Supporting Information

Energetic Butterfly: Heat-Resistant Diaminodinitro *trans*-Bimane

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1. **^{1}H NMR Spectroscopy**.

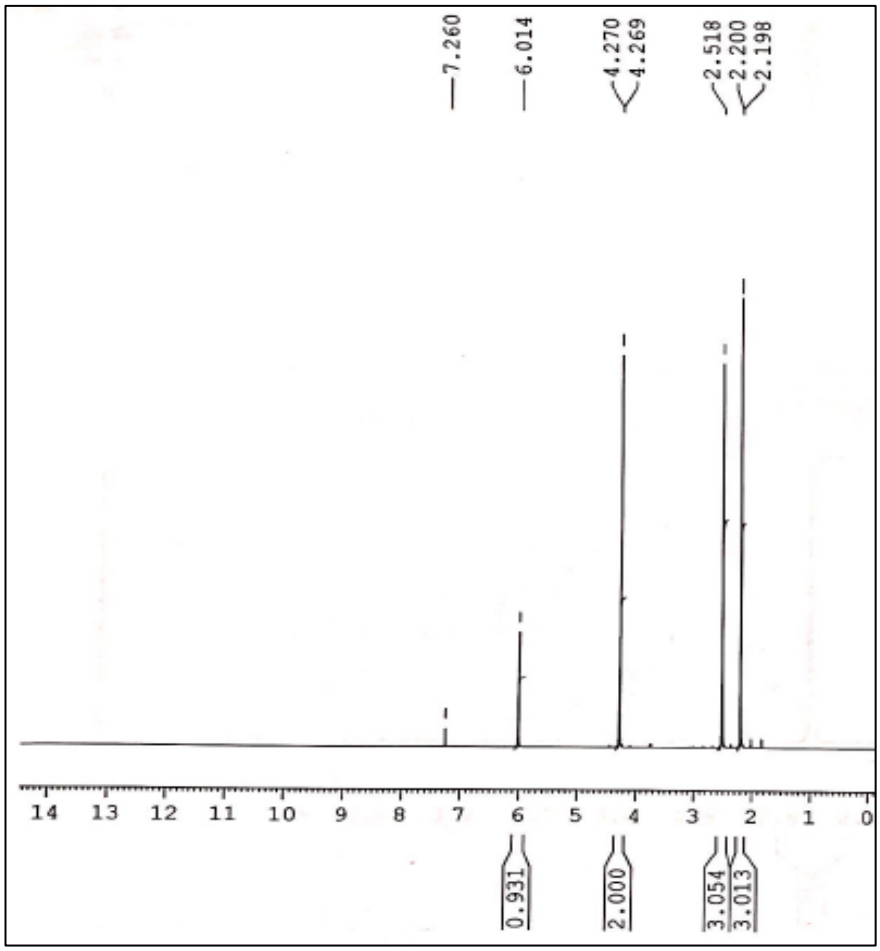

Figure S1. ^{1}H NMR spectrum of compound **1**.

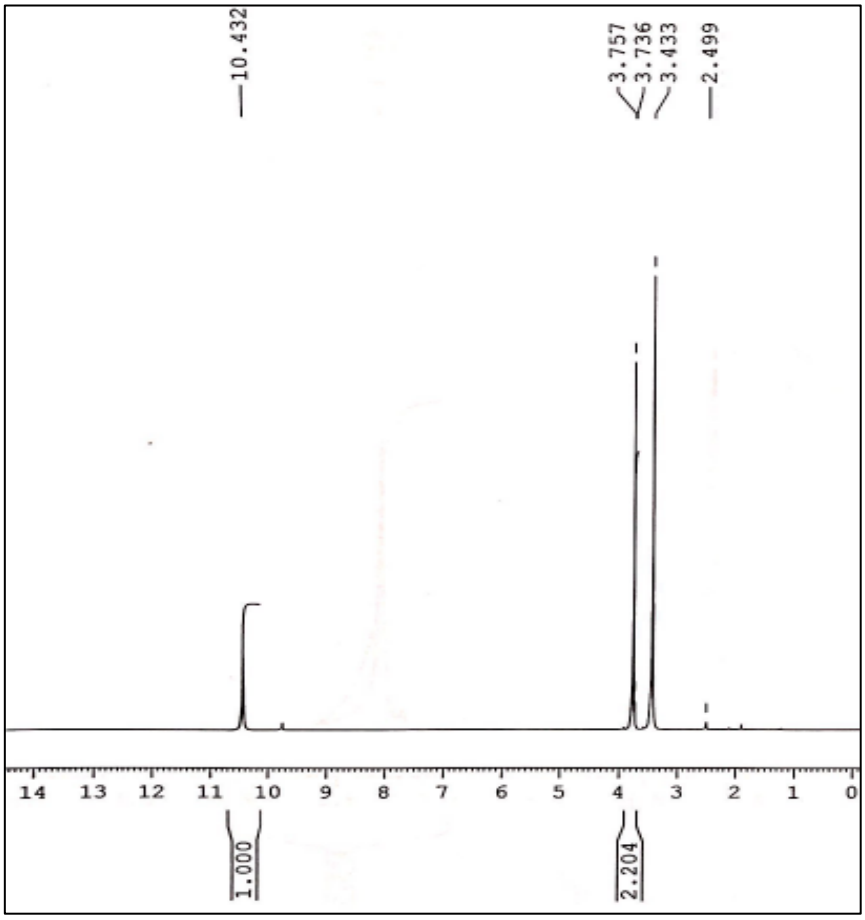

Figure S2. ^{1}H NMR spectrum of compound **2**.

