

Supplementary Information

Table S1: Crystal data and refinement details of complexes **1**, **2** and **3**

	1	2	3
Formula	C ₁₆ H ₁₂ C ₁₂ CuN ₂ O ₆	C ₁₆ H ₁₀ ClCuN ₅ O	C ₁₈ H ₁₆ ClCuN ₂ O ₃
Formula Weight	462.73	387.29	407.33
Temperature (K)	150(2)	296	296
Crystal System	Triclinic	Triclinic	Monoclinic
Space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>C</i> ₂ / <i>c</i>
<i>a</i> (Å)	7.1589(12)	7.8516(2)	18.2712(4)
<i>b</i> (Å)	10.1414(12)	9.3769(2)	10.8166(4)
<i>c</i> (Å)	12.8984(16)	11.8132(3)	18.3726(6)
α (°)	67.555(12)	97.965(1)	90
β (°)	73.912(13)	108.633(1)	110.640(2)
γ (°)	78.022(12)	111.107(1)	90
<i>Z</i>	2	2	8
<i>d</i> _{cal} (g cm ⁻³)	1.860	1.746	1.592
μ (mm ⁻¹)	1.685	1.678	1.462
F(000)	466	390	1664
Total reflection	4797	11132	26030
Unique Reflections	3797	2810	3508
Observed	2620	2614	3148
R(int)	0.069	0.021	0.028
R1, wR2 (all data)	0.1121, 0.2511	0.0261, 0.0662	0.0324, 0.0813
R1, wR2 [<i>I</i> > 2 σ (<i>I</i>)]	0.0890, 0.2181	0.0240, 0.0649	0.0284, 0.0788

Table S2: Selected bond lengths (Å) and bond angles (°) for complexes **1**, **2** and **3**

	1	2	3
Cu(1)–O(1)	1.999(5)	–	2.2738(17)
Cu(1)–O(11)	1.894(5)	1.8872(14)	1.9088(14)
Cu(1)–O(21)	2.595(6)	–	–
Cu(1)–N(1)	–	1.9549(19)	–
Cu(1)–N(19)	1.963(6)	1.9605(16)	1.9792(16)
Cu(1)–N(28)	1.965(6)	1.9880(16)	1.9968(17)
Cu(1)–Cl(1)	–	–	2.3343(6)
Cu(1)–O(22)*	2.539(6)	–	–
O(1)–Cu(1)–O(11)	89.6(2)	–	87.03(6)
O(1)–Cu(1)–O(21)	80.14(19)	–	–
O(1)–Cu(1)–N(19)	172.4(2)	–	104.47(7)
O(1)–Cu(1)–N(28)	94.4(2)	–	91.10(7)
Cl(1)–Cu(1)–O(1)	–	–	108.22(4)
Cl(1)–Cu(1)–O(11)	–	–	93.73(5)
Cl(1)–Cu(1)–N(19)	–	–	146.91(5)
Cl(1)–Cu(1)–N(28)	–	–	92.27(5)
O(1)–Cu(1)–O(22)*	82.72(18)	–	–
O(11)–Cu(1)–N(1)	–	91.71(7)	–
O(11)–Cu(1)–O(21)	85.78(18)	–	–
O(11)–Cu(1)–N(19)	93.8(2)	93.76(6)	92.91(6)
O(11)–Cu(1)–N(28)	174.0(2)	175.85(7)	173.99(7)
O(11)–Cu(1)–O(22)*	92.74(19)	–	–
O(21)–Cu(1)–N(19)	106.9(2)	–	–
O(21)–Cu(1)–N(28)	90.4(2)	–	–
O(21)–Cu(1)–O(22)*	162.80(19)	–	–
N(1)–Cu(1)–N(19)	–	171.53(9)	–
N(1)–Cu(1)–N(28)	–	92.06(8)	–
N(19)–Cu(1)–N(28)	82.8(3)	82.70(7)	82.02(7)

Symmetry transformation * = 1+x, y, z

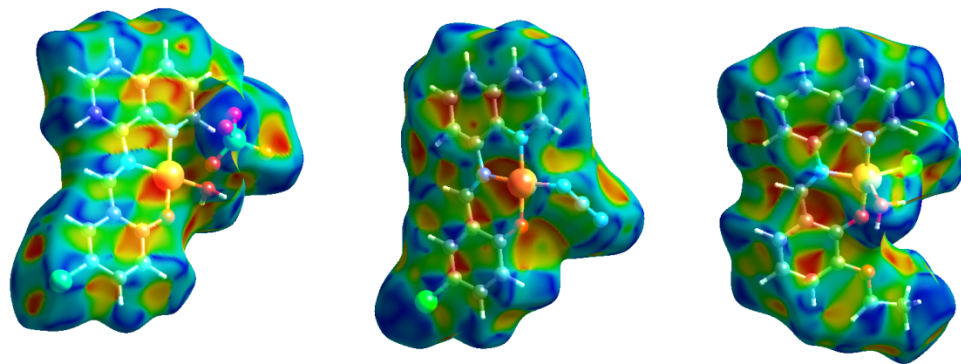


Fig. S1: Hirshfeld surfaces mapped over shape index for complexes **1** (left), **2** (middle) and **3** (right).

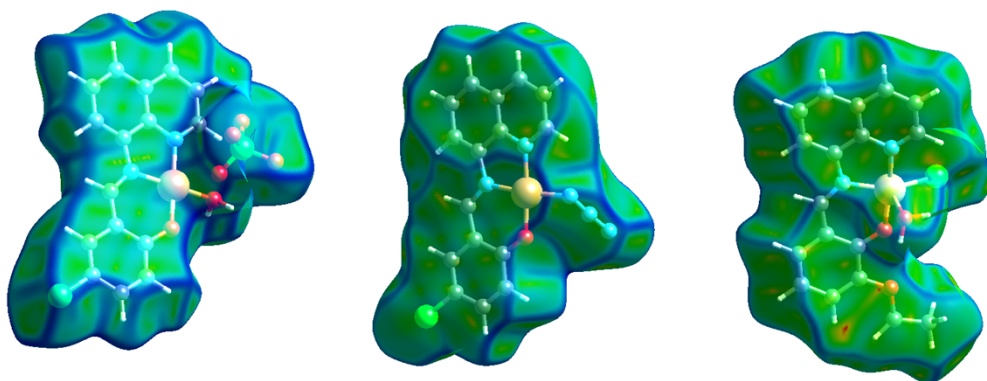


Fig. S2: Hirshfeld surfaces mapped over curvedness for complexes **1** (left), **2** (middle) and **3** (right).