Structural elucidation by 1D/ 2D NMR, FTIR, and mass spectrometry analyses

Table 1. ^{1}H and ^{13}C NMR analysis

^{1}H NMR analysis	
Chemical shift (δ, ppm)	**Assignment(s)**
1.2 (t)	$-\mathrm{C}\boldsymbol{H}^{1}{}_{2}-$ of the cyclopropane ring
1.6 (t)	$-\mathrm{C}\boldsymbol{H}^{2}{}_{2}-$ of the cyclopropane ring
2.5–2.9 (m)	$>\mathrm{C}\boldsymbol{H}^{3}-$ of the cyclopropane ring
7.2–7.4 (m)	$\boldsymbol{H}^{4}/\boldsymbol{H}^{5}$ of benzene ring
8.5–8.8 (br, s)	$-\mathrm{N}\boldsymbol{H}^{6}{}_{2}$
^{13}C NMR analysis	
12	$>\boldsymbol{C}^{3}\mathrm{H}-$ of the cyclopropane ring
21	$-\boldsymbol{C}^{1}\mathrm{H}_{2}$ of the cyclopropane ring
31	$-\boldsymbol{C}^{2}\mathrm{H}_{2}$ of the cyclopropane ring
120–125	$\boldsymbol{C}^{4}$, $\boldsymbol{C}^{5}$, and $\boldsymbol{C}^{6}$ of the benzene ring
138	$\boldsymbol{C}^{7}$ of the benzene ring

br = broad, m = medium, s = singlet, and t = triplet

Peaks assignment:

^{1}H NMR ($CDCl_3$, 0.05% v/v TMS, 300MHz, δ ppm): 1.2 (2H, t), 1.6 (2H, t), 2.5–2.9 (1H, m), 7.2–7.4 (4H, m), and 8.5–8.8 (br, s)

^{13}C NMR ($CDCl_3$, 0.05% v/v TMS, 300MHz, δ ppm): 12 ($>\boldsymbol{C}^{3}\mathrm{H}-$), 21 ($-\boldsymbol{C}^{1}\mathrm{H}_{2}$), 31 ($-\boldsymbol{C}^{2}\mathrm{H}_{2}$), 120–125 ($>\boldsymbol{C}^{4/5/7}-$), and 138 ($\boldsymbol{C}^{6}$)

Discussions of results:

Herein, the presence of two $-CH_2-$ protons (H^1 and H^2) was confirmed from the ^{1}H NMR peaks at 1.2 and 1.6 ppm (Figure 1 and Table 1). In ^{1}H-^{1}H COSY spectrum, the cross peaks between 1.2 and 1.6 ppm confirm the direct interaction between these two protons, which eventually confirms the presence of $-CH_2-CH_2-$ in the molecule (Figure 2 and Table 1). Interestingly, peaks within 2.5–2.9 ppm interact with both H^1 and H^2, confirming the presence of the cyclopropane ring in the structure (Figure 2). Furthermore, the peaks within 7.2–7.4 ppm confirm the existence of the benzene ring with para substitutions. The presence of $-NH_2$ group was confirmed from the broad/ singlet peak within 8.5–8.8 ppm. In ^{13}C NMR spectrum (with DEPT-135), the $-\boldsymbol{C}^{1}\mathrm{H}_{2}-$/ $-\boldsymbol{C}^{2}\mathrm{H}_{2}-$ peaks were confirmed from the negative signals at 21/ 31 ppm (Figure 3 and Table 1). In this context, the attachment between the protons and the carbon atoms is confirmed from the ^{1}H-^{13}C HETCOR analysis (Figure 4). Therefore, the benzene ring carbons are assigned to the ^{13}C peaks within 120–125 ppm, while the peaks within 10–31 ppm are assigned to the aliphatic regions of the cyclopropane ring (Figure 4 and Table 1). Therefore, the presence of one cyclopropane ring, benzene ring, and $-NH_2$ group was confirmed in the structure of the molecule. Furthermore, the molecular ion peak at 133 corresponds to the structure of 4-cyclopropylaniline (Figure 5).

FTIR analysis

Table 2. FTIR analysis of 4-cyclopropylaniline

peaks (cm^{-1})	**Assignment(s)**
3467 and 3421 (br)	–NH_2 group was confirmed from the broad peaks
2901 (w)	C–H *str.* of aromatic benzene ring
2619 and 2495 (w)	N–H *str.* of the amine salts
1950 (m)	Tertiary ammonium ion specific peak
1683 (s)	
1606 (m)	
1583 (s)	
1570 (m)	C–H *def.* of cyclopropane ring
1498 (s)	C–C *str.* of benzene ring
1464 (s)	>CH_2 *bending* of cyclopropane ring
1443 (m)	In plane C–H *bending* and torsional C–C *bending* of the aromatic ring
1406 (m)	
1388 (m)	C–H *rocking vib.* of cyclopropane ring
1341 (s)	C–N *str.* of primary aromatic amine
1229 (m)	
1193 (m)	
1151 (m)	
1085 (m)	In plane C–H *bending* of benzene ring
1060 (m)	
1049 (m)	
1033 (m)	In plane C–H *bending* of benzene ring
1013 (m)	In plane C–H *bending* of cyclopropane ring
999 (m)	
936 (m)	C–C *str.* of cyclopropane ring
913 (m)	
897 (s)	
886 (s), 800 (s), and 754 (s)	C–H *wagging* of benzene ring
742 (s)	Out of the plane C–H *bending* of benzene ring
695 (s), 573 (m), 530 (m)	Ring in plane bending of benzene ring

Herein, the presence of –NH_2 group was confirmed from the N–H *str.* within 3467–3421 cm^{-1}, C–N *str.* of primary aromatic amine at 1341 cm^{-1}, tertiary ammonium ion specific peak at 1950 cm^{-1}, and N–H *str.* of the amine salts within 2619–2495 cm^{-1} (Figure 6). The presence of cyclopropane ring was confirmed from the >CH_2 *bending* at 1464 cm^{-1} and in plane >CH– *bending* at 1013 cm^{-1} (Figure 6 and Table 2). The peaks at 2901, 1498, 1085, 1033, 886/ 800/ 754, and 742 cm^{-1} were ascribed to the C–H *str.*, C–C *str.*, in plane C–H *bending*, C–H *wagging*, and out of the plane C–H *bending* of the benzene ring, respectively (Figure 6 and Table 2). Furthermore, the ring in plane *bending* of the benzene ring was assigned to 695/ 573/ 530 cm^{-1} (Figure 6 and Table 2). In this context, the peak at 1443 cm^{-1} was ascribed to the in plane C–H *bending* and torsional C–C *bending* of the aromatic ring (Table 2).

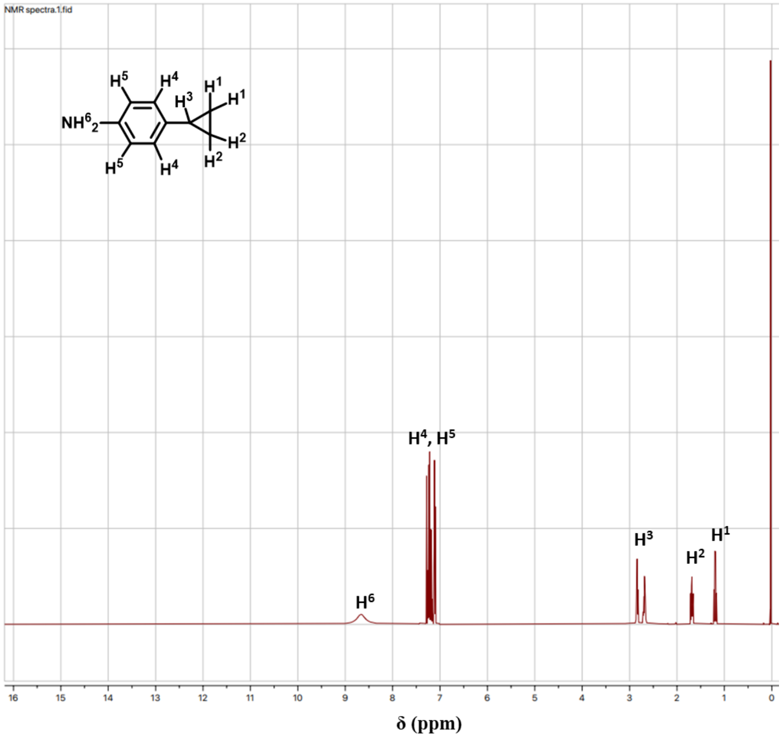


Figure 1. ^{1}H NMR spectrum of 4-cyclopropylaniline

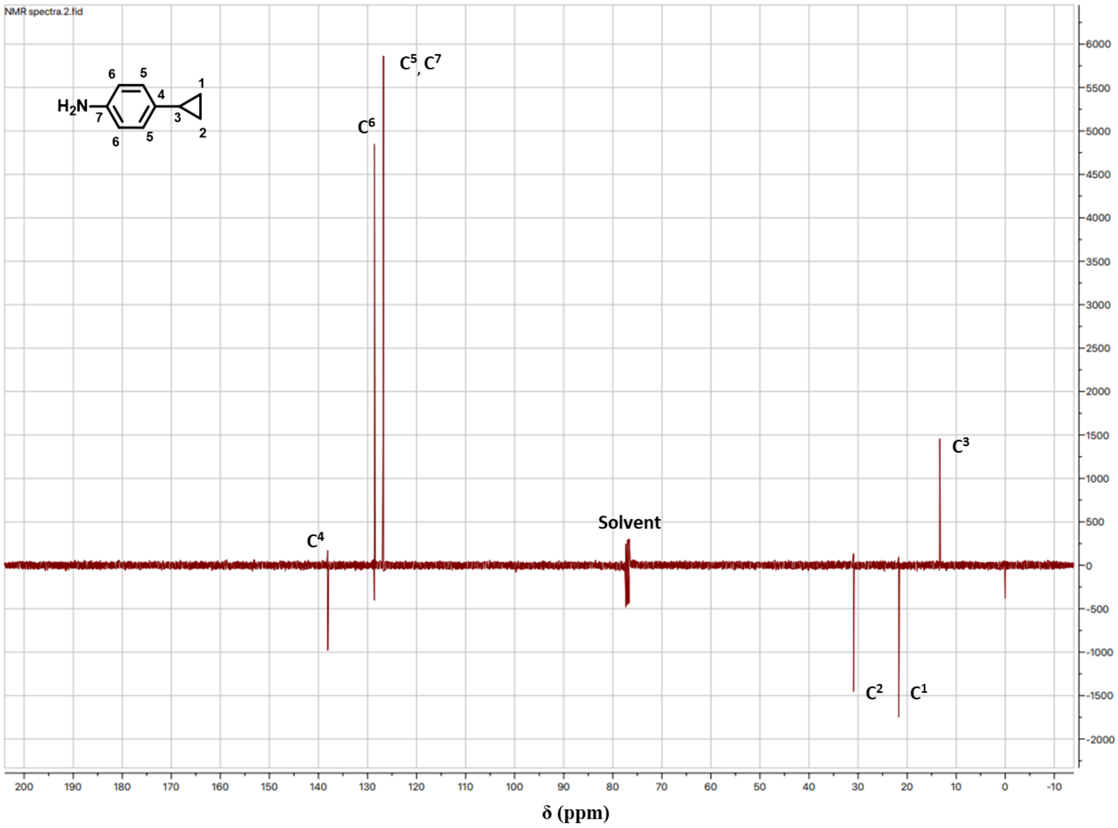
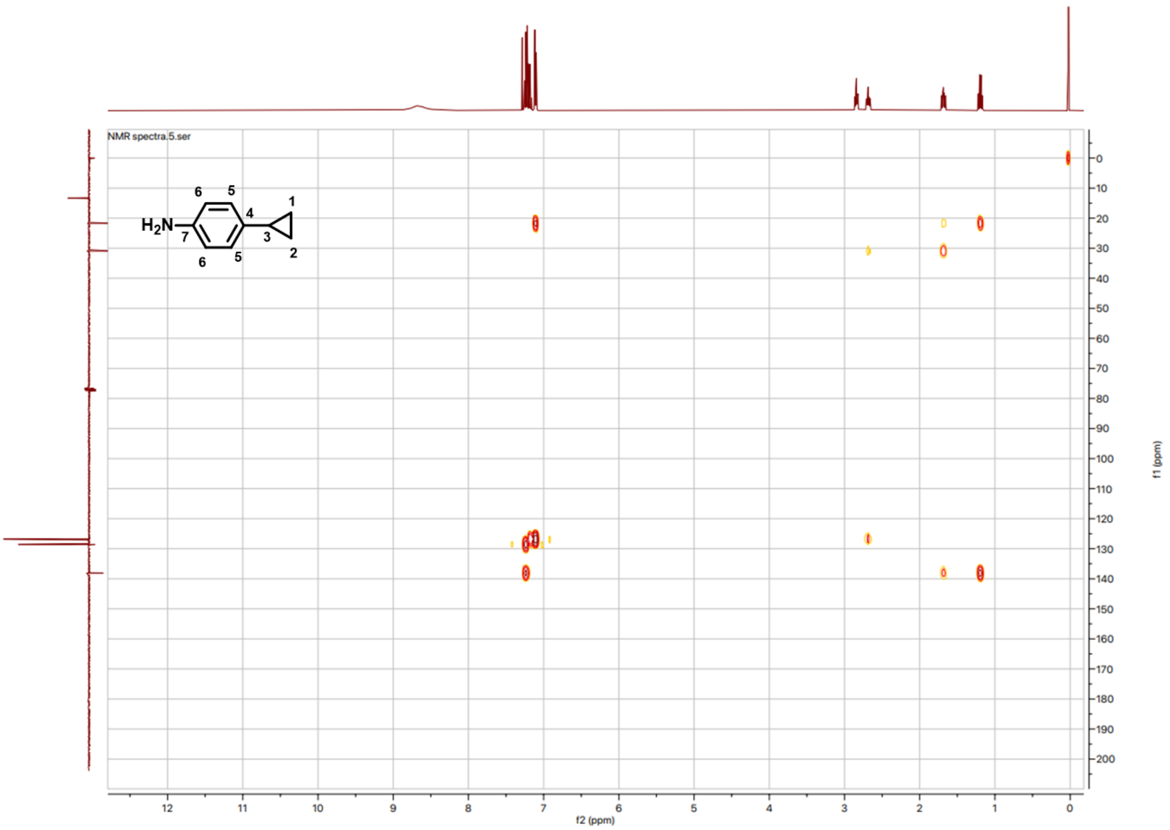


Figure 3. ^{13}C NMR spectrum of 4-cyclopropylaniline



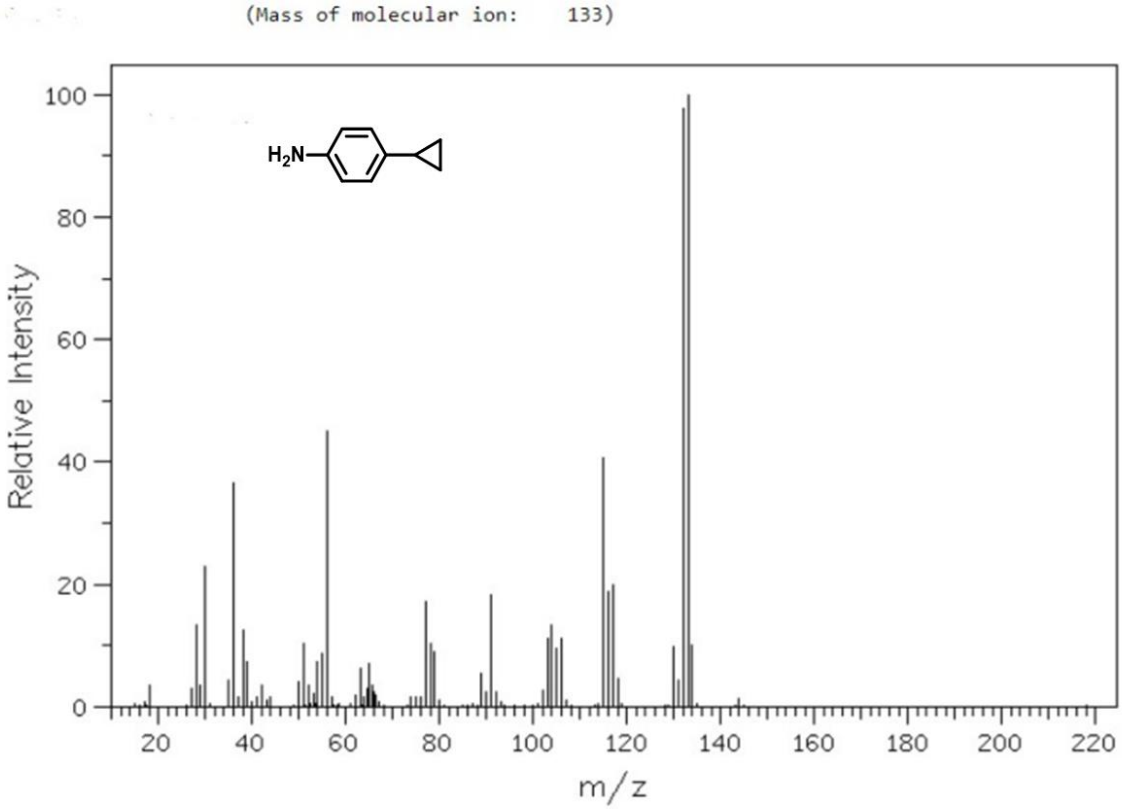
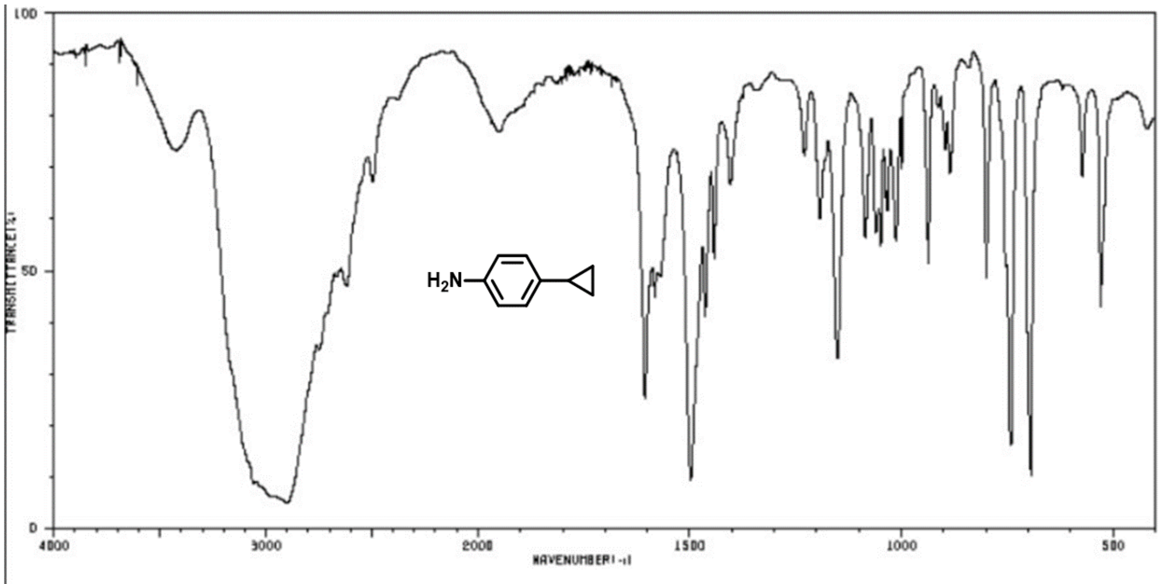


Figure 5. Mass spectrum of 4-cyclopropylaniline



3467	72	1606	24	1388	77	1049	53	886	66
3421	70	1583	43	1341	81	1033	60	800	47
2901	4	1570	47	1229	70	1013	55	754	49
2619	46	1498	9	1193	68	999	68	742	16
2495	64	1464	39	1151	32	936	49	695	10
1950	74	1443	50	1085	55	913	79	573	66
1683	81	1406	64	1060	66	897	70	530	42

Figure 6. FTIR spectrum of 4-cyclopropylaniline