

SUPPORTING INFORMATION

Microstructural investigation and magnetic studies on sonochemically synthesized Ni substituted copper zinc ferrite nanoparticles for Heterogeneous Green Catalytic Click Chemistry and Dye Degradation

Sunil Mukherjee,^a Rahul Kumar Das,^a Atul Bandyopadhyay,^b Bhaskar Jyoti Sarkar^{c,*} and Ujjal Kanti Roy^{a,*}

^a Department of Chemistry, Kazi Nazrul University, Asansol, Paschim Bardhaman, W.B. 713340, India.

^bDepartment of Physics, University of Gour Banga, Mokdumpur, Malda, W.B. 732103, India.

^cDepartment of Physics, Vivekananda Mahavidyalaya, Burdwan, Purba Bardhaman, W.B. 713103, India

*Corresponding authors Email address:

bhaskar.dbm@gmail.com (Bhaskar Jyoti Sarkar)

uroccu@gmail.com (Ujjal Kanti Roy)

Contents	Page no.
1. Table S1	S2
2. Table S2	S2
3. Stability of the catalyst	S3
4. Analytical data	S3-S5
5. Spectra of Products	S6-S15

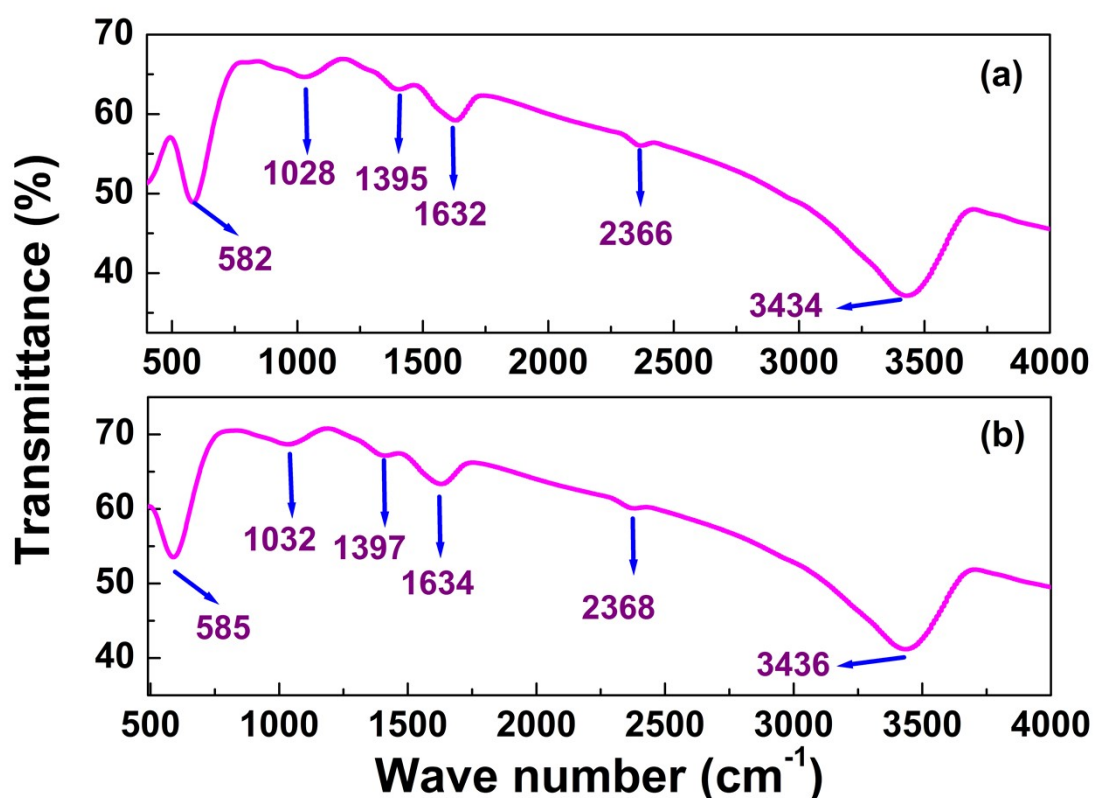
Table S1: Structural and microstructural parameters along with metal-oxygen (M-O) bond lengths of the sample obtained from Rietveld analysis of PXRD pattern of the sample by MAUD software.

