Firstly, the α_0 values of the four molecules are close. Secondly, the β_{tot} values of the pure cage-like radicals $C_{59}B$ and $C_{59}N$ are close to each other. Interestingly, when one Li atom encapsulated into the cage-like radicals $C_{59}B$ and $C_{59}N$, the β_{tot} value of Li@$C_{59}N$ increases. However, the β_{tot} value of Li@$C_{59}B$ sharply decreases. It is clear that the encapsulated Li atom has a large contribution to the β_{tot} value. We hope the present work can provide a novel strategy for enhancing the first hyperpolarizability by altering the molecular structure, which may be beneficial to experimentalists for designing high-performance nonlinear optical materials.

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