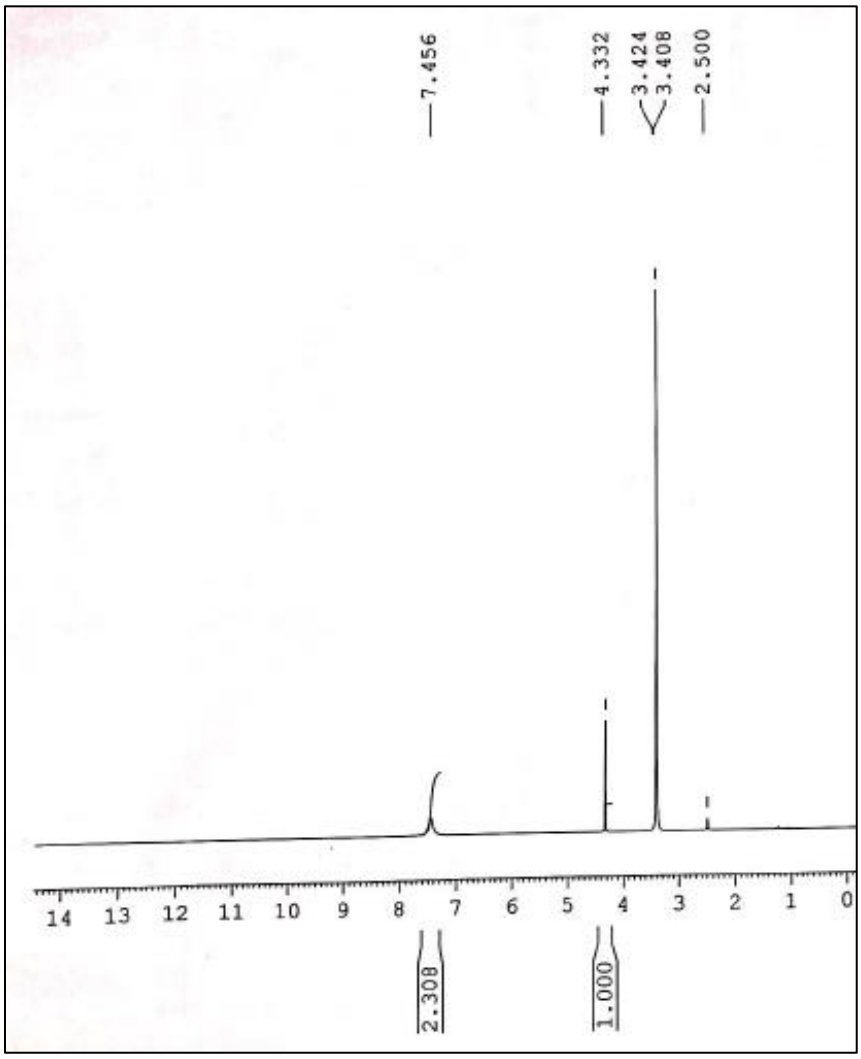

Figure S3. ^{1}H NMR spectrum of compound **3**.

