



IJSRM

INTERNATIONAL JOURNAL OF SCIENCE AND RESEARCH METHODOLOGY

An Official Publication of Human Journals



Human Journals

Research Article

December 2016 Vol.:5, Issue:2

© All rights are reserved by Dr. V. J. NAUKUDKAR et al.

Theoretical and Infrared Studies of O-Dichlorobenzene and O-Chlorophenol with Acetone, Acetophenone, Cyclohexanone and Cyclohexane



IJSRM

INTERNATIONAL JOURNAL OF SCIENCE AND RESEARCH METHODOLOGY

An Official Publication of Human Journals



Dr. V. J. NAUKUDKAR

*Head, Department of Chemistry, K. V. N. Naik, Arts,
Commerce & Science College, Nashik, 422 002,
Maharashtra, India.*

Submission: 7 December 2016

Accepted: 12 December 2016

Published: 25 December 2016



HUMAN JOURNALS

www.ijsrm.humanjournals.com

Keywords: Infrared spectroscopy, Theoretical studies, DFT/B3LYP method, 6-31G (d) basis set, o-dichlorobenzene, o-chlorophenol, Ketones, Cyclohexane, Molecular Interactions

ABSTRACT

Binary mixtures of o-dichlorobenzene and o-chlorophenol with acetone, acetophenone, cyclohexanone and cyclohexane have been prepared at room temperature for entire concentrations. These binary mixtures studied by Infrared spectroscopy. The data have been utilized to compute the infrared studies correlate to theoretical calculations. The results have been interpreted in terms of molecular interactions existing between the components of the mixtures.

1. INTRODUCTION

The composition dependence of thermodynamic properties has proved to be very useful tools in understanding the nature and extent of pattern of molecular aggregation resulting from intermolecular interaction between components^{1,2}. In the present paper binary liquid mixture of *o*-dichlorobenzene (ODB) and *o*-chlorophenol (OCP) with acetone (AC), acetophenone (AP), cyclohexanone (CYNO) and cyclohexane (CYN) have been studied. Theoretical and Infrared studies of *o*-dichlorobenzene (ODB) and *o*-chlorophenol (OCP) with above ketones have been studied over the entire composition range.

2. EXPERIMENTAL

The entire chemical used was of A. R. grade with purity >99% are used as such. Binary mixtures were prepared by mixing a known mass of each liquid in an airtight, stoppered glass bottle. I.R. measurement through liquid mixtures provides an excellent tool to investigate inter and intramolecular interactions between like and unlike molecules. I.R. Spectroscopy studies of pure and binary mixtures of ODB and OCP with ketones have been recorded over the whole composition range at room temperature and atmospheric pressure. FTIR spectra were recorded on a FTIR spectrometer (Model: SIMADZU 8400S PC) by using KBr pellet in the region 400-4000cm⁻¹ with 4.0 cm⁻¹ resolution. The transmission values were read in steps of 5%. The spectrometer possesses out to aligned energy optimization and dynamically aligned interferometer. It is fitted with KBr beam splitter, a DLATGS detector. A baseline correction was made for the spectra recorded. The data have been utilized to compute the infrared studies correlate to theoretical calculations.

3. THEORY

An IR is widely used for: (1) identification and determination of structure (2) determining the purity and quantitative analysis (3) following the course of reaction (4) hydrogen bonding (5) molecular geometry and conformational analysis (6) chemistry of organic polymers and (7) reactions of reactive species like free radicals and ions.

The stretching frequency of chemical bond depends upon (i) bond strength (ii) reduced masses of the atoms forming bond. Any factor which will increase bond strength will increase stretching frequency of the bond, and if the mass of atoms forming the chemical bond is increased, the reduced mass will increase and stretching frequency will decrease. The

following factors affect the IR absorption frequency: (a) Inductive and resonance effect (b) Conjugation (c) size of the ring and (d) hydrogen bonding.

The free (non-bonded) -OH group is observed only in very dilute solution in non-polar solvent. The free O-H stretching band appears at about 3600cm^{-1} . Intermolecular H-bonding increases with the increase in concentration of solution. A broad O-H stretching vibration is obtained for intermolecular hydrogen bonding in the range from $3400\text{-}3200\text{cm}^{-1}$. In short, H-bonding decreases the O-H stretch frequency. Intermolecular hydrogen bonding weakens the O-H bond, thereby shifting the band to lower frequency.

4. RESULTS AND DISCUSSION

In recent years, experimental results have been frequently supported with spectroscopic/theoretical calculations which have proved quite helpful in explaining the comparative relativities and many other properties of the organic molecules/complexes. Hydrogen bonding is of central importance in the molecular sciences for both practical and theoretical reasons³⁻¹⁰. Hydrogen bonding has held particular interest in recent years due to the central role it plays with regard to molecular recognition in both biological and artificial systems¹¹⁻¹⁴.

There has been increasing interest in C-H...O hydrogen bonds recently, both theoretically and experimentally¹⁵⁻¹⁷. Because carbon is not particularly electronegative, the ability of the C-H group to serve as a proton donor in hydrogen bonding depends on the carbon hybridization [C (sp)-H > C (sp²)-H > C (sp³)-H] and on the electron withdrawing strength of adjacent substituent¹⁸⁻²⁰. Although the C-H...O interaction energy varies and is much weaker than conventional hydrogen bonds, it can play important role in molecular conformation²¹, crystal packing²² and protein folding²³. Close C-H...O contracts have been observed widely in high-resolution protein structures. Extensive calculations are carried out to determine the optimized geometries, and electronic structure and thermochemical data. On the basis of semi-empirical calculations, the reactivity of heterocyclic compounds towards electrophilic substitution has been predicted²⁴⁻²⁹.

