

Thermodynamic functions and IR modes Calculation for newly Azo compounds by Using DFT Model

د. حميدة عيدان سلمان م.م. خضير عبد الحسين م.م. مثنى ناهض علي
جامعة كربلاء / كلية التربية / قسم الكيمياء

الخلاصة :-

تضمن البحث اعتماد برنامج كاوس (Gaussian 03) لاستخدام طريقة الحساب التام على وفق نظرية دوال الكثافة (DFT) وبأسلوب (B3LYP) وباستعمال عناصر القاعدة (STO-3G) وذلك لغرض حساب الأبعاد الهندسية (أطوال وزوايا التآصر) عند الشكل الهندسي المتوازن ، الشحنات ، الدوال الترموديناميكية وكذلك حساب وتصنيف الأنماط الاهتزازية العائدة لطيف الأشعة تحت الحمراء تكافؤياً وتمائلياً وبعده (3N-6) لاثنتين من جزيئات الأزو الغير محضرة سابقاً (التي يرمز لها اختصاراً B , A) ، كما وتم اعتماد برنامج الموباك (MOPAC 2000) لاستخدام طريقة الحساب التقريبية شبه التجريبية (PM3) لحساب حرارة التكوين ، عزم ثنائي القطب ، طاقة المدارات (HOMO, LUMO) وطاقة التأين . وقد وجد إن المركب (B) أكثر استقراراً لكونه يمتلك أقل حرارة تكوين وأيضاً أقل انتروبي ويكون أسهل تأيئاً ، كما تبين من خلال ملاحظة النتائج بان ذرات النتروجين العائدة للمركب (B) تكون أعلى كثافة الكترونية أي أكثر منح للالكترونات لذا نستنتج عند سلوكه كليكاند يكون معقدات أكثر استقراراً . كما أظهرت النتائج بان التردد الأعلى لكلا المركبين (A, B) يكون للمط الاهتزازي الأساسي لمجموعة إل (O-H) .

Abstract

Depended on (Gaussian 03) program for using Density Function Theory calculations (DFT/B3LYP) have been done after complete optimization of geometry on the newly azo (A, B) molecules . The geometric parameter (bond lengths and bond angles) , charge , thermodynamic data and the fundamental vibration frequencies (3N-6) along with their assignments and the corresponding IR absorption intensities for each one of the two molecules where , also, The MOPAC Computational Packages (semi-empirical method , PM3 model) employed through out this study to compute the heats of formations, dipole moments, orbital energies (HOMO, LUMO) and ionization energies . The compound –B is more stability because it has less heats of formation and entropy , and easier ionization than compound-A , the shown results that each one nitrogen atom of compound-B highest electron densities than compound-A . The higher frequencies values for the (O-H) stretch fundamental vibration mode.

Keyword: DFT study, thermodynamic functions, IR studies.

Introduction

Azo compounds, with tow phenyl rings separated by an azo (-N=N-) group, this molecules are a very important in research both fundamental and application.

Azo compounds have been used for a long time as dyes in industry [1]. In addition, azo compounds are used in analytical chemistry as indicators in pH, redox, or complexometric titration [2,3]. Some azo compounds have shown a good antibacterial activity [4,5]. The existence of an azo moiety in different types of compounds has caused them to show pesticidal activity [6]. Because of the good thermal stability of azo compound, one of the most important applications of azo compound is in the optical properties in applications such as optical recording medium [7-9], toner [10,11], ink-jet

printing [12,13], and oil-soluble lightfast dyes [14]. Recently, azo metal chelates have also attracted increasing attention due to their interesting electronic and geometrical features in connection with their application for molecular memory storage, nonlinear optical elements, and printing systems [8,10,15]. Metal azo complex dyes are used for DVD-R (digital versatile disc-recordable) as recording layer.

The aim of present work is to report the optimized geometries, heats of formations, dipole moments, orbital energies (HOMO, LUMO), ionization energies, charge, thermodynamic data and the fundamental vibration frequencies (3N-6) along with their assignments and the corresponding IR absorption intensities for each one of the tow molecules (Fig. 1) by calculation based on the (DFT/B3LYP) and (MINDO/3 model).