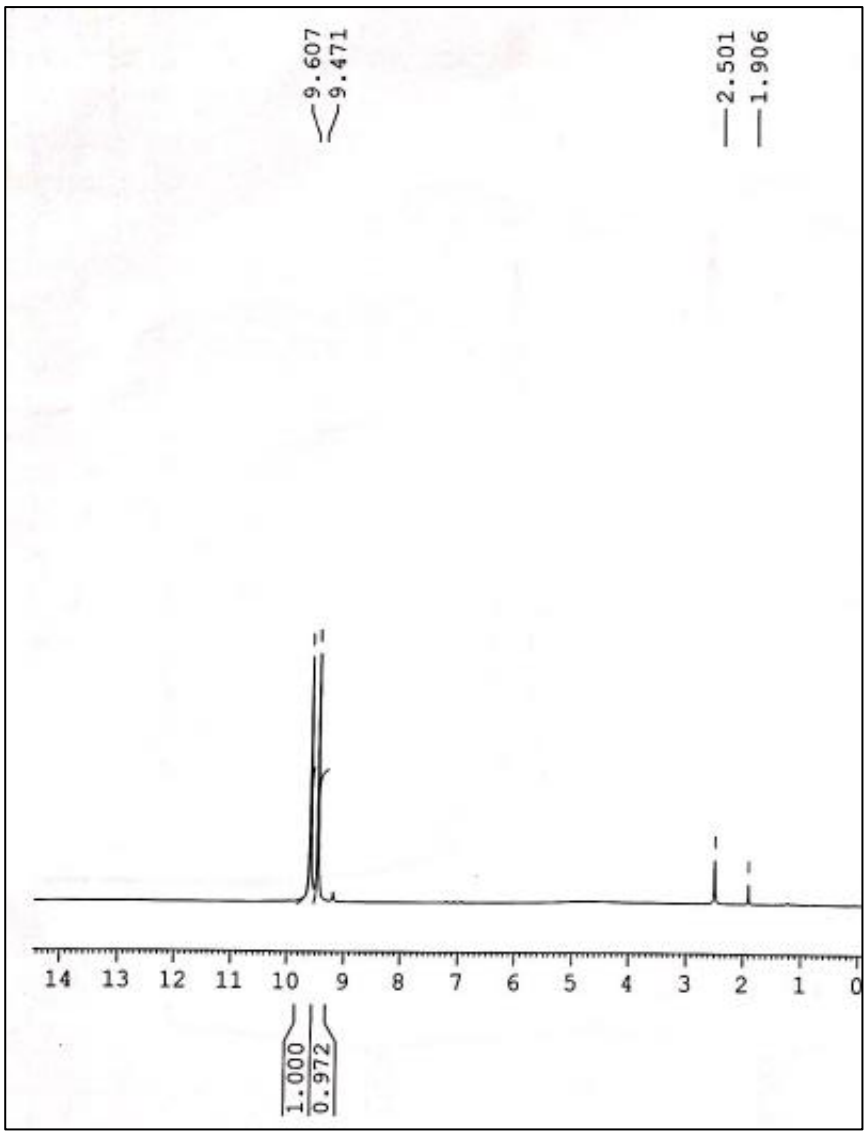

Figure S4. ^{1}H NMR spectrum of compound **4**.

2. **^{13}C NMR Spectroscopy**.

