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## Theoretical DFT study of Cannizzaro reaction mechanism: A mini perspective

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## RESEARCH ARTICLE



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## ABSTRACT

In regards to the Cannizzaro reaction and its peculiar mechanism, some researchers have presented a free radical mechanism for the Cannizzaro reaction, while others have found that it is feasible through an ionic mechanism, but the actual mechanism has not been finalized yet. The researchers have given the proof of both the mechanisms through their papers published. Actually, Cannizzaro reaction may occur through both mechanisms depending on both molecular structure and different conditions which are yet to be explained. Recently published papers describe that free radical mechanism occurs only in a heterogeneous medium, while an ionic mechanism occurs in a homogeneous medium. We revealed no explanation of the molecular structure-based reason, responsible for a radical or an ionic mechanism. The present paper reviews not only homogeneous/heterogeneous medium conditions but also molecular structure-based facts, which may be responsible for the Cannizzaro reaction to occur through the radical or ionic mechanism, and that may be acceptable to the scientific society. Besides, Density Functional Theory study using Gaussian software was also involved in the explanation of the molecular structure, responsible for one of the two mechanisms. Also, the present paper specifies all points related to future perspectives on which additional studies are required to understand the actual mechanism with a definite molecular structure in the different reaction media.

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## 1. Introduction

It is well understood that the disproportionation of an aldehyde to a primary alcohol and the respective carboxylic salt is involved in the Cannizzaro reaction. Another well-understood point is that this reaction occurs only in those aldehydes which do not have  $\alpha$ -hydrogen [1] such as aromatic aldehyde. In aromatic aldehydes, this reaction occurs [2] as follows:



For a long time, scientists have been curious about the actual mechanism of Cannizzaro reaction because there are a variety of mechanisms given for Cannizzaro reaction to occur [2]. Many attempts have been made to the novel kind of the reaction in the past years using microwave irradiation [3], ultrasound mediation [4], cation templates [5], solid-supported reagents [6], solvent-free conditions [7], crossed Cannizzaro version of the reaction [8], gas-phase process [9] and photo induction [10].

## 1.1. The rate law for Cannizzaro reaction

Kinetics is an important aspect of any reaction; especially for organic reactions [11-15]. The kinetics give us important data about the reaction. Although this reaction also occurs in aliphatic aldehydes having no  $\alpha$ -hydrogen, still aromatic aldehydes are the best option to study the kinetics of the Cannizzaro reaction [16]. The reaction is usually brought about in a homogeneous medium having a strongly basic solution or in a heterogeneous system consisting of the benzaldehyde phase having a strongly basic aqueous phase [2]. The reported conditions under which kinetics of Cannizzaro reaction is studied are 0.60 M benzaldehyde and 0.25 M NaOH in 74%  $\text{CH}_3\text{OH}$ -26% water at 100 °C. Under these conditions, the reactants exist predominantly as free benzaldehyde (not as hydrate or hemiacetal),  $\text{Na}^+$  and  $\text{OH}^-$ . Under these conditions, the reaction is second order with respect to benzaldehyde, and first order with respect to the base. The principal products are benzyl alcohol and benzoate ion. Hence, the reaction rate may be represented by the following equation [17].

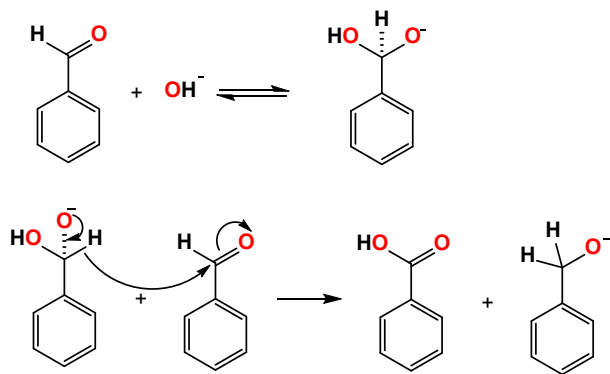


Figure 1. An ionic mechanism for Cannizzaro reaction.

