

Supporting informations

Table S1. Crystal data and structure refinement for the hybrid compound (HQ)₂[ZnCl₄] and the HQCl salt.

	(HQ) ₂ [ZnCl ₄]	HQCl
Empirical formula	C ₁₈ H ₁₆ Cl ₄ N ₂ O ₂ Zn	C ₉ H ₁₀ Cl ₁ N ₁ O ₂
Fw	499.52	199.63
Crystal colour	yellow	yellow
Wavelength (Å)	0.71073	0.71073
Temperature (K)	298	100
Crystal system, Z	Monoclinic, 4	Triclinic, 2
Space group	<i>C2/c</i>	<i>P-1</i>
a (Å)	15.2108(17)	7.2651(8)
b (Å)	8.1418(8)	8.2751(9)
c (Å)	16.7204(19)	8.4760(9)
α (°)	90	78.281(3)
β (°)	91.503(7)	86.099(3)
γ (°)	90	66.537(3)
V (Å ³)	2070.0(4)	457.65(9)
ρ _{calc} (g.cm ⁻³)	1.603	1.449
μ(MoKα) (mm ⁻¹)	1.718	0.381
θ range (°)	2.437–32.458	2.454– 45.405
Data collected	12032	59879
Data unique	3700	7659
Data observed	1816	6366
R(int)	0.0796	0.0437
Nb of parameters / restraints	125/0	158/0
R1 [F ² > 2s(F ²)], ^a	0.1186 [0.0488]	0.0466 [0.0339]
wR2 [F ² > 2s(F ²)], ^b	0.1390 [0.1100]	0.1066 [0.0954]
S(F ²), ^c	0.954	0.987

^aR1(F) = Σ||F₀| - |F_C||/Σ|F₀|; ^bwR2(F²) = [Σw(F₀²-F_C²)²/ΣwF₀⁴]^{1/2}; ^cS(F²) = [Σw(F₀²-F_C²)²/(n+r-p)]^{1/2}.

Table S2. Selected bond distances for the hybrid compound (HQ)₂[ZnCl₄].

Bond	Length (Å)
Zn-Cl1	2.2725(8)
Zn-Cl2	2.2654(9)
N5-H5...Cl2	2.3444(9)
O4-H4...Cl1	2.2846(9)

Table S3. Selected bond distances for the HQCl salt.

Bond	Length (Å)
O1-H8...Ow1	1.70(3)
C1-H2...Cl	2.74(1)
C1-H2...Cl	2.91(2)
N1-H1...Cl	2.36(1)
C9-H5...Ow	2.59(1)
C3-H4...Cl	2.74(2)

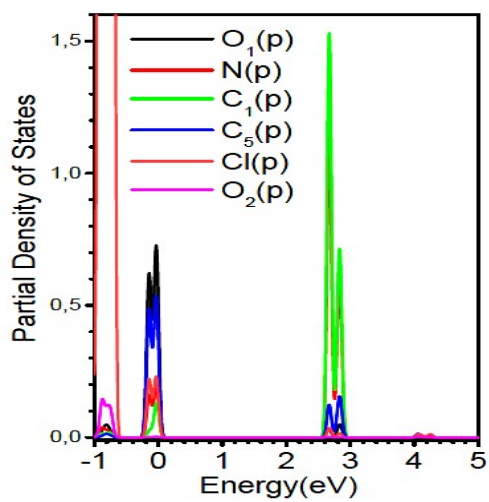


Figure S1. Calculated electronic density of states of (HQ.Cl) salt.