

The difference of reaction mechanism between 2, 4-di-tert-butylphenol and 2, 6-di-tert-butylphenol in the synthesis of salicylic acid

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Abstract

Although the Kolbe-Schmidt reaction has been studied in industrial production for more than 100 years, it is surprising that the scientific research in the theoretical stage has not attracted enough attention. Theoretical research is indispensable for the guidance and deepening of industrial production. In this paper, the carboxylation reaction characteristics of 2, 4-di-tert-butylphenol and 2, 6-di-tert-butylphenol were effectively studied at the atomic scale for the first time. The results show that the reaction of tert-butylphenol and CO_2 is an exothermic reaction, and the product of 2, 4-di-tert-butylphenol O^- is more exothermic and more stable in structure. However, compared with 2, 6-di-tert-butylphenol O^- , the energy barrier needed to overcome in the reaction process is larger. Therefore, in order to achieve a considerable rate and conversion rate, industrial production needs to be carried out at high temperature and high pressure. This study provides a strategic direction for further understanding and optimizing the industrial application of the Kolbe-Schmitt reaction.

1. Introduction

Excessive consumption of fossil fuels has led to a rapid increase in atmospheric CO_2 levels, global warming and environmental degradation^[1, 2]. Based on the national policy of “carbon peak by 2030, carbon neutrality by 2050”, the rational utilization and transformation of CO_2 is the focus of current research^[3, 4]. Among the many types of CO_2 catalytic conversion, the formation of C-C bonds is considered to be an ideal way to utilize carbon dioxide, because the newly generated C-C bonds have higher energy density and broader development prospects, the Kolbe-Schmitt reaction conforms to this feature^[5]. The Kolbe-Schmidt reaction is a carboxylation reaction of alkali metal phenol salt and CO_2 to produce hydroxybenzoic acid^[6, 7]. Kolbe-Schmitt reaction has been used for carboxylation synthesis for 150 years(Fig. 1a)^[8–10]. The reaction has been widely used in the industrial production of aromatic carboxylic acids such as salicylic acid, 3-hydroxy-2-naphthoic acid, and 6-hydroxy-2-naphthoic acid, because hydroxybenzoic acid is a key compound in food, medicine, materials and so on^[11, 12].

Although a century has passed since its inception, there are still some challenges. The reaction temperature ($> 120^\circ\text{C}$) and CO_2 pressure ($> 20 \text{ atm}$) are high^[13–15]. In order to reduce the temperature and pressure under the determined industrial conditions, the most advantageous way is to choose the electron-rich phenols^[16, 17]. As shown in Fig. 1b, Larrosa et al. proposed one of the most significant advances in the Kolbe-Schmidt reaction. The results showed that under atmospheric pressure, the addition of 2, 4, 6-trimethylphenol significantly improved the efficiency of phenol carboxylation reaction due to the electron-donating characteristics of methyl. However, the reaction temperature (185°C) is high, sensitive to water, and needs to be carried out in the glove box, resulting in limited practicality^[18]. In addition, the methyl group in 2, 4, 6-trimethylphenol is small, and CO_2 can attack more sites, resulting in an increase in by-products and a decrease in the selectivity of the main product. Methyl has $\alpha\text{-H}$, which is easily oxidized to $\text{-CH}_2\text{OH}$, -CHO , -COOH under strong alkali and high temperature, resulting in many by-

products and complex product distribution. Therefore, the key to this reaction is the selection of excellent electron-donating groups.

Among the many electron-donating groups, tert-butyl has very obvious advantages. Firstly, the +I effect of tert-butyl is stronger, which makes the phenolic oxygen anion more stable and the reaction more likely to occur. Secondly, tert-butyl has a large volume, which can fix the phenoxy anion configuration and increase the probability of CO₂ attacking the ortho position, so that the yield of salicylic acid is increased. Thirdly, tert-butyl has no α-H, is not easy to be oxidized, and the product purity is high. Fourth, the tert-butyl substituted salicylic acid has large steric hindrance, good crystallinity and is easy to be separated by crystallization. At present, there are many related studies in industry, but the reaction mechanism has not been reported from a scientific point of view. So, the mechanism of tert-butylphenol reaction has been a hot topic in experimental and theoretical research. For the accuracy of the study, the microscopic mechanism of 2, 4-di-tert-butylphenol and 2, 6-di-tert-butylphenol is based on the results of the Kolbe Schmitt reaction.