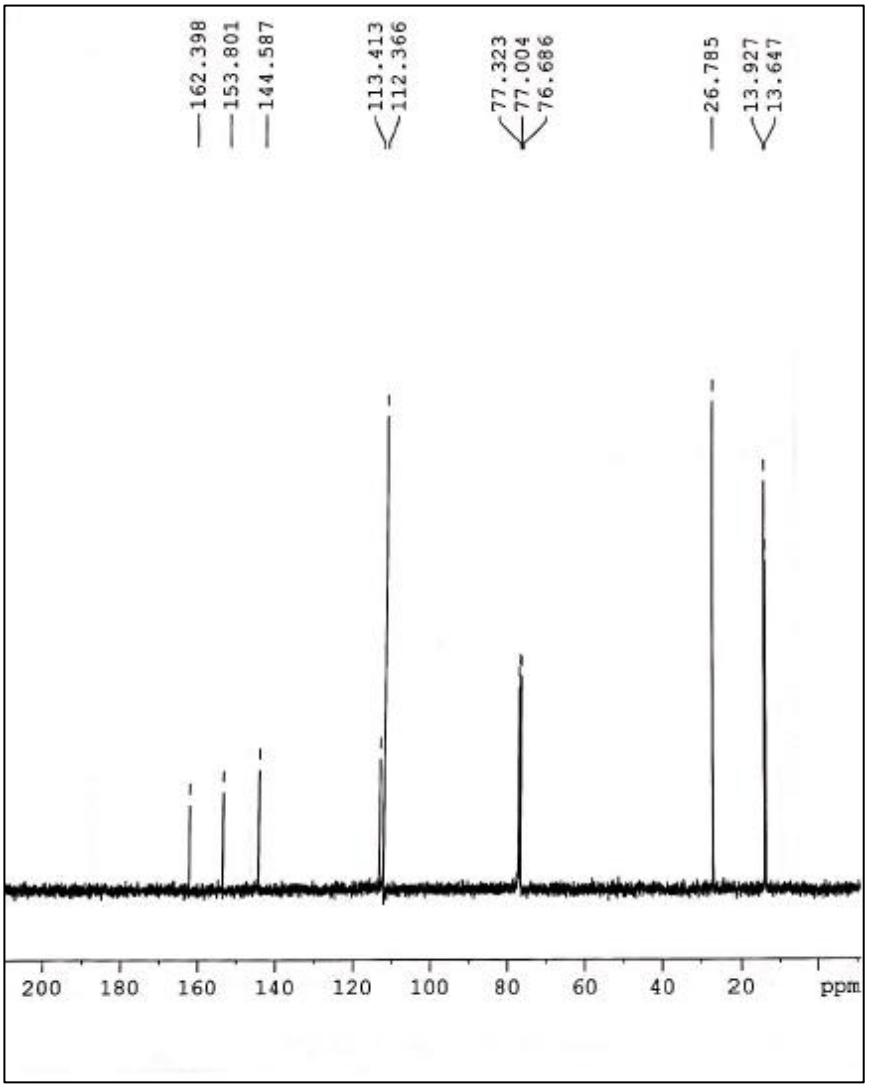

Figure S5. ^{13}C NMR spectrum of compound **1.**

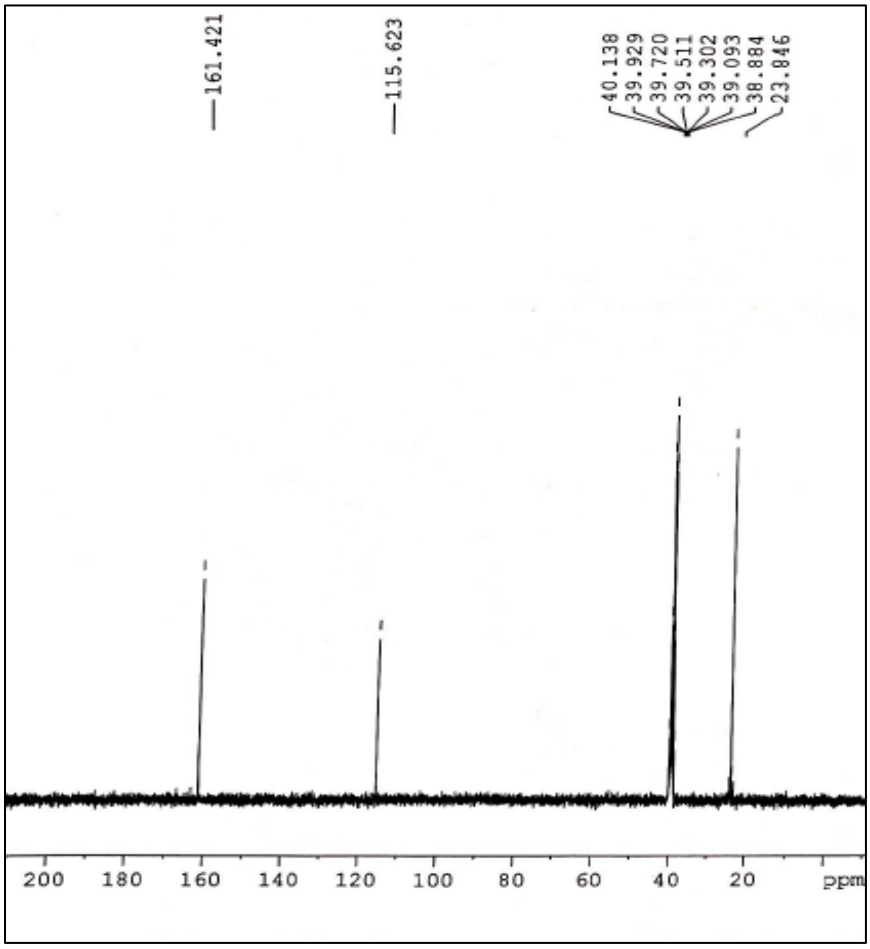

Figure S6. ^{13}C NMR spectrum of compound **2.**