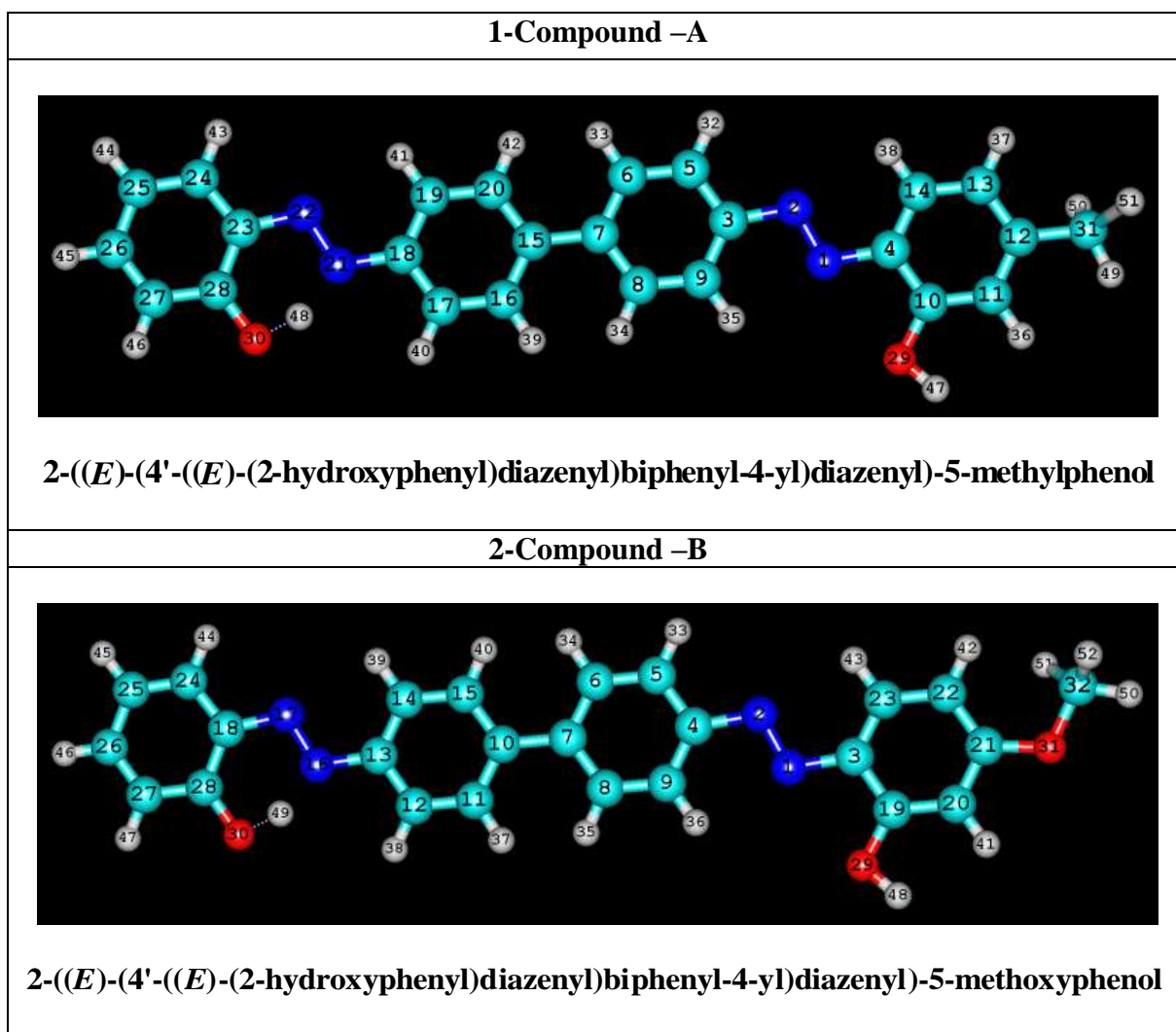


Fig 1: compounds A and B.

Results and Discussion

For the A and B molecules , the calculated geometric parameters (bond lengths and bond angles), According to the results of the calculated geometric parameters (table.1) , show that each one of a bond length ($C_{11}-C_{12}$, $C_{12}-C_{13}$) in compound-A smaller than their identical in compound-B ($C_{20}-C_{21}$, $C_{21}-C_{22}$), and the bond angle value which is located the group substituted in compound-A ($\angle C_{11}C_{12}C_{13}$) bigger than identical in compound-B ($\angle C_{20}C_{21}C_{22}$), whereas each one of the bond angles values ($\angle C_{13}C_{12}C_{31}$, $\angle N_2N_1C_4$) in compound-A smaller than their identical in compound-B ($\angle C_{22}C_{21}O_{31}$, $\angle N_2N_1C_3$), and all this might due to Resonance effect of Methoxy group which is stronger pushing of electrons than Methyl group. And the calculated some physical properties; heats of formation (ΔH_f , kcal.mol⁻¹), Dipole moments (μ in Debye), energies (eV) of the High Occupied Molecular Orbital (HOMO) and the Lower Unoccupied Molecular Orbital (LUMO), ionization energies (eV), the shown this results (table.2) that compound-B has lower heat of formation ΔH_f , (kcal/mol), that means it is more stability than compound-A, due to the same previous reason, in addition to that compound-B has highest E_{HOMO} and lowest E_{LUMO} and ionization energy IP, (eV), which indicates that compound-B is easier ionization than compound-A .

The results of the calculated thermodynamics data (Table.3), show the entropy value (S^0) less to compound-B , and it has highest heat capacity value, and which agree with the results of the calculated heat of formation, the reason as it is mentioned before.

In a comparison between every nitrogen atom in compound-A with their identical in compound-B is found that all the nitrogen atoms in compound-B (N_1 , N_2 , N_{21} , N_{22}) has lower charge values (highest electronic density) than the nitrogen atoms in compound-A (N_1 , N_2 , N_{16} , N_{17}) (Table.4), the reason of this due to the high pushing of electrons effect of the Methoxy group comparing with Methyl group, so we can conclude compound-B form complexes more stability than compound-A because it has atoms give more electrons.

The compound-A belongs to the C_s symmetry point group and it is has ($3N-6=147$) fundamental vibration modes, whereas compound-B belong to the C_1 symmetry point group and it is has ($3N-6=150$) fundamental vibration modes . From the character table, it is shown that all the modes have the (A' , A'') symmetry for compound A and the (A) symmetry for compound B . The frequency values for all of these modes along with their assignments and the corresponding IR absorption intensities for the A and B compounds where listed in table 5 and 6 respectively.

From these two tables it was shown that the frequency with the higher value is that of ν_1 , (O-H) st.; calculated with about the same value for the tow molecules . The next higher frequency values where these of the (C-H) stretch fundamental vibrations . The (CH_3 st., ν_3 , ν_{19}) and (CH_3 sciss., ν_{29}) frequencies values in compound-A bigger than its identical in compound-B (ν_{15} , ν_{19}) and (ν_{29}) respectively .

Table 1. Calculated geometric parameters (bond lengths in Angstrom and bond angles in degrees) of the Azo compounds .

