With the aim of finding a suitable synthesizable superalkali species, using the B3LYP/6-31G* density functional level of theory we provide results for the interaction between the buckminsterfullerene C_{60} and the superalkali Li_3F_2. We show that this endofullerene is stable and provides a closed environment in which the superalkali can exist and interact with CO_2. It is worthwhile to mention that the optimized Li_3F_2 structure inside C_{60} is not the most stable C_2v isomer found for the “free” superalkali but the D_{3h} geometry. The binding energy at 0 K between C_{60} and Li_3F_2 (D_{3h}) is computed to be 119 kJ mol^{-1}. Once CO_2 is introduced in the endofullerene, it is activated, and the \hat{\text{O}}\text{C}=\text{O} angle is bent to 132°. This activation does not follow the previously studied CO_2 reduction by an electron transfer process from the superalkali, but it is rather an actual reaction where a F (from Li_3F_2) atom is bonded to the CO_2. From a thermodynamic analysis, both CO_2 and the encapsulated [Li_3F_2·CO_2] are destabilized in C_{60} with solvation energies at 0 K of 147 and < −965 kJ mol^{-1}, respectively.

Keywords: CO_2 activation, superalkali, endofullerene, ionization energy, solvation energy

INTRODUCTION

In 1985, Kroto and co-workers discovered an extremely stable cluster consisting of 60 carbon atoms during a study of long-chain carbon molecules. (Kroto et al., 1985) This cluster, called fullerenes, has a football shape with 12 pentagonal and 20 hexagonal rings. (Kroto et al., 1985) Shortly after, a study presenting successful formation of fullerenes with a lanthanum atom trapped in the cavity of C_{60}, called endofullerene, C_{60}La, was published. (Heath et al., 1985) Another consequent experiment proved the stability of C_{60}La against H_2, O_2, NO, and NH_3. (Weiss et al., 1988) This suggested that the lanthanum atom can be “protected” by being encapsulated in the fullerene. Since then, a number of studies focusing on novel properties of C_{60} and its interactions with other species have been carried out. (Ruoff et al., 1993; Diederich and Gómez-López, 1999; Bakry et al., 2007; Mignolet et al., 2013; Wang et al., 2014; Elliott et al., 2018; Kouřil et al., 2018) Some investigations concentrated on medical applications, hydrogen storage, and various endofullerene. (Wang et al., 2013; Srivastava et al., 2016; Srivastava et al., 2017; Elliott et al., 2018; Kouřil et al., 2018) Due to the fullerene’s unique cage-like cavity, a procedure called molecular surgery can be performed to entrap an atom or molecule. (Murata et al., 2006; Krachmalnicoff et al., 2016) Utilizing this technique, encapsulation of molecular hydrogen and HF were successfully achieved. (Murata et al., 2006; Krachmalnicoff et al., 2016) In addition, a recent paper by Jana and Chattaraj (2020) describes the effects of a molecular reaction environment, dodecahedrane, on the He dimer bonding. Also, theoretical studies of a new type of endofullerenes with superalkali have been performed. (Srivastava et al., 2016; Srivastava et al., 2017) Superalkalis are clusters with very low adiabatic ionization energies. (Gutsev and Boldyrev, 1982; Gutsev and Boldyrev, 1983; Gutsev and Boldyrev, 1987; Lia et al., 1988; Gutsev and Boldyrev, 1990;
Tong et al., 2013a; Tong et al., 2013b). The first and most common superalkalis have the formula $M_{n+1}L$, where $M$ is an alkali atom with valence $k$ and $L$ is an electronegative atom. (Gutsev and Boldyrev, 1985; Gutsev and Boldyrev, 1987; Zhao et al., 2017). Nambari et al. (2021) showed the importance of these compounds through a density functional computational study to improve the efficacy of reox reactions.

The concentration of carbon dioxide (CO$_2$) in the atmosphere has been increasing constantly since the early 20$^{th}$ century with rapid industrialization. (D’Amato and Akdas, 2020; Kuzovkin and Semenov, 2020). This is a globally recognized issue as CO$_2$ contributes significantly to the greenhouse effect and the acidification of the oceans. (Crowley and Berner, 2001; Hönisch et al., 2012). Increment of atmospheric temperature causes climate change that threatens the overall ecosystem. To capture CO$_2$ molecules present in the air, various methods have been employed such as packed column of monoethanolamine and metal-organic frameworks. (Lv et al., 2015; Li et al., 2019; Li et al., 2020). The next step is activating CO$_2$ molecules and converting them to value-added chemicals such as hydrocarbon fuels. (Hu et al., 2013). The activation of CO$_2$ is extremely complex due to its stability and much efforts have been made by researchers to directly convert it into liquid hydrocarbons, useful for the aviation sector as novel jet fuels (Boreriboon et al., 2018; Vogt et al., 2019; Yao et al., 2020) or into oxygenates, such as ethanol. (Song et al., 2016; Bai et al., 2017; Wang et al., 2018). This conversion, whether it involves a direct CO$_2$ hydrogenation route or not, entails the usage of metal-based catalysts to ensure an overall reasonable efficiency. (Yao et al., 2020).

