# Supplementary Information

## Thiocyanato-bridged new copper(II) 1D polymeric chains: structures, electrical properties, catecholase activity and DFT studies

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## Figures with Captions

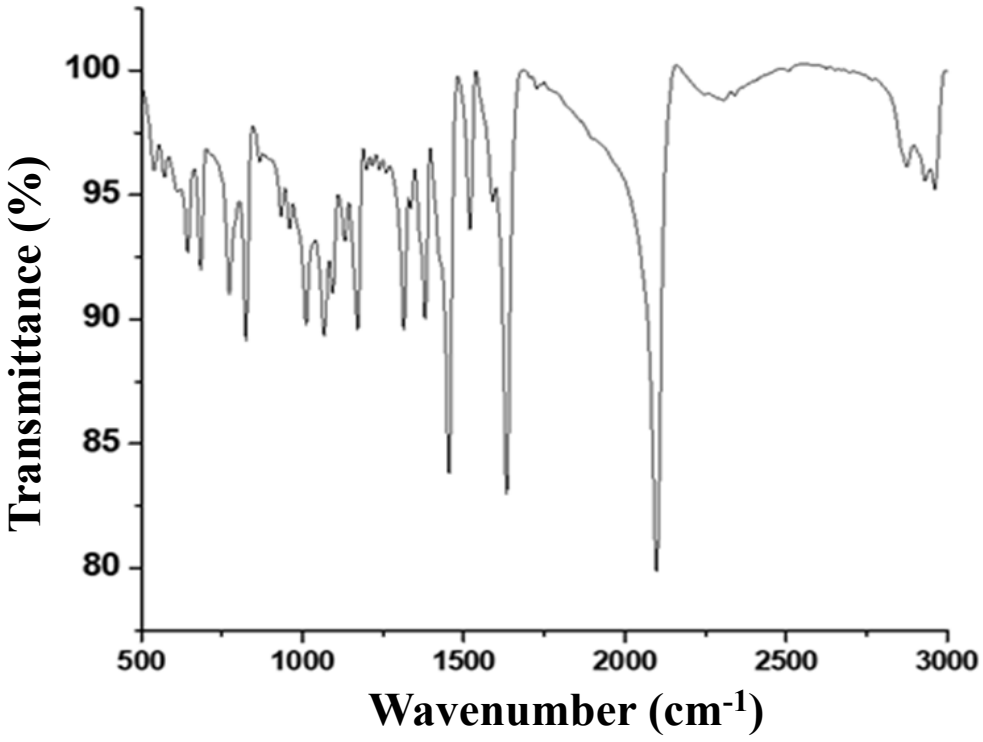



**Fig. S1** FTIR spectrum of complex **1**.

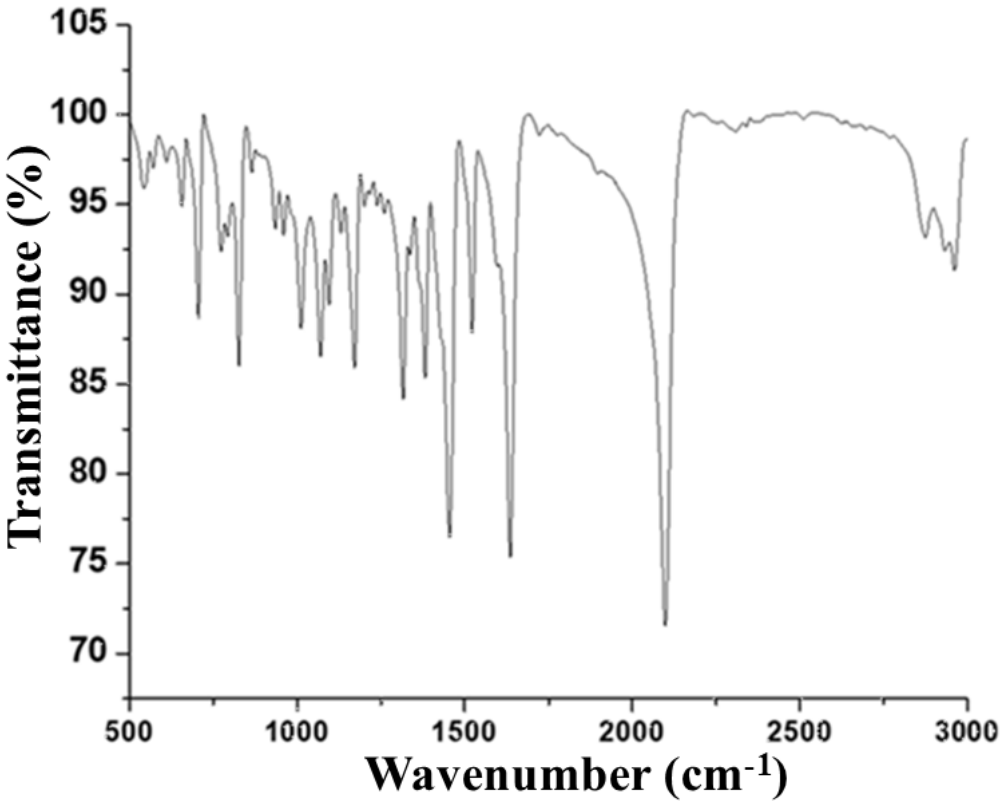