Geometric parameter	Compound -A-	Geometric parameter	Compound -B-
N ₁ -N ₂	1.350	N ₁ -N ₂	1.352
N ₁ -C ₄	1.487	N ₁ -C ₃	1.481
N ₂ -C ₃	1.496	N ₂ -C ₄	1.495
C ₃ -C ₅	1.419	C ₃ -C ₁₉	1.441
C ₃ -C ₉	1.421	C ₃ -C ₂₃	1.418
C ₄ -C ₁₀	1.436	C ₄ -C ₅	1.419
C ₄ -C ₁₄	1.420	C ₄ -C ₉	1.421
C ₅ -C ₆	1.403	C ₅ -C ₆	1.402
C ₅ -H ₃₂	1.099	C ₅ -H ₃₃	1.099
C ₆ -C ₇	1.425	C ₆ -C ₇	1.425
C ₆ -H ₃₃	1.096	C ₆ -H ₃₄	1.096
C ₇ -C ₈	1.428	C ₇ -C ₈	1.428
C ₇ -C ₁₅	1.513	C ₇ -C ₁₀	1.512
C ₈ -C ₉	1.400	C ₈ -C ₉	1.400
C ₈ -H ₃₄	1.096	C ₈ -H ₃₅	1.096
C ₉ -H ₃₅	1.099	C ₉ -H ₃₆	1.099
C ₁₀ -C ₁₁	1.423	C ₁₀ -C ₁₁	1.426
C ₁₀ -O ₂₉	1.408	C ₁₀ -C ₁₅	1.428
C ₁₁ -C ₁₂	1.408	C ₁₁ -C ₁₂	1.401
C ₁₁ -H ₃₆	1.099	C ₁₁ -H ₃₇	1.096
C ₁₂ -C ₁₃	1.423	C ₁₂ -C ₁₃	1.420
C ₁₂ -C ₃₁	1.539	C ₁₂ -H ₃₈	1.098
C ₁₃ -C ₁₄	1.400	C ₁₃ -C ₁₄	1.421
C ₁₃ -H ₃₇	1.097	C ₁₃ -N ₁₆	1.465
C ₁₄ -H ₃₈	1.099	C ₁₄ -C ₁₅	1.400
C ₁₅ -C ₁₆	1.426	C ₁₄ -H ₃₉	1.098
C ₁₅ -C ₂₀	1.428	C ₁₅ -H ₄₀	1.096
C ₁₆ -C ₁₇	1.401	N ₁₆ -N ₁₇	1.364
C ₁₆ -H ₃₉	1.096	N ₁₇ -C ₁₈	1.452
C ₁₇ -C ₁₈	1.420	C ₁₈ -C ₂₄	1.431
C ₁₇ -C ₄₀	1.098	C ₁₈ -C ₂₈	1.460
C ₁₈ -C ₁₉	1.421	C ₁₉ -C ₂₀	1.413
C ₁₈ -N ₂₁	1.465	C ₁₉ -O ₂₉	1.408
C ₁₉ -C ₂₀	1.400	C ₂₀ -C ₂₁	1.422
C ₁₉ -H ₄₁	1.098	C ₂₀ -H ₄₁	1.098
C ₂₀ -H ₄₂	1.096	C ₂₁ -C ₂₂	1.428
N ₂₁ -N ₂₂	1.364	C ₂₁ -C ₃₁	1.416

N ₂₁ – H ₄₈	1.451	C ₂₂ – C ₂₃	1.400
C ₂₂ – C ₂₃	1.431	C ₂₂ – H ₄₂	1.094
C ₂₃ – C ₂₄	1.460	C ₂₃ – H ₄₃	1.099
C ₂₃ – C ₂₈	1.392	C ₂₄ – C ₂₅	1.392
C ₂₄ – C ₂₅	1.099	C ₂₄ – H ₄₄	1.099
C ₂₄ – H ₄₃	1.429	C ₂₅ – C ₂₆	1.429
C ₂₅ – C ₂₆	1.097	C ₂₅ – H ₄₅	1.097
C ₂₅ – H ₄₄	1.392	C ₂₆ – C ₂₇	1.392
C ₂₆ – C ₂₇	1.099	C ₂₆ – H ₄₆	1.099
C ₂₆ – H ₄₅	1.442	C ₂₇ – C ₂₈	1.442
C ₂₇ – C ₂₈	1.097	C ₂₇ – H ₄₇	1.097
C ₂₇ – H ₄₆	1.364	C ₂₈ – O ₃₀	1.364
C ₂₈ – O ₃₀	1.027	O ₂₉ – H ₄₈	1.027
O ₂₉ – H ₄₇	1.100	O ₃₁ – C ₃₂	1.476
O ₃₀ – H ₄₈	1.103	C ₃₂ – H ₅₀	1.106
C ₃₁ – H ₄₉	1.103	C ₃₂ – H ₅₁	1.110
C ₃₁ – H ₅₀	1.095	C ₃₂ – H ₅₂	1.110
C ₃₁ – H ₅₁	1.092	O ₃₀ – H ₄₉	1.095
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		<H ₅₀ C ₃₂ H ₅₁	109.1
		<H ₅₁ C ₃₂ H ₅₂	109.1

Table 2. Calculated heats of formation (in kcal/mole), dipole moments (in Debye), orbital energies (HOMO,LUOMO, in eV) and ionization energies (IP, in eV) for Azo compounds .

Parameter	Compound -A	Compound -B
ΔH_f (kcal/mol)	83.925	54.846
Dipole moment (μ in Debye)	3.524	4.501
HOMO energies (eV)	-8.688	-8.654
LUMO energies (eV)	1.211	1.196
Ionization potential IP, (eV)	8.688	8.653

Table 3. The calculated standard thermodynamics functions at 298.15° K of the Azo compounds .

Thermodynamic Data	Compound -A	Compound -B
U ⁰ (kcal/mol)	277.223	280.237
H ⁰ (kcal/mol)	277.815	280.829
S ⁰ (kcal mol ⁻¹ deg ⁻¹)	182.051	181.938
G ⁰ (kcal/mol)	-54000	-53964
A ⁰ (kcal/mol)	-54001	-53965
C _v (kcal mol ⁻¹ deg ⁻¹)	97.107	100.473

Table 4. Calculated charge for the Azo compounds (See Table 1 for numbering) .

A- COMPOUND				B-COMPOUND			
Atom Symb.	Charge	Atom Symb.	Charge	Atom Symb.	Charge	Atom Symb.	Charge
N ₁	-0.1191	C ₂₇	-0.0986	N ₁	-0.1212	C ₂₇	-0.0987
N ₂	-0.1282	C ₂₈	0.0979	N ₂	-0.1337	C ₂₈	0.0977
C ₃	0.0554	O ₂₉	-0.1939	C ₃	0.0300	O ₂₉	-0.1939
C ₄	0.0356	O ₃₀	-0.2282	C ₄	0.0554	O ₃₀	-0.2285
C ₅	-0.0735	C ₃₁	-0.2230	C ₅	-0.0746	O ₃₁	-0.1570
C ₆	-0.0761	H ₃₂	0.0908	C ₆	-0.0765	C ₃₂	-0.1220
C ₇	-0.0015	H ₃₃	0.0805	C ₇	-0.0027	H ₃₃	0.0895
C ₈	-0.0749	H ₃₄	0.0807	C ₈	-0.0753	H ₃₄	0.0797
C ₉	-0.0766	H ₃₅	0.1037	C ₉	-0.0774	H ₃₅	0.0800
C ₁₀	0.0898	H ₃₆	0.0682	C ₁₀	0.0009	H ₃₆	0.1031
C ₁₁	-0.1125	H ₃₇	0.0781	C ₁₁	-0.0740	H ₃₇	0.0835
C ₁₂	0.0147	H ₃₈	0.1015	C ₁₂	-0.0762	H ₃₈	0.0889
C ₁₃	-0.0921	H ₃₉	0.0837	C ₁₃	0.0669	H ₃₉	0.1022
C ₁₄	-0.0738	H ₄₀	0.0892	C ₁₄	-0.0765	H ₄₀	0.0835
C ₁₅	0.0007	H ₄₁	0.1025	C ₁₅	-0.0733	H ₄₁	0.0767
C ₁₆	-0.0737	H ₄₂	0.0837	N ₁₆	-0.1764	H ₄₂	0.0785
C ₁₇	-0.0761	H ₄₃	0.0905	N ₁₇	-0.1079	H ₄₃	0.1026
C ₁₈	0.0674	H ₄₄	0.0792	C ₁₈	0.0182	H ₄₄	0.0903
C ₁₉	-0.0763	H ₄₅	0.0834	C ₁₉	0.0922	H ₄₅	0.0790
C ₂₀	-0.0730	H ₄₆	0.0860	C ₂₀	-0.1262	H ₄₆	0.0831
N ₂₁	-0.1765	H ₄₇	0.2047	C ₂₁	0.0939	H ₄₇	0.0858
N ₂₂	-0.1076	H ₄₈	0.2463	C ₂₂	-0.1148	H ₄₈	0.2052
C ₂₃	0.0184	H ₄₉	0.0802	C ₂₃	-0.0700	H ₄₉	0.2463
C ₂₄	-0.0683	H ₅₀	0.0860	C ₂₄	-0.0684	H ₅₀	0.0964
C ₂₅	-0.0936	H ₅₁	0.0860	C ₂₅	-0.0938	H ₅₁	0.0887
C ₂₆	-0.0677			C ₂₆	-0.0679	H ₅₂	0.0887

