

Supplementary Information

Table S1. Protonation constants of ligands **L1-L4** in NMe₄NO₃ 0.1 M, 298.1 K.

Reaction	L1	L2	L3	L4
$L + H^+ = HL^+$	9.52(2)	9.91(3)	9.98(3)	10.39(3)
$HL^+ + H^+ = H_2L^{2+}$	9.23(2)	9.43(3)	7.73(3)	9.01(2)
$H_2L^{2+} + H^+ = H_3L^{3+}$	5.88(3)	6.05(3)	4.11(2)	7.35(2)
$H_3L^{3+} + H^+ = H_4L^{4+}$	4.60(3)	5.22(4)		6.02(4)

Table S2. Formation constants of the ATP complexes with ligands **L1-L4** (A = ATP, L = **L1-L4**) in NMe₄NO₃ 0.1 M, 298.1 K.

Reaction	L1	L2	L3	L4
$L + 2H^+ + A^{4-} = H_2LA^{2-}$	23.07(5)	24.74(7)	21.95(3)	22.24(8)
$L + 3H^+ + A^{4-} = H_3LA^-$	30.28(6)	31.18(7)	28.07(3)	30.99(2)
$L + 4H^+ + A^{4-} = H_4LA$	36.98(3)	37.86(6)	32.53(2)	39.41(2)
$L + 5H^+ + A^{4-} = H_5LA^+$	41.91(4)	42.49(6)		45.24(4)
$L + 6H^+ + A^{4-} = H_6LA^{2+}$				47.66(5)
$H_2L^{2+} + A^{4-} = H_2LA^{2-}$	4.32(5)	5.40(7)	4.24(3)	2.84(8)
$H_2L^{2+} + HA^{3-} = H_3LA^-$	4.70(6)	5.01(7)	3.53(3)	
$H_3L^{3+} + A^{4-} = H_3LA^-$				4.24(2)
$H_3L^{3+} + HA^{3-} = H_4LA$	5.52(3)	5.64(6)	3.88(2)	5.83(2)
$H_4L^{4+} + HA^{3-} = H_5LA^+$	5.85(4)	5.05(6)		5.64(4)
$H_4L^{4+} + H_2A^{2-} = H_6LA^{2+}$				4.03(5)

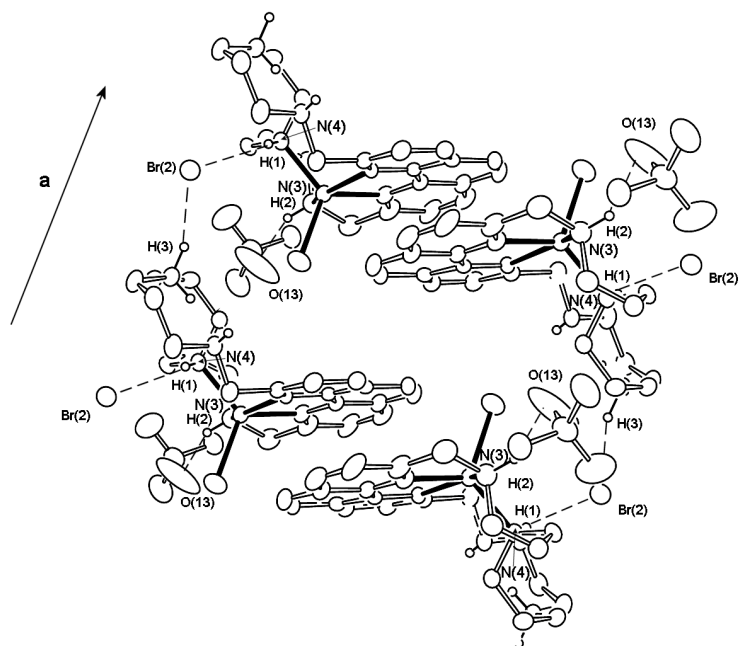


Figure S1. Crystal packing of the $[\text{ZnHL4Br}]\text{Br}(\text{ClO}_4)$ complex, displaying the pillared structure of $[\text{ZnHL4Br}]^+$ cations, associated *via* hydrogen bonds with the Br(2) anion and π -stacking interactions between the phenanthroline moieties