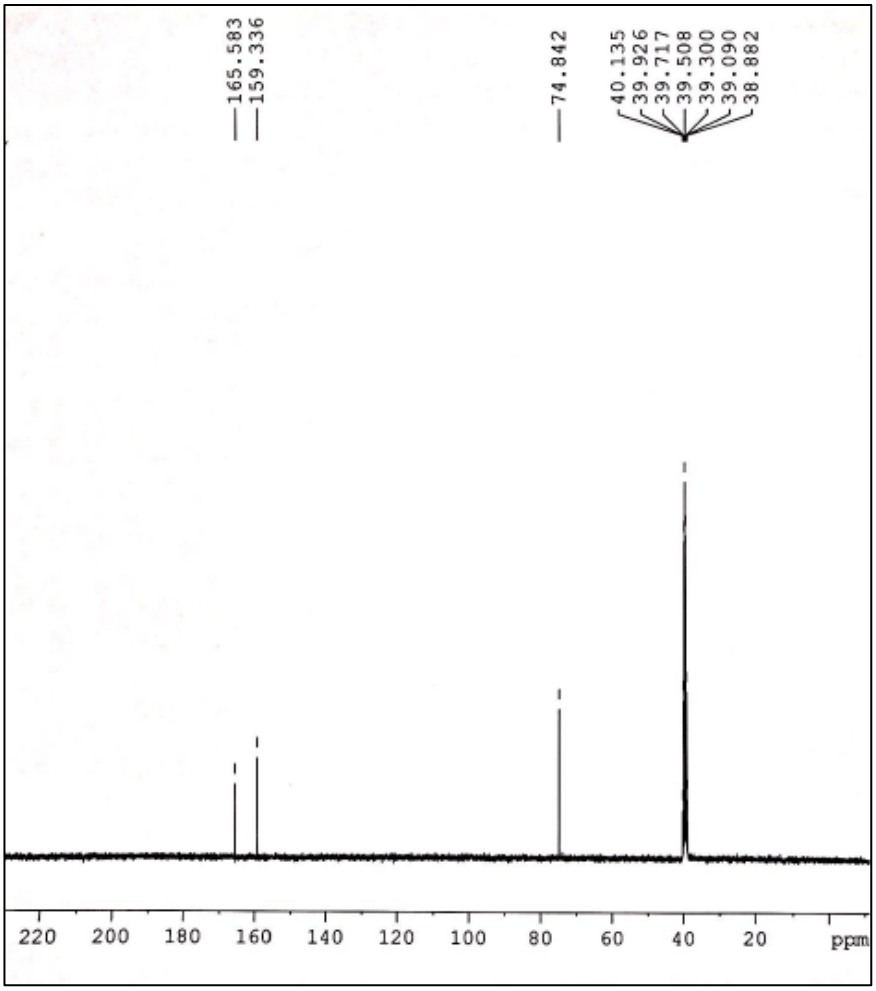

Figure S7. ^{13}C NMR spectrum of compound **3.**

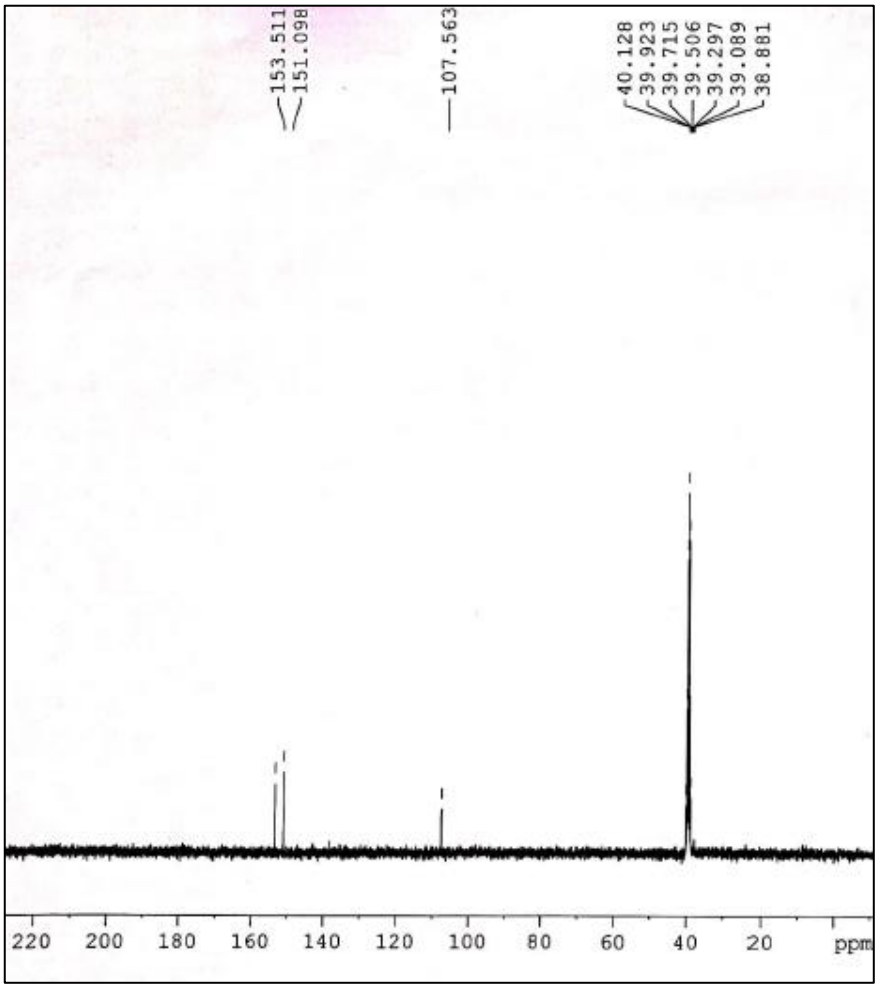

Figure S8. ^{13}C NMR spectrum of compound **4**.

3. **FTIR Spectroscopy**.