Table 5. The calculated fundamental vibration frequencies (ν in cm^{-1}) along with their assignments and the corresponding infrared absorption intensities (ir intensities in km. mol^{-1}) for the A molecule .

No. of Freq.	Freq. cm^{-1}	Intensity km mol^{-1}	Assignments
In plane, A'			
v ₁	3714	5.6618	(O-H) st.
v ₂	3485	0.2568	Ring (C-H) st.
v ₃	3484	1.4594	CH ₃ st.
v ₄	3482	20.3900	Ring (C-H) st.
v ₅	3479	16.1540	Hydroxybenzene (C-H) st.
v ₆	3479	4.9932	Ring (C-H) st.
v ₇	3476	1.5379	Ring (C-H) st.
v ₈	3472	9.7005	Hydroxymethylbenzene (C-H) st.
v ₉	3469	10.1187	Hydroxybenzene (C-H) st.
v ₁₀	3466	5.5586	Ring (C-H) st.
v ₁₁	3463	4.1486	Ring (C-H) st.
v ₁₂	3459	0.2515	Ring (C-H) st.
v ₁₃	3458	2.6425	Ring (C-H) st.
v ₁₄	3456	2.1345	Hydroxymethylbenzene (C-H) st.
v ₁₅	3456	7.9894	Hydroxybenzene (C-H) st.
v ₁₆	3454	0.2343	Ring (C-H) st.
v ₁₇	3447	2.4926	Hydroxybenzene (C-H) st.
v ₁₈	3434	0.8622	Ring (C-H) st.
v ₁₉	3303	0.5035	CH ₃ st.
v ₂₀	2619	81.1289	(O-H) st.
v ₂₁	1881	104.8377	δ (O-H) + Ring (δ CCC)
v ₂₂	1738	100.3480	δ -Hydroxybenzene
v ₂₃	1732	65.2590	δ -Hydroxymethylbenzene + δ -Ring
v ₂₄	1731	5.0362	δ -Ring + δ -Hydroxymethylbenzene
v ₂₅	1722	33.1666	δ (O-H) + Ring (δ CCC)
v ₂₆	1710	2.5669	Ring (δ CH)
v ₂₇	1695	2.0157	Ring (δ CH)
v ₂₈	1677	21.4059	δ -Ring
v ₂₉	1672	22.2003	CH ₃ scis.
v ₃₀	1637	37.2929	δ -Hydroxybenzene
v ₃₁	1634	3.4880	δ -Ring
v ₃₂	1625	3.7556	δ -Hydroxymethylbenzene
v ₃₃	1600	55.1361	δ -Ring
v ₃₄	1579	68.7489	δ -Hydroxybenzene
v ₃₅	1543	65.7152	δ -Hydroxymethylbenzene + δ -Ring
v ₃₆	1535	46.8499	δ -Hydroxybenzene + δ -Ring
v ₃₇	1532	16.9868	δ -Hydroxybenzene + δ -Ring
v ₃₈	1491	50.6271	δ -Ring
v ₃₉	1466	36.6582	δ (O-H) + δ -Ring
v ₄₀	1435	20.8787	δ -Hydroxybenzene + δ (N=N)
v ₄₁	1415	14.3420	δ -Ring + δ (N=N)