In our previous studies, successful activation of CO$_2$ with a superalkali species, Li$_3$F$_2$, were presented. (Park and Meloni, 2017). The computational study showed charge transfer from Li$_3$F$_2$ to CO$_2$, which indicates migration of the unpaired electron from Li$_3$F$_2$ to CO$_2$. The activated CO$_2$ showed geometric change such as bent OCO angle. The activated CO$_2$ then can be transformed to other organic molecules with catalysis. (Liu et al., 2016; Luc et al., 2017). Removing the unpaired electron from [Li$_3$F$_2$-CO$_2$] cluster weakens the interaction between Li$_3$F$_2$ and CO$_2$ and geometry of CO$_2$ returns back to the linear form. (Park and Meloni, 2017). The superalkali Li$_3$F$_2$ was observed and characterized experimentally. (Yokoyama et al., 2000; Haketa et al., 2002). They also confirmed three stable Li$_3$F$_2$ structures through a computational density functional approach. (Haketa et al., 2002). In this investigation, the Li$_3$F$_2$-doped fullerene and its endo-reaction with CO$_2$ has been characterized using the B3LYP/6-31G$^*$ level of theory. These results are explained in terms of energetics and molecular orbitals of the species involved. In addition, these findings will be beneficial in providing insights for CO$_2$ reduction and in helping the exploration of new materials with tailored properties.

**Computational Methods**

Geometries and total electronic energies of the investigated species were calculated at the B3LYP/6-31G$^*$ level of theory (Becke, 1988; Lee et al., 1988) using the computational software Gaussian09. (Frisch et al., 2016). B3LYP is one of the most commonly used density functional theory (DFT) methods that employs a three-parameter exchange functional developed by Becke (1992) and Becke (1993) with a correlational functional proposed by Lee, Yang, and Parr (LYP) Becke (1988) to approximate the exchange-correlation energy. The B3LYP/6-31G$^*$ level has been employed to study endofullerene systems because it yields reliable geometries and energies. (Wang et al., 2013; Srivastava et al., 2016; Srivastava et al., 2017). Partial atomic charges are calculated based on the Mulliken population analysis (Mulliken, 1955) and natural bond orbital (NBO) population analysis. (Reed et al., 1985).

The adiabatic ionization energy (AIE) is calculated by taking the zero-point energy corrected electronic energy difference between the optimized neutral and cation, whereas the adiabatic electron affinity (AEA) is obtained by subtracting the zero-point-energy corrected electronic energy of the optimized anion and neutral. All the optimized structures have real vibrational frequencies and their Cartesian coordinates have been reported in the Supplementary Material.

**RESULTS AND DISCUSSION**

The main intent of this computational investigation is to study the interactions relevant to the reduction of CO$_2$ by the superalkali Li$_3$F$_2$ inside our molecular reaction vessel, i.e., C$_{60}$, and see how this environment affects the CO$_2$ activation. The system is fairly large and, therefore, computationally challenging to investigate. We have analyzed the possible interactions between the fullerene and the two reactants, CO$_2$ and Li$_3$F$_2$. All the computed energetics are reported in Table 1 together with the available literature (experimental and computed) values.