IR spectroscopy is the leading method for identification of hydrogen bonds. For instance, the formation of an O-H...O hydrogen bond elongates and weakens the O-H bond. The resulting redshift of the O-H bond stretching frequency can be easily detected in the IR spectra and its magnitude indicates the strength of the hydrogen bond³⁰. This phenomenon is called anti-

hydrogen bond³¹⁻³². However, Scheiner *et al.*³³ have concluded, from a set of careful calculations that “antihydrogen” bonds do not differ fundamentally from conventional hydrogen bonds. According to their results, the electron density redistribution upon hydrogen bond formation is similar for both the C-H--O and O-H--O interactions. The amount of charge transferred from a donor to an acceptor is roughly proportional to the bonding strength. The solvent structure determines the nature of molecular interaction. Spectral changes are caused by hydrogen bonding, van der Waals interactions, dipole-dipole interactions, induced-dipole interactions etc. Information about hydrogen bonding is derived from the bond width, position and intensity of the first overtone bands of the -OH band (intensity of first overtone band decreases)³⁴.

Spectrum of some OCP + ketones shows two absorption bands -OH. The sharp band is due to free -OH while weak band is due to hydrogen bonded -OH. Presence of hydrogen bonding between -OH of OCP with oxygen of studied ketones and absence of hydrogen bonding in systems of ODB + ketones is confirmed by FTIR. In case of ODB + Ketones, carbonyl stretching frequency is not so affected but slightly increases at $x_1 \approx 0.8$ and 0.9 .

The interesting behavior of intramolecular hydrogen bonds both from the practical and theoretical points of view has received increased attention in recent years³⁵⁻⁴³. This can be attributed to the fact that the value of hydrogen bond energy is only a few kilocalories per mole and can readily perturb by any change in its environment. This is especially important in studies of weakly bound complexes of ketones and OCP.

4.1 Infrared studies

The FTIR absorption frequencies of the binary mixtures of ODB and OCP with ketones over the entire range at room temperature are listed in Tables 1.0-3.0.

4.1.1 ODB + Ketones

C=O stretching vibrations: The band due to C=O stretching vibration is observed in the region $1650-1850\text{ cm}^{-1}$. For aliphatic ketone C=O stretching vibration is at $1710-1720\text{ cm}^{-1}$ and for aromatic ketone C=O stretching vibration it is observed at around $1680-1690\text{ cm}^{-1}$ due to conjugation effect. From Table 1.0, it is observed that C=O stretching frequency is almost same from $x_1 \approx 0.1-0.9$ for ODB + AC, ODB + AP and ODB + CYNO. Lower C=O stretching frequency is observed at $x_1 \approx 0.1$ and higher C=O stretching frequency is observed

at $x_1 \approx 0.8$ and 0.9 for all systems. The frequency follows the order: ODB + AC > ODB + CYNO > OCP + CYNO > ODB + AP.

Table 1. IR stretching frequencies of C=O (cm^{-1}) in (x_1) ODB and ($1-x_1$) ketones systems.

x_1	ODB+AC	ODB +AP	ODB +CYNO
0	1714.6(w)	1683.7(s)	1710.7(s)
0.1	1714.6(w)	1683.7(s)	1712.8(s)
0.2	1714.6(w)	1683.7(s)	1712.8(s)
0.3	1714.6(w)	1683.7(s)	1712.8(s)
0.4	1714.6(w)	1683.7(s)	1712.8 (s)
0.5	1714.6(w)	1685.7(s)	1712.8(s)
0.6	1714.6(s)	1683.7 (s)	1712.8(s)
0.7	1714.6(s)	1685.7(s)	1712.8(s)
0.8	1714.6(s)	1685.7(s)	1712.8(s)
0.9	1714.6(m)	1683.7(m)	1712.8(m)
1.0	1714.6(w)	----	----

w = weak absorption, s = strong absorption, m = medium absorption.

4.1.2 OCP + Ketones

C=O stretching vibrations: From Table 2.0, it is observed that C=O stretching frequency decreases from $x_1 \approx 0.1$ to 0.9 for OCP + AC, OCP + AP and OCP + CYNO. Higher C=O stretching frequency observed at $x_1 \approx 0.1$ and lower for all above systems except OCP + AC. The frequency follows the order: OCP + AC > OCP + CYNO > OCP + AP.

Table 2. IR stretching frequencies of C=O (cm⁻¹) in (x₁) OCP and (1-x₁) ketones systems.

