Supporting Information

for

Aromatic C-nitrosation by a Copper(II)-nitrosyl complex

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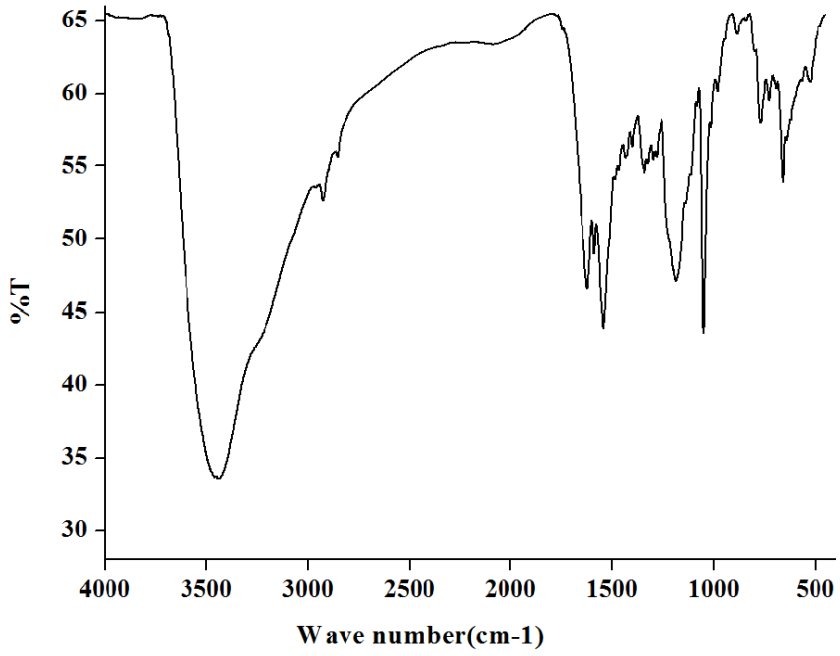


Figure S1. FT-IR spectrum of complex **1** in KBr pallet.

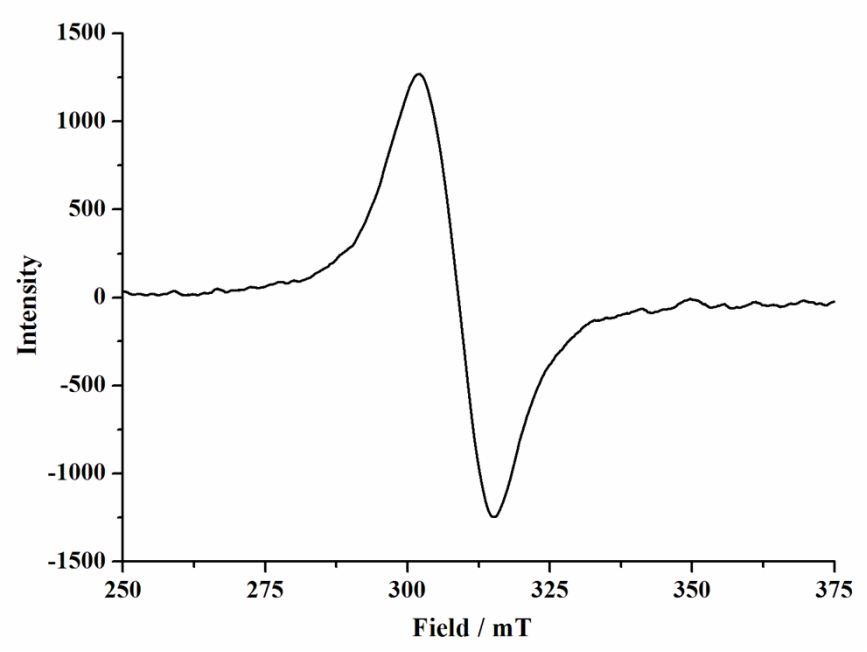


Figure S2. X-Band EPR spectrum of complex **1** in methanol at room temperature.

