

A Theoretical Study on Vibration Frequencies of Some Aniline Derivatives and Correlations with Experimental Data

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In this work, a theoretical study on the vibrational frequencies of all possible isomers of some aniline derivatives with general formula $C_6H_{5-n}X_nNH_2$ ($n = 1-5$; $X = F, Cl, Br$) is reported. Calculations have been done at B3LYP employing the 6-31G(d), 6-31G(d,p), 6-31++G(d,p) and 6-311++G(d,p) levels of theory. The optimized structures were used for calculation of vibrational frequencies at B3LYP/6-311++G(d,p) level of theory. The resulting data were scaled by 0.952 for N-H stretching bond and 0.981 for C-N, C-X ($X = F, Cl, Br$), C=C, N-H (bending) bonds. The results showed that, there is a good agreement between the scaled theoretical frequencies and experimental data for this type of compounds.

Key Words: DFT, Halo aniline derivatives, Infrared spectra, Vibrational frequencies.

INTRODUCTION

In recent years, aniline and its derivatives have been subjected to many different types of scientific studies¹. They have been widely used in a variety of industrial and commercial purposes, including dyestuff, pesticide and pharmaceuticals manufacturing². Some of the *para*-substituted derivatives of anilines are local anesthetics and the amino group in these molecules plays an important role in the interaction with the receptor³. The inclusion of a substituent group in aniline leads to the variation of charge distribution in the molecule and consequently this greatly affects the structural, electronic and vibrational parameters⁴⁻⁷. This work is a series of previous works for predicting of the experimental parameters of some known compounds using theoretical calculation⁸⁻¹⁰. To best of our knowledge, the first complete study on aniline has carried out by Evans¹¹, the assignments of the infrared spectra in the vapour, solution and liquid phases and the Raman spectra in the liquid state have been reported by other authors¹²⁻¹⁴. It is well known that adequate prediction and interpretation of the vibrational spectra requires the use of quantum chemical methods¹⁵.

Density functional theory (DFT) used in physics and chemistry to investigate the electronic structure of many-particle systems. It has already been successfully used in the prediction of structures, reaction mechanism, IR and NMR¹⁶⁻²¹.

CALCULATIONS METHODS

In this work, DFT studies with Becke's three parameter hybrid functional using the Lee, Yang and Parr correlation functional (B3LYP)²²⁻²⁴, have been performed on the equilibrium geometries and the harmonic-vibrational frequencies of all halo aniline derivatives at 6-31G(d), 6-31G(d,p), 6-31++G(d,p) and 6-311++G(d,p) levels of theory. The result show that the B3LYP//6-311++G(d,p) level of theory is better than other levels. Thus we take into account B3LYP/6-311++G(d,p) level of theory for all calculations in the present discussion. The frequencies calculated at B3LYP/6-311++G (d,p) level were scaled by 0.952 for N-H stretching bond and 0.981 for C-N, C-X (X = F, Cl, Br), C=C, N-H (bending) bonds. All the calculations are performed by using GAUSSSIAN 98²⁵ program package on the personal computer.

RESULTS AND DISCUSSION

The geometrical structures such as bond lengths and bond angles of all halo aniline derivatives are given in supplementary data.

The comparison of the frequencies calculated at the DFT using B3LYP 6-311++G (d,p) level and scaled data with experimental values for all fluoro aniline derivatives are given in Table-1. Anyway, notwithstanding the level of calculations, it is customary to scale down the calculated harmonic frequencies in order to improve the agreement with the experiment. In this work we select the *para*-halo aniline and 2,5-di halo aniline for present studies to show the correlations of the theoretical and experimental frequencies (Fig. 2). As it can be seen in this Figure, there is a good correlation between the experimental and calculated frequencies for latter components.

The calculated, scaled and experimental vibrations frequencies for chloro aniline derivatives with the some aniline derivatives with the general formula $C_6H_{5-n}X_nNH_2$ ($n = 1-5$; $X = F, Cl, Br$) compounds are given in Table-2. The comparison of experimental and calculated IR spectra for *para*-chloro aniline and 2,5-dichloro aniline are shown in Fig. 3. As it can be seen in the Fig. 4, there is a good correlation between the experimental and calculated frequencies.

