

JANUARY

2026 V 1.0

CHEMICAL SCIENCE

PAPER EDITING

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CHEMICAL SCIENCE RESEARCH PAPER EDITING SAMPLE

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

ABSTRACT

This study ~~uses the~~used DFT ~~method for 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 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 ° and 119.36 °, ~~respectively~~. The HOMO-LUMO energy gap is 6.331 eV, which ~~corresponds is~~ 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⁻¹, 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 ~~region regions~~ and ~~its their~~ reactive natures. ~~The~~ FT-IR spectroscopy shows strong C-H vibrations at 3186-3093 cm⁻¹, methyl group vibration at 3091-3078 cm⁻¹ and ~~the~~ ring vibrations at 1641-1482 cm⁻¹. The heat capacity at constant

volume and ~~at~~ constant pressure, internal energy, enthalpy, ~~and~~ entropy increase with increasing temperature. However, ~~Gibb's~~Gibbs 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, Sivaranjani 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 ~~Cumene~~cumene formation through benzene alkylation with propylene on ~~the~~a new three-dimensional catalyst (Jansang et al., 2006). Al-Khattaf & de Lasa (2001) ~~found~~studied the ~~process of~~catalytic cracking of ~~Cumene~~cumene. Petroselli ~~and colleagues~~et al. (2017) proposed a report ~~wherein which~~ a new class ~~of lipophilic~~of lipophilic N-hydroxyphthalimides catalysts, designed for the aromatic oxidation of ~~Cumene in~~cumene under solvent-free conditions, were synthesized and tested. Luyben studied the chemical process to form ~~Cumene~~cumene with the interaction of benzene and propylene and again with the repellent of ~~Cumene~~cumene with propylene to shape the formation of p-diisopropylbenzene (Luyben, 2010). In 2016, the ~~research of~~chemical kinetics ~~on of the~~ thermal decomposition of ~~Cumene~~cumene hydroperoxide in ~~Cumene~~cumene by calorimetry ~~was were~~ studied ~~where, and~~ the compound was noted to have a catalytic product reaction (Duh, 2016). ~~Even though~~Although the literature review reveals different research regarding the atoms, electrons, and overall molecular structure of ~~Cumene~~cumene, it can be observed that no research ~~for on the~~ molecular structure, electronic structure, spectroscopic analysis, and thermodynamic properties ~~have has~~ been performed using the B3LYP/6-311++G(d,p) basis set. ~~So~~Therefore, 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 ~~behaviour~~behavior, 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 analysed~~were analyzed using the thermodynamic parameters, and notable thermodynamic changes ~~are seen~~were observed in ~~its~~the 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) ~~represents~~shows the correlation graphs of ~~the~~heat capacity at constant volume (Cv) and heat capacity at constant pressure (Cp) with respect to ~~the~~temperature range ~~in of~~ 50 K—500 K. It shows that ~~the~~Cv and Cp increase ~~along with the increase in increasing~~ 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 ~~along with the increase in increasing~~ temperature starting from ~~50 K~~50 K. Figure 9(c) ~~represents~~shows the graphs of entropy (S) and ~~Gibb's~~Gibbs free energy (G) with respect to temperature ~~within~~ the range of 50 K—500 K. In this Figure, S also increases with ~~increase in increasing~~ 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 ~~relation~~relationship between Sand G. Furthermore, the change ~~of Hand in H and~~ S ~~represent~~indicates that these parameters ~~changing depend~~change depending on the temperature ~~due, owing~~ to which these parameters change their thermodynamic system ~~on in~~ 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)
Abstract	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.
Abstract	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.
Abstract	Broken sentence/word fusion	“arewere...”, “eVandeV...”	Clean separation: “were ... eV and ... Debye”	Eliminates “track-change collision” errors that damage readability and reviewer trust.
Abstract	Unit/notation duplication	“1.39 ÅÅ and 1.08 ÅÅ”	“1.39 Å and 1.08 Å”	Unit duplication looks careless; bond lengths must use Å once (or pm) consistently.

Abstract	Wrong symbol for angles	unit for “angleangles... 120.10 Å° ...”	“bond angles ... 120.10 ° ...”	Angles are measured in degrees (°), not Å; this is a technical credibility fix.
Abstract	Subject–verb agreement	“which corresponds very close...”	“which corresponds closely...”	Grammar accuracy is a basic gatekeeper for peer review; improves fluency and tone.
Abstract	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.
Abstract	Duplicate terms	“Mulliken chargescharge analysis”; “indicateindicat ed that...”	“Mulliken charge analysis indicated that...”	Removes duplication and ensures the correct scientific noun form (“charge analysis”).
Abstract	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.
Abstract	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.

Abstract	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.
Abstract	Technical term formatting	“Gibb’sGibbs free energy”	“Gibbs free energy”	Correct naming is important; “Gibbs” is standard (no apostrophe) in most chemistry writing.
Abstract	Word choice / logic connector	“insights according tointo the change...”	“insights into the change...”	Eliminates incorrect phrase blending; improves logical flow in the final abstract sentence.
Introduction	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.
Introduction	Article/preposition error	“propylone 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.
Introduction	Merged verbs / unclear action	“Al-Khattaf... foundstudied the process...”	“Al-Khattaf... studied/investigated the process...”	Clarifies the research action; correct verb choice strengthens literature narration.

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

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

				essential for interpreting thermodynamic correlations.
Discussion	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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