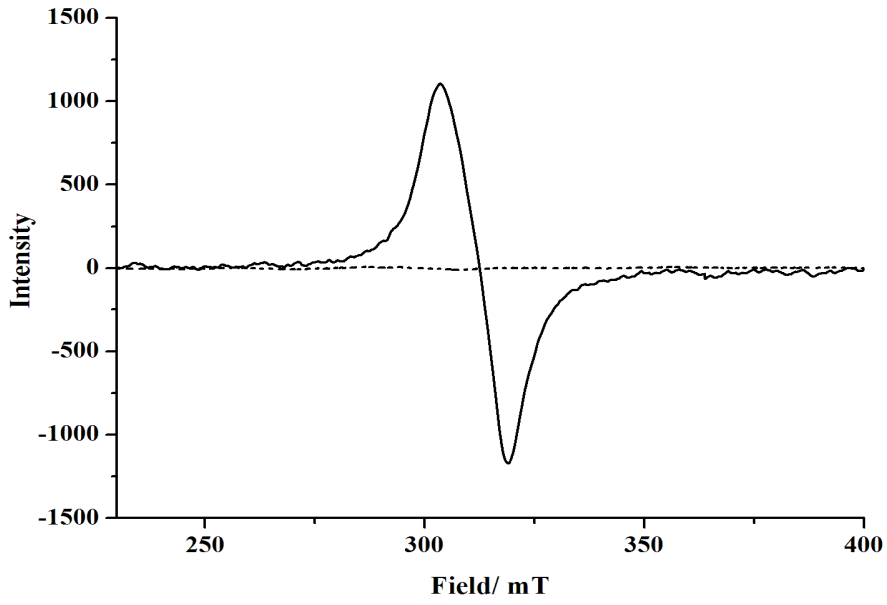


Figure S3. X-Band EPR spectra of complex **1**before (solid line) and after (dotted line) purging nitric oxide in methanol.

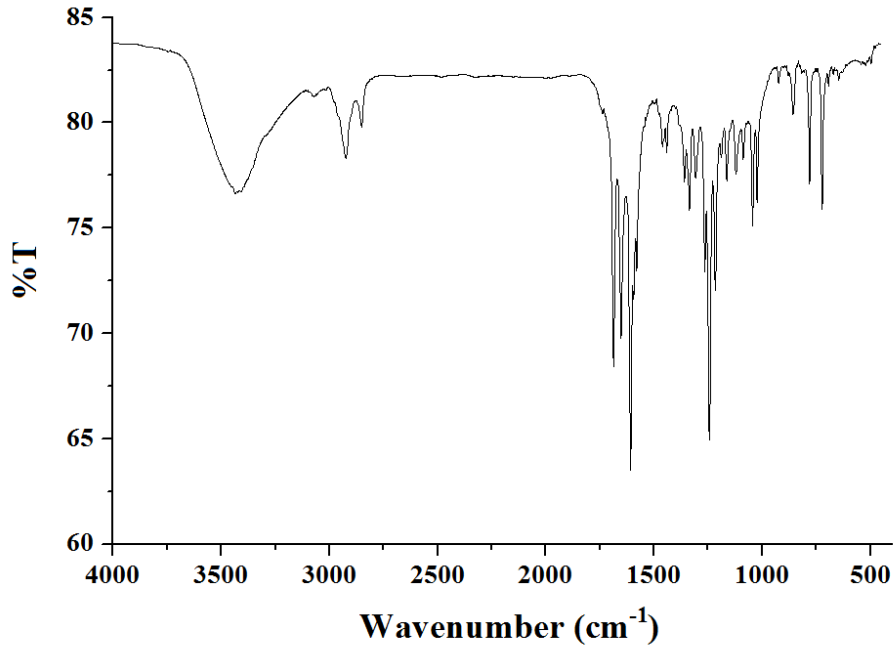


Figure S4. FT-IR spectrum of **L**/ in KBr pellet.

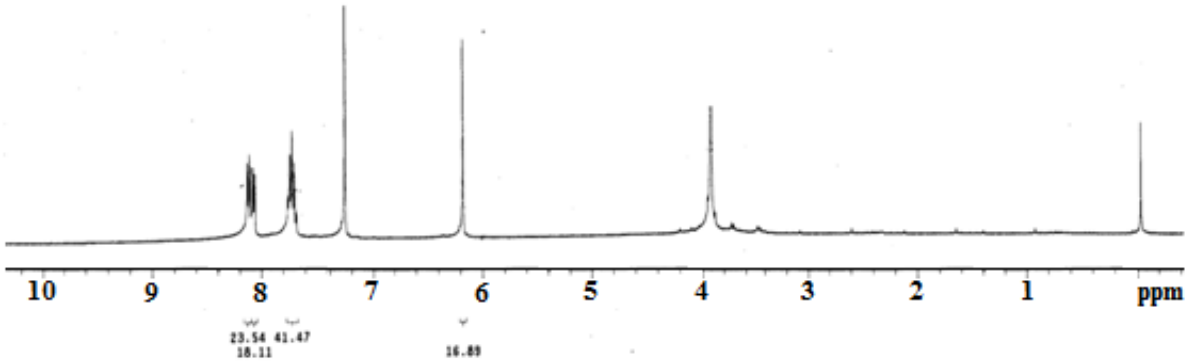


Figure S5. ^{1}H- NMR spectrum of **L/** in $CDCl_3$.

