

Hydrosoluble Cu(I)-DAPTA complexes: Synthesis, characterization, luminescence thermochromism and catalytic activity for microwave-assisted three-component azide-alkyne cycloaddition click reaction

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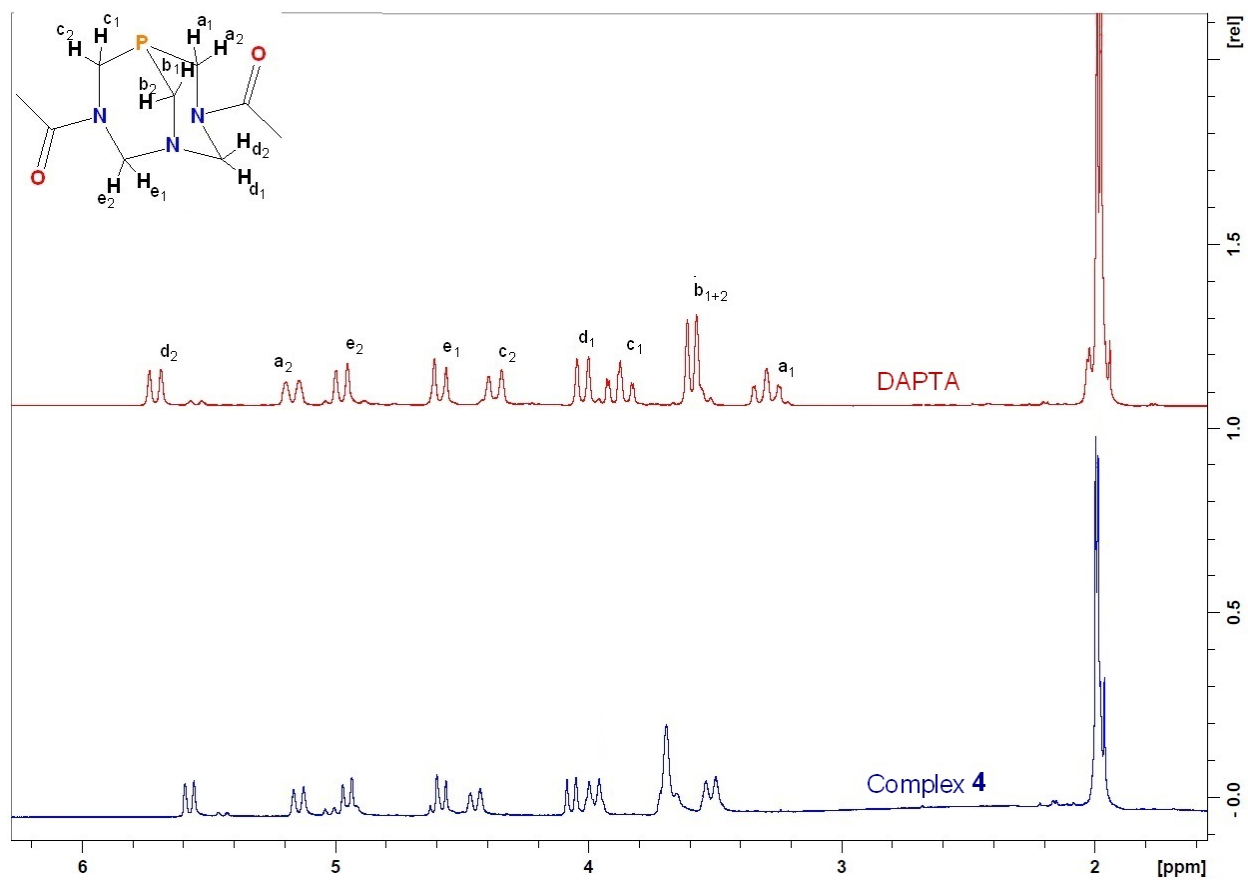


Figure S1: ^1H NMR spectra of DAPTA (top) and complex **4** (bottom) in acetonitrile- d_3 .