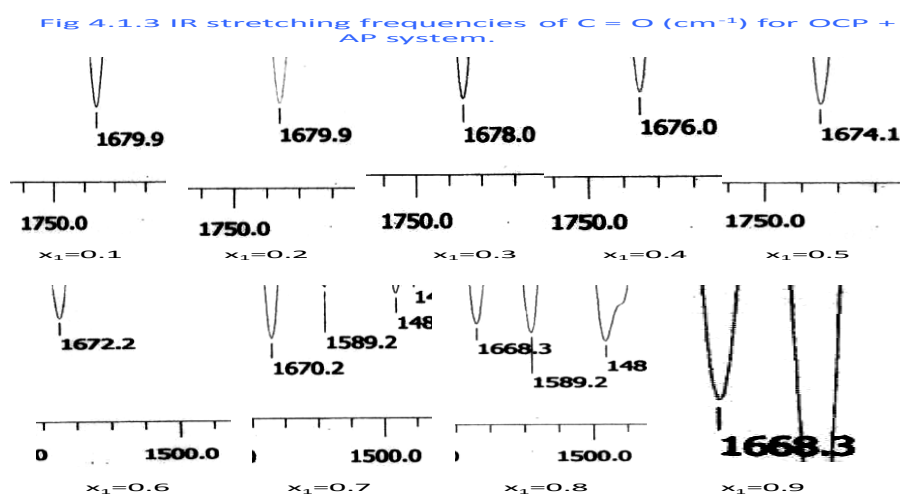
x ₁	OCP+AC	OCP+AP	OCP+CYNO
0	1714.6(w)	1683.7(s)	1710.7(s)
0.1	1714.6(s)	1679.9(s)	1712.8(s)
0.2	1706.9(s)	1679.9(s)	1712.8(s)
0.3	1701.1(s)	1678.0(s)	1705.1(s)
0.4	1701.1(s)	1676.0(s)	1701.2(s)
0.5	1701.1(s)	1674.1(s)	1697.4(s)
0.6	1705.0(s)	1672.2(s)	1697.4(s)
0.7	1699.2(s)	1670.0(s)	1697.4(m)
0.8	1697.2(s)	1668.3(s)	1697.4(m)
0.9	1701.1(m)	1668.3(s)	1693.5(m)
1.0	----	----	----

O-H stretching vibrations: The non-hydrogen-bonded hydroxyl group of phenol absorbs strongly in the 3584-3650 cm⁻¹ region. The sharp free hydroxyl bands are observed in the vapor phase and in dilute solution in non-polar solvent⁴⁴. Intermolecular hydrogen bonding increases as the concentration of solution increases and additional bands appear at lower frequencies 3200-3500 cm⁻¹. Hence in the present investigations (Table 3.0); phenolic O-H frequency decreases from x₁ ≈ 0.1 - 0.6 and increases from x₁ ≈ 0.7 - 0.9 for OCP + AC. This frequency increases from x₁ ≈ 0.1 - 0.9 for OCP + AP. The O-H frequency decreases from x₁ ≈ 0.1 - 0.4 and increases from x₁ ≈ 0.5 - 0.9 for OCP + CYNO. For OCP systems the sharp band is due to free -OH, while weak band is due to hydrogen bonded -OH. Two bands are observed in OCP + CYNO in x₁ ≈ 0.6 - 0.9 and one sharp band is recorded for OCP +AC and OCP + AP over entire range of composition.

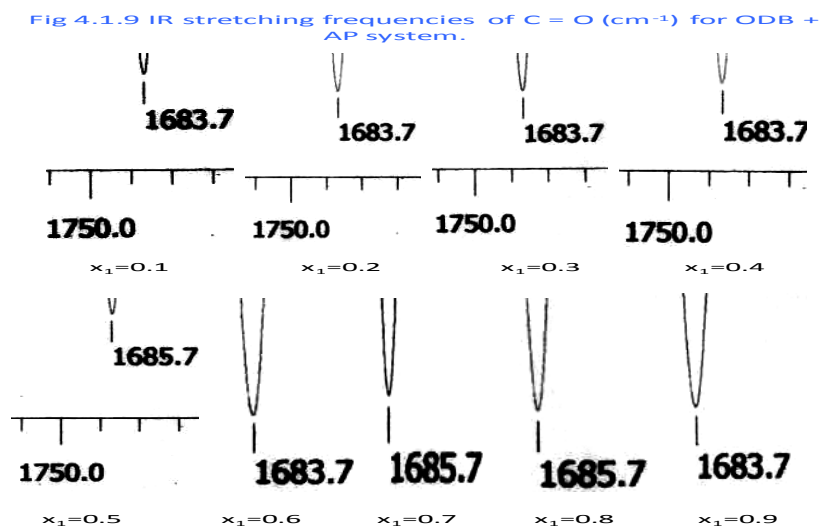
Table 3. IR stretching frequencies of O-H (cm^{-1}) in (x_1) OCP and ($1-x_1$) ketones systems.

x_1	OCP+AC	OCP+AP	OCP+CYNO
0	----	----	----
0.1	3460.1(s)	3355.9(s)	3404.4(s)3255.9(m)
0.2	3402.2(s)	3352.1(s)	3400.6 (s)3255.9(s)
0.3	3442.7(s)	3354.0(s)	3277.1(s)3265.5(s)
0.4	3400.3(s)	3392.8(s)	3265.5(s)
0.5	3394.5(s)	3398.3(s)	3369.7(s)3294.5(s)
0.6	3386.8(s)	3404.1(s)	3369.7(s)3302.2(m)
0.7	3444.6(s)	3409.9(s)	3400.6(s)3381.3(s)
0.8	3454.3(s)	3425.3(s)	3524.0(m)3431.4(s)
0.9	3427.3(s)	3438.8(s)	3524.0(s)3448.84(m)
1.0	3456.2(s)	3456.2(s)	3456.2(s)