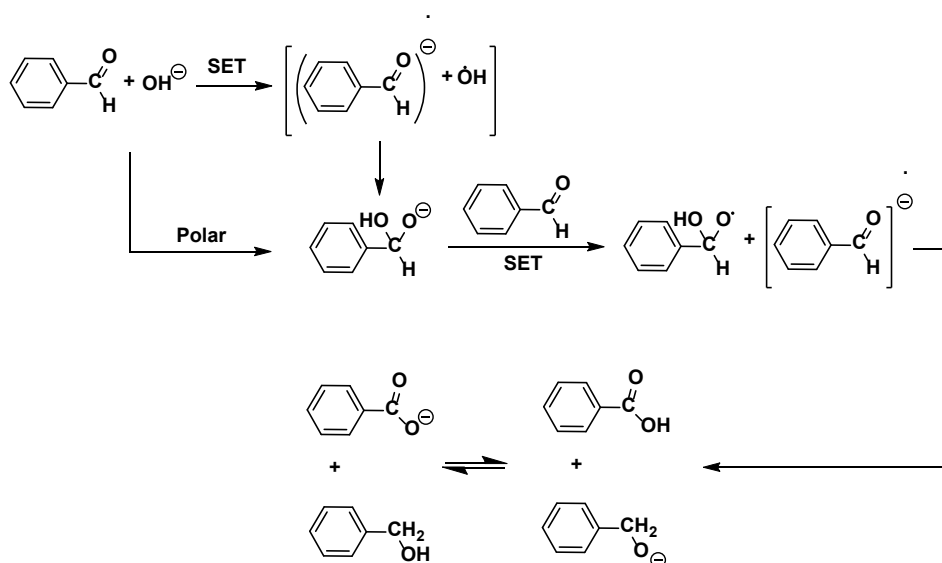


Figure 2. Single-electron transfer (SET) mechanism for Cannizzaro reaction.

$$\text{Rate} = k \times [\text{PhCHO}]^2 \times [\text{OH}^-] \quad (2)$$

Another interesting point is that the order of reaction varies in case of furfural and formaldehyde, from first to second in the base, hence third to fourth overall depending on the conditions; sodium *m*-formyl-benzenesulfonate also gives a fourth-order reaction,  $K_4 \times [\text{RCHO}]^2 \times [\text{Base}]^2$ , under certain conditions [2]. Therefore, the results obtained were fascinating in different conditions.

### 1.2. Mechanisms for Cannizzaro reaction

Many observers [17-23] have demonstrated that this reaction occurs through the ionic mechanism (Figure 1). According to an ionic mechanism, the addition of  $\text{OH}^-$  ion to benzaldehyde yields a tetrahedral adduct which then undergoes nucleophilic addition with a second molecule of benzaldehyde. Hydroxyl transfer following hydride migration within this intermediate initiate disproportionation to form benzyl alcohol and benzoate ion. Before this proposal, the first mechanistic proposal for this reaction was also given [2] but the first mechanistic proposal was proven wrong [8] experimentally. The isolation of benzyl benzoate as a minor product added credence to this proposal [8]. It is now considered that the mechanism of the Cannizzaro reaction occurs through an ionic mechanism shown in Figure 1.

On the other hand, some researchers have proposed a radical mechanism or Single Electron Transfer (SET)

mechanism (Figure 2) for Cannizzaro reaction with an experimental proof [16,19-29].

Now, the most interesting point is that both the mechanisms ionic and SET have their evidences to be true which are as follows:

#### 1.2.1. Evidence supporting the ionic mechanism

Before the SET mechanism, radical chain mechanisms were also suggested, but have been discounted on the basis that neither radical initiators (such as benzoyl or sodium peroxide) nor inhibitors (such as hydroquinone or diphenyl amine) have a decisive effect on the rate of reaction [18,19]. Besides, a radical chain mechanism with all evidences is excluded under homogeneous conditions consisting of benzaldehyde (0.495 M) and sodium hydroxide (0.250 M) at 100 °C in 74% (vol.) aqueous methanol [19].

