

JANUARY

2026 V 1.0

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# CHEMICAL SCIENCE RESEARCH PAPER EDITING SAMPLE

*Prepared By – ResearchEdit4u Solutions*

*(Includes language, grammar, and punctuation extensive editing in American English)*

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## ABSTRACT

This study uses the used DFT method to investigate the investigation of optimized structure, electronic structures, charge analysis, FT-IR, FT-Raman spectroscopic analysis, and thermodynamic properties. The optimized energy and dipole moment are were - 9531.775 eV and 0.3818 Debye, respectively. The bond lengths of Cl-C2 and Cl-H7 molecules inside the benzene ring are observed to be were 1.39 Å and 1.08 Å, respectively. The bond angle angles of Cl-C2-C3 and C2-Cl-C6 are found to be were 120.10 Å and 119.36 Å, respectively. The HOMO-LUMO energy gap is 6.331 eV, which corresponds very close to the 6.321 eV energy gap of 6.321 eV obtained from the density of states. The global parameters with ionization energy value 6.747 eV, electron affinity with of 0.4152 eV, chemical potential of with -3.5811 eV, electronegativity with of 3.5811 eV, global hardness with of 3.1659 eV, softness with of 0.3148 ev<sup>-1</sup>, and electrophilicity index with of 2.0253 eV are were obtained. The Mulliken charges/charge analysis indicate indicated that most of the carbon atoms, except C4 and C12 – are found to carry, carried negative charges where, whereas all of the H-atoms are were found having to have positive charge/charges. The molecular electrostatic potential, electrostatic potential, and electron density identify different electrophilic and nucleophilic regions and its their reactive natures. The FT-IR spectroscopy shows strong C-H vibrations at 3186-3093 cm<sup>-1</sup>, methyl group vibration at 3091-3078 cm<sup>-1</sup> and the ring vibrations at 1641-1482 cm<sup>-1</sup>. The heat capacity at constant

volume and ~~at~~-constant pressure, internal energy, enthalpy, and entropy increase with increasing temperature. However, Gibb'sGibbs free energy shows the opposite nature, providing very important insights according to into the change in temperature.

*Keywords:* density functional theory, density of state, molecular electrostatic potential, IR-spectroscopy, thermodynamic properties

## INTRODUCTION **EXCERPT**

Various studies, research and report have been made till date regarding the study of Cumene molecule. In 2015, Sivarajani et al., did an investigation on Cumene obtaining FT-IR, FT-Raman, NMR and UV spectra through various spectroscopic techniques. Researchers in 2006 reported the process of Cumenecumene formation through benzene alkylation with propylene on thea new three-dimensional catalyst (Jansang et al., 2006). Al-Khattaf & de Lasa (2001) foundstudied the processof catalytic cracking of Cumenecumene. Petroselli and colleagueset al. (2017) proposed a report wherein which a new class oflipophilicof lipophilic N-hydroxyphthalimides catalysts, designed for the aromatic oxidation of Cumeneincumene under solvent-free conditions, were synthesized and tested. Luyben studied the chemical process to form Cumenecumene with the interaction of benzene and propylene and again with the repellent of Cumenecumene with propylene to shape the formation of p-diisopropylbenzene (Luyben, 2010). In 2016, the researchof chemical kinetics onof the thermal decomposition of Cumenecumene hydroperoxide in Cumenecumene by calorimetry waswere studied where, and the compound was noted to have a catalytic product reaction (Duh, 2016). EventhoughAlthough the literature review reveals different research regarding the atoms, electrons, and overall molecular structure of Cumenecumene, it can be observed that no research foron the molecular structure, electronic structure, spectroscopic analysis, and thermodynamic properties havehas been performed using the B3LYP/6-311++G(d,p) basis set. SoTherefore, our objectives are to investigate the optimization energy and its steps, bond length, bond angle, dihedral angle, highest occupied molecular orbitals and lowest unoccupied molecular

orbital orbitals (HOMO-LUMO), density of states (DOS), global reactivity parameters, Mulliken charges, molecular electrostatic potential (MEP), electrostatic potential (ESP), electron density (ED), vibrational behaviourbehavior, and thermodynamic parameters of Cumenecumene using the B3LYP/6-311++G(d,p) basis set, filling the research gap identified in the literature review regarding the calculation and analysis of these properties.