Parameters	Values
Formula Weight	238.143
Crystal System	cubic
Space group	Fd-3m
Lattice parameter (Å)	8.35
Volume (Å ³)	582.20
Metal-Oxygen bond length (Å)	1.807(A-site) 2.08(B-site)
Metal-Oxygen bond angle	109.47° (A-site) 90.1° (B-site)
R _{wp} (%)	1.620
R _{exp} (%)	1.0766
GOF (sig)	1.505

Table S2: Fractional coordinates and occupancy of different ions obtained from the Rietveld refinement by MAUD software.

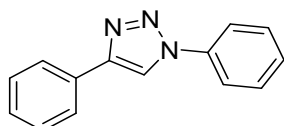
Ions	x	y	z	Occupancy (± 0.002)
Zn (A)	0	0	0	0.2
Fe (A)	0	0	0	0.8
Cu (B)	0.625	0.625	0.625	0.25
Ni(B)	0.625	0.625	0.625	0.15
Fe (B)	0.625	0.625	0.625	0.6
O	0.375	0.375	0.375	1.00

Stability of the catalyst: To determine the stability of the catalyst FTIR after three run has been performed and compared to fresh. It shows that the catalyst is fairly stable (please see supporting information). The FTIR spectra of the fresh catalyst (Fig. a) and the used catalyst (Fig. b) exhibit the same characteristic absorption pattern. Only minor shifts in wave numbers and slight variations in transmittance are observed in Fig. b compared to Fig. a. These small changes indicate that no significant structural alteration has occurred during the reaction. Therefore, the catalyst can be considered **structurally stable** under the reaction conditions.

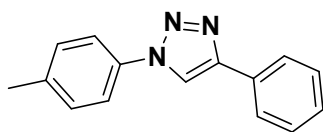


FTIR spectra of the fresh catalyst (Fig. a) and the used catalyst (Fig. b)

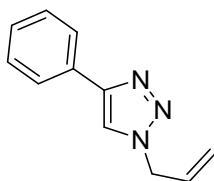
Analytical data of the synthesized organic compounds:



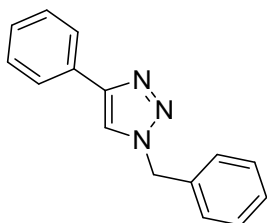
1,4-diphenyl-1H-1,2,3-triazole (P₁): white solid, ¹H NMR (d₆-DMSO, 400 MHz) δ 7.35 (t, J = 6 Hz, 1H), 7.37-7.54 (m, 3 H), 7.64 (t, J = 7.5 Hz, 2H), 7.94-7.97 (m, 4H), 9.31 (s, 1H). ¹³C NMR (CDCl₃, 100 MHz) δ 117.6, 120.5, 125.8, 128.4, 128.8, 128.9, 129.7, 130.0, 137.0. 148.5. LC-MS Calcd. for C₁₄H₁₁N₃ m/z 221.1, found (M+H) 222.1.



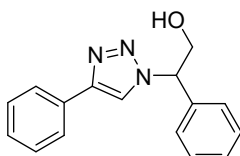
4-phenyl-1-(p-tolyl)-1H-1,2,3-triazole (*P*₂): ¹H NMR (CDCl₃, 400 MHz) δ: 2.40 (s, 3H); 7.36-7.51 (m, 5H), 7.83 (d, J = 8.2 Hz, 2H), 7.94 (d, J = 7.6 Hz, 2H), 9.3 (s, 1H). ¹³C NMR (CDCl₃, 100 MHz) δ 21.1, 117.6, 120.6, 125.8, 128.3, 128.8, 130.2, 134.7, 138.8, 148.2. LC-MS Calcd. for C₁₅H₁₃N₃ m/z 235.1, found (M+H) 236.3.



1-Allyl-4-phenyl-1H-[1,2,3]triazole (*P*₃): ¹H NMR (400 MHz, d₆-DMSO): δ: 4.90-5.08 (m, 2H), 5.22-5.32 (m, 2H), 6.07-6.15 (m, 1H), 7.31-7.35 (m, 1H), 7.43-7.53 (m, 2H), 7.86 (d, 2H, J=7.2), 8.55 (s, 1H). ¹³C NMR (100 MHz, CDCl₃) δ= 51.7, 118.7, 121.2, 125.0, 127.7, 128.7, 131.0, 130.6, 132.5, 146.35. Anal. (C₁₁H₁₁N₃) calcd, C: 71.33; H: 5.99; N: 22.69; found, C: 71.35; H: 6.04; N: 22.72.