#### 1.2.2. Evidence supporting SET mechanism

The main evidence supporting the radical mechanism for the Cannizzaro reaction is EPR signals (Table 1) obtained from chemical species taken for this reaction [16]. On the basis of the EPR spectroscopic study, an electron-transfer pathway (Figure 2) was suggested for the Cannizzaro reaction [16]. Radical species were detected [25-28] by EPR spectroscopy in the Cannizzaro reaction involving various substituted benzaldehydes with NaOH in THF/HMPA (9:1, v:v).

**Table 1.** EPR signals in benzaldehyde and substituted benzaldehyde [25].

Compounds	EPR signal
<i>para</i> -Chlorobenzaldehyde	Observed
<i>para</i> -Trifluoromethylbenzaldehyde	Observed
<i>para</i> -Cyanobenzaldehyde	Observed
Benzaldehyde	Uncertain
<i>para</i> -Nitrobenzaldehyde	Observed
<i>ortho</i> -Methyl benzaldehyde	Uncertain
2,4,6-Trimethylbenzaldehyde	No signal

Besides, the spectra obtained were identical to the spectra produced from the reaction of sodium metal with each respective aldehyde in the same solvent system [30]. Further, the same pieces of evidence were obtained [16] again for the existence of paramagnetic species during the Cannizzaro reaction by ESR spectroscopic examination when benzaldehyde and several substituted benzaldehydes were allowed to react with NaOH in THF/HMPA (9:1, v:v), and the resulting heterogeneous mixtures were studied by ESR spectroscopy. The results obtained during the Cannizzaro reaction are shown in Table 1.

Moreover, the same results in favor of radical mechanism were obtained [27] during the observation and characterization of radical transients for a variety of N-heterocyclic carbenes and aldehydes in the benzoin condensation reaction. In that reaction, *para*-substituted benzoate obtained from aromatic aldehyde was Cannizzaro adduct. He also recorded the EPR spectrum of a solution of *p*-nitrobenzaldehyde.

### 1.3. Conditions for the radical and ionic mechanism

After exhaustive literature survey of papers supporting the radical mechanism as well as an ionic mechanism for Cannizzaro reaction, we focused on the conditions encouraging radical mechanism and also on those conditions which are responsible for an ionic mechanism. Finally, we have found that an ionic mechanism takes place in a homogeneous medium [19], and the radical mechanism in the heterogeneous medium [16]. Also, we have noted that the role of the molecular structure was nullified for Cannizzaro reaction to occur through the radical mechanism or an ionic mechanism. Actually, the molecular structure also plays an important role for both mechanisms. The medium and molecular structure-based conditions, responsible for both mechanisms are as follows:

#### 1.3.1. Conditions for the radical mechanism

As we have described that there are many pieces of evidence in support of radical mechanism for Cannizzaro reaction, but it has been excluded in the case of homogeneous medium i.e., the radical mechanism is possible only through the heterogeneous medium. Another point which we noticed in the radical mechanism supporting papers is that the ESR spectra were well resolved only when electron-withdrawing groups (EWGs) such as *p*-chloro-, *p*-trifluoromethyl-, and *p*-cyanobenzaldehyde were attached to aromatic aldehyde. On the other hand, the ESR spectrum was not observed in the absence of the electron-withdrawing group. Hence, radical mechanism depends not only on the reaction medium but also on the groups attached to aromatic aldehyde. It can be considered that through the inductive (-I) effect, the electron-withdrawing group withdraws electrons from the benzene ring and prevents the electron shift occurring through electrometric effect from benzene to the aldehyde group. Therefore, the radical formation may occur due to the presence of an electron-withdrawing group attached to aromatic aldehyde. EPR signals were observed only in the presence of those electron-withdrawing groups whose

inductive effect is greater than that of hydrogen as shown in relative inductive effects measured experimentally with reference to hydrogen:  $-\text{NH}_3^+ > -\text{NO}_2 > -\text{SO}_2\text{R} > -\text{CN} > -\text{SO}_3\text{H} > -\text{CHO} > -\text{CO}- > -\text{COOH} > -\text{COCl} > -\text{CONH}_2 > -\text{F} > -\text{Cl} > -\text{Br} > -\text{I} > -\text{OH} > -\text{OR} > -\text{NH}_2 > -\text{C}_6\text{H}_5 > -\text{CH}=\text{CH}_2 > -\text{H}$ .