The calculated, scaled and experimental vibrations frequencies of bromo aniline derivatives with the title compound are given in Table-3. The comparison of IR spectra of calculated and experimental of *para*-bromo aniline and 2,5-di bromo aniline are shown in Fig. 5. It can also be seen in the Fig. 6, there is a good correlation between the theoretical and experimental frequencies of N-H stretching and bending vibrations, C=C stretching vibrations, C-N stretching vibrations and C-Br stretching vibrations.

One substitute of halo aniline derivatives the trends of frequency for N-H bending-X (X = F, Cl, Br), C-N in *ortho*, *meta* and *para* positions are:

$$V_{(F)} > V_{(Cl)} > V_{(Br)}$$

The trends of frequency for two substitute of halo aniline derivatives for N-H bending-X (X = F, Cl, Br), C-N bonding in (2,3), (2,5), (2,6),(3,4) and (3,5) positions are:

TABLE-1
THEORETICAL AND EXPERIMENTAL IR DATA FOR FLUORO ANILINE DERIVATIVES

Mode	ν_{\max} (cm ⁻¹)														
	<i>ortho</i> -Fluoro aniline			<i>meta</i> -Fluoro aniline			<i>para</i> -Fluoro aniline			2,3-di fluoro aniline			2,4-di fluoro aniline		
	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a
N-H stretching	3618.92	3445.21	3457.00	3611.42	3438.07	3461.00	3615.03	3441.51	3442.00	3616.18	3442.60	3477.00	3620.76	3446.96	-
N-H bending	1661.38	1629.81	1631.00	1660.60	1629.05	1633.00	1662.38	1630.79	1624.00	1634.73	1603.67	1599.00	1633.82	1602.78	-
C-F stretching	1181.04	1158.60	1154.00	1170.52	1148.28	1146.00	1178.72	1156.33	1155.00	1186.90	1164.35	1163.00	1240.64	1217.07	-
C=C	1539.56	1510.31	1508.00	1522.65	1493.72	1495.00	1541.55	1512.26	1510.00	1508.38	1479.72	1481.00	1544.22	1514.88	-
C-N	1051.19	1031.22	1026.00	1022.00	1002.58	1000.00	1034.87	1015.21	1010.00	1070.86	1050.51	1053.00	1038.16	1018.44	-
	2,5-di fluoro aniline			2,6-di fluoro aniline			3,4-di fluoro aniline			3,5-di fluoro aniline			2,3,4-tri fluoro aniline		
	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a
N-H stretching	3617.28	3443.65	3481.00	3623.81	3449.87	3475.00	3613.62	3440.17	-	3610.92	3437.60	3445.00	3618.99	3445.28	3469.00
N-H bending	1676.08	1644.23	1642.00	1664.87	1633.24	1639.00	1667.32	1635.64	-	1665.01	1633.37	1633.00	1636.60	1605.50	1608.00
C-F stretching	1184.54	1162.03	1157.00	1178.17	1155.78	1160.00	1186.02	1163.48	-	1189.53	1166.93	1159.00	1188.35	1165.77	1171.00
C=C	1542.04	1512.74	1514.00	1539.11	1509.87	1506.00	1546.39	1517.01	-	1501.85	1473.31	1466.00	1539.69	1510.44	1513.00
C-N	1053.39	1033.37	1068.00	1077.05	1056.59	1057.00	1054.55	1034.52	-	1029.49	1009.93	1014.00	1007.52	988.38	981.00
	2,3,5-tri fluoro aniline			2,4,5-tri fluoro aniline			2,4,6-tri fluoro aniline			2,3,5,6-tetra fluoro aniline			2,3,4,5,6-penta fluoro aniline		
	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a
N-H stretching	3614.74	3441.23	-	3620.78	3446.98	3439.00	3625.85	3451.81	3445.00	3619.00	3445.29	3417.00	3620.03	3446.27	3420.00
N-H bending	1627.45	1596.53	-	1637.26	1606.15	1607.00	1630.47	1599.49	1610.00	1636.26	1605.17	1618.00	1642.78	1611.57	1612.00
C-F stretching	1147.66	1125.85	-	1189.07	1166.48	1166.00	1139.75	1118.09	1113.00	1105.60	1084.59	1090.00	1158.64	1136.62	1125.00
C=C	1546.31	1516.93	-	1554.21	1524.68	1525.00	1544.75	1515.40	1520.00	1530.04	1500.97	1507.00	1539.99	1510.73	1525.00
C-N	1053.65	1033.63	-	1123.92	1102.57	1107.00	1126.76	1105.35	1113.00	1102.86	1081.91	1090.00	1105.60	1084.59	1083.00

