



Research Article

Theoretical and experimental study of infrared spectral data of 2-bromo-4-chlorobenzaldehyde

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Abstract

Infrared (IR) spectroscopy is one of the most common spectroscopic techniques and serves as an effective tool for characterizing compound and solvent interactions. In this research, experimental and theoretical spectral investigation and conformational analysis of 2-bromo-4-chlorobenzaldehyde were performed by IR spectroscopy and density functional theory (DFT). The solvent effect on carbonyl stretching vibration and the correlations between the experimental IR data for different solvents scales were also investigated. The reliability of a suitable theoretical model for the solvent effect was evaluated using experimental data. The scale from linear solvation energy relationships obtained using both experimental and theoretical data is useful to study solvent effect.

Keywords IR spectra · Di-halogenated benzaldehydes · Solvent effect · DFT · LSER

1 Introduction

IR spectroscopy is a useful analytical technique for both qualitative and quantitative analysis and it is based on molecular vibrational transitions. Powders, films, liquids, solutions, pastes, fibres, gases and surfaces can all be examined with IR technique. It is a useful tool to identify functional groups in organic and inorganic compounds. Different functional groups absorb different ranges of frequencies. The polarity of the solvent has influence on IR spectra of the compounds because of the interaction between solvent and compound and this is known as solvent effect. Solvent effects on IR data are well known [1–3] and characteristic IR stretching vibrations have been investigated [4, 5].

Benzaldehyde derivatives (aromatic aldehydes) are commonly employed in the field of pharmaceutical chemistry and in the chemical industry in the production of flavoring agents, agrochemicals, cosmetics, textiles, dyes

as well as ligands in metal coordination chemistry. For example, substituted benzaldehydes can be designed to increase the oxygen affinity of human hemoglobin and to inhibit the sickle erythrocytes. Further, substituted chalcones obtained by using with benzaldehydes derivatives show anti-bacterial, anti-tumor, anti-inflammatory, anti-fungal, anti-microbial and anti-oxidant properties [6, 7].

Benzaldehyde and its derivatives have been the subject of several spectroscopic studies [6–19]. On the other hand, there are several approaches such as Kirkwood-Bauer-Magat (KBM) [20], solvent acceptor number (AN) [21], Swain [22] and linear solvation energy relationships (LSER) [23] scales in order to determine solvent influence on IR and Raman spectra. The KBM scale presented in 1937 was the first theoretical equation. Other scales were also developed between 1978 and 1983. These solvent parameters have been used to explain solvent effect for a variety of the compounds. In 2001, the theoretical carbonyl stretching frequencies of dialkyl ketones in seven different

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organic solvents were investigated by KBM and AN [24]. In 2002–2013, only the experimental carbonyl stretching frequencies of 5-methyl-7-methoxy-iso-flavone [25], 2-acetylthiophene [26], trimethyl phosphate [27], methyl methacrylate [28], 1,3-indanedione [29], butyl methacrylate [30], ethyl methacrylate [31], N-tert-butylacetamide [32] in various solvents were investigated by LSER, KBM or AN. Both experimental and theoretical studies employing these equations between 2012 and 2015 were related to flurbiprofen [33] and vinyl acetate [34]. Recently, theoretically, some IR and NMR shifts of the benzyne (KBM and AN) [35] and carbene (KBM and LSER) [36] complexes were investigated by LSER, KBM or AN whereas NH and carbonyl stretching frequencies of 1-(4-pyridyl) piperazine [37] and 4-bromo-2-halogenobenzaldehyde [38] correspondingly were investigated by Swain, LSER, KBM and AN.

Even though, as outlined above, influences of different substituents on benzaldehydes such as dihydroxybenzaldehydes, fluorobenzaldehydes or 2-bromo-5-fluorobenzaldehyde [6–19] were studied by vibrational spectroscopy and density functional theory (DFT), to the best of our knowledge, in literature, there is no experimental and theoretical IR spectral investigation of 2-bromo-4-chlorobenzaldehyde (Cas No: 84459-33-6). The current investigation is in continuation with our interests in studying the experimental vibrational spectra of di-halogenated benzaldehydes as 4-chloro-3-fluorobenzaldehyde [6] and 2-fluoro-4-bromobenzaldehyde [7], and the theoretical solvent effect on carbonyl stretching of 4-chloro-3-halogenobenzaldehydes [39] and 4-bromo-2-halogenobenzaldehyde (Cas No: 158435-41-7 of 4-bromo-2-chlorobenzaldehyde) [38]. The main aim of this research was to characterize the IR bands of 2-bromo-4-chlorobenzaldehyde by experimental (IR spectroscopy) and DFT methods. Further, solvent effect on carbonyl stretching of the compound was studied.

2 Experimental

All solvents and 2-bromo-4-chlorobenzaldehyde were purchased from Merck and Sigma-Aldrich Co., respectively. IR spectra of 2-bromo-4-chlorobenzaldehyde in solid phase and in n-hexane, cyclohexane, chloroform, benzene, toluene as non-polar solvents and ethanol, 2-propanol, methanol as polar solvents were recorded by Bruker Optics IFS66v/s FTIR spectrometer and Perkin Elmer FTIR spectrophotometer correspondingly. All spectra were reported in the region of $4000\text{--}400\text{ cm}^{-1}$ at 2 cm^{-1} resolutions. Concentrations of the compound in solutions were between 0.21 and 0.25 mol/l.