Markovic et al. used Gaussian 98 software package for quantum mechanics calculation, three intermediate species and corresponding transition states were proposed^[19]. Subsequently, Stanescu groups performed chemical calculations using the Jaguar 4.2 calculation program to further verify the accuracy of the mechanism^[20]. Based on the previous mechanism results, what is the effect of different tert-butyl positions in 2, 4-di-tert-butylphenol and 2, 6-di-tert-butylphenol on the reaction mechanism, and what is the essence of tert-butyl promoting the reaction?

To fill the relevant research gaps, in this paper, the microscopic mechanism of the reaction of 2, 4-di-tert-butylphenol and 2, 6-di-tert-butylphenol with CO₂ to form the corresponding salicylic acid was systematically studied at the atomic scale. CO₂ will attack the ortho-position of 2, 4-di-tert-butylphenol and the para-position of 2, 6-di-tert-butylphenol to form a triplet anion. The study found that 2, 4-di-tert-butylphenol is particularly effective in CO₂ conversion, and the lower reaction energy barrier indicates that the reaction can be carried out at a milder temperature and pressure. A para-selective Kolbe-Schmidt reaction form that can be carried out at lower temperatures and pressures is revealed. The accurate determination of the energy barrier of each key point promotes a deeper understanding of the reaction mechanism at the atomic level. Therefore, the reaction substrates involved in this paper maybe provide a more practical and mild alternative to the traditional Kolbe-Schmidt reaction.

In this paper, the microscopic mechanism of the reaction of 2, 4-di-tert-butylphenol O- and 2, 6-di-tert-butylphenol O- with CO₂ was systematically studied. Firstly, the active sites of CO₂ attack were predicted by analyzing the structural differences between the two substrates. The optimal reaction mechanism was determined by the frontier molecular orbital hybridization and differential charge of the substrate and CO₂. Finally, the reaction pathways corresponding to the two substrates were clearly analyzed. The first step is the reaction of carbon dioxide molecules with delocalized phenoxy anions in the oxidation of ionic compounds. The carbon dioxide molecule electrophilically attacks the phenyl carbon in the anion to

form the intermediate OPh-CO₂ complex. In the subsequent steps, an electrophilic carbon atom mainly attacks the ortho and para positions of the benzene ring, resulting in the formation of two new intermediates. The final product salicylic acid is generated by H proton transfer, in which protons are transferred from carbon atoms to oxygen atoms.

2. Computational methods

Density Functional Theory (DFT) calculations were performed using the Gaussian 09 program package^[21]. B3LYP/6-311 + G(d, p) basis set is used due to the effective balance between the computational accuracy and the amount of computation^[22]. All stationary points are either stable structures without imaginary frequencies or transition states with only one. In order to judge the accuracy of the transition state, the intrinsic reaction coordinate (IRC) calculation was carried out to verify the effective correlation between the transition state and the corresponding product^[23].