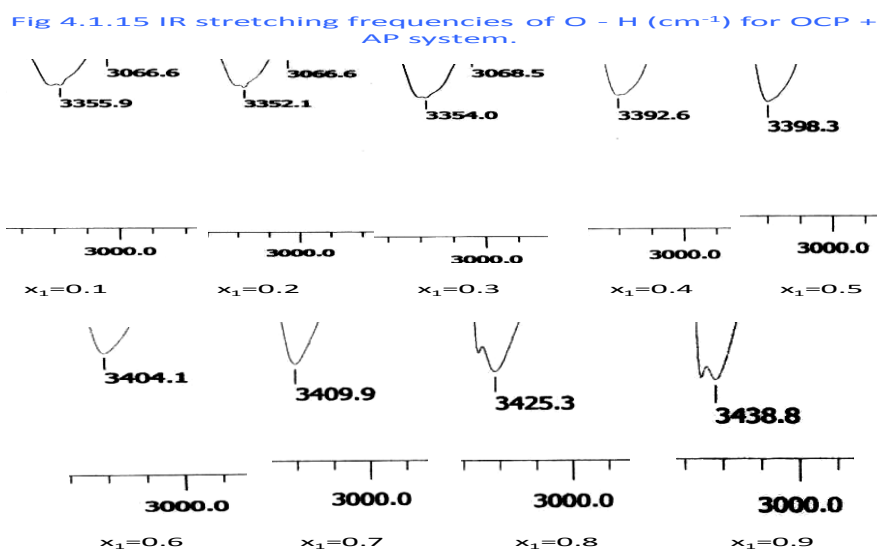
The position and breadth of an -OH absorption band depend on the concentration of the solution. The more concentrated solution and the more -OH containing molecules form intermolecular hydrogen bonds. It is easier to stretch an O-H bond if it is hydrogen bonded because the hydrogen is attached to oxygen of a neighboring molecule. Therefore, the stretch of a concentrated (hydrogen bonded) solution of OCP occurs at 3427.3 cm^{-1} , whereas the stretch of a dilute solution (with little or no hydrogen bonding) occurs at 3460.1 cm^{-1} for OCP + AC system. However, no such dilution effect is observed in other binary mixture. But other all systems show hydrogen bond effect at higher concentration ($x_1 \approx 0.1$ to 0.6) of OCP.



It is seen that the O-H stretching frequency increases when mole fraction of OCP decreases. Higher values of O-H stretching frequency is observed at high mole fraction and lower values of O-H stretching frequency is recorded in between 0.2 to 0.5 mole fractions of OCP. This may be due to hydrogen bonding between phenolic O-H group and carbonyl group. The O-H stretching frequency of OCP is 3456.2 cm^{-1} , which gets decrease in presence of ketone because of intermolecular hydrogen bonding between them. The binaries OCP + AP and OCP + CYNO show large decrease in the O-H stretching frequency.



Spectrum of some OCP + ketones shows two absorption bands -OH. The sharp band is due to free -OH while weak band is due to hydrogen bonded -OH. Presence of hydrogen bonding between -OH of OCP with oxygen of studied ketones and absence of hydrogen bonding in systems of ODB + ketones is confirmed by FTIR. In case of ODB + Ketones, carbonyl stretching frequency is not so affected.



The interesting behavior of intramolecular hydrogen bonds both from the practical and theoretical points of view has received increased attention in recent years³⁵⁻⁴³. This can be attributed to the fact that the value of hydrogen bond energy is only a few kilocalories per mole and can readily perturb by any change in its environment. This is especially important in studies of weakly bound complexes of ketones and OCP.

o-dichlorobenzene (ODB) and o-chlorophenol (OCP) with acetone (AC), acetophenone (AP), cyclohexanone (CYNO) and cyclohexane (CYN)

4.2 THEORETICAL STUDIES

All the theoretical calculations on OCP/ODB and their mixtures with ketones were performed by the use of G03W series of programs⁴⁴. Geometries of optimizations for all the investigated molecules in this work were carried out using the DFT/B3LYP method with medium size 6-31G (d) basis set.

The difference between the observed and scaled frequency values of most of the fundamentals in many cases is very small. Any discrepancy noted between the observed and calculated frequencies may be due to the fact that the calculations have been actually done on the single molecule/complex between two molecules in the gaseous state contrary to the experimental values recorded in the presence of intermolecular interactions. Therefore the assignment made at higher levels of theory with only reasonable deviations from the experimental values seem to be correct.

4.2.1 Hydrogen bond (Table 4.2.1)

Weak intermolecular hydrogen bonds are also seen in Cis-OCP + AC and Cis-OCP + AP. Strong intermolecular hydrogen bonds are also observed for Trans-OCP + CYNO.

Table 4.2.1: Optimized atomic distances of systems at B3LYP level using 6-31G (d) basis set.

