2 July 2025

DFT Investigation of 1-Hydroxycyclohexyl Phenyl Ketone (Irgacure 184): Unraveling Molecular Structure and Chemical Reactivity

MANJEET BHATIA[1]

1. Quantumsimm

Abstract

In this study, quantum mechanical calculations are performed using the density functional theory (DFT) method B3 LYP functional and the set of 6-311 ++ G (d, p) basis to investigate the structural, chemical reactivity, and stability properties of 1-hydroxycyclohexyl phenyl ketone (Irgacure 184). 1-hydroxycyclohexyl phenyl ketone is a widely used photoinitiator in UV- curable formulations, playing a crucial role in initiating polymerization reac- tions. Through a comprehensive computational analysis, the electronic struc- ture and reactivity parameters, such as proton affinity, ionization potential (IP), chemical potential (μ), chemical hardness (#) and softness (#), frontier molecular orbitals of HOMO-LUMO, electrophilic index (#) and electronega- tivity (#) of 1-hydroxycyclohexyl phenyl ketone have been elucidated in gas and aqueous medium. Molecular stability arising from delocalization or hyper- conjugation interactions and charge delocalization has been investigated using natural bond orbital (NBO) analysis. From the reported data, it is observed that the data on chemical reactivity from Koopmans' approximation hold well with the DFT-computed data in aqueous medium calculations.

Keywords

Chemical reactivity, natural bond orbital, density functional theory, photoinitiators, dispersion correction

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Abstract

In this study, quantum mechanical calculations are performed using the density functional theory (DFT) method B_3 LYP functional and the set of 6-311 ++ G (d, p) basis to investigate the structural, chemical reactivity, and stability properties of 1-hydroxycyclohexyl phenyl ketone (Irgacure 184). 1-hydroxycyclohexyl phenyl ketone is a widely used photoinitiator in UV-curable formulations, playing a crucial role in initiating polymerization reactions. Through a comprehensive computational analysis, the electronic structure and reactivity parameters, such as proton affinity, ionization potential (IP), chemical potential (μ), chemical hardness (η) and softness (σ), frontier molecular orbitals of HOMO-LUMO, electrophilic index (ω) and electronegativity (χ) of 1-hydroxycyclohexyl phenyl ketone have been elucidated in gas and aqueous medium. Molecular stability arising from delocalization or hyperconjugation interactions and charge delocalization has been investigated using natural bond orbital (NBO) analysis. From the reported data, it is observed that the data on chemical reactivity from Koopmans' approximation hold well with the DFT-computed data in aqueous medium calculations.

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1 Introduction

Photoinitiators are among the major constituents of ultraviolet (UV)-cured inks used in the printing industry. These compounds absorb the UV energy and generate free

radicals. Through a free-radical mechanism, they promote rapid drying of the ink, leading to a faster curing process (*1*, *2*). Due to the added advantages of UV-cured inks, such as high production efficiency, energy saving, and low environmental pollution, photoinitiators are widely used in the printing of packaging for foodstuff (*2*) and in the production of a wide range of products for medical applications (*3*, *4*). However, the photoinitiators are not always completely utilized or removed after the printing process. These unused traces of photoinitiators, especially low molecular weight from the ink on the package surface, have the potential to migrate into food and contaminate food (*5*, *6*).

1-Hydroxycyclohexyl phenyl ketone, also known as Irgacure 184, is a photoinitiator widely used in various industries for initiating UV-curable formulations and polymerization reactions (*7*). 1-Hydroxycyclohexyl phenyl ketone is one of the essential components in UV-curing processes, where UV light is used to initiate and control the polymerization of coatings, inks, adhesives, and other materials (*8*). In the context of food packaging, the potential for 1-Hydroxycyclohexyl phenyl ketone to migrate into food products is a critical concern. Analytical methods, such as gas chromatography-mass spectrometry (GC-MS) and liquid chromatography-mass spectrometry (LC-MS), can be employed to detect and quantify the presence of 1-Hydroxycyclohexyl phenyl ketone or its degradation products in food samples (*5*, *9*, *10*). Understanding its molecular structure, chemical reactivity, stability, and interaction with different packaging materials, and addressing challenges such as potential food contaminants is a continuing field of exploration.