The above order clearly shows that all groups which were present at the *para* position of benzaldehyde in the experiment [25] have greater -I effect with respect to hydrogen and caused radical formation. On the other hand, it can also be seen that the methyl group has a lesser -I effect than that of hydrogen that is why no EPR signal was observed when methyl group was present at the *ortho* position in benzaldehyde in the experiment performed [25]. Hence, an electron-donating nature of groups attached to benzaldehyde did not cause radical formation i.e., no EPR signal. Besides, the free radical formation may occur due to the reagents taken for this reaction to provide heterogeneous conditions.

#### 1.3.2. Conditions for the ionic mechanism

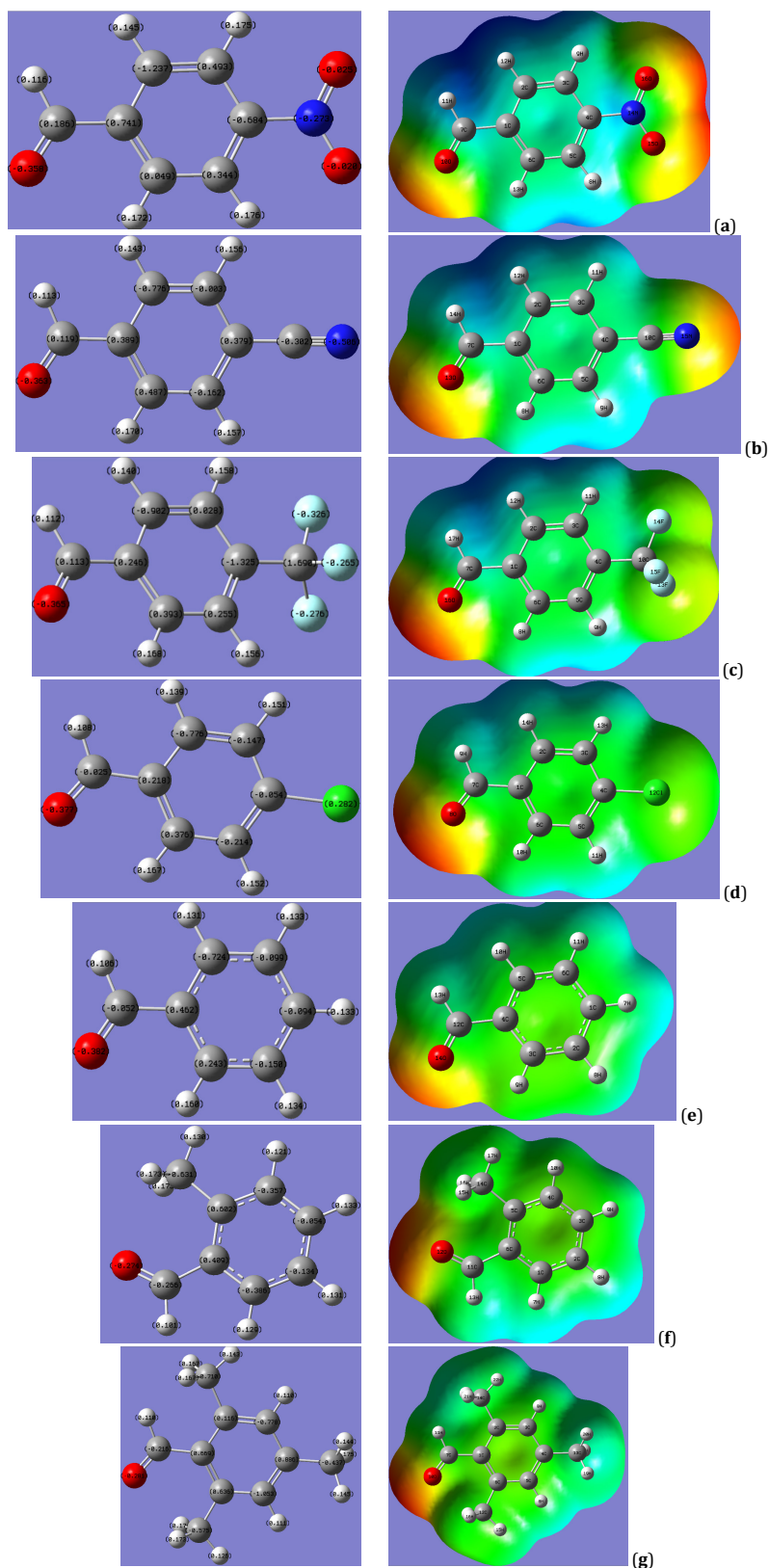
Cannizzaro reaction may occur through ionic mechanism but only in a homogeneous medium [18] as it has been shown [31] that the yield of the reaction product is lowered considerably or sometimes the reaction doesn't occur or even inhibited completely by employing peroxide-free aldehyde. The purpose of this experiment was to study the Cannizzaro reaction with benzaldehyde in a homogeneous medium under peroxide-free conditions and in the presence of added peroxides or peroxide inhibitors.