^aExp = Ref [27]. A = DFT/ B3Lyp 6-311++G**; B = Scaled, according to correlation equation: $\nu(\text{corr}) = \nu(\text{cal}) * 0.952$ for N-H stretching and $\nu(\text{corr}) = \nu(\text{cal}) * 0.981$ for N-H bending, C-F stretching, C=C and C-N.

TABLE-2
THEORETICAL AND EXPERIMENTAL IR DATA FOR CHLORO ANILINE DERIVATIVES

Mode	ν_{\max} (cm ⁻¹)											
	<i>ortho</i> -Chloro aniline			<i>meta</i> -Chloro aniline			<i>para</i> -Chloro aniline			2,3-di chloro aniline		
	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a
N-H stretching	3608.30	3435.10	–	3608.84	3435.62	–	3610.97	3484.59	3473.00	3607.27	3434.12	3482.00
N-H bending	1654.32	1622.89	–	1658.26	1626.75	–	1659.74	1628.20	1618.00	1651.76	1620.37	1615.00
C-Cl stretching	685.14	672.12	–	698.80	685.52	–	645.33	633.07	640.00	781.54	766.69	769.00
C=C	1519.50	1490.63	–	1512.89	1484.15	–	1523.48	1494.54	1494.00	1493.62	1465.24	1465.00
C-N	1061.56	1041.39	–	1090.93	1070.20	–	1097.70	1076.84	1089.00	1115.23	1094.04	1098.00
2,4-di chloro aniline			2,5-di chloro aniline			2,6-di chloro aniline			3,4-di chloro aniline			
	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a
N-H stretching	3607.44	3434.28	3462.00	3605.50	3432.44	3434.00	3604.88	3431.85	3432.00	3609.30	3436.05	3404.00
N-H bending	1656.31	1624.84	1620.00	1654.37	1622.94	1616.00	1650.20	1618.85	1618.00	1630.44	1599.46	1600.00
C-Cl stretching	727.68	713.85	716.00	801.52	786.29	784.00	738.15	724.13	711.00	701.05	687.73	685.00
C=C	1513.85	1485.09	1480.00	1511.48	1482.76	1466.00	1498.08	1469.62	1470.00	1505.53	1476.93	1478.00
C-N	1065.91	1045.66	1046.00	1067.41	1047.13	1046.00	1092.83	1072.07	1068.00	1053.60	1033.58	1030.00
3,5-di chloro aniline			2,3,4-tri chloro aniline			2,3,5-tri chloro aniline			2,4,5-tri chloro aniline			
	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a
N-H stretching	3608.61	3435.40	3491.00	3606.31	3433.21	–	3605.11	3529.40	–	3608.27	3532.49	–
N-H bending	1659.76	1628.22	1621.00	1653.36	1621.95	–	1652.15	1617.46	–	1661.58	1626.69	–
C-Cl stretching	684.65	671.64	671.00	686.66	673.62	–	713.72	698.73	–	656.53	642.74	–
C=C	1475.46	1447.43	1461.00	1485.89	1457.66	–	1575.64	1542.56	–	1569.67	1536.71	–
C-N	1121.15	1099.85	1100.00	1096.16	1075.33	–	1132.27	1108.49	–	1163.30	1138.87	–
2,3,4,5-tetra chloro aniline			2,3,4,6-tetra chloro aniline			2,3,5,6-tetra chloro aniline			2,3,4,5,6-penta chloro aniline			
	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a
N-H stretching	3604.23	3431.23	–	3601.78	3428.89	–	3600.55	3427.72	–	3600.98	3428.13	–
N-H bending	1652.45	1621.05	–	1647.27	1615.97	–	1643.48	1612.25	–	1644.21	1612.97	–
C-Cl stretching	699.76	686.46	–	741.42	727.33	–	659.00	646.48	–	668.77	656.06	–
C=C	1459.71	1431.98	–	1474.99	1446.97	–	1454.29	1426.66	–	1445.91	1418.44	–
C-N	1098.28	1077.41	–	1072.80	1052.42	–	1162.33	1061.77	–	1089.83	1069.12	–