Global reactivity descriptors are theoretical concepts based on the Koopmans' theorem (*11*) used in computational chemistry to provide insights into the reactivity and chemical behavior of molecules (*12*). The chemical reactivity parameters, such as chemical potential (μ), ionization potential (I), chemical hardness (η) and softness (σ), electrophilicity index (ω), electronegativity (χ), and HOMO-LUMO energy are generally investigated from conceptual density functional theory (C-DFT) (*13–15*). These parameters offer valuable information about the potential applications and behavior of 1-Hydroxycyclohexyl Phenyl Ketone. Chemical potential (μ) and ionization potential (IP) provide insights into the molecule's electron-donating and accepting tendencies. Hardness implies stability and resistance to chemical changes. A high hardness means high stability and low chemical reactivity, while a low value of the hardness parameter signifies the high reactivity of a molecular system. Softness is the reciprocal of hardness and indicates the ease of deformation and chemical change. A higher electrophilicity index suggests a greater tendency to undergo nucleophilic attacks, which is relevant in applications where reactions with electron-rich species are desirable. It can help predict regions of high and low electron density, which is relevant for understanding sites of potential reactivity.

It's important to note that these global reactivity descriptors are theoretical and should be interpreted alongside experimental data and chemical intuition. Depending on the specific applications of the molecular system, certain descriptors may be more relevant than others. Additionally, the accuracy of these descriptors depends on the

computational method used and the specific context of their application.

2 Computational Method

DFT calculations were performed on the Gaussian 16 code (*16*) using the B_3LYP functional (*17*) in conjunction with the 6-311++G(d, p) basis set and D3 dispersion correction. The basis sets include both polarization and diffuse functions for hydrogen and heavy atoms to account for the behavior of electrons farther from the atomic nucleus and electron density variations due to molecular geometry changes. This approach allowed us to accurately model the electronic structure and reactivity of 1-Hydroxycyclohexyl phenyl ketones. Geometry optimization and frequency calculations were carried out to obtain the ground-state molecular structure and vibrational frequencies. To analyze the effect of solvent, the molecular structure is optimized at B_3LYP/6-311++G(d, p) theory in water employing PCM method using the Gaussian 16 suite of code. The D3 dispersion correction, also known as the Grimme dispersion correction (*18*), is added along with the Becke-Johnson damping term (*19*) to the DFT calculations to account for van der Waals interactions and dispersion forces that are not adequately captured by standard DFT functionals. This correction improves the accuracy of calculated binding energies, molecular geometries, and interaction energies in systems where dispersion forces play a significant role.

3 Results and Discussion

The molecular structure of the investigated molecule is optimized at B_3LYP/6-311++G(d, p) DFT method in the gas phase, and the true minima is confirmed by the absence of negative vibrational frequencies. The optimized structural parameters are reported in Table 1. Figure 1 shows the fully optimized structure of 1-Hydroxycyclohexyl Phenyl Ketone molecule.

All the parameters are then computed using B_3LYP/6-311++G(d, p) DFT method. The proton affinity (PA) is a measure of the probability of a chemical group being protonated. While, ionization energy and electron affinity (EA) measure the energy needed to remove an electron and the energy released during electron addition to the neutral system, respectively.

NBO population charges are reported in Table 2 for neutral and O2-protonated molecules in the gas and aqueous media. O1 and O2 sites of the neutral molecule carry the highest negative charges in the gas phase, -0.7393 and -0.5615, respectively. All other carbon atoms are electronegative except C3 and C9, which are bonded to electronegative oxygen atoms and carry positive charges. Similarly, the charge on O2 decreases upon protonation in gas and aqueous phases because some negative charge is shared by the protonated H atom. One of the useful aspects of NBO analysis is that it provides information about interactions in both filled and virtual orbitals,