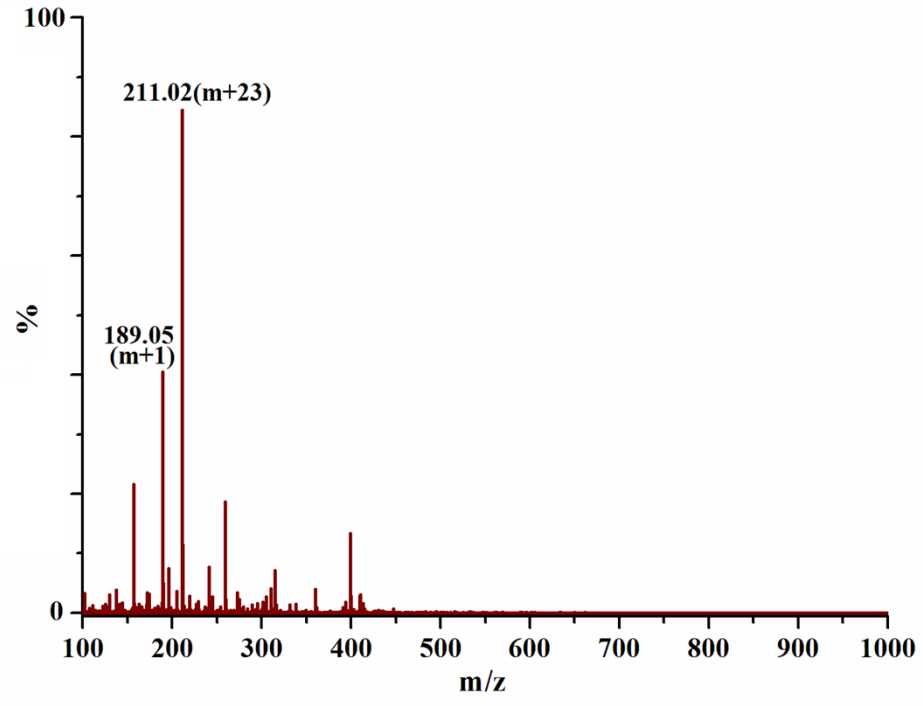


Figure S6. ESI mass spectrum of **L/** in methanol.

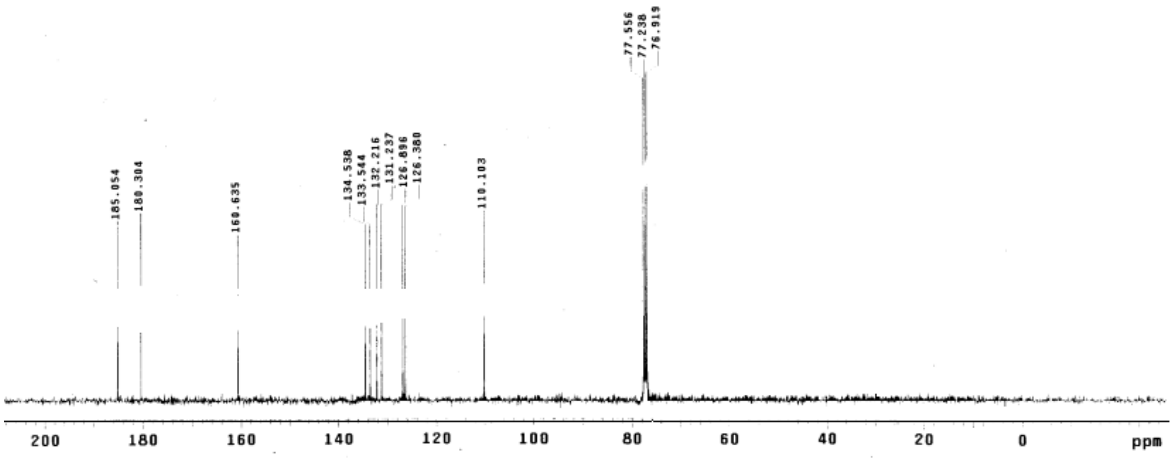


Figure S7. ^{13}C- NMR spectrum of **L**/ in $CDCl_3$.

