

Supporting Information

[Cu^{II}(N–N)(HIMC[−])(Sol)] complexes, their anti-cancer activities, ΔG , ΔE , and solid luminescence

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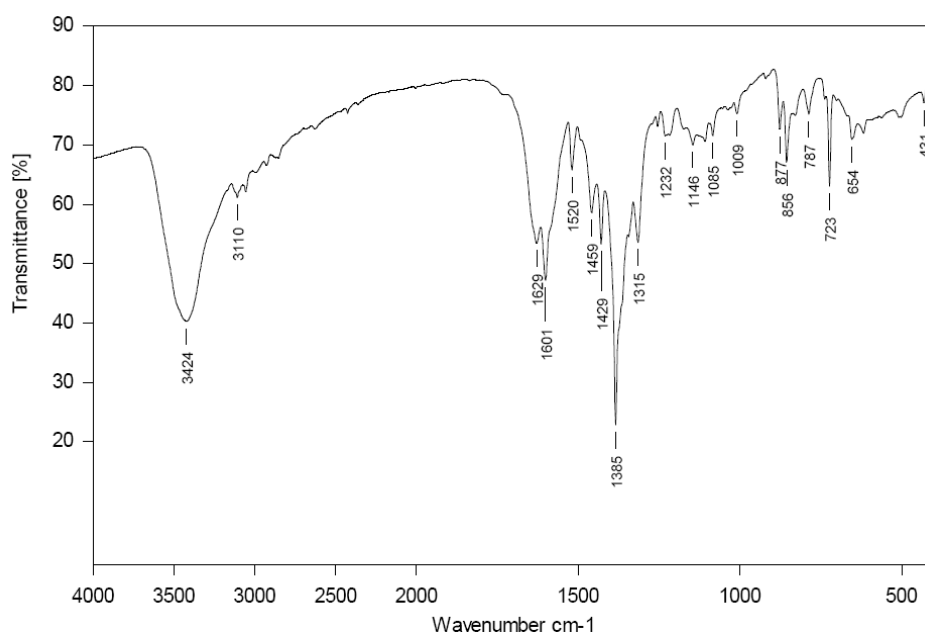


Figure S1. IR spectrum of compound 1.

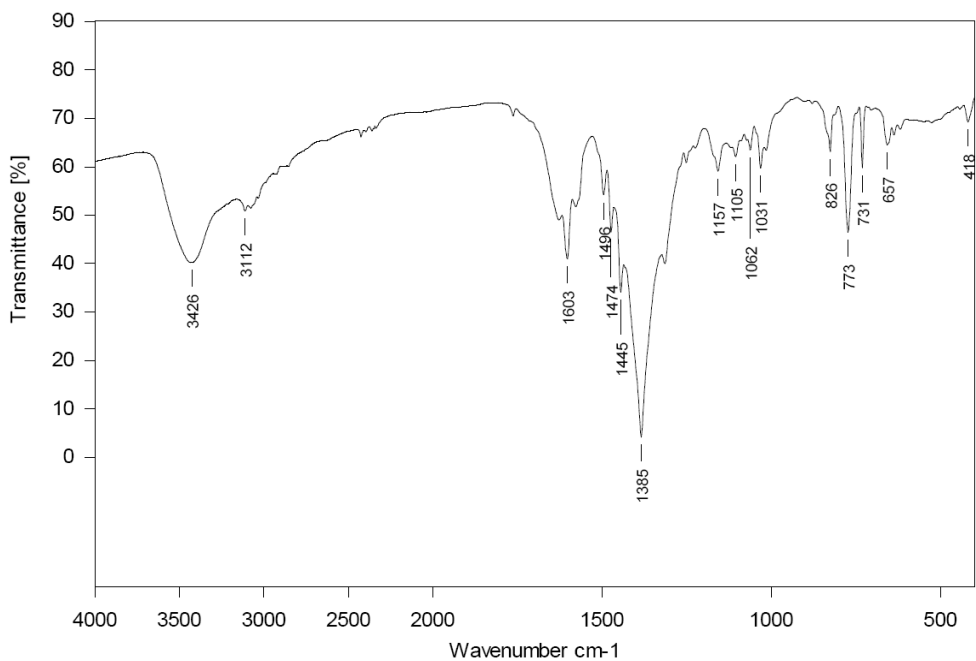


Figure S2. IR spectrum of compound 2.

Table S1. The crystallographic data and structure refinement parameters for complex 2

Complex 2	
CCDC number	874756
Empirical formula	C ₁₄ H ₁₇ CuN ₅ O ₈
Formula weight	446.87
Temperature/K	298(2)
Crystal system	Monoclinic
Space group	Cc
a/nm	8.3328(9)
b/nm	35.658(3)
c/nm	7.1036(6)
α/(°)	90.00
β/(°)	114.269(2)
γ/(°)	90.00
Volume/Å ³	1924.2(3)
Z	4
ρ calc/mg · mm ⁻³	1.543
2θ range for data collection	4.56 to 50.04°
Goodness-of-fit on F ²	1.061
Reflections collected	4541
Independent reflections	2314
Absorption coefficient /mm ⁻¹	1.187
Final R1 indexes [I>2σ (I)] ^a	0.1085
Final wR2 indexes [I>2σ (I)] ^b	0.2543
Final R1indexes [all data]	0.1507
Final wR2 indexes [all data]	0.2837

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

Table S2 Selected bond lengths and angles of complex 2

Compound 2			
Selected bond lengths/Å			
Cu(1)-O(1)	1.986(13)	Cu(1)-N(1)	2.082(16)
Cu(1)-N(4)	2.003(17)	Cu(1)-O(6)	2.414(13)
Cu(1)-N(3)	2.054(14)		
Selected bond angles/(°)			
O(1)-Cu(1)-N(4)	173.2(6)	N(3)-Cu(1)-N(1)	173.6(6)
O(1)-Cu(1)-N(3)	91.0(5)	O(1)-Cu(1)-O(6)	90.2(5)
N(4)-Cu(1)-N(3)	82.6(6)	N(4)-Cu(1)-O(6)	92.1(6)
O(1)-Cu(1)-N(1)	83.4(6)	N(3)-Cu(1)-O(6)	91.8(5)
N(4)-Cu(1)-N(1)	103.0(6)	N(1)-Cu(1)-O(6)	91.1(5)