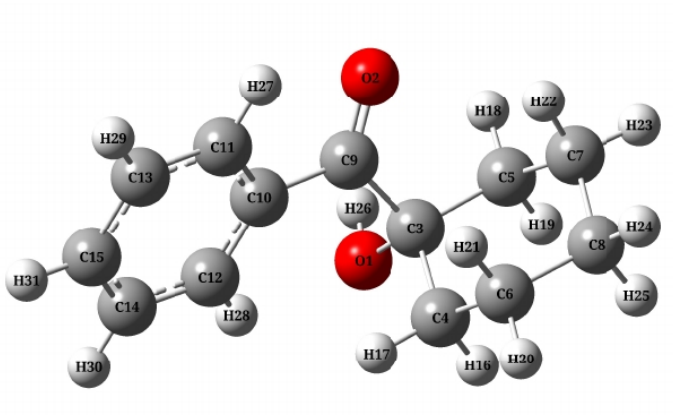


Figure 1: Optimized equilibrium structure of ground neutral 1-Hydroxycyclohexyl Phenyl Ketone molecule with B_3LYP/6-311++G(d, p) theory.

which further advances the analysis of intra and intermolecular interactions. NBO analysis has confirmed that the electron delocalization from O1 is mainly concentrated at antibonding C3-C9 and C3-C5 orbitals, while the electron lone pair of O2 is delocalized mainly on antibonding C3-C9 and C9-C10 orbitals. Apart from the small donor-acceptor interactions of the O2 lone pair with antibonding orbitals of C3-C9 (85.48 KJ/mol), bonding of C14-C15 with antibonding C10-C12 (92.80 KJ/mol), bonding C11-C13 with antibonding orbitals of C14-C15 (90.92 KJ/mol), and bonding orbitals of C10-C12 with antibonding of C11-C13 (85.56 KJ/mol), there is higher interaction between antibonding orbitals of O2-C9 with antibonding C10-C12 orbitals seen to give strong stabilization (472.50 KJ/mol). Understanding these patterns is crucial in the evaluation of chemical reactivity, stability, and biological activity of a molecule. The electron delocalization primarily arises from the conjugation of pi (π) electrons across its aromatic rings and the oxygen atoms within the molecule. The molecule under study has two potential electrostatic potential (ESP) regions with higher negative charges at O1 and O2, see Figure 2. It can be seen that the electrons are mainly concentrated in the region (red color) close to O1 and O2. Similarly, an electron-deficient region is represented by a light blue region. The region with negative ESP is susceptible to electrophilic attack, while the region of higher positive charge is more likely susceptible to nucleophilic attack. The reactivity of a molecule is influenced by the distribution of electron density due to electron delocalization. The O1 and O2 atoms within 1-Hydroxycyclohexyl Phenyl Ketone can act as electron-rich sites and function as nucleophiles in certain reactions, especially under basic conditions.

The computed quantities, such as PA, IE, electric dipole moment, and polarizability, are important for accurate identification and quantification of the molecule using chemical ionization mass spectrometry (CI-MS). It is worthwhile to mention that a higher PA value (872.49 KJ/mol) is obtained when a proton attaches to the O2 position than to the O1 position (825.75 KJ/mol). A higher PA value which

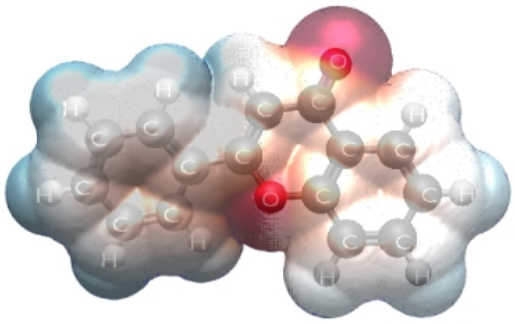
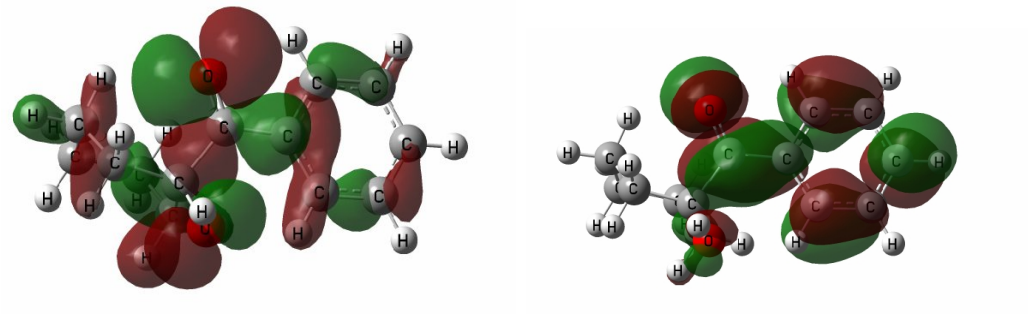


Figure 2: Electrostatic potential surface (ESP) and charge density distribution of 1-Hydroxycyclohexyl Phenyl Ketone.