1-Benzyl-4-phenyl-1H-1,2,3-triazole (*P*₄): ¹H NMR (600 MHz, CDCl₃): δ: 5.59 (s, 2H), 7.32–7.345 (m, 3H), 7.38–7.434 (m, 5H), 7.68 (s, 1H), 7.80–7.82 (m, 2H). ¹³C NMR (150 MHz, CDCl₃): δ: 147.79, 134.23, 130.07, 128.71, 128.36, 127.62, 127.61, 125.25, 119.04, 53.79. Anal. (C₁₅H₁₃N₃) calcd, C: 76.57; H: 5.57; N: 17.86; found, C: 76.61; H: 5.60; N: 17.89.

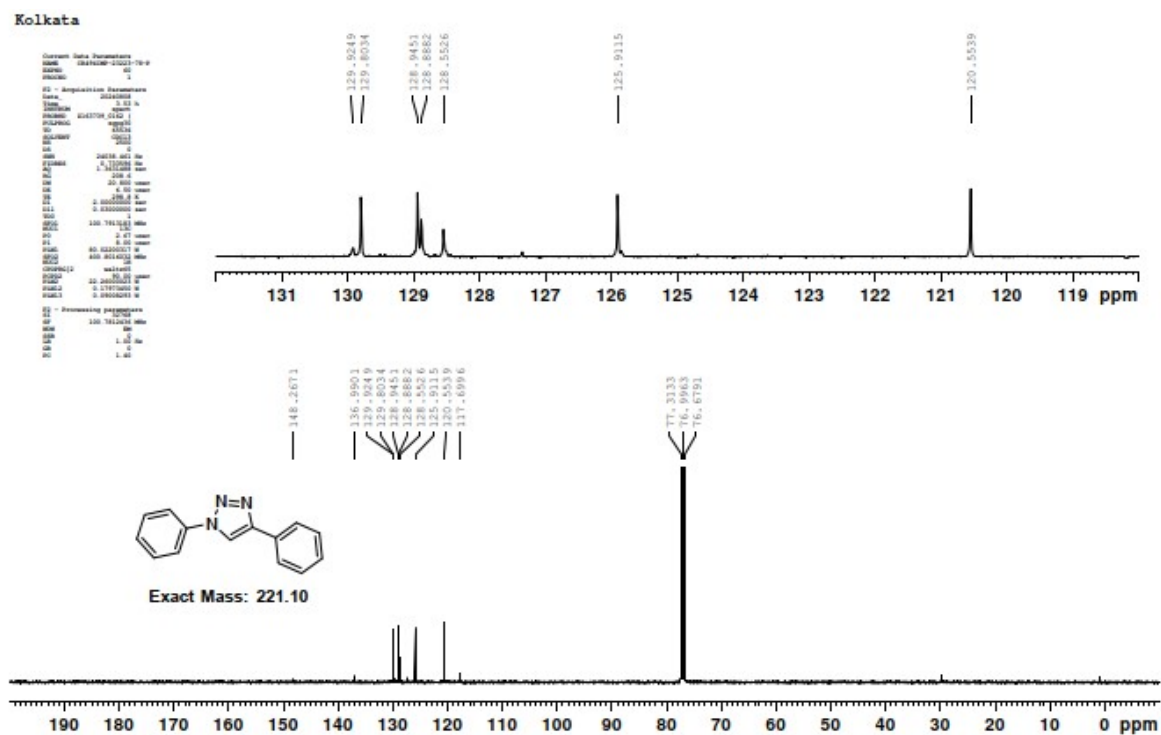


2-phenyl-2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethan-1-ol (*P*₅):