Sr. No.	System	O-H	C-Cl	C=O	=C-O	O--H	Cl--O=C
1.	ODB	--	1.81381	--	--	--	--
2.	Trans-OCP+AC	0.98481	1.75638	1.22532	1.35291	1.81189	5.69423
3.	Trans-OCP+AP	0.98210	1.75650	1.23038	1.35395	1.81440	5.71295
4.	Trans-OCP+CYNO	0.98566	1.75663	1.22648	1.35201	1.80296	5.69902
5.	Trans-OCP+CYN	0.96954	1.75164	--	1.36207	--	--
6.	Cis-OCP+AC	0.98437	1.76249	1.22249	1.35124	1.88585	3.37004
7.	Cis-OCP+AP	0.98447	1.76195	1.22911	1.35097	1.88027	3.35123
8.	Cis-OCP+CYNO	0.98510	1.76221	1.22344	1.35074	1.87075	3.35404
9.	Cis-OCP+CYN	--	--	--	--	--	--
10.	ODB+AC	--	1.75187 1.74477	1.21723	--	--	3.10374 5.48618
11.	ODB+AP	--	1.74462 1.75168	1.22322	--	--	3.11168 5.52234
12.	ODB+CYNO	--	1.75199 1.74489	--	--	--	3.11471
13.	ODB+CYN	--	1.74854 1.74824	--	--	--	--

Hydrogen bond: $O_{(C=O \text{ of KETONE})} \cdots H_{(OH \text{ of OCP})}$.

4.2.2 Atomic Charges (Table 4.2.2)

Atomic charges unlike the electron density are not a quantum mechanical observable and are not unambiguously practicable. Gaussian jobs perform a Mulliken population analysis, which partitions the total charge among the atoms in the molecule/complex. Mulliken population analysis is an arbitrary scheme for assigning charges. Both chlorine atom of free ODB shows positive charge. In present investigation (Table 4.2.2), for ODB + AC, ODB + AP and ODB + CYNO system, only one of the chlorine atom shows positive charge and other shows negative charge. In ODB + CYN both chlorine atom of ODB show positive value but lower than that of free ODB.

In case of ketones, negative charge is estimated on oxygen of C=O. It is maximum negative charge for AP and minimum for AC. For other complexes minimum for Cis-OCP + AC. In case of OCP, negative charge is noted on oxygen of -OH. In all complex system, Trans-OCP + CYN shows lowest negative charge on oxygen of -OH. In Cis-OCP + AP; positive charge

on hydrogen atom of -OH increases. In all complex system, Trans-OCP + CYN shows lowest value positive charge on hydrogen atom of -OH. Chlorine of OCP shows negative charge for all Cis/Trans-OCP + Ketone systems in present investigation (Table 4.2.2). It is observed that maximum negative charge for complex Cis-OCP + AC. In OCP + CYN, chlorine atom of OCP shows lowest negative value. In case of ketones, positive charge on carbon of C=O is minimum for AP.

Table 4.2.2: Optimized Mulliken atomic charges of systems at B3LYP level using 6-31G (d) basis set.

Sr. No.	System	O _(OH)	H _(OH)	Cl _(OCP)	Cl _(ODB)	O _(C=O)	C _(C=O)
1	ODB	-	--	--	0.121	--	--
2	AC	--	--	--	--	-0.430	--
3	AP	--	--	--	--	-0.452	0.408
4	CYNO	--	--	--	--	-0.446	0.452
5	CYN	--	--	--	--	--	--
6	Trans-OCP+AC	-0.672	0.449	-0.023	--	-0.454	0.471
7	Trans-OCP+AP	-0.671	0.460	-0.023	--	-0.484	0.417
8	Trans-OCP+CYNO	-0.673	0.451	-0.024	--	-0.475	0.472
9	Trans-OCP+CYN	-0.621	0.414	-0.000	--	--	--
10	Cis-OCP+AC	-0.676	0.460	-0.035	--	-0.442	0.471
11	Cis-OCP+AP	-0.676	0.463	-0.033	--	-0.476	0.425
12	Cis-OCP+CYNO	--	--	--	--	--	--
13	Cis-OCP+CYN	-0.642	0.434	-0.031	--	--	--
14	ODB+AC	--	--	--	0.040	-0.423	0.457
					-0.001		
15	ODB+AP	--	--	--	0.041	-0.450	0.413
					-0.001		
16	ODB+CYNO	--	--	--	0.041	-0.444	0.456
					-0.002		
17	ODB+CYN	--	--	--	0.016	-	--
					0.014		

4.2.3 Energy and dipole moment (Table 4.2.3)

Negative value of energy indicates the stability. For individual molecules, it follows: ODB > AP > CYNO > CYN > AC. The most stable complexes are ODB + ketones which are in the order: ODB + AP > ODB + CYNO > ODB + CYN > ODB + AC. Cis-OCP + AC complex is least is least stable.

Complexes having maximum dipole moment follow: Trans-OCP + AP > Trans-OCP + AC.

Table 4.2.3: Optimized energy and dipole moment of systems at B3LYPLevel using 6-31G (d) basis set.

Sr. No.	Name of system	Energy (a. u.)	Dipole Moment(Debye)
1	ODB	-1151.3433	3.5027
2	AC	-193.1546	2.7383
3	AP	-384.8959	2.9969
4	CYNO	-309.8912	3.0732
5	CYN	-235.8804	0.0002
6	<i>Trans</i> -OCP+AC	-960.2312	5.5213
7	<i>Trans</i> -OCP+AP	-1151.9707	6.2009
8	<i>Trans</i> -OCP+CYNO	-1076.9673	5.9452
9	<i>Trans</i> -OCP+CYN	-1076.9074	5.9452
10	<i>Cis</i> -OCP+AC	-960.2302	3.4140
11	<i>Cis</i> -OCP+AP	-1151.9704	3.9839
12	<i>Cis</i> -OCP+CYNO	-1076.9662	--
13	<i>Cis</i> -OCP+CYN	-1002.9449	0.9121
14	ODB+AC	-1344.5940	0.8799
15	ODB+EMK	-1383.9061	0.9261
16	ODB+AP	-1536.3340	0.6741
17	ODB+CYNO	-1461.3296	1.1681
18	ODB+CYN	-1387.3164	2.9289