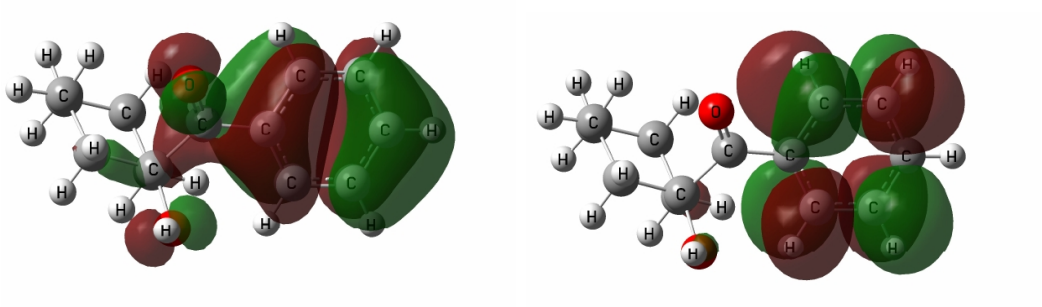


(a) (b)

Figure 3: Schematic representation of the outermost molecular orbitals of neutral 1-Hydroxycyclohexyl Phenyl Ketone (3a) HOMO, (3b) LUMO states.

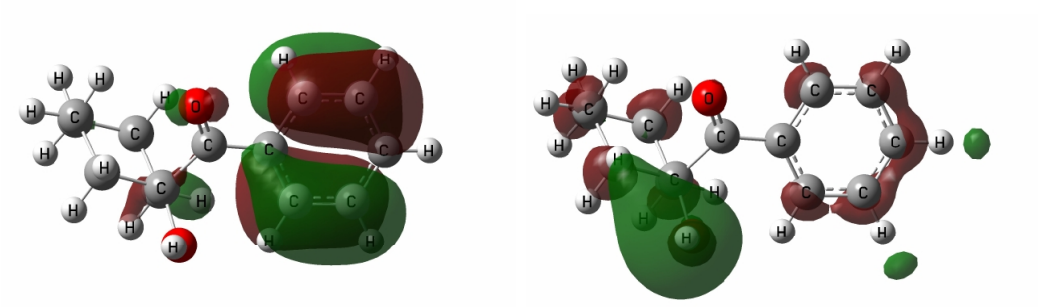
indicates a higher propensity to protonation, is reported in Table 3. The aqueous medium calculations anticipate higher PA and EA values, while lower ionization energy values are due to solvation. The electric dipole moment and polarizability values are higher in aqueous medium.

The chemical reactivity of a molecular system is governed by the frontier molecular orbitals (FMO). The highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbitals (LUMO) determine the chemical reactivity and stability of molecules. The energy of HOMO represents the capability of a molecule to donate electrons, while LUMO energy indicates the ability to accept electrons. HOMO-LUMO energy gap ($\Delta\varepsilon_{\text{gap}}$) determines the chemical reactivity and stability of the molecule. A higher $\Delta\varepsilon_{\text{gap}}$ means lower reactivity and high stability. Because a higher $\Delta\varepsilon_{\text{gap}}$ doesn't favor frequent electron transfer from HOMO to LUMO orbitals as compared to molecules with lower $\Delta\varepsilon_{\text{gap}}$. A pictorial representation of HOMO LUMO molecular orbitals is given in Figures 3 to 5. HOMO corresponds to the occupied pi-type molecular orbitals and the electron density is concentrated at O2=C9



(a) (b)

Figure 4: Molecular orbitals of neutral 1-Hydroxycyclohexyl Phenyl Ketone in (4a) HOMO-1, (4b) LUMO+1 states.



(a) (b)

Figure 5: Molecular orbitals of neutral 1-Hydroxycyclohexyl Phenyl Ketone molecule in (5a) HOMO-2, (5b) LUMO+2 states.