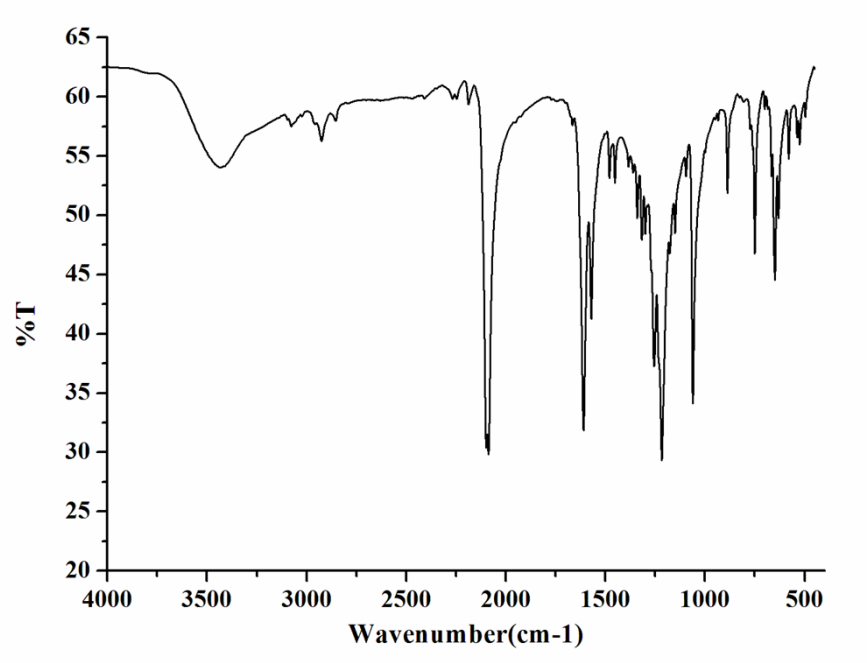


Figure S8: FT-IR spectrum of **L**// in KBr pellet.

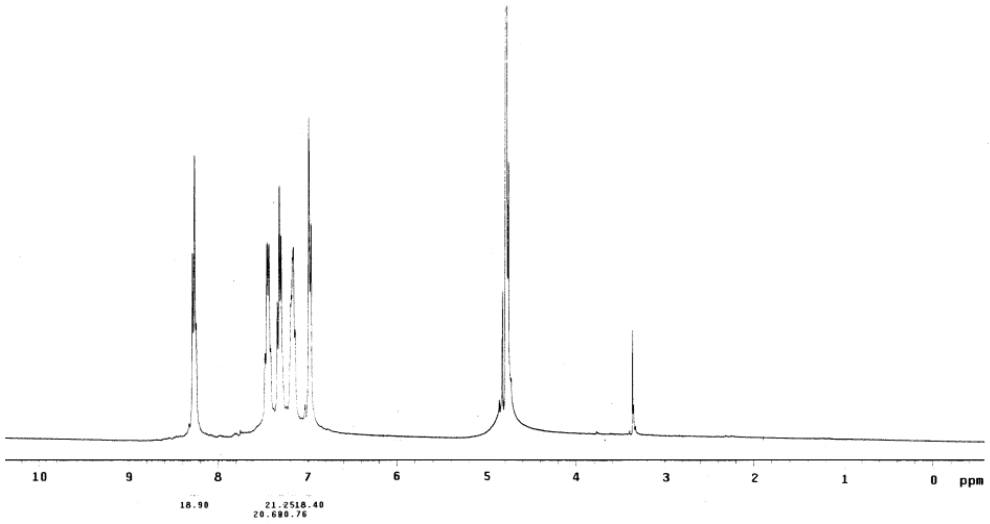


Figure S9: ^{1}H-NMR spectrum of **L**$^{//}$ in D_2O.

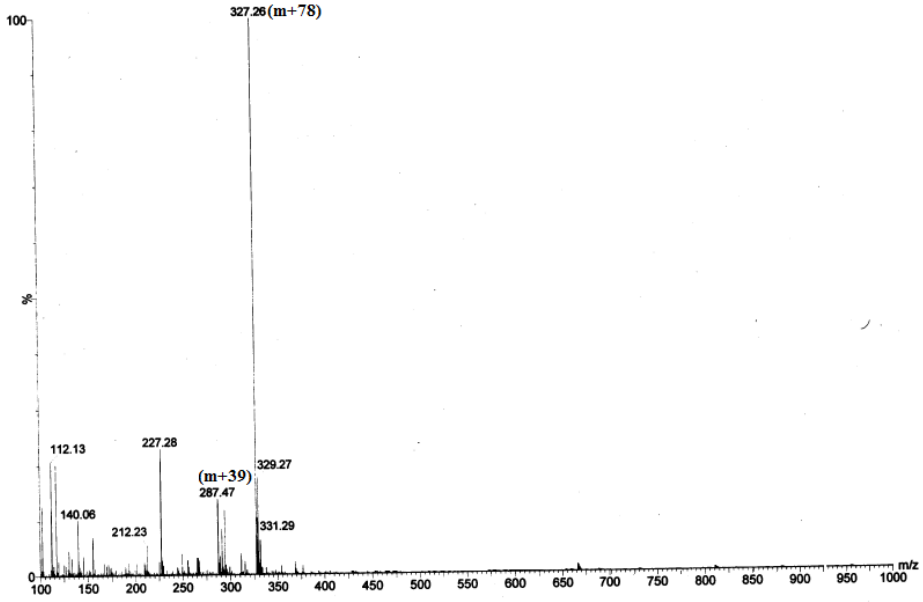


Figure S10: ESI-mass spectrum of **L**$^{//}$ in methanol.