^aExp : Ref [27]; A = DFT/ B3Lyp 6-311++G**. B = Scaled, according to correlation equation: $\nu(\text{corr}) = \nu(\text{cal}) * 0.952$ for N-H stretching and $\nu(\text{corr}) = \nu(\text{cal}) * 0.981$ for N-H bending, C-Cl stretching, C=C and C-N.

TABLE-3
THEORETICAL AND EXPERIMENTAL IR DATA FOR BROMO ANILINE DERIVATIVES

Mode	ν_{\max} (cm ⁻¹)											
	<i>ortho</i> -Bromo aniline			<i>meta</i> -Bromo aniline			<i>para</i> -Bromo aniline			2,3-di bromo aniline		
	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a
N-H stretching	3597.92	3425.22	3467.00	3608.72	3435.50	3451.00	3609.87	3436.60	3475.00	3595.54	3422.95	-
N-H bending	1651.61	1620.23	1615.00	1657.42	1625.93	1620.00	1649.14	1617.81	1614.00	1647.62	1616.32	-
C-Br stretching	667.70	655.01	657.00	680.74	667.81	671.00	611.99	600.36	605.00	702.90	689.55	-
C=C	1515.03	1486.24	1483.00	1510.84	1482.13	1480.00	1521.38	1492.47	1489.00	1454.59	1426.96	-
C-N	1064.55	1044.32	1043.00	1084.66	1064.05	1066.00	1084.28	1063.68	1066.00	1064.37	1044.15	-
	2,4-di bromo aniline			2,5-di bromo aniline			2,6-di bromo aniline			3,4-di bromo aniline		
	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a
N-H stretching	3596.71	3424.07	3492.00	3595.71	3423.12	3421.00	3587.91	3415.69	3426.00	3608.77	3435.55	-
N-H bending	1651.35	1619.97	1615.00	1610.93	1580.33	1584.00	1646.39	1615.11	1613.00	1659.83	1628.29	-
C-Br stretching	693.91	680.73	673.00	798.53	783.36	778.00	715.60	702.00	710.00	686.35	673.31	-
C=C	1508.40	1479.74	1481.00	1506.24	1477.62	1475.00	1491.07	1462.74	1466.00	1498.52	1470.05	-
C-N	1055.63	1035.57	1033.00	1054.57	1034.53	1023.00	1054.17	1034.14	1030.00	1124.73	1103.36	-
	3,5-di bromo aniline			2,3,4-tri bromo aniline			2,3,5-tri bromo aniline			2,4,5-tri bromo aniline		
	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a
N-H stretching	3607.42	3434.26	-	3594.93	3422.37	-	3593.40	3420.92	-	3595.79	3423.19	-
N-H bending	1658.84	1627.32	-	1648.17	1616.85	-	1647.16	1615.86	-	1651.68	1620.30	-
C-Br stretching	676.24	663.39	-	730.12	716.25	-	770.60	755.96	-	712.13	698.60	-
C=C	1577.87	1547.89	-	1477.40	1449.33	-	1562.88	1533.19	-	1559.90	1530.26	-
C-N	1115.04	1093.85	-	1075.84	1055.40	-	1069.56	1049.24	-	1063.30	1043.09	-
	2,3,4,5-tetra bromo aniline			2,3,4,6-tetra bromo aniline			2,3,5,6-tetra bromo aniline			2,3,4,5,6-penta bromo aniline		
	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a	A	B	Exp ^a
N-H stretching	3655.82	3480.34	-	3583.60	3411.59	-	3581.44	3409.53	-	3581.67	3409.75	-
N-H bending	1694.16	1661.97	-	1641.43	1610.24	-	1636.33	1605.24	-	1635.91	1604.83	-
C-Br stretching	696.43	683.20	-	684.93	671.92	-	830.75	814.97	-	686.05	673.02	-
C=C	1546.68	1517.29	-	1463.42	1435.62	-	1547.78	1518.37	-	1552.65	1523.15	-
C-N	1078.46	1057.97	-	1076.23	1055.78	-	1077.72	1057.24	-	1085.46	1064.84	-