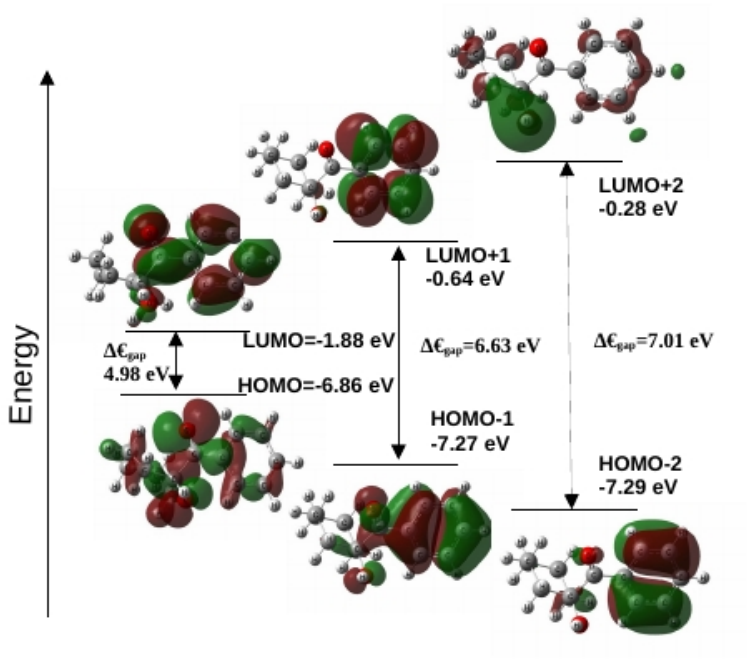


Figure 6: complete energy variation of orbitals for 1-Hydroxycyclohexyl Phenyl Ketone.

double bond and O1-C3 single bond. HOMO orbital energy mainly comes from pi-orbitals of O2=13.7 and O1=3.45 eV. The distribution of pi-electrons in the HOMO orbital is important because these electrons are available to participate in chemical reactions. The site, where the highest occupied orbital is localized, is considered a good nucleophilic site. Similarly, LUMO can be described by the pi-orbitals of the following atoms with corresponding orbital energies: C9=7.69, O2=5.00, C15=4.14, C12=2.79 eV, respectively. The lowest unoccupied molecular orbital site is treated as a good electrophilic site. Other occupied and unoccupied orbitals, such as HOMO-1, HOMO-2, LUMO+1, and LUMO+2 are also shown in Figures 4 and 5. A complete energy variation of orbitals for 1-Hydroxycyclohexyl Phenyl Ketone is shown in Figure 6.

The chemical reactivity of the molecular systems is determined by the C-DFT, which gives very effective results for predicting global chemical reactivity and stability behaviors of molecular structures. According to, Koopmans' theorem for closed-shell molecules, which assumes that if removing or adding an electron to a molecule does not significantly change the molecular orbitals of the system then the I and A can be expressed in terms of the energy of HOMO ($-\varepsilon_{\mathrm{HOMO}}$=I) and LUMO ($-\varepsilon_{\mathrm{LUMO}}$=A) molecular orbitals. Based on the Koopmans' approximation, other reactivity parameters such as chemical potentials (μ), chemical hardness (η) and softness (σ),

electrophilic index (ω), and electronegativity (χ) can be derived as:

$$\mu = \frac{\mathrm{I} + \mathrm{A}}{2} \tag{1}$$

$$\eta = \frac{\mathrm{I} - \mathrm{A}}{2} \tag{2}$$

$$\sigma = \frac{1}{2\eta} \tag{3}$$

$$\omega = \frac{\mu^2}{2\eta} \tag{4}$$

The electronegativity (χ) can be represented as -μ. Molecular reactivity parameters as obtained from B_3LYP/6-311++G(d, p) DFT method are reported in Table 3. Chemical potential (μ) measures the escaping tendency of an electron in a molecule. As μ becomes higher (more negative), it is difficult to lose an electron, but easier to gain one instead. 1-Hydroxycyclohexyl Phenyl Ketone possess μ value=-4.3725 eV, which is equivalent to the electronegativity of χ=4.3725 eV. A high χ means a higher ability to attract electrons. Similarly, chemical hardness (η) and softness (σ) can be understood in terms of the HOMO-LUMO energy gap. A hard molecule can be labeled as low reactive, and highly stable with a large HOMO-LUMO energy gap. On an equitable basis, a soft molecule is one with a very low HOMO-LUMO gap, is highly reactive, and is considered less stable. The electrophilic index (ω) of a molecule estimates stabilization energy when the system gets saturated by electrons. A good electrophile must have high, ω while a good nucleophile means low ω values. In aqueous medium, the DFT computed IE and EA values are 7.04 and 2.09 which are similar to the values obtained from the HOMO and LUMO energies (Koopmans' approximations) thus almost identical global reactivity parameters (values in brackets Table 3) can be obtained via both methods, i.e., from DFT and C-DFT. These results have demonstrated that the Koopmans' theorem is valid and can be applied in conjunction with DFT method B_3LYP/6-311++G(d, p) to investigate related molecules in aqueous medium.

4 Conclusions

DFT calculations using B_3LYP/6-311++G(d, p) combination, structural and chemical reactivity parameters are obtained for 1-Hydroxycyclohexyl Phenyl Ketone. This compound is widely used as a Photoinitiators in the printing industry and printing of food packages. The knowledge of the chemical reactivity, stability, and electron-rich and electron-deficient sites of 1-Hydroxycyclohexyl Phenyl Ketone is crucial as it allows us to understand interactions, especially in food package surface reactions, with components of food during storage and packaging. Parameters like PA, IE, dipole moment, and polarizability of a molecule are critical in finding the concentration of a compound using analytic techniques (CI-MS). Global reactivity descriptors, such

as chemical potential (μ), ionization potential (IP), chemical hardness (η) and softness (σ), electrophilicity index (ω), electronegativity (χ), and HOMO-LUMO energy are computed for 1-Hydroxycyclohexyl Phenyl Ketone molecule in gas and aqueous phases. The computed results have confirmed that Koopmans' theorem predicts molecular reactivity similar to that of DFT in aqueous medium. Since no comprehensive data on the molecular properties of the investigated molecule is available in the literature, these reactivity descriptors offer a quantitative framework to analyze and predict molecular behavior, guide the design of new molecules for photoinitiating applications with tailored properties, and advance our understanding of reaction mechanisms in gas and aqueous phases.

In conclusion, 1-Hydroxycyclohexyl Phenyl Ketone has emerged as a valuable photoinitiator for UV-curable coatings applied to food packaging materials. Its ability to efficiently initiate polymerization, along with its safety approvals, positions it as a key component in the development of sustainable and high-performance food packaging solutions. Research continues to explore the optimization of UV-curable coatings containing 1-Hydroxycyclohexyl Phenyl Ketone for food packaging. This includes fine-tuning the electronic and chemical properties and understanding their interaction with different packaging materials.

5 Declarations

Ethical Approval
Not applicable

Competing interests
Not applicable

Authors' contributions
Not applicable

Funding
Not applicable

Availability of data and materials
Data is available on request from the author.

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Table 1: Molecular structure parameters of optimized 1-Hydroxycyclohexyl Phenyl Ketone. Bond lengths are in Å and bond angles are in degrees.

1-Hydroxycyclohexyl Phenyl Ketone					
O1-H26	0.964	C9-O2	1.217	C8-H25	1.097
C3-O1	1.443	C9-C10	1.499	C8-H24	1.094
C3-C9	1.555	C10-C11	1.402	C7-C8	1.532
C3-C4	1.533	C10-C12	1.402	C6-C8	1.532
C3-C5	1.534	C11-H27	1.083	C6-H21	1.097
C5-H18	1.094	C12-H28	1.080	C6-H20	1.094
C5-H19	1.095	C11-C13	1.389	C7-H23	1.094
C4-H16	1.095	C12-C14	1.392	C15-H31	1.084
C4-H17	1.090	C14-H30	1.084	C7-H22	1.092
C5-C7	1.536	C13-H29	1.084	C14-C15	1.393
C4-C6	1.533	C13-C15	1.395	H27-C11-C10	118.54
H29-C13-C11	119.93	H29-C13-C15	120.13	H31-C15-C14	120.06
O2-C9-C3	120.11	H26-O1-C3	108.18	C11-C10-C9	116.89
H18-C5-H19	107.84	H22-C7-H23	106.84	H24-C8-H25	106.74
H21-C6-H20	106.38	H17-C4-H16	107.15	C4-C3-C5	109.88
C3-C5-C7	113.62	C5-C7-C8	111.71	C8-C6-C4	111.08
O2-C9-C10	119.72	C11-C10-C12	119.13	C14-C12-C10	120.09

Table 2: DFT computed natural charges of 1-Hydroxycyclohexyl Phenyl Ketone ($C_{13}H_{16}O_2$) at equilibrium ground state and protonated O2 site in gas phase and in water. The natural charges are represented in atomic units.