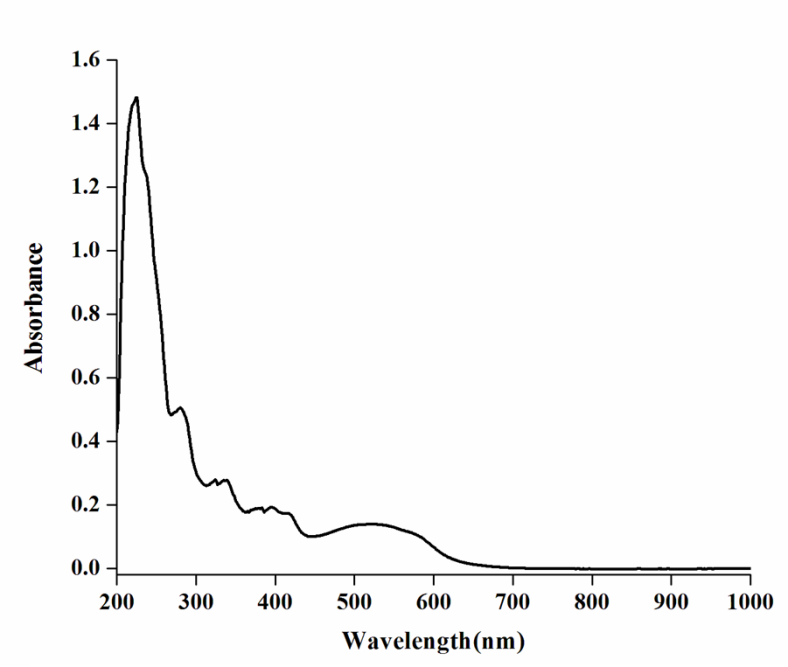
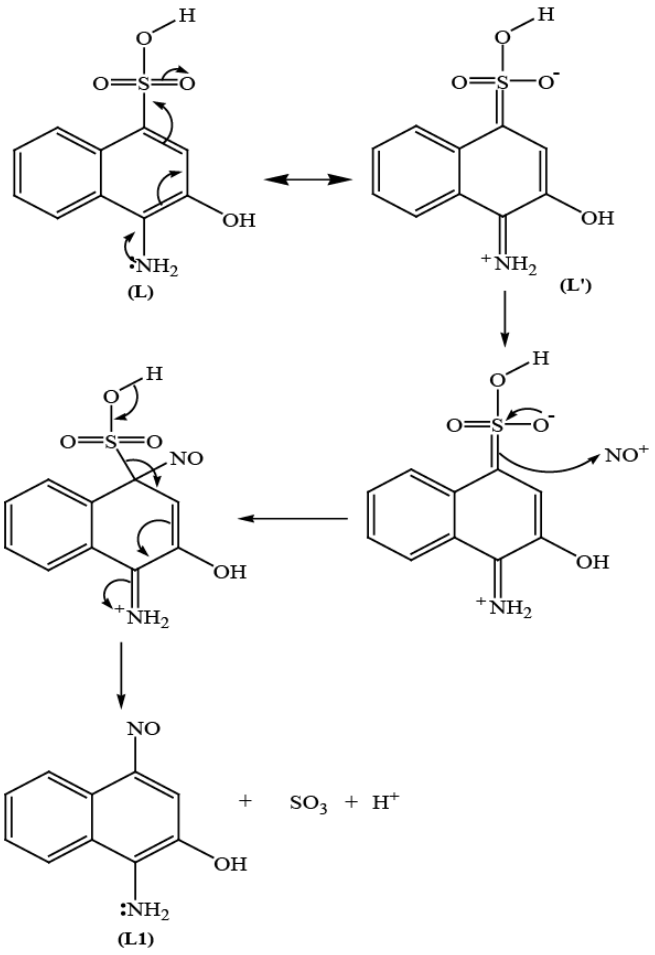
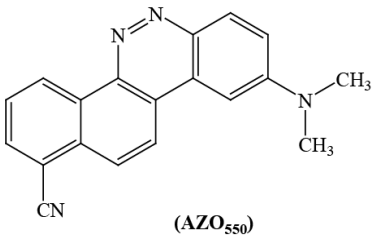


Figure S11: UV-visible spectrum of **L**$^{//}$ in methanol.