^aExp: Ref [27]; A = DFT/ B3Lyp 6-311++G**. B = Scaled, according to correlation equation: $\nu(\text{corr}) = \nu(\text{cal}) * 0.952$ for N-H stretching and $\nu(\text{corr}) = \nu(\text{cal}) * 0.981$ for N-H bending, C-Br stretching, C=C and C-N.

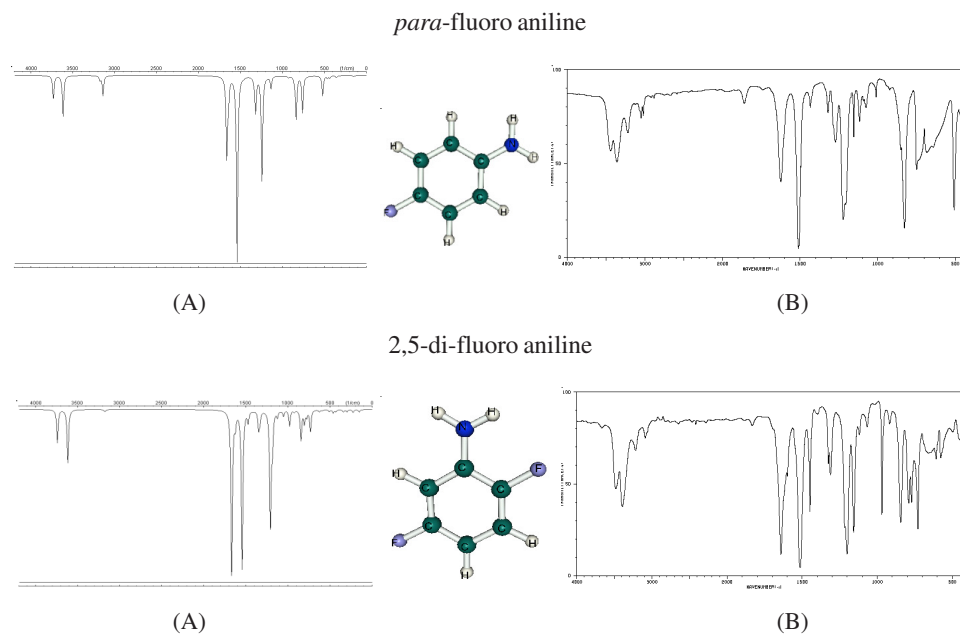


Fig. 1. (A) Theoretical IR spectra, optimized structure by DFT//((B3LYP//6-311++G(d,p)) and (B) experimental IR spectra of *para*-fluoro aniline and *2,5*-di-fluoro aniline derivatives

