

Characterization and Computational analysis of unsymmetrical azines

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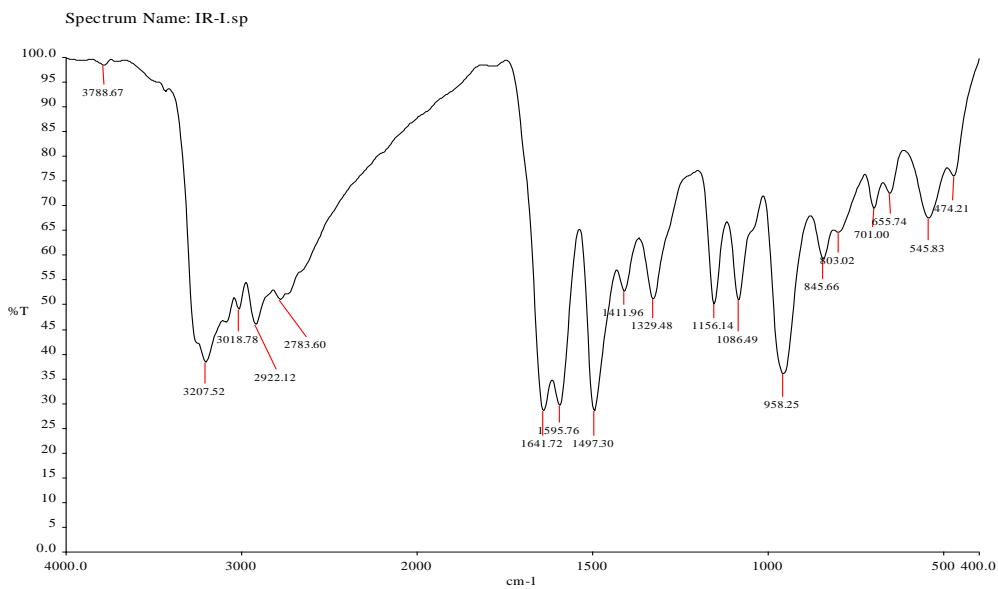


Figure 1. FT-IR Spectrum of azine 1

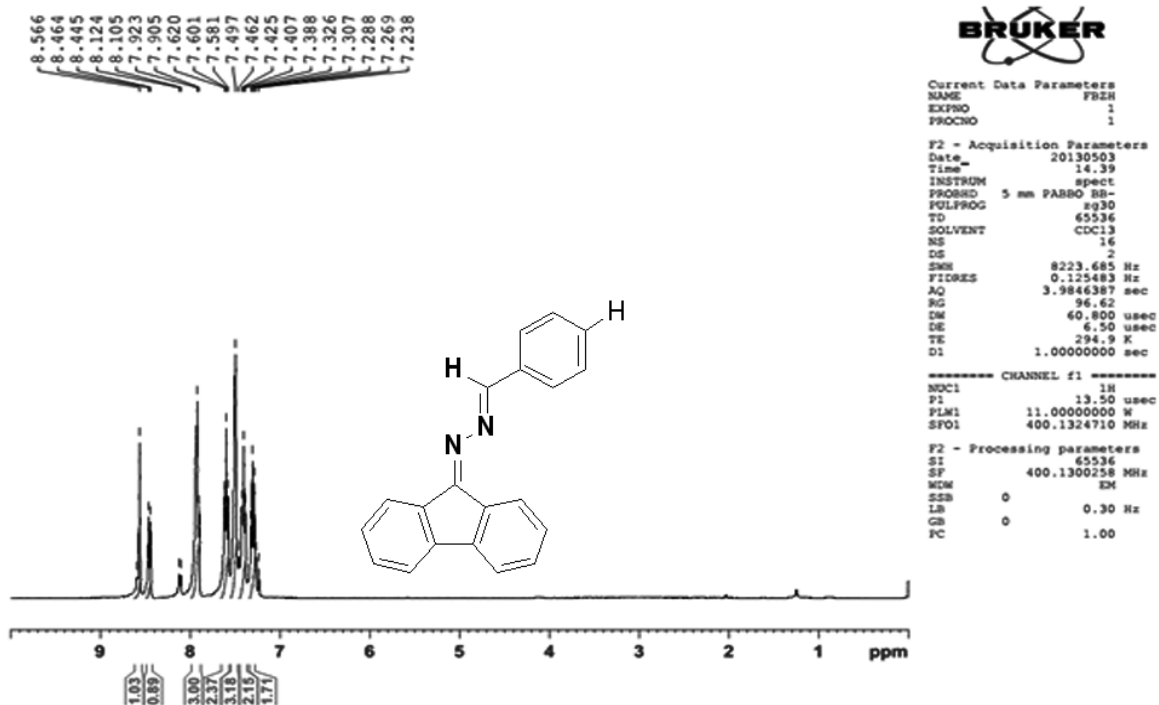


Figure 2. ¹H NMR Spectrum of 1 in CDCl₃

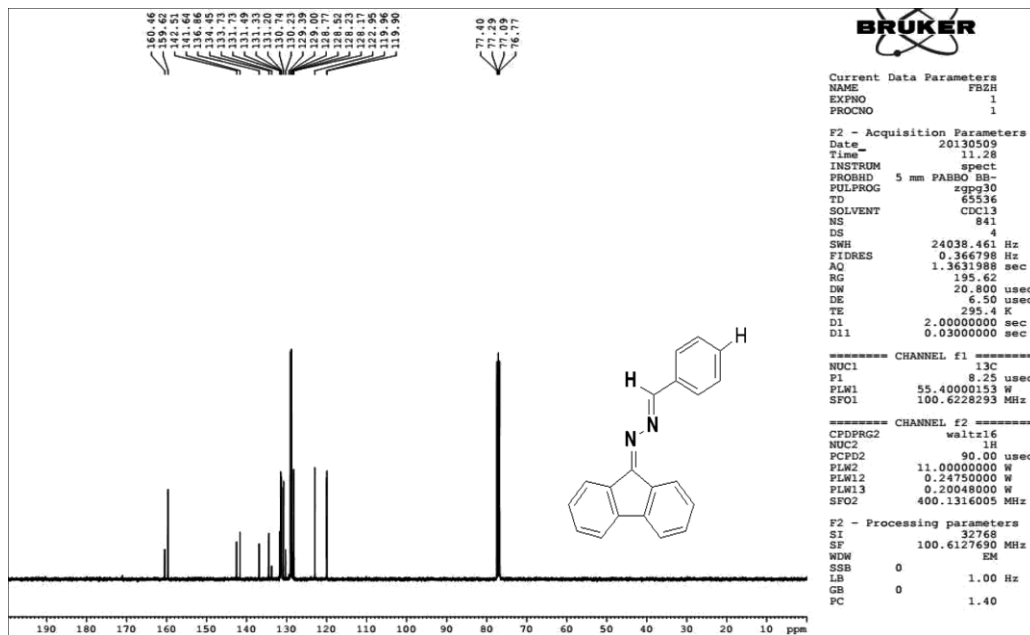


Figure 3. ^{13}C NMR Spectrum of 1 in CDCl_3

Table 1: FT-IR frequency and yield of azines 1-6

Azines	IR frequency (cm^{-1})						Yield (%)
	CH=N	CH	N-N	SP ³ (CH)	SP ³ (C-O)	SCH ₃	
1	1641	3018	1086	-	-	-	98
2	1604	3044	1093	2911	-	-	96
3	1661	3151	1013	-	1115	-	96
4	1660	3150	1075	-	-	630	97
5	1617	3068	1023	-	-	-	95
6	1600	3050	1095	-	-	-	95

Table 2: ^1H NMR data of azines 1-6

^1H NMR (CDCl_3 , 400 MHz) (δ , ppm)						
Azine	1	2	3	4	5	6
CH=N	8.556	8.556	8.562	8.540	8.511	8.546
Aromatic proton	7.269-8.464	7.315-8.502	7.007-8.535	7.282-8.487	7.292-8.385	7.181-8.440
CH ₃	-	2.446	-	-	-	-
OCH ₃	-	-	3.875		-	-
SCH ₃				2.552		

Table 3: ^{13}C NMR data of azines 1-6

Azine	^{13}C NMR (CDCl_3 , 100MHz, ppm)					
	1	2	3	4	5	6
Azomethene	159.62	159.83	160.12	159.54	158.27	159.54
C=N	160.46	160.31	160.40	160.43	160.54	160.42
Aromatic carbon	119.90- 142.51	119.86- 142.43	114.29- 162.32	119.88- 143.35	119.93- 142.57	116.13- 142.53
CH ₃	-	21.74	-	-	-	-
OCH ₃	-	-	55.49	-	-	-
SCH ₃	-	-	-	15.13	-	-
C-Br	-	-	-	-	125.81	-
C-F	-	-	-	-	-	165.94, 163.42