Scheme. Most probable mechanism for the desulphonation of the ligand by NO^+.



(AZO$_{550}$)

Figure S12. AZO$_{550}$

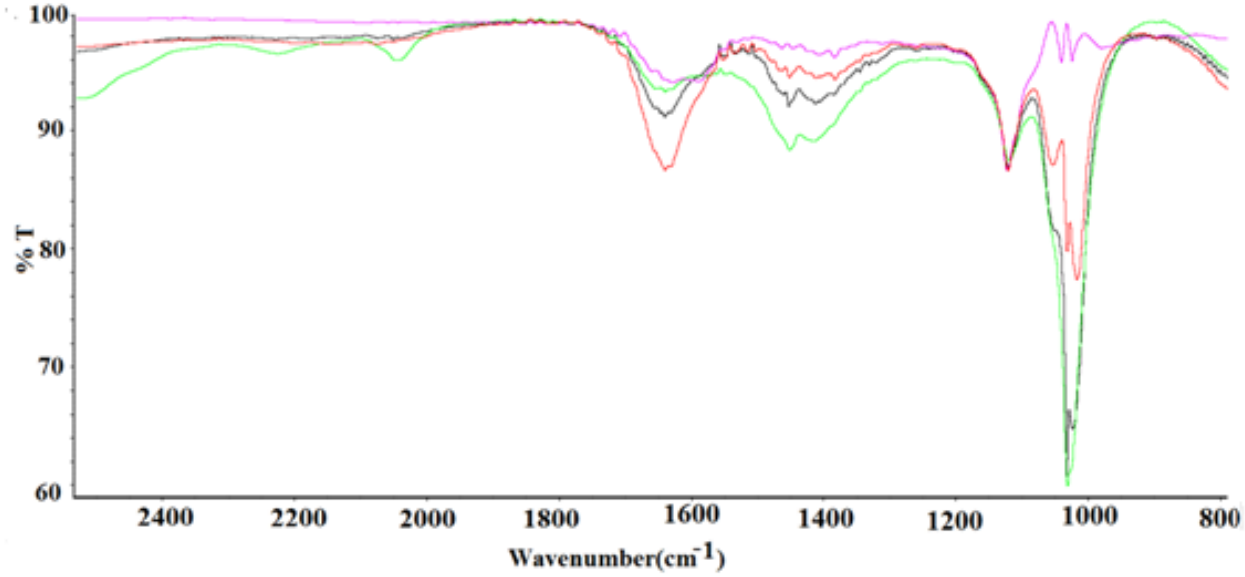


Figure S13: Solution FT- IR of [Cu-NO] complex. The band ~1650 cm^{-1} decays gradually with time indicating the unstable nature of the intermediate (red , immediate after purging NO into the methanol solution of complex **1**; black, after 10 mint; green after, 20 mint and pink, after 30 mint of NO purging).