**Figure 1** reports the optimized geometries for CO$_2$ and CO$_2$, Li$_3$F$_2$(C$_{2v}$), Li$_3$F$_2$(D$_{3h}$) and their cations. The structures of CO$_2$ and CO$_2$ reproduce well the literature experimental values for both bond distances and bond angles. In fact, for CO$_2$ we have r$_{C-O}$ = 1.17 Å (1.16 Å) (Herzberg, 1966) and for CO$_2$, we have r$_{C-O}$ = 1.25 Å (1.25 Å) (Hartman and Hisatsune, 1966) and αOCO$^\prime$ = 134° (127 ± 7°) . (Hartman and Hisatsune, 1966). Both the geometries of the lowest energy Li$_3$F$_2$(C$_{2v}$) isomer, trigonal bipyramidal Li$_3$F$_2$(D$_{3h}$), and their cations are in agreement with our previous work. (Park and Meloni, 2017; Cochran and Meloni, 2014). **Figure 2** shows the two superalkali isomers reducing the CO$_2$. The geometry for the previously studied C$_{2v}$ isomer interacting with CO$_2$ is in agreement with our previous results, (Park and Meloni, 2017), whereas the D$_{3h}$CO$_2$ species is reported for the first time. When the D$_{3h}$ structure reacts with CO$_2$, the trigonal bipyramidal geometry is distorted by increasing two “equatorial” Li-Li distances, maintaining only the Li(1)-Li(2) distance of 2.30 Å, with Li(3) being closer to the CO$_2$, Li(3)-O(7) = Li(3)-O(8) = 2.03 Å and increasing the axial F-F distance from 2.40 to 2.68 Å. The αOCO’ bond angle is 128° and the C-O bond length is 1.26 Å. The Li$_3$F$_2$ isomers have similar binding energy with CO$_2$, with the C$_{2v}$ isomer...
presenting a stronger interaction of 184 kJ mol\(^{-1}\). These clusters can be defined as “free” or “naked” because they are isolated in the gas phase. The presented energy values are calculated at the B3LYP/6-31G* level and are within 10% from the literature reported quantities, whether they are experimental or computed at very high level of theory.
When a molecule is inserted in the fullerene (yielding an endofullerene), the chemical system is not free, but it will be subjected to the interactions with the carbon cage (“solvation effects”). In Figure 3, the two endofullerenes with CO$_2$ and Li$_3$F$_2$ are shown. In the case of carbon dioxide, it is clear from the energetics presented in Table 1 that CO$_2$ is destabilized by C$_{60}$ having a negative binding energy at 0 K of $-147$ kJ mol$^{-1}$ or a solvation energy at 0 K of $147$ kJ mol$^{-1}$, calculated as $E_0$(CO$_2$) $+ E_0$(C$_{60}$) $- E_0$(C$_{60}$·CO$_2$). The CO$_2$ occupies the center of the C$_{60}$, aligned with the C$_3$ axis passing through a hexagonal face, minimizing its interactions with the C cage. The solvation energy is more properly defined as the Gibbs free energy change associated with the transfer of a molecule from the gas phase into a solvent, i.e., it provides the relative equilibrium populations of a species between gas phase and the solvent. Therefore, we should also know the entropy change connected with this process. The values that we are reporting in this investigation are at 0 K, so that $\Delta_{solv}H_0^0 = \Delta_{solv}G_0^0 = -BE$(solvent−species), from which we can see that negative binding energies correspond to positive solvation energies (destabilizing effect). For the encapsulated superalkali two main findings can be noticed. First, the superalkali inside the fullerene is “forced” to assume a D$_{3h}$
geometry, a structure almost identical to the free D₃h cluster but less stable than the free Cᵥ cluster. Despite having started the Li₂F₂ geometry optimization from different initial configurations, the optimized structure inside the fullerene resulted in the trigonal bipyramidal geometry. The Li-F distances are shortened in C₆₀ from 1.83 (free superalkali) to 1.77 Å, which corresponds to a compression along the F-F distance from 2.40 to 2.21 Å, and the two Li-Li bonds elongate to 2.40 Å. The second result is that C₆₀ interacts strongly with Li₃F₂ with a binding energy at 0 K of 119 kJ mol⁻¹ or solvation energy at 0 K of −119 kJ mol⁻³, calculated as $E_{\text{Li}_3\text{F}_2(D_{3h})} + E_{\text{C}_6\text{O}} - E_{\text{C}_6\text{O}+\text{Li}_3\text{F}_2(D_{3h})}$. This interaction is not a reduction of C₆₀, where the electron from the superalkali is transferred to the fullerene. In fact, upon ionization of C₆₀·Li₃F₂(D₃h), the encapsulated Li₃F₂ retains its trigonal bipyramidal structure, just slightly distorted (as described above) due to the interactions with C₆₀. In addition, looking at the Mulliken population and the natural orbital population neither the endo-Li₃F₂(D₃h) nor the C₆₀ show an increase or change of electron charges. The C₆₀·Li₃F₂ HOMO, the main contribution of which is given by C 2p AO’s, is delocalized almost entirely on the fullerene (Figure 4). The fact that the C₆₀·Li₃F₂ AIE is much lower than C₆₀ AIE, 5.64 vs. 7.08 eV, respectively, can be explained using a molecular orbital character argument. The interaction of C₆₀ with the superalkali makes the HOMO of fullerene less bonding, and consequently, most of the C-C bonds are elongated by 0.1–0.2 Å. Upon ionization, the C-C bonds in C₆₀·Li₃F₂ are shortened on average by 0.1 Å, which can be interpreted as the removal of an electron from a HOMO with antibonding character.