4.2.4 HOMO and LUMO

The HOMO is the orbital that could act as an electron donor since it is the outermost (highest energy) orbital containing electrons. The LUMO is the orbital that could act as the electron acceptor since it is the innermost (lowest energy) orbital that has room to accept electrons. Hardness is dependent on the closeness of the frontier orbitals. When the HOMO and LUMO are close together, the energy difference between the two is very low and the absolute hardness is low. In this case, molecule/s can easily share orbitals to create covalent bonds/complexing. In other words, we can say strong intermolecular interactions. When the frontier orbitals are far apart, their difference in energy is large. Typically, the ionization energy in the LUMO is high in this situation. In such molecules, the absolute hardness is high and they are not willing to share covalent bonds i.e. weak intermolecular interactions.

Generally, polarizable molecules form strong bonds with other polarizable molecules, whereas unpolarizable molecules form strong bonds with other unpolarizable molecules.

4.2.4.1 HOMO:

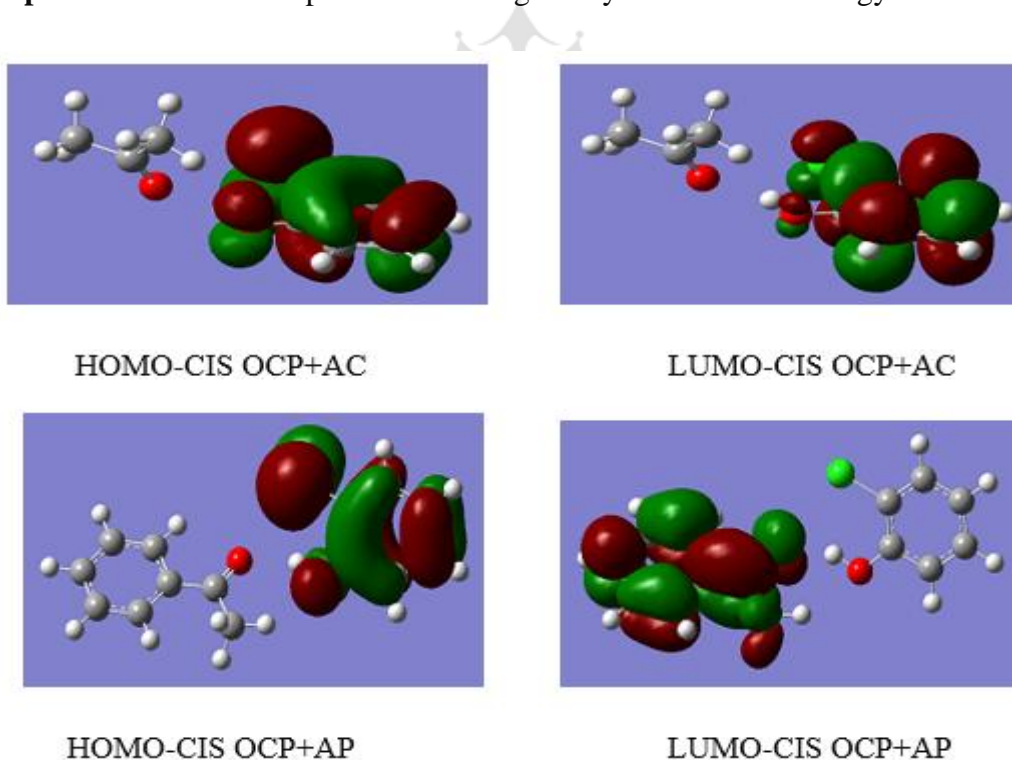
I) Individual: For individual negative value as follows: AP > AC > CYNO > ODB > CYN. High negative value is observed in the case of AP and low value is observed in the case of CYN.

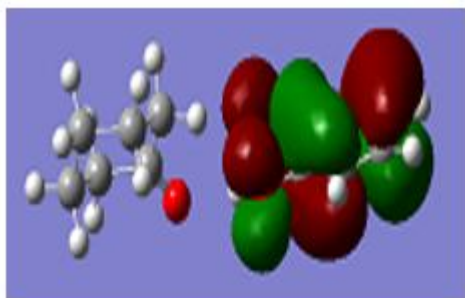
II) Complexes: All complexes show lower negative value as compared to the corresponding individual molecules of ketones.

4.2.4.2 LUMO:

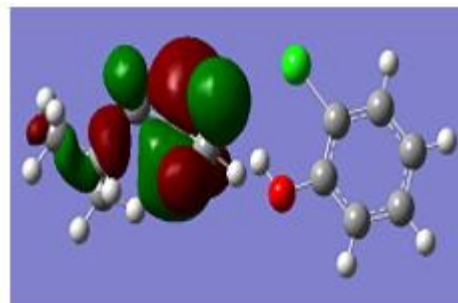
I) Individual: For individual negative value as follows: AP > CYNO > ODB > AC > CYN. Negative value is low observed in the case of CYN.

II) Complexes: All ODB complexes are having nearly same LUMO energy with individuals.

