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Supplementary Information

Ethambutol Analysis by Copper Complexation in Pharmaceutical Formulations: Spectrophotometry and Crystal Structure

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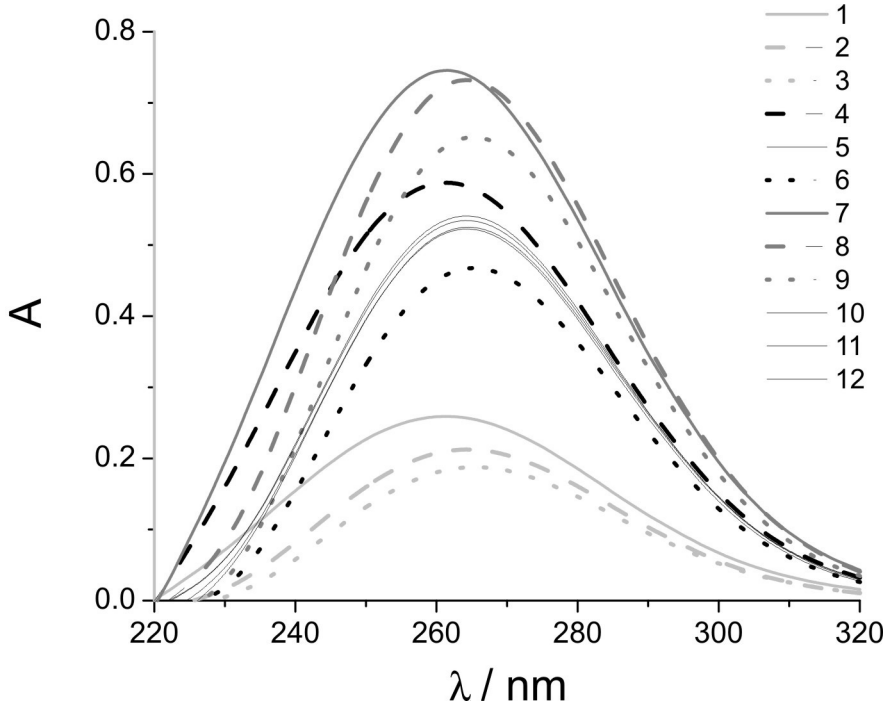

Figure S1. CuETB UV-Vis spectra obtained for 3^2 experimental design.

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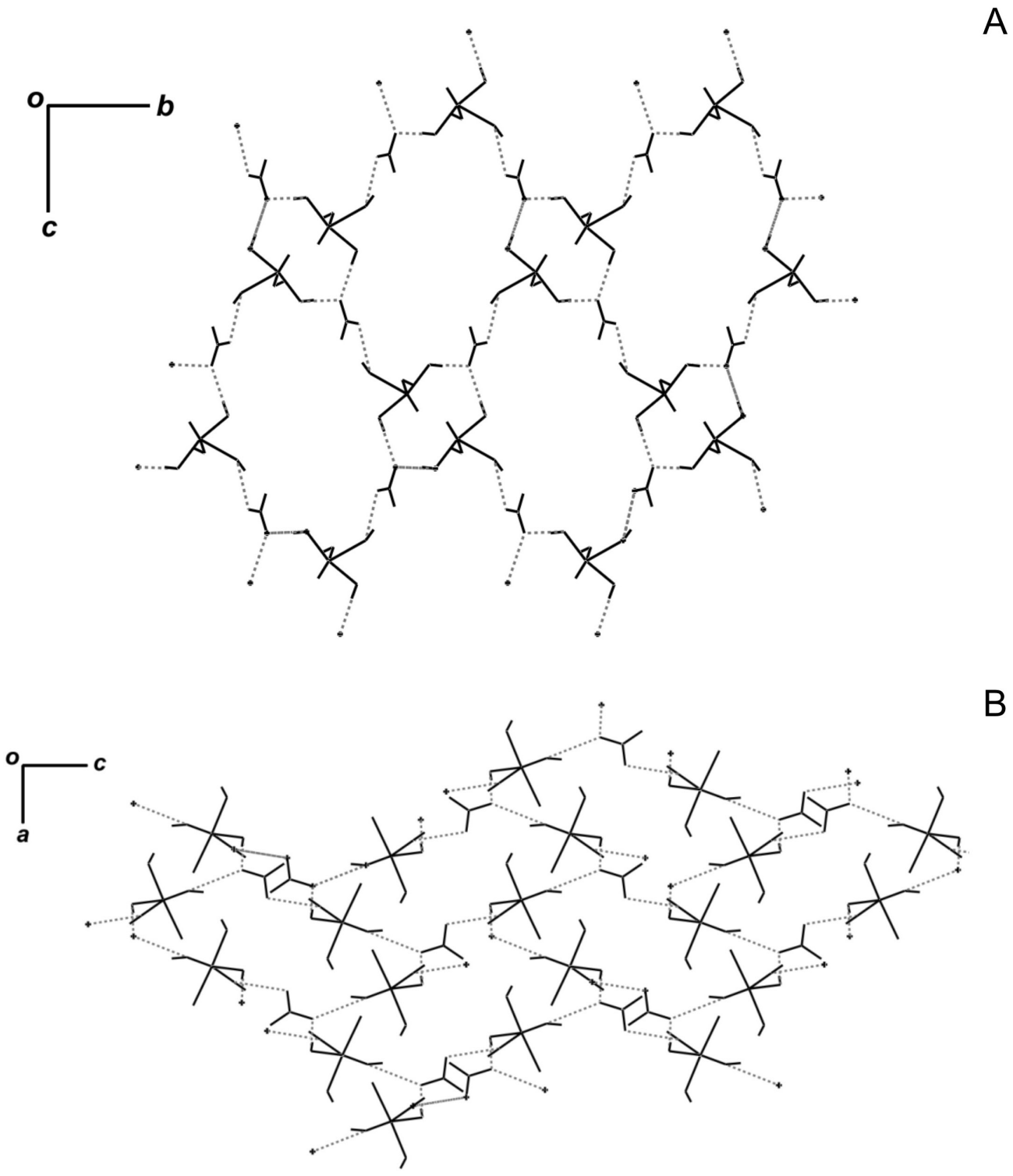