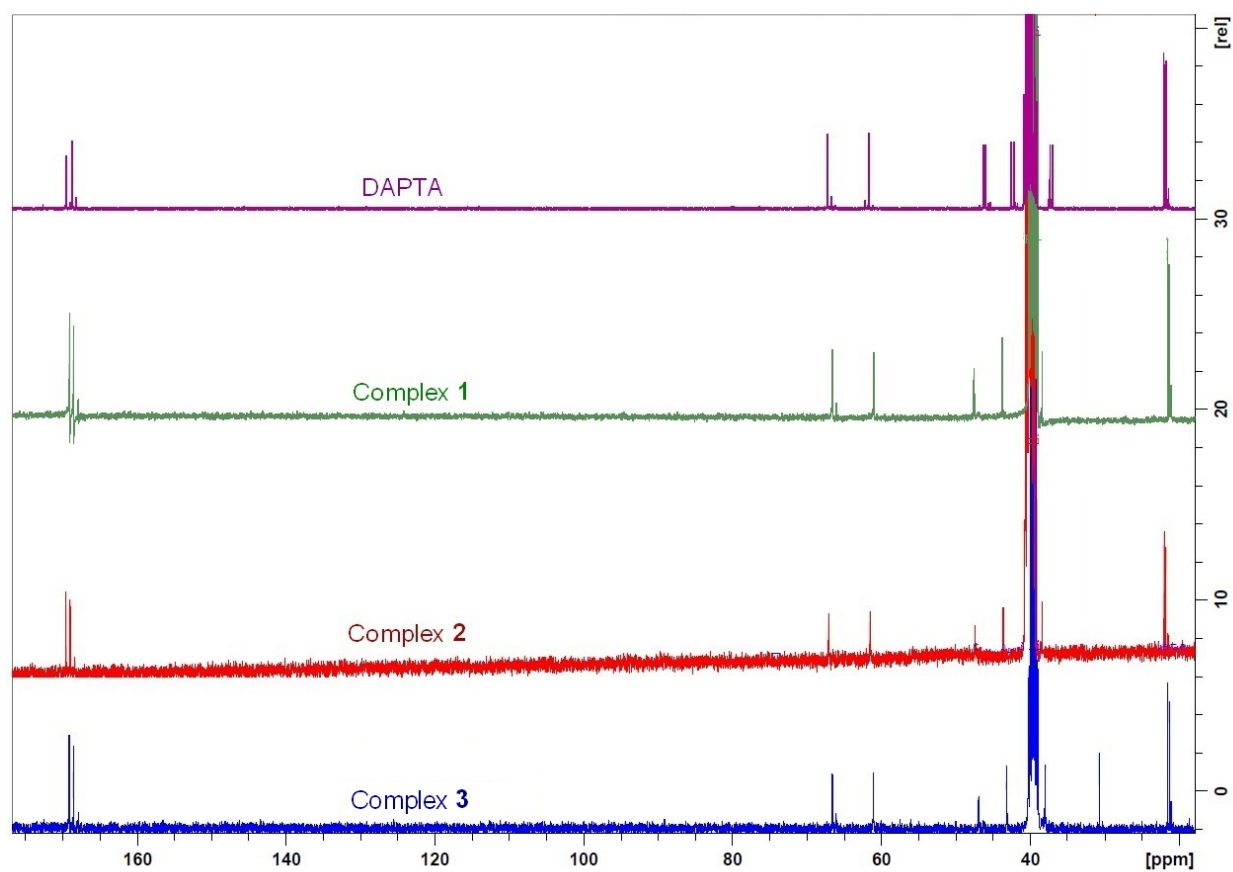


Figure S2: $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of DAPTA and complexes **1-3** in $\text{DMSO-}d_6$.