The insertion of CO₂ within C₆₀·Li₃F₂(D₃h) produces an unexpected result (Figure 5). In previous computational studies, (Zhao et al., 2017; Park and Meloni, 2017; Sikorska and Gaston, 2020), naked superalkali have been shown to be capable of reducing carbon dioxide by transferring an electron and yielding an activated bent CO$_2^-$, which is not observed in this investigation. Upon ionization, the C-C bonds in C₆₀·Li₃F₂ are shortened on average by 0.1 Å, which can be interpreted as the removal of an electron from a HOMO with antibonding character. The insertion of CO₂ within C₆₀·Li₃F₂(D₃h) produces an unexpected result (Figure 5). In previous computational studies, (Zhao et al., 2017; Park and Meloni, 2017; Sikorska and Gaston, 2020), naked superalkali have been shown to be capable of reducing carbon dioxide by transferring an electron and yielding an activated bent CO$_2^-$, which is not observed in this investigation. Upon ionization, the C-C bonds in C₆₀·Li₃F₂ are shortened on average by 0.1 Å, which can be interpreted as the removal of an electron from a HOMO with antibonding character. The insertion of CO₂ within C₆₀·Li₃F₂(D₃h) produces an unexpected result (Figure 5). In previous computational studies, (Zhao et al., 2017; Park and Meloni, 2017; Sikorska and Gaston, 2020), naked superalkali have been shown to be capable of reducing carbon dioxide by transferring an electron and yielding an activated bent CO$_2^-$, which is not observed in this investigation. Upon ionization, the C-C bonds in C₆₀·Li₃F₂ are shortened on average by 0.1 Å, which can be interpreted as the removal of an electron from a HOMO with antibonding character. The insertion of CO₂ within C₆₀·Li₃F₂(D₃h) produces an unexpected result (Figure 5). In previous computational studies, (Zhao et al., 2017; Park and Meloni, 2017; Sikorska and Gaston, 2020), naked superalkali have been shown to be capable of reducing carbon dioxide by transferring an electron and yielding an activated bent CO$_2^-$, which is not observed in this investigation. Upon ionization, the C-C bonds in C₆₀·Li₃F₂ are shortened on average by 0.1 Å, which can be interpreted as the removal of an electron from a HOMO with antibonding character. The insertion of CO₂ within C₆₀·Li₃F₂(D₃h) produces an unexpected result (Figure 5). In previous computational studies, (Zhao et al., 2017; Park and Meloni, 2017; Sikorska and Gaston, 2020), naked superalkali have been shown to be capable of reducing carbon dioxide by transferring an electron and yielding an activated bent CO$_2^-$, which is not observed in this investigation. Upon ionization, the C-C bonds in C₆₀·Li₃F₂ are shortened on average by 0.1 Å, which can be interpreted as the removal of an electron from a HOMO with antibonding character. The insertion of CO₂ within C₆₀·Li₃F₂(D₃h) produces an unexpected result (Figure 5). In previous computational studies, (Zhao et al., 2017; Park and Meloni, 2017; Sikorska and Gaston, 2020), naked superalkali have been shown to be capable of reducing carbon dioxide by transferring an electron and yielding an activated bent CO$_2^-$, which is not observed in this investigation. Upon ionization, the C-C bonds in C₆₀·Li₃F₂ are shortened on average by 0.1 Å, which can be interpreted as the removal of an electron from a HOMO with antibonding character. The insertion of CO₂ within C₆₀·Li₃F₂(D₃h) produces an unexpected result (Figure 5). In previous computational studies, (Zhao et al., 2017; Park and Meloni, 2017; Sikorska and Gaston, 2020), naked superalkali have been shown to be capable of reducing carbon dioxide by transferring an electron and yielding an activated bent CO$_2^-$, which is not observed in this investigation. Upon ionization, the C-C bonds in C₆₀·Li₃F₂ are shortened on average by 0.1 Å, which can be interpreted as the removal of an electron from a HOMO with antibonding character.
(trigonal pyramidal) FCO$_2$ that interacts with what it looks like a FLI$_3$ species. All the attempts to optimize this structure outside C$_{60}$ as free endo-Li$_3$F$_2$-CO$_2$ returned a Li$_3$F$_2$ (D$_{3h}$)-CO$_2$ geometry. Unfortunately, this prevents us from quantifying the interaction of Li$_3$F$_2$ (D$_{3h}$) with CO$_2$ inside C$_{60}$. In fact, the reaction we need is:

$$C_{60} \cdot [SA \cdot CO_2] \rightarrow C_{60} \cdot Li_3F_2(D_{3h}) + C_{60} \cdot CO_2 \quad (1)$$

from which the interaction of Li$_3$F$_2$ (D$_{3h}$) with CO$_2$ can be derived if we were able to find the [SA-CO$_2$] reaction product as a free species and then its binding energy (or negative solvation energy) with C$_{60}$, i.e.,

$$C_{60} \cdot [SA \cdot CO_2] \rightarrow C_{60} + [SA \cdot CO_2] \quad (2)$$

In fact, the interaction of Li$_3$F$_2$ (D$_{3h}$) with CO$_2$ inside fullerene can be calculated as:

$$\Delta H^\circ (1) - BE(C_{60} \cdot CO_2) - BE(C_{60} \cdot Li_2F_3(D_{3h})) + BE(C_{60} \cdot [SA \cdot CO_2]) \quad (3)$$

In other words, this expression tells us that the interaction between endo-Li$_3$F$_2$ (D$_{3h}$) and endo-CO$_2$, i.e., the BE of superalkali-CO$_2$ in fullerene, is equal to the enthalpy of reaction (1) plus the solvation energies of CO$_2$ and Li$_3$F$_2$ (D$_{3h}$) minus the solvation energy of [SA-CO$_2$]. Because we cannot derive this last solvation energy absolute value due to the impossibility of optimizing the free endo-[SA-CO$_2$] species, we can estimate this interaction by performing a single-point energy calculation of the free [SA-CO$_2$] optimized inside C$_{60}$. This structure necessarily represents a higher energy structure than a real minimum and, therefore, the estimated BE of superalkali-CO$_2$ in fullerene would denote an upper bound providing us some insights on this interaction. From this computation we get an upper bound for BE(C$_{60} \cdot [SA \cdot CO_2]$) of -965 kJ mol$^{-1}$, which tells us that this endo-product is highly destabilized by C$_{60}$!

## CONCLUSION

The activation of CO$_2$ by the Li$_3$F$_2$ superalkali within C$_{60}$ has been investigated at the B3LYP/6-31G* level of theory. C$_{60}$ has been utilized as a reaction vessel and its interaction with the reactants, superalkali and carbon dioxide, have been computed. C$_{60}$ is capable of forcing a superalkali geometry, which does not present the global minimum in the gas phase. Specifically, Li$_3$F$_2$ takes the D$_{3h}$ structure. C$_{60}$ has a stabilizing effect on the superalkali but a destabilizing effect on the CO$_2$, as it can be deduced by the binding energies of these two systems, $BE(C_{60}\cdot CO_2) = -147$ kJ mol$^{-1}$ and $BE(C_{60}\cdot Li_3F_2) = 119$ kJ mol$^{-1}$. Upon interaction of Li$_3$F$_2$ (D$_{3h}$) with CO$_2$ inside fullerene, CO$_2$ is clearly activated showing a C-O-C bond angle of 132° and C-O bond lengths of 1.20 Å, 0.03 Å longer than r$_{C-O}$ in CO$_2$ but 0.06 Å shorter than r$_{C-O}$ in the free Li$_3$F$_2$ (D$_{3h}$)-CO$_2$ species. The activation of CO$_2$ is achieved by a F transfer from Li$_3$F$_2$ to CO$_2$ with the formation of a C-F bond of 1.38 Å. Due to the impossibility of optimizing a free superalkali-CO$_2$ complex, [SA-CO$_2$], resembling the one optimized within the C$_{60}$, a single-point energy calculation has been performed on the free [SA-CO$_2$]. This energy has been utilized to provide an upper bound for the binding energy of Li$_3$F$_2$ (D$_{3h}$) with CO$_2$ within C$_{60}$ of -965 kJ mol$^{-1}$, showing that C$_{60}$ destabilizes the reaction product.

## DATA AVAILABILITY STATEMENT

The original contribution presented in the study are included in the article/Supplementary Material, further inquiries can be directed to the corresponding author.

## AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

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## SUPPLEMENTARY MATERIAL

The Supplementary Material for this article can be found online at: https://www.frontiersin.org/articles/10.3389/fchem.2021.712960/full#supplementary-material

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Conflict of Interest: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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