V ₄₂	1403	9.3215	δ-Ring
V ₄₃	1394	64.1438	δ-Hydroxymethylbenzene
V ₄₄	1385	24.3654	δ-Hydroxymethylbenzene
V ₄₅	1380	5.4003	δ-Ring + δ(N=N)
V ₄₆	1353	7.4277	δ-Ring
V ₄₇	1349	63.7841	δ-Ring
V ₄₈	1339	6.4088	δ-Ring + δ(N=N)
V ₄₉	1336	141.6631	Ring (δCCC) + δ(O-H) + δ(N=N)
V ₅₀	1329	35.1281	δ-Ring + δ(N=N) + δ(O-H)
V ₅₁	1316	55.2878	δ-Ring + δ(N=N) + δ(O-H)
V ₅₂	1300	63.5003	δ-Hydroxybenzene + δ-Ring
V ₅₃	1288	25.1431	Ring (δCH) + δ(O-H)
V ₅₄	1279	24.3582	δ-Ring + δ(O-H)
V ₅₅	1257	27.9144	δ-Ring + δ(O-H)
V ₅₆	1251	116.6396	δ-Ring + δ(O-H)
V ₅₇	1235	2.1758	δ-Ring
V ₅₈	1229	24.9266	δ-Hydroxymethylbenzene
V ₅₉	1207	189.7887	δ-Hydroxybenzene + δ(N=N)
V ₆₀	1202	50.8668	δ-Ring + δ(O-H)
V ₆₁	1190	3.6971	δ-Ring
V ₆₂	1183	265.7362	δ-Hydroxybenzene + δ(N=N)
V ₆₃	1176	8.2524	Ring (δCH)
V ₆₄	1151	53.0147	Ring (δCH) + δ(C-N) + δ(O-H)
V ₆₅	1100	20.1831	ρCH ₃ + δ(O-H) + Ring (δCH)
V ₆₆	1084	13.5376	Ring (δCH)
V ₆₇	1081	11.2942	δ-Ring
V ₆₈	1064	2.0926	δ-Ring
V ₆₉	1052	17.0718	δ-Ring
V ₇₀	997	1.8548	δ-CH ₃ + Ring (δCH)
V ₇₁	993	5.7769	δ(N=N) + Ring (δCH) + δ(O-H)
V ₇₂	936	3.3940	δ(N=N) + Ring (δCH)
V ₇₃	905	25.7455	Ring (δCCC) + Ring (δCH) + δ(N=N)
V ₇₄	838	35.7639	Ring (δCH) + δ(N=N)
V ₇₅	805	1.0317	Ring (δCH) + δ(O-H) + δ(N=N)
V ₇₆	757	3.3802	Ring (δCCC) + δ-CH ₃
V ₇₇	747	12.8726	Ring (δCH) + δ-CH ₃
V ₇₈	678	0.4546	Ring (δCH)
V ₇₉	677	0.6464	δ-Ring + δ(O-H)
V ₈₀	658	0.0053	δ-Ring
V ₈₁	608	13.1065	Ring (δCH)
V ₈₂	586	19.2956	δ-Ring + δ(N=N) + δ(O-H)
V ₈₃	577	19.0588	δ-Ring + δ(O-H) + δ(N=N)
V ₈₄	548	25.5553	δ(O-H) + δ(N=N) + δ-Ring
V ₈₅	529	5.1969	δ-CH ₃ + δ-Ring + δ(O-H)
V ₈₆	515	5.4754	Ring (δCH) + δ(O-H)
V ₈₇	487	2.7418	δ(O-H) + Ring (δCH)
V ₈₈	454	12.3881	Ring (δCH) + δ(O-H) + δ-CH ₃

V ₈₉	407	3.4041	δ-Ring + δ(O-H)
V ₉₀	384	1.3995	δ-Ring + δ-CH ₃
V ₉₁	306	0.7707	δ-CH ₃ + δ-Ring + δ(O-H)
V ₉₂	294	2.9114	δ-CH ₃ + δ-Ring + δ(O-H)
V ₉₃	230	1.1195	δ(O-H) + δ-Ring
V ₉₄	212	2.2970	Ring (δCH) + δ(O-H)
V ₉₅	128	0.9081	δ(O-H) + δ-Ring
V ₉₆	117	0.3728	δ-Ring + δ-CH ₃
V ₉₇	55	0.1792	δ-Ring + δ(O-H)
V ₉₈	26	0.2116	δ-CH ₃ + δ(O-H) + δ-Ring
Out of plane, A''			
V ₉₉	1669	3.9395	ωCH ₃
V ₁₀₀	1565	9.5390	ωCH ₃
V ₁₀₁	1184	85.5990	γ(O-H)
V ₁₀₂	1142	6.5679	τCH ₃
V ₁₀₃	1045	0.1767	Ring (γCH)
V ₁₀₄	1040	0.0104	Ring (γCH)
V ₁₀₅	1033	0.2637	Ring (γCH)
V ₁₀₆	1030	0.6673	Ring (γCH)
V ₁₀₇	1020	0.3843	Ring (γCH)
V ₁₀₈	1015	0.5004	γ-Ring
V ₁₀₉	1014	0.5891	Ring (γCH)
V ₁₁₀	904	2.5361	Ring (γCH)
V ₁₁₁	900	1.3292	Ring (γCH)
V ₁₁₂	896	0.1268	Ring (γCH)
V ₁₁₃	888	0.1573	Ring (γCH)
V ₁₁₄	878	3.8539	Ring (γCH)
V ₁₁₅	870	54.2377	Ring (γCH)
V ₁₁₆	864	13.2858	Ring (γCH)
V ₁₁₇	796	30.6621	Ring (γCH)
V ₁₁₈	774	0.0555	Ring (γCH)
V ₁₁₉	760	8.0183	γ-Ring
V ₁₂₀	751	0.2556	Ring (γCH) + γ-CH ₃
V ₁₂₁	744	0.0159	γ-Ring
V ₁₂₂	600	0.0840	Ring (γCH) + τCH ₃
V ₁₂₃	574	0.0073	Ring (γCH)
V ₁₂₄	559	0.0587	Ring (γCH)
V ₁₂₅	528	2.5374	γ-Ring
V ₁₂₆	498	46.2411	γ(O-H)
V ₁₂₇	477	18.3269	γ(O-H) + γ-Ring
V ₁₂₈	461	13.8353	γ-Ring
V ₁₂₉	424	0.4870	Ring (γCH)
V ₁₃₀	413	0.5130	Ring (γCH)
V ₁₃₁	410	0.9710	γ-Ring
V ₁₃₂	362	0.8974	γ-Ring + γ-CH ₃ + γ(O-H)
V ₁₃₃	330	1.0525	γ(N=N) + Ring (γCH) + γ(O-H)
V ₁₃₄	302	0.3722	γ(N=N) + γ-Ring

V ₁₃₅	217	0.9940	$\gamma(\text{N}=\text{N}) + \gamma\text{-Ring}$
V ₁₃₆	215	0.0225	$\gamma\text{-Hydroxymethylbenzene}$
V ₁₃₇	207	0.0118	$\gamma\text{-Hydroxybenzene}$
V ₁₃₈	169	0.0015	$\gamma(\text{N}=\text{N}) + \gamma\text{-CH}_3 + \text{Ring} (\gamma\text{CH}) + \gamma(\text{O-H})$
V ₁₃₉	140	0.0175	$\gamma(\text{N}=\text{N}) + \text{Ring} (\gamma\text{CH})$
V ₁₄₀	91	0.1485	$\gamma(\text{N}=\text{N}) + \text{Ring} (\gamma\text{CH})$
V ₁₄₁	64	0.9724	$\gamma\text{-CH}_3 + \text{Ring} (\gamma\text{CH})$
V ₁₄₂	35	0.1163	$\text{Ring} (\gamma\text{CH}) + \gamma\text{-CH}_3$
V ₁₄₃	29	0.0766	$\text{Ring} (\gamma\text{CH})$
V ₁₄₄	13	0.0776	τCH_3
V ₁₄₅	11	0.1011	$\gamma(\text{O-H}) + \text{Ring} (\gamma\text{CH})$
V ₁₄₆	10	0.1550	$\gamma\text{-CH}_3$
V ₁₄₇	6	0.0218	$\text{Ring} (\gamma\text{CH})$

Where; st. stretching; δ , in plane binding; γ , out of plane binding; scis., scissoring; ρ , rock; τ , twist; ω , waging.