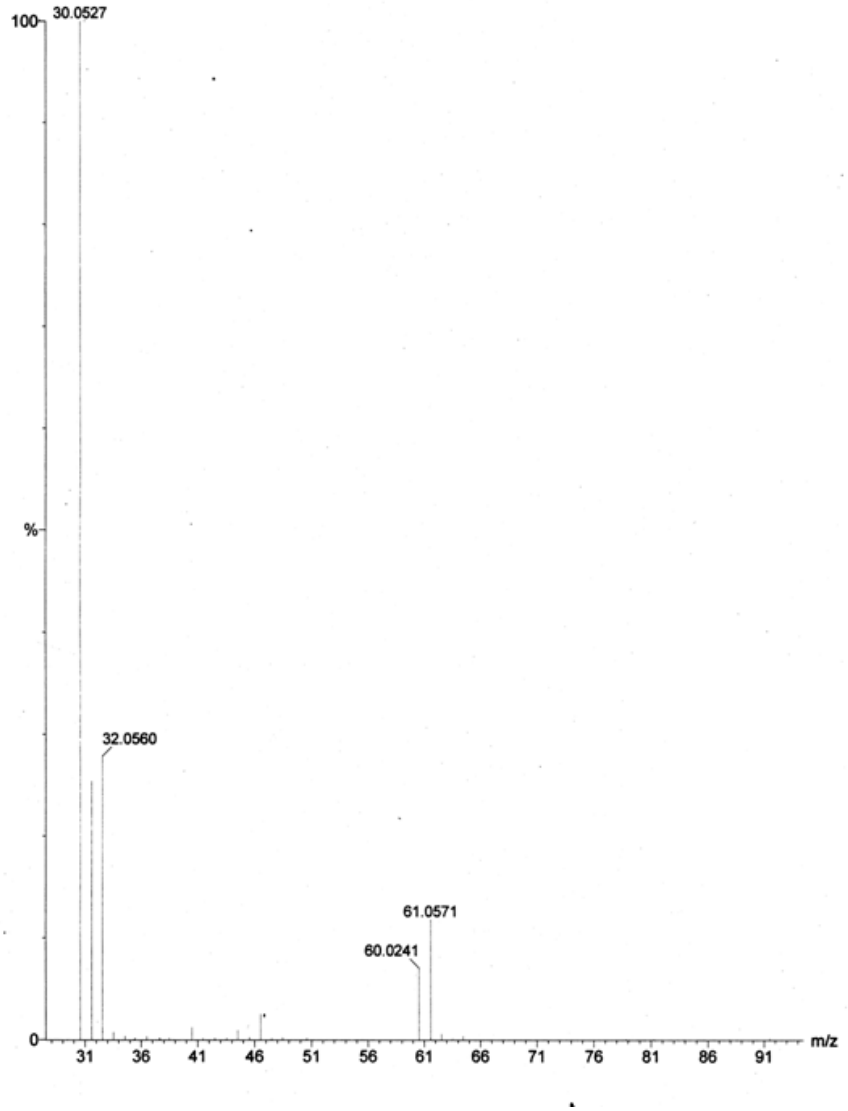


Figure S14: GC-Mass spectrum of $MeNO_2$.

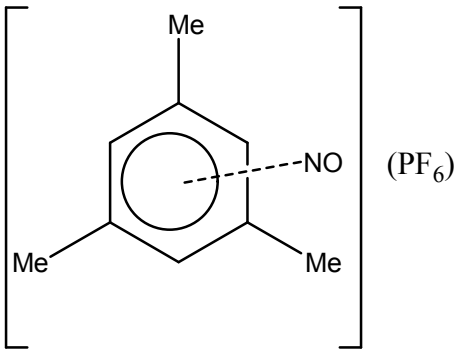


Figure S15: $[1,3,5\text{-}Me_3C_6H_3NO]PF_6$

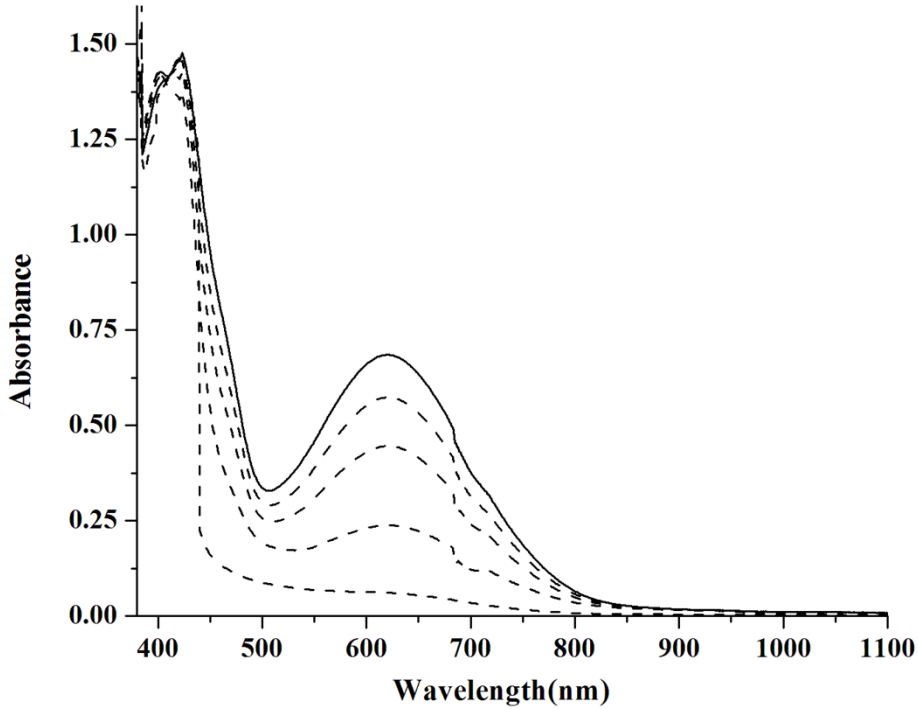


Figure S16. UV-Visible spectra of intermediate [Cu^{II}-NO] species (solid line) and it's decay (dotted line) in methanol**.** The band at ~430 nm remains even after reduction of the Cu(II) to Cu(I).