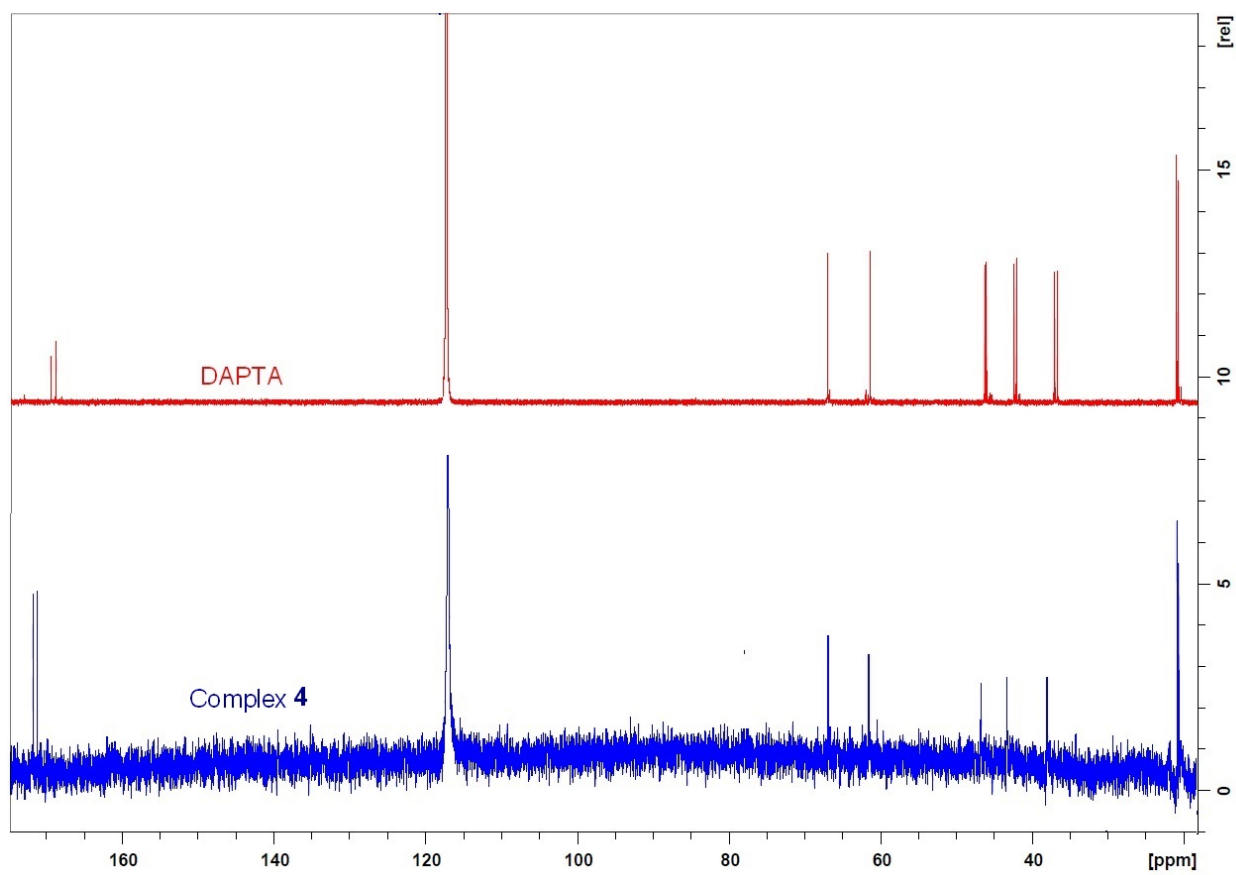


Figure S3: $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of DAPTA (top) and complexes **4** (bottom) in acetonitrile- d_3 .