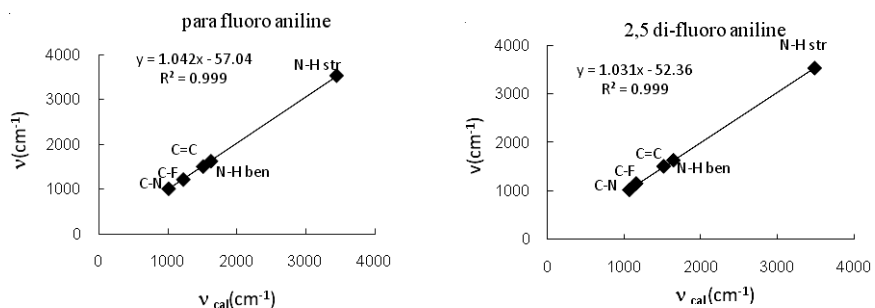
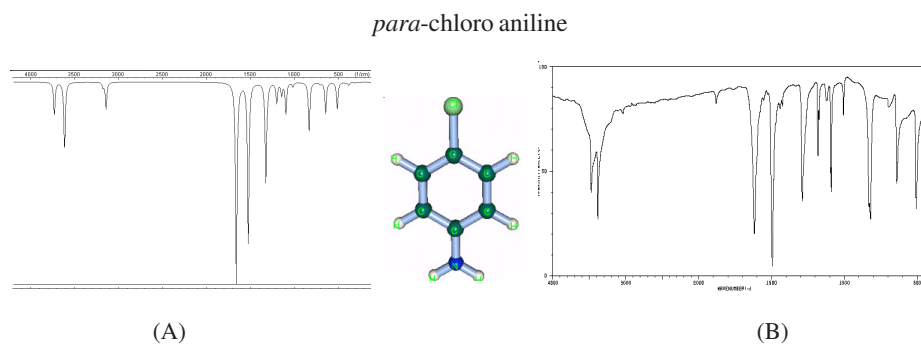


Fig. 2. Correlation of the theoretical and experimental vibrational frequency of *para*-fluoro aniline and *2,5*-di-fluoro aniline derivatives by DFT//((B3LYP//6-311++G(d,p))



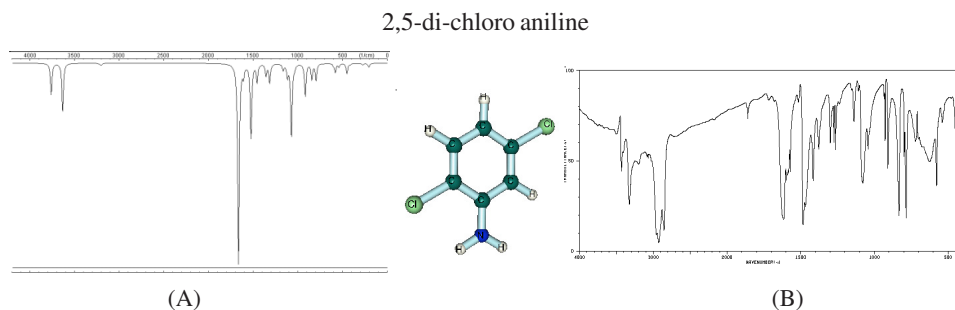


Fig. 3. (A) Theoretical IR spectra, optimized structure by DFT//((B3LYP//6-311++G(d,p)) and (B) experimental IR spectra of *para*-chloro aniline and 2,5-di-chloro aniline derivatives

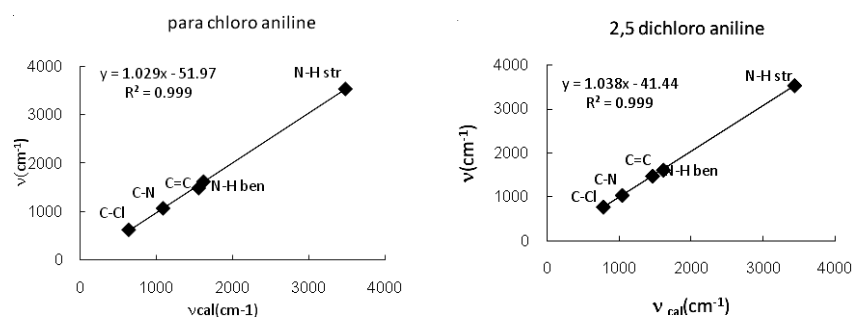


Fig. 4. Correlation of the theoretical and experimental vibrational frequency of *para*-chloro aniline and 2,5-di-chloro aniline derivatives by DFT//((B3LYP//6-311++G(d,p))