1-Hydroxycyclohexyl Phenyl Ketone*				
	Neutral		O2-protonated	
Atom no	Gas	Water	Gas	Water
O1	-0.7393	-0.7529	-0.7098	-0.7247
O2	-0.5615	-0.5923	-0.5608	-0.5515
C3	0.2023	0.2036	0.2150	0.2158
C4	-0.3967	-0.3982	-0.3943	-0.3931
C5	-0.4077	-0.4085	-0.4183	-0.4151
C6	-0.3843	-0.3852	-0.3881	-0.3890
C7	-0.3853	-0.3842	-0.3856	-0.3863
C8	-0.3789	-0.3804	-0.3854	-0.3821
C9	0.5539	0.5695	0.6555	0.6591
C10	-0.1536	-0.1595	-0.2100	-0.2032
C11	-0.1540	-0.1620	-0.1466	-0.1289
C12	-0.1758	-0.1774	-0.1011	-0.1070
C13	-0.2054	-0.2092	-0.1861	-0.1942
C14	-0.2058	-0.2087	-0.1892	-0.1983
C15	-0.1784	-0.1807	-0.0897	-0.1020

Table 2: continued

1-Hydroxycyclohexyl Phenyl Ketone*				
	Neutral		O2-protonated	
Atom no	Gas	Water	Gas	Water
H16	0.2082	0.2098	0.2303	0.2239
H17	0.2160	0.2168	0.2168	0.2212
H18	0.2131	0.2141	0.2168	0.2220
H19	0.2037	0.2079	0.2279	0.2242
H20	0.2038	0.2078	0.2265	0.2172
H21	0.1924	0.1923	0.1844	0.1949
H22	0.2090	0.2003	0.1946	0.2000
H23	0.1998	0.2034	0.2245	0.2136
H24	0.2013	0.2030	0.2196	0.2093
H25	0.1853	0.1891	0.2012	0.1947
H26	0.4619	0.4761	0.4804	0.4872
H27	0.2228	0.2220	0.2094	0.2240
H28	0.2344	0.2346	0.2538	0.2493
H29	0.2070	0.2167	0.2358	0.2343
H30	0.2066	0.2163	0.2360	0.2326
H31	0.2053	0.2158	0.2320	0.2291
H32	—	—	0.5041	0.5229

Table 3: DFT evaluated the molecular properties of 1-Hydroxycyclohexyl Phenyl Ketone ($C_{13}H_{16}O_2$) using B_3LYP/6-311++G(d, p) method in the gas phase and in solvent (water). Except for proton affinity, dipole moment, and polarizability, all other values are in eV. Reactivity parameters in brackets are computed from IE and EA values in aqueous media.

1-Hydroxycyclohexyl Phenyl Ketone*					
	Gas	Water		Gas	Water
PA[a]	872.49	1038.59	LUMO+1	-0.64	-0.71
IE	8.65	7.04	LUMO+2	-0.28	-0.22
EA	0.18	2.09	$\Delta\varepsilon_{\text{gap}}$	4.98	5.05 (4.95)
μ_D[b]	1.40	2.09	μ	-4.3725	-4.5209 (-4.5650)
α[c]	22.88	31.13	η	2.4900	2.5228 (2.4750)
HOMO	-6.86	-7.04	σ	0.2008	0.1982 (0.2020)
LUMO	-1.88	-2.00	ω	3.8391	4.0508 (4.2099)
HOMO-1	-7.27	-7.35	χ	4.3725	4.5209 (4.5650)
HOMO-2	-7.29	-7.37			

*CAS Number (947-19-3) and Molecular Mass=204.26 g/mol
[a]KJ/mol
[b]Debye
[c]Å^3