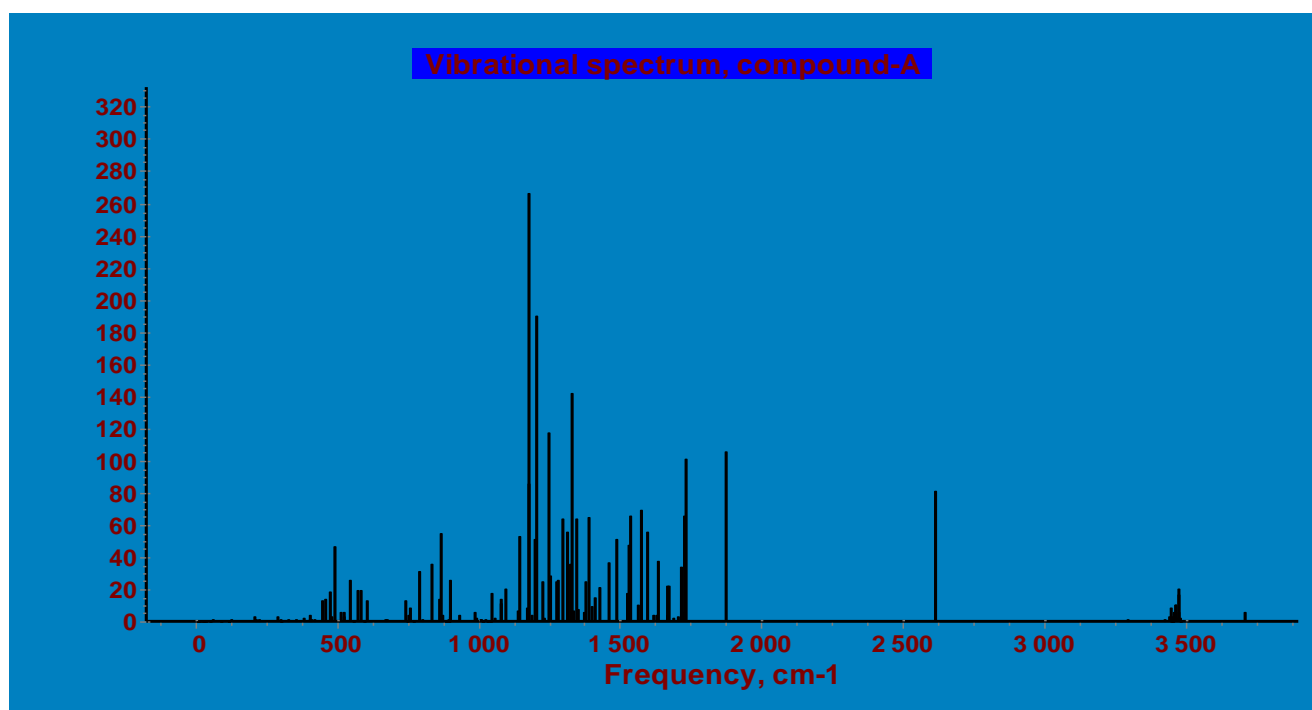


Fig.2: The vibration spectrum of the compound-A .

Table 6. The calculated fundamental vibration frequencies (ν in cm^{-1}) along with their assignments and the corresponding infrared absorption intensities (ir intensities in km. mol^{-1}) for the B molecule .

No. of freq.	Freq. cm^{-1}	Intensity km mol^{-1}	Assignments
In plane, A			
ν_1	3715	6.8100	(O-H) st.
ν_2	3491	8.6613	Ring (C-H) st.
ν_3	3485	0.3448	Ring (C-H) st.
ν_4	3482	19.6165	Ring (C-H) st.
ν_5	3479	15.9420	Ring (C-H) st.
ν_6	3478	5.0684	Ring (C-H) st.
ν_7	3476	1.7122	Ring (C-H) st.
ν_8	3469	10.0212	Ring (C-H) st.
ν_9	3466	5.3720	Ring (C-H) st.
ν_{10}	3463	3.6000	Ring (C-H) st.
ν_{11}	3461	3.9941	Ring (C-H) st.
ν_{12}	3459	0.3190	Ring (C-H) st.
ν_{13}	3457	2.8060	Ring (C-H) st.
ν_{14}	3455	7.6612	Ring (C-H) st.
ν_{15}	3449	0.3516	CH_3 st.
ν_{16}	3447	2.5007	Ring (C-H) st.
ν_{17}	3446	4.7832	Ring (C-H) st.
ν_{18}	3409	3.7062	CH_3 st.
ν_{19}	3255	18.7841	CH_3 st.
ν_{20}	2617	83.3689	(O-H) st.
ν_{21}	1882	106.1954	$\delta(\text{O-H})$
ν_{22}	1738	99.4511	δ -Hydroxybenzene
ν_{23}	1732	17.0723	Ring (δCH)
ν_{24}	1720	350.9322	Ring (δCH) + Ring (CCC) st. + $\delta(\text{O-H})$
ν_{25}	1710	27.1434	Ring (δCH)
ν_{26}	1706	56.9708	$\delta(\text{O-H})$ + Ring (CCC) st.
ν_{27}	1695	8.2097	Ring (δCH) + $\delta(\text{O-H})$
ν_{28}	1677	24.4626	δ -Ring
ν_{29}	1652	38.3161	CH_3 scis.