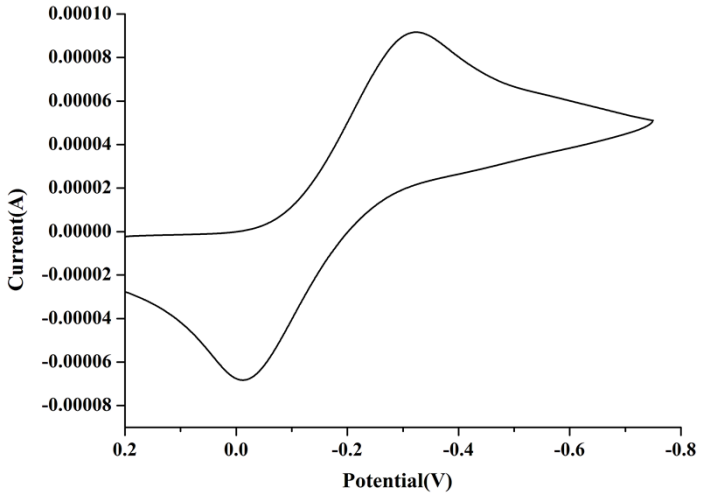
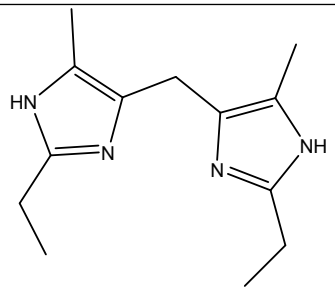
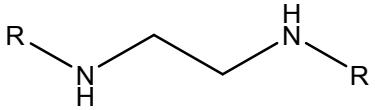
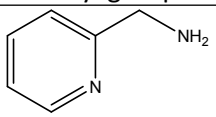
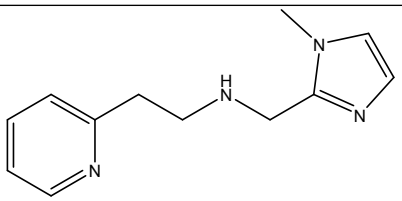
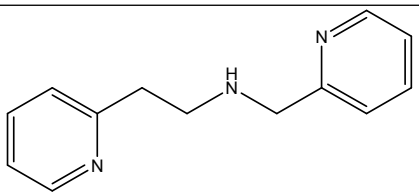
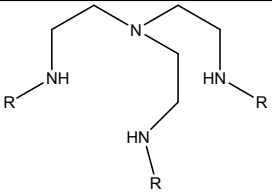


Figure S17. Cyclic voltammogram of the complex in methanol with glassy carbon working electrode, Ag/Ag^{+} reference electrode, tetrabutylammonium perchlorate (TBAP) supporting electrolyte, scan rate: 05 v/s.

Proposed and isolated Cu(II)-nitrosyl intermediates

Sl. No.	Ligand	Cu(II)-nitrosyl	Reference
1		Isolated	*Chem. Commun.*, **2012,** 48, 1251
2	 R = alkyl group	proposed	*Dalton Trans*., **2012**, *41*, 2927
3		proposed	*Inorg. Chem*. **2011**, *50*, 3206
4		proposed	*Dalton Trans*., **2011**, *40*, 8656
5		proposed	*Chem. Commun*, **2011**, *47*, 2964
6	 R = ethyl, isopropyl	proposed	*J. Am. Chem. Soc*. **2010**, *132*, 7846

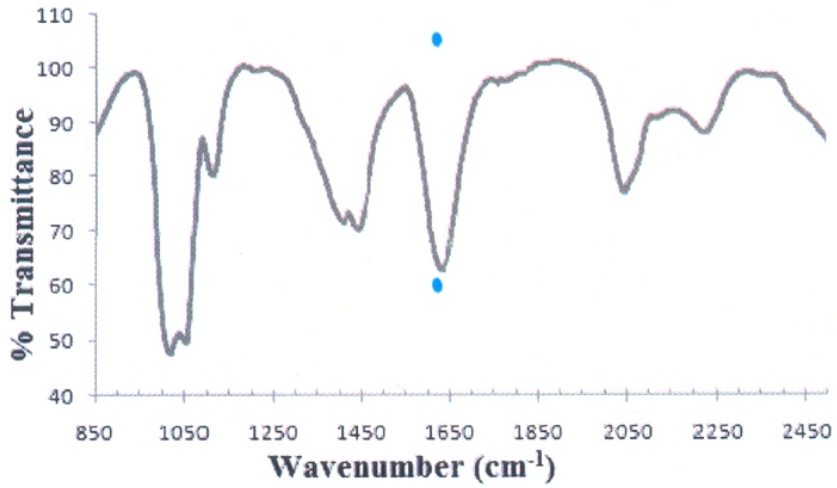


Figure S18: Solution FT-IR of the [Cu-NO] intermediate generated from the reaction of the complex with ^{15}NO in methanol at room temperature.