3. Results and discussion

3.1 Microstructure of the substrate

The basic structural skeletons of 2, 4-di-tert-butylphenol and 2, 6-di-tert-butylphenol are phenol derivatives, the benzene ring is a planar structure, and -OH is directly connected to the aromatic ring. The difference is that the two-C(CH₃)₃ are replaced at different positions (**Fig. S1**). In the structure of 2, 4-tert-butylphenol, there is an obvious spatial repulsion between the ortho-tert-butyl group and the hydroxyl group, which makes the hydroxyl group slightly deviate from the benzene ring plane. The para-tert-butyl group is far away from the hydroxyl group, and the spatial interference of the hydroxyl group is small. Therefore, the steric hindrance of the whole molecule is medium. The two tert-butyl groups in the structure of 2, 6-tert-butylphenol are located at the ortho position of hydroxyl group. Two bulky tert-butyl groups form a “pinch” effect on both sides of the hydroxyl group, and the steric hindrance is very large. The hydroxyl group was severely squeezed, significantly deviated from the benzene ring plane, and the O-H bond pointed away from the aromatic ring. The molecule as a whole is “umbrella” structure, and the hydroxyl group is very tightly protected by two tert-butyl groups.

In actual industrial production, phenol is not used as raw material, but phenol salt solution. Therefore, the structure involved in this paper is phenol O⁻. Compared with 2, 6-di-tert-butylphenol anion (**Fig. 2c**, 121°), the angle of 2,4-di-tert-butylphenol anion is larger (**Fig. 2a**, 124°). This is because the asymmetric steric hindrance of 2, 4-di-tert-butyl leads to the deviation of O from the benzene ring plane, the p-π conjugation is weakened, and the electronic contribution of O to the aromatic ring is more biased towards the induction effect. It is worth noting that the C-O bond length of phenol (**Fig. S1**, 1.4 Å) is longer than the O-bond length of phenol (**Fig. 2**, 1.2 Å), because the O atom in phenol is closer to the sp³ hybridization, and the C-O is more like a single bond. Phenolic oxygen anions are more willing to push electrons to the

ring, O is closer to sp^2 hybridization, p orbital and benzene ring π system overlap better, C-O double bond composition increases, bond order is higher, bond is shorter.

3.2 Determination of CO₂ attack site

The carboxylation of 2, 4-di-tert-butylphenol and 2, 6-di-tert-butylphenol with CO₂ is essentially the orbital interaction between the highest occupied molecular orbital (HOMO) of phenol and the lowest unoccupied molecular orbital (LUMO) of CO₂. This is because the LUMO of phenoxy oxygen anion is located on tert-butyl (**Fig. S2**), the HOMO orbital energy is higher and easier to be excited, it is the “offensive side” that actually participates in the reaction. As shown in Fig. 3a, b, the HOMO of the phenoxy anion exhibits delocalization on adjacent carbon-carbon bonds and oxygen atom. The LUMO of CO₂ is π^* , and delocalized at all atoms, but the contribution of C atom is more prominent, while the HOMO of CO₂ is located on two oxygen atoms (**Fig. S2**). So, it is easier to accept the electron density. The electron transfer from the HOMO of the phenolic oxygen anion to the LUMO of CO₂ leads to the activation of the C = O bond of CO₂, and finally carboxylation occurs at the ortho or para position of the aromatic ring.

In order to further verify the accuracy of the frontier molecular orbital analysis, the differential charge is performed. It can be clearly seen from Fig. 4 that the carbon end of the CO₂ molecule is close to the main structure of 2, 6-di-tert-butylphenol oxygen anion, and a distinct yellow region appears, indicating that the electron is transferred to the CO₂. The area around 2, 6-di-tert-butylphenol oxygen anion is cyan, indicating that it is the electron donor. This charge transfer is the key to the activation of CO₂ and the formation of stable binding with phenol oxygen anion. The nature of the interaction between CO₂ and phenolate adsorbents was revealed.

3.3 Exploration of reaction microscopic mechanism

Figure 5 shows the thermodynamic and kinetic characteristics of 2, 4-di-tert-butylbenzene O⁻ and CO₂. The ordinate represents the energy level relative to the reactant. The abscissa represents the reaction process, from left to right is the reactant→the first intermediate→the transition state→the product. Rea. (reactant) energy is set as the reference point (0 KJ/mol), which is the initial state of the reaction. IM1 represents the first intermediate with an energy 24 KJ/mol lower than the reactant, representing a relatively stable intermediate state. In TS1, the structure of CO₂ changes from linear to curved, and the bond angle changes from 180° to 128°. At this time, the molecule is in an unstable state of old bond breaking and new bond forming. The C atom in CO₂ forms a C-C chemical bond with the C atom at the ortho-position of phenylphenanthrene O⁻, and the bond length is 1.5 Å. At the same time, the C-H bond length is stretched from 1.0 to 1.3 Å. TS1 is the rate-determining step of the reaction, which needs to cross the energy barrier of 176 KJ/mol. It is the highest energy point of the whole reaction and determines the activation energy of the reaction.