## DISCUSSION ~~EXCERPT~~

### *Thermodynamic Parameters Analysis*

The thermodynamic properties are analysedwere analyzed using the thermodynamic parameters\_ and notable thermodynamic changes are seenwere observed in itsthe structure as per the change in with temperature. The Gaussian DFT B3LYP/6-311++G(d, p) basis set\_ following the Moltran software\_ was used to calculate the thermodynamic properties. Figure 9(a) representsshows the correlation graphs of the heat capacity at constant volume (C<sub>v</sub>) and heat capacity at constant pressure (C<sub>p</sub>) with respect to the temperature range inof 50 K—500 K. It shows that the C<sub>v</sub> and C<sub>p</sub> increase alongwith the increase inincreasing temperature. Figure 9(b) represents the graphs of internal energy (U) and enthalpy (H) with respect to temperature in the range of 50 K—500 K. This Figure shows that U and H also increase alongwith the increase inincreasing temperature starting from 50K50 K. Figure 9(c) representsshows the graphs of entropy (S) and Gibb'sGibbs free energy (G) with respect to temperature within the range of 50 K—500 K. In this Figure, S also increases with increase inincreasing temperature. However, the G decreases relentlessly as it depends upon Sand Hof the system that shows the amount of useful work with respect to temperature where its maximum value was recorded at 50 K with the value of 481.445 kJ/mol and minimum at the maximum temperature 500 K with the value of 307.166 kJ/mol. The correlation plot of G and S shows that the two lines intersect at a certain point, which verifies the relationrelationship between Sand G. Furthermore, the change ofand H and S representindicates that these parameters changingdependchange depending on the temperature dueowing to which these parameters change their thermodynamic system onin their own ways (Gauli et al., 2023; Seshadri & Mp, 2018).

## WHY THE CHANGES WERE MADE AND WHERE THEY?

Excerpt	Error type	Original (before) example	RE4U fix (after) – example	Why this matters (Chemical Sciences / journal style)
<b>Abstract</b>	Redundancy + incorrect infinitive	“uses the used DFT method for to investigate the investigation of...”	“used the DFT method to investigate ...”	Removes repeated meaning and fixes grammar; abstracts must be concise and professionally phrased.
<b>Abstract</b>	Tense consistency (scientific reporting)	“This study uses...” (present) while results are reported later	Shifted to past: “This study used...”	Computational work is completed work, so journals typically prefer past tense for methods/results.
<b>Abstract</b>	Broken sentence/word fusion	“are were...”, “eVandeV...”	Clean separation: “were ... eV and ... Debye”	Eliminates “track- change collision” errors that damage readability and reviewer trust.
<b>Abstract</b>	Unit/notation duplication	“1.39 Å and 1.08 Å”	“1.39 Å and 1.08 Å”	Unit duplication looks careless; bond lengths must use Å once (or pm) consistently.

<b>Abstract</b>	Wrong symbol for angles	“angleangles... 120.10 Å° ...”	“bond angles ... 120.10 ° ...”	Angles are measured in degrees (°), not Å; this is a technical credibility fix.
<b>Abstract</b>	Subject–verb agreement	“which corresponds very close...”	“which corresponds closely...”	Grammar accuracy is a basic gatekeeper for peer review; improves fluency and tone.
<b>Abstract</b>	Preposition errors (quantitative parameters)	“global parameters withof 0.4152 eV...”	“global parameters with 0.4152 eV...”	Prevents awkward phrasing around numbers; helps keep the sentence scientifically readable.
<b>Abstract</b>	Duplicate terms	“Mulliken chargescharge analysis”; “indicateindicated that...”	“Mulliken charge analysis indicated that...”	Removes duplication and ensures the correct scientific noun form (“charge analysis”).
<b>Abstract</b>	Faulty parallel structure	“carbon atoms... are found to carry, carried negative charges— where, whereas ...”	“carbon atoms... were found to carry negative charges, whereas ...”	Ensures clean contrast logic; reviewers expect tight, parallel scientific statements.
<b>Abstract</b>	Incorrect verb pattern	“H-atoms... were found having to have positive...”	“H atoms were found to have positive...”	Fixes unnatural verb construction; improves clarity of charge-distribution claims.