V ₃₀	1642	5.0202	CH ₃ scis.
V ₃₁	1637	37.5624	δ-Hydroxybenzene
V ₃₂	1634	0.8109	Ring (δCH)
V ₃₃	1622	56.5582	δ-Hydroxymethylbenzene
V ₃₄	1600	57.5817	Ring (δCH)
V ₃₅	1579	68.3842	δ-Hydroxybenzene
V ₃₆	1569	72.3193	CH ₃ scis.
V ₃₇	1546	70.6883	δ-Hydroxymethylbenzene
V ₃₈	1536	46.2466	δ-Hydroxybenzene + δ-Ring
V ₃₉	1533	18.6818	δ-Hydroxybenzene + δ-Ring
V ₄₀	1492	46.2417	Ring (δCH)
V ₄₁	1458	55.7358	δ(O-H) + Ring (δCH) + δ-CH ₃
V ₄₂	1434	20.4117	δ-Hydroxybenzene
V ₄₃	1415	0.6730	Ring (δCH) + δ(N=N)
V ₄₄	1404	144.4004	Ring (δCH) + δ(N=N) + δ(O-H)
V ₄₅	1398	178.3608	δ-Hydroxymethylbenzene
V ₄₆	1385	19.0405	δ-Hydroxybenzene + δ(N=N)
V ₄₇	1378	17.1190	Ring (δCH) + δ(N=N)
V ₄₈	1354	34.2971	Ring (δCH) + δ(N=N)
V ₄₉	1349	67.4009	Ring (δCH) + δ(N=N)
V ₅₀	1346	322.2940	δ-Hydroxymethylbenzene + δ(N=N)
V ₅₁	1339	14.5917	Ring (δCH) + δ(N=N)
V ₅₂	1329	21.9933	Ring (δCH) + δ(N=N)
V ₅₃	1316	59.0833	δ-Ring + δ(N=N)
V ₅₄	1300	82.3882	Ring (δCH)
V ₅₅	1287	125.6677	Ring (δCH) + δ-OCH ₃ + δ(O-H)
V ₅₆	1279	20.0249	Ring (δCH) + δ-OCH ₃ + δ(O-H)
V ₅₇	1260	54.5446	Ring (δCH) + δ(O-H) + δ-OCH ₃
V ₅₈	1255	176.2497	Ring (δCH) + δ(O-H) + δ-CH ₃
V ₅₉	1253	8.2539	Ring (δCH) + δ-CH ₃ + δ(O-H)
V ₆₀	1235	1.4897	Ring (δCH)
V ₆₁	1229	7.7699	ρCH ₃ + Ring (δCH)
V ₆₂	1208	215.1202	Ring (δCH)
V ₆₃	1202	23.0639	Ring (δCH) + δ(O-H)
V ₆₄	1190	4.7917	Ring (δCH)
V ₆₅	1183	263.0470	Ring (δCH) + δ(N=N)

V ₆₆	1176	11.9002	Ring (δ CH)
V ₆₇	1169	0.5088	ρ CH ₃
V ₆₈	1152	182.5279	Ring (δ CH) + δ -CH ₃ + δ (N=N)
V ₆₉	1106	1.9090	Ring (δ CH) + δ -OCH ₃
V ₇₀	1085	13.8510	Ring (δ CH)
V ₇₁	1082	11.0273	δ -Ring
V ₇₂	1064	2.1092	Ring (δ CH)
V ₇₃	1052	17.2218	Ring (δ CH)
V ₇₄	993	6.2278	δ (N=N) + δ -Ring
V ₇₅	983	1.4661	Ring (δ CH) + δ -OCH ₃
V ₇₆	938	1.3653	δ (N=N) + Ring (δ CH)
V ₇₇	905	26.4107	Ring (δ CH) + δ (N=N)
V ₇₈	837	28.6560	δ -Ring + δ (O-H) + δ (N=N)
V ₇₉	805	1.3245	δ -Hydroxybenzene + δ (N=N)
V ₈₀	755	1.4680	Ring (δ CH) + δ -CH ₃ + δ -Ring
V ₈₁	742	2.7973	Ring (δ CH) + δ -CH ₃ + δ -Ring
V ₈₂	678	0.3494	δ -Ring
V ₈₃	674	1.5239	δ -Ring + δ -OCH ₃
V ₈₄	658	0.1021	δ -Ring
V ₈₅	606	3.4171	δ -Ring + δ -OCH ₃ + δ (N=N)
V ₈₆	602	16.1252	δ -OCH ₃ + δ (O-H) + δ (N=N)
V ₈₇	580	15.6587	δ -OCH ₃ + Ring (δ CH)
V ₈₈	576	39.4576	δ (N=N) + Ring (δ CH)
V ₈₉	545	27.9798	δ (O-H) + δ (N=N)
V ₉₀	510	5.2071	δ (O-H) + Ring (δ CH) + δ -Ring
V ₉₁	487	18.6077	δ (O-H) + δ (N=N)
V ₉₂	475	15.9346	δ (N=N) + δ -Hydroxybenzene + δ -Ring
V ₉₃	420	2.0345	δ -Ring + δ (N=N) + δ -OCH ₃
V ₉₄	382	0.2506	δ -Hydroxymethylbenzene + δ -Hydroxybenzene
V ₉₅	372	1.0273	δ (O-H) + δ -OCH ₃ + δ (N=N)
V ₉₆	300	2.3671	δ -Ring + δ (N=N) + δ (O-H)
V ₉₇	256	6.0527	δ -OCH ₃ + δ (O-H) + δ (N=N)
V ₉₈	225	0.1372	δ (O-H) + δ (N=N) + δ -CH ₃ + δ -Ring
V ₉₉	204	1.9504	δ -OCH ₃ + δ -Ring
V ₁₀₀	127	1.1673	δ (O-H) + δ (N=N) + δ -Ring
V ₁₀₁	108	0.2443	δ (N=N) + δ -Ring