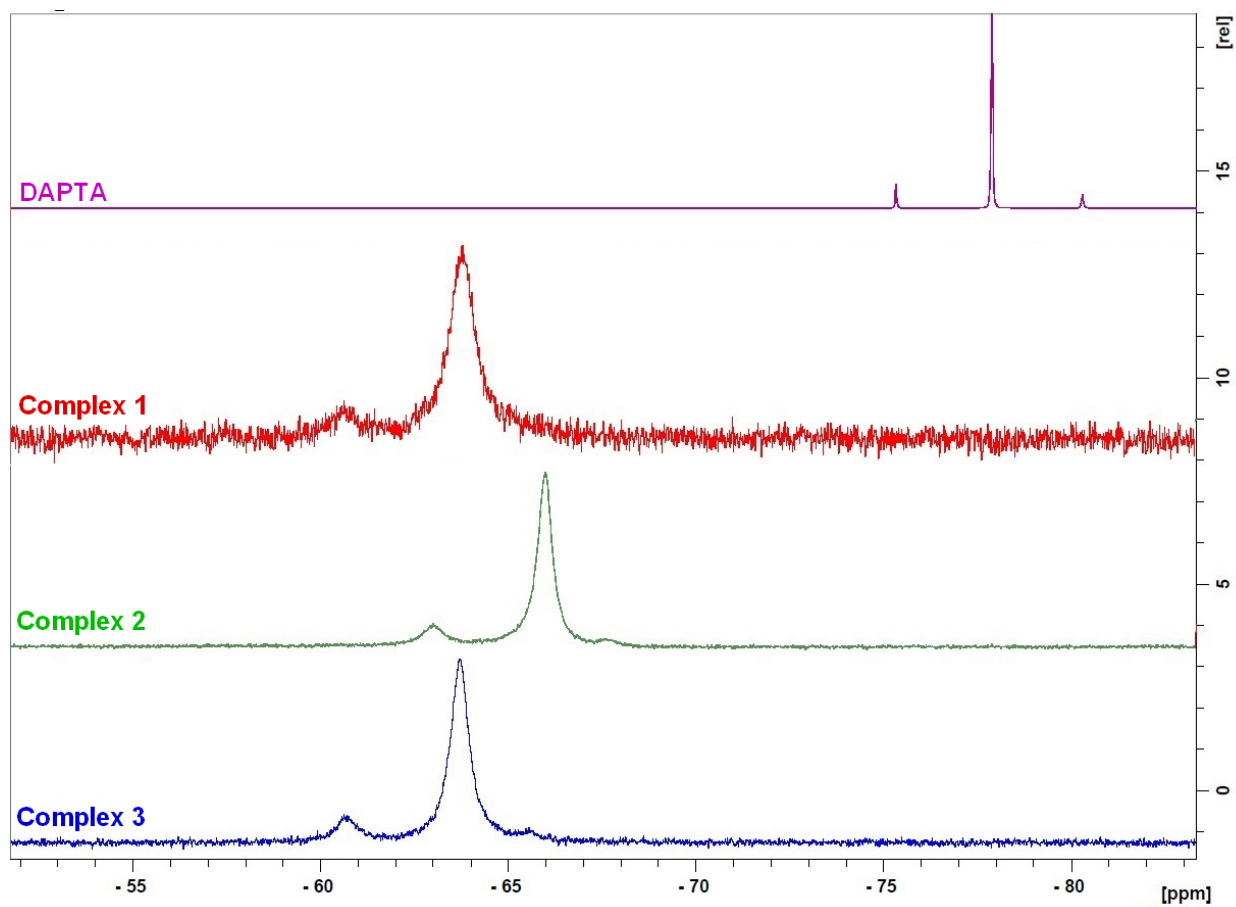


Figure S4: $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of DAPTA and complexes 1-3 in $\text{DMSO}-d_6$.