<b>Abstract</b>	Pronoun mismatch	“regions regions and its their reactive natures”	“regions and their reactive nature(s)”	Removes ambiguity (what “its” refers to) and aligns with formal scientific English.
<b>Abstract</b>	Technical term formatting	“Gibb’s Gibbs free energy”	“Gibbs free energy”	Correct naming is important; “Gibbs” is standard (no apostrophe) in most chemistry writing.
<b>Abstract</b>	Word choice / logic connector	“insights according to into the change...”	“insights into the change...”	Eliminates incorrect phrase blending; improves logical flow in the final abstract sentence.
<b>Introduction</b>	Duplicate chemical name	“process of Cumene cumene formation ...”	“process of cumene formation ...”	Chemical names should not be duplicated; also common names are usually lowercase mid-sentence.
<b>Introduction</b>	Article/preposition error	“propylene on the a new three-dimensional catalyst...”	“... on a new three-dimensional catalyst...”	Fixes basic grammar and prevents “non-native” tone that reviewers often flag.
<b>Introduction</b>	Merged verbs / unclear action	“Al-Khattaf... found studied the process...”	“Al-Khattaf... studied/investigated the process...”	Clarifies the research action; correct verb choice strengthens literature narration.

<b>Introduction</b>	Faulty relative clause	“proposed a report wherein in which ...”	“reported/proposed that ...” or “in which ...” (single form)	Avoids duplicated structures; improves scholarly style in literature review sections.
<b>Introduction</b>	Repeated descriptor	“class of lipophilic of lipophilic ... catalysts”	“class of lipophilic catalysts”	Removes duplication; keeps technical descriptors precise and readable.
<b>Introduction</b>	Connector logic	“Even though Although the literature review reveals...”	“Although ...” (or “Even though...”, one only)	Prevents double-connector errors; improves argumentative clarity of the research gap.
<b>Introduction</b>	Research-gap sentence grammar	“no research for on ... have has been performed”	“no research on ... has been performed”	Research gap must be unmistakable; correct grammar increases persuasiveness and credibility.
<b>Introduction</b>	Objective statement clarity	“So Therefore, our objectives are...”	“Therefore, our objectives are...”	Removes duplicated transition and makes the study aim sound authoritative.
<b>Introduction</b>	Terminology consistency	“orbital orbitals (HOMO-LUMO)”	“molecular orbitals (HOMO-LUMO)”	Ensures correct pluralization and standard typography (often an en dash HOMO–LUMO).
<b>Discussion</b>	Tense + US/UK consistency	“properties are analysed ...”	“properties were analyzed ...”	Results/discussion typically use

				past tense; consistent spelling (analyzed/analyse d) avoids editorial inconsistency.
<b>Discussion</b>	Wordiness + wrong phrasing	“observed... as per the change in with temperature”	“observed... with temperature”	“As per” is non-standard in journals; tightened phrasing improves professional tone.
<b>Discussion</b>	Figure callout verb	“Figure 9(a) represents shows ...”	“Figure 9(a) shows ...”	Removes redundancy; figure descriptions should be direct and precise.
<b>Discussion</b>	Range formatting + prepositions	“range inof 50 K—500 K”	“range of 50–500 K”	Correct range style is expected (often en dash); improves technical presentation.
<b>Discussion</b>	Repetition in trend description	“increase along with the increase increasing temperature”	“increase with increasing temperature”	Standard scientific phrasing; avoids repetitive, awkward constructions.
<b>Discussion</b>	Spacing/units	“from 50K50 K”	“from 50 K”	Correct SI spacing (number + space + unit) is a common journal requirement.
<b>Discussion</b>	Duplicate/garbled phrasing	“verifies the relate relationship...”	“verifies the relationship ...”	Removes duplication and restores meaning;

				essential for interpreting thermodynamic correlations.
<b>Discussion</b>	Grammar in cause–effect	“parameters changing dependchange depending on...”	“parameters change depending on...”	Fixes sentence structure so the temperature-dependence claim is scientifically interpretable.

# THANK YOU

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