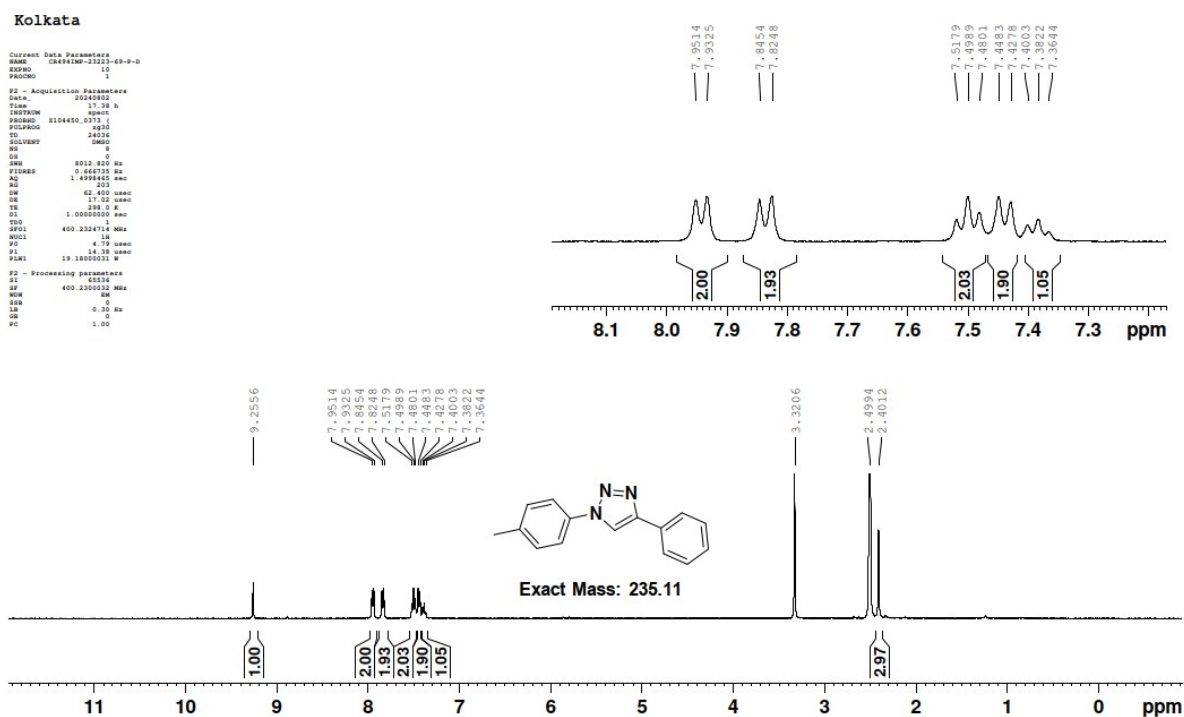
White solid, ^1H NMR (400 MHz, DMSO) δ 3.99 – 4.09 (m, 1H), 4.27 – 4.38 (m, 1H), 5.36 (t, $J = 5.5$ Hz, 1H), 5.79 – 5.87 (m, 1H), 7.29 – 7.50 (m, 8H), 7.87 (d, $J = 7.7$ Hz, 2H), 8.82 (s, 1H). ^{13}C NMR (100 MHz, d_6 -DMSO): δ 63.06, 66.33, 120.81, 125.0, 127.03, 127.71, 128.17, 128.60, 130.74, 137.22, 146.09. LC-MS Calcd. for $\text{C}_{16}\text{H}_{15}\text{N}_3\text{O}$ m/z 265.12, found (M+H) 266.2. LC-MS Calcd. for $\text{C}_{16}\text{H}_{15}\text{N}_3\text{O}$ m/z 265.12, found (M+H) 266.2.

[illegible]