In order to ensure the accuracy of the reaction mechanism, the energy evolution process of each elementary chemical reaction from reactant to product is demonstrated. As shown in **Fig. S3**, the abscissa represents the intrinsic reaction path (IRC), which describes the progress of the reaction along the lowest energy path. The ordinate represents the total energy of the whole reaction system, the value is more negative and the system is more stable. The reactant is located at IRC = 1.1, and the energy is about - 810.22 Hartree. The transition state is located at IRC = 0, which is the highest energy point of the whole path, (about - 810.21 Hartree). It is the energy barrier of the reaction and the most difficult step to cross. The product is located at IRC = -1.1, and the energy is about - 810.25 Hartree, which is the lowest and most stable state of the whole system. From the energy trend in the reaction process, it can be seen that the reactants need to absorb energy to reach the transition state, and then release energy to form a more stable product. The results compound scientific laws and prove the accuracy of the mechanism. On the whole, the product energy is lower than the reactant, indicating that this is an exothermic reaction.

Through TS1, H atoms migrate to the O atoms of CO₂, and the **Pro.** (product) is formed. The energy is 81 KJ/mol lower than the reactant, indicating that the whole reaction is exothermic and the product is more stable than the reactant. Therefore, from the thermodynamic point of view, the Kolbe-Schmitt reaction is spontaneous in energy. However, high temperature and high pressure conditions are still needed in actual industrial production. According to the reaction mechanism, the bottleneck of this reaction is the transition state TS1, and its high energy means that the outside world needs to provide enough energy to react. High temperature can provide sufficient kinetic energy to allow the reactant molecules to overcome this high activation energy barrier, and the reaction rate is significantly accelerated. High pressure can increase the concentration of reactants and promote the balance to move in the direction of the generated product. Therefore, exothermic does not mean that the reaction does not need to be heated. The heat release only indicates that the final state of the reaction is lower than the initial state energy, but it does not mean that the reaction can proceed spontaneously and quickly. High temperature is to accelerate the reaction rate, and high pressure is to increase the concentration of CO₂ and promote the equilibrium, both of which ensure the efficiency and yield of industrial production.

Compared with 2, 4-di-tert-butylphenol oxygen anion, the reaction mechanism of 2, 6-di-tert-butylphenol oxygen anion is more complex. As shown in Fig. 6, it is a three-step reaction (reactant → IM1 → TS1 → IM2 → TS2 → product), including two intermediates (IM1, IM2) and two transition states (TS1, TS2). The reaction steps are more and the path is longer. The energy of the ortho-product formed by 2, 4-di-tert-butylphenylphenoxy anion is -81 KJ/mol, which is a strong exothermic reaction, while the energy of the para-product formed by 2, 6-di-tert-butylphenylphenoxy anion is -24 KJ/mol, which is a weak exothermic reaction. The TS1 of 2, 4-di-tert-butylphenol O⁻ is the only high energy bottleneck, while the TS2 of 2, 6-di-tert-butylphenol O⁻ is the highest energy barrier (rate-determining step) of the whole reaction. Similarly, in order to prove the accuracy of the microscopic path, the TS1 (**Fig. S4**) and TS2 (**Fig. S5**) of 2, 6-di-tert-butylphenol oxygen anion were tested by IRC. By comparing the energy of the rate-determining step, it can be seen that under the same reaction conditions, di-tert-butylphenol O⁻ is more likely to produce

para-salicylic acid than ortho-salicylic acid. However, the stability of di-tert-butyl ortho-salicylic acid is very strong.