**Fig. S2** FTIR spectrum of complex **2.**

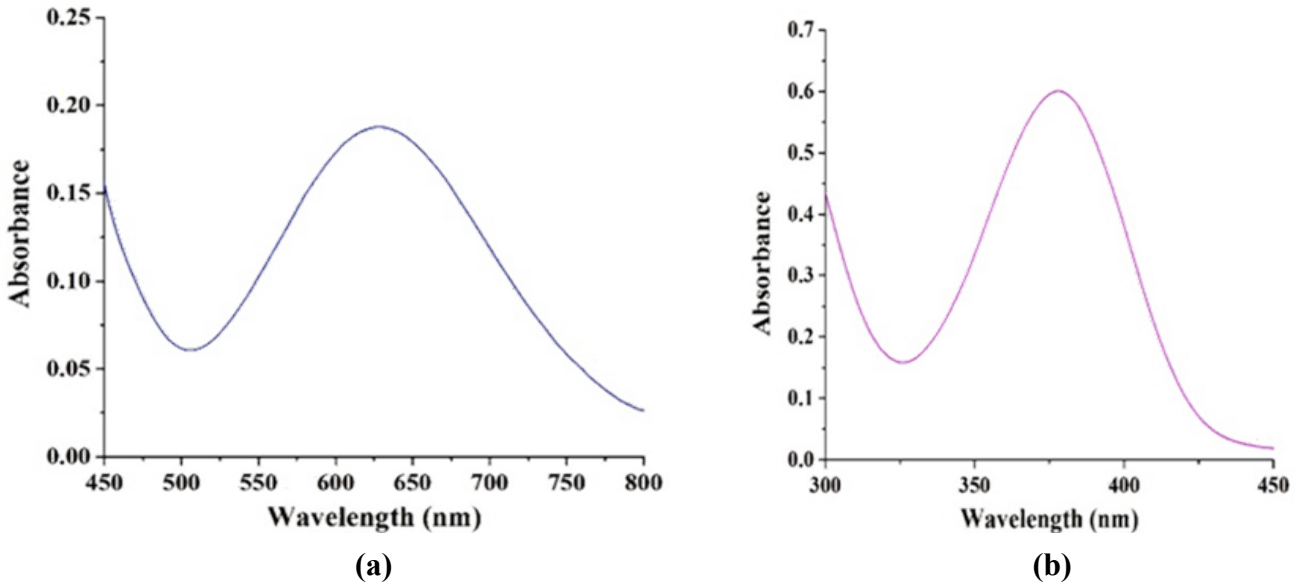
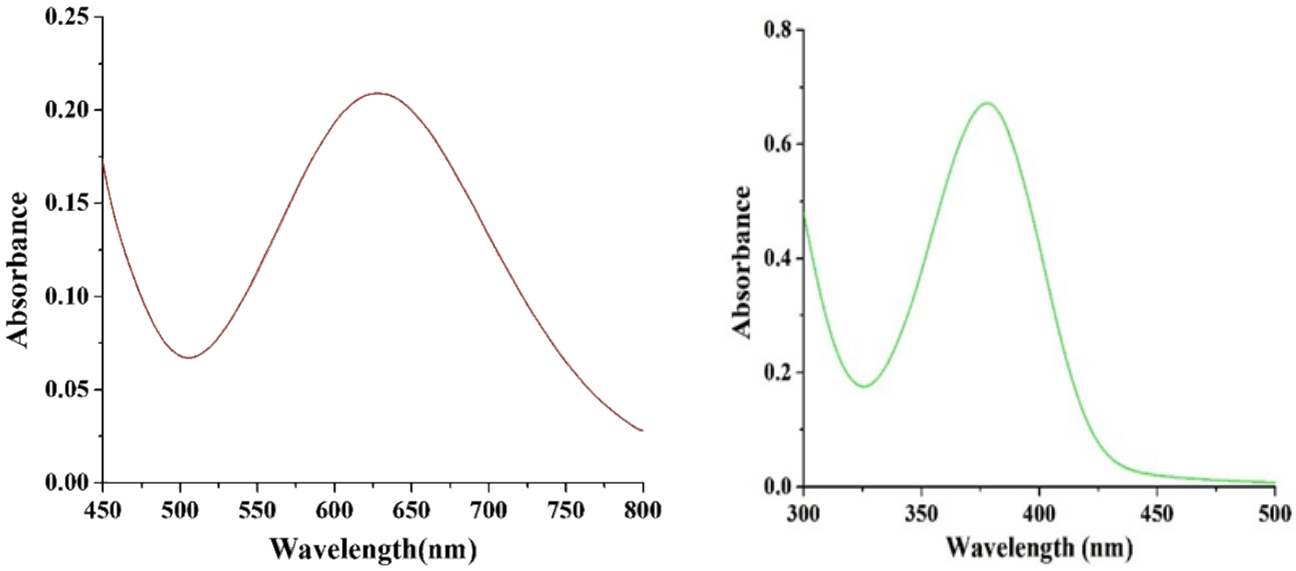



**Fig. S3** UV-Vis spectra of complex **1** at (a) $10^{-3}$ (M) and (b) $10^{-4}$ (M) in MeOH.




**(a)** **(b)**

**Fig. S4** UV-Vis spectra of complex **2** at (a) $10^{-3}$ (M) and (b) $10^{-4}$ (M) in MeOH.

**(a)** **(b)**

**Fig. S5** UV-Vis spectra of complex **1** at (a) $10^{-3}$ (M) and (b) $10^{-4}$ (M) in MeOH at different time intervals.

**(a)** **(b)**

**Fig. S6** UV-Vis spectra of complex **2** at (a) $10^{-3}$ (M) and (b) $10^{-4}$ (M) in MeOH at different time intervals.