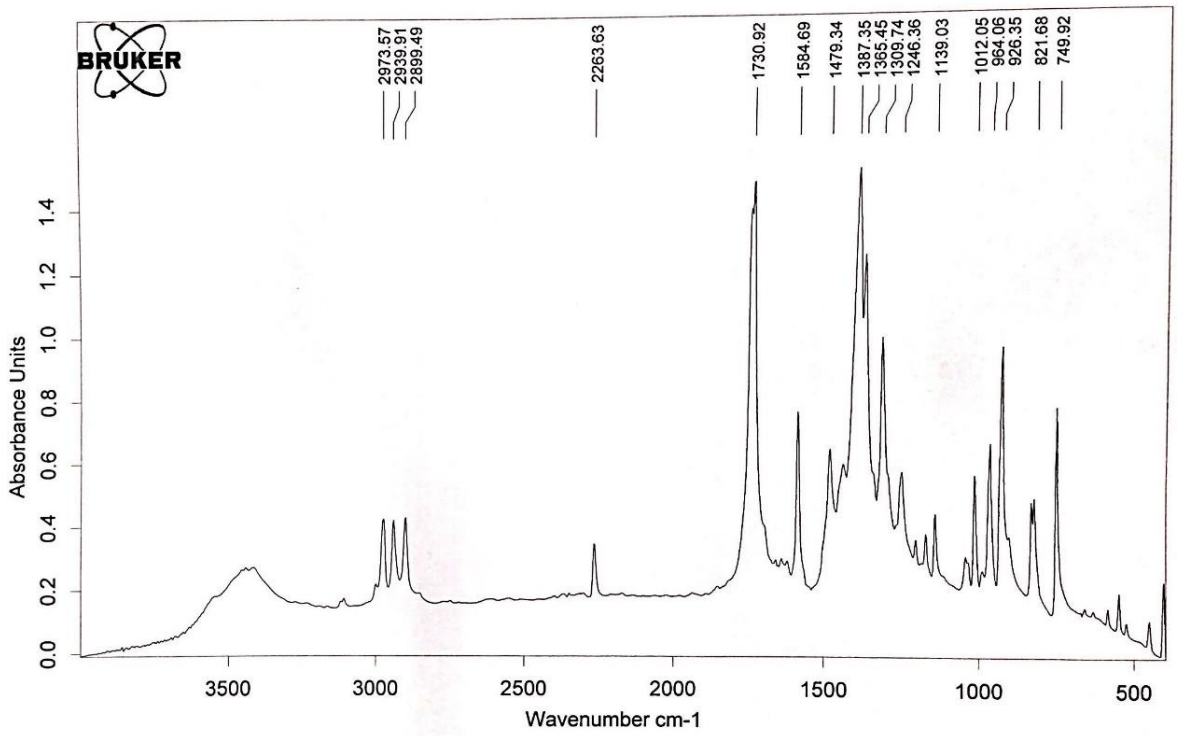

Figure S9. FTIR spectra of compound **1.**

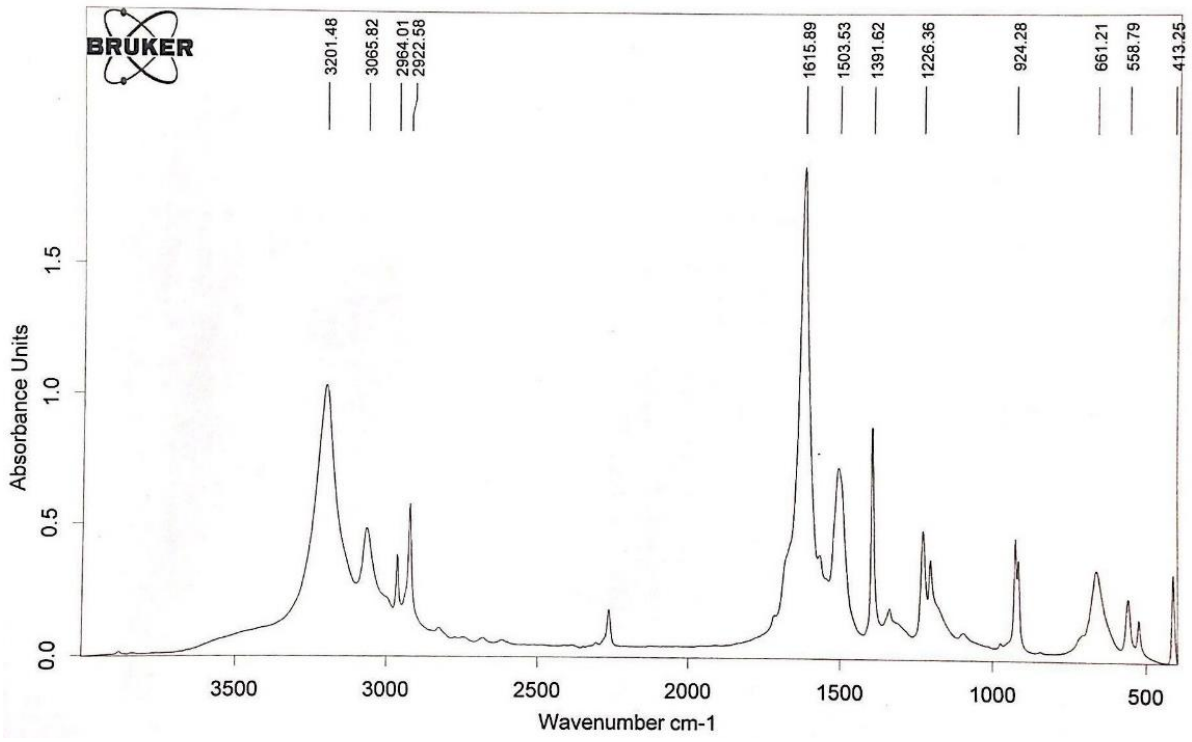

Figure S10. FTIR spectra of compound **2.**

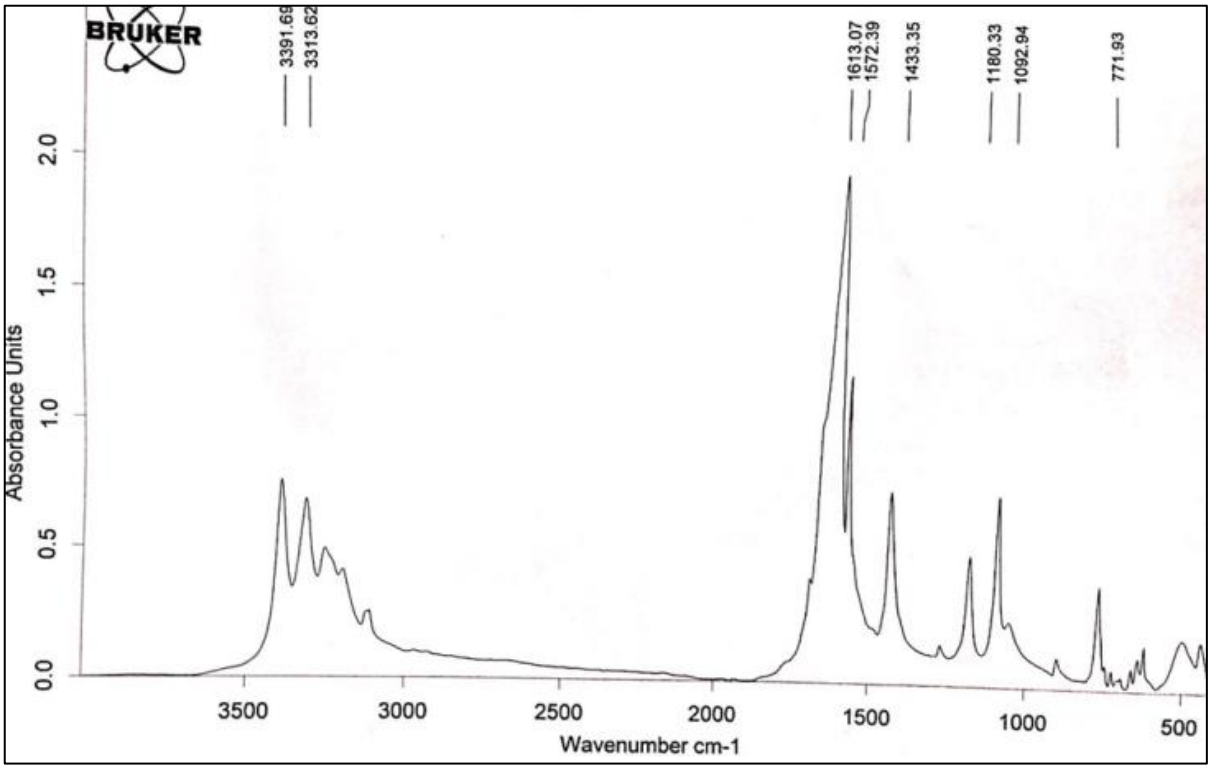

Figure S11. FTIR spectra of compound **3.**

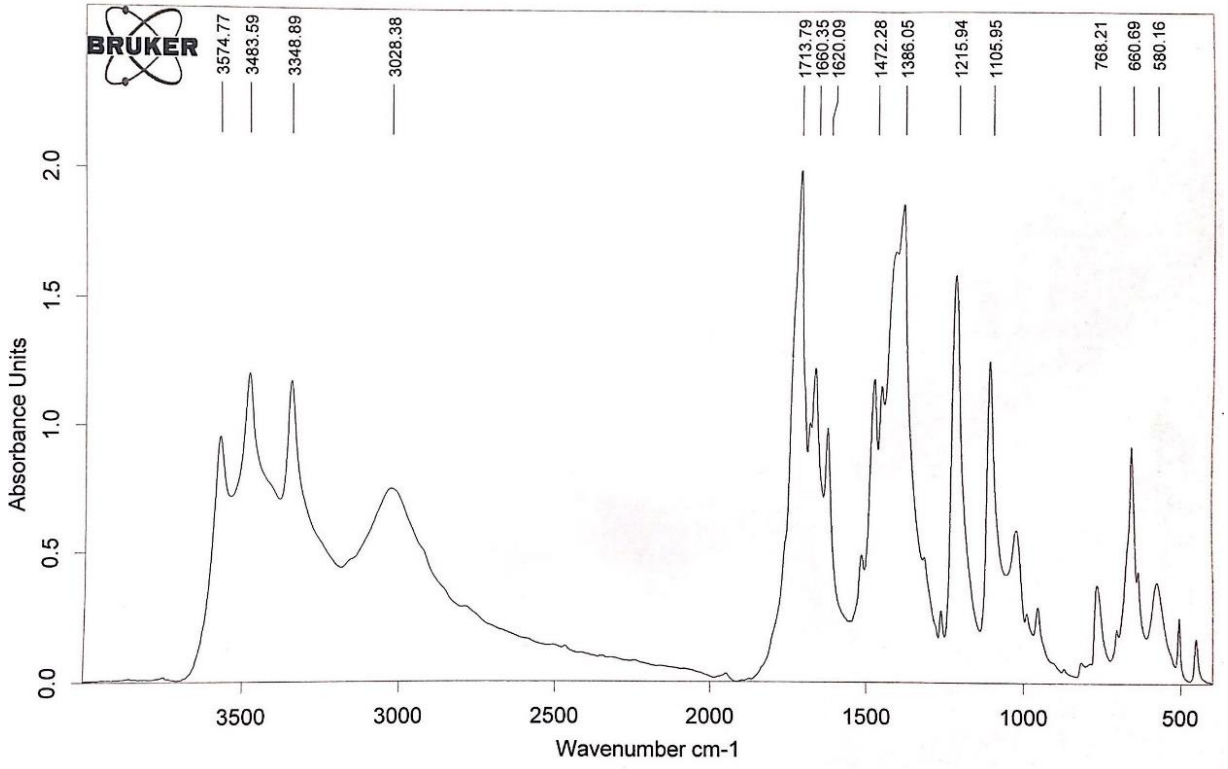

Figure S12. FTIR spectra of compound **4.**

4. X-ray crystallography data

Table S1 Crystal data and structure refinement for compound 4.

Parameter	**4**
Formula	$C_6H_4N_6O_6$
Mr	292.18
T /K	173
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.220(2)
b/Å	9.605(2)
c/Å	6.5492(15)
a/°	90
b/°	92.304(5)
g/°	90
Volume	516.7(2)
Z	2
ρ/g·cm^{-3}	1.878
Mu/mm^{-1}	0.175
F(000)	300
Crystal size/mm3	0.18 × 0.11 × 0.08
Radiation	MoKα (λ = 0.71073)
2θ /° range for data collection	3.525 to 25.561