4. Conclusion

Studies have shown that the Kolbe-Schmidt carboxylation reaction of 2, 4-di-tert-butylphenol includes one discrete transition state and one transient intermediate, while 2, 6-di-tert-butylphenol includes two corresponding transition states and two transient intermediates. The initiation process is that the ortho-position and para-position of benzene are attacked by CO_2 , respectively, and the $\text{PhO}^- \text{-CO}_2$ complex intermediate is formed. In the final step, the intermediate undergoes H proton transfer from its carbon nucleus to the oxygen nucleus and is finally converted to ortho-hydroxybenzoic acid. The process requires a large activation energy, the total reaction rate is limited. Compare the whole reaction mechanism, it can be seen that due to the steric hindrance effect, 2, 4-di-tert-butylphenol O^- is easy to form ortho-products, while 2, 6-di-tert-butylbenzophenone O^- is easy to form para-products. Through this theoretical exploration, the formation pathways of intermediate species involved in the carboxylation of 2, 4-di-tert-butylphenol and 2, 6-di-tert-butylphenol have been further understood. This work provides valuable theoretical guidance for promoting the understanding and optimization of this key industrial process.

Declarations

Ethics approval

Not applicable.

Consent to participate

Not applicable.

Consent for publication

The authors consent for publication.

Conflict of interest

The authors declare no competing interests.

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Author Contribution

MingZe Kou: Writing-original draft, Writing-review & editing. Qiao Li: Writing-original draft, Software. Yongning Yuan: Writing-review & editing, Resources.

Availability of data and materials

Data and material sharing is not applicable to this article as no datasets were generated or analysed during the current study.

Data availability statement

The datasets generated during the current study are available from the corresponding author on reasonable request.

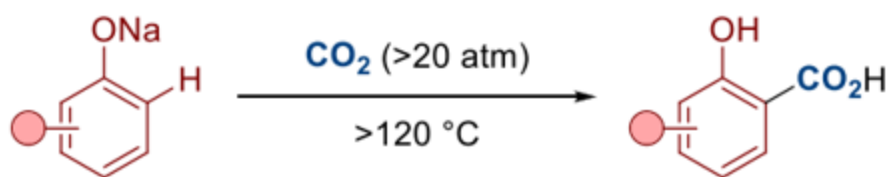
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Figures

a) The Kolbe-Schmitt Reaction



b) Kolbe-Schmitt-type carboxylation at 1 atm

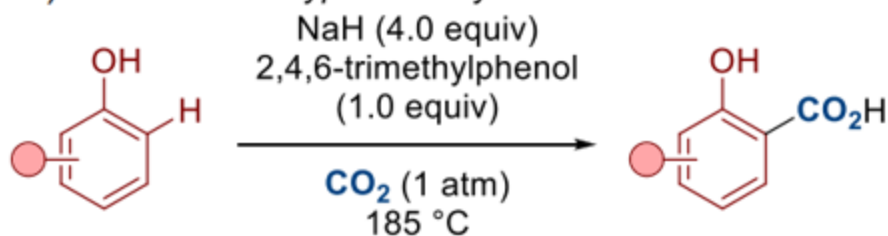


Figure 1

The previous Kolbe-Schmitt-type reactions

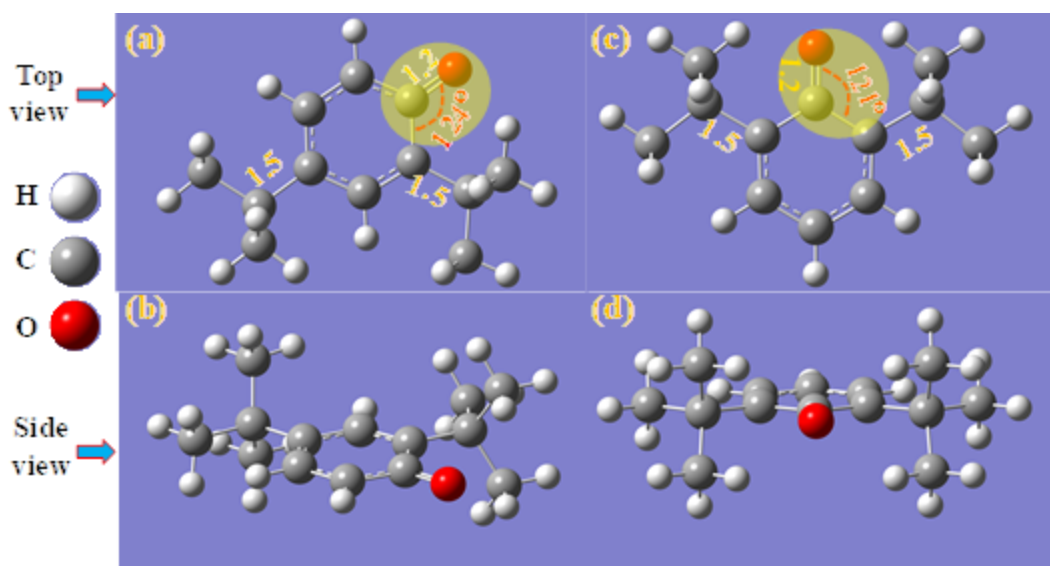


Figure 2

Top view and side view of phenolic oxygen anion. **(a, b)** 2, 4-tert-phenolic oxygen anion; **(c, d)** 2, 6-tert-phenolic oxygen anion (The number represents the chemical bond length, and the unit is Å).

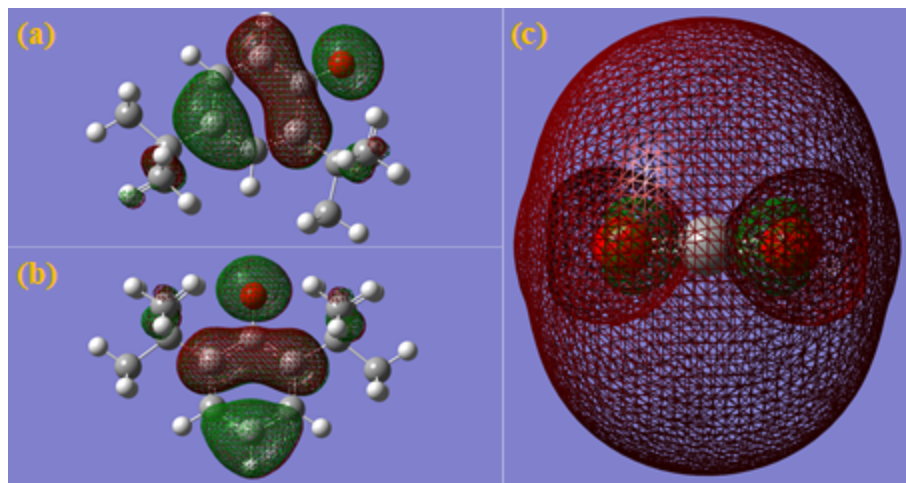


Figure 3

Front molecular orbitals of reactants, red represents the positive phase (+) of the wave function, green represents the negative phase (-) of the wave function. **(a, b)** HOMO of 2, 4-di-tert-butylphenol and 2, 6-di-tert-butylphenol; **(c)** LUMO of CO₂.

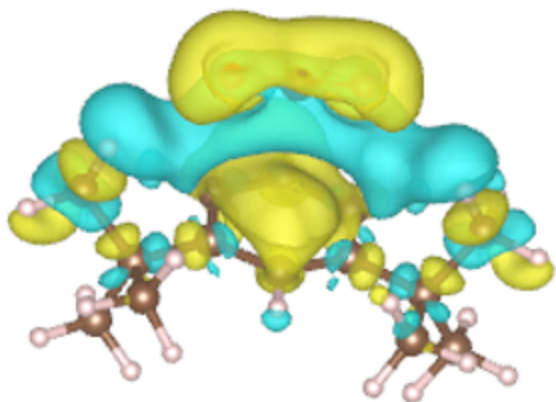


Figure 4

Differential charge of 2, 6-di-tert-butyloxycyanide and CO₂ complex. The yellow area represents charge aggregation, and the cyan area represents charge loss.

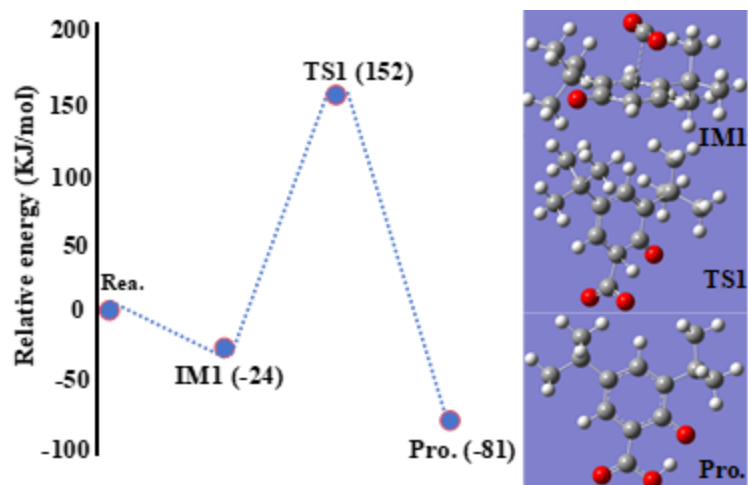


Figure 5

Potential energy diagram for the reaction of 2, 4-di-tert-butylphenol with CO_2 (left) and schematic diagram of key structures in the corresponding reaction pathway (right). IM1 represents the intermediate, and TS1 corresponds to the transition state. **Pro.** represents the final product of the reaction salicylic acid. The number in brackets represents the relative energy value.

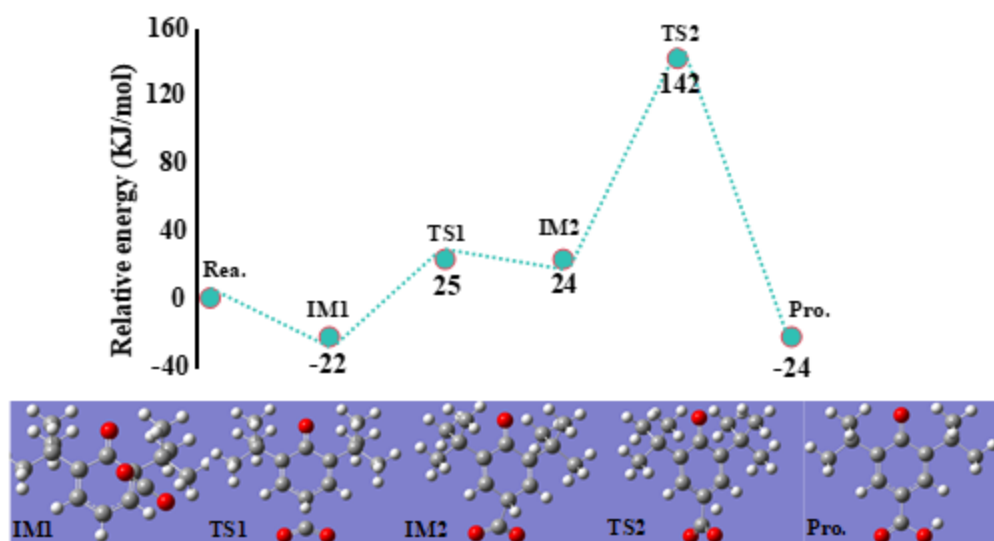


Figure 6

Potential energy diagram for the reaction of 2, 6-di-tert-butylphenol with CO_2 and schematic diagram of key structures in the corresponding reaction pathway.

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