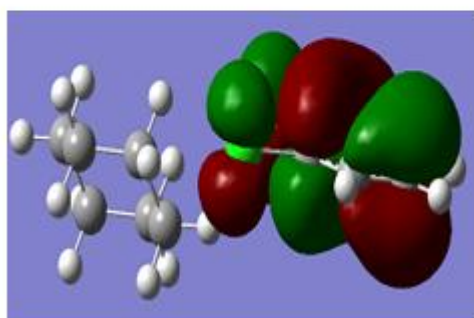




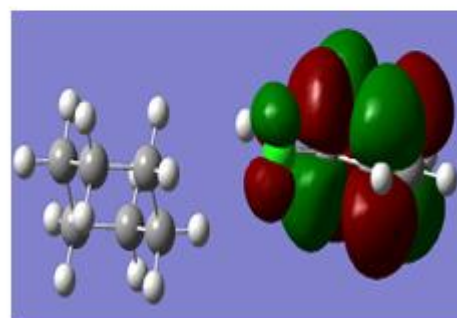
HOMO-CIS OCP+CYNO



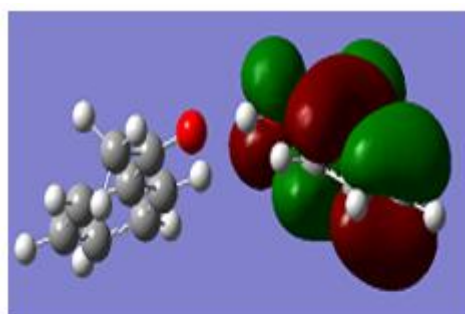
LUMO-CIS OCP+CYNO



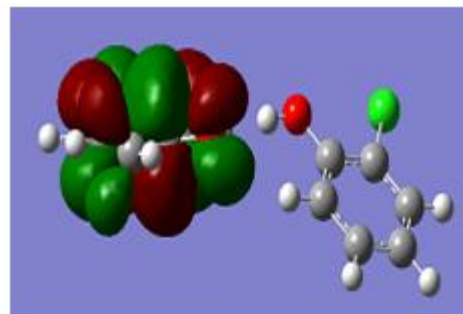
HOMO-CIS OCP+CYN



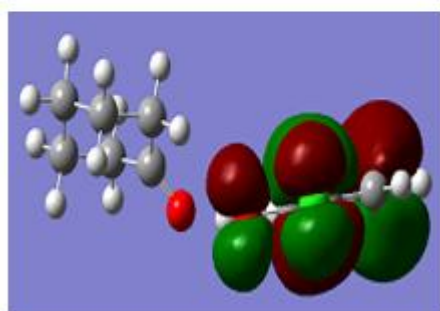
LUMO-CIS OCP+CYN



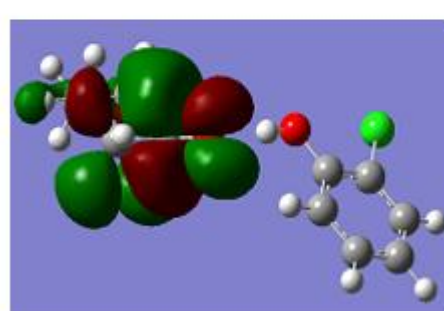
HOMO-TRANS OCP+AP



LUMO-TRANS OCP+AP



HOMO-TRANS OCP+CYNO



LUMO-TRANS OCP+CYNO

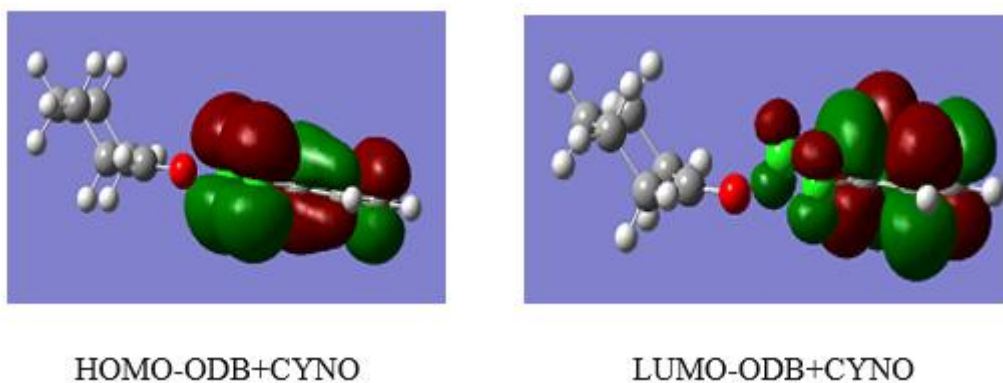


Fig 4.2: Optimized geometries of molecule by DFT method atB3LYP/6-31G (d) level.

CONCLUSIONS

The compound data provide evidence for the existence of interactions between ODB and OCP with ketones studied by using IR Spectroscopy and theoretical Chemistry. Spectrum of some OCP + Ketones shows to absorption bands for -OH. The Sharp band is due to free -OH while weak band is due to H-bonded -OH. Presence of hydrogen bonding between -OH of OCP with carbonyl oxygen of studied ketones and absence of hydrogen bonding in systems of ODB+ketones is confirmed by FTIR. Gaussian also predicts dipole moments and higher multipole moments. This term indicates the nature i.e. polar or nonpolar. The dipole moment is the first derivative of the energy with respect to an applied electric field. It is a measure of the asymmetry in the molecular charge distribution and is given a vector in three dimensions. Generally, polarizable molecules form strong bonds with other polarizable molecules, whereas unpolarizable molecules form strong bonds with other unpolarizable molecules.