## 2. The density functional theory studies

The simulation study is also very helpful in understanding the reaction mechanism and organic synthesis [32-41]. In the present work, the Milliken atomic charge in coulomb's acquired by an oxygen atom in different chemical species taken for the Cannizzaro reaction [25] was calculated by DFT method in the ground state by using the Gaussian(R) 03 program [42]. The basis set used was 6-311+G(d,p) using Becke's three parameter hybrid functionals [43] with Lee, Yang, and Parr correlation functional methods (B3LYP) [44]. The interpretation in this study clearly explained the results mentioned in Table 1. The calculated results were visualized by means of GaussView 6.0 [45].

## 3. Results

Results obtained after optimization showed, an electron-withdrawing group (EWG) decreased the charge on an aldehydic oxygen atom while an electron-donating group (EDG) increased the charge on an aldehydic oxygen atom. We know that the tendency of an electronegative element to attract electron pair towards itself, depends on the charge acquired by itself. Theoretical results clearly showed that all the groups/elements present in *para*-nitrobenzaldehyde, *para*-cyanobenzaldehyde, *para*-trifluoromethyl benzaldehyde and *para*-chlorobenzaldehyde (Figure 3a-d) having more inductive effect (-I) with respect to hydrogen, reduced the charge on an oxygen atom which caused radical formation.



**Figure 3.** Gaussian calculation results for charge acquired by an oxygen atom of benzaldehyde with different groups at para position (a) -NO<sub>2</sub>, (b) -CN (c) -CF<sub>3</sub>, (d) -Cl, (e) Hydrogen atom, (f) -CH<sub>3</sub> at ortho and (g) -CH<sub>3</sub> at 2,4,6-positions.

Due to this reason, EPR signals were observed in the Cannizzaro reaction. On the other hand, all such groups/elements present in *ortho*-methylbenzaldehyde and 2,4,6-trimethylbenzaldehyde (Figures 3f and 3g) which have less

inductive effect (-I) with respect to hydrogen, increased the charge on an oxygen atom which caused ionic formation. Due to this reason, EPR signals were not observed in the Cannizzaro reaction.

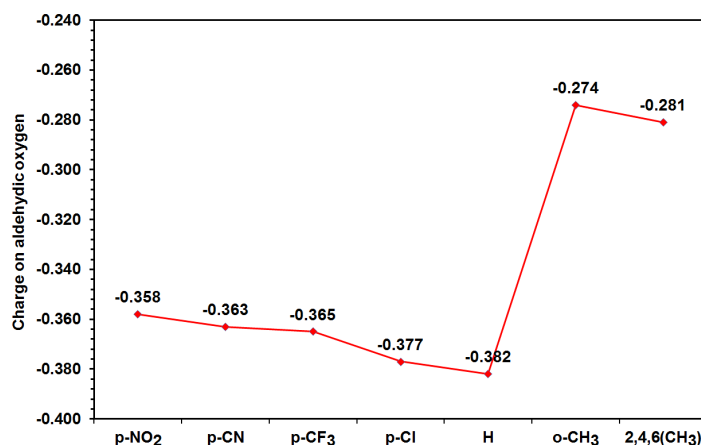


Figure 4. Charge variation on the oxygen atom of benzaldehyde with different groups attached.