reflections collected	1061
Independent reflections	1061 [R_{sigma} = 0.0200]
data/restraints/parameters	1061/0/94
GOF on F^2	1.099
R_1 [I>2σ(I)]	0.0504
wR_2 [I>2σ(I)]	0.1608
R_1 (all data)	0.0559
wR_2 (all data)	0.1657
largest diff. peak and hole [e Å^{-3}]	0.51/-0.42
CCDC	1955362

Table S2 Bond Lengths for 4.

Atom	Atom	Length/Å
O1	N1	1.246(2)
O2	N1	1.230(2)
O3	C3	1.215(3)
N1	C2	1.386(2)
N2	C1	1.301(3)
N4	N4[1]	1.390(3)
N4	C1	1.359(2)
N4	C3[1]	1.397(3)
C1	C2	1.413(3)
C2	C3	1.442(3)

[1]1-X,1-Y,1-Z

Table S3 Bond Angles for compound 4.

Atom	Atom	Atom	Angle/°
O1	N1	C2	117.12(18)
O2	N1	O1	122.88(17)
O2	N1	C2	120.00(17)
N4[1]	N4	C3[1]	110.66(19)
C1	N4	N4[1]	109.92(19)
C1	N4	C3[1]	139.36(16)
N2	C1	N4	122.02(17)
N2	C1	C2	132.08(17)
N4	C1	C2	105.91(15)