ACKNOWLEDGMENT

The author is thankful to Research guide; Dr. A. B. Sawant, President of K. V. N. Naik Shikshan Prasarak Sanstha's Nashik & Principal of K. V. N. Naik College, Nashik for promoting research.

REFERENCES

1. Ezhil Pavai R, Vasantharani P & Kannappan A N, Indian J Pure Appl Phys, 2007, **45**, 587.
2. Ali A, Yasmin A & Nain A K, Indian J Pure Appl Phys, 2002, **40**, 315.
3. Pimental G C and McClellan A L; "Hydrogen Bond", W H Freeman, San Francisco (1960).
4. Josesten M D and Schaad L; "Hydrogen Bonding", Marcel Dekker, New York (1974).
5. Vinogradov S N and Linnell R H; "Hydrogen Bonding", Van NostandReinhold, New York (1971).
6. Legon A C and Millen D; J ChemSoc Rev, 21 (1992) 71.
7. Scheiner S; Acc Chem Res, 27 (1994) 402.

8. Etter M C; Acc Chem Res, 23 (1990) 120.
9. Gordon M S and Jenson J H; Acc Chem Res, 29 (1996) 536.
10. Hibbert F and Emsley J; Adv Phys Org Chem, 26 (1990) 255.
11. Kirby A J; Acc Chem Res 30 (1997) 290.
12. Desirajau G R; Crystal Engineering: "The design of Organic Solids", Elsevier Amsterdam (1989).
13. Jeffery G A and Saenger W; "Hydrogen Bonding in Biological Structures", Springer-verlag Barlin,(1991).
14. Gerit J A, Kreevoy M M, Cleland W W and Frey P A; Chem Biol, (1997)250.
15. Green R D; "Hydrogen Bonding by C-H Groups", Willey: New York, 974.
16. Steinger T and Saenger S; J Am Chem Soc, 114 (1992) 10146.
17. Gu Y, Kar T and Scheiner S; J Am Chem Soc, 121 (1999) 9411.
18. Allerhand A and Schleyer P V R; Am Chem Soc, 85 (1963) 1715.
19. Turi L and Dannenberg J J; Phy Chem, 99 (1995) 639.
20. Scheiner S, Grabowski S J and Kar T; J Phy Chem, 105 (2001) 10607.
21. Muchall H M; J PhyChem, 105 (2001) 632.
22. Desiraju G R; Acc Chem Res, 29 (1996) 441.
23. Derewenda Z S, Lee L and Derewenda U; J Mol Bio, 252 (1995) 248.
24. Metzger J and Pullman A; Bull Soc Chim France, 1166 (1948).
25. Zahradnik R and Kontecki J; Coll Czech Chem Comm, 26 (1961) 156.
26. Vitry J and Metzger J; Bull SocChim France, 1784 (1963).
27. Bansal R K, Karaghiosoff K, Gupta N, Schmidpeter A and Spindler C; Chem Ber, 124 (1991) 475.
28. Bansal R K, Gupta N, Kabra V, Spindler C, Karaghiosoff K and Schmidpeter A; Heteroatom Chem, 3(1992)259.
29. Gupta N, Jain C B, Heinicke J, Bharatiya N, Bansal RK and Jones P G; Heteroatom Chem, 9(1998) 259.
30. Wang B, Hinton J F and Polay P; J Phy Chem, 107 (2003) 4683.
31. Cubero E, Orozco M, Hobza P and Luque F J; Phys Chem, A 103(1999) 6394.
32. Hobza P and Havlas Z; Chem Phys Lett, 303 (1999) 447.
33. Scheiner S and Kr T; J Phy Chem, A 106 (2002) 1784.
34. Kadam U B, Hasan Mehdi and Sawant A B, International Journal of Chemical Sciences 4 (2) (2006) 458.
35. Nazir H, Yildiz M, Yilmaz H, Tahir M N and Ulku D; J Mol Struct, 524 (2000) 241.
36. Cuma M, Scheiner S and Kar T; J Am Chem Soc, 120 (1998) 10497.
37. Filarowski A, Glowiak T and Koll A; J Mol Struct, 484 (1999) 75.
38. Raissi H, Moshfeghi E, Jalbout A F, Hosseini M S and Fazli M; Int J Quant. Chem,107 (2007) 1835.
39. Cuma M, Scheiner S and Kar T; J Mol Struct, (Theochem) 467 (1999) 37.
40. Chung G, Kwon O and Kwon Y; J Phys Chem, A 102 (1998) 2381.
41. Fores M and Scheiner S; Chem Phys 246 (1999) 65.
42. Cheng C, Shyu S F and Hsu F S; Int J Quant Chem, 74 (1999) 395.
43. Barone V, Palma P and Sanna N; PhysLett, 381 (2003) 45.
44. R M Silverstein and F X Webster; "Spectrometric Identification of Organic Compounds" 6thed New York (2006).
45. Frisch M J, Trucks G W, Schlegel H B, Scuseria G E, Gill P M W, Johnson B, Chen W, Wong M W, Gonzalez C and Pople J A; Gaussian, Inc., Wallingford CT, 2004.