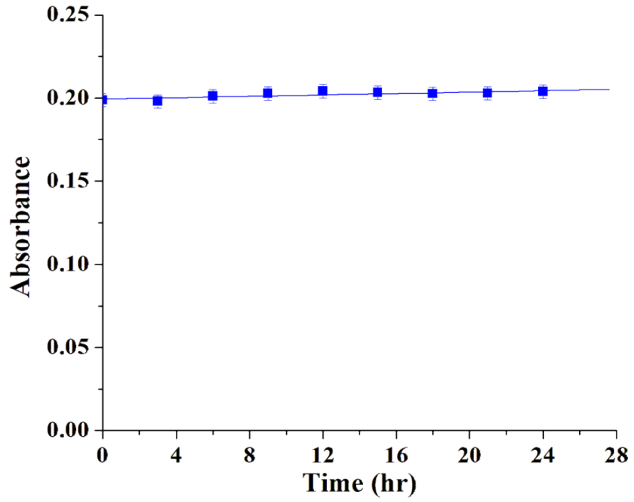



**Fig. S7** Absorbance *vs.* time plots monitored at 629 nm for ~24 h obtained from UV-Vis spectra of complex **1** at $10^{-3}$ (M) in methanol solution.

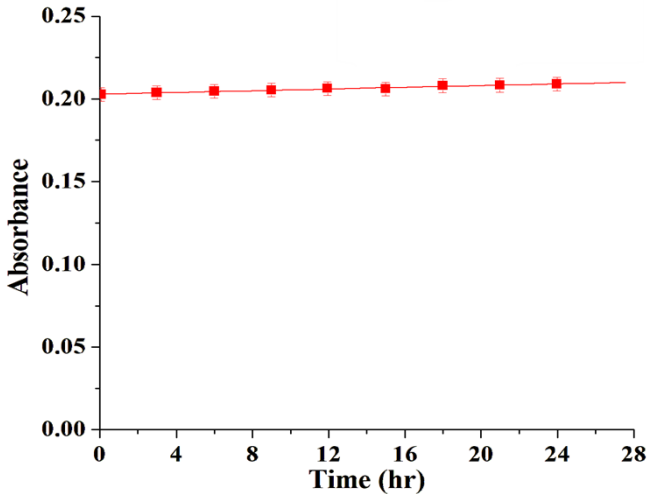



**Fig. S8** Absorbance *vs.* time plots monitored at 630 nm for ~24 h obtained from UV-Vis spectra of complex **2** at $10^{-3}$ (M) in methanol solution.

**Table S1** Bond distances and angles in complexes **1** and **2**

| Bond distances (Å) | | |
|---|---|---|
| | **1** | **2** |
| Cu1-N1 | 1.938(2) | 1.947(3) |
| Cu1- N2 | 2.053(2) | 2.065(3) |
| Cu1- N3 | 1.962(2) | 1.965(3) |
| Cu1- S1[a] | 2.9476(7) | 2.940(2) |
| Cu1- O1 | 1.902(2) | 1.914(2) |
| N3-C13 | 1.154(3) | 1.168(4) |
| C13-S1 | 1.637(2) | 1.639(3) |
| N1-C7 | 1.278(3) | 1.286(4) |
| N1-C8 | 1.467(3) | 1.472(4) |
| N2-C9 | 1.485(3) | 1.490(4) |
| N2-C10 | 1.478(3) | 1.479(4) |
| O1-C1 | 1.299(3) | 1.312(4) |
| Bond angles (deg) | | |
| N1-Cu1-N2 | 84.36(8) | 84.5(1) |
| N1-Cu1-N3 | 175.98(8) | 174.8(1) |
| N1-Cu1-S1 | 85.67(6) | 87.02(7) |
| O1-Cu1-N1 | 92.34(8) | 92.1(1) |
| O1-Cu1-N2 | 171.45(8) | 171.9(1) |
| O1-Cu1-N3 | 87.99(8) | 88.4(1) |
| O1-Cu1-S1 | 95.25(6) | 95.09(7) |
| N2-Cu1-N3 | 94.75(8) | 94.3(1) |
| N2-Cu1-S1 | 92.37(6) | 92.13(7) |
| N3-Cu1-S1 | 98.3(1) | 98.12(8) |
| O1-C1-C6 | 124.6(2) | 124.7(2) |
| N3-C13-S1 | 179.3(2) | 178.9(3) |