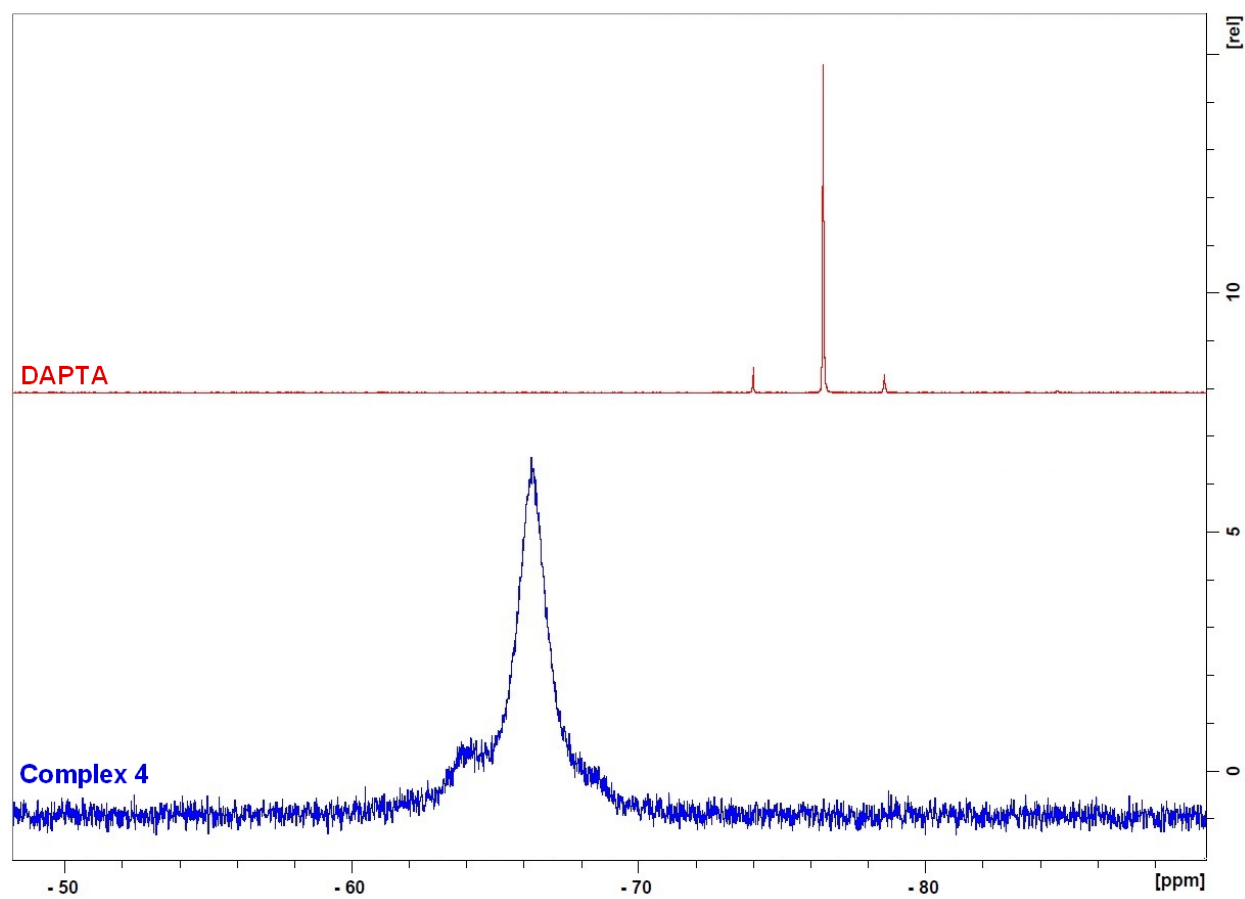


Figure S5: $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of DAPTA (top) and complex **4** (bottom) in acetonitrile- d_3 .

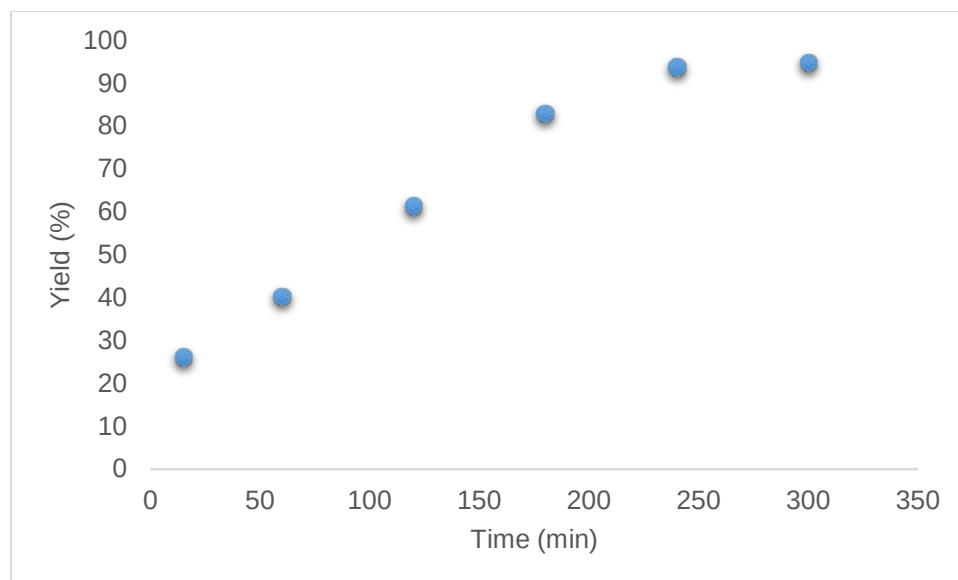


Figure S6: Plot of yield vs. time for the CuAAC reaction in water:MeCN mixtures (1:1 ratio) using 0.5 mol% of catalyst **2**, 125 °C and microwave irradiation (30 W).

Table S1. Crystal data and structure refinement summary for **4**.

Empirical formula	C ₃₆ H ₆₄ Cu ₂ I ₂ N ₁₂ O ₈ P ₄
Formula Weight	1297.75
Crystal system	triclinic
Space group	<i>P</i> $\bar{1}$
Temperature/K	296 (2)
<i>a</i> /Å	7.7429(11)
<i>b</i> /Å	12.6570(18)
<i>c</i> /Å	13.3551(19)
α /°	107.207(5)
β /°	98.563(4)
γ /°	99.439(5)
<i>V</i> (Å ³)	1205.9(3)
<i>Z</i>	1
<i>D</i> _{calc} (g cm ⁻³)	1.787
<i>F</i> 000	652
μ (Mo K α) (mm ⁻¹)	2.356
Rfls. collected/unique/observed	19488/ 4410/ 3216
<i>R</i> _{int}	0.0514
Final <i>R</i> 1 ^a , <i>wR</i> 2 ^b (<i>I</i> ≥ 2σ)	0.0841, 0.1779
Goodness-of-fit on <i>F</i> ²	1.113

^a $R = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$; ^b $wR(F^2) = [\Sigma w(|F_o|^2 - |F_c|^2)^2 / \Sigma w|F_o|^4]^{1/2}$