V ₁₀₂	53	0.1812	$\delta(N=N) + \delta\text{-Ring}$
V ₁₀₃	24	0.3455	$\delta\text{-CH}_3 + \delta(N=N)$
Out of plane, A			
V ₁₀₄	1184	85.5512	$\gamma(O-H)$
V ₁₀₅	1044	0.1772	Hydroxybenzene (γCH)
V ₁₀₆	1040	0.0114	Ring (γCH)
V ₁₀₇	1033	0.2541	Ring (γCH)
V ₁₀₈	1020	0.7150	Ring (γCH)
V ₁₀₉	1017	0.4961	Ring (γCH)
V ₁₁₀	1015	0.5149	Hydroxybenzene (γCH) + Ring (γCH)
V ₁₁₁	1014	0.6262	Hydroxybenzene (γCH) + Ring (γCH)
V ₁₁₂	900	1.3185	Hydroxybenzene (γCH)
V ₁₁₃	896	0.0322	Ring (γCH)
V ₁₁₄	888	0.0279	Ring (γCH)
V ₁₁₅	878	3.9176	Ring (γCH)
V ₁₁₆	875	19.2015	Ring (γCH)
V ₁₁₇	866	54.4395	Ring (γCH)
V ₁₁₈	836	15.1374	Ring (γCH)
V ₁₁₉	796	30.7789	Ring (γCH)
V ₁₂₀	773	0.0644	Ring (γCH)
V ₁₂₁	759	8.0894	Ring (γCH)
V ₁₂₂	749	0.8838	Ring (γCH)
V ₁₂₃	738	1.8192	Ring (γCH)
V ₁₂₄	625	0.0895	$\gamma(O-H) + \text{Ring} (\gamma\text{CH})$
V ₁₂₅	575	0.0006	Ring (γCH)
V ₁₂₆	559	0.0828	Ring (γCH)
V ₁₂₇	528	2.6384	Ring (γCH)
V ₁₂₈	497	54.6243	$\gamma(O-H)$
V ₁₂₉	477	11.4285	$\gamma(O-H) + \text{Ring} (\gamma\text{CH})$
V ₁₃₀	461	10.3663	$\gamma(O-H) + \text{Ring} (\gamma\text{CH})$
V ₁₃₁	426	0.0632	Ring (γCH)
V ₁₃₂	417	0.0038	Ring (γCH)
V ₁₃₃	412	0.0086	Ring (γCH)
V ₁₃₄	371	0.3130	$\gamma\text{-Ring}$
V ₁₃₅	331	2.1893	$\gamma\text{-Hydroxybenzene}$
V ₁₃₆	306	1.8112	$\gamma(N=N) + \gamma\text{-OCH}_3 + \gamma\text{-Ring}$

v ₁₃₇	248	0.7030	τCH_3
v ₁₃₈	227	0.8850	$\tau\text{CH}_3 + \gamma\text{-Hydroxymethoxybenzene}$
v ₁₃₉	216	1.3273	$\gamma(\text{N}=\text{N}) + \gamma\text{-Hydroxybenzene} + \gamma\text{-CH}_3 + \gamma\text{-Ring}$
v ₁₄₀	206	0.1348	$\gamma\text{-Hydroxybenzene} + \gamma\text{-Ring} + \gamma(\text{N}=\text{N}) + \gamma\text{-CH}_3$
v ₁₄₁	169	1.0167	$\gamma(\text{N}=\text{N}) + \tau\text{CH}_3$
v ₁₄₂	143	0.0216	$\gamma(\text{N}=\text{N}) + \gamma\text{-Ring}$
v ₁₄₃	100	1.9120	$\gamma\text{-OCH}_3 + \gamma(\text{N}=\text{N}) + \gamma\text{-Ring}$
v ₁₄₄	89	0.0167	$\gamma\text{-OCH}_3 + \gamma\text{-Ring}$
v ₁₄₅	60	0.7371	$\gamma\text{-OCH}_3 + \gamma\text{-Ring}$
v ₁₄₆	35	0.0549	$\gamma\text{-Ring}$
v ₁₄₇	29	0.1373	$\gamma\text{-Ring}$
v ₁₄₈	12	0.0000	$\gamma(\text{O-H}) + \gamma\text{-Ring}$
v ₁₄₉	10	0.1983	$\gamma\text{-OCH}_3 + \gamma\text{-Ring}$
v ₁₅₀	6	0.0220	$\gamma\text{-Ring}$

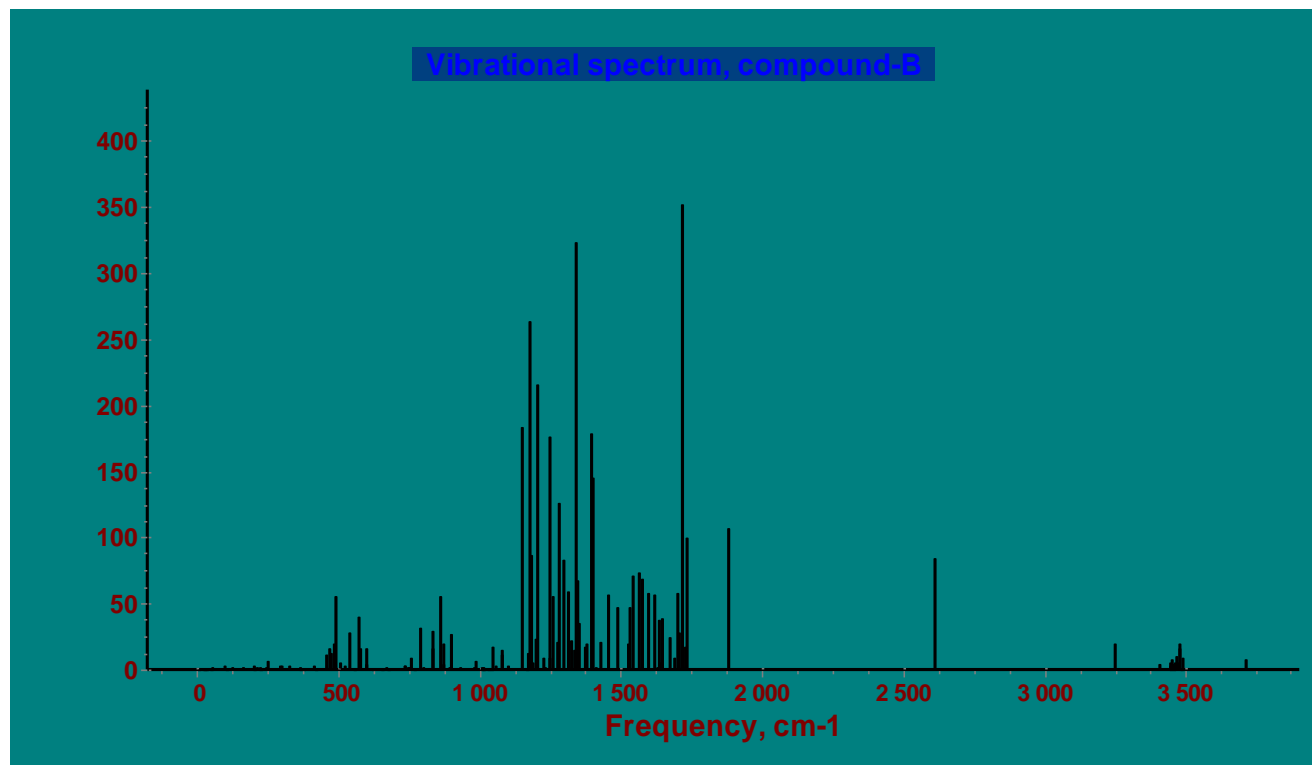


Fig.3: The vibration spectrum of the compound-B .

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