3 Calculations

DFT methods are widely used for the quantum mechanical calculations of the different structures. The accuracy of theoretical predictions strongly depends on chosen functional and basis set. Methods, functional and basis sets chosen in this search showed quite accurate results for parameters of the experimentally single crystal structures of these type compounds [6, 7]. Gas phase optimization process of trans and cis forms of 2-bromo-4-chlorobenzaldehyde in C_s symmetry (Fig. 1) was performed at the HF, MP2 and B3LYP level of theory using the aug-cc-pVDZ basis set in Gaussian 09 [40]. For the gas phase optimization, 6-311+G(3df,p) and 6-31G(d,p) basis sets were also used with B3LYP. The computations for the liquid phase in the non-polar or polar solvents were conducted using B3LYP/6-31G(d,p) method and the polarizable continuum model. Potential energy distribution (PED) was computed by the program of vibrational energy distribution analysis 4 [41]. Experimental and theoretical carbonyl stretching frequency was correlated by KBM, AN, Swain and LSER solvent models as described earlier [39]. The solvent parameters of these models for the solvents used were taken from Ref. [39].

4 Results and discussion

4.1 Structural analysis

The conformational energy parameters of the trans and cis forms of 2-bromo-4-chlorobenzaldehyde in the gas phase are given in Table 1. We reported the conformational analyses of 4-bromo-2-chlorobenzaldehyde [38] and 4-chloro-3-bromobenzaldehyde [39], related to bromo- and chloro-substituted benzaldehydes and showed that

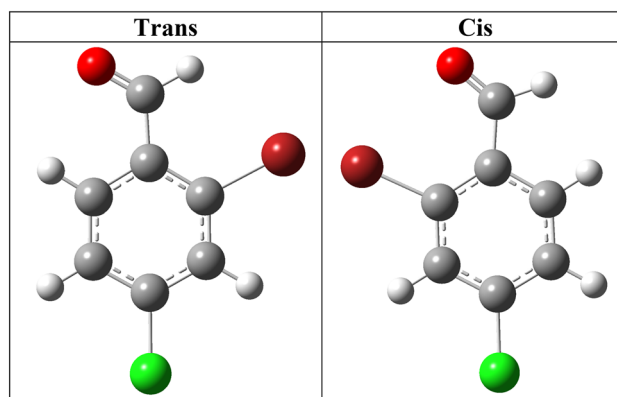


Fig. 1 Conformations of 2-bromo-4-chlorobenzaldehyde

Table 1 Conformational energy parameters in the gas phase

Method	Conformer	Energy (Hartree)	Relative energy (kcal/mol)	Mole fraction (%)	Dipole moment (Debye)
HF/aug-cc-pVDZ	Trans	-3374.19196835	0.00	99.8	1.65
	Cis	-3374.18618258	3.63	0.2	3.54
MP2/aug-cc-pVDZ	Trans	-3375.61202079	0.00	98.7	2.01
	Cis	-3375.60795523	2.55	1.3	3.72
B3LYP/aug-cc-pVDZ	Trans	-3378.78588833	0.00	98.8	1.91
	Cis	-3378.78170327	2.63	1.2	3.22
B3LYP/6-311 + G(3df,p)	Trans	-3378.85926055	0.00	98.5	1.96
	Cis	-3378.85529502	2.49	1.5	3.21
B3LYP/6-31G(d,p)	Trans	-3376.27565886	0.00	99.2	1.60
	Cis	-3376.27115219	2.83	0.8	3.95

the trans isomer is more stable in the gas phase and in solutions for both compounds. For all levels of theory, the trans conformer of 2-bromo-4-chlorobenzaldehyde is more stable than cis and its relative percentage is almost 100%. Further, gas phase computations using MP2, HF and B3LYP with the aug-cc-pVDZ basis set and the use of B3LYP with the 6-311 + G(3df,p) and 6-31G(d,p) basis sets do not show any change. On comparing the results of expensive MP2/aug-cc-pVDZ calculations, it is seen that other levels of theory can be used for such classes of compounds. Turning to the conformer in solutions of 2-bromo-4-chlorobenzaldehyde, the energetic parameters are listed in Table 2. Trans forms of the compound in the solutions are also more stable than cis like in the gas phase. According to

the energy calculations from hexane to dimethylsulfoxide, the compound prefers the trans conformer in the solutions with approximate probabilities of 98–93%. Conformations with higher dipole moment are commonly less stable [6]. The results are similar for the compound in all solvents.