Besides, EPR signals were uncertain in benzaldehyde and *ortho*-methylbenzaldehyde as shown in Table 1. It was also explained on the basis of theoretical data. Figures 3e and 3f clearly showed that delocalization of electron around the benzene ring was not disturbed by the presence of group/element attached to benzaldehyde and *ortho*-methylbenzaldehyde. It means that the delocalized electrons were not involved in the radical formation that is why EPR signal was uncertain. Hence, optimization results were also in support of both mechanisms depending on the nature of groups attached to aromatic aldehyde. Therefore, it can be concluded that the nature of groups attached to aromatic aldehyde directly affects the charge on an oxygen atom as well as reaction mechanism. The outstanding point after the whole calculation of charge on an aldehydic oxygen atom was that an oxygen atom should have more negative charge in Figure 3g because of the presence of three electron-donating groups attached to aromatic aldehyde but the theoretical results were just opposite of it. It was because of the steric inhibition [46-49] whose intervention disturbs the inductive effect of an individual group whether it is an electron-withdrawing group or an electron-donating group.

#### 4. Future perspective

Having read research papers regarding the mechanism of Cannizzaro reaction, we observed many interesting points which we explained on the basis of theoretical data. Another most interesting point which this review shows is that free radical formation depends upon not only heat or light but also on molecular structure, reagent or reaction conditions because this reaction was carried out in dark [25] at room temperature [50], and EPR signals were observed indicating chemical species with free radical. Hence, the factor for free radical formation in that reaction is the point that needs to be addressed. Either it was molecular structure or reagent or reaction medium. Also, we observed some other complicated points which need more efforts on the mechanism of this reaction. For instance, what would be the mechanism if:

- Benzaldehyde substituted at para position with EWG is taken in the homogeneous medium for Cannizzaro reaction because this chemical species is not taken for Cannizzaro reaction in the homogeneous medium yet.
- Benzaldehyde substituted at *meta* position with either EWG or EDG is taken in the homogeneous medium for Cannizzaro reaction.
- Benzaldehyde substituted at *meta* position with either EWG or EDG is taken in the heterogeneous medium for Cannizzaro reaction because this chemical species is not

taken for Cannizzaro reaction in the heterogeneous medium yet.

- Besides, it will also be very intriguing to note that EPR signals would be observed or not from such species during the reaction.

#### 5. Conclusion

Based on the discussions, we can conclude that the Cannizzaro reaction mechanism depends on the reaction medium (homogeneous or heterogeneous) as well as the nature of the group i.e. electron-withdrawing or donating attached to the aromatic aldehyde. For the ionic mechanism, the medium should be homogeneous while in the case of radical mechanism, the medium should be heterogeneous, and the group attached to aromatic aldehyde should be electron-withdrawing. Therefore, the mechanism of the Cannizzaro reaction may take place through both ionic as well as the radical mechanism that depends on the reaction medium as well as the nature of the group attached to aromatic aldehyde. Besides, another point to be kept in mind is that the radical mechanism may produce many by-products because of the combination of radical species with itself or another radical species present in the reaction mixture. Hence, this fact may be considered as a disadvantage of a radical mechanism. On the other hand, it does not occur in an ionic mechanism. Finally, the curtain on the mechanism of this reaction needs to be removed completely as soon as possible by considering the interesting points mentioned in the future perspective.

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#### Disclosure statement

Conflict of interests: The authors declare that they have no conflict of interest.

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Ethical approval: All ethical guidelines have been adhered.

Sample availability: Samples of the compounds are available from the author.

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