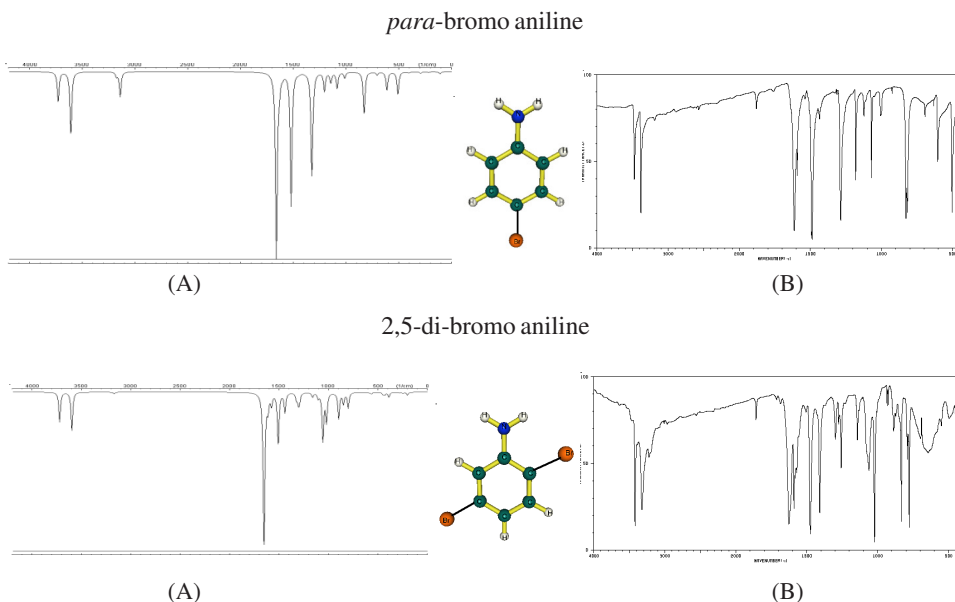


Fig. 5. (A) Theoretical IR spectra, optimized structure by DFT//((B3LYP//6-311++G(d,p)) and (B) experimental IR spectra of *para*-bromo aniline and 2,5-di-bromo aniline derivatives

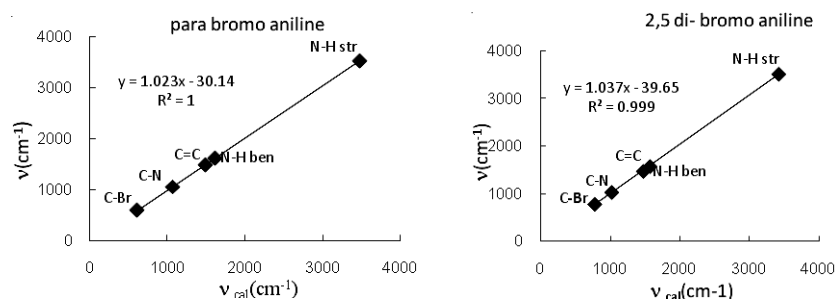


Fig. 6. Correlation of the theoretical and experimental vibrational frequency of *para*-bromo aniline and 2,5 di-bromo aniline derivatives by DFT/(B3LYP//6-311++G(d,p))

$$V_{(F)} > V_{(Cl)} > V_{(Br)}$$

In the three substitute of halo aniline the trends of frequency for N-H bending and C-N bonding in the (2,3,4),(2,3,5) and (2,4,5) are:

$$V_{(Cl)} > V_{(Br)} > V_{(F)}$$

And the trends of frequency for C-X (X = F, Cl, Br) bonding are:

$$V_{(F)} > V_{(Br)} > V_{(Cl)}$$

Conclusion

Comparison of the observed fundamental vibrational frequencies of halo aniline derivatives with calculated vibrational frequencies by DFT/B3LYP at different base sets indicates that the density functional methods are reliable and provides valuable information for understanding the vibrational spectra of halo aniline derivatives molecule. The trends of vibrational frequencies are depended on the substitute of halogen, the number of halogen and electronegativity of halogen in aniline ring.

Appendix A: Supplementary data

Geometrical parameters of all component, figures of vibrational frequencies of experimental and theoretical, figures of correlation between experimental and theoretical data, the IR data of all components at the B3LYP/6-31G(d), 6-31G(d,p), 6-31++G(d,p), 6-311++G(d,p) base set are gathered in supplementary data.

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