The computed bond lengths are in good agreement with our previous experimental values [6, 7]. For example, carbonyl bond lengths of 4-chloro-3-fluorobenzaldehyde and 2-fluoro-4-bromobenzaldehyde in solid were found as 1.206 Å and 1.233 Å [6, 7]. For the compound studied in this work, this bond length has been computed as 1.217 Å and 1.218–1.220 Å (Table 3) in gas phase and in solutions, respectively. Similarly, C–Cl and C–Br bond lengths of these compounds were experimentally reported as

Table 2 Conformational energy parameters in solution

Solvent	B3LYP/6-31G(d,p)	ϵ	Energy (Hartree)		%	
			Cis	Trans	Cis	Trans
n-Hexane		1.89	-3376.27359817	-3376.27753691	1.5	98.5
n-Heptane		1.92	-3376.27365157	-3376.27757651	1.5	98.5
Cyclohexane		2.02	-3376.27383332	-3376.27771085	1.6	98.4
1,4-Dioxane		2.21	-3376.27413369	-3376.27793136	1.7	98.3
Tetrachloromethane		2.24	-3376.27415981	-3376.27795045	1.8	98.2
Benzene		2.28	-3376.27422004	-3376.27799440	1.8	98.2
Toluene		2.38	-3376.27435953	-3376.27809591	1.9	98.1
Diethylether		4.26	-3376.27588425	-3376.27917904	2.9	97.1
Chloroform		4.81	-3376.27610524	-3376.27933203	3.2	96.8
Tetrahydrofuran		7.52	-3376.27688429	-3376.27986329	4.1	95.9
Dichloromethane		9.08	-3376.27712873	-3376.28002741	4.4	95.6
2-Butanol		17.26	-3376.27768876	-3376.28039879	5.3	94.7
2-Propanol		18.60	-3376.27781738	-3376.28048318	5.6	94.4
Acetone		21.01	-3376.28050768	-3376.27785483	5.7	94.3
Ethanol		24.60	-3376.27795873	-3376.28057552	5.9	94.1
Methanol		32.60	-3376.27807666	-3376.28065225	6.1	93.9
Acetonitrile		36.64	-3376.27810951	-3376.28067357	6.2	93.8
Dimethylsulfoxide		47.00	-3376.27819302	-3376.28072768	6.4	93.6

Table 3 Carbonyl bond length (Å), frequency (cm⁻¹) and dipole moment (Debye) of the compound

Medium B3LYP/6-31G(d,p)	Dipole moment	Bond length	$\nu(\text{C}=\text{O})$ Theo.I ^a	$\nu(\text{C}=\text{O})$ Theo.II ^a	$\nu(\text{C}=\text{O})$ Exp.
Solid	–	–	–	–	1690
Gas	1.60	1.217	1717	1723	–
n-Hexane	1.78	1.218	1709	1715	1706
n-Heptane	1.78	1.218	1709	–	–
Cyclohexane	1.79	1.218	1709	1714	1705
1,4-Dioxane	1.81	1.218	1708	–	–
Tetrachloromethane	1.81	1.218	1708	–	–
Benzene	1.82	1.218	1707	1713	1701
Toluene	1.83	1.218	1707	1713	1701
Diethylether	1.93	1.219	1702	–	–
Chloroform	1.95	1.219	1701	1707	1699
Tetrahydrofuran	2.00	1.220	1699	–	–
Dichloromethane	2.01	1.220	1698	–	–
2-Butanol	2.05	1.220	1697	–	–
2-Propanol	2.06	1.220	1696	1702	1704
Acetone	2.06	1.220	1696	–	–
Ethanol	2.07	1.220	1696	1701	1703
Methanol	2.07	1.220	1695	1701	1702
Acetonitrile	2.08	1.220	1695	–	–
Dimethylsulfoxide	2.08	1.220	1695	–	–

^aScaled frequencies with 0.9595 and 0.9627 [42] for B3LYP/6-31G(d,p)

1.732 Å and 1.893 Å whereas these bond lengths were computed as 1.750–1.753 Å and 1.915–1.916 Å in the gas phase or in solutions.

4.2 IR study

Experimental and theoretical IR data of 2-bromo-4-chlorobenzaldehyde are listed in Table 4 and the frequencies were scaled by 0.9683 [42]. The compound consists of fourteen atoms and has thirty-six normal vibrational modes. These modes by C_s point group are given as $\Gamma_v = 25A' + 11A''$ irreducible representations. Experimental and simulated IR spectra of 2-bromo-4-chlorobenzaldehyde are shown in Fig. 2.

For the high frequency region, CH stretching vibrations of 4-chloro-3-fluorobenzaldehyde and 2-fluoro-4-bromobenzaldehyde were observed at 3094, 3069, 3042 cm⁻¹ and 3086, 3075, 3032 cm⁻¹, respectively [6, 7]. The corresponding bands of the title compound are observed in the expected region as 3100, 3088, 3019 cm⁻¹. One of the most important functional groups of the compound is the formyl group. Carbonyl and CH stretching vibrations of this group are observed at 1690 cm⁻¹ and 2873 cm⁻¹. Theoretical values were computed at 1709 cm⁻¹ and 2878 cm⁻¹. Observed band about 2932 cm⁻¹ in IR spectrum is due to the Fermi resonance which occurs between CH stretching fundamental and overtone of CHO deformation band [6,

7]. The IR bands observed at 1392 cm⁻¹ and 1001/988 cm⁻¹ are assigned to CH rocking and wagging of formyl group. Theoretical values are found at 1380 cm⁻¹ and 1000 cm⁻¹. All peaks are observed in the expected region [6–19]. CF stretching vibration of para chloro–meta fluoro compound [6] was shown as 1253 cm⁻¹. For the current study, CBr stretching vibration of para chloro–ortho bromo compound are dominated in two different bands as 1251 and 568 cm⁻¹. Further, it can be mentioned that the CBr stretching of para bromo–ortho fluoro compound [7] were shown as 658 cm⁻¹.