Figure S2. Hydrogen bond design in CuETB crystal structure view along of (A) *a* axis and (B) *b* axis. The C atoms were omitted to clarity.

Table S1. Crystal data of CuETB

Compound	CuETB
Formula	$C_{10}H_{24}ClCuN_3O_5$
Formula weight (g mol^{-1})	365.31
Crystal System	Orthorhombic
Space Group	$P2_12_12_1$
a / Å	6.7029(5)
b / Å	13.929(1)
c / Å	18.094(1)
V / Å^3	1689.4(2)
Z	4
Crystal size (mm)	$0.20 \times 0.07 \times 0.05$
Crystal color	blue
Dcalc (g cm^{-3})	1.436
μ(Mo-K_α) (cm^{-1})	1.470
Transmission factors (min / max)	0.805 / 0.929
Reflections measured / unique	9232 / 3643
R_{int} / R_σ	0.0522 / 0.0645
Observed reflections[$F_o^2 > 2\sigma(F_o^2)$]	2986
No. of refined parameters	181
R [$F_o > 2\sigma(F_o)$]	0.0427
wR [$F_o^2 > 2\sigma(F_o)^2$]	0.0940
S	1.067
Density difference max / min	0.713 / –0.547
RMS peak (e Å^{-3})	0.071

Table S2. Select bond distance and bond angles for CuETB

Bond Distance / Å			
Cu1 – N1	2.006(3)	Cu1 – O2	2.421(3)
Cu1 – N2	2.032(3)	Cu1 – Cl1	2.263(1)
Cu1 – O1	2.004(3)		
Bond Angle / °			
N1-Cu-N2	86.1(1)	N2-Cu-O2	75.2(1)
N1-Cu-O1	82.3(1)	N2-Cu-Cl1	97.7(1)
N1-Cu-O2	91.1(1)	O1-Cu-O2	95.5(1)
N1-Cu-Cl1	171.72(9)	O1-Cu-Cl1	95.18(8)
N2-Cu-O1	164.9(1)	O2-Cu-Cl1	97.04(8)

Hydrogen bond		
D-H···A	D···A / Å	D-H···A / °
O1-H1O···O5^{i}	2.691(5)	171.00
O2-H2O···O3	2.789(5)	139.00
N2-H2N···O5^{ii}	3.035(5)	147.00

Symmetry code: *i*: 1 - *x*, ½ + *y*, ½ - *z*; *ii*: ½ - *x*, 1 - *y*, ½ + *z*.