N1	C2	C1	123.86(18)
N1	C2	C3	125.58(19)
C1	C2	C3	110.56(16)
O3	C3	N4[1]	122.29(17)
O3	C3	C2	134.80(18)
N4[1]	C3	C2	102.91(17)

[1]1-X,1-Y,1-Z

Table S4 Torsion Angles for 4.

A	B	C	D	Angle/°
O1	N1	C2	C1	-0.8(3)
O1	N1	C2	C3	178.47(18)
O2	N1	C2	C1	179.19(16)
O2	N1	C2	C3	-1.5(3)
N1	C2	C3	O3	0.7(3)
N1	C2	C3	N41	-178.93(17)
N2	C1	C2	N1	0.4(3)
N2	C1	C2	C3	-178.92(18)
N41	N4	C1	N2	177.98(19)
N41	N4	C1	C2	-1.8(3)
N4	C1	C2	N1	-179.78(16)
N4	C1	C2	C3	0.8(2)
C1	C2	C3	O3	-179.9(2)
C1	C2	C3	N41	0.42(18)
C31	N4	C1	N2	1.2(4)
C31	N4	C1	C2	-178.6(2)

[1]1-X,1-Y,1-Z

Table S5 Hydrogen Atom Coordinates (Å×104) and Isotropic Displacement Parameters (Å2×103) for 4.

Atom	x	y	z	U(eq)
H2A	2853.5	2395.29	6029.59	29
H2B	1424.94	3258.69	6734.24	29
H5A	1840.47	96.92	6438.64	63
H5B	3278.11	-346.82	5777.08	63