Table 3 gives experimental and theoretical data for solvent effect on carbonyl stretching frequency as one of the most important functional groups of the compounds. Figure 3 shows the experimental carbonyl stretching bands of 2-bromo-4-chlorobenzaldehyde in non-polar and polar solvents. The carbonyl stretching bands in solutions appear in the region of 1699–1706 cm⁻¹. Theoretical frequencies (I) and (II) were multiplied by the scaling factor of 0.9595 and 0.9627 for the B3LYP/6-31G(d,p) method, which were obtained in this study and reported [42]. These bands in the solvents were computed as the region of 1695–1709 cm⁻¹ and 1701–1715 cm⁻¹, respectively. These results show an obvious correlation for carbonyl frequency. The root mean square deviations (RMSD) of the theoretical and experimental frequencies for carbonyl stretching were found as 5.73 cm⁻¹ and 8.09 cm⁻¹

Table 4 Comparison of the experimental and computed vibrational frequencies (cm^{-1})

Mode	Assignment	Experimental	B3LYP/6-311+G(3df,p)	
			Trans	
	PED ($\geq 10\%$)	IR	IR	I_{IR}
1 (A')	v(CH) (95)	3100	3113	2.93
2 (A')	v(CH) (95)	3088	3106	2.82
3 (A')	v(CH) (94)	3019	3087	0.08
4 (A')	v(CH) (100)	2873	2878	43.64
5 (A')	v(C=O) (92)	1690	1709	284.79
6 (A')	v(CC) (95)	1578	1561	209.52
7 (A')	v(CC) (85) + β (CH) (10)	1554/1508	1530	29.95
8 (A')	v(CC) (42) + β (CH) (42)	1460/1442	1441	35.57
9 (A')	ρ (CH) (45) + v(CC) (40)	1392	1380	3.49
10 (A')	v(CC) (45) + ρ (CH) (41)	1372	1362	57.53
11 (A')	v(CC) (88)	1283	1269	3.58
12 (A')	v(CBr) (43) + v(CC) (40)	1251	1239	32.44
13 (A')	β (CH) (45) + v(CC) (42)	1198	1178	51.85
14 (A')	β (CH) (70) + v(CC) (157)	1123	1110	23.46
15 (A')	v(CC) (51) + β (CH) (29) + v(CCl) (10)	1098/1085/1067	1077	66.74
16 (A')	β (CC) (51) + v(CC) (30) + v(CCl) (10)	1035	1019	29.60
17 (A'')	ω (CH) (91)	1001/988	1000	0.60
18 (A'')	γ (CH) (90)	949	964	0.04
19 (A'')	γ (CH) (94)	865	870	11.80
20 (A')	v(CC) (15) + v(C-CHO) (15) + v(CBr) (10)	836	822	94.53
21 (A'')	γ (CH) (91)	822	821	24.13
22 (A')	β (CC) (52) + v(CC) (30)	734	716	15.94
23 (A'')	γ (CC) (90)	692	692	0.84
24 (A')	β (CC) (86) + v(CCl) (10)	657/645	649	1.93
25 (A')	β (CC) (40) + v(CBr) (40) + v(CCl) (10)	568	553	10.53
26 (A'')	γ (CC) (85) + γ (C-CHO) (10)	542	546	2.00
27 (A'')	γ (CC) (68) + γ (C-CHO) (18)	436	440	6.90

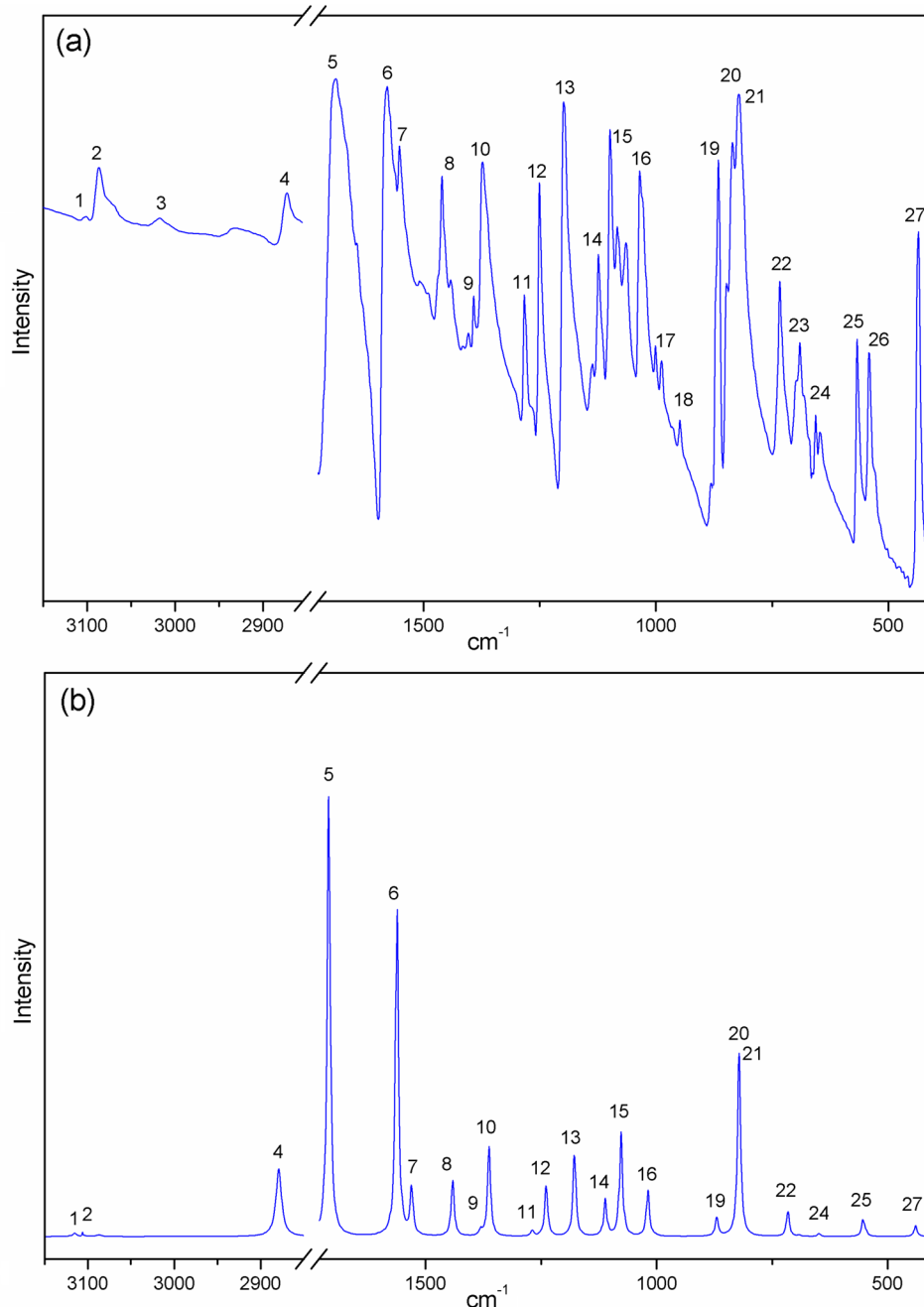
v, β , γ , ρ , ω and τ denote stretching, in plane bending, out of plane bending, rocking, wagging and torsion, respectively

according to the scaling factors of the present study and literature whereas it was computed as 33 cm^{-1} for this level in literature [42].

Turning to the solvent scales for the carbonyl stretching frequencies, there is a linear correlation between theoretical frequencies and KBM parameters for both 18 solvents ($1718.58 - 48.60 f(\epsilon)$ and $R^2: 0.99698$) and for 8 solvents employed ($1718.47 - 48.54 f(\epsilon)$ and $R^2: 0.99637$). There is a good relationship and the negative slope in these equations show that all theoretical frequencies are red shifted while the dielectric constants of solvents increase. KBM considers only the dielectric constant of the solvent and the good correlation shows that PCM model is suitable to probe dielectric constant-induced solvent effects. However, when the experimental data of 2-bromo-4-chlorobenzaldehyde are evaluated by KBM, there is no linear correlation between experimental

frequencies and the KBM parameters. It means that specific and nonspecific solvent effects collectively contribute to solute-solvent interactions and it is inadequate to use single solvent parameter to describe them. Therefore, the single-parameter KBM equation is insufficient to provide an overall description of solvent effects of 2-bromo-4-chlorobenzaldehyde. Similar results were reported for both experimental [25, 27, 29, 31, 33, 34] and theoretical data [34-37] of KBM scales of various compounds. Meanwhile, the AN scale which handles only acidity of the solvent shows poor correlation ($1706.92 - 0.34 \text{ AN}$ and $R^2: 0.57360$) for theoretical frequencies of 18 solvent systems as shown previously [25-27, 31-33, 37] whereas there is a linear correlation between theoretical frequencies and AN' parameters for the system of 8 solvents ($1709.42 - 0.36 \text{ AN}$ $R^2: 0.98894$). However, analogously there is no linear

Fig. 2 Experimental (a) and theoretical (b) IR spectra of 2-bromo-4-chlorobenzaldehyde



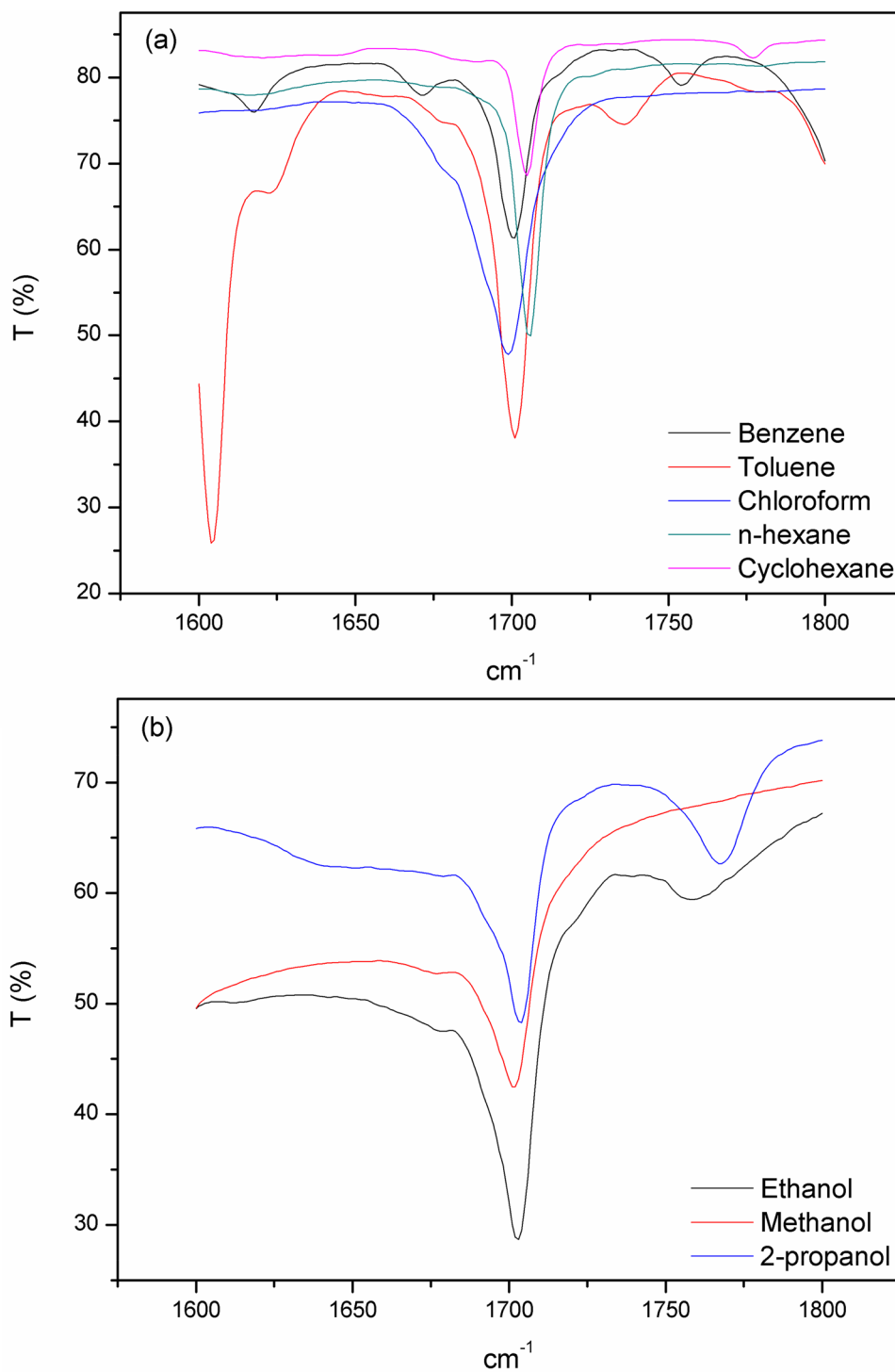
correlation between the experimental frequencies and parameters of AN equation.

Moving to the theoretical carbonyl stretching frequencies both for 18 solvents ($1710.08 - 16.28 A_j - 7.51 B_j$ and $R^2: 0.73485$) and for 8 solvents employed ($1709.22 - 20.92 A_j + 1.02 B_j$ and $R^2: 0.98511$) of Swain equation which considers only specific solute-solvent interactions such as acidity and basicity, the experimental data ($1705.92 + 2.13 A_j - 9.74 B_j$ and $R^2: 0.90560$) help to achieve a realistic assessment. Although the correlation of Swain equation with the experimental data is poor, it is better than those obtained

with KBM and AN [34]. Positive and negative signs of the coefficients represent the blue and red frequency shifts due to the solvent acidity and basicity.

Turning to the LSER solvent scale which considers both specific and non-specific interaction parameters, there are linear and good correlations between theoretical and experimental carbonyl stretching frequencies for the 8 solvents employed whereas there is poor correlation for theoretical data of the 18 solvents. Theoretical and experimental LSER equations are given as follows;

Fig. 3 Experimental IR spectra of carbonyl stretching vibration of 2-bromo-4-chlorobenzaldehyde in non-polar (a) and polar (b) solvents



$$1709.07 - 13.34\pi^* + 5.13\delta - 4.39\alpha - 3.73\beta \quad (R^2 : 0.8143 \text{ for 18 solvents theoretically})$$

$$1708.49 - 23.46\pi^* + 12.18\delta + 3.76\alpha - 4.57\beta \quad (R^2 : 0.98810 \text{ for 8 solvents theoretically})$$

$$1705.15 - 16.67\pi^* + 4.74\delta + 3.76\alpha + 4.78\beta \quad (R^2 : 0.97203 \text{ for 8 solvent experimentally})$$

Negative π^* coefficients as non-specific solvent effect mean that frequencies shift the red region. Hence, the parameters of non-specific interaction such as dielectric constant on the carbonyl stretching frequencies displays a larger effect than parameters of specific interaction such as acidity or basicity. Positive and negative signs represent blue and red shifts of the carbonyl frequencies. When comparing the acidity and basicity regression coefficients, it is concluded that carbonyl frequencies are more susceptible to basicity of the solvents than the acidity.

Both the Swain and LSER models exhibit linear correlations together with experimental data whereas theoretical values show linear correlations with KBM scale. LSER model have also shown similar and good linear results in previous studies [25–27, 29, 31–37]. These indicate that specific and non-specific solute–solvent interactions collectively contribute to the solvent interaction.

5 Conclusions

An experimental and theoretical study of the IR spectral data, solvent effect on carbonyl stretching and conformer of 2-bromo-4-chlorobenzaldehyde can be summarized as the follows:

1. Conformational preference is independent on the solvent and theory employed.
2. Carbonyl frequencies exhibit linear correlations with dipole moment of the compound (R^2 : 0.99746).
3. The computation of 6-311 + G(3df,p) basis set with B3LYP functional for the gas phase is reliable and complement the understanding of IR spectra. The R-square values for IR data is found to be 0.99964. RMSD value for theoretical and experimental frequencies is found as 12.47 cm^{-1} .
4. B3LYP/6-31G(d,p) calculations in solutions show excellent agreement with the experimental data for the carbonyl stretching frequencies. Scaling factor for this level is computed as 0.9595. RMSD value for the experimental and theoretical carbonyl stretching frequencies is found as 5.73 cm^{-1} .
5. With the help of experimental data, an excellent correlation is observed between carbonyl frequencies and LSER parameters while KBM scale show successful correlation together with the theoretical values. Thus, LSER scale gives physically meaningful explanation of solute–solvent interaction and it proves a quantitatively accurate and allows the theoretical prediction for such classes of the compound.

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Compliance with ethical standards

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

References

1. Lobato Silva LF, Paschoal W Jr, Pinheiro GS, da Silva Filho JG, Freire PTC, de Sousa FF, Moreira SGC (2019) Understanding the effect of solvent polarity on the polymorphism of octadecanoic acid through spectroscopic techniques and DFT calculations. *CrystEngComm* 21:297–309
2. Seitsonen AP, Idrissi A, Protti S, Mezzetti A (2019) Solvent effects on the vibrational spectrum of 3-hydroxyflavone. *J Mol Liq* 275:723–728
3. Bilkhan MT, Şahin O, Yurdakul Ş (2017) Experimental and DFT studies of solvent effects on molecular structure and physical properties of dipyrindylamine pyridine based ligand. *J Mol Struct* 1133:580–590
4. Davies JA, Besley NA, Nicholas A, Yang SF, Ellis AM (2019) Infrared spectroscopy of a small ion solvated by helium: OH stretching region of $\text{He}_N\text{-HOCO}^+$. *J Chem Phys* 151:194307
5. Smith BC (2017) The carbonyl group, part I: introduction. *Spectroscopy* 32:31–36
6. Parlak C, Kumar CSC, Fun HK, Kesan G, Rhyman L, Ramasami P, Chandrāju S, Quah CK (2014) 4-chloro-3-fluorobenzaldehyde: experimental (XRD, FT-IR and Raman) and DFT studies. *J Fluor Chem* 163:7–15
7. Tursun M, Kumar CSC, Bilge M, Rhyman L, Fun HK, Parlak C, Ramasami P, Chandrāju S, Quah CK (2015) Crystal structure, vibrational spectra and DFT simulations of 2-fluoro-4-bromobenzaldehyde. *Spectrochim Acta A* 146:342–349
8. Aralakkanavar MK, Katti NR, Jeergal PR, Kalkoti GB, Rao R, Shashidhar MA (1992) $\pi^* \leftarrow \pi$ systems in the electronic absorption spectra of some trisubstituted benzenes. *Spectrochim Acta A* 48:983–991
9. Samdal S, Strand TG, Tafipolsky MA, Vilkov LV, Popik MV, Volden HV (1997) The molecular structure of benzene derivatives part 1. 4-fluorobenzaldehyde by joint analysis of gas electron diffraction, microwave spectroscopy and ab initio molecular orbital calculations. *J Mol Struct* 435:89–99
10. Mollendal H, Gundersen S, Tafipolsky MA, Volden HV (1998) The molecular structure of benzene derivatives, part 2: 4-chlorobenzaldehyde by joint analysis of gas electron diffraction, microwave spectroscopy and ab initio molecular orbital calculations. *J Mol Struct* 444:47–56
11. Anjaneyulu A, Rao GR (1999) Vibrational analysis of substituted benzaldehydes: part I. Vibrational spectra, normal co-ordinate analysis and transferability of force constants of monohalogenated benzaldehydes. *Spectrochim Acta A* 55:749–760
12. Marques MPM, Amorim da Costa AM, Ribeiro-Claro PJA (2001) Evidence of C-H...O hydrogen bonds in liquid 4-ethoxybenzaldehyde by NMR and vibrational spectroscopies. *J Phys Chem A* 105:5292–5297
13. Akai N, Kudoh S, Takayanagi M, Nakata M (2002) Photoinduced rotational isomerization mechanism of 2-chlorobenzaldehyde in low-temperature rare-gas matrices by vibrational and electronic spectroscopies. *J Photochem Photobiol, A* 150:93–100

14. Bednarek P, Bally T, Gebicki J (2002) Characterization of rotameric mixtures in o- and m-substituted benzaldehydes by matrix isolation IR spectroscopy. *J Org Chem* 67:1319–1322
15. Rao PVR, Rao GR (2002) Vibrational analysis of substituted phenols: part II. Transferability of valence force constants. *Spectrochim Acta A* 58:3205–3221
16. Speakman LD, Papas BN, Woodcock HL, Schaefer HF (2004) The microwave and infrared spectroscopy of benzaldehyde: conflict between theory and experimental deductions. *J Chem Phys* 120:4247–4250
17. Qayyum M, Reddy BV, Rao GR (2004) Vibrational analysis of mononitro substituted benzamides, benzaldehydes and toluenes: part I. Vibrational spectra, normal coordinate analysis and transferability of force constants of nitrobenzamides, nitrobenzaldehydes and nitrotoluenes. *Spectrochim Acta A* 60:279–290
18. Itoh T, Akai N, Ohno K (2006) Infrared spectra of p-, m- and o-fluorobenzaldehyde in low temperature argon matrices. *J Mol Struct* 786:39–45
19. Hiremath CS, Yenagi J, Tonannavar J (2007) FT-Raman and infrared spectra and vibrational assignments for 3-chloro-4-methoxybenzaldehyde, as supported by ab initio, hybrid density functional theory and normal coordinate calculations. *Spectrochim Acta A* 68:710–717
20. Kirkwood JG, Edwards RT (1937) The infrared absorption spectrum of hydrogen chloride in solution. *J Chem Phys* 5:14–22
21. Gutmann V, Resch G (1978) The donor-acceptor interactions. Plenum Press, New York
22. Swain CG, Swain MS, Powell AL, Alunni S (1983) Solvent effects on chemical reactivity. Evaluation of anion- and cation-solvation components. *J Am Chem Soc* 105:502–513
23. Kamlet MJ, Abboud JLM, Abraham MH, Taft RW (1983) Linear solvation energy relationships. 23. A comprehensive collection of the solvatochromic parameters, π^* , α , and β , and some methods for simplifying the generalized solvatochromic equation. *J Org Chem* 48:2877–2887
24. Cappelli C, Silva CO, Tomasi J (2001) Solvent effects on vibrational modes: ab initio calculations, scaling and solvent functions with applications to the carbonyl stretch of dialkyl ketones. *J Mol Struct* 544:191–203
25. Liu Q, Sang W, Xu X (2002) Solvent effects on infrared spectra of 5-methyl-7-methoxy-iso-flavone in single solvent systems. *J Mol Struct* 608:253–257
26. Liu Q, Xu X, Sang W (2003) Solvent effects on infrared spectra of 2-acetylthiophene in organic solvents. *Spectrochim Acta A* 59:471–475
27. Tekin N, Cebe M (2004) Solvents effect on infrared spectra of trimethyl phosphate in organic solvents. *Vib Spectrosc* 36:129–133
28. Liu Q, Zheng JP, Fang DJ (2004) Solvent effects on infrared spectra of methyl methacrylate. *Spectrosc Lett* 37:225–233
29. Tekin N, Namli H, Turhan O (2005) Solvents effect on infrared spectra of 1, 3-indanedione in organic solvents. *Vib Spectrosc* 39:214–219
30. Dharmalingam K, Ramachandran K, Sivagurunathan P (2006) FTIR study of molecular interaction in butyl methacrylate-organic solvents mixtures. *Z Phys Chem* 220:739–748
31. Ji X, Li Y, Zheng J, Liu Q (2011) Solvent effects of ethyl methacrylate characterized by FTIR. *Mater Chem Phys* 130:1151–1155
32. Jovic B, Nikolic A, Petrovic S (2013) FTIR spectroscopic study of hydrogen bonding and solvent induced frequency shifts of N-tert-butylacetamide. *J Mol Struct* 1044:140–143
33. Tekin N, Pir H, Sagdin S (2012) Study of the solvent effects on the molecular structure and CO stretching vibrations of flurbiprofen. *Spectrochim Acta A* 98:122–131
34. Chen Y, Zhang H, Liu Q (2014) FT-IR spectroscopy combined with DFT calculation to explore solvent effects of vinyl acetate. *Spectrochim Acta A* 126:122–128
35. Shabani M, Ghiasi R, Yousefi M, Ketabi S (2017) A computational understanding of solvent effect on the structure, electronic, thermochemical, and spectroscopic properties of Ni(η^2 -C₆H₄)(H₂PCH₂CH₂PH₂) complex. *J Chin Chem Soc* 64:925–933
36. Ghiasi R (2018) Exploration of solvent effects on the spectroscopic properties (Ir and ¹³C NMR) in the OsCl₃(≡CCH₂CMe₃)(PH₃)₂ carbyne complex. *J Struct Chem* 59:1052–1057
37. Parlak C (2017) Solvent effects on the NH stretching of 1-(4-pyridyl) piperazine. *J Struct Chem* 58:167–172
38. Fernández D, Parlak C, Bilge M, Kaya MF, Tursun M, Keşan G, Rhyman L, Ramasami P, Şenyel M (2017) Molecular, vibrational and electronic structure of 4-bromo-2-halogenobenzaldehydes: halogen and solvent effects. *Phys Sci Rev* 2:20170058
39. Tursun M, Parlak C (2015) Conformation stability, halogen and solvent effects on CO stretching of 4-chloro-3-halogenobenzaldehydes. *Spectrochim Acta A* 141:58–63
40. Frisch MJ, Trucks GW, Schlegel HB et al (2009) Gaussian 09, revision A.1. Gaussian Inc., Wallingford
41. Jamróz MH (2013) Vibrational energy distribution analysis (VEDA): scopes and limitations. *Spectrochim Acta A* 114:220–230
42. Merrick JP, Moran D, Radom L (2007) An evaluation of harmonic vibrational frequency scale factors. *J Phys Chem A* 111:11683–11700

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