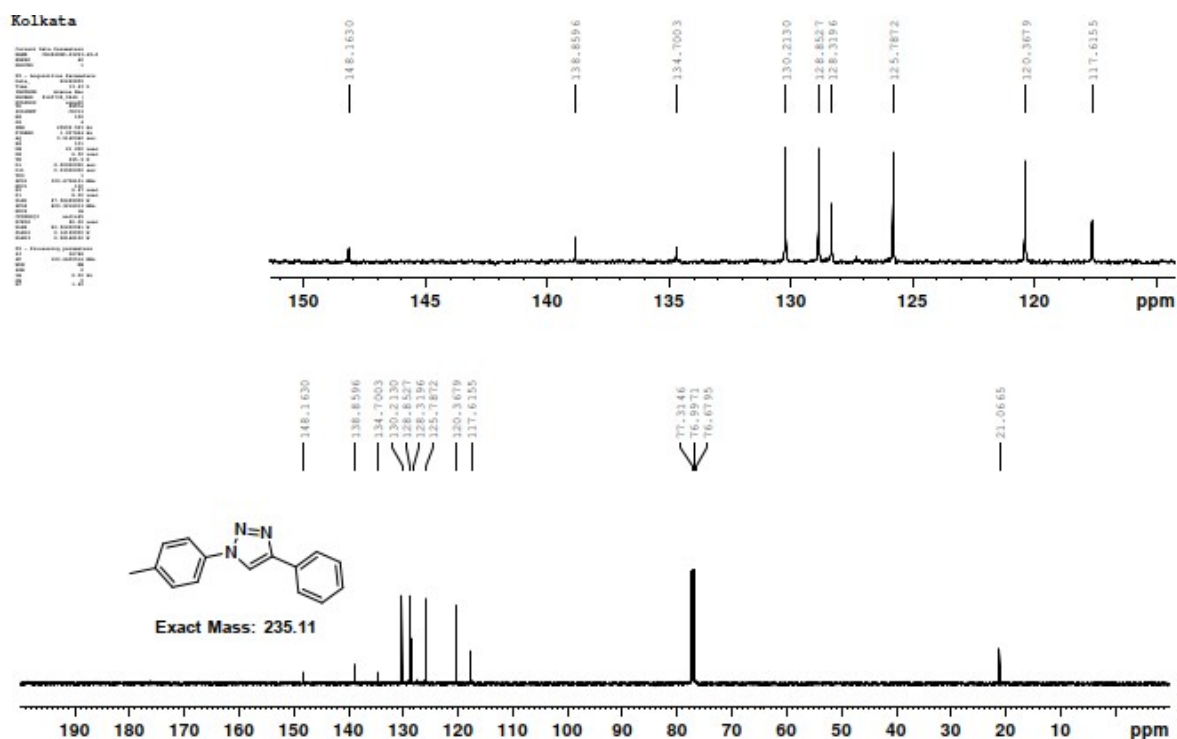
¹³C NMR Spectrum of the Compound 1,4-diphenyl-1H-1,2,3-triazole (P₁) :



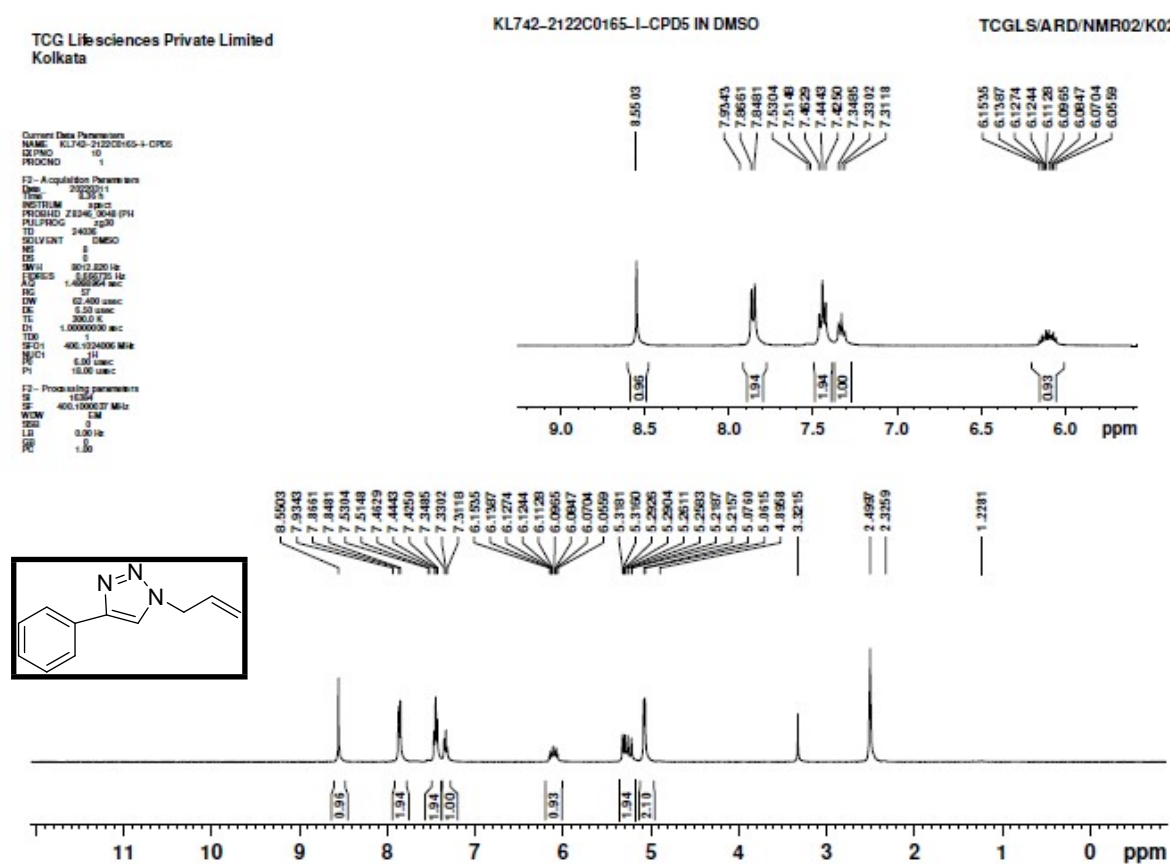
¹H NMR Spectra of Compound P₂:



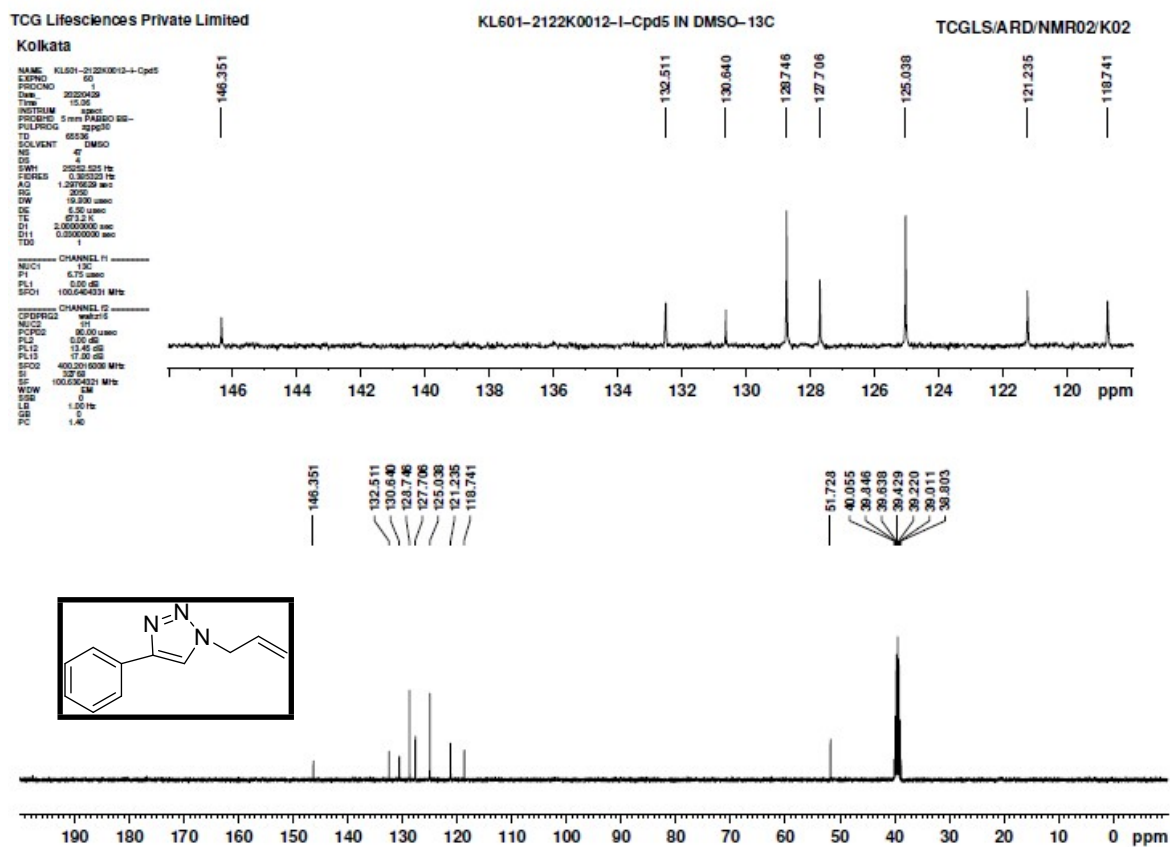
¹³C NMR Spectra of Comp P₂:



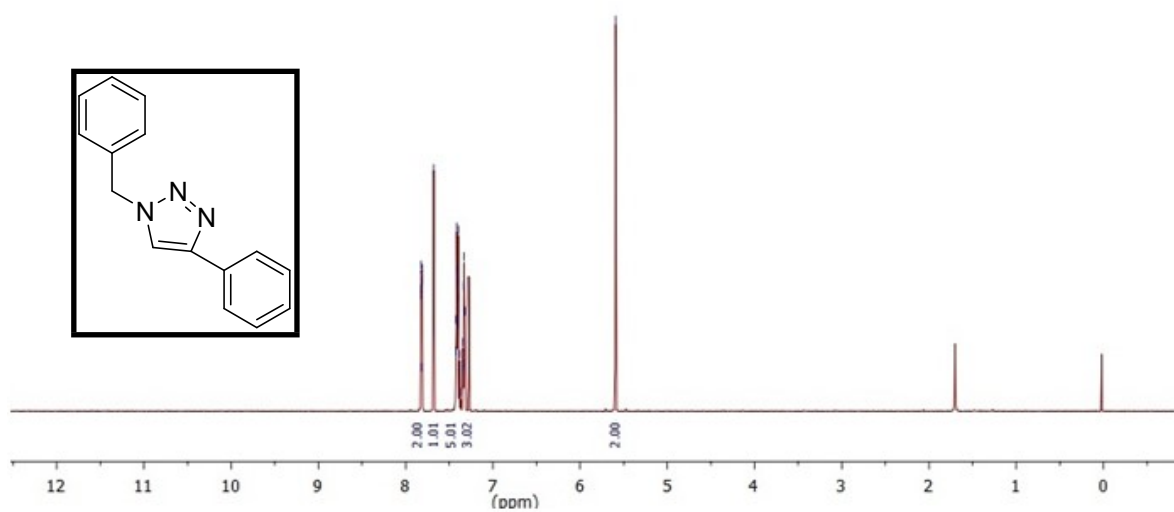
¹H NMR spectra of the compound **P₃**:



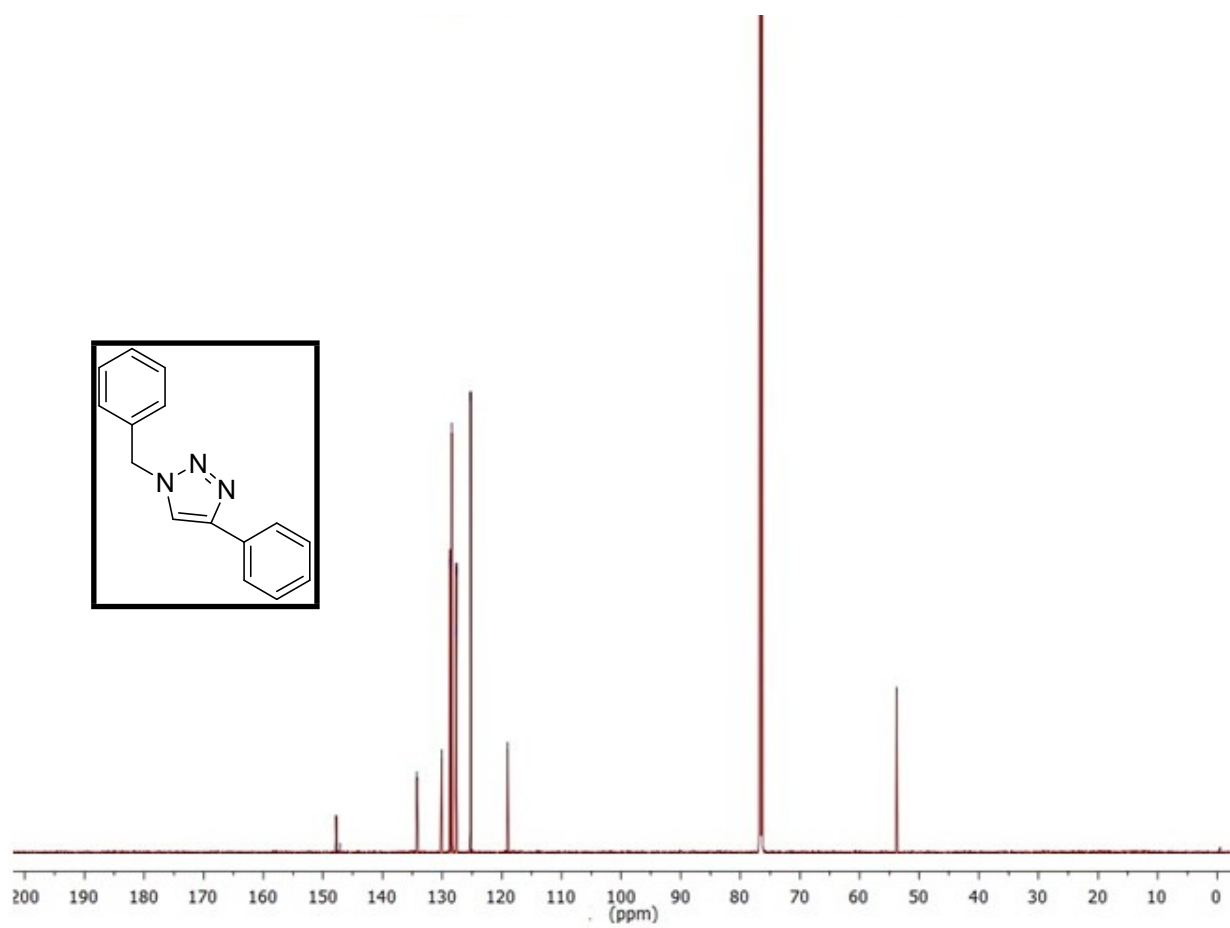
^{13}C NMR spectra of the compound P₃:



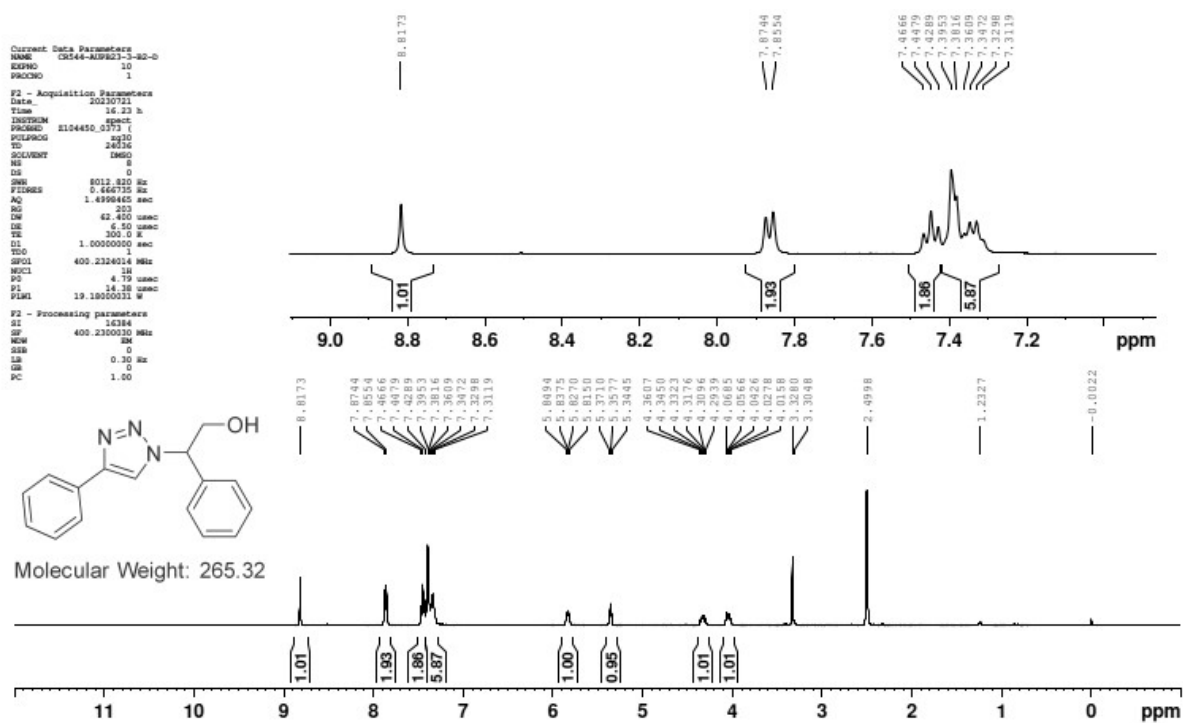
^{13}C NMR spectrum of the compound P₄:



^{13}C NMR spectrum of the compound P₄:



¹H NMR Spectrum of the Compound P₅:



¹³C NMR of the compound P₅:

