Electronic Supplementary Information

Tuning ESIPT-coupled luminescence by expanding π-conjugation of a proton acceptor moiety in ESIPT-capable zinc(II) complexes with 1-hydroxy-1*H*-imidazole-based ligands

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Experimental part

X-ray crystal structure data

Table S1. Crystal data and structure refinement for **HL^q** and **$[Zn(HL^q)Hal_2]$**.

Empirical formula	$C_{18}H_{14}N_4O$	$C_{18}H_{14}Cl_2N_4OZn$	$C_{18}H_{14}Br_2N_4OZn$	$C_{18}H_{14}I_2N_4OZn$
Formula weight	302.33	438.60	527.52	621.50
Crystal system	Monoclinic	Triclinic	Triclinic	Triclinic
Space group	$P2_1/n$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a(Å)	12.6436(8)	7.7585(4)	8.6131(1)	7.8596(3)
b(Å)	3.8107(3)	8.8124(3)	8.8588(2)	8.1625(3)
c(Å)	29.172(2)	14.2538(6)	13.9114(3)	16.6942(7)
α(°)		73.240(1)	100.513(1)	93.867(2)
β(°)	90.800(2)	85.065(2)	95.759(1)	99.890(2)
γ(°)		69.358(1)	116.975(0)	111.278(2)
V(Å^3)	1405.4(2)	873.11(7)	909.57(3)	973.29(7)
Z	4	2	2	2
d_{Calc}(g/cm^3)	1.429	1.668	1.926	2.121
μ (mm^{-1})	0.093	1.728	5.758	4.448
F(000)	632	444	516	588
Crystal size	0.20 x 0.06 x 0.04	0.25 x 0.12 x 0.06	0.24 x 0.08 x 0.05	0.25 x 0.08 x 0.08
Theta range for data collection (°)	2.661 – 25.706	2.570 – 26.372	2.670 – 26.333	2.502 – 26.372
Index ranges	$-15 \le h \le 13$ $-4 \le k \le 4$ $-35 \le l \le 32$	$-9 \le h \le 9$ $-11 \le k \le 10$ $-17 \le l \le 17$	$-10 \le h \le 10$ $-10 \le k \le 10$ $-17 \le l \le 17$	$-9 \le h \le 9$ $-9 \le k \le 10$ $-20 \le l \le 20$
Reflections collected	7072	6770	8945	17112
Independent reflections (R_{int})	2647 (R_{int} = 0.0403)	3561 (R_{int} = 0.0237)	3650 (R_{int}= 0.0274)	3984 (R_{int} = 0.0465)
Completeness to theta = 25.25°(%)	98.9	99.8	99.6	100.0
Data / restraints / parameters	2647 / 0 / 210	3561 / 0 / 236	3650 / 0 / 239	3984 / 0 / 239
Goodness-of-fit on F^2	1.005	1.087	0.899	1.095
Final *R* indices ($I>2\sigma_I$)	R_1 = 0.0457 wR_2 = 0.1182	R_1 = 0.0305 wR_2 = 0.0781	R_1 = 0.0191 wR_2 = 0.0580	R_1 = 0.0309 wR_2 = 0.0733
R indices (all data)	R_1 = 0.0660 wR_2 = 0.1301	R_1 = 0.0379 wR_2 = 0.0808	R_1 = 0.0217 wR_2 = 0.0596	R_1 = 0.0387 wR_2 = 0.0766
Largest diff. peak and hole (e/Å^3)	0.197 and -0.272	0.594 and -0.244	0.411 and -0.345	1.265 and -0.724

Table S2. Bond lengths d [Å]and angles ω [°] for **HL^{q}**.

Bond	d	Bond	d
O(1)-N(1)	1.382(2)	C(4)-C(5)	1.419(2)
N(1)-C(1)	1.350(2)	C(5)-C(6)	1.362(3)
N(1)-C(3)	1.375(2)	C(6)-C(7)	1.416(2)
N(2)-C(3)	1.325(2)	C(7)-C(9)	1.410(3)
N(2)-C(2)	1.374(2)	C(7)-C(8)	1.422(2)
N(3)-C(4)	1.330(2)	C(8)-C(12)	1.410(2)
N(3)-C(8)	1.371(2)	C(9)-C(10)	1.371(3)
N(4)-C(17)	1.335(2)	C(10)-C(11)	1.407(3)
N(4)-C(13)	1.349(2)	C(11)-C(12)	1.366(3)
C(1)-C(2)	1.393(2)	C(13)-C(14)	1.397(3)
C(1)-C(18)	1.487(2)	C(14)-C(15)	1.370(3)
C(2)-C(13)	1.461(2)	C(15)-C(16)	1.383(3)
C(3)-C(4)	1.447(3)	C(16)-C(17)	1.381(3)
Angle	ω	Angle	ω
C(1)-N(1)-C(3)	110.27(14)	C(5)-C(6)-C(7)	119.94(17)
C(1)-N(1)-O(1)	123.55(14)	C(9)-C(7)-C(6)	123.48(17)
C(3)-N(1)-O(1)	126.18(15)	C(9)-C(7)-C(8)	118.41(17)
C(3)-N(2)-C(2)	105.55(15)	C(6)-C(7)-C(8)	118.11(17)
C(4)-N(3)-C(8)	119.01(15)	N(3)-C(8)-C(12)	119.10(16)
C(17)-N(4)-C(13)	117.38(16)	N(3)-C(8)-C(7)	121.18(16)
N(1)-C(1)-C(2)	103.36(15)	C(12)-C(8)-C(7)	119.72(17)
N(1)-C(1)-C(18)	121.95(16)	C(10)-C(9)-C(7)	120.64(18)
C(2)-C(1)-C(18)	134.69(17)	C(9)-C(10)-C(11)	120.67(18)
N(2)-C(2)-C(1)	111.34(16)	C(12)-C(11)-C(10)	120.13(17)
N(2)-C(2)-C(13)	120.98(15)	C(11)-C(12)-C(8)	120.43(17)
C(1)-C(2)-C(13)	127.67(16)	N(4)-C(13)-C(14)	122.00(17)
N(2)-C(3)-N(1)	109.47(15)	N(4)-C(13)-C(2)	117.01(16)
N(2)-C(3)-C(4)	128.29(16)	C(14)-C(13)-C(2)	120.99(16)
N(1)-C(3)-C(4)	122.24(15)	C(15)-C(14)-C(13)	119.22(18)
N(3)-C(4)-C(5)	122.91(17)	C(14)-C(15)-C(16)	119.30(18)
N(3)-C(4)-C(3)	116.76(16)	C(17)-C(16)-C(15)	118.04(18)
C(5)-C(4)-C(3)	120.33(16)	N(4)-C(17)-C(16)	124.04(18)
C(6)-C(5)-C(4)	118.83(17)		

Table S3. Bond lengths d [Å] and angles ω [°] for **[Zn(HL^{q})Cl$_2$]**.

Bond	d	Bond	d	Bond	d
Zn(1)-N(4)	2.0526(18)	N(3)-C(8)	1.373(3)	C(7)-C(9)	1.419(3)
Zn(1)-N(2)	2.0908(18)	N(4)-C(17)	1.339(3)	C(7)-C(8)	1.425(3)
Zn(1)-Cl(2)	2.2124(6)	N(4)-C(13)	1.361(3)	C(8)-C(12)	1.408(3)
Zn(1)-Cl(1)	2.2229(7)	C(1)-C(2)	1.382(3)	C(9)-C(10)	1.373(4)
N(1)-C(1)	1.360(3)	C(1)-C(18)	1.493(3)	C(10)-C(11)	1.405(4)
N(1)-C(3)	1.366(3)	C(2)-C(13)	1.461(3)	C(11)-C(12)	1.368(4)
N(1)-O(1)	1.376(2)	C(3)-C(4)	1.455(3)	C(13)-C(14)	1.399(3)
N(2)-C(3)	1.329(3)	C(4)-C(5)	1.422(3)	C(14)-C(15)	1.385(3)
N(2)-C(2)	1.382(3)	C(5)-C(6)	1.364(3)	C(15)-C(16)	1.377(3)
N(3)-C(4)	1.325(3)	C(6)-C(7)	1.407(3)	C(16)-C(17)	1.387(3)
Angle	ω	Angle	ω	Angle	ω

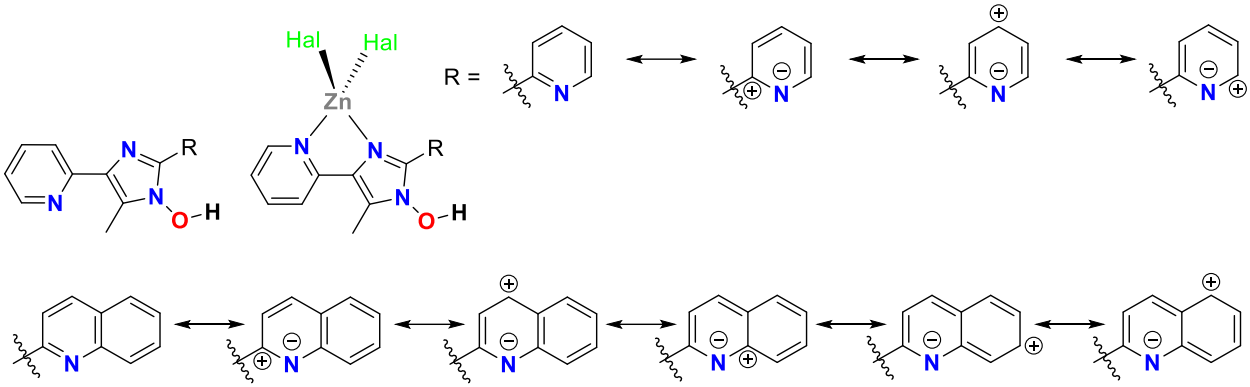
N(4)-Zn(1)-N(2)	81.06(7)	N(1)-C(1)-C(2)	104.19(18)	C(9)-C(7)-C(8)	119.0(2)
N(4)-Zn(1)-Cl(2)	114.50(6)	N(1)-C(1)-C(18)	121.9(2)	N(3)-C(8)-C(12)	119.5(2)
N(2)-Zn(1)-Cl(2)	115.84(5)	C(2)-C(1)-C(18)	133.9(2)	N(3)-C(8)-C(7)	120.9(2)
N(4)-Zn(1)-Cl(1)	114.26(5)	C(1)-C(2)-N(2)	109.85(19)	C(12)-C(8)-C(7)	119.6(2)
N(2)-Zn(1)-Cl(1)	105.99(5)	C(1)-C(2)-C(13)	131.41(19)	C(10)-C(9)-C(7)	119.8(2)
Cl(2)-Zn(1)-Cl(1)	118.91(3)	N(2)-C(2)-C(13)	118.59(18)	C(9)-C(10)-C(11)	120.7(2)
C(1)-N(1)-C(3)	110.58(18)	N(2)-C(3)-N(1)	108.32(18)	C(12)-C(11)-C(10)	120.9(2)
C(1)-N(1)-O(1)	123.23(17)	N(2)-C(3)-C(4)	129.10(19)	C(11)-C(12)-C(8)	119.9(2)
C(3)-N(1)-O(1)	126.18(18)	N(1)-C(3)-C(4)	122.6(2)	N(4)-C(13)-C(14)	120.7(2)
C(3)-N(2)-C(2)	107.05(17)	N(3)-C(4)-C(5)	123.1(2)	N(4)-C(13)-C(2)	114.51(18)
C(3)-N(2)-Zn(1)	142.10(14)	N(3)-C(4)-C(3)	115.70(19)	C(14)-C(13)-C(2)	124.7(2)
C(2)-N(2)-Zn(1)	109.15(14)	C(5)-C(4)-C(3)	121.2(2)	C(15)-C(14)-C(13)	118.9(2)
C(4)-N(3)-C(8)	119.28(19)	C(6)-C(5)-C(4)	117.9(2)	C(16)-C(15)-C(14)	119.9(2)
C(17)-N(4)-C(13)	119.45(18)	C(5)-C(6)-C(7)	120.9(2)	C(15)-C(16)-C(17)	118.7(2)
C(17)-N(4)-Zn(1)	126.50(15)	C(6)-C(7)-C(9)	123.2(2)	N(4)-C(17)-C(16)	122.3(2)
C(13)-N(4)-Zn(1)	114.05(14)	C(6)-C(7)-C(8)	117.8(2)		

Table S4. Bond lengths d [Å] and angles ω [°] for **[Zn(HL^{q})Br$_2$]**.

Bond	d	Bond	d	Bond	d
Zn(1)-N(4)	2.0568(14)	N(3)-C(8)	1.364(2)	C(7)-C(9)	1.420(3)
Zn(1)-N(2)	2.0755(15)	N(4)-C(17)	1.340(2)	C(7)-C(8)	1.426(3)
Zn(1)-Br(2)	2.3518(3)	N(4)-C(13)	1.353(2)	C(8)-C(12)	1.410(2)
Zn(1)-Br(1)	2.3522(3)	C(1)-C(2)	1.381(2)	C(9)-C(10)	1.364(3)
N(1)-C(1)	1.354(2)	C(1)-C(18)	1.494(2)	C(10)-C(11)	1.413(3)
N(1)-C(3)	1.368(2)	C(2)-C(13)	1.458(2)	C(11)-C(12)	1.366(3)
N(1)-O(1)	1.3756(19)	C(3)-C(4)	1.454(2)	C(13)-C(14)	1.400(2)
N(2)-C(3)	1.324(2)	C(4)-C(5)	1.415(2)	C(14)-C(15)	1.377(3)
N(2)-C(2)	1.378(2)	C(5)-C(6)	1.367(3)	C(15)-C(16)	1.387(3)
N(3)-C(4)	1.326(2)	C(6)-C(7)	1.401(3)	C(16)-C(17)	1.375(3)
Angle	ω	Angle	ω	Angle	ω
N(4)-Zn(1)-N(2)	80.94(6)	N(1)-C(1)-C(2)	104.28(14)	C(9)-C(7)-C(8)	118.73(17)
N(4)-Zn(1)-Br(2)	112.28(4)	N(1)-C(1)-C(18)	121.72(16)	N(3)-C(8)-C(12)	119.64(16)
N(2)-Zn(1)-Br(2)	116.27(4)	C(2)-C(1)-C(18)	134.00(17)	N(3)-C(8)-C(7)	120.91(16)
N(4)-Zn(1)-Br(1)	116.35(4)	N(2)-C(2)-C(1)	109.67(16)	C(12)-C(8)-C(7)	119.45(16)
N(2)-Zn(1)-Br(1)	105.27(4)	N(2)-C(2)-C(13)	118.42(15)	C(10)-C(9)-C(7)	120.54(18)
Br(2)-Zn(1)-Br(1)	119.372(10)	C(1)-C(2)-C(13)	131.90(16)	C(9)-C(10)-C(11)	120.21(17)
C(1)-N(1)-C(3)	110.60(15)	N(2)-C(3)-N(1)	108.08(15)	C(12)-C(11)-C(10)	121.01(18)
C(1)-N(1)-O(1)	123.59(14)	N(2)-C(3)-C(4)	129.24(15)	C(11)-C(12)-C(8)	120.04(17)
C(3)-N(1)-O(1)	125.80(15)	N(1)-C(3)-C(4)	122.66(16)	N(4)-C(13)-C(14)	120.83(16)
C(3)-N(2)-C(2)	107.36(14)	N(3)-C(4)-C(5)	123.24(16)	N(4)-C(13)-C(2)	114.56(15)
C(3)-N(2)-Zn(1)	140.75(12)	N(3)-C(4)-C(3)	115.60(15)	C(14)-C(13)-C(2)	124.56(16)
C(2)-N(2)-Zn(1)	110.34(11)	C(5)-C(4)-C(3)	121.16(16)	C(15)-C(14)-C(13)	118.98(17)
C(4)-N(3)-C(8)	119.23(15)	C(6)-C(5)-C(4)	117.97(17)	C(14)-C(15)-C(16)	119.87(17)
C(17)-N(4)-C(13)	119.17(15)	C(5)-C(6)-C(7)	120.66(17)	C(17)-C(16)-C(15)	118.26(18)
C(17)-N(4)-Zn(1)	126.33(12)	C(6)-C(7)-C(9)	123.34(17)	N(4)-C(17)-C(16)	122.88(17)
C(13)-N(4)-Zn(1)	114.44(12)	C(6)-C(7)-C(8)	117.93(16)		

Table S5. Bond lengths d [Å] and angles ω [°] for **[Zn(HL^{q})I$_2$]**.

Bond	d	Bond	d	Bond	d
Zn(1)-N(4)	2.051(4)	N(3)-C(8)	1.371(5)	C(7)-C(9)	1.407(6)
Zn(1)-N(2)	2.058(3)	N(4)-C(17)	1.335(5)	C(7)-C(8)	1.419(6)
Zn(1)-I(1)	2.5362(6)	N(4)-C(13)	1.356(5)	C(8)-C(12)	1.408(6)
Zn(1)-I(2)	2.5520(5)	C(1)-C(2)	1.391(6)	C(9)-C(10)	1.376(6)
N(1)-C(3)	1.355(5)	C(1)-C(18)	1.483(6)	C(10)-C(11)	1.405(7)
N(1)-C(1)	1.356(5)	C(2)-C(13)	1.460(6)	C(11)-C(12)	1.374(6)
N(1)-O(1)	1.375(4)	C(3)-C(4)	1.460(6)	C(13)-C(14)	1.381(6)
N(2)-C(3)	1.325(5)	C(4)-C(5)	1.416(6)	C(14)-C(15)	1.388(7)
N(2)-C(2)	1.380(5)	C(5)-C(6)	1.373(6)	C(15)-C(16)	1.382(7)
N(3)-C(4)	1.328(5)	C(6)-C(7)	1.411(6)	C(16)-C(17)	1.390(7)
Angle	ω	Angle	ω	Angle	ω
N(4)-Zn(1)-N(2)	81.83(14)	N(1)-C(1)-C(2)	104.1(4)	C(9)-C(7)-C(8)	118.4(4)
N(4)-Zn(1)-I(1)	109.60(10)	N(1)-C(1)-C(18)	122.5(4)	N(3)-C(8)-C(12)	118.7(4)
N(2)-Zn(1)-I(1)	111.64(9)	C(2)-C(1)-C(18)	133.4(4)	N(3)-C(8)-C(7)	121.0(4)
N(4)-Zn(1)-I(2)	112.64(10)	N(2)-C(2)-C(1)	109.5(4)	C(12)-C(8)-C(7)	120.3(4)
N(2)-Zn(1)-I(2)	112.43(10)	N(2)-C(2)-C(13)	119.3(4)	C(10)-C(9)-C(7)	121.1(4)
I(1)-Zn(1)-I(2)	121.74(2)	C(1)-C(2)-C(13)	131.0(4)	C(9)-C(10)-C(11)	119.6(4)
C(3)-N(1)-C(1)	110.5(3)	N(2)-C(3)-N(1)	109.0(4)	C(12)-C(11)-C(10)	121.2(4)
C(3)-N(1)-O(1)	127.0(3)	N(2)-C(3)-C(4)	129.2(4)	C(11)-C(12)-C(8)	119.3(4)
C(1)-N(1)-O(1)	122.5(3)	N(1)-C(3)-C(4)	121.7(4)	N(4)-C(13)-C(14)	121.2(4)
C(3)-N(2)-C(2)	106.8(3)	N(3)-C(4)-C(5)	122.7(4)	N(4)-C(13)-C(2)	114.0(4)
C(3)-N(2)-Zn(1)	143.1(3)	N(3)-C(4)-C(3)	114.9(4)	C(14)-C(13)-C(2)	124.7(4)
C(2)-N(2)-Zn(1)	110.0(3)	C(5)-C(4)-C(3)	122.4(4)	C(13)-C(14)-C(15)	119.7(5)
C(4)-N(3)-C(8)	119.5(4)	C(6)-C(5)-C(4)	118.5(4)	C(16)-C(15)-C(14)	118.7(5)
C(17)-N(4)-C(13)	119.2(4)	C(5)-C(6)-C(7)	120.2(4)	C(15)-C(16)-C(17)	119.1(4)
C(17)-N(4)-Zn(1)	126.6(3)	C(6)-C(7)-C(9)	123.6(4)	N(4)-C(17)-C(16)	122.1(4)
C(13)-N(4)-Zn(1)	114.2(3)	C(6)-C(7)-C(8)	118.1(4)		



Scheme S1. Resonance structures showing the delocalization of the charge over the pyridine-2-yl group in **HL^{p}** and quinolin-2-yl group in **HL^{q}**.

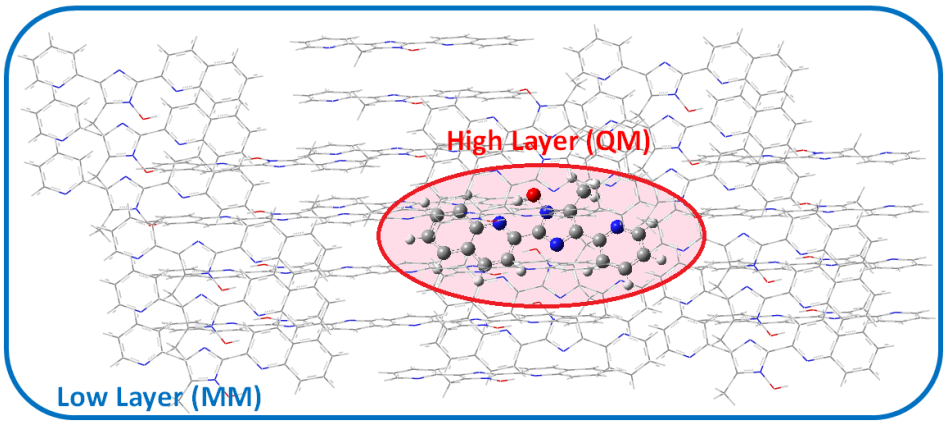


Figure S1. The ONIOM model for the quantum chemical calculations of **HL^{q}**.

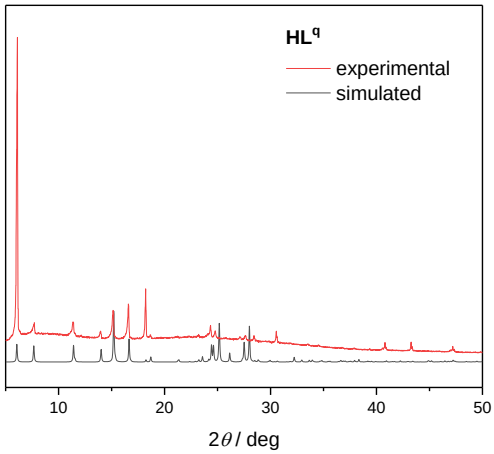


Figure S2. X-ray powder diffraction patterns of HL^{q}.

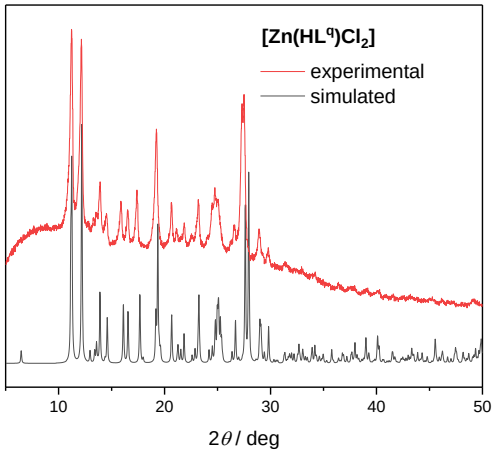


Figure S3. X-ray powder diffraction patterns of [Zn(HL^q)Cl$_2$].

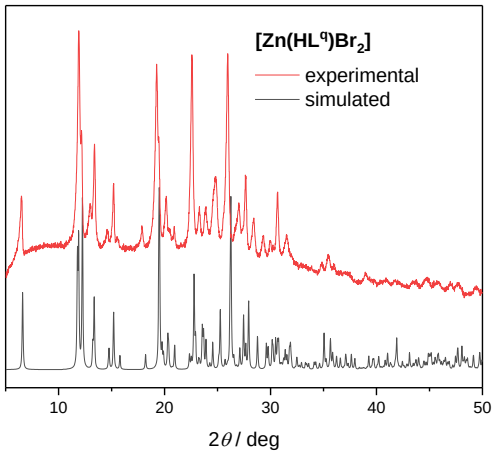


Figure S4. X-ray powder diffraction patterns of [Zn(HL^q)Br$_2$].

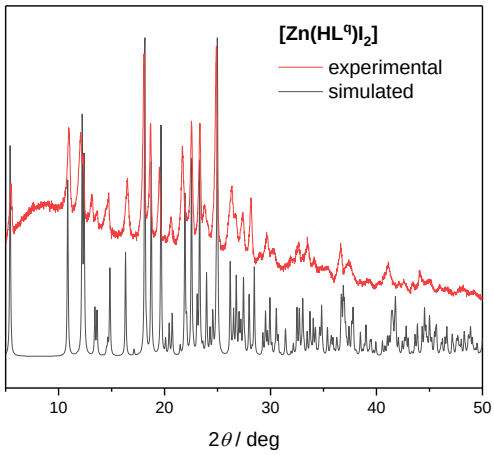


Figure S5. X-ray powder diffraction patterns of [Zn(HL^q)I$_2$].

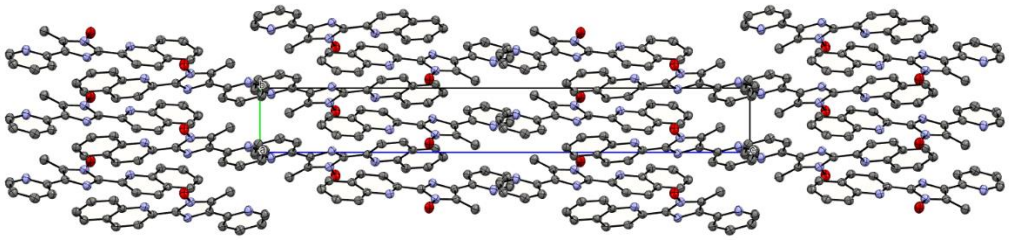


Figure S6. Packing of **HL^{q}** (view along the *a* axis).

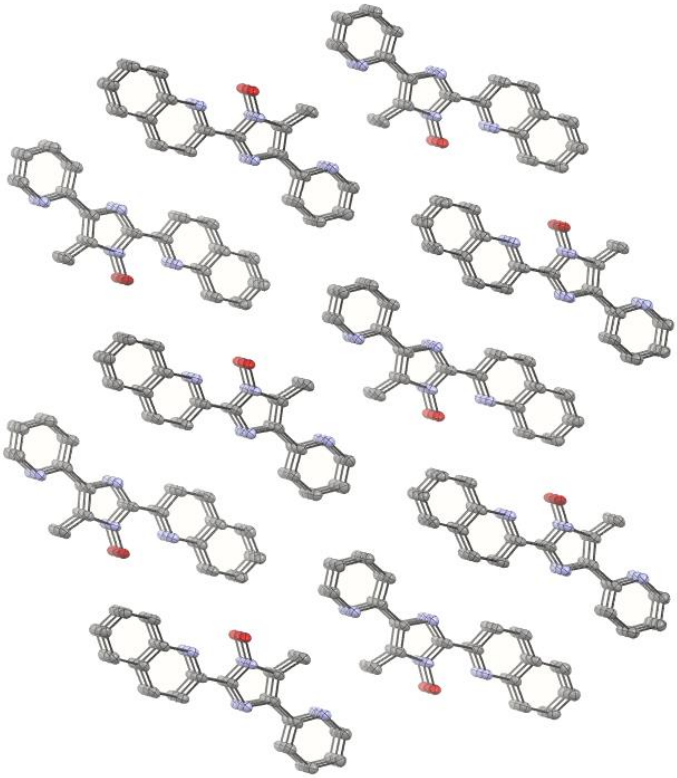


Figure S7. Packing of **HL^{q}** (view along the *b* axis).

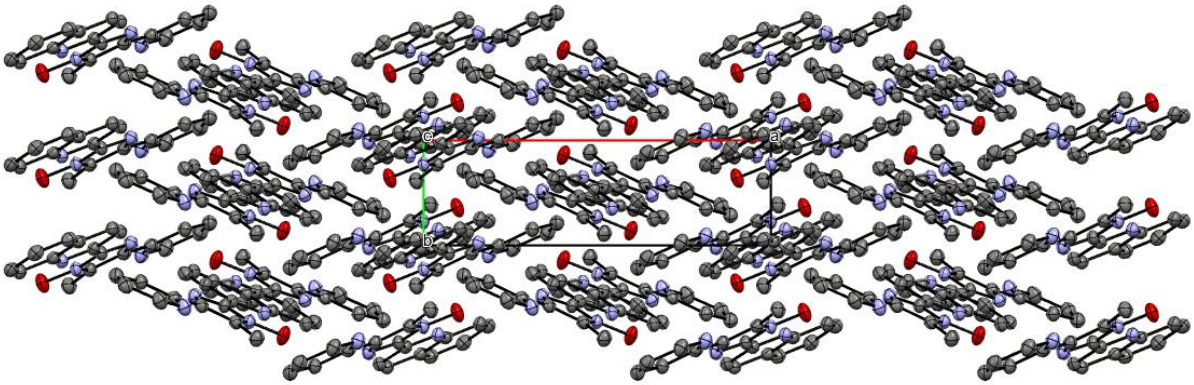


Figure S8. Packing of **HL^{q}** (view along the *c* axis).

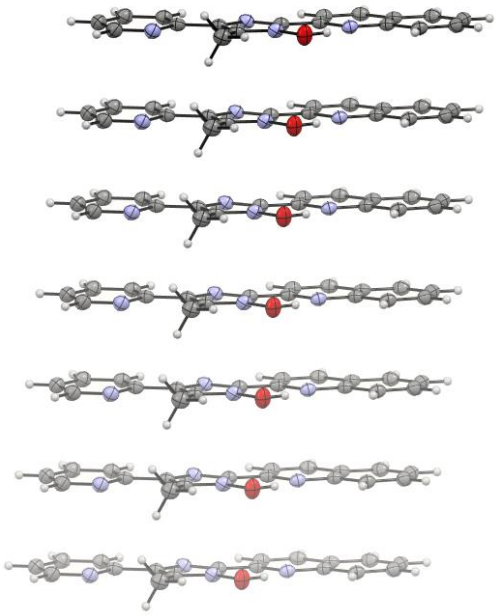


Figure S9. A supramolecular chain in the structure of **HL^{q}**.

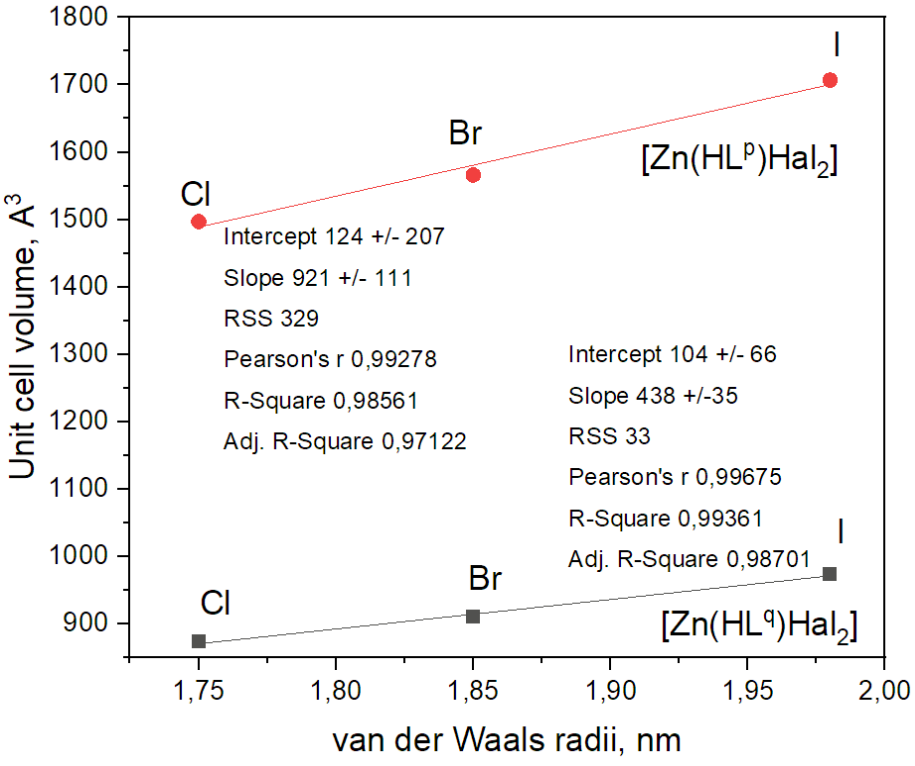


Figure S10. The correlation between the unit cell volume and the van der Waals radii of halogenido anions for **[Zn(HL^{p})Hal$_2$]** and **[Zn(HL^{q})Hal$_2$]**.

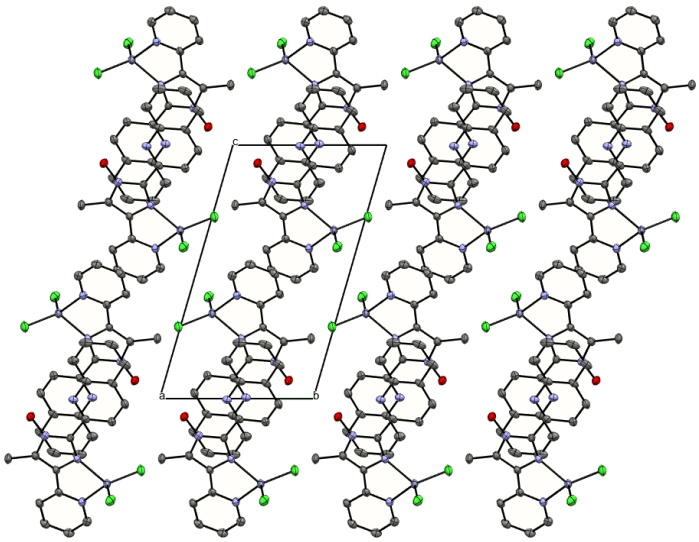


Figure S11. Packing of **[Zn(HL^{q})Cl$_2$]** (view along the a axis).

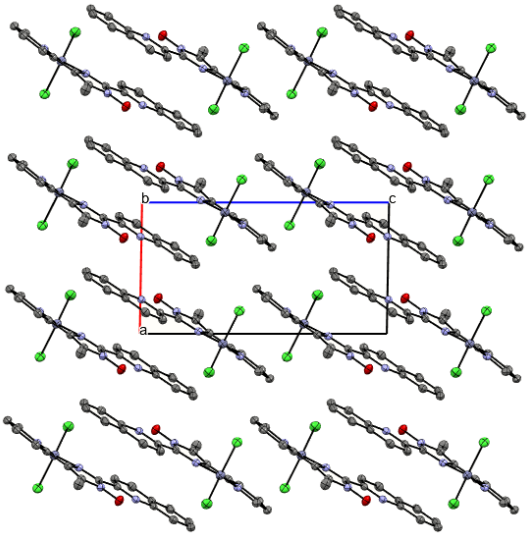


Figure S12. Packing of **[Zn(HL^{q})Cl$_2$]** (view along the b axis).

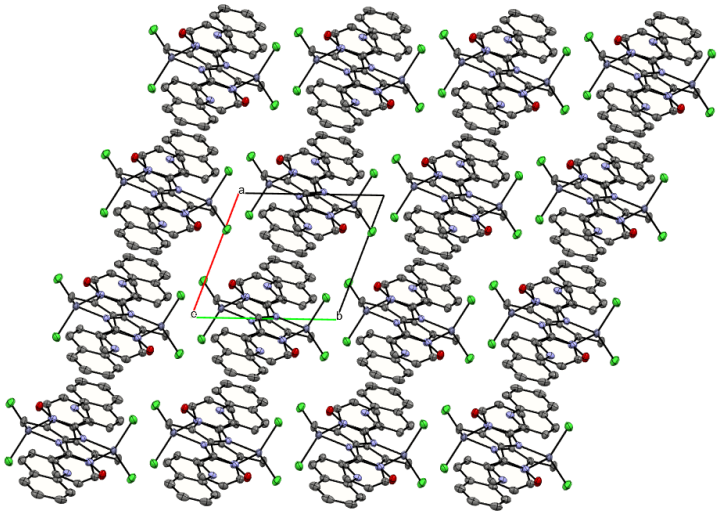


Figure S13. Packing of **[Zn(HL^{q})Cl$_2$]** (view along the c axis).

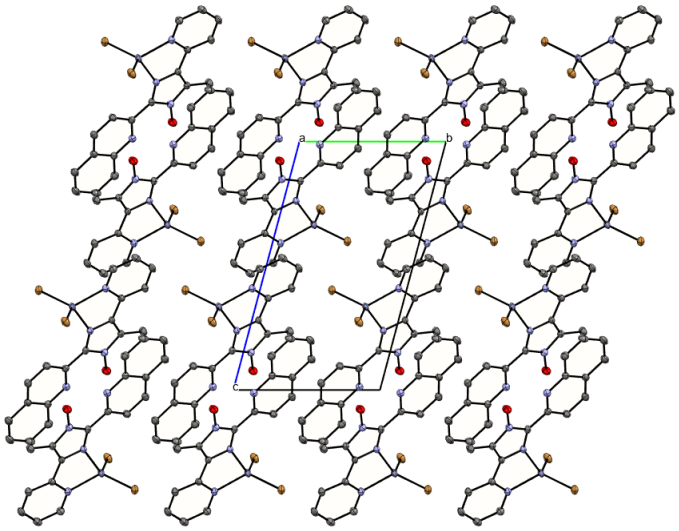


Figure S14. Packing of **[Zn(HL^{q})Br$_2$]** (view along the a axis).

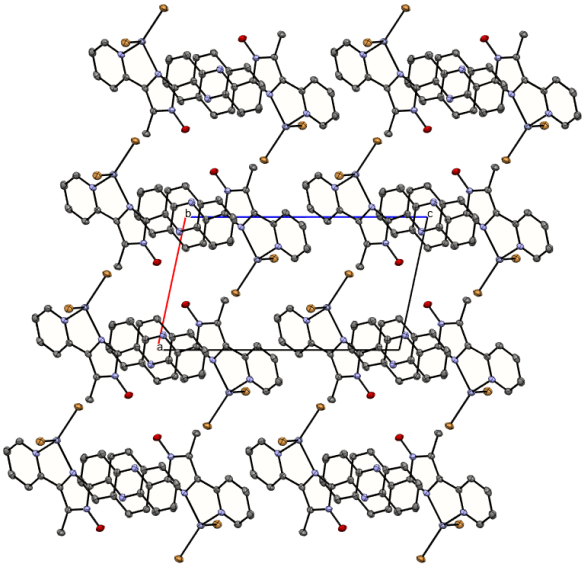


Figure S15. Packing of **[Zn(HL^{q})Br$_2$]** (view along the b axis).

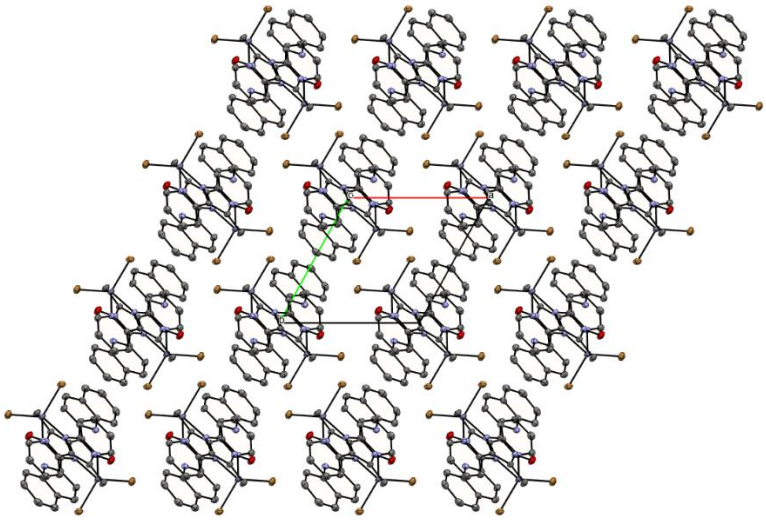


Figure S16. Packing of **[Zn(HL^{q})Br$_2$]** (view along the c axis).

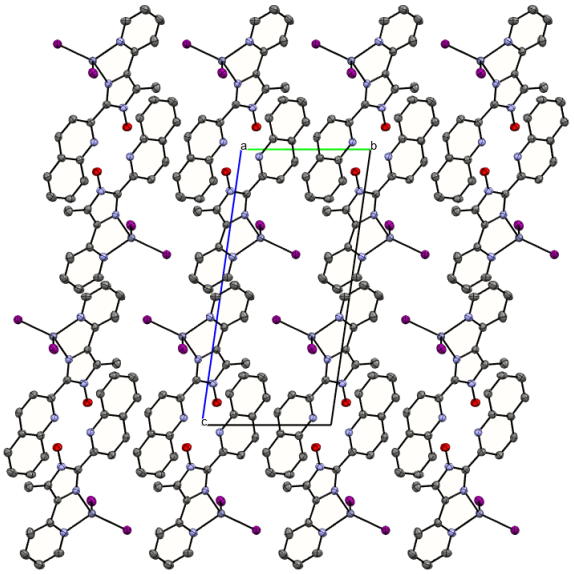


Figure S17. Packing of **[Zn(HL^{q})I$_2$]** (view along the a axis).

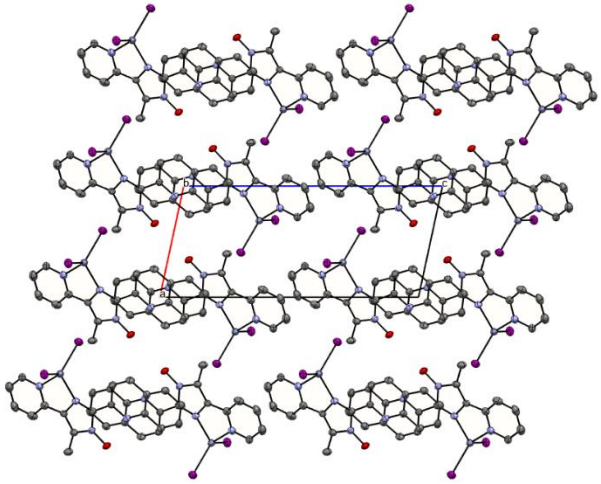


Figure S18. Packing of **[Zn(HL^{q})I$_2$]** (view along the a axis).

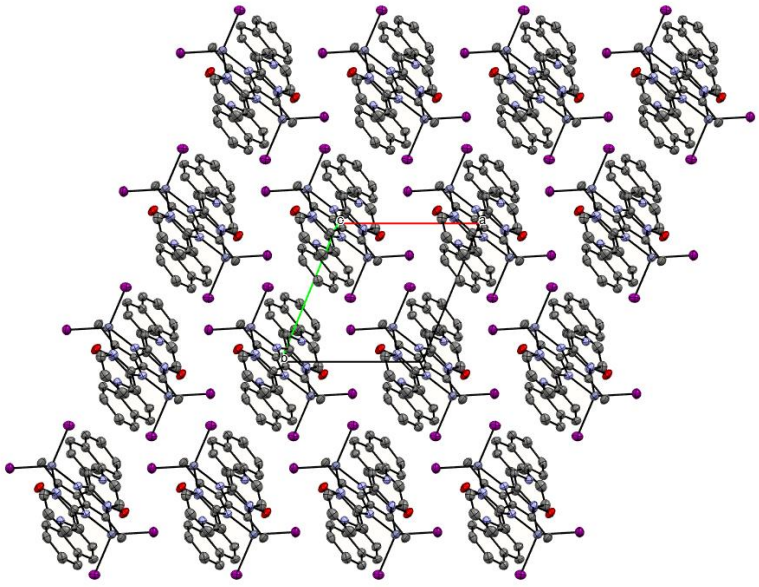


Figure S19. Packing of **[Zn(HL^{q})I$_2$]** (view along the c axis).

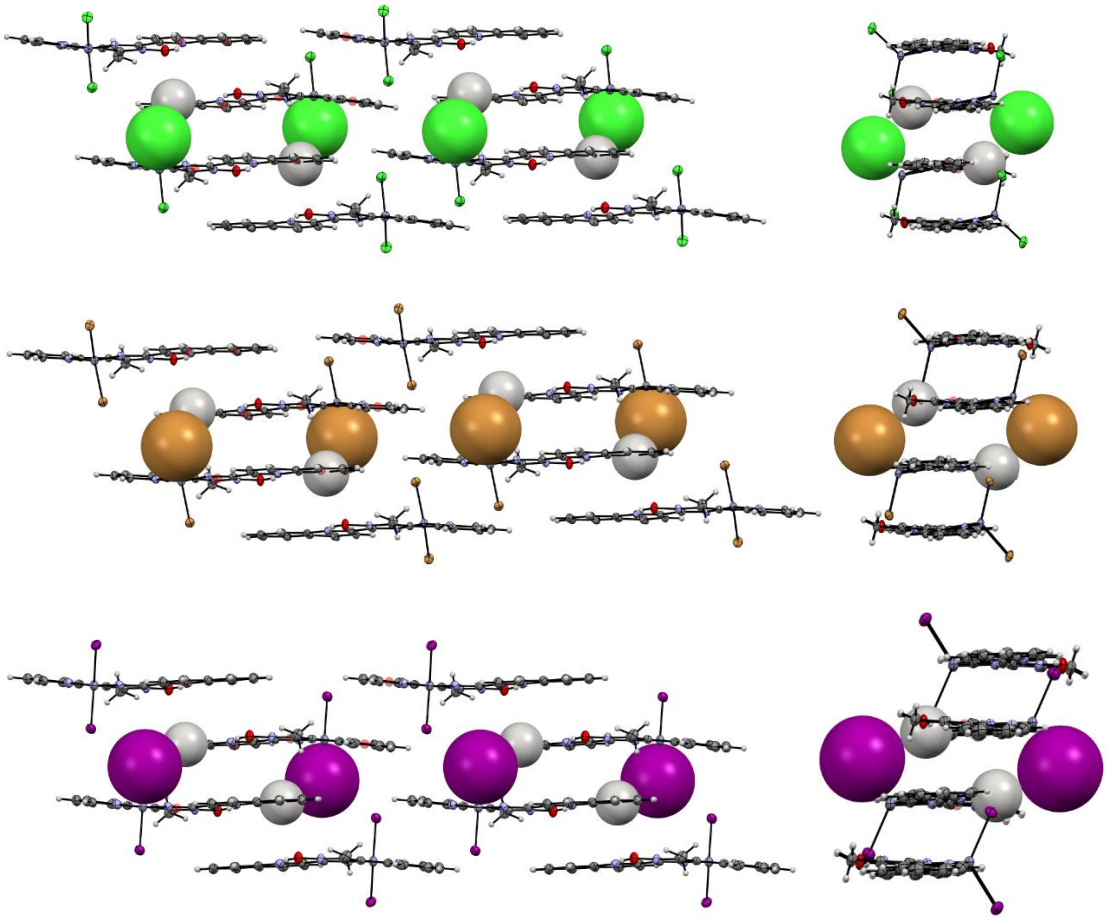
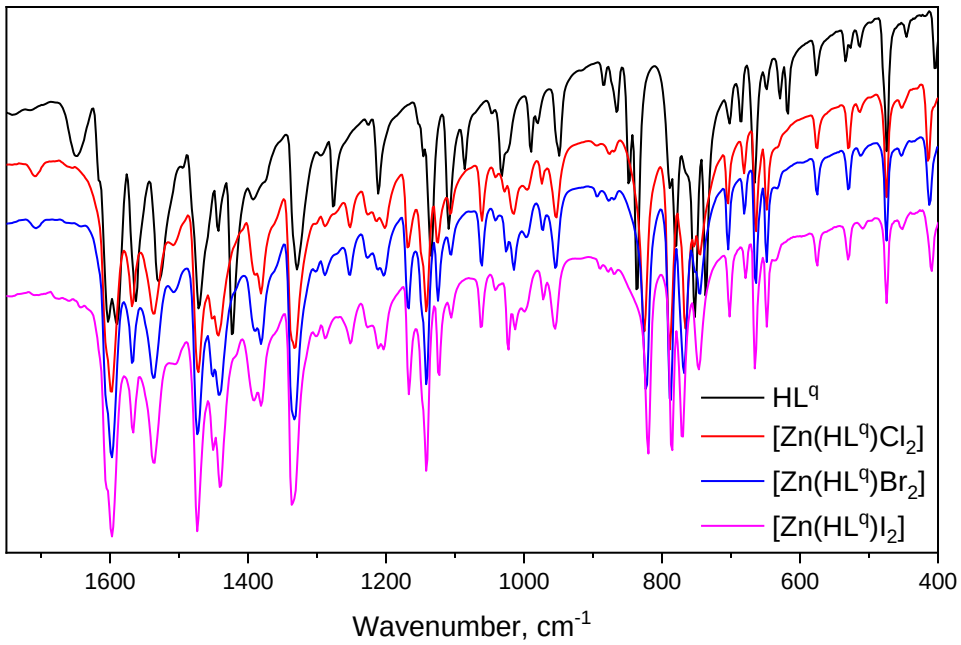


Figure S20. The packing of dimeric associates in the structures of **[Zn(HL^{q})Hal$_2$]**.

IR spectra



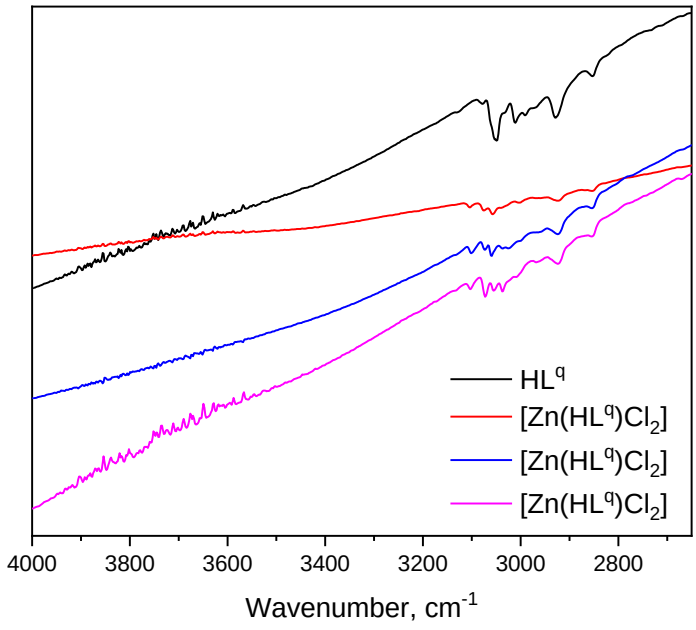


Figure S21. IR spectra of HL^q, $[Zn(HL^q)Cl_2]$, $[Zn(HL^q)Br_2]$ and $[Zn(HL^q)I_2]$ in KBr (top) and fluorinated oil (bottom).

Photoluminescence data

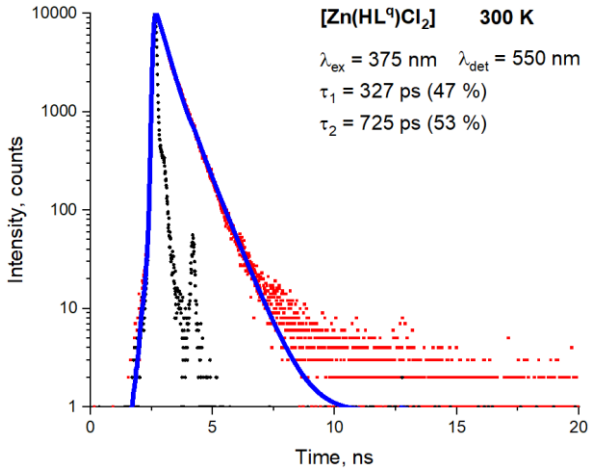
Table S6. Photoluminescence lifetimes recorded for **HL^q**, **[Zn(HL^q)Cl$_2$]**, **[Zn(HL^q)Br$_2$]** and **[Zn(HL^q)I$_2$]** in the solid state. All compounds were excited with λ_{ex} = 375 nm.

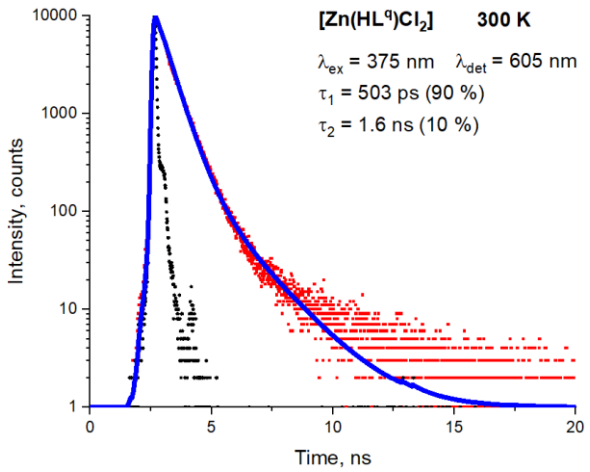
Compound	T, K	λ_{det}, nm[a]	τ[b]
HL^q	300	650	74 ps, 1.1 ns, 107.5 ns
	77	650	14 ps, 2.8 ns, 39.0 ns
[Zn(HL^q)Cl$_2$]	300	550	327 ps, 725 ps
		605	503 ps, 1.6 ns
		670	522 ps, 1.8 ns
		730	540 ps. 3.2 ns
	77	560	143 ps, 1.0 ns, 3.0 ns
		600	148 ps, 1.1 ns, 3.7 ns
		650	156 ps, 1.1 ns, 3.8 ns
		700	173 ps, 1.0 ns, 3.6 ns
[Zn(HL^q)Br$_2$]	300	550	553 ps, 1.0 ns
		605	652 ps, 2.5 ns
		670	690 ps, 3.1 ns
		730	722 ps, 2.8 ns
	77	560	173 ps, 1.2 ns, 3.9 ns
		600	129 ps, 1.2 ns, 3.1 ns
		650	117 ps, 1.2 ns, 3.2 ns
		700	154 ps, 1.3 ns, 3.3 ns
[Zn(HL^q)I$_2$]	300	550	281 ps, 670 ps
		605	559 ps. 1.4 ns
		670	574 ps, 1.7 ns
		730	579 ps, 1.8 ns
	77	545	164 ps, 1.1 ns, 2.2 ns
		585	123 ps, 1.1 ns, 2.7 ns
		640	172 ps, 1.2 ns, 3.1 ns
		700	156 ps, 1.2 ns, 3.3 ns

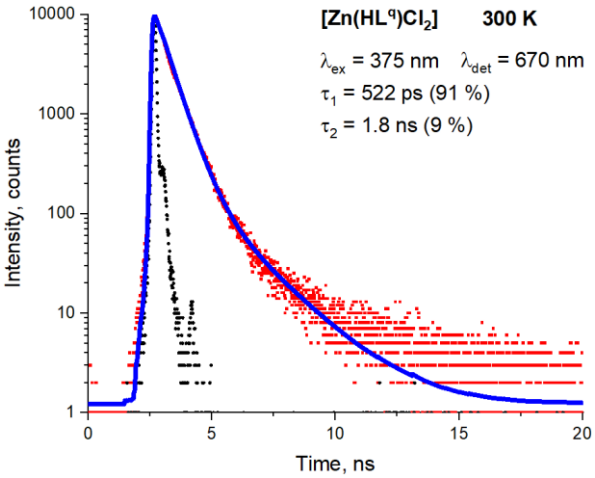
a – detection wavelength

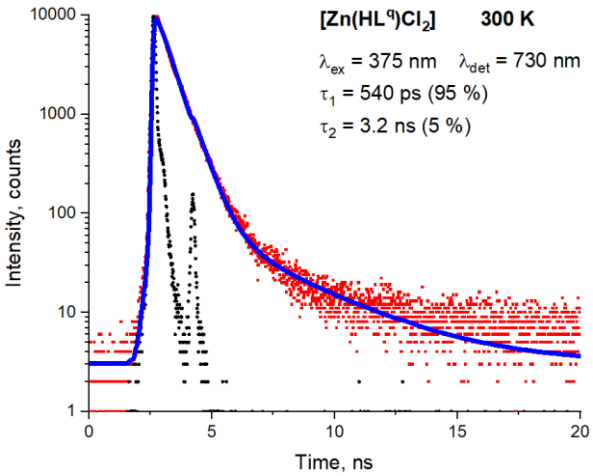
b – emission decay was analyzed with two or three components : $I = \sum_i A_i \exp\left(^{-t}/_{\tau_i}\right)$

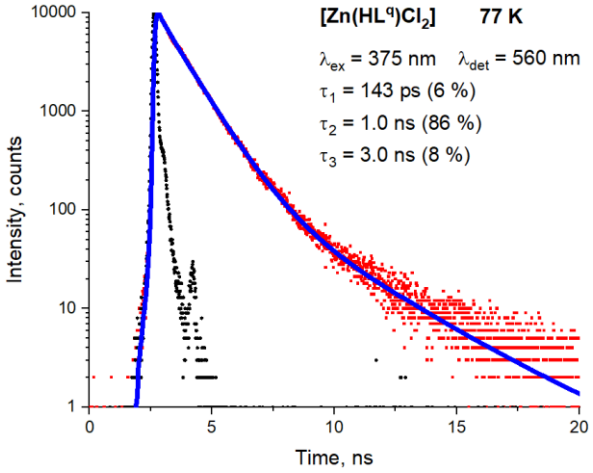
Fluorescence decay curves recorded for **HL^q**, **[Zn(HL^q)Cl$_2$]**, **[Zn(HL^q)Br$_2$]** and **[Zn(HL^q)I$_2$]** in the solid state: approximation (blue), experimental points (red) and instrument response function (black).

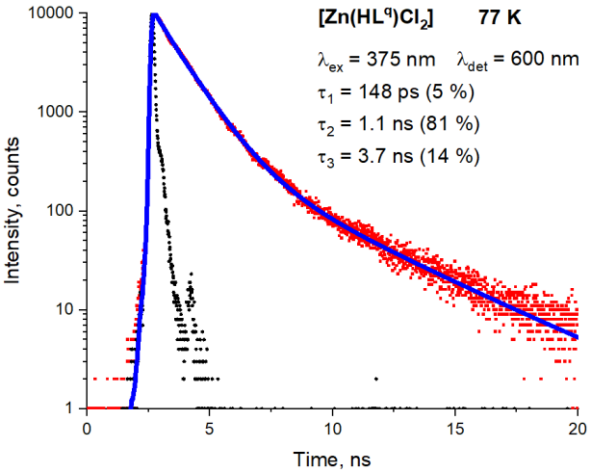

[Zn(HL^q)Cl2] 300 K
λex = 375 nm λdet = 550 nm
τ1 = 327 ps (47 %)
τ2 = 725 ps (53 %)
Intensity, counts
Time, ns

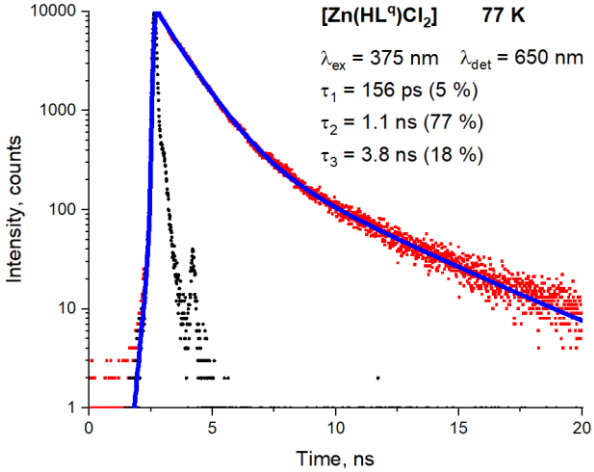

[Zn(HL^q)Cl2] 300 K
λex = 375 nm λdet = 605 nm
τ1 = 503 ps (90 %)
τ2 = 1.6 ns (10 %)
Intensity, counts
Time, ns

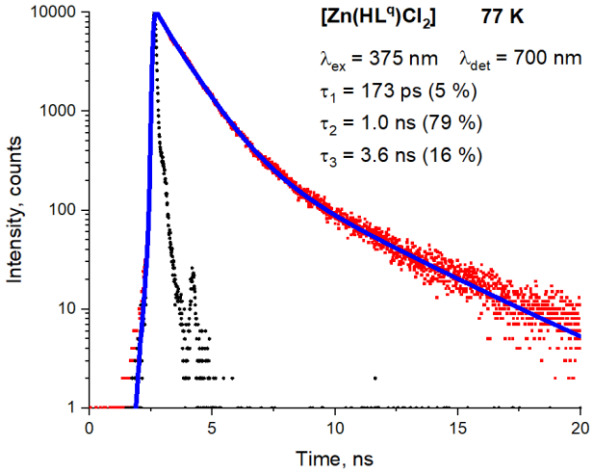

[Zn(HL^q)Cl2] 300 K
λex = 375 nm λdet = 670 nm
τ1 = 522 ps (91 %)
τ2 = 1.8 ns (9 %)
Intensity, counts
Time, ns

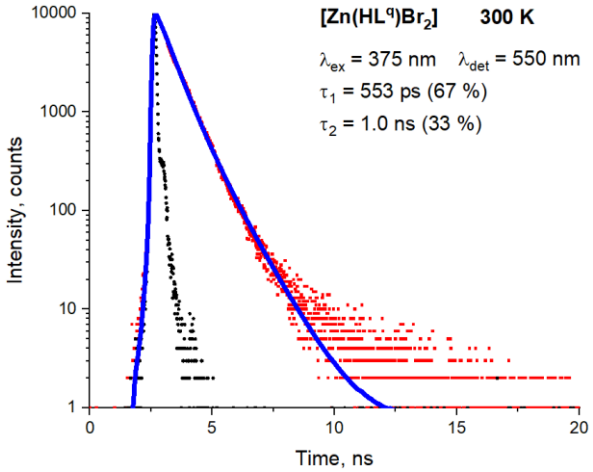

[Zn(HL^q)Cl2] 300 K
λex = 375 nm λdet = 730 nm
τ1 = 540 ps (95 %)
τ2 = 3.2 ns (5 %)
Intensity, counts
Time, ns

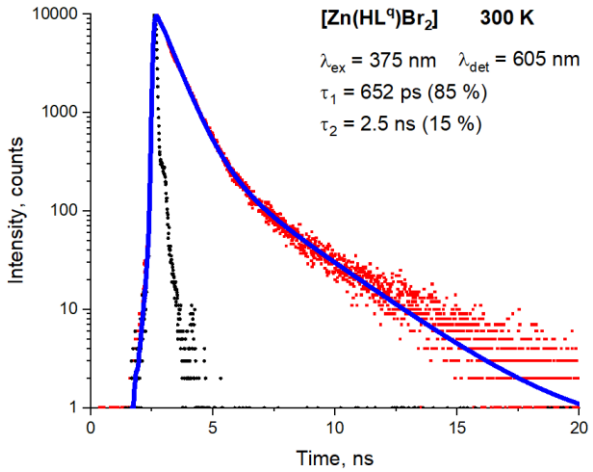

[Zn(HL^q)Cl2] 77 K
λex = 375 nm λdet = 560 nm
τ1 = 143 ps (6 %)
τ2 = 1.0 ns (86 %)
τ3 = 3.0 ns (8 %)
Intensity, counts
Time, ns

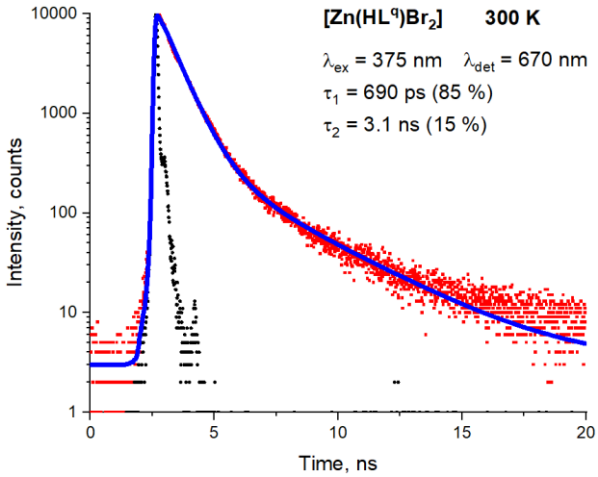

[Zn(HL^q)Cl2] 77 K
λex = 375 nm λdet = 600 nm
τ1 = 148 ps (5 %)
τ2 = 1.1 ns (81 %)
τ3 = 3.7 ns (14 %)
Intensity, counts
Time, ns

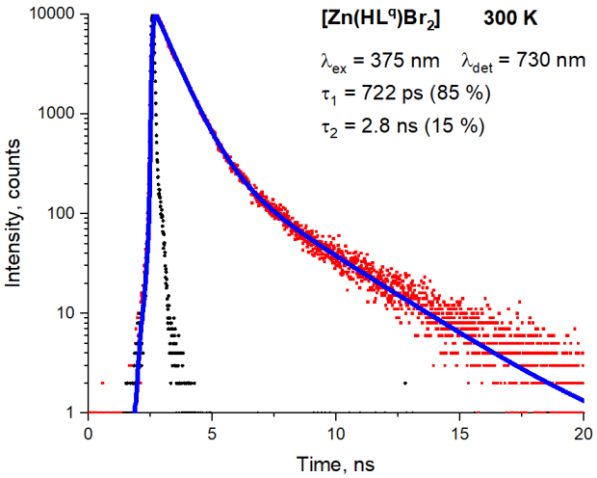

[Zn(HL^q)Cl2] 77 K
λex = 375 nm λdet = 650 nm
τ1 = 156 ps (5 %)
τ2 = 1.1 ns (77 %)
τ3 = 3.8 ns (18 %)
Intensity, counts
Time, ns

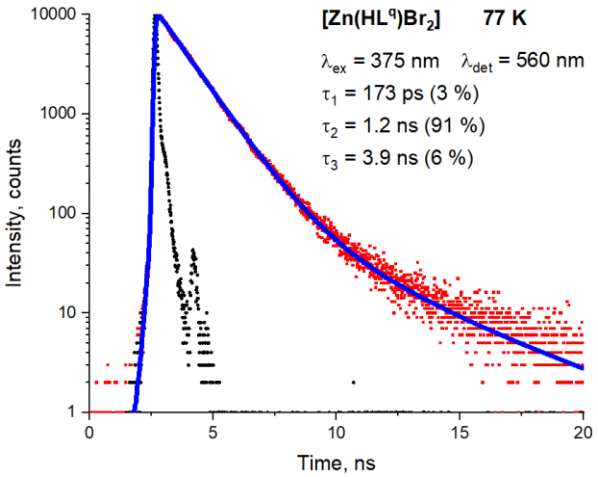

[Zn(HL^q)Cl2] 77 K
λex = 375 nm λdet = 700 nm
τ1 = 173 ps (5 %)
τ2 = 1.0 ns (79 %)
τ3 = 3.6 ns (16 %)
Intensity, counts
Time, ns

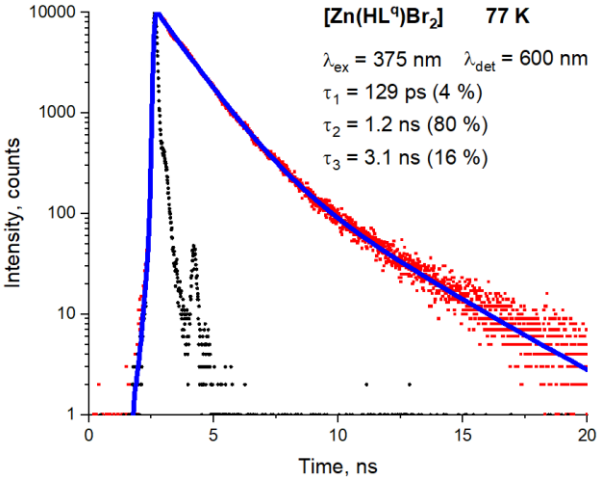

[Zn(HL^q)Br2] 300 K
λex = 375 nm λdet = 550 nm
τ1 = 553 ps (67 %)
τ2 = 1.0 ns (33 %)
Intensity, counts
Time, ns

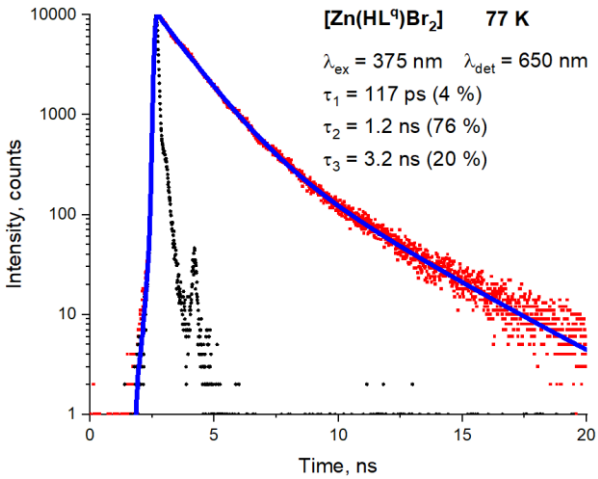

[Zn(HL^q)Br2] 300 K
λex = 375 nm λdet = 605 nm
τ1 = 652 ps (85 %)
τ2 = 2.5 ns (15 %)
Intensity, counts
Time, ns

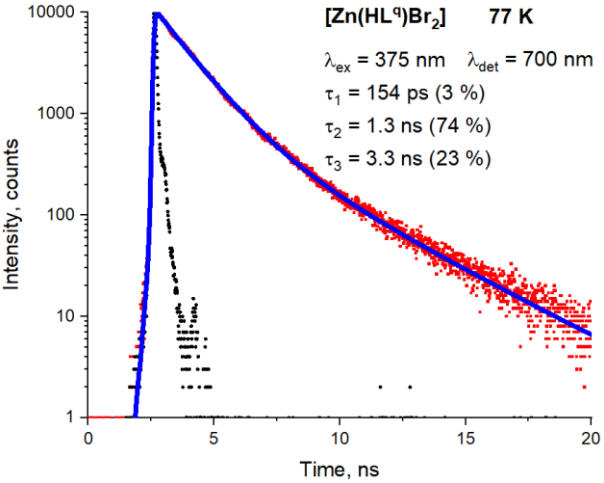

[Zn(HL^q)Br2] 300 K
λex = 375 nm λdet = 670 nm
τ1 = 690 ps (85 %)
τ2 = 3.1 ns (15 %)
Intensity, counts
Time, ns

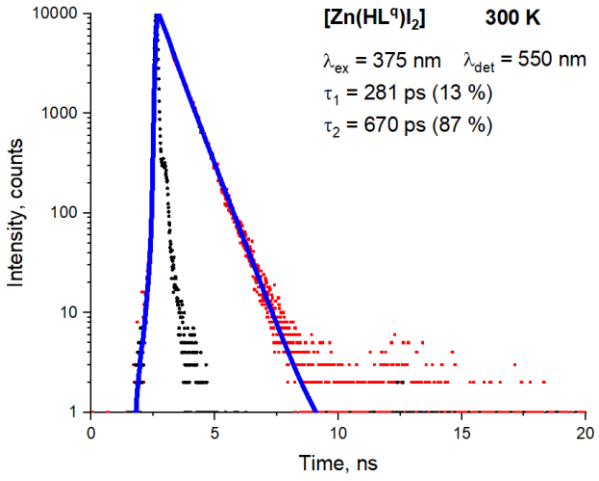

[Zn(HL^q)Br2] 300 K
λex = 375 nm λdet = 730 nm
τ1 = 722 ps (85 %)
τ2 = 2.8 ns (15 %)
Intensity, counts
Time, ns

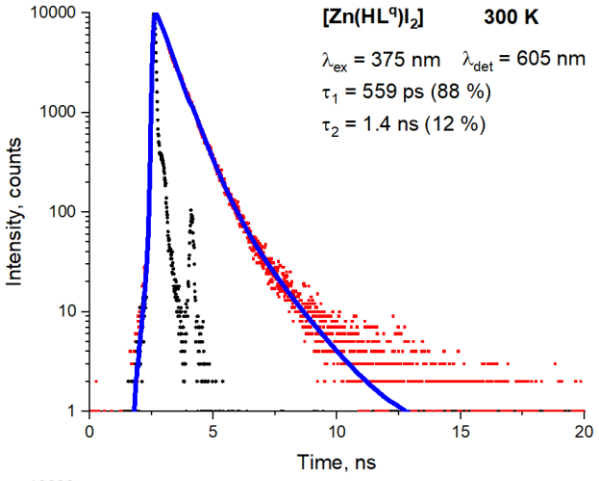

[Zn(HL^q)Br2] 77 K
λex = 375 nm λdet = 560 nm
τ1 = 173 ps (3 %)
τ2 = 1.2 ns (91 %)
τ3 = 3.9 ns (6 %)
Intensity, counts
Time, ns

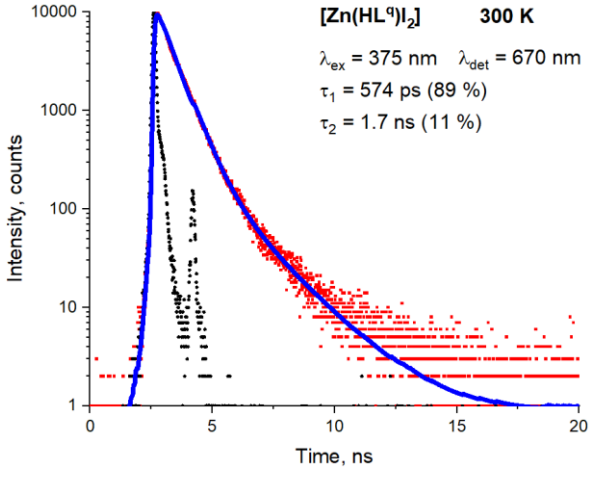

[Zn(HL^q)Br2] 77 K
λex = 375 nm λdet = 600 nm
τ1 = 129 ps (4 %)
τ2 = 1.2 ns (80 %)
τ3 = 3.1 ns (16 %)
Intensity, counts
Time, ns

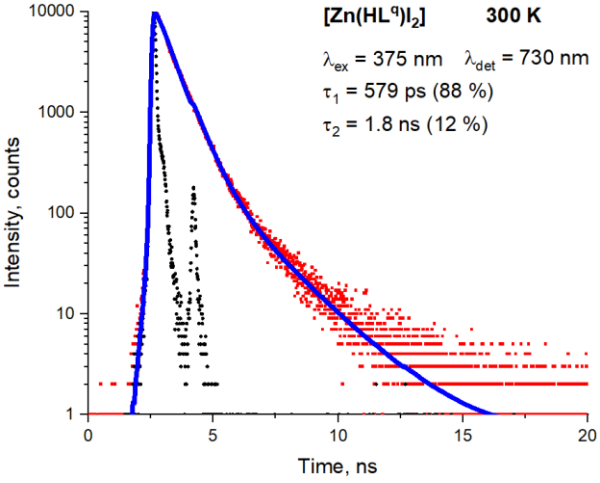

[Zn(HL^q)Br2] 77 K
λex = 375 nm λdet = 650 nm
τ1 = 117 ps (4 %)
τ2 = 1.2 ns (76 %)
τ3 = 3.2 ns (20 %)
Intensity, counts
Time, ns

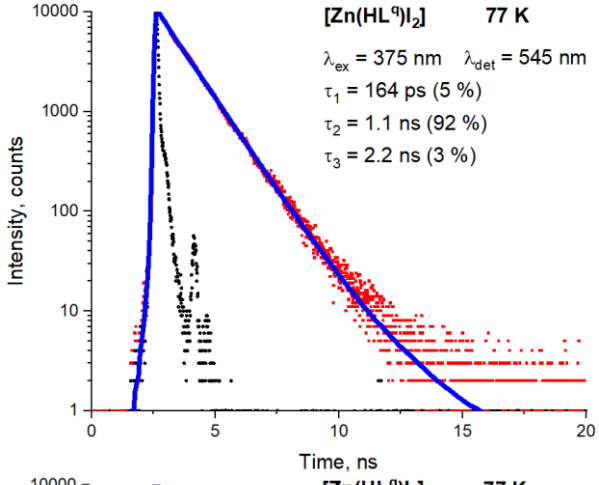

[Zn(HL^q)Br2] 77 K
λex = 375 nm λdet = 700 nm
τ1 = 154 ps (3 %)
τ2 = 1.3 ns (74 %)
τ3 = 3.3 ns (23 %)
Intensity, counts
Time, ns

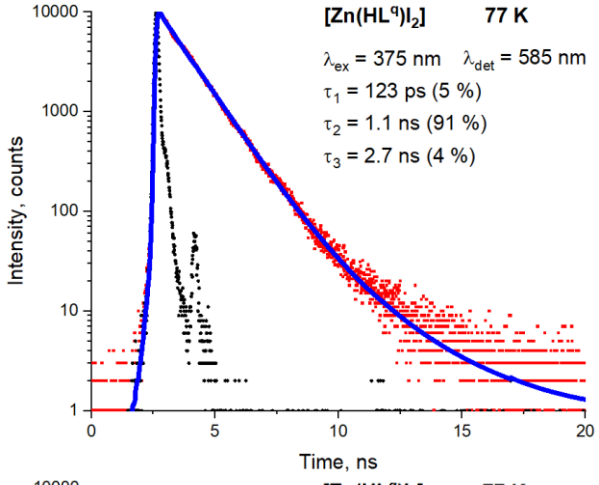

[Zn(HL^q)I2] 300 K
λex = 375 nm λdet = 550 nm
τ1 = 281 ps (13 %)
τ2 = 670 ps (87 %)
Intensity, counts
Time, ns

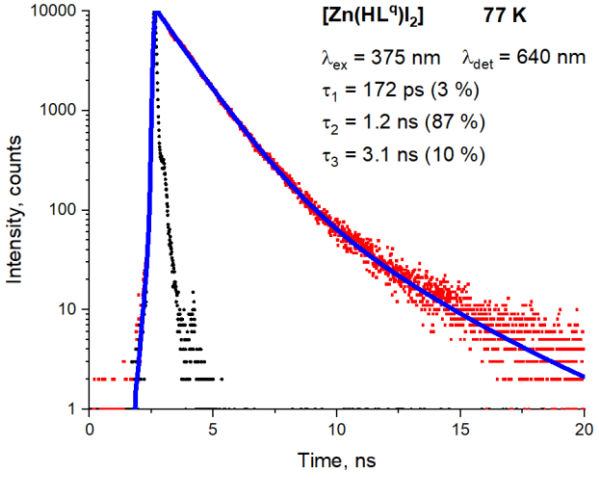

[Zn(HL^q)I2] 300 K
λex = 375 nm λdet = 605 nm
τ1 = 559 ps (88 %)
τ2 = 1.4 ns (12 %)
Intensity, counts
Time, ns

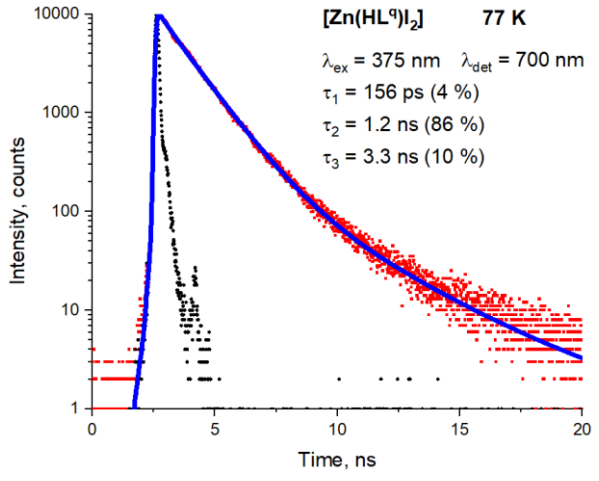

[Zn(HL^q)I2] 300 K
λex = 375 nm λdet = 670 nm
τ1 = 574 ps (89 %)
τ2 = 1.7 ns (11 %)
Intensity, counts
Time, ns


[Zn(HL^q)I2] 300 K
λex = 375 nm λdet = 730 nm
τ1 = 579 ps (88 %)
τ2 = 1.8 ns (12 %)
Intensity, counts
Time, ns


[Zn(HL^q)I2] 77 K
λex = 375 nm λdet = 545 nm
τ1 = 164 ps (5 %)
τ2 = 1.1 ns (92 %)
τ3 = 2.2 ns (3 %)
Intensity, counts
Time, ns


[Zn(HL^q)I2] 77 K
λex = 375 nm λdet = 585 nm
τ1 = 123 ps (5 %)
τ2 = 1.1 ns (91 %)
τ3 = 2.7 ns (4 %)
Intensity, counts
Time, ns


[Zn(HL^q)I2] 77 K
λex = 375 nm λdet = 640 nm
τ1 = 172 ps (3 %)
τ2 = 1.2 ns (87 %)
τ3 = 3.1 ns (10 %)
Intensity, counts
Time, ns


[Zn(HL^q)I2] 77 K
λex = 375 nm λdet = 700 nm
τ1 = 156 ps (4 %)
τ2 = 1.2 ns (86 %)
τ3 = 3.3 ns (10 %)
Intensity, counts
Time, ns

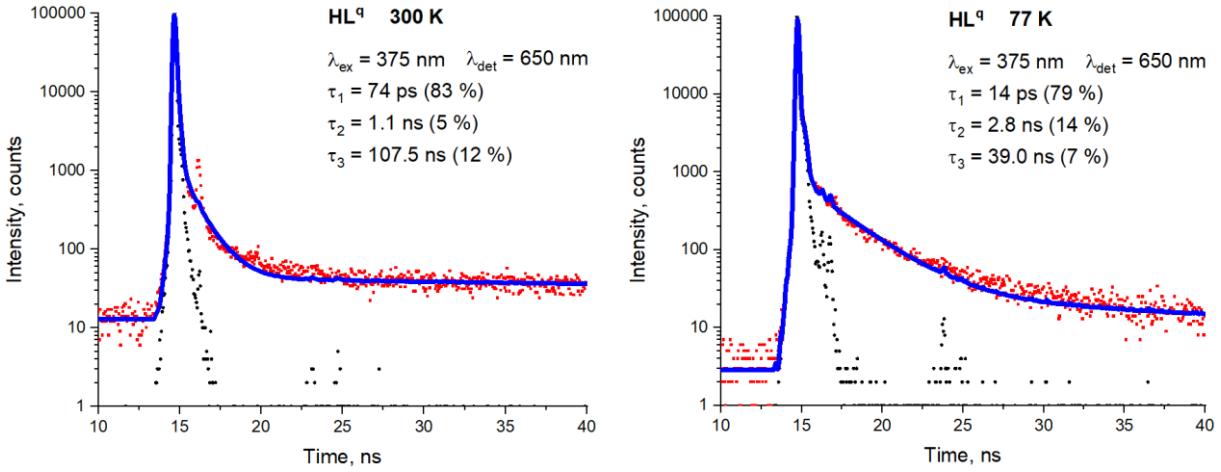


Table S7. Photoluminescence quantum yields (PLQY) recorded for **HL^q**, **[Zn(HL^q)Cl$_2$]**, **[Zn(HL^q)Br$_2$]** and **[Zn(HL^q)I$_2$]** in the solid state.

Compound	T, K	λ_{ex}, nm[a]	PLQY, %
HL^q	300	560	<1
		600	<1
[Zn(HL^q)Cl$_2$]	300	300	1
		420	3
		560	11
	77	300	1
		420	4
		560	6
[Zn(HL^q)Br$_2$]	300	300	<1
		420	3
		500	4
	77	300	<1
		420	4
		500	3
[Zn(HL^q)I$_2$]	300	320	<1
		480	4
		550	5
	77	320	<1
		480	7
		550	3

a – excitation wavelength

Theoretical part

Table S8. Optimized geometries of the ground and excited states of **HL^q** using QM/MM method and in CH_2Cl_2 solvation continuum model. The dihedral angles between the planes of quinoline and imidazole heterocycles are shown as well as the O···N and O–H distances.

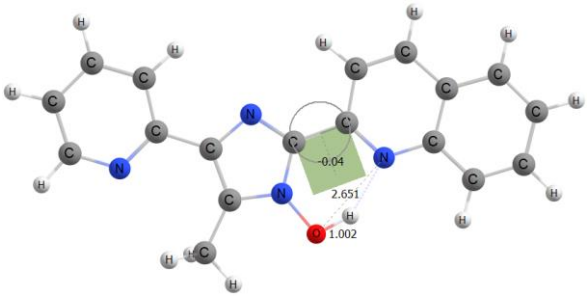
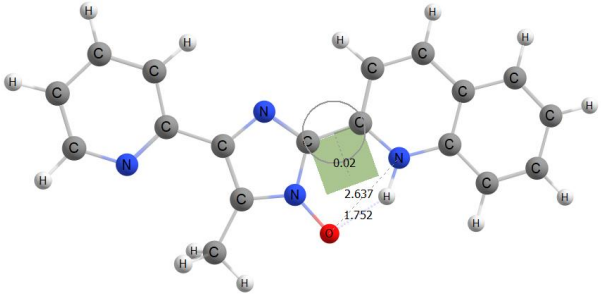
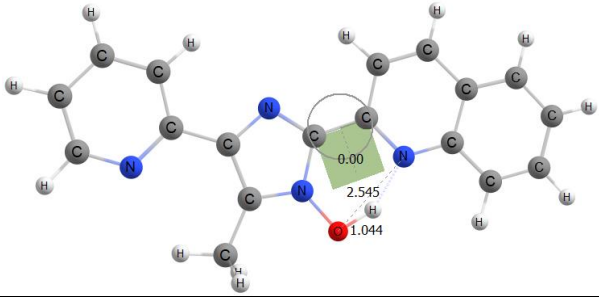
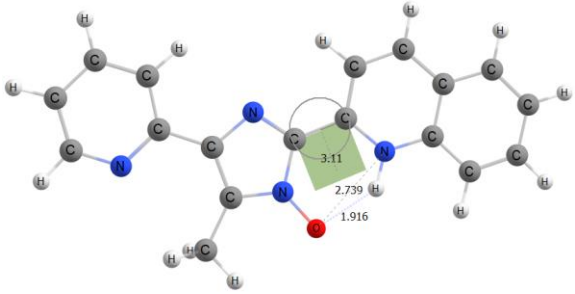
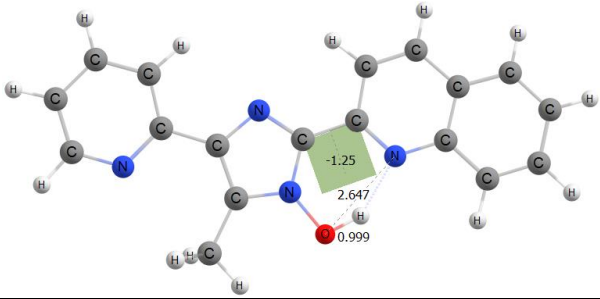
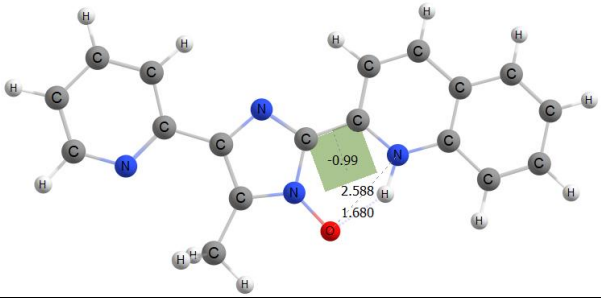
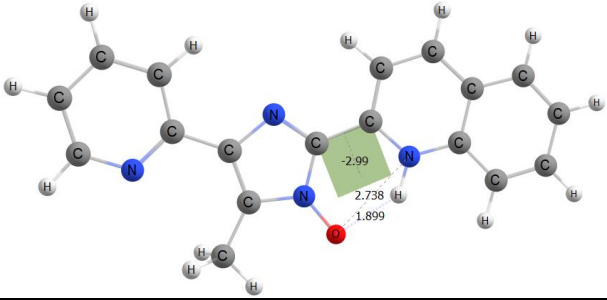
Normal form, ground state (S_0^N) **CH_2Cl_2** 	**Tautomeric form, ground state (S_0^T)** **CH_2Cl_2** 
Normal form, first singlet excited state (S_1^N) **CH_2Cl_2** 	**Tautomeric form, first singlet excited state (S_1^T)** **CH_2Cl_2** 
Normal form, ground state (S_0^N) **QM/MM** 	**Tautomeric form, ground state (S_0^T)** **QM/MM** 
Tautomeric form, first singlet excited state (S_1^T) **QM/MM** 	

Table S9. Optimized geometries of the ground and excited states of **[Zn(HL^{q})Cl$_2$]** using QM/MM method and in CH_2Cl_2 solvation continuum model. The dihedral angles between the planes of quinoline and imidazole heterocycles are shown as well as the O···N and O–H distances.

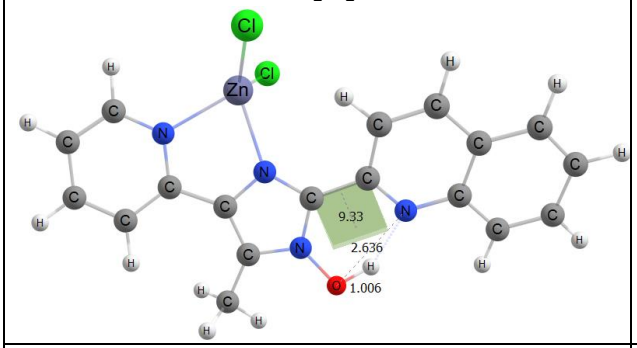
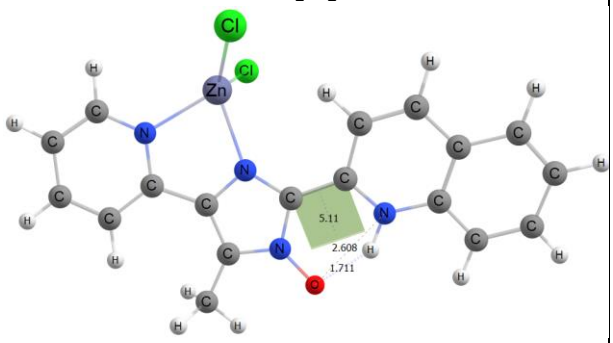
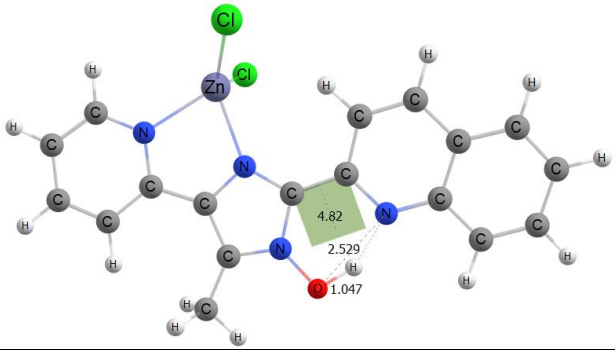
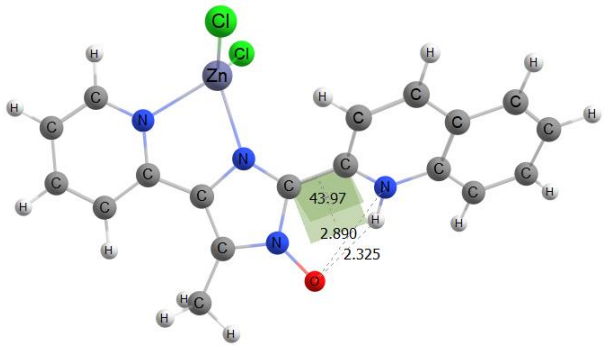
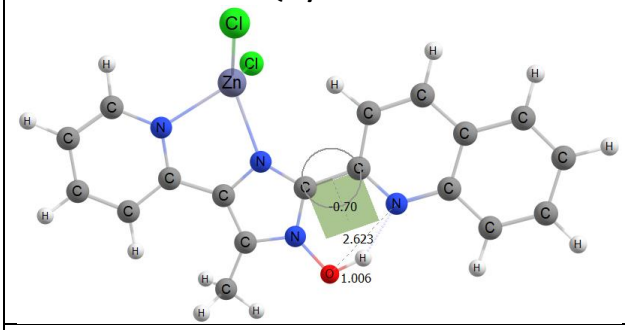
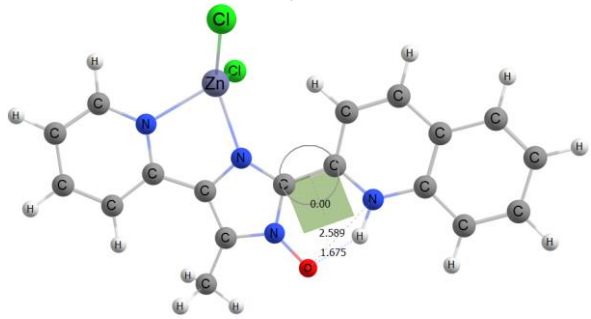
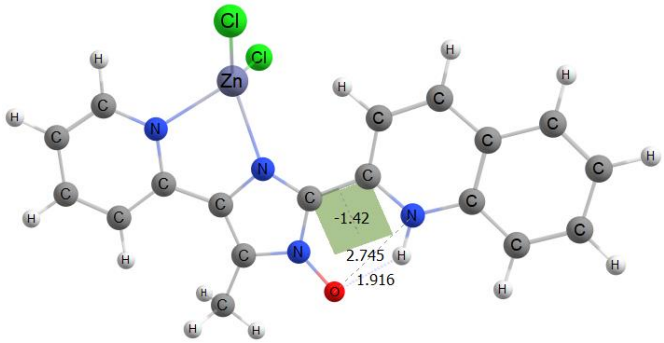
Normal form, ground state (S_0^N) **CH_2Cl_2** 	**Tautomeric form, ground state (S_0^T)** **CH_2Cl_2** 
Normal form, first singlet excited state (S_1^N) **CH_2Cl_2** 	**Tautomeric form, first singlet excited state (S_1^T)** **CH_2Cl_2** 
Normal form, ground state (S_0^N) **QM/MM** 	**Tautomeric form, ground state (S_0^T)** **QM/MM** 
Tautomeric form, first singlet excited state (S_1^T) **QM/MM** 	

Table S10. Optimized geometries of the ground and excited states of **[Zn(HL^{q})Br$_2$]** using QM/MM method and in CH_2Cl_2 solvation continuum model. The dihedral angles between the planes of quinoline and imidazole heterocycles are shown as well as the O···N and O–H distances.

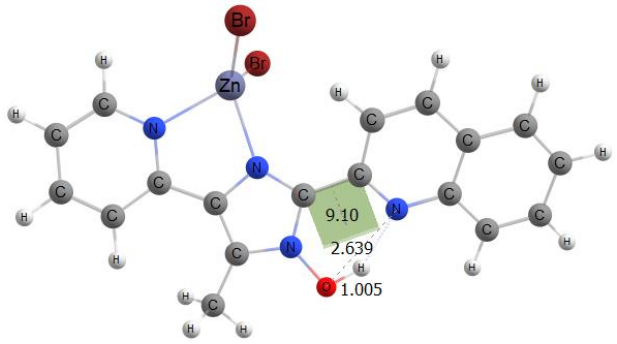
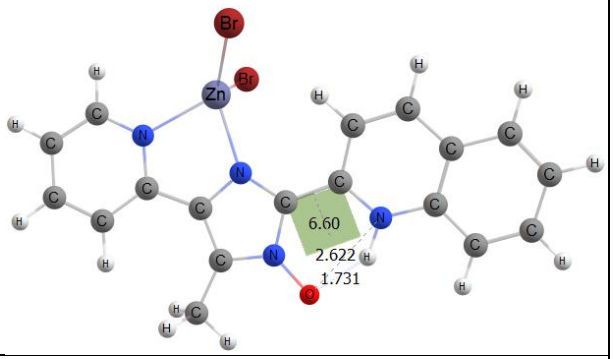
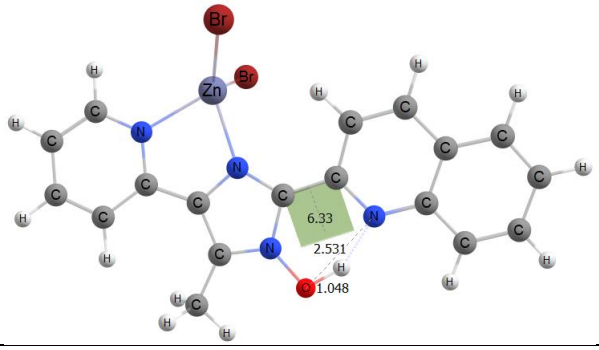
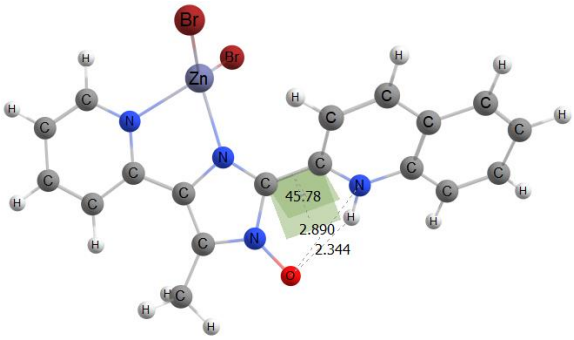
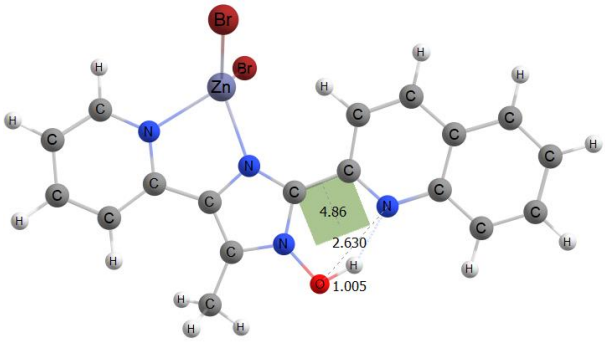
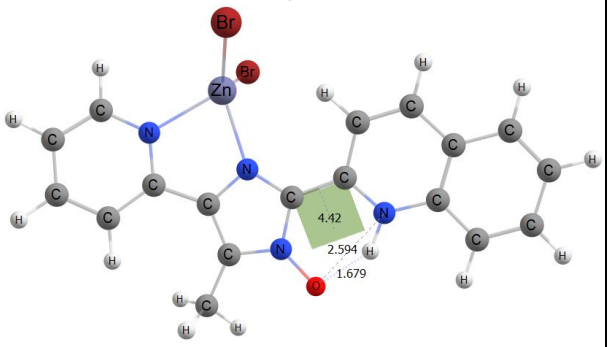
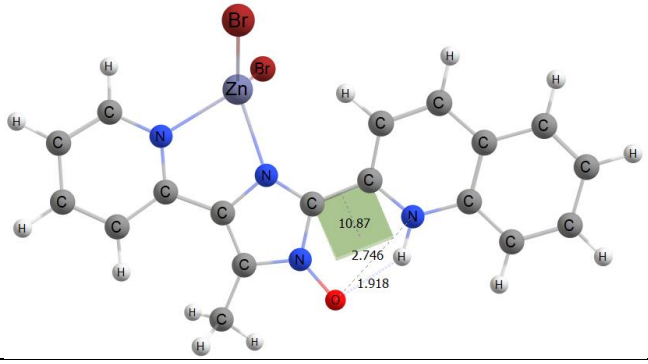
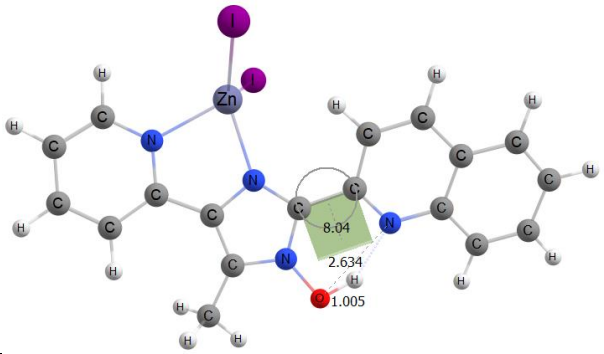
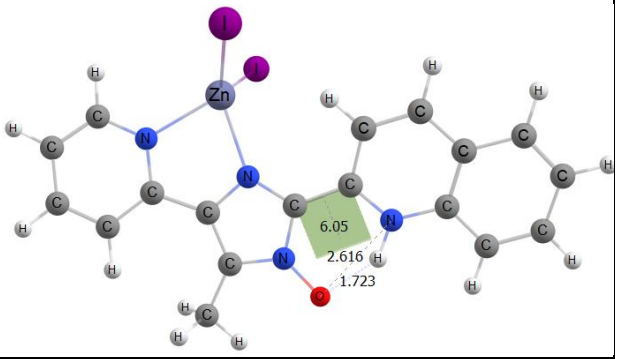
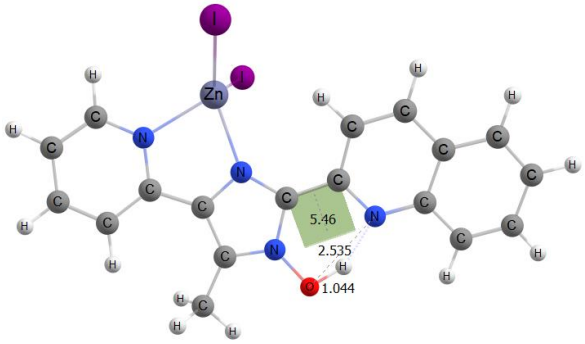
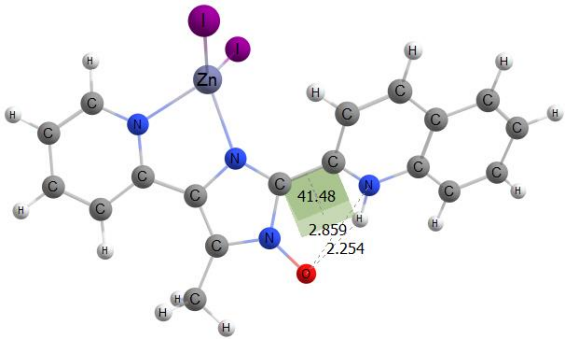
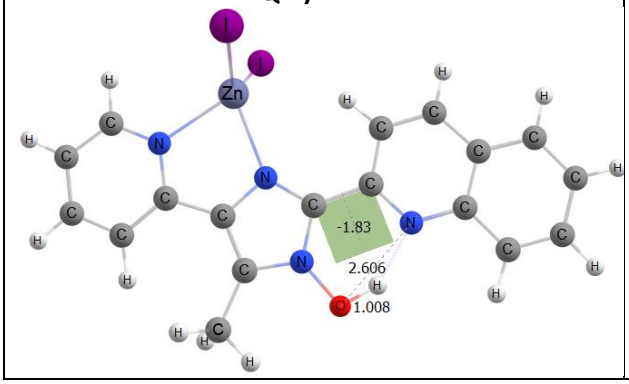
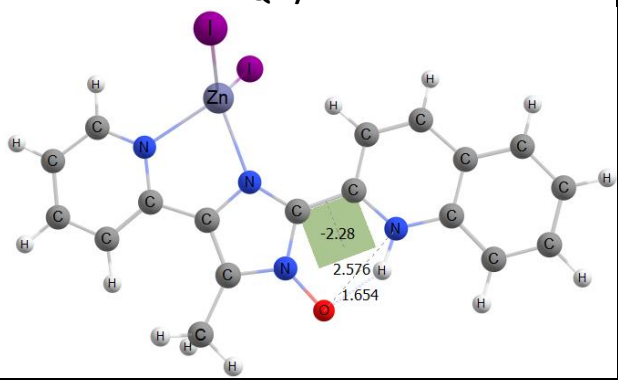
Normal form, ground state (S_0^N) **CH_2Cl_2** 	**Tautomeric form, ground state (S_0^T)** **CH_2Cl_2** 
Normal form, first singlet excited state (S_1^N) **CH_2Cl_2** 	**Tautomeric form, first singlet excited state (S_1^T)** **CH_2Cl_2** 
Normal form, ground state (S_0^N) **QM/MM** 	**Tautomeric form, ground state (S_0^T)** **QM/MM** 
Tautomeric form, first singlet excited state (S_1^T) **QM/MM** 	

Table S11. Optimized geometries of the ground and excited states of **[Zn(HL^{q})I$_2$]** using QM/MM method and in CH_2Cl_2 solvation continuum model. The dihedral angles between the planes of quinoline and imidazole heterocycles are shown as well as the O···N and O–H distances.

Normal form, ground state (S_0^N) **CH_2Cl_2**	**Tautomeric form, ground state (S_0^T)** **CH_2Cl_2**
	
Normal form, first singlet excited state (S_1^N) **CH_2Cl_2**	**Tautomeric form, first singlet excited state (S_1^T)** **CH_2Cl_2**
	
Normal form, ground state (S_0^N) **QM/MM**	**Tautomeric form, ground state (S_0^T)** **QM/MM**
	

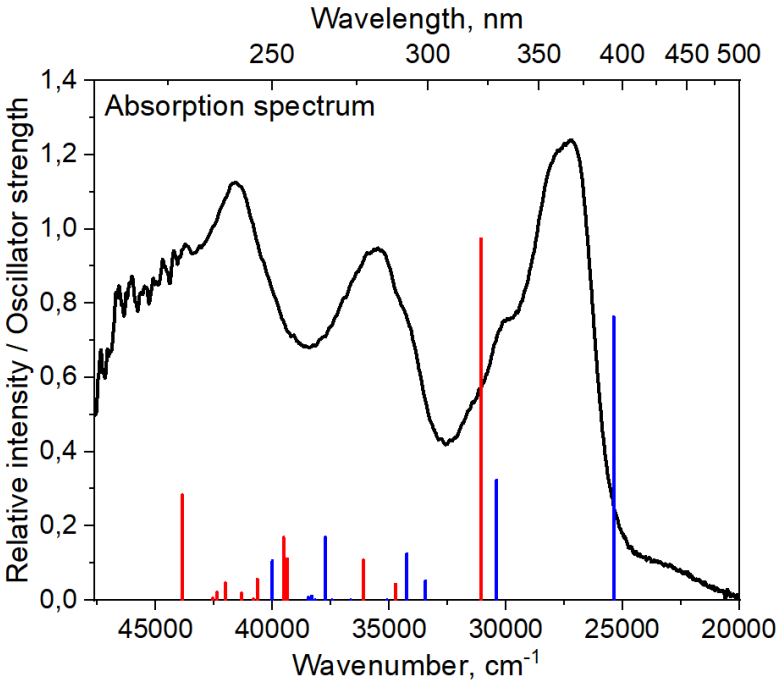


Figure S22. Absorption spectrum of **[Zn(HL^{q})Br$_2$]** (black). Vertical bars display the positions and oscillator strengths of the electronic transitions from the global energy minima of the normal (red) and tautomeric (blue) forms.

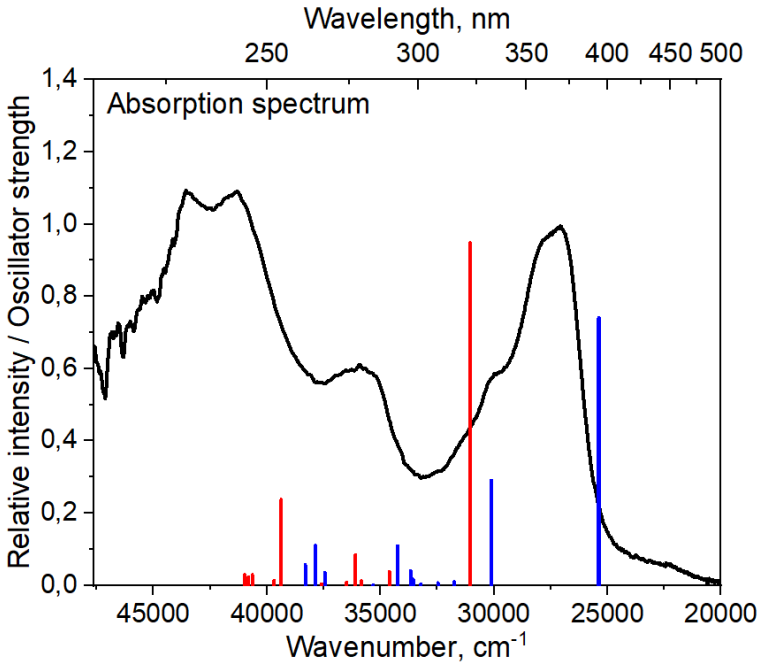
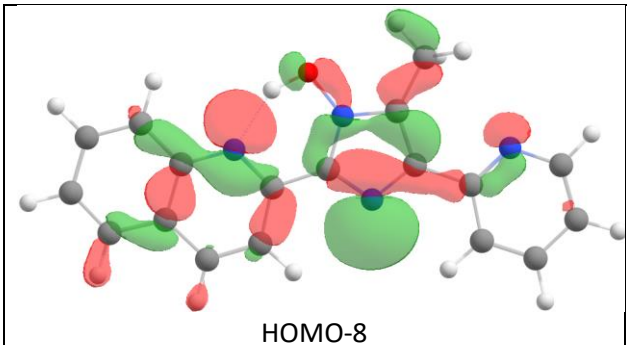


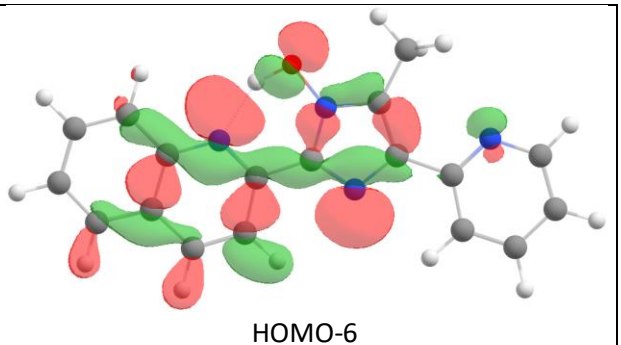
Figure S23. Absorption spectrum of **[Zn(HL^{q})I$_2$]** (black). Vertical bars display the positions and oscillator strengths of the electronic transitions from the global energy minima of the normal (red) and tautomeric (blue) forms.

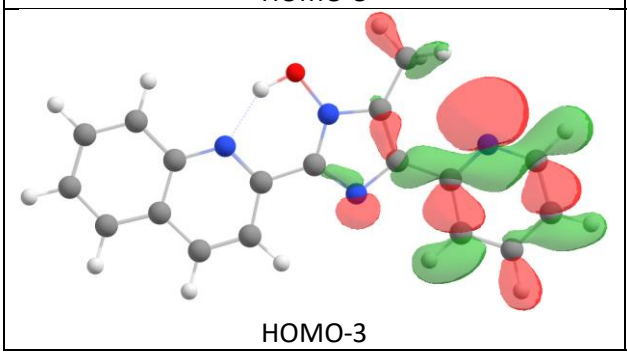
Table S12. Excited state properties of **HL^q** at the relaxed ground state geometry (**normal form**, **S_0^N**) as calculated in Gaussian at the BMK/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**. Transitions with contribution >10% are shown.

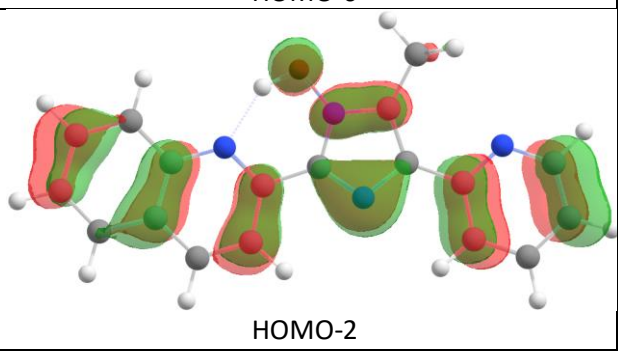
State	Energy (eV)	Energy (nm)	Contributions (%)	Oscillator strength	Character
S1	3.6641	338	HOMO -> LUMO (94.0 %)	0.8688	π – π*
S2	4.3675	284	HOMO-1 -> LUMO (19.2 %) HOMO -> LUMO+1 (61.5 %)	0.1871	π – π*
S3	4.5642	272	HOMO-1 -> LUMO (53.7 %) HOMO -> LUMO+1 (16.5 %) HOMO -> LUMO+2 (23.5 %)	0.2785	π – π*
S4	4.7372	262	HOMO-1 -> LUMO (17.9 %) HOMO -> LUMO+2 (56.1 %)	0.0826	π – π*
S5	4.9129	252	HOMO-2 -> LUMO (54.5 %) HOMO-1 -> LUMO+1 (10.4 %) HOMO -> LUMO+1 (11.8 %)	0.0798	π – π*
S6	4.9222	252	HOMO-8 -> LUMO (11.6 %) HOMO-6 -> LUMO (79.9 %)	0.0028	σ – π* + n – π*
S7	4.9902	248	HOMO-3 -> LUMO+1 (16.8 %) HOMO-3 -> LUMO+2 (67.8 %)	0.0033	σ – π* + n – π*
S8	5.0839	244	HOMO -> LUMO+3 (68.1 %)	0.2217	π – π*

Table S13. Isosurface contour plots of the molecular orbitals of **HL^q** at the relaxed ground state geometry (**normal form**, **S_0^N**) as calculated in Gaussian at the BMK/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.


HOMO-8


HOMO-6


HOMO-3


HOMO-2

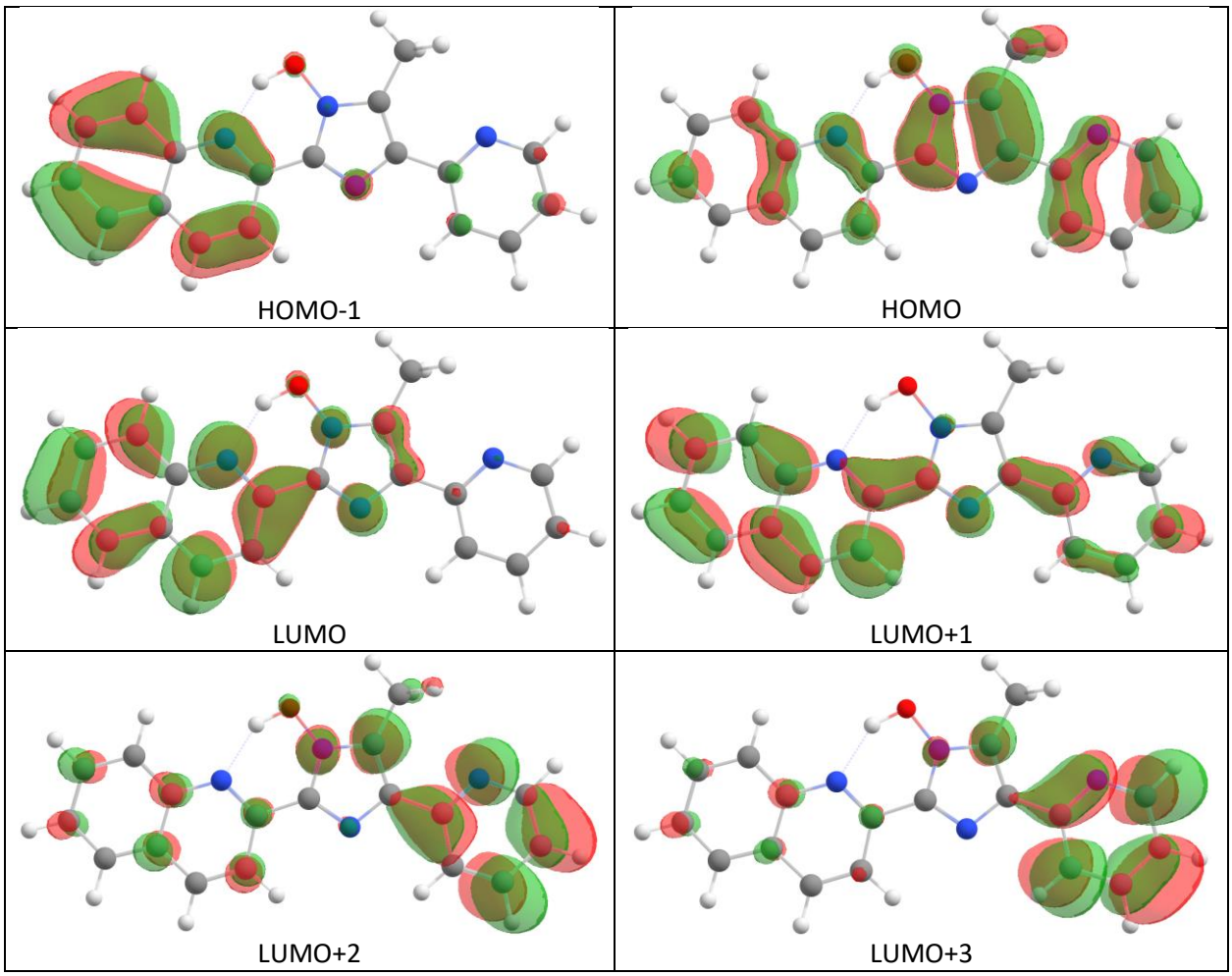


Table S14. Excited state properties of **HL^{q}** at the relaxed ground state geometry (**tautomeric form**, **S_0^T**) as calculated in Gaussian at the BMK/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**. Transitions with contribution >10% are shown.

State	Energy (eV)	Energy (nm)	Contributions (%)	Oscillator strength	Character
S1	2.9911	415	HOMO -> LUMO (96.7 %)	0.7768	π – π*
S2	3.5853	346	HOMO-1 -> LUMO (97.0 %)	0.3275	π – π*
S3	4.0709	305	HOMO -> LUMO+1 (92.8 %)	0.2227	π – π*
S4	4.1898	296	HOMO-5 -> LUMO (19.5 %) HOMO-3 -> LUMO (72.6 %)	0.0002	σ – π* + n – π*
S5	4.4327	280	HOMO-2 -> LUMO (86.9 %)	0.1490	π – π*
S6	4.6502	267	HOMO -> LUMO+2 (82.8 %)	0.1455	π – π*
S7	4.7215	263	HOMO-4 -> LUMO (26.6 %) HOMO-1 -> LUMO+1 (51.0 %)	0.0284	π – π*
S8	4.7915	259	HOMO-5 -> LUMO (40.8 %) HOMO-5 -> LUMO+2 (21.5 %) HOMO-3 -> LUMO+2 (13.3 %)	0.0017	σ – π* + n – π*

Table S15. Isosurface contour plots of the molecular orbitals of **HL^{q}** at the relaxed ground state geometry (**tautomeric form**, **S_0^T**) as calculated in Gaussian at the BMK/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.

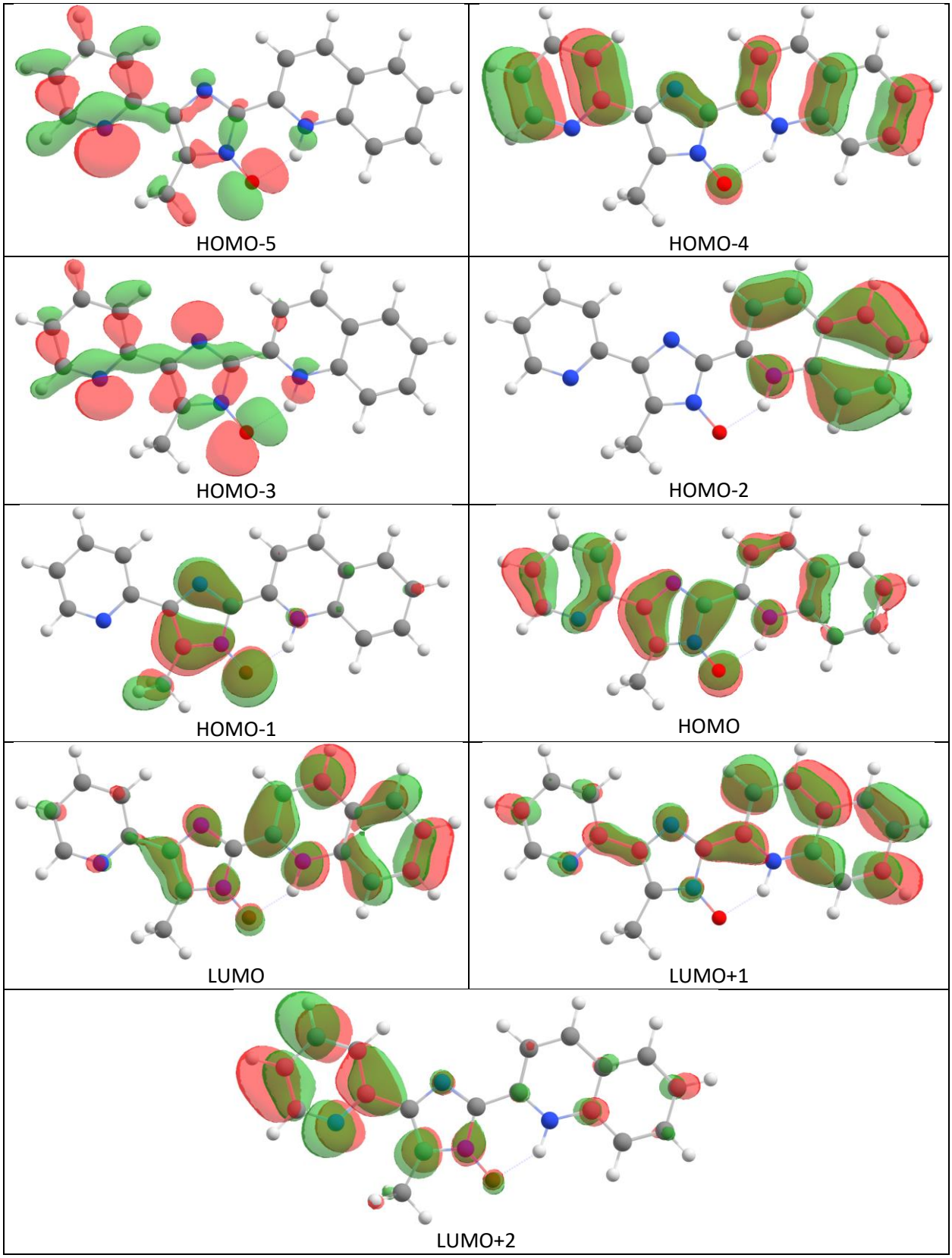
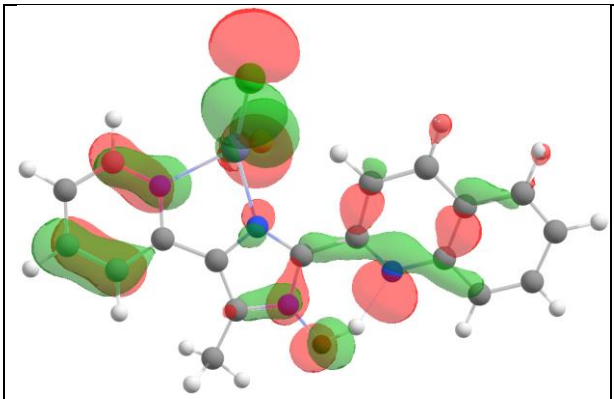


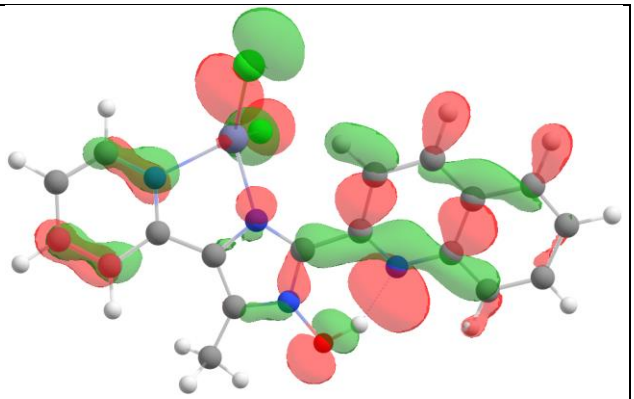
Table S16. Excited state properties of **[Zn(HL^{q})Cl$_2$]** at the relaxed ground state geometry (**normal form**, **S$_0^N$**) as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**. Transitions with contribution >10% are shown.

State	Energy (eV)	Energy (nm)	Contributions (%)	Oscillator strength	Character
S1	3.8624	321	HOMO -> LUMO (92.7 %)	0.9831	π – π*
S2	4.3060	288	HOMO-1 -> LUMO (72.7 %)	0.0440	π – π*
S3	4.4719	277	HOMO-1 -> LUMO (12.1 %) HOMO -> LUMO+1 (72.4 %)	0.1138	π – π*
S4	4.8946	253	HOMO-8 -> LUMO (10.3 %) HOMO -> LUMO+2 (38.1 %)	0.2422	π – π*
S5	4.9010	253	HOMO-9 -> LUMO (19.7 %) HOMO-8 -> LUMO (50.9 %)	0.0414	XLCT + σ – π* + n – π*
S6	5.0474	246	HOMO -> LUMO+2 (16.9 %) HOMO -> LUMO+3 (56.3 %)	0.0696	π – π*
S7	5.2185	238	HOMO-2 -> LUMO (40.6 %) HOMO -> LUMO+2 (16.4 %) HOMO -> LUMO+3 (24.3 %)	0.0764	π – π*
S8	5.4368	228	HOMO-4 -> LUMO (15.6 %) HOMO-2 -> LUMO (14.9 %) HOMO-1 -> LUMO+1 (15.2 %)	0.2606	XLCT + π – π*

Table S17. Isosurface contour plots of the molecular orbitals of **[Zn(HL^{q})Cl$_2$]** at the relaxed ground state geometry (**normal form**, **S$_0^N$**) as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.



HOMO-9



HOMO-8

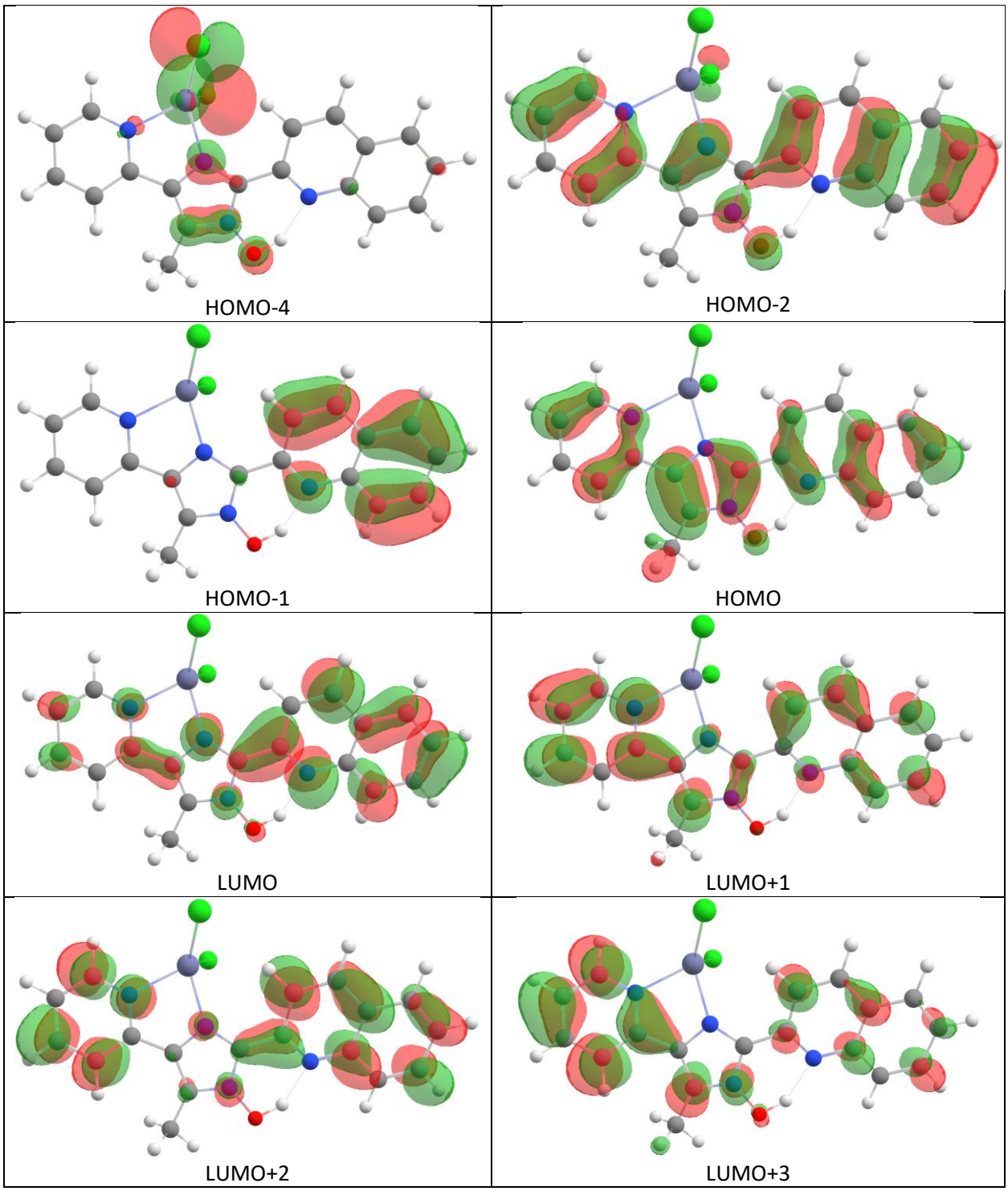
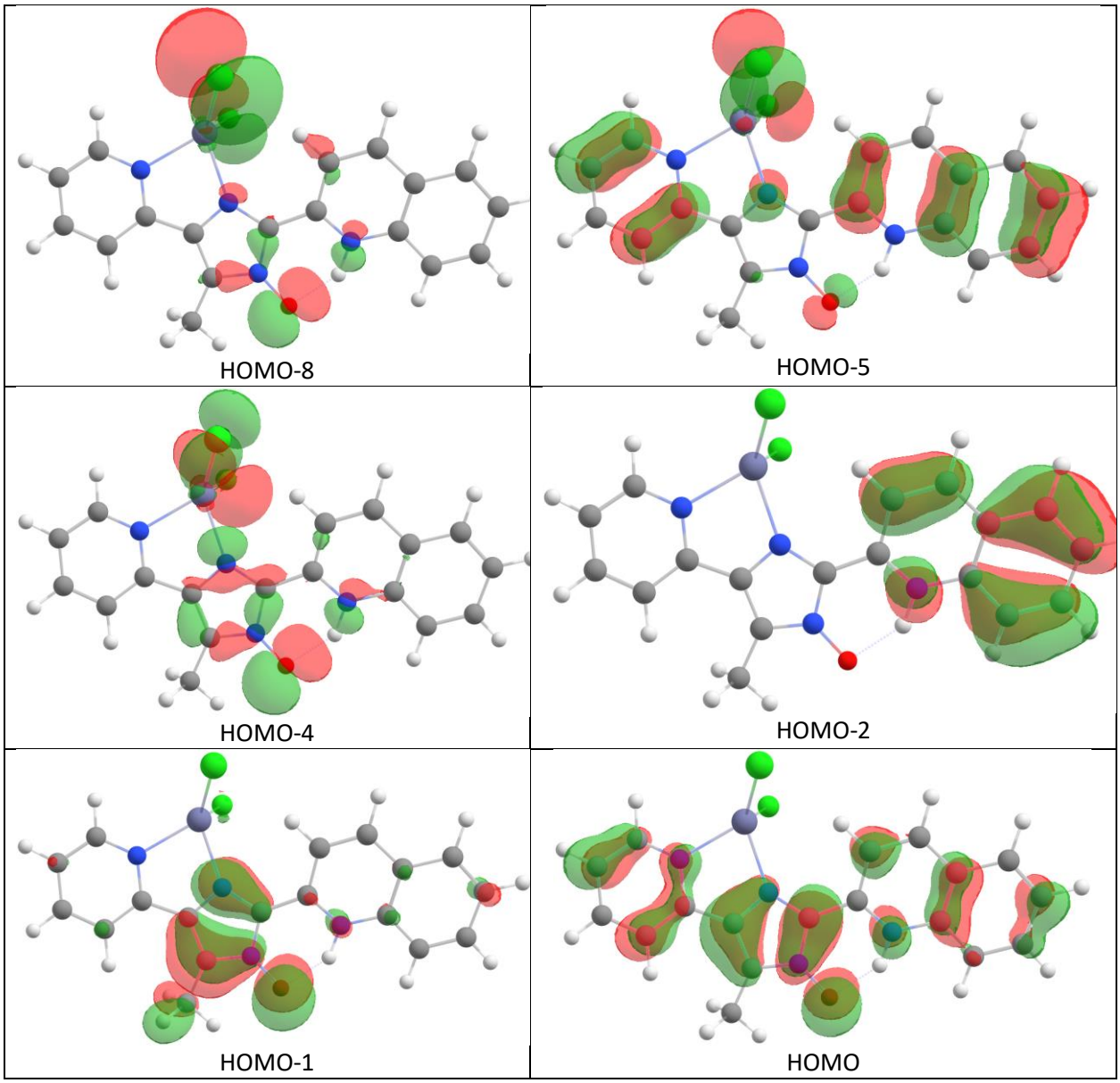


Table S18. Excited state properties of **[Zn(HL^{q})Cl$_2$]** at the relaxed ground state geometry (**tautomeric form**, **S$_0^T$**) as calculated in Gaussian at the BMK/LANL2DZ /6-31+g(d) level of theory **in CH$_2$Cl$_2$ continuum solvation model**. Transitions with contribution >10% are shown.

State	Energy (eV)	Energy (nm)	Contributions (%)	Oscillator strength	Character
S1	3.1540	393	HOMO -> LUMO (97.1 %)	0.7769	π – π*
S2	3.7805	328	HOMO-1 -> LUMO (96.8 %)	0.3242	π – π*
S3	4.1577	298	HOMO-2 -> LUMO (42.9 %) HOMO -> LUMO+1 (51.8 %)	0.0565	π – π*

S4	4.2504	292	HOMO-2 -> LUMO (48.4 %) HOMO -> LUMO+1 (41.7 %)	0.1319	π – π*
S5	4.3662	284	HOMO-8 -> LUMO (16.1 %) HOMO-4 -> LUMO (58.8 %)	0.0006	XLCT + σ – π* + n – π*
S6	4.6883	264	HOMO -> LUMO+2 (80.0 %)	0.1754	π – π*
S7	4.7520	261	HOMO-5 -> LUMO (22.1 %) HOMO-1 -> LUMO+1 (37.1 %)	0.0146	XLCT + π – π*
S8	4.9589	250	HOMO-5 -> LUMO (11.3 %) HOMO -> LUMO+3 (54.2 %)	0.1150	π – π*

Table S19. Isosurface contour plots of the molecular orbitals of **[Zn(HL^{q})Cl$_2$]** at the relaxed ground state geometry (**tautomeric form**, **S$_0^T$**) as calculated in Gaussian at the BMK/LANL2DZ /6-31+g(d) level of theory **in CH$_2$Cl$_2$ continuum solvation model**.



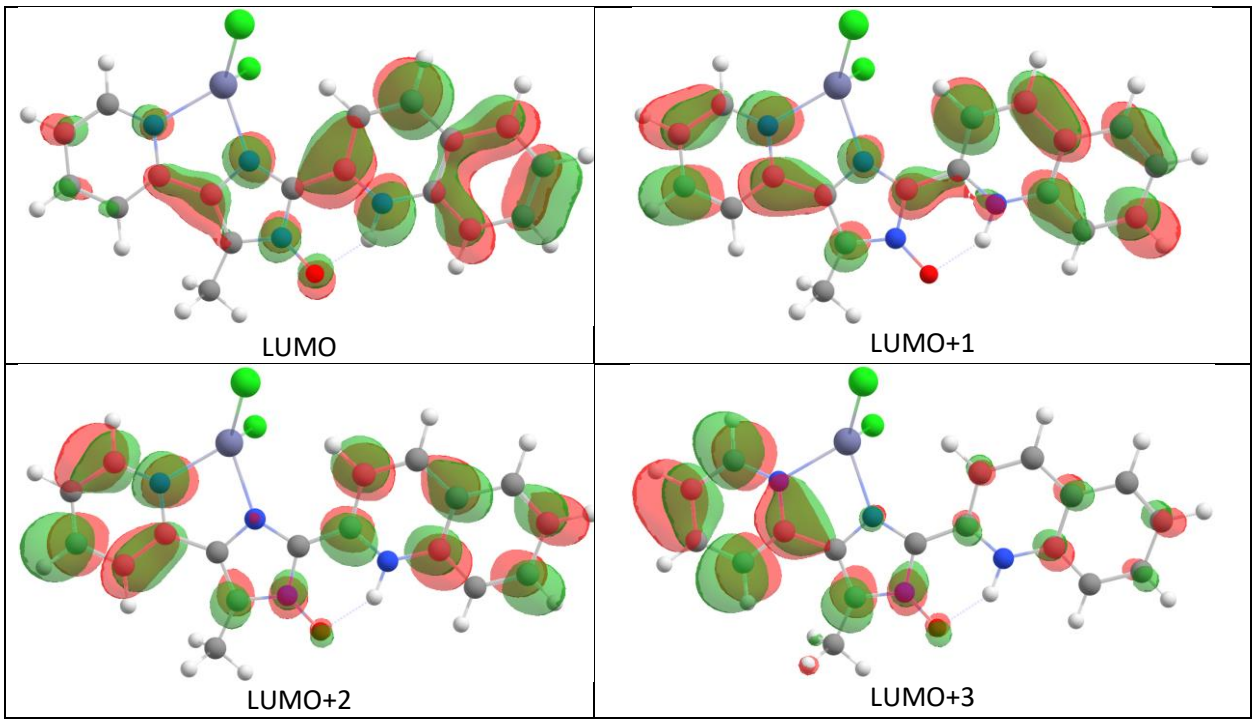
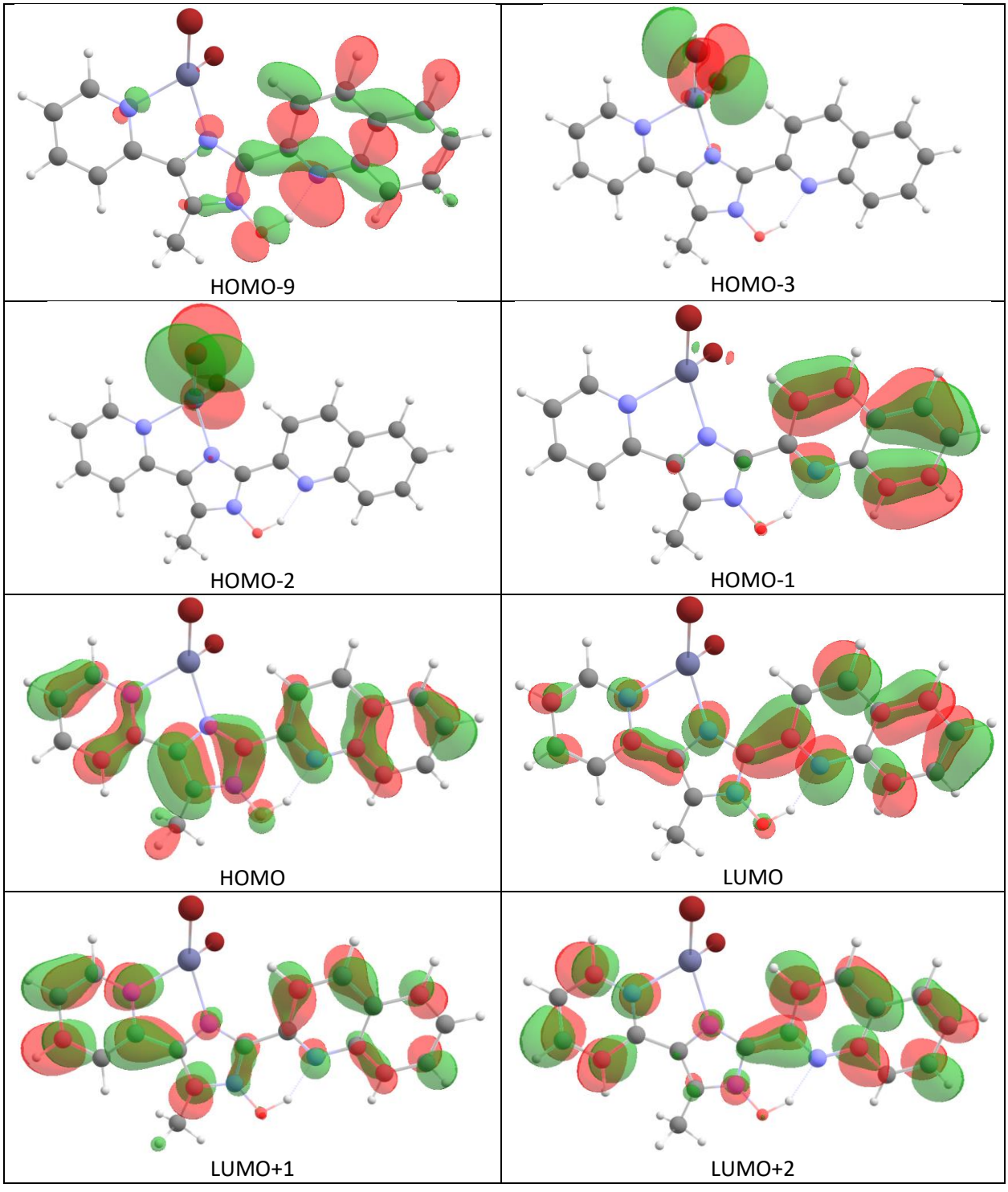
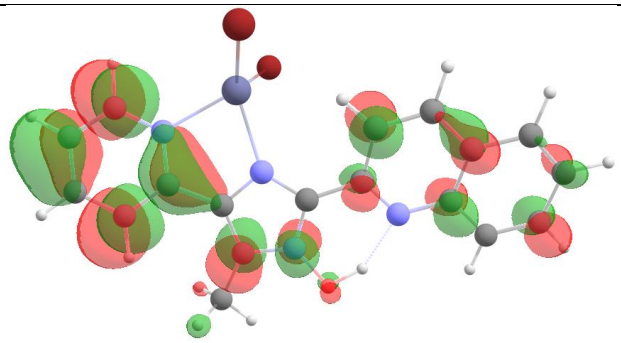


Table S20. Excited state properties of **[Zn(HL^{q})Br$_2$]** at the relaxed ground state geometry (**normal form**, **S$_0^N$**) as calculated in Gaussian at the BMK/LANL2DZ /6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**. Transitions with contribution >10% are shown.

State	Energy (eV)	Energy (nm)	Contributions (%)	Oscillator strength	Character
S1	3.8557	322	HOMO -> LUMO (92.8 %)	0.9739	π – π*
S2	4.3022	288	HOMO-1 -> LUMO (72.3 %)	0.0426	π – π*
S3	4.4694	277	HOMO-1 -> LUMO (12.1 %) HOMO -> LUMO+1 (72.0 %)	0.1072	π – π*
S4	4.8873	254	HOMO-9 -> LUMO (47.0 %) HOMO -> LUMO+2 (18.5 %)	0.1114	σ – π* + n – π* + π – π*
S5	4.8966	253	HOMO-9 -> LUMO (32.9 %) HOMO -> LUMO+2 (25.3 %)	0.1691	σ – π* + n – π* + π – π*
S6	5.0369	246	HOMO -> LUMO+2 (16.4 %) HOMO -> LUMO+3 (51.2 %)	0.0566	π – π*
S7	5.0624	245	HOMO-2 -> LUMO (88.9 %)	0.0026	XLCT
S8	5.1305	242	HOMO-3 -> LUMO (73.8 %)	0.0186	XLCT

Table S21. Isosurface contour plots of the molecular orbitals of **[Zn(HL^{q})Br$_2$]** at the relaxed ground state geometry (**normal form**, **S$_0^N$**) as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.



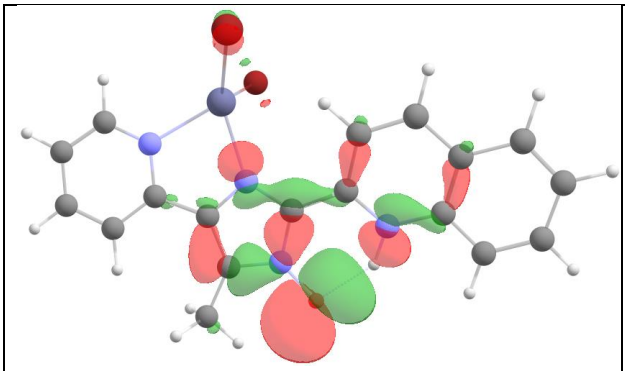


LUMO+3

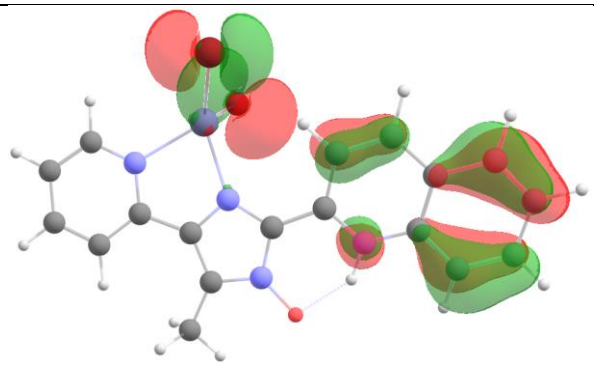
Table S22. Excited state properties of **[Zn(HL^{q})Br$_2$]** at the relaxed ground state geometry (**tautomeric form**, **S$_0^T$**) as calculated in Gaussian at the BMK/LANL2DZ /6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**. Transitions with contribution >10% are shown.

State	Energy (eV)	Energy (nm)	Contributions (%)	Oscillator strength	Character
S1	3.1451	394	HOMO -> LUMO (97.1 %)	0.7628	π – π*
S2	3.7666	329	HOMO-1 -> LUMO (96.6 %)	0.3226	π – π*
S3	4.1516	298	HOMO-4 -> LUMO (17.7 %) HOMO-3 -> LUMO (25.3 %) HOMO -> LUMO+1 (50.4 %)	0.0512	π – π* + XLCT
S4	4.2435	292	HOMO-4 -> LUMO (17.4 %) HOMO-3 -> LUMO (27.8 %) HOMO -> LUMO+1 (43.0 %)	0.1248	π – π* + XLCT
S5	4.3524	285	HOMO-8 -> LUMO (78.1 %)	0.0006	σ – π* + n – π*
S6	4.5398	273	HOMO-2 -> LUMO (98.7 %)	0.0004	XLCT
S7	4.6451	267	HOMO-4 -> LUMO (49.5 %) HOMO-3 -> LUMO (41.0 %)	0.0002	π – π* + XLCT
S8	4.6832	265	HOMO -> LUMO+2 (80.0 %)	0.1689	π – π*

Table S23. Isosurface contour plots of the molecular orbitals of **[Zn(HL^{q})Br$_2$]** at the relaxed ground state geometry (**tautomeric form**, **S$_0^T$**) as calculated in Gaussian at the BMK/LANL2DZ /6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.



HOMO-8



HOMO-4

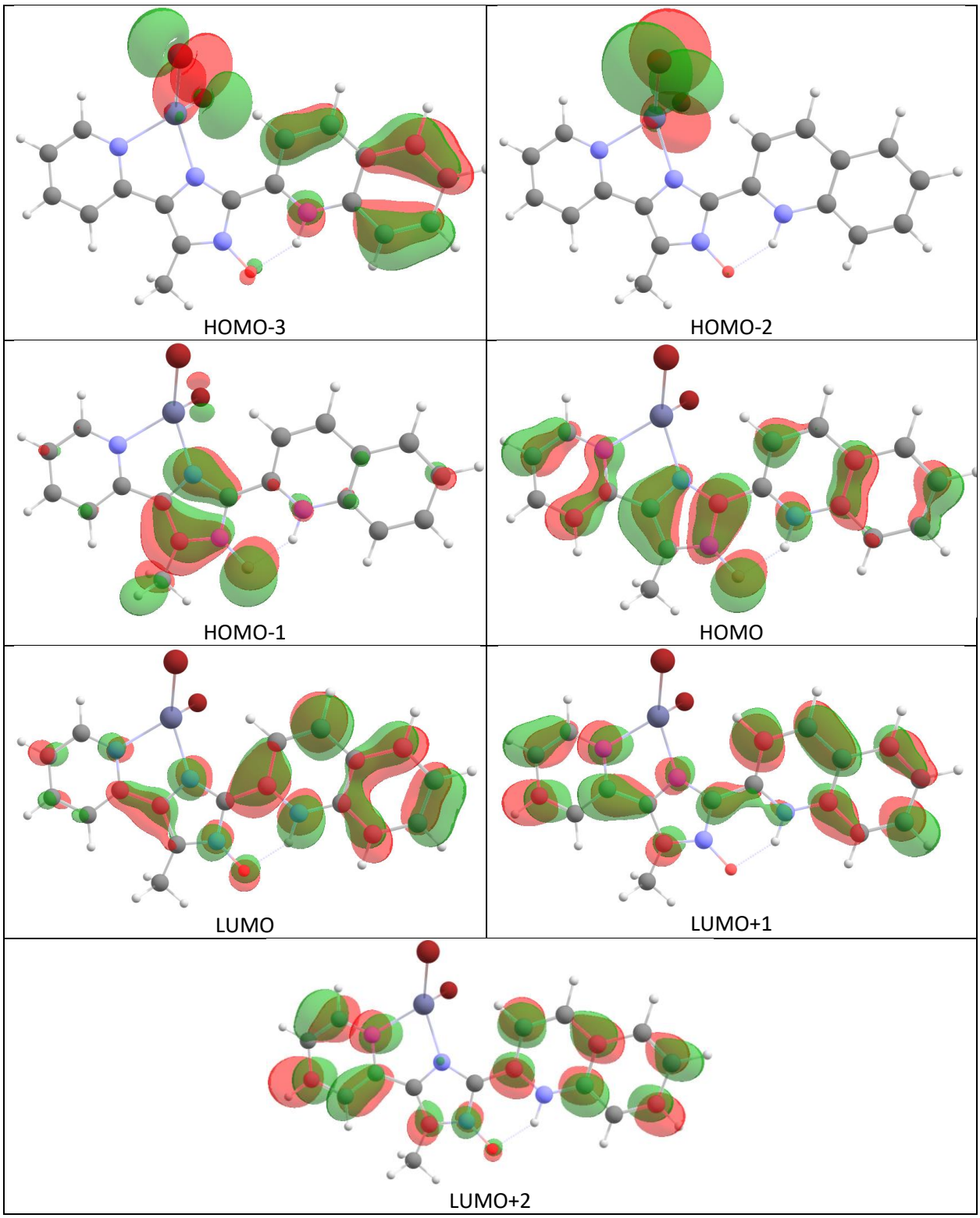
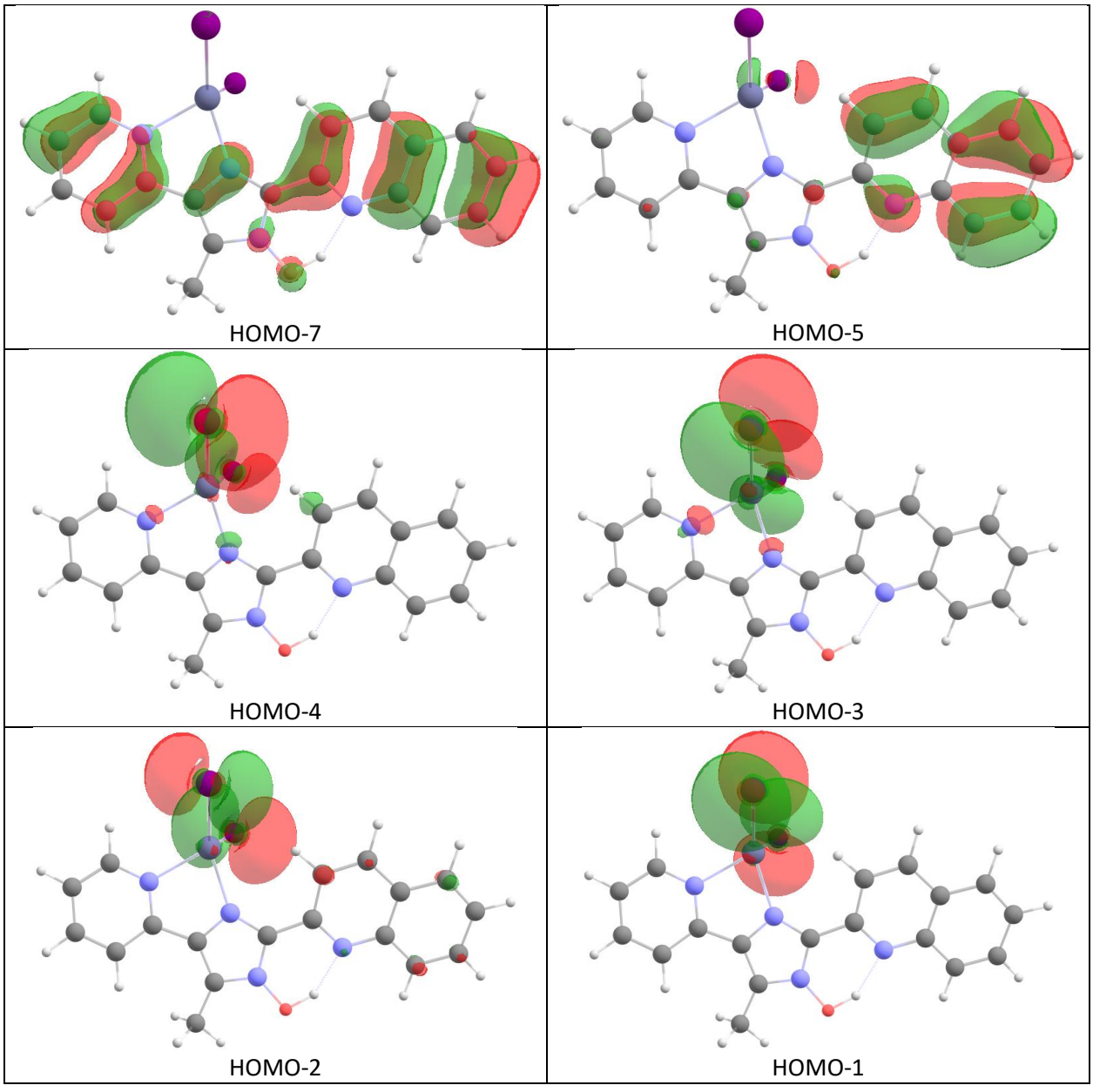


Table S24. Excited state properties of **[Zn(HL^{q})I$_2$]** at the relaxed ground state geometry (**normal form**, **S$_0^N$**) as calculated in Gaussian at the BMK/LANL2DZ /6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**. Transitions with contribution >10% are shown.

State	Energy (eV)	Energy (nm)	Contributions (%)	Oscillator strength	Character
S1	3.8467	322	HOMO -> LUMO (92.8 %)	0.9484	π – π*
S2	4.2879	289	HOMO-5 -> LUMO (58.1 %)	0.0377	π – π* + XLCT

			HOMO-2 -> LUMO (14.8 %)		
S3	4.4466	279	HOMO-1 -> LUMO (84.3 %)	0.0124	XLCT
S4	4.4690	277	HOMO-1 -> LUMO (10.4 %) HOMO -> LUMO+1 (65.2 %)	0.0845	π – π*
S5	4.5310	274	HOMO-5 -> LUMO (19.1 %) HOMO-2 -> LUMO (73.7 %)	0.0084	XLCT + π – π*
S6	4.6624	266	HOMO-3 -> LUMO (89.8 %)	0.0040	XLCT
S7	4.6866	265	HOMO-4 -> LUMO (89.8 %)	0.0000	XLCT
S8	4.8834	254	HOMO-7 -> LUMO (9.9 %) HOMO-5 -> LUMO+1 (10.1 %) HOMO -> LUMO+2 (44.0 %)	0.2375	π – π*

Table S25. Isosurface contour plots of the molecular orbitals of **[Zn(HL^{q})I$_2$]** at the relaxed ground state geometry (**normal form**, **S$_0^N$**) as calculated in Gaussian at the BMK/LANL2DZ /6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.



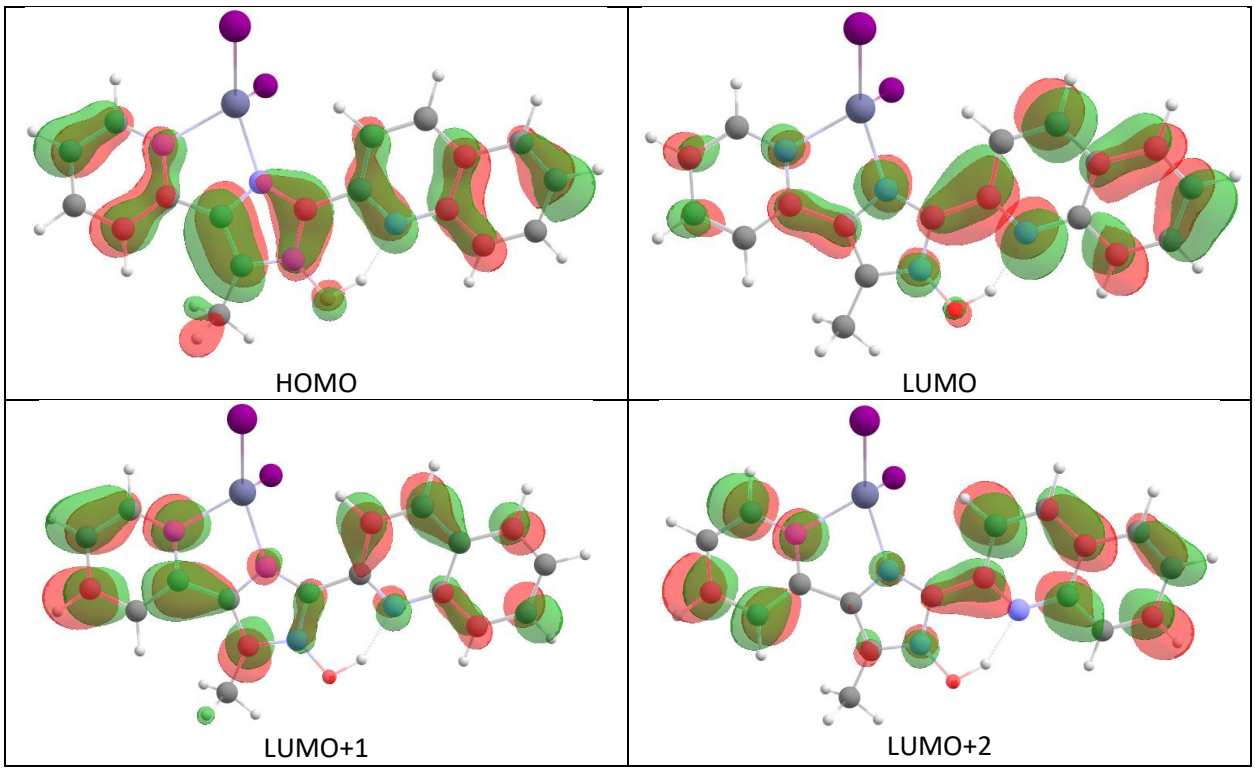
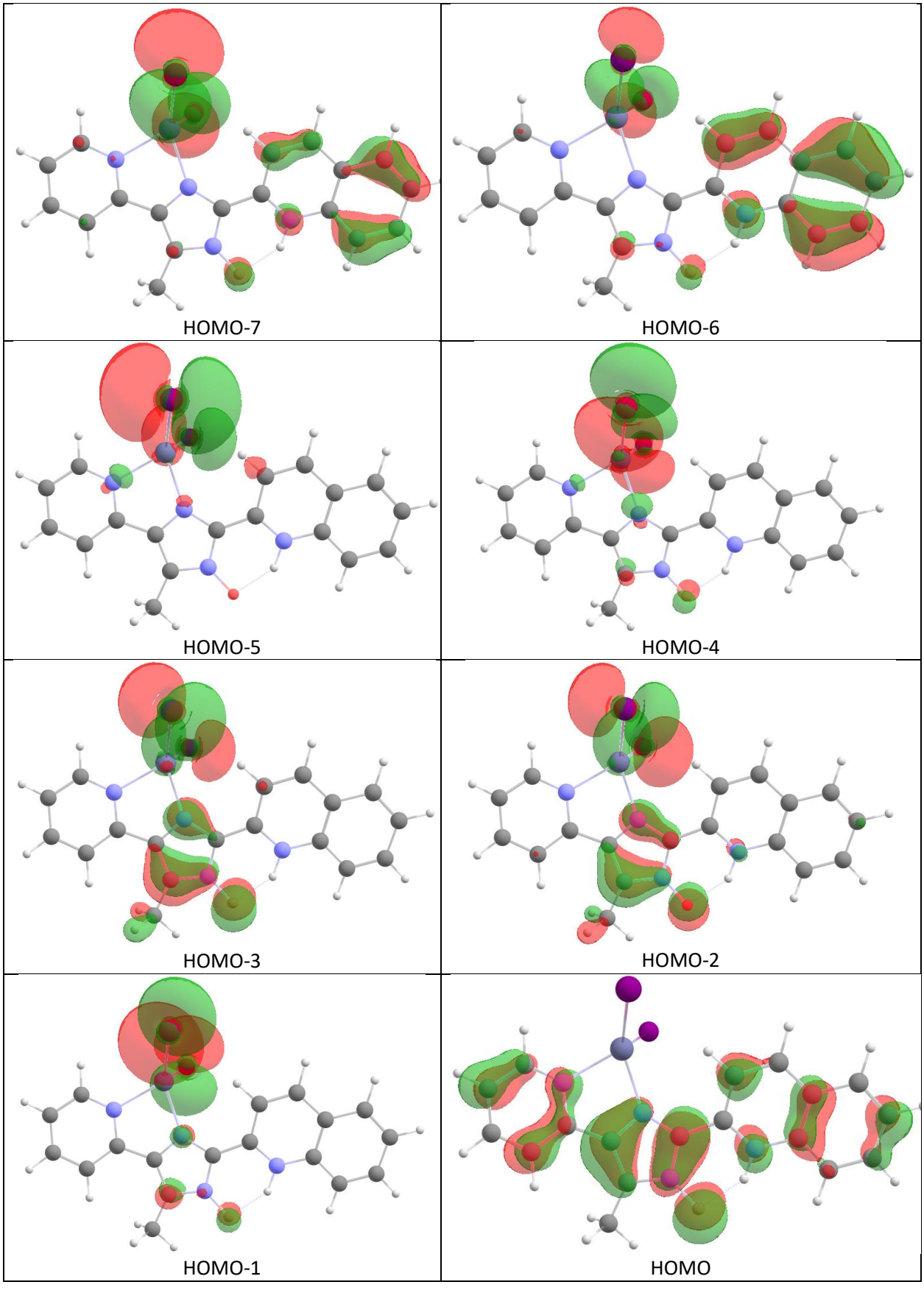


Table S26. Excited state properties of **[Zn(HL^{q})I$_2$]** at the relaxed ground state geometry (**tautomeric form**, **S$_0^T$**) as calculated in Gaussian at the BMK/LANL2DZ /6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**. Transitions with contribution >10% are shown.

State	Energy (eV)	Energy (nm)	Contributions (%)	Oscillator strength	Character
S1	3.1443	394	HOMO -> LUMO (97.1 %)	0.7402	π – π*
S2	3.7375	332	HOMO-3 -> LUMO (31.1 %) HOMO-2 -> LUMO (43.2 %) HOMO-1 -> LUMO (20.4 %)	0.2905	π – π* + XLCT
S3	3.9405	315	HOMO-2 -> LUMO (18.9 %) HOMO-1 -> LUMO (76.7 %)	0.0098	XLCT
S4	4.0234	308	HOMO-3 -> LUMO (53.5 %) HOMO-2 -> LUMO (34.8 %)	0.0072	XLCT + π – π*
S5	4.1157	301	HOMO-5 -> LUMO (18.8 %) HOMO-4 -> LUMO (68.5 %)	0.0036	XLCT
S6	4.1538	298	HOMO-5 -> LUMO (53.9 %) HOMO-4 -> LUMO (10.0 %) HOMO -> LUMO+1 (18.6 %)	0.0171	XLCT + π – π*
S7	4.1638	298	HOMO-6 -> LUMO (14.5 %) HOMO-5 -> LUMO (25.1 %) HOMO -> LUMO+1 (38.0 %)	0.0401	XLCT + π – π*
S8	4.2508	292	HOMO-7 -> LUMO (11.7 %) HOMO-6 -> LUMO (41.5 %) HOMO -> LUMO+1 (35.6 %)	0.1088	XLCT + π – π*

Table S27. Isosurface contour plots of the molecular orbitals of **[Zn(HL^{q})I$_2$]** at the relaxed ground state geometry (**tautomeric form**, **S$_0^T$**) as calculated in Gaussian at the BMK/LANL2DZ /6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.



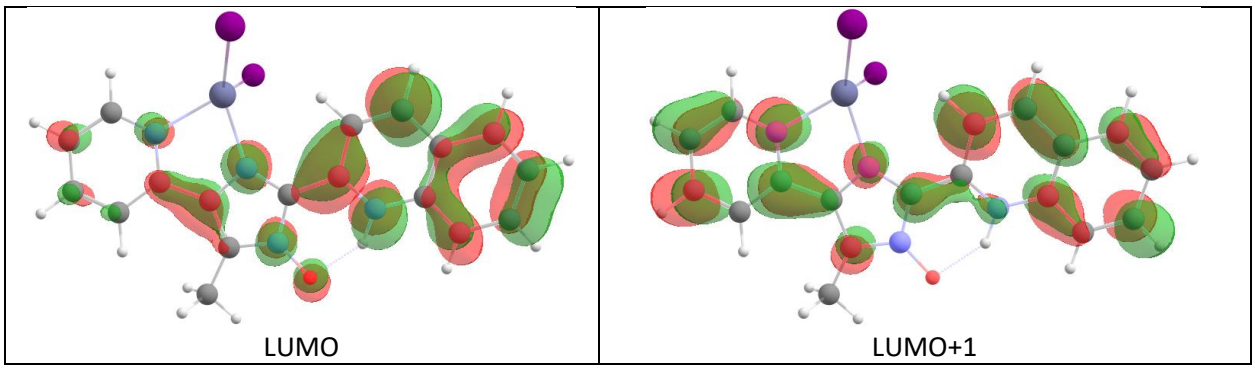


Table S28. Isosurface contour plots of the molecular orbitals of **HL^q** at the relaxed **first singlet excited state** geometry (**normal form**, **S_1^N**) as calculated in Gaussian at the BMK/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.

$S_1^N \rightarrow S_0^N$ is LUMO → HOMO transition (95.9%), λ = 399 nm, f = 1.1385

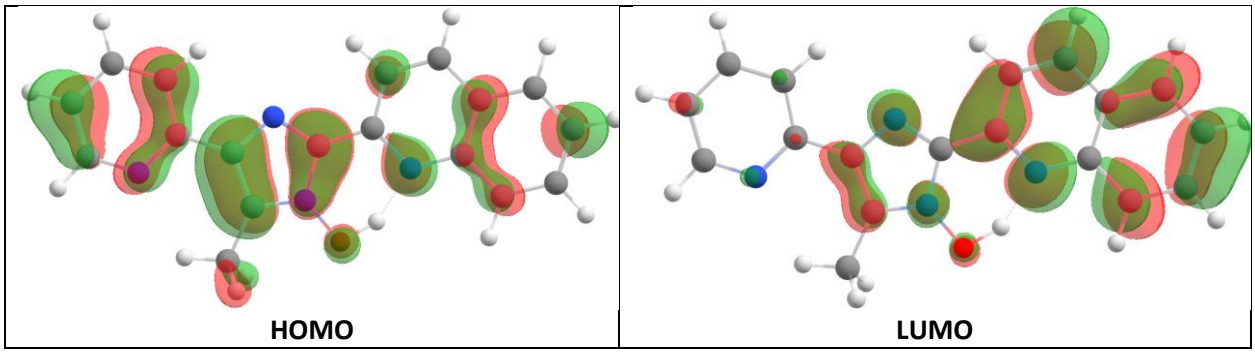


Table S29. Isosurface contour plots of the molecular orbitals of **[$Zn(HL^q)Cl_2$]** at the relaxed **first singlet excited state** geometry (**normal form**, **S_1^N**) as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.

$S_1^N \rightarrow S_0^N$ is LUMO → HOMO transition (96.6%), λ = 387 nm, f = 1.3890

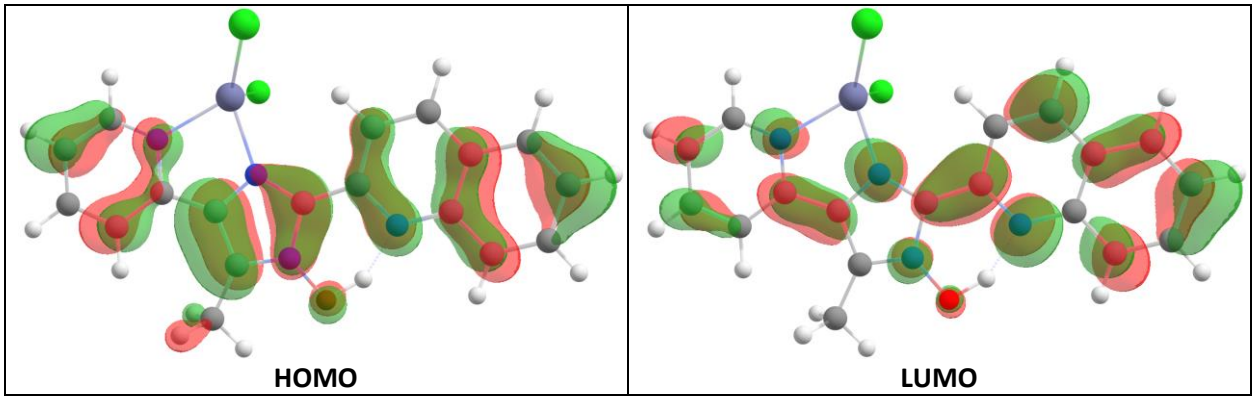


Table S30. Isosurface contour plots of the molecular orbitals of **[$Zn(HL^q)Br_2$]** at the relaxed **first singlet excited state** geometry (**normal form**, **S_1^N**) as calculated in Gaussian at the BMK/LANL2DZ /6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.

$S_1^N \rightarrow S_0^N$ is LUMO → HOMO transition (96.6%), λ = 387 nm, f = 1.3714

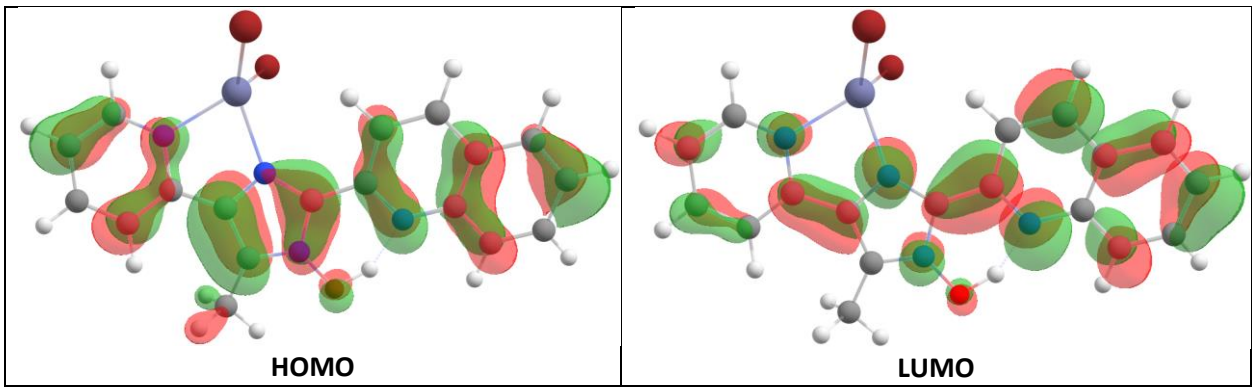


Table S31. Isosurface contour plots of the molecular orbitals of **[Zn(HL^{q})I$_2$]** at the relaxed **first singlet excited state** geometry (**normal form**, **S$_1^N$**) as calculated in Gaussian at the BMK/LANL2DZ /6-31+g(d) level of theory **in CH$_2$Cl$_2$ continuum solvation model**.

S$_1^N$ → S$_0^N$ is LUMO → HOMO transition (96.6%), λ = 387 nm, f = 1.3540

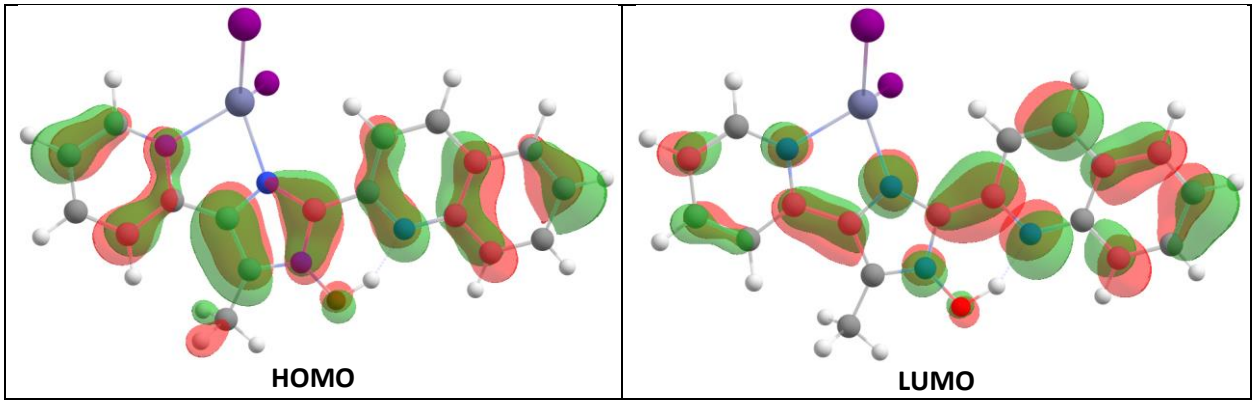


Table S32. Isosurface contour plots of the molecular orbitals of **HL^{q}** at the relaxed **first singlet excited state** geometry (**tautomeric form**, **S$_1^T$**) as calculated in Gaussian at the BMK/6-31+g(d) level of theory **in CH$_2$Cl$_2$ continuum solvation model**.

S$_1^T$ → S$_0^T$ is LUMO → HOMO transition (98.2%), λ = 522 nm, f = 0.5597

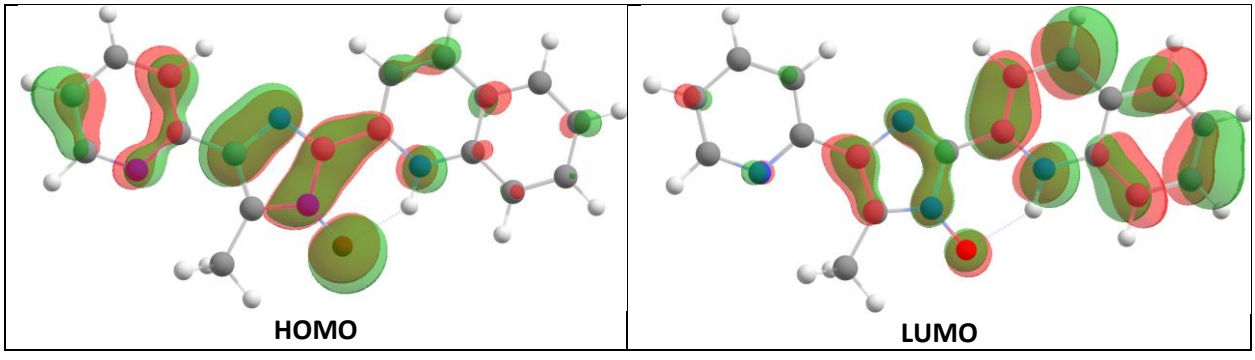


Table S33. Isosurface contour plots of the molecular orbitals of **[Zn(HL^{q})Cl$_2$]** at the relaxed **first singlet excited state** geometry (**tautomeric form**, **S$_1^T$**) as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **in CH$_2$Cl$_2$ continuum solvation model**.

S$_1^T$ → S$_0^T$ is LUMO → HOMO transition (98.0%), λ = 576 nm, f = 0.2749

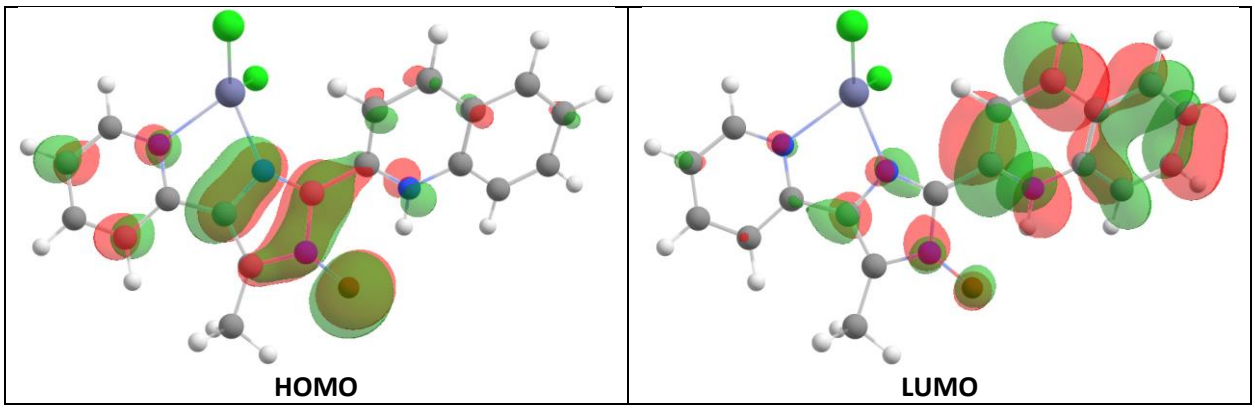


Table S34. Isosurface contour plots of the molecular orbitals of **[Zn(HL^{q})Br$_2$]** at the relaxed **first singlet excited state** geometry (**tautomeric form**, **S_1^T**) as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.

$S_1^T \rightarrow S_0^T$ is LUMO → HOMO transition (98.0%), λ = 587 nm, f = 0.2443

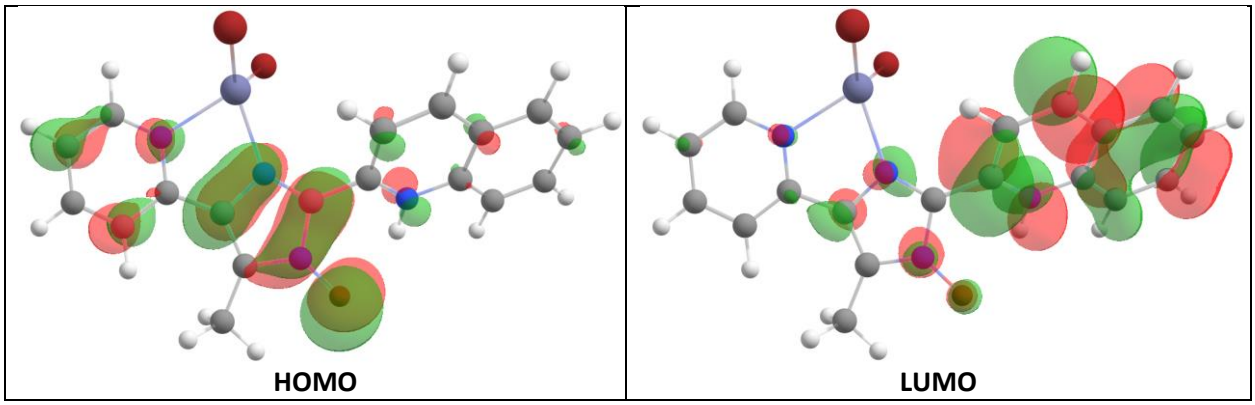


Table S35. Isosurface contour plots of the molecular orbitals of **[Zn(HL^{q})I$_2$]** at the relaxed **first singlet excited state** geometry (**tautomeric form**, **S_1^T**) as calculated in Gaussian at the BMK/LANL2DZ /6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.

$S_1^T \rightarrow S_0^T$ is LUMO → HOMO transition (98.0%), λ = 568 nm, f = 0.2786

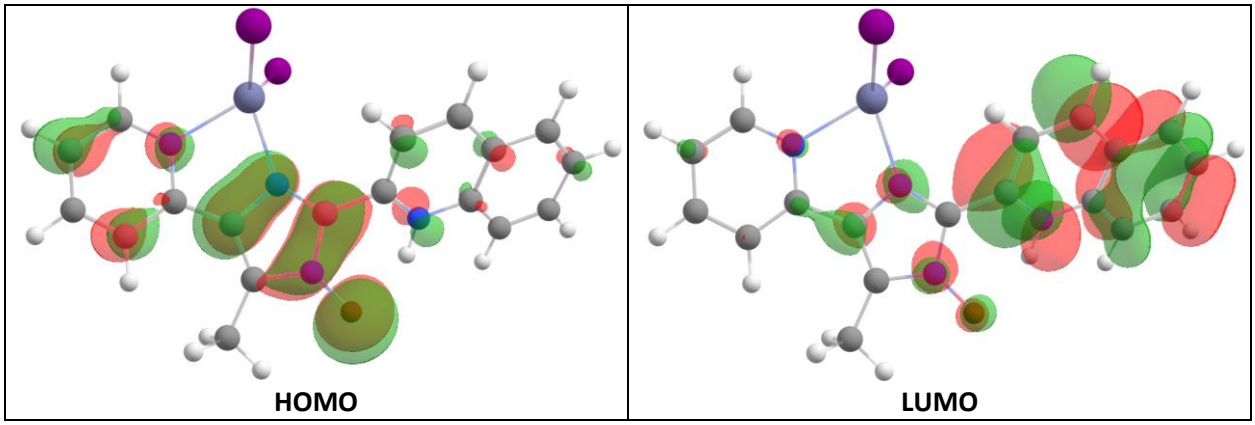
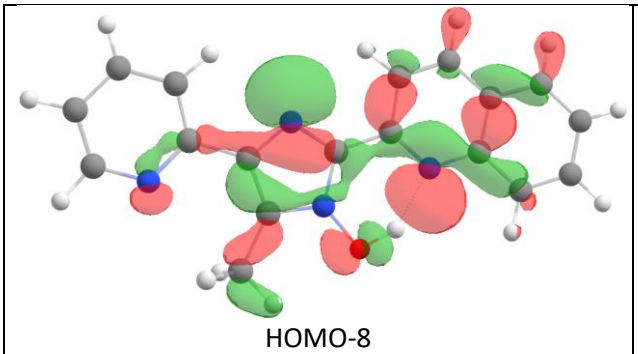
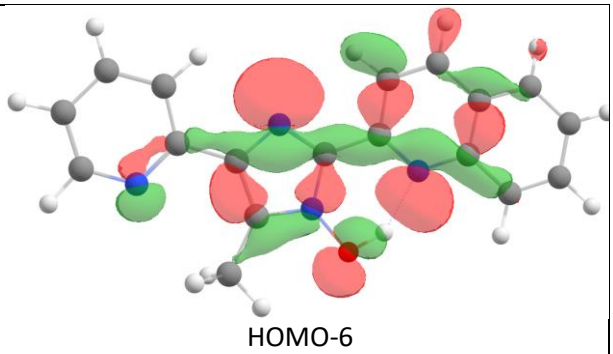


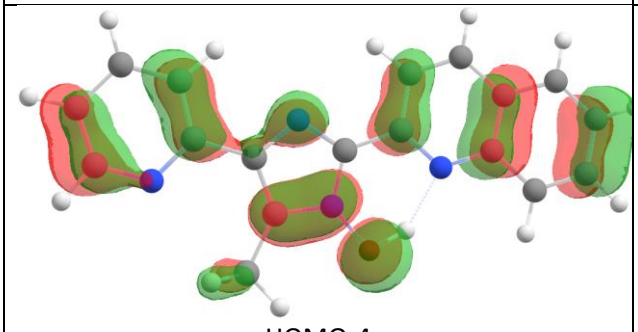
Table S36. Excited state properties of **HL^q** at the relaxed ground state geometry (**normal form**, **S_0^N**) as calculated in Gaussian at the BMK/6-31+g(d) level of theory **using the QM/MM method**. Transitions with contribution >10% are shown.

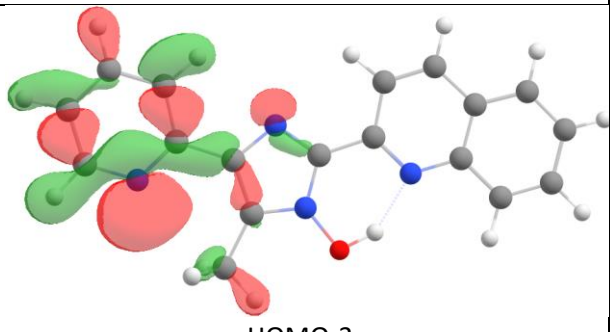
State	Energy (eV)	Energy (nm)	Contributions (%)	Oscillator strength	Character
S1	3.5883	345	HOMO -> LUMO (95.5 %)	0.6410	π – π*
S2	4.3080	288	HOMO-2 -> LUMO (12.0 %) HOMO -> LUMO+1 (78.9 %)	0.2591	π – π*
S3	4.6518	267	HOMO-2 -> LUMO (33.1 %) HOMO-1 -> LUMO (25.8 %) HOMO -> LUMO+2 (29.6 %)	0.2059	π – π*
S4	4.7614	260	HOMO-1 -> LUMO (36.9 %) HOMO -> LUMO+2 (39.5 %)	0.0872	π – π*
S5	4.8117	258	HOMO-2 -> LUMO (37.4 %) HOMO-1 -> LUMO (21.7 %) HOMO -> LUMO+1 (10.1 %) HOMO -> LUMO+2 (10.8 %)	0.0912	π – π*
S6	4.8894	254	HOMO-8 -> LUMO (21.6 %) HOMO-6 -> LUMO (66.9 %)	0.0022	σ – π* + n – π*
S7	4.9509	250	HOMO-3 -> LUMO+1 (10.1 %) HOMO-3 -> LUMO+2 (70.7 %)	0.0020	σ – π* + n – π*
S8	5.0927	243	HOMO-4 -> LUMO (20.9 %) HOMO -> LUMO+3 (41.2 %)	0.1139	π – π*

Table S37. Isosurface contour plots of the molecular orbitals of **HL^q** at the relaxed ground state geometry (**normal form**, **S_0^N**) as calculated in Gaussian at the BMK/6-31+g(d) level of theory **using the QM/MM method (QM region)**.


HOMO-8


HOMO-6


HOMO-4


HOMO-3

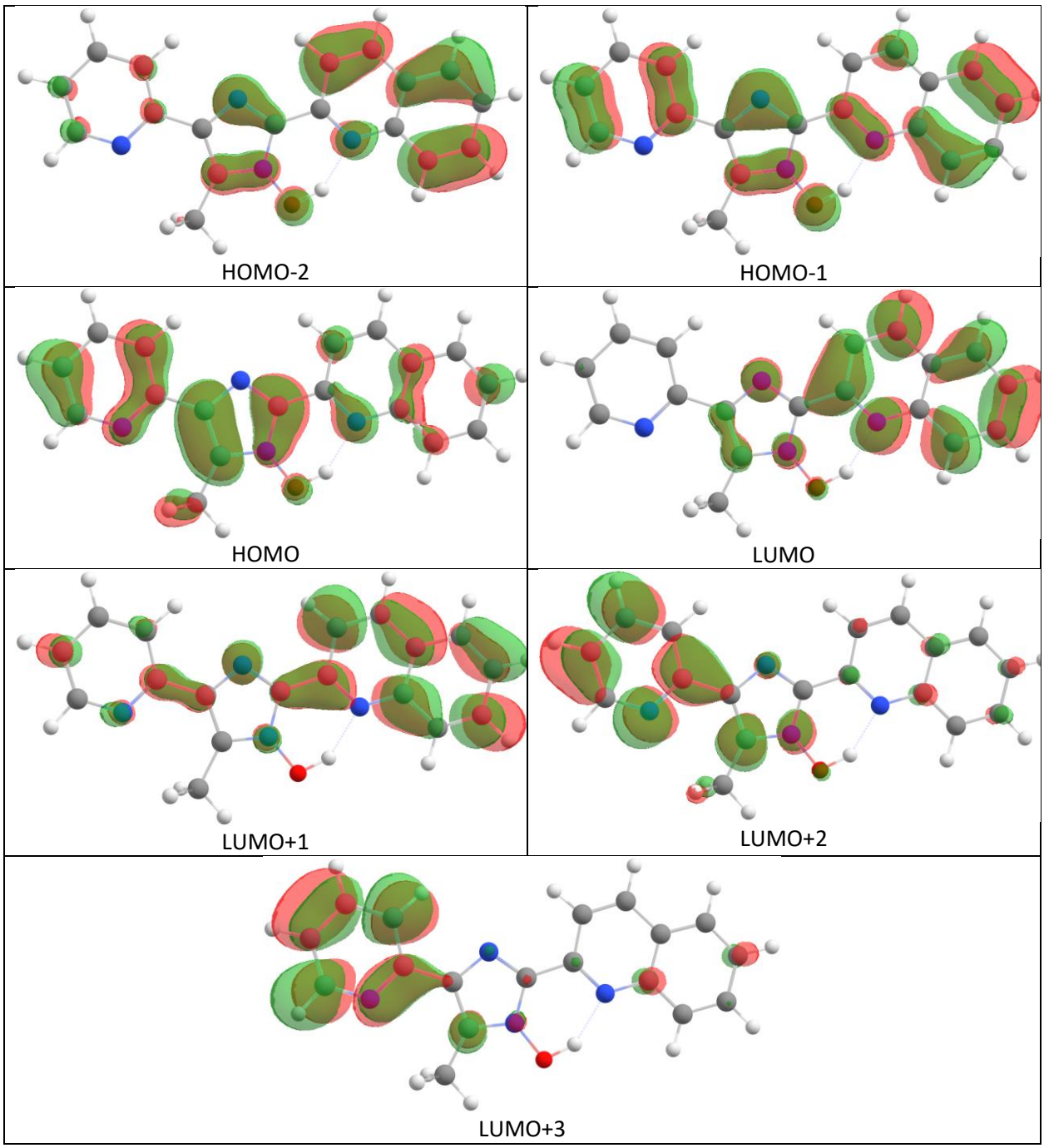
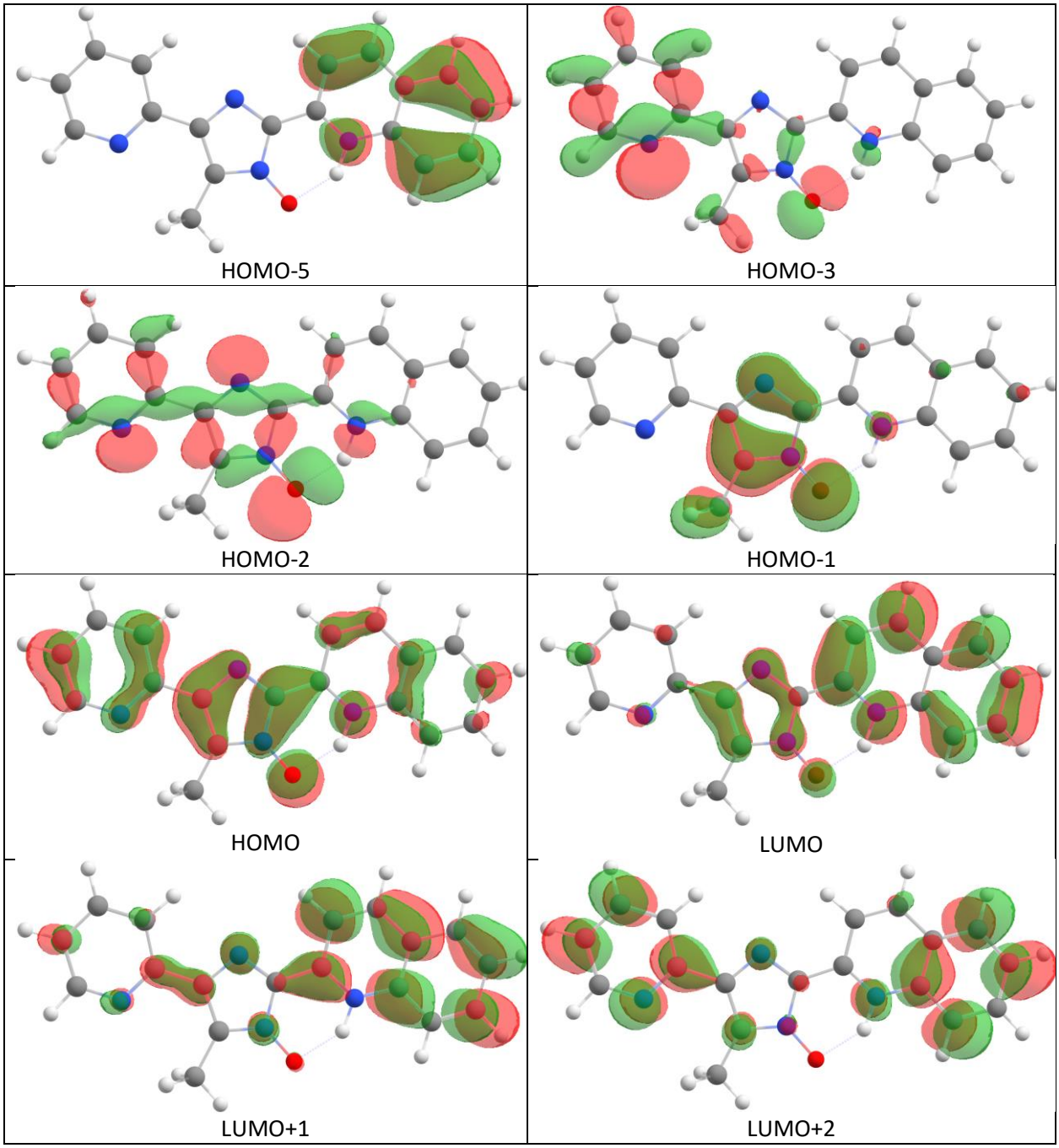


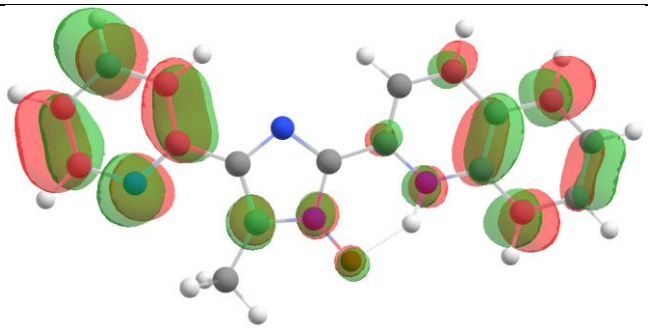
Table S38. Excited state properties of **HL^q** at the relaxed ground state geometry (**tautomeric form**, **S_0^T**) as calculated in Gaussian at the BMK/6-31+g(d) level of theory **using the QM/MM method**. Transitions with contribution >10% are shown.

State	Energy (eV)	Energy (nm)	Contributions (%)	Oscillator strength	Character
S1	2.9016	427	HOMO -> LUMO (92.0 %)	0.4404	π – π*
S2	3.3610	369	HOMO-1 -> LUMO (91.4 %)	0.3891	π – π*
S3	3.8479	322	HOMO -> LUMO+1 (95.6 %)	0.3105	π – π*
S4	3.8812	319	HOMO-3 -> LUMO (10.7 %) HOMO-2 -> LUMO (80.6 %)	0.0001	σ – π* + n – π*
S5	4.4396	279	HOMO-1 -> LUMO+1 (91.1 %)	0.0336	π – π*
S6	4.6097	269	HOMO-3 -> LUMO (55.6 %)	0.0054	σ – π* + n – π*

S7	4.6173	269	HOMO-5 -> LUMO (61.2 %) HOMO -> LUMO+2 (22.3 %)	0.1998	π – π*
S8	4.7259	262	HOMO-5 -> LUMO (12.5 %) HOMO -> LUMO+2 (19.9 %) HOMO -> LUMO+3 (54.1 %)	0.0812	π – π*

Table S39. Isosurface contour plots of the molecular orbitals of **HL^{q}** at the relaxed ground state geometry (**tautomeric form**, **S_0^T**) as calculated in Gaussian at the BMK/6-31+g(d) level of theory **using the QM/MM method (QM region)**.



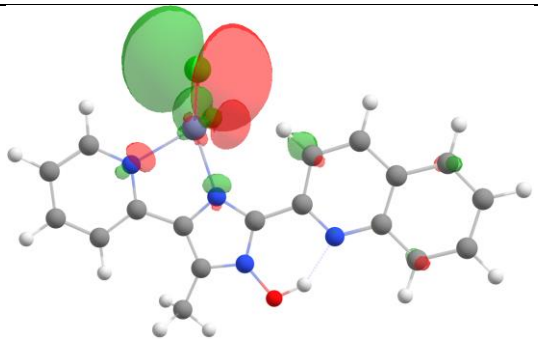


LUMO+3

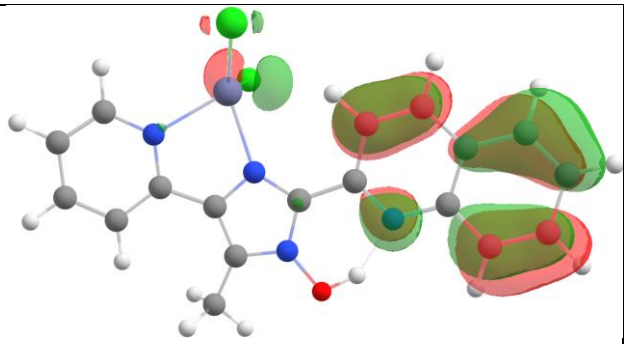
Table S40. Excited state properties of **[Zn(HL^{q})Cl$_2$]** at the relaxed ground state geometry (**normal form**, **S$_0^N$**) as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **using the QM/MM method**. Transitions with contribution >10% are shown.

State	Energy (eV)	Energy (nm)	Contributions (%)	Oscillator strength	Character
S1	3.9436	314	HOMO -> LUMO (92.0 %)	0.7733	π – π*
S2	4.3633	284	HOMO-4 -> LUMO (56.0 %) HOMO -> LUMO+1 (12.5 %)	0.0444	π – π*
S3	4.5216	274	HOMO-1 -> LUMO (58.7 %) HOMO -> LUMO+1 (24.7 %)	0.0322	Halide-to-ligand charge transfer (XLCT) + π – π*
S4	4.5446	273	HOMO-1 -> LUMO (34.9 %) HOMO -> LUMO+1 (42.5 %)	0.0575	XLCT + π – π*
S5	4.6373	267	HOMO-4 -> LUMO (13.9 %) HOMO-2 -> LUMO (76.3 %)	0.0088	XLCT
S6	4.7224	263	HOMO-3 -> LUMO (88.6 %)	0.0035	XLCT
S7	4.8350	256	HOMO-5 -> LUMO (81.7 %)	0.0003	XLCT
S8	4.9356	251	HOMO -> LUMO+2 (53.1 %)	0.1906	π – π*

Table S41. Isosurface contour plots of the molecular orbitals of **[Zn(HL^{q})Cl$_2$]** at the relaxed ground state geometry (**normal form**, **S$_0^N$**) as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **using the QM/MM method (QM region)**.



HOMO-5



HOMO-4

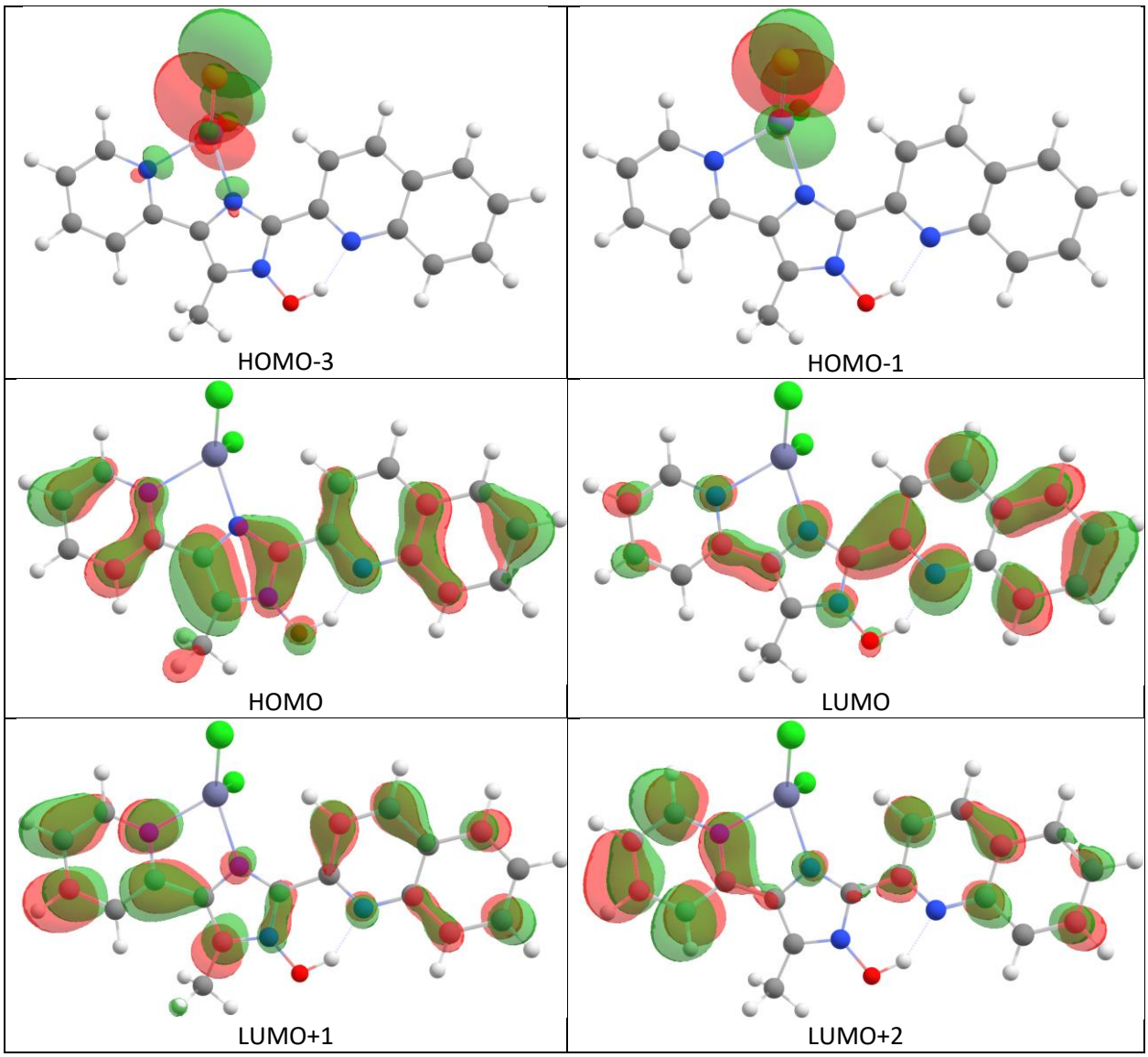
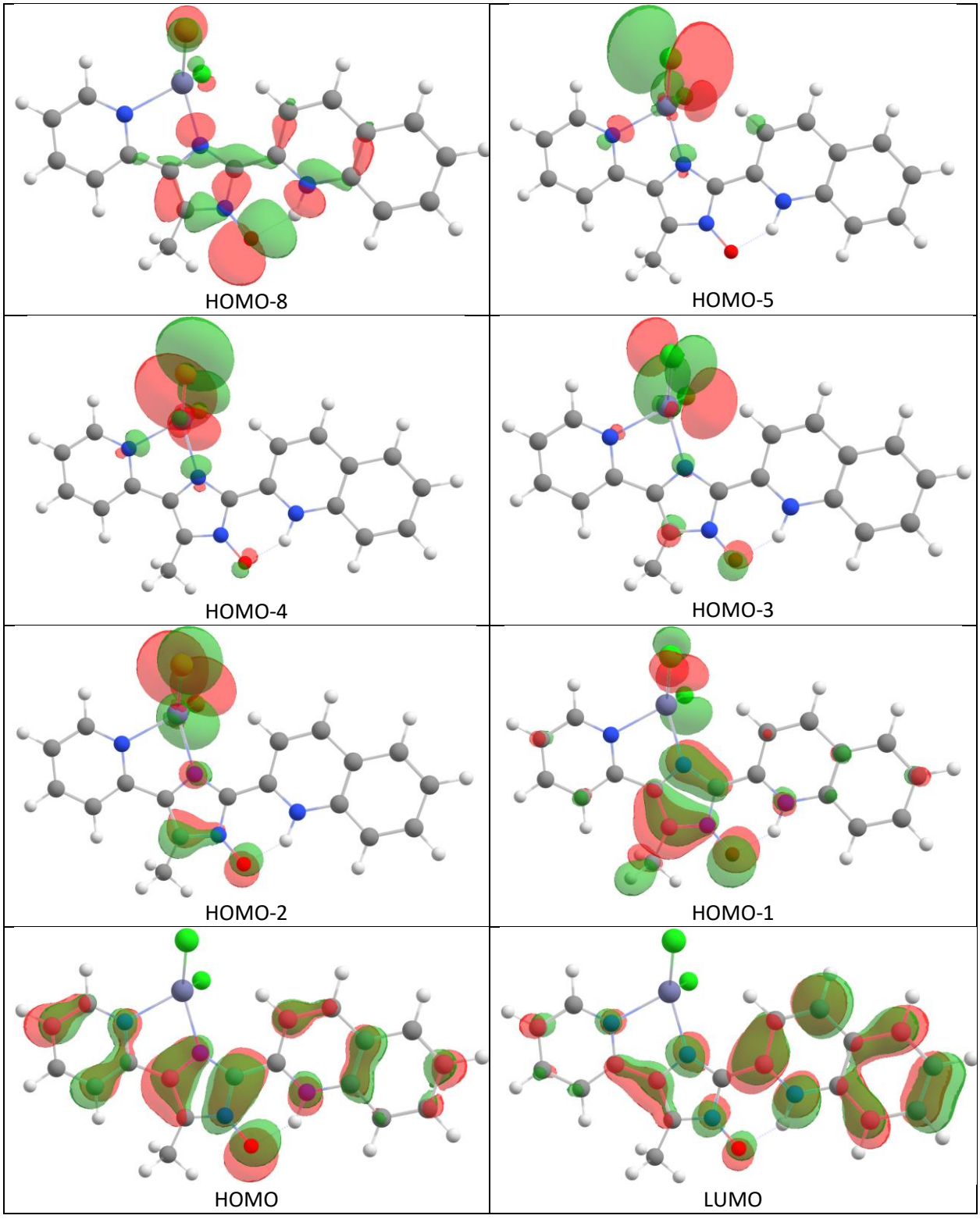


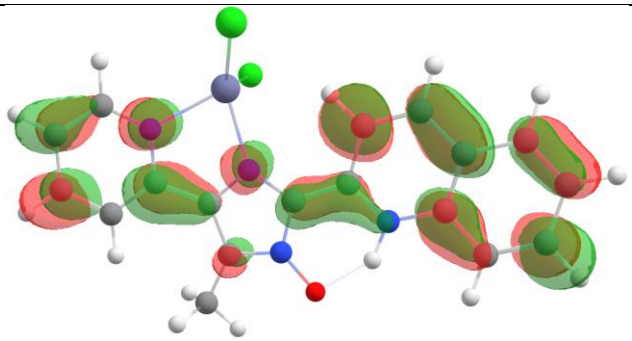
Table S42. Excited state properties of **[Zn(HL^{q})Cl$_2$]** at the relaxed ground state geometry (**tautomeric form**, **S$_0^T$**) as calculated in Gaussian at the BMK/LANL2DZ /6-31+g(d) level of theory **using the QM/MM method**. Transitions with contribution >10% are shown.

State	Energy (eV)	Energy (nm)	Contributions (%)	Oscillator strength	Character
S1	3.1145	398	HOMO -> LUMO (96.7 %)	0.4946	π – π*
S2	3.6506	340	HOMO-1 -> LUMO (87.5 %)	0.3662	π – π*
S3	3.9511	314	HOMO-2 -> LUMO (88.5 %)	0.0051	XLCT
S4	4.0463	306	HOMO-8 -> LUMO (11.4 %) HOMO-4 -> LUMO (11.4 %) HOMO-3 -> LUMO (69.9 %)	0.0010	XLCT
S5	4.1007	302	HOMO-8 -> LUMO (20.0 %) HOMO-4 -> LUMO (44.4 %) HOMO-3 -> LUMO (23.3 %)	0.0026	XLCT
S6	4.1209	301	HOMO -> LUMO+1 (86.9 %)	0.1211	π – π*
S7	4.2413	292	HOMO-8 -> LUMO (40.6 %) HOMO-5 -> LUMO (14.7 %)	0.0010	XLCT + σ – π* + n – π*

			HOMO-4 -> LUMO (37.9 %)		
S8	4.3054	288	HOMO-8 -> LUMO (15.1 %) HOMO-5 -> LUMO (80.1 %)	0.0000	XLCT

Table S43. Isosurface contour plots of the molecular orbitals of **[Zn(HL^{q})Cl$_2$]** at the relaxed ground state geometry (**tautomeric form**, **S$_0^T$**) as calculated in Gaussian at the BMK/LANL2DZ /6-31+g(d) level of theory **using the QM/MM method (QM region)**.



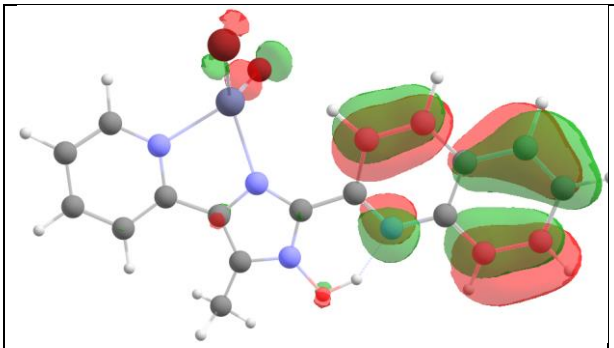


LUMO+1

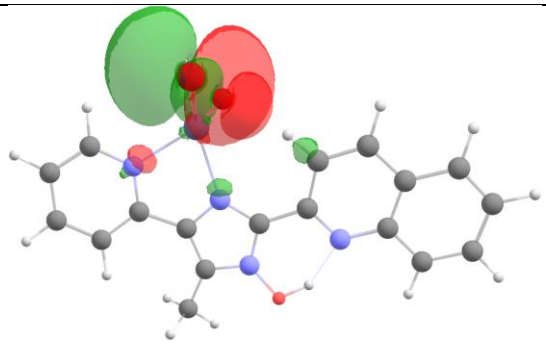
Table S44. Excited state properties of **[Zn(HL^{q})Br$_2$]** at the relaxed ground state geometry (**normal form**, **S$_0^N$**) as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **using the QM/MM method**. Transitions with contribution >10% are shown.

State	Energy (eV)	Energy (nm)	Contributions (%)	Oscillator strength	Character
S1	3.9496	314	HOMO-2 -> LUMO (80.9 %)	0.7239	π – π*
S2	4.0479	306	HOMO -> LUMO (93.0 %)	0.0133	XLCT
S3	4.1811	297	HOMO-2 -> LUMO (9.7 %) HOMO-1 -> LUMO (85.1 %)	0.0110	XLCT
S4	4.2805	290	HOMO-3 -> LUMO (93.1 %)	0.0024	XLCT
S5	4.3709	284	HOMO-5 -> LUMO (53.3 %) HOMO-4 -> LUMO (11.2 %)	0.0342	π – π*
S6	4.3754	283	HOMO-4 -> LUMO (82.9 %)	0.0036	XLCT
S7	4.5392	273	HOMO-5 -> LUMO (16.8 %) HOMO-2 -> LUMO+1 (64.2 %)	0.0878	π – π* + XLCT
S8	4.5952	270	HOMO -> LUMO+1 (94.1 %)	0.0018	XLCT

Table S45. Isosurface contour plots of the molecular orbitals of **[Zn(HL^{q})Br$_2$]** at the relaxed ground state geometry (**normal form**, **S$_0^N$**) as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **using the QM/MM method (QM region)**.



HOMO-5



HOMO-4

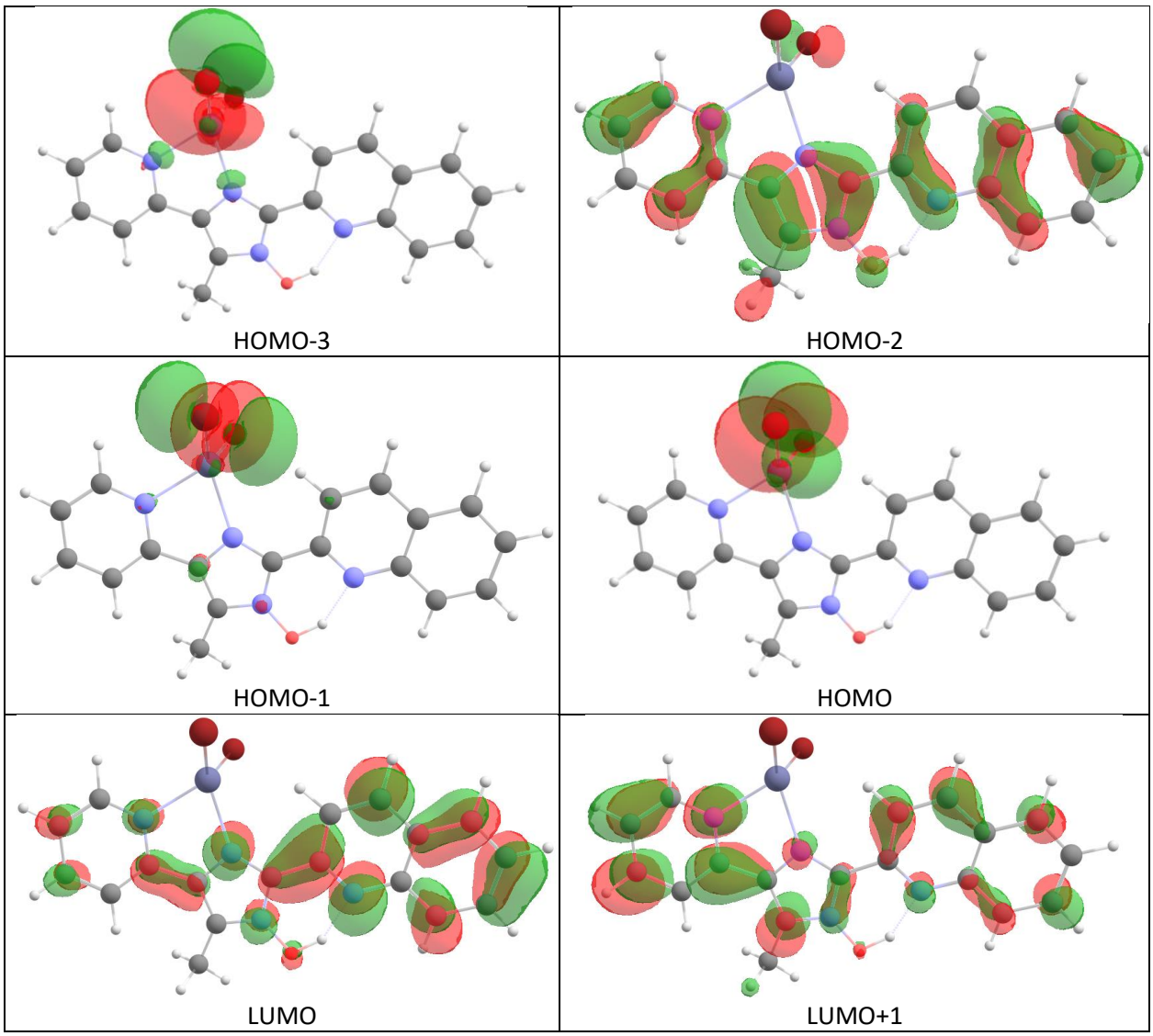
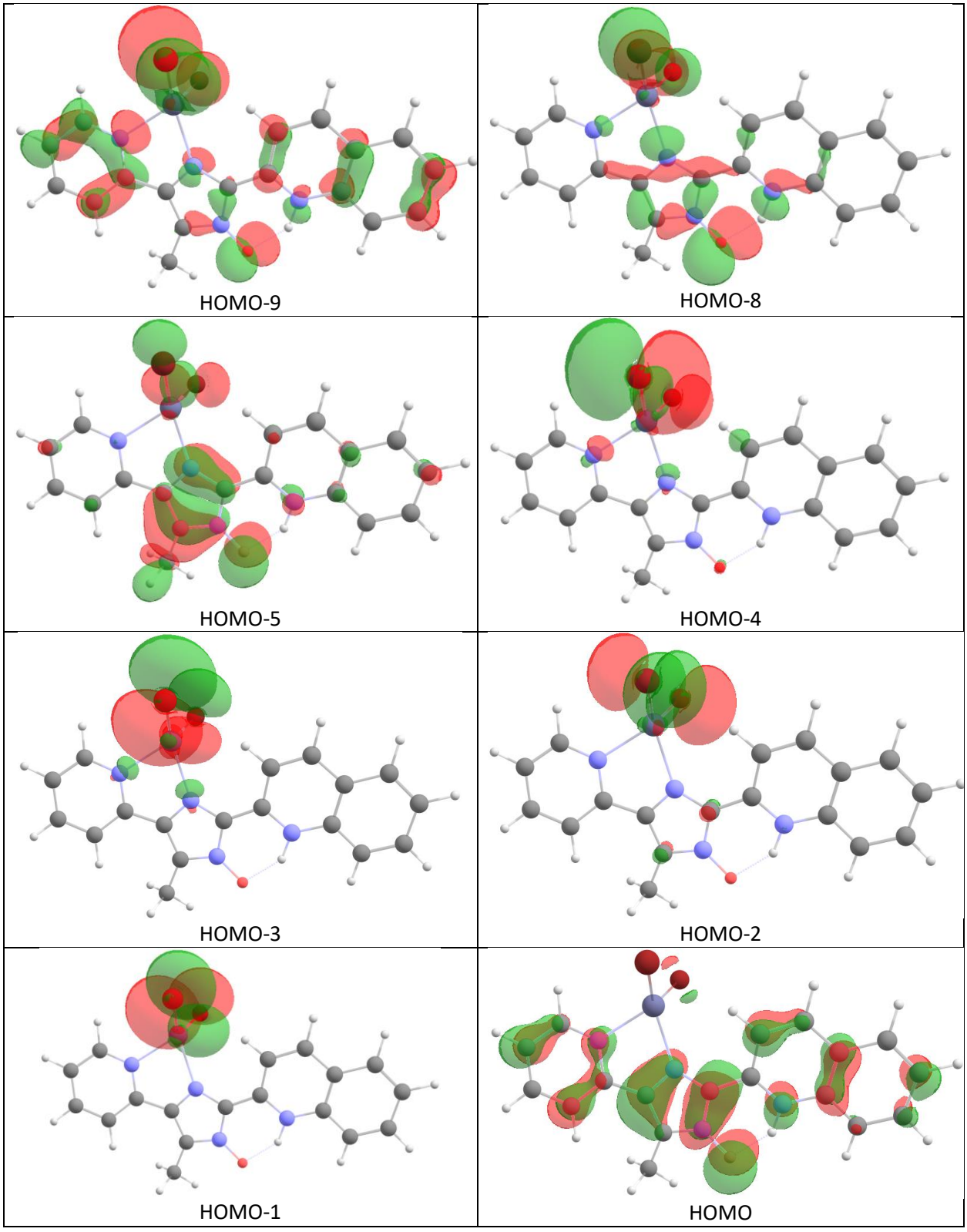
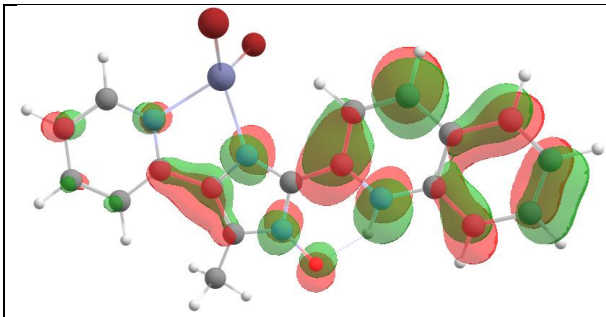


Table S46. Excited state properties of **[Zn(HL^{q})Br$_2$]** at the relaxed ground state geometry (**tautomeric form**, **S$_0^T$**) as calculated in Gaussian at the BMK/LANL2DZ /6-31+g(d) level of theory **using the QM/MM method**. Transitions with contribution >10% are shown.

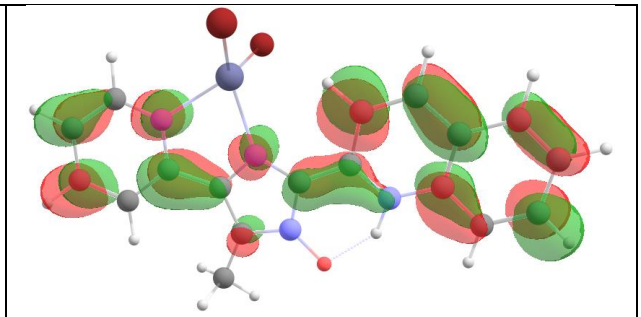
State	Energy (eV)	Energy (nm)	Contributions (%)	Oscillator strength	Character
S1	3.1146	398	HOMO -> LUMO (96.3 %)	0.4776	π – π*
S2	3.4435	360	HOMO-1 -> LUMO (97.3 %)	0.0210	XLCT
S3	3.5859	346	HOMO-5 -> LUMO (9.6 %) HOMO-2 -> LUMO (87.0 %)	0.0897	XLCT
S4	3.6733	338	HOMO-5 -> LUMO (78.6 %) HOMO-2 -> LUMO (11.2 %)	0.2394	π – π* + XLCT
S5	3.6896	336	HOMO-3 -> LUMO (92.5 %)	0.0049	XLCT
S6	3.8038	326	HOMO-4 -> LUMO (95.3 %)	0.0013	XLCT
S7	4.1258	301	HOMO -> LUMO+1 (90.5 %)	0.1062	π – π*
S8	4.1887	296	HOMO-9 -> LUMO (11.8 %) HOMO-8 -> LUMO (72.0 %)	0.0004	XLCT + σ – π* + n – π*

Table S47. Isosurface contour plots of the molecular orbitals of **[Zn(HL^{q})Br$_2$]** at the relaxed ground state geometry (**tautomeric form**, S_0^T) as calculated in Gaussian at the BMK/LANL2DZ /6-31+g(d) level of theory **using the QM/MM method (QM region)**.





LUMO

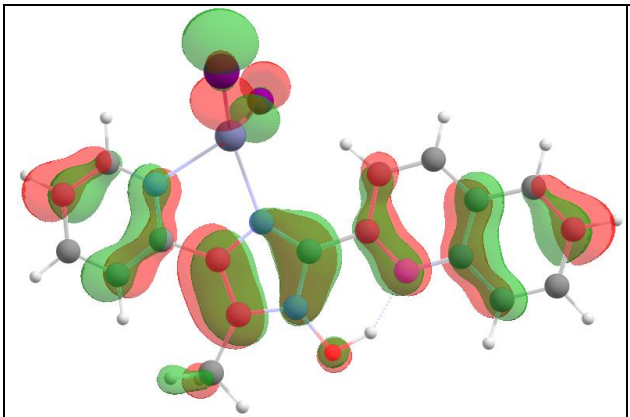


LUMO+1

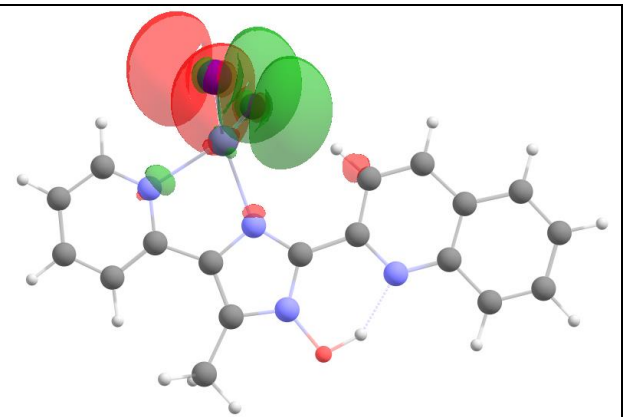
Table S48. Excited state properties of **[Zn(HL^{q})I$_2$]** at the relaxed ground state geometry (**normal form**, **S$_0^N$**) as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **using the QM/MM method**. Transitions with contribution >10% are shown.

State	Energy (eV)	Energy (nm)	Contributions (%)	Oscillator strength	Character
S1	3.5220	352	HOMO -> LUMO (96.1 %)	0.0013	XLCT
S2	3.6472	340	HOMO-1 -> LUMO (95.3 %)	0.0034	XLCT
S3	3.7366	332	HOMO-2 -> LUMO (94.6 %)	0.0021	XLCT
S4	3.8138	325	HOMO-3 -> LUMO (93.7 %)	0.0138	XLCT
S5	3.9274	316	HOMO-4 -> LUMO (87.4 %)	0.6869	$\pi - \pi^*$
S6	4.0916	303	HOMO -> LUMO+1 (95.3 %)	0.0017	XLCT
S7	4.2162	294	HOMO-1 -> LUMO+1 (92.0 %)	0.0133	XLCT
S8	4.2997	288	HOMO-2 -> LUMO+1 (87.4 %)	0.0026	XLCT

Table S49. Isosurface contour plots of the molecular orbitals of **[Zn(HL^{q})I$_2$]** at the relaxed ground state geometry (**normal form**, **S$_0^N$**) as calculated in Gaussian at the BMK/LANL2DZ /6-31+g(d) level of theory **using the QM/MM method (QM region)**.



HOMO-4



HOMO-3

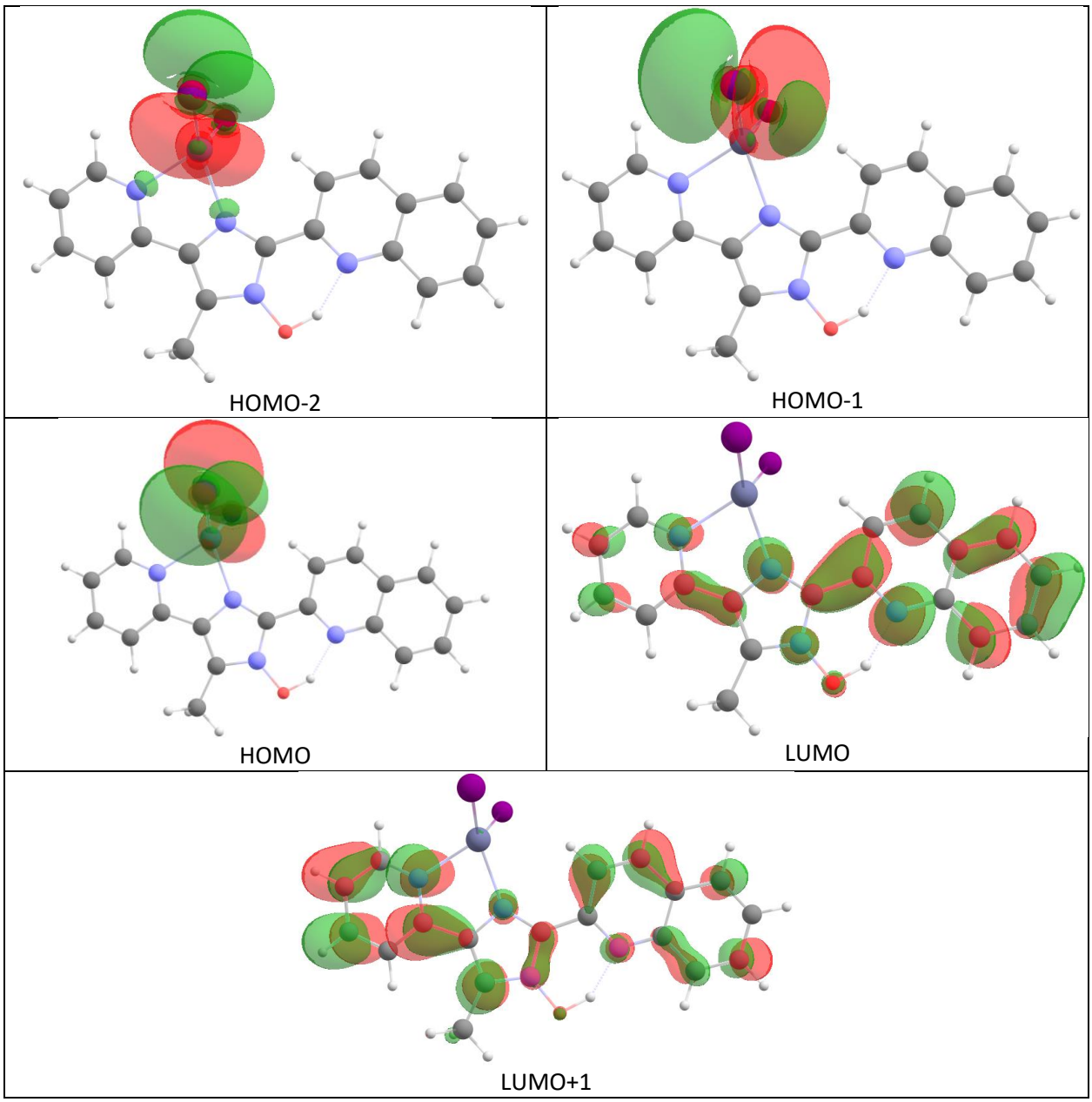
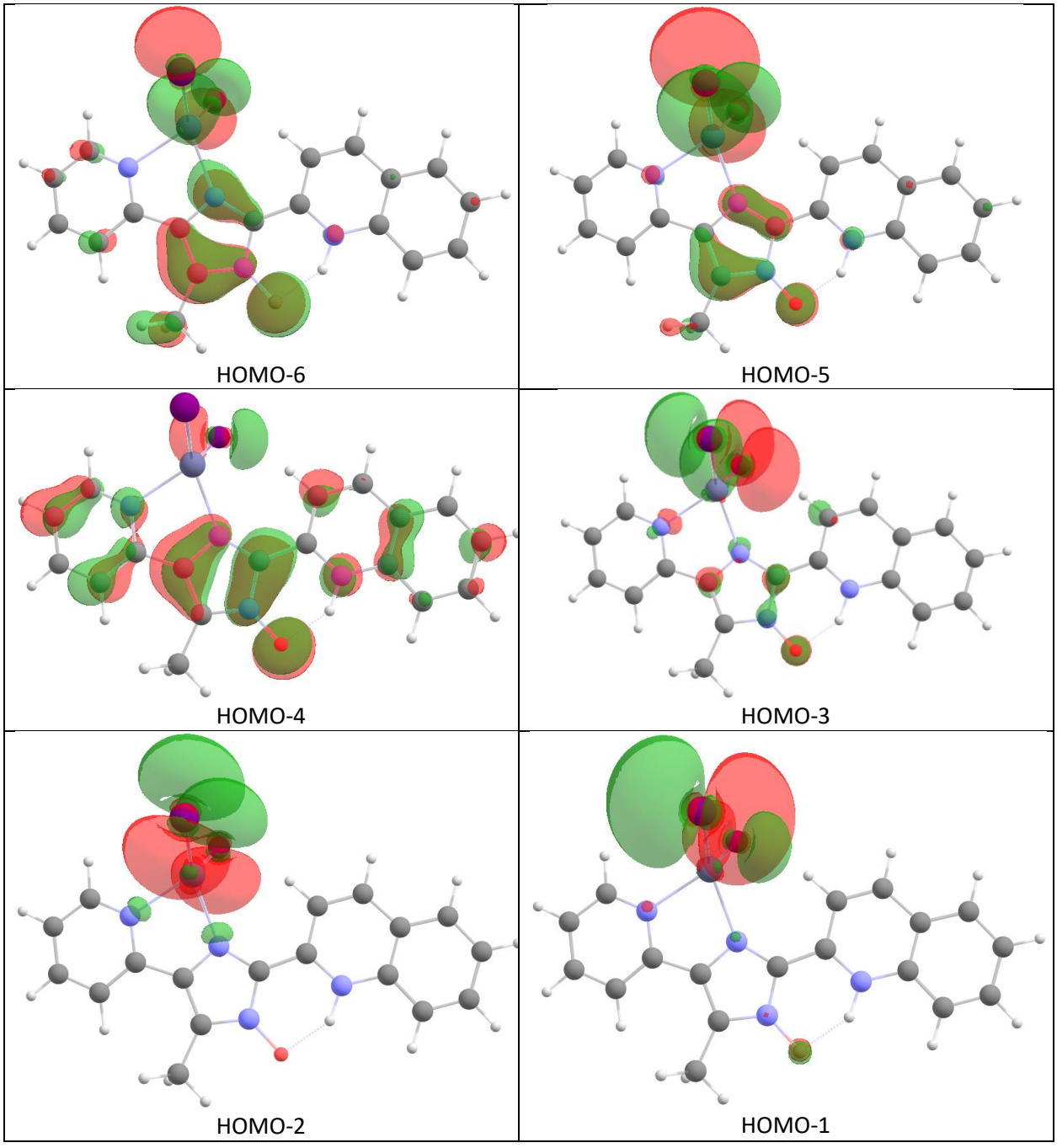


Table S50. Excited state properties of **[Zn(HL^{q})I$_2$]** at the relaxed ground state geometry (**tautomeric form**, **S$_0^T$**) as calculated in Gaussian at the BMK/LANL2DZ /6-31+g(d) level of theory **using the QM/MM method**. Transitions with contribution >10% are shown.

State	Energy (eV)	Energy (nm)	Contributions (%)	Oscillator strength	Character
S1	2.9381	422	HOMO -> LUMO (98.0 %)	0.0021	XLCT
S2	3.0549	406	HOMO-4 -> LUMO (10.4 %) HOMO-1 -> LUMO (82.6 %)	0.1130	XLCT + π – π*
S3	3.1461	394	HOMO-4 -> LUMO (68.8 %) HOMO-3 -> LUMO (9.7 %) HOMO-1 -> LUMO (15.1 %)	0.3463	π – π*
S4	3.1613	392	HOMO-2 -> LUMO (92.2 %)	0.0149	XLCT
S5	3.2576	381	HOMO-4 -> LUMO (16.1 %) HOMO-3 -> LUMO (80.4 %)	0.0066	XLCT
S6	3.5615	348	HOMO-6 -> LUMO (11.1 %)	0.2330	π – π*

			HOMO-5 -> LUMO (85.9 %)		
S7	3.9223	316	HOMO-6 -> LUMO (84.4 %) HOMO-5 -> LUMO (12.0 %)	0.1145	π – π*
S8	3.9823	311	HOMO -> LUMO+1 (95.0 %)	0.0027	XLCT

Table S51. Isosurface contour plots of the molecular orbitals of **[Zn(HL^{q})I$_2$]** at the relaxed ground state geometry (**tautomeric form**, **S$_0^T$**) as calculated in Gaussian at the BMK/LANL2DZ /6-31+g(d) level of theory **using the QM/MM method (QM region)**.



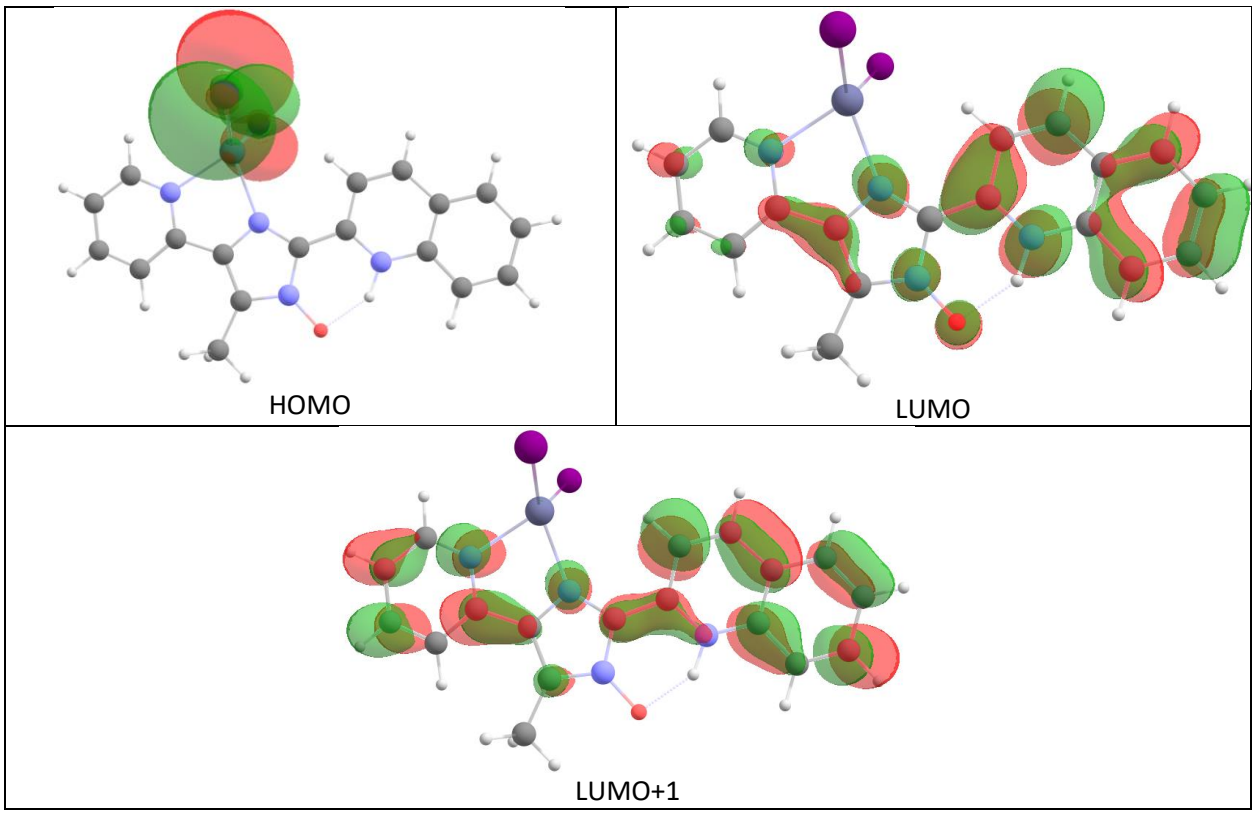


Table S52. Isosurface contour plots of the molecular orbitals of **HL^q** at the relaxed **first singlet excited state** geometry (**tautomeric form**, **S_1^T**) as calculated in Gaussian at the BMK/6-31+g(d) level of theory **using the QM/MM method (QM region)**.

$S_1^T \rightarrow S_0^T$ is LUMO → HOMO transition (97.4%), λ = 643 nm, f = 0.1134

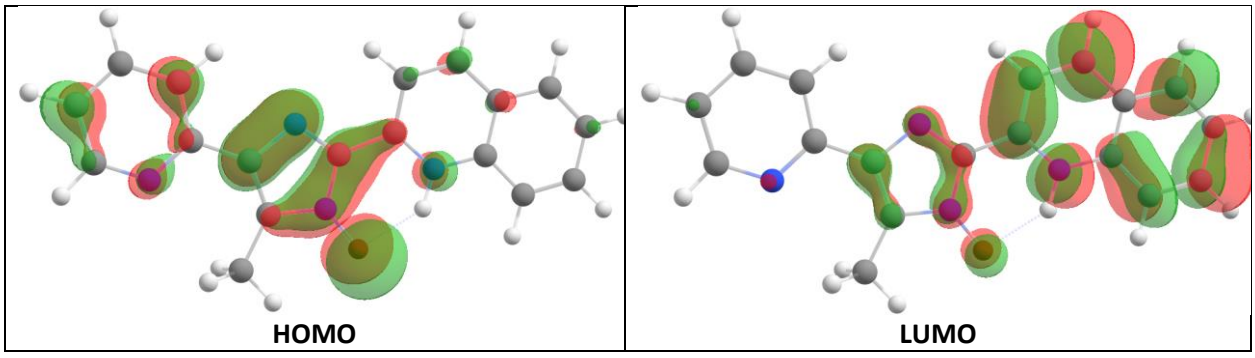


Table S53. Isosurface contour plots of the molecular orbitals of **$[Zn(HL^q)Cl_2]$** at the relaxed **first singlet excited state** geometry (**tautomeric form**, **S_1^T**) as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **using the QM/MM method (QM region)**.

$S_1^T \rightarrow S_0^T$ is LUMO → HOMO transition (98.8%), λ = 520 nm, f = 0.2003

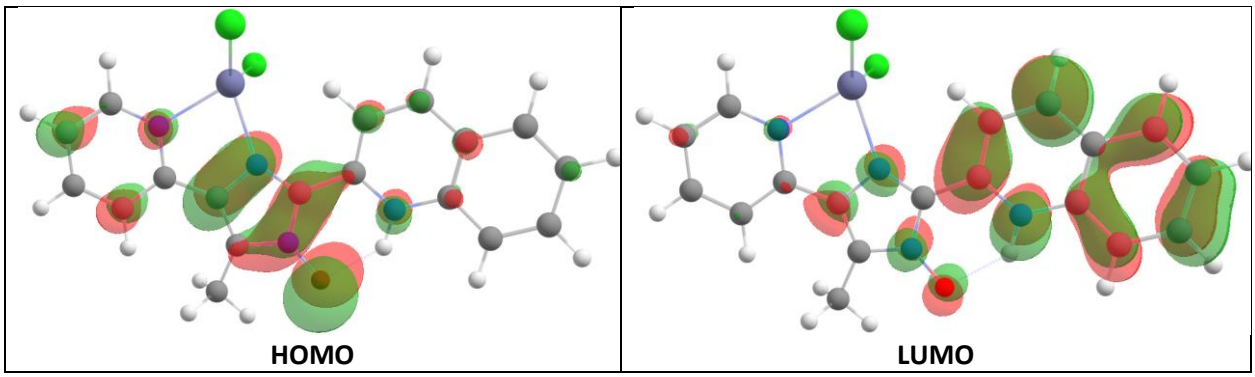


Table S54. Isosurface contour plots of the molecular orbitals of **[Zn(HL^{q})Br$_2$]** at the relaxed **first singlet excited state** geometry (**tautomeric form**, **S$_1^T$**) as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **using the QM/MM method (QM region)**.

S$_1^T$ → S$_0^T$ is LUMO → HOMO transition (98.6%), λ = 524 nm, f = 0.1925

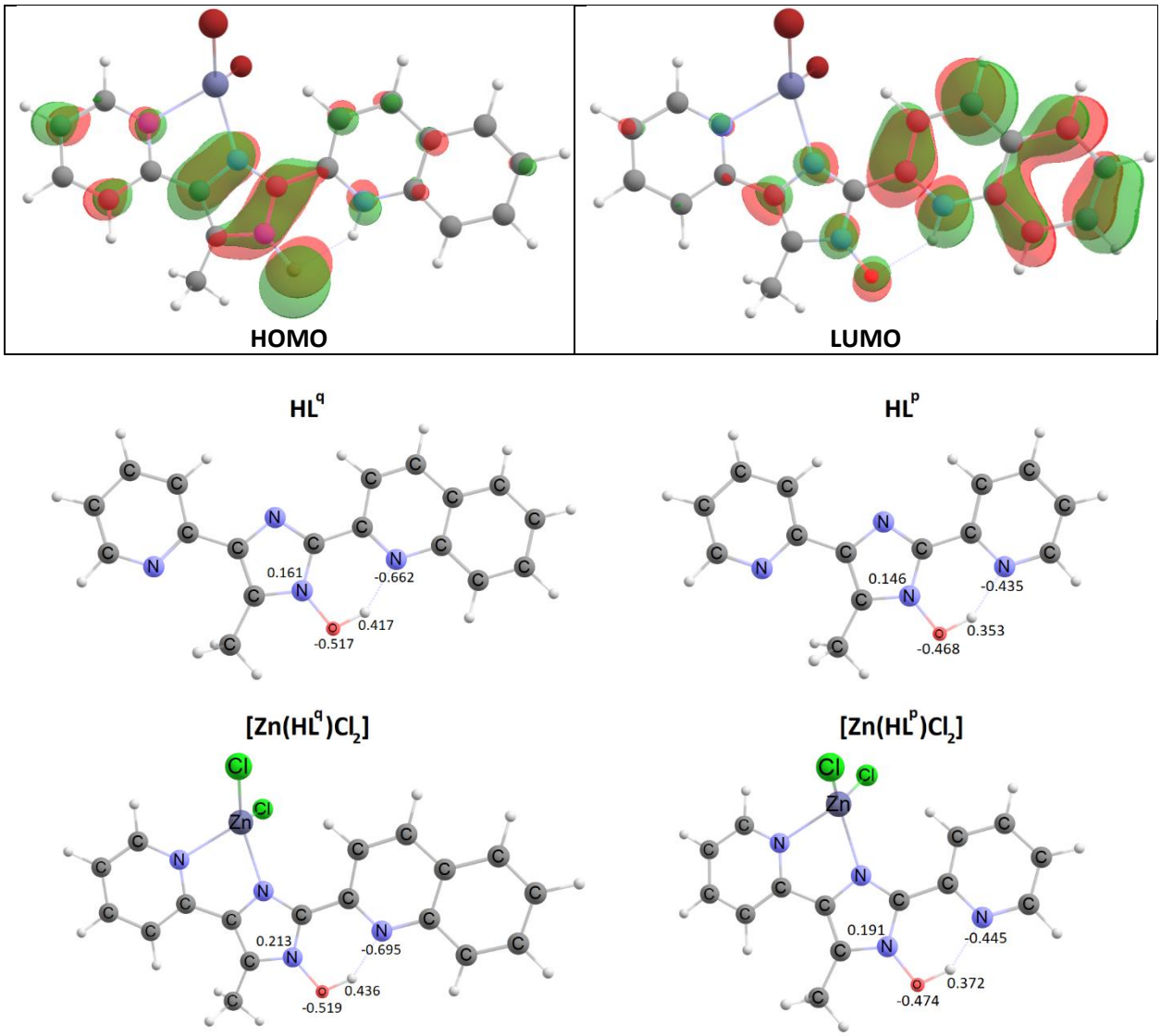


Figure S24. Merz–Singh–Kollman atomic charges on the most relevant atoms of **HL^{q}**, **[Zn(HL^{q})Hal$_2$]**, **HL^{p}** and **[Zn(HL^{p})Hal$_2$]**.

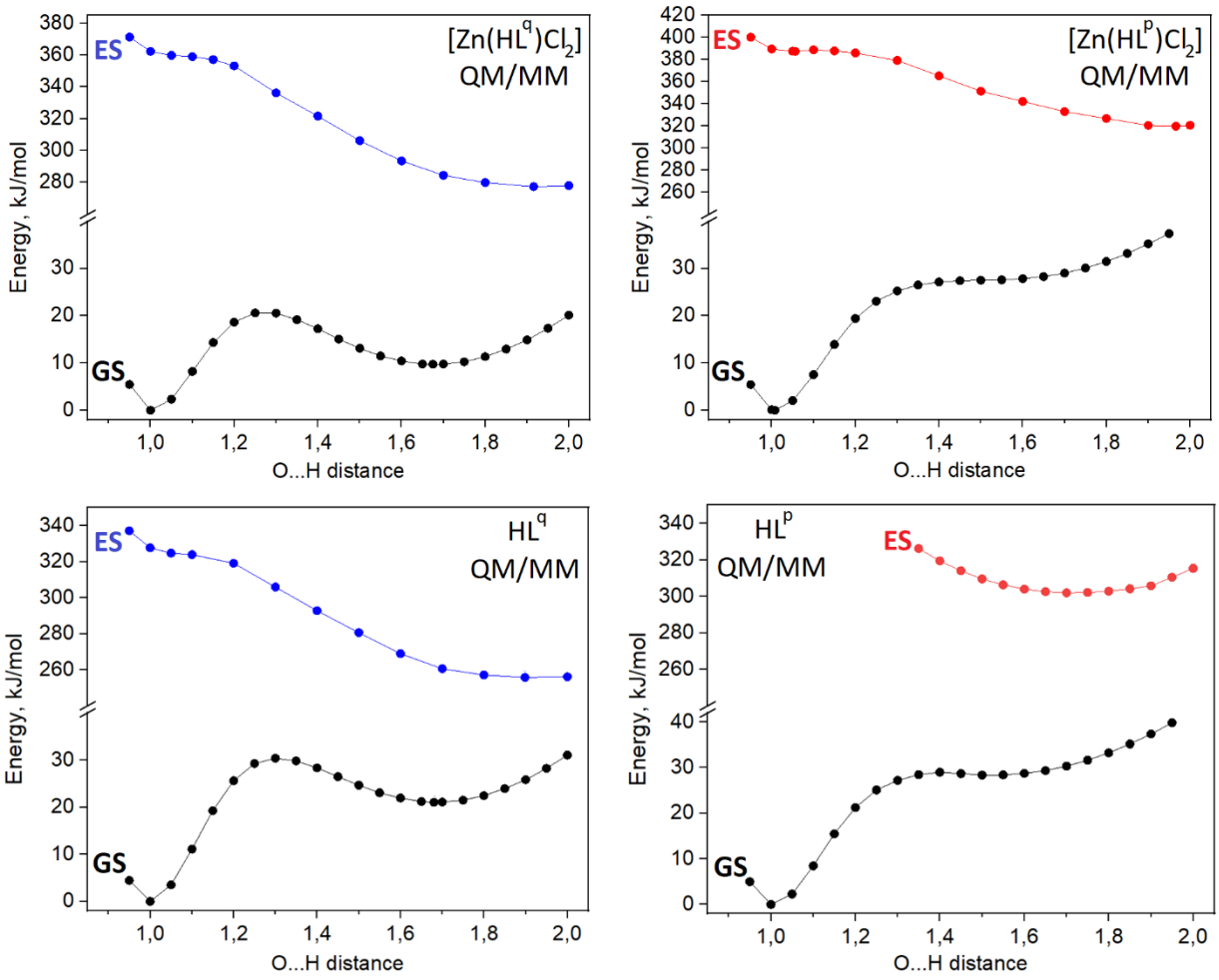


Figure S25. Potential energy curves of the ground (GS) and excited (ES) states of **HL^q**, **[Zn(HL^q)Hal$_2$]**, **HL^p** and **[Zn(HL^p)Hal$_2$]**.

Table S55. Optimized geometry of the **ground state** of **HL^q** (**normal form**, **S_0^N**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/6-31+g(d) level of theory **using the QM/MM method (QM region)**.

O	2.467059000000	2.081848000000	-1.342294000000
H	1.569856000000	1.660380000000	-1.216842000000
N	3.328992000000	1.052105000000	-1.064920000000
N	7.483748000000	0.356709000000	-0.951371000000
N	0.650570000000	0.221902000000	-0.842869000000
N	4.085710000000	-0.943713000000	-0.530515000000
C	4.671354000000	1.184915000000	-1.091302000000
C	5.132066000000	-0.099786000000	-0.746910000000
C	2.986437000000	-0.226274000000	-0.728923000000
C	5.339627000000	2.477749000000	-1.435952000000
H	5.915984000000	2.371061000000	-2.359990000000
H	6.052781000000	2.748895000000	-0.653433000000
H	4.592318000000	3.268759000000	-1.553112000000
C	6.532515000000	-0.542711000000	-0.649155000000
C	6.835844000000	-1.862895000000	-0.263201000000
H	6.018170000000	-2.540452000000	-0.036265000000
C	8.173444000000	-2.246958000000	-0.195294000000

H	8.447615000000	-3.259755000000	0.090524000000
C	9.167026000000	-1.310002000000	-0.506697000000
H	10.221736000000	-1.566478000000	-0.463110000000
C	8.760919000000	-0.025228000000	-0.881278000000
H	9.498637000000	0.734598000000	-1.139120000000
C	1.602162000000	-0.675141000000	-0.622686000000
C	1.328049000000	-2.035985000000	-0.284896000000
H	2.169974000000	-2.701783000000	-0.129631000000
C	0.020095000000	-2.430709000000	-0.177251000000
H	-0.236922000000	-3.458282000000	0.072383000000
C	-1.028850000000	-1.486084000000	-0.397413000000
C	-2.406640000000	-1.818901000000	-0.297481000000
H	-2.684112000000	-2.847401000000	-0.075841000000
C	-3.374886000000	-0.852521000000	-0.484969000000
H	-4.426480000000	-1.105910000000	-0.394103000000
C	-3.001771000000	0.481801000000	-0.799092000000
H	-3.777941000000	1.233492000000	-0.921955000000
C	-1.672916000000	0.829487000000	-0.937988000000
H	-1.374453000000	1.845821000000	-1.182810000000
C	-0.656379000000	-0.146673000000	-0.733839000000

Table S56. Optimized geometry of the **ground state** of **HL^q** (**tautomeric form**, **S_0^T**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/6-31+g(d) level of theory **using the QM/MM method (QM region)**.

O	2.418775000000	2.014454000000	-1.326855000000
H	1.001024000000	1.144745000000	-1.090350000000
N	3.311692000000	1.070670000000	-1.072923000000
N	7.476601000000	0.348635000000	-0.954297000000
N	0.652169000000	0.186065000000	-0.845697000000
N	4.106528000000	-0.965636000000	-0.524833000000
C	4.646843000000	1.182255000000	-1.098013000000
C	5.123689000000	-0.121100000000	-0.745352000000
C	2.994189000000	-0.231388000000	-0.726296000000
C	5.320069000000	2.468932000000	-1.444493000000
H	5.897315000000	2.362423000000	-2.368553000000
H	6.033033000000	2.746696000000	-0.663226000000
H	4.559070000000	3.246793000000	-1.564276000000
C	6.529498000000	-0.552540000000	-0.647103000000
C	6.837981000000	-1.869927000000	-0.253826000000
H	6.021702000000	-2.547453000000	-0.022357000000
C	8.176118000000	-2.250026000000	-0.185004000000
H	8.453744000000	-3.260396000000	0.106149000000
C	9.165785000000	-1.310545000000	-0.502526000000
H	10.221464000000	-1.563238000000	-0.458631000000
C	8.755246000000	-0.028831000000	-0.883173000000
H	9.490689000000	0.731839000000	-1.144817000000
C	1.657884000000	-0.683560000000	-0.620631000000
C	1.340720000000	-2.038358000000	-0.274839000000
H	2.175859000000	-2.709600000000	-0.111340000000
C	0.033873000000	-2.415752000000	-0.169250000000

H	-0.227643000000	-3.439855000000	0.089136000000
C	-1.029246000000	-1.471207000000	-0.396029000000
C	-2.399541000000	-1.806591000000	-0.291851000000
H	-2.671679000000	-2.834564000000	-0.062607000000
C	-3.376788000000	-0.842925000000	-0.483850000000
H	-4.426505000000	-1.100518000000	-0.388250000000
C	-3.007786000000	0.483579000000	-0.805478000000
H	-3.782583000000	1.235538000000	-0.932288000000
C	-1.675125000000	0.838937000000	-0.950974000000
H	-1.386702000000	1.856147000000	-1.204906000000
C	-0.675540000000	-0.138067000000	-0.740669000000

Table S57. Optimized geometry of the **ground state** of **[Zn(HL^{q})Cl$_2$]** (**normal form**, **S$_0^N$**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **using the QM/MM method (QM region)**.

Zn	-2.252506000000	-2.491687000000	0.674322000000
Cl	-2.043836000000	-2.826458000000	2.873190000000
Cl	-1.838031000000	-3.988345000000	-0.934722000000
N	-1.532895000000	-0.504016000000	0.230965000000
N	-4.078389000000	-1.424019000000	0.263547000000
O	0.190959000000	2.551797000000	0.191164000000
H	1.076481000000	2.077935000000	0.129268000000
C	-2.556534000000	0.400392000000	0.277350000000
C	-3.944118000000	-0.085310000000	0.214593000000
C	-5.280495000000	-1.985538000000	0.128816000000
H	-5.306602000000	-3.071811000000	0.141681000000
C	-6.440682000000	-1.229143000000	-0.035968000000
H	-7.406191000000	-1.712605000000	-0.125202000000
C	-6.319941000000	0.161723000000	-0.077506000000
H	-7.203059000000	0.776566000000	-0.215226000000
C	-5.060265000000	0.749999000000	0.043717000000
H	-4.944390000000	1.827820000000	-0.005129000000
C	-2.040115000000	1.697688000000	0.292730000000
C	-2.646330000000	3.063039000000	0.371581000000
H	-1.868746000000	3.802484000000	0.583873000000
H	-3.389328000000	3.105294000000	1.173882000000
H	-3.135944000000	3.326988000000	-0.573612000000
N	-0.698538000000	1.510865000000	0.227441000000
C	-0.400303000000	0.184354000000	0.191992000000
C	0.969792000000	-0.331552000000	0.110489000000
C	1.225143000000	-1.732539000000	0.105616000000
H	0.404023000000	-2.442590000000	0.077180000000
C	2.535615000000	-2.144847000000	0.120492000000
H	2.782904000000	-3.202955000000	0.152135000000
C	3.585990000000	-1.186245000000	0.081122000000
C	3.223278000000	0.194903000000	0.011704000000
C	4.239976000000	1.179350000000	-0.118257000000
H	3.948161000000	2.224617000000	-0.178529000000
C	5.560098000000	0.790932000000	-0.177915000000
H	6.325178000000	1.537269000000	-0.344203000000

C	5.933380000000	-0.577037000000	-0.053097000000
H	6.987257000000	-0.845866000000	-0.066782000000
C	4.961958000000	-1.547596000000	0.079553000000
H	5.221246000000	-2.599863000000	0.177041000000
N	1.923221000000	0.586790000000	0.057720000000

Table S58. Optimized geometry of the **ground state** of **[Zn(HL^{q})Cl$_2$]** (**tautomeric form**, **S$_0^T$**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **using the QM/MM method (QM region)**.

Zn	-2.264403000000	-2.495033000000	0.683633000000
Cl	-2.035293000000	-2.840082000000	2.880057000000
Cl	-1.798875000000	-3.988866000000	-0.918109000000
N	-1.549785000000	-0.521754000000	0.234851000000
N	-4.087467000000	-1.435120000000	0.266215000000
O	0.220991000000	2.492038000000	0.189384000000
H	1.597748000000	1.544184000000	0.081506000000
C	-2.552765000000	0.382100000000	0.276103000000
C	-3.943443000000	-0.096119000000	0.215140000000
C	-5.291851000000	-1.989257000000	0.128873000000
H	-5.325605000000	-3.075222000000	0.144465000000
C	-6.447074000000	-1.225890000000	-0.041541000000
H	-7.414994000000	-1.703658000000	-0.134187000000
C	-6.317307000000	0.164166000000	-0.082715000000
H	-7.196225000000	0.784101000000	-0.223122000000
C	-5.054396000000	0.745253000000	0.043015000000
H	-4.929773000000	1.822192000000	-0.002253000000
C	-2.026248000000	1.692170000000	0.288554000000
C	-2.626328000000	3.057846000000	0.371087000000
H	-1.817626000000	3.776187000000	0.539298000000
H	-3.336673000000	3.126087000000	1.201699000000
H	-3.146202000000	3.319693000000	-0.558754000000
N	-0.684462000000	1.528192000000	0.225592000000
C	-0.410733000000	0.182983000000	0.197746000000
C	0.920926000000	-0.340234000000	0.115028000000
C	1.214002000000	-1.735898000000	0.100790000000
H	0.398027000000	-2.451739000000	0.067400000000
C	2.525373000000	-2.134255000000	0.115396000000
H	2.773660000000	-3.192104000000	0.142675000000
C	3.589697000000	-1.178955000000	0.079191000000
C	3.245351000000	0.198149000000	0.013117000000
C	4.243260000000	1.188523000000	-0.113133000000
H	3.959117000000	2.236266000000	-0.169455000000
C	5.566041000000	0.792126000000	-0.173504000000
H	6.329288000000	1.539847000000	-0.337779000000
C	5.937079000000	-0.571702000000	-0.054819000000
H	6.989883000000	-0.842540000000	-0.071295000000
C	4.960630000000	-1.542834000000	0.073994000000
H	5.217036000000	-2.595811000000	0.165632000000
N	1.925171000000	0.547169000000	0.063804000000

Table S59. Optimized geometry of the **ground state** of **HL^{q}** (**normal form**, **S_0^N**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.

O	-0.421806000000	-2.482719000000	-0.004767000000
H	-1.324578000000	-2.047823000000	-0.006731000000
N	0.431616000000	-1.403824000000	-0.001517000000
N	4.597073000000	-0.607594000000	0.039152000000
N	-2.256606000000	-0.569855000000	0.000509000000
N	1.161249000000	0.670155000000	0.006306000000
C	1.782012000000	-1.521977000000	-0.007530000000
C	2.225197000000	-0.186460000000	-0.000214000000
C	0.070330000000	-0.085551000000	0.005739000000
C	2.470666000000	-2.852281000000	-0.021992000000
H	2.974718000000	-3.038184000000	0.934972000000
H	3.237625000000	-2.869842000000	-0.802940000000
H	1.743121000000	-3.650600000000	-0.201563000000
C	3.612723000000	0.307726000000	-0.000182000000
C	3.874225000000	1.693373000000	-0.038835000000
H	3.043149000000	2.392550000000	-0.070186000000
C	5.199400000000	2.126481000000	-0.035805000000
H	5.429858000000	3.190153000000	-0.063839000000
C	6.226408000000	1.172996000000	0.003523000000
H	7.274327000000	1.463266000000	0.007314000000
C	5.863414000000	-0.178130000000	0.038954000000
H	6.628362000000	-0.954241000000	0.070403000000
C	-1.319850000000	0.368376000000	0.007334000000
C	-1.614501000000	1.766778000000	0.014073000000
H	-0.794564000000	2.479300000000	0.019325000000
C	-2.932030000000	2.153436000000	0.013065000000
H	-3.202325000000	3.208651000000	0.017527000000
C	-3.965144000000	1.167288000000	0.006063000000
C	-5.350488000000	1.494317000000	0.004760000000
H	-5.644418000000	2.543155000000	0.009107000000
C	-6.303194000000	0.493239000000	-0.001882000000
H	-7.361348000000	0.746507000000	-0.002841000000
C	-5.906583000000	-0.874315000000	-0.007420000000
H	-6.667720000000	-1.652356000000	-0.012382000000
C	-4.569391000000	-1.222536000000	-0.006523000000
H	-4.252007000000	-2.263414000000	-0.010714000000
C	-3.570372000000	-0.207350000000	0.000129000000

Table S60. Optimized geometry of the **ground state** of **HL^{q}** (**tautomeric form**, **S_0^T**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.

O	0.444124000000	2.450093000000	-0.000042000000
H	1.932141000000	1.525913000000	0.000506000000
N	-0.427592000000	1.442207000000	0.000536000000
N	-4.596731000000	0.614000000000	0.006324000000
N	2.263397000000	0.540541000000	0.001178000000
N	-1.180180000000	-0.672155000000	0.002190000000
C	-1.773817000000	1.532111000000	-0.000900000000
C	-2.225014000000	0.179203000000	0.000543000000
C	-0.083175000000	0.105176000000	0.002186000000
C	-2.469907000000	2.856427000000	-0.005649000000
H	-3.084892000000	2.978440000000	0.894211000000
H	-3.138450000000	2.940851000000	-0.870260000000
H	-1.718532000000	3.652261000000	-0.042798000000
C	-3.616827000000	-0.306882000000	-0.000013000000
C	-3.886957000000	-1.691891000000	-0.006569000000
H	-3.059651000000	-2.396225000000	-0.011634000000
C	-5.214164000000	-2.117651000000	-0.006330000000
H	-5.450694000000	-3.180337000000	-0.011071000000
C	-6.236036000000	-1.157521000000	0.000038000000
H	-7.285665000000	-1.441686000000	0.000480000000
C	-5.865477000000	0.192055000000	0.006011000000
H	-6.626034000000	0.973104000000	0.011081000000
C	1.266825000000	-0.360378000000	0.002278000000
C	1.592385000000	-1.753226000000	0.002914000000
H	0.775151000000	-2.467493000000	0.003822000000
C	2.907843000000	-2.134062000000	0.002100000000
H	3.171880000000	-3.190450000000	0.002396000000
C	3.961020000000	-1.157889000000	0.000756000000
C	5.338481000000	-1.497592000000	-0.000286000000
H	5.621243000000	-2.548947000000	-0.000045000000
C	6.303531000000	-0.503488000000	-0.001618000000
H	7.358623000000	-0.767046000000	-0.002450000000
C	5.919437000000	0.862118000000	-0.001885000000
H	6.684448000000	1.635775000000	-0.002894000000
C	4.581943000000	1.227995000000	-0.000884000000
H	4.282025000000	2.273998000000	-0.001076000000
C	3.595437000000	0.215321000000	0.000388000000

Table S61. Optimized geometry of the **ground state** of **[Zn(HL^{q})Cl$_2$]** (**normal form**, **S$_0^N$**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **in CH$_2$Cl$_2$ continuum solvation model**.

Zn	-1.573971000000	-1.502061000000	0.209032000000
Cl	-1.165174000000	-1.841538000000	2.429121000000
Cl	-1.195151000000	-3.068394000000	-1.408428000000
N	-0.711826000000	0.380511000000	-0.269718000000
N	-3.329543000000	-0.296253000000	-0.064308000000
O	1.312525000000	3.224049000000	0.009637000000
H	2.138356000000	2.658399000000	0.110054000000

C	-1.646114000000	1.379910000000	-0.195185000000
C	-3.071715000000	1.020294000000	-0.215513000000
C	-4.591522000000	-0.738308000000	-0.079990000000
H	-4.726122000000	-1.810834000000	0.042953000000
C	-5.680948000000	0.120293000000	-0.241509000000
H	-6.692532000000	-0.275697000000	-0.245106000000
C	-5.427592000000	1.488413000000	-0.401579000000
H	-6.247929000000	2.189345000000	-0.539792000000
C	-4.108388000000	1.948326000000	-0.395279000000
H	-3.885340000000	3.000274000000	-0.544480000000
C	-1.004653000000	2.614270000000	-0.066095000000
C	-1.479404000000	4.026465000000	0.089184000000
H	-0.672572000000	4.645925000000	0.493971000000
H	-2.330861000000	4.067672000000	0.778219000000
H	-1.787984000000	4.449381000000	-0.876384000000
N	0.316507000000	2.288424000000	-0.076901000000
C	0.487836000000	0.946266000000	-0.203914000000
C	1.801439000000	0.293796000000	-0.251537000000
C	1.923083000000	-1.083227000000	-0.597963000000
H	1.046356000000	-1.668826000000	-0.864535000000
C	3.184980000000	-1.631024000000	-0.619985000000
H	3.327087000000	-2.677321000000	-0.886213000000
C	4.318384000000	-0.826362000000	-0.307870000000
C	4.091979000000	0.550679000000	0.013050000000
C	5.198984000000	1.392819000000	0.321498000000
H	5.007478000000	2.434997000000	0.568687000000
C	6.479140000000	0.876132000000	0.308212000000
H	7.324730000000	1.518761000000	0.545032000000
C	6.709857000000	-0.493946000000	-0.013174000000
H	7.727588000000	-0.878487000000	-0.018306000000
C	5.651905000000	-1.328178000000	-0.314858000000
H	5.817528000000	-2.375669000000	-0.562545000000
N	2.835598000000	1.073124000000	0.030020000000

Table S62. Optimized geometry of the **ground state** of **[Zn(HL^{q})Cl$_2$]** (**tautomeric form**, **S$_0^T$**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.

Zn	-1.667068000000	1.517456000000	-0.112492000000
Cl	-1.358144000000	2.146298000000	-2.288696000000
Cl	-1.117492000000	2.904918000000	1.616561000000
N	-0.712951000000	-0.368221000000	0.169393000000
N	-3.364660000000	0.242435000000	0.076087000000
O	1.368876000000	-3.166255000000	-0.076519000000
H	2.666816000000	-2.052877000000	-0.125415000000
C	-1.618886000000	-1.379317000000	0.127898000000
C	-3.055890000000	-1.068884000000	0.157453000000
C	-4.641425000000	0.639420000000	0.100560000000
H	-4.813414000000	1.711543000000	0.032957000000
C	-5.700644000000	-0.264267000000	0.205370000000
H	-6.725707000000	0.094771000000	0.219123000000

C	-5.397107000000	-1.628684000000	0.292065000000
H	-6.191952000000	-2.366096000000	0.379760000000
C	-4.062557000000	-2.040469000000	0.271546000000
H	-3.806558000000	-3.091604000000	0.350459000000
C	-0.954583000000	-2.617227000000	0.029936000000
C	-1.416693000000	-4.037214000000	-0.069454000000
H	-0.549673000000	-4.671965000000	-0.278222000000
H	-2.148325000000	-4.156658000000	-0.878556000000
H	-1.876658000000	-4.374015000000	0.869472000000
N	0.366104000000	-2.301582000000	0.012030000000
C	0.501628000000	-0.939144000000	0.104197000000
C	1.782715000000	-0.274011000000	0.145002000000
C	1.940346000000	1.125088000000	0.357629000000
H	1.074696000000	1.750930000000	0.546420000000
C	3.207276000000	1.658753000000	0.367786000000
H	3.342727000000	2.726071000000	0.533407000000
C	4.359182000000	0.835853000000	0.175728000000
C	4.155730000000	-0.559688000000	-0.010868000000
C	5.250305000000	-1.439408000000	-0.187540000000
H	5.072161000000	-2.503568000000	-0.327227000000
C	6.532151000000	-0.917280000000	-0.179755000000
H	7.381717000000	-1.582693000000	-0.316082000000
C	6.756118000000	0.475473000000	0.002009000000
H	7.773910000000	0.858237000000	0.002613000000
C	5.689241000000	1.337426000000	0.177702000000
H	5.847605000000	2.404905000000	0.319310000000
N	2.874087000000	-1.036891000000	-0.017282000000

Table S63. Optimized geometry of the **first singlet excited state** of **HL^q** (**normal form**, **S_1^N**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.

O	0.456587000000	2.388146000000	0.000239000000
H	1.370294000000	1.882986000000	0.000441000000
N	-0.423716000000	1.348591000000	-0.006157000000
N	-4.597189000000	0.636754000000	-0.018943000000
N	2.224097000000	0.556370000000	-0.002874000000
N	-1.205789000000	-0.743797000000	-0.016202000000
C	-1.743581000000	1.500903000000	-0.008544000000
C	-2.241038000000	0.139148000000	-0.015172000000
C	-0.081539000000	-0.018745000000	-0.010723000000
C	-2.367781000000	2.854064000000	-0.004058000000
H	-2.037773000000	3.410666000000	0.884766000000
H	-3.453548000000	2.763106000000	-0.007554000000
H	-2.032966000000	3.418839000000	-0.885885000000
C	-3.623778000000	-0.304396000000	-0.020133000000
C	-3.911017000000	-1.691940000000	-0.025899000000
H	-3.092873000000	-2.406166000000	-0.026464000000
C	-5.244540000000	-2.098578000000	-0.030693000000
H	-5.496714000000	-3.157075000000	-0.035241000000
C	-6.249173000000	-1.122962000000	-0.029534000000

H	-7.302970000000	-1.390606000000	-0.033136000000
C	-5.861623000000	0.231940000000	-0.023494000000
H	-6.616391000000	1.018143000000	-0.022315000000
C	1.279095000000	-0.454421000000	-0.009136000000
C	1.623828000000	-1.827957000000	-0.013526000000
H	0.829067000000	-2.570536000000	-0.018369000000
C	2.957047000000	-2.187532000000	-0.011546000000
H	3.258769000000	-3.232923000000	-0.014756000000
C	3.968900000000	-1.157722000000	-0.005063000000
C	5.348935000000	-1.439064000000	-0.002723000000
H	5.669867000000	-2.480445000000	-0.005968000000
C	6.298652000000	-0.409188000000	0.003647000000
H	7.360534000000	-0.647527000000	0.005367000000
C	5.874310000000	0.939441000000	0.007845000000
H	6.614502000000	1.738212000000	0.012817000000
C	4.520786000000	1.259059000000	0.005698000000
H	4.185339000000	2.294643000000	0.008878000000
C	3.529267000000	0.227604000000	-0.000816000000

Table S64. Optimized geometry of the **first singlet excited state** of **HL^q** (**tautomeric form**, **S_1^T**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.

O	4.780940000000	2.335407000000	24.727360000000
H	4.796145000000	2.792872000000	22.867333000000
N	5.923161000000	2.842643000000	25.094551000000
N	8.346337000000	3.463095000000	28.527431000000
N	5.468023000000	3.220255000000	22.227736000000
N	7.901098000000	3.852217000000	24.890471000000
C	6.432433000000	2.863000000000	26.357848000000
C	7.672986000000	3.499650000000	26.227688000000
C	6.853481000000	3.457657000000	24.224060000000
C	5.684217000000	2.273519000000	27.511281000000
H	5.350674000000	3.059905000000	28.200067000000
H	6.331857000000	1.595968000000	28.077286000000
H	4.810673000000	1.729867000000	27.136752000000
C	8.655758000000	3.798763000000	27.254334000000
C	9.881094000000	4.418843000000	26.911229000000
H	10.083488000000	4.669757000000	25.874104000000
C	10.800494000000	4.689853000000	27.924398000000
H	11.751111000000	5.165811000000	27.691270000000
C	10.479140000000	4.340109000000	29.241626000000
H	11.163025000000	4.531476000000	30.064938000000
C	9.235346000000	3.728617000000	29.480355000000
H	8.951100000000	3.443282000000	30.493294000000
C	6.658926000000	3.627643000000	22.779438000000
C	7.632921000000	4.197483000000	21.964452000000
H	8.564872000000	4.515415000000	22.422857000000
C	7.400848000000	4.350782000000	20.592883000000
H	8.156843000000	4.796156000000	19.950753000000
C	6.159836000000	3.917421000000	20.022520000000

C	5.845313000000	4.030863000000	18.645571000000
H	6.583302000000	4.472167000000	17.977496000000
C	4.618480000000	3.587590000000	18.150403000000
H	4.396105000000	3.683335000000	17.089639000000
C	3.667173000000	3.015856000000	19.019656000000
H	2.711565000000	2.669944000000	18.630957000000
C	3.941081000000	2.887694000000	20.384492000000
H	3.211704000000	2.447066000000	21.062123000000
C	5.177044000000	3.333517000000	20.891249000000

Table S65. Optimized geometry of the **first singlet excited state** of **[Zn(HL^{q})Cl$_2$]** (**normal form**, **S$_1^N$**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.

Zn	-1.695028000000	-1.557796000000	0.083712000000
Cl	-1.394923000000	-2.189569000000	2.259019000000
Cl	-1.203303000000	-2.902851000000	-1.691237000000
N	-0.713922000000	0.328771000000	-0.170748000000
N	-3.353536000000	-0.230086000000	-0.102981000000
O	1.409339000000	3.144231000000	0.006621000000
H	2.238418000000	2.505072000000	0.038356000000
C	-1.606633000000	1.360599000000	-0.128681000000
C	-3.024132000000	1.094072000000	-0.142111000000
C	-4.636248000000	-0.592376000000	-0.120265000000
H	-4.834746000000	-1.661863000000	-0.085128000000
C	-5.683923000000	0.336218000000	-0.179684000000
H	-6.714013000000	-0.008424000000	-0.192975000000
C	-5.363050000000	1.704378000000	-0.220641000000
H	-6.146643000000	2.456741000000	-0.269214000000
C	-4.024880000000	2.090735000000	-0.203191000000
H	-3.756293000000	3.140744000000	-0.244051000000
C	-0.898503000000	2.611954000000	-0.044384000000
C	-1.339549000000	4.034691000000	0.046621000000
H	-0.469302000000	4.680060000000	0.194191000000
H	-2.028920000000	4.167306000000	0.889786000000
H	-1.852039000000	4.339315000000	-0.875701000000
N	0.381578000000	2.258731000000	-0.043449000000
C	0.527485000000	0.859582000000	-0.131353000000
C	1.796176000000	0.235249000000	-0.167456000000
C	1.957758000000	-1.175650000000	-0.358199000000
H	1.092320000000	-1.806646000000	-0.541300000000
C	3.221934000000	-1.705811000000	-0.349005000000
H	3.378818000000	-2.772236000000	-0.498158000000
C	4.362443000000	-0.844697000000	-0.150258000000
C	4.114872000000	0.578093000000	0.007887000000
C	5.235499000000	1.457292000000	0.184202000000
H	5.041081000000	2.521964000000	0.298937000000
C	6.523179000000	0.950774000000	0.206920000000
H	7.366432000000	1.625519000000	0.342779000000
C	6.759738000000	-0.441801000000	0.056797000000

H	7.778386000000	-0.823413000000	0.078218000000
C	5.686587000000	-1.319496000000	-0.120565000000
H	5.863950000000	-2.387855000000	-0.238403000000
N	2.874052000000	1.082516000000	-0.006006000000

Table S66. Optimized geometry of the **first singlet excited state** of **[Zn(HL^{q})Cl$_2$]** (**tautomeric form**, **S$_1^T$**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **in CH$_2$Cl$_2$ continuum solvation model**.

Zn	-1.447130000000	-1.440297000000	0.262550000000
Cl	-1.118614000000	-1.879743000000	2.493413000000
Cl	-1.172503000000	-2.789461000000	-1.572864000000
N	-0.648127000000	0.489299000000	-0.170868000000
N	-3.223176000000	-0.223604000000	0.142480000000
O	1.290594000000	3.246913000000	-0.751754000000
H	2.735564000000	1.964259000000	0.541990000000
C	-1.625561000000	1.497065000000	-0.203294000000
C	-3.017938000000	1.103247000000	-0.032886000000
C	-4.464394000000	-0.686854000000	0.307300000000
H	-4.561965000000	-1.761403000000	0.445657000000
C	-5.584906000000	0.150876000000	0.307664000000
H	-6.577493000000	-0.268385000000	0.445600000000
C	-5.386414000000	1.526447000000	0.130205000000
H	-6.230653000000	2.212003000000	0.126069000000
C	-4.090011000000	2.013726000000	-0.043338000000
H	-3.909566000000	3.074374000000	-0.184950000000
C	-1.018668000000	2.728422000000	-0.404159000000
C	-1.519007000000	4.134334000000	-0.519997000000
H	-0.667786000000	4.806250000000	-0.670051000000
H	-2.047633000000	4.436033000000	0.392969000000
H	-2.201465000000	4.238978000000	-1.372919000000
N	0.318058000000	2.432007000000	-0.526350000000
C	0.507958000000	1.050508000000	-0.377981000000
C	1.819533000000	0.408242000000	-0.458955000000
C	2.008606000000	-0.825840000000	-1.081647000000
H	1.163067000000	-1.296084000000	-1.578398000000
C	3.258708000000	-1.439244000000	-1.049707000000
H	3.413705000000	-2.403959000000	-1.525592000000
C	4.354636000000	-0.794605000000	-0.379002000000
C	4.129240000000	0.471611000000	0.251196000000
C	5.173307000000	1.143378000000	0.914841000000
H	4.980072000000	2.105034000000	1.386806000000
C	6.445763000000	0.570162000000	0.956631000000
H	7.252150000000	1.093818000000	1.465279000000
C	6.687906000000	-0.677793000000	0.345436000000
H	7.682004000000	-1.117737000000	0.384732000000
C	5.656128000000	-1.347450000000	-0.310329000000
H	5.836397000000	-2.309876000000	-0.786402000000
N	2.865205000000	1.018478000000	0.199937000000

Table S67. Optimized geometry of the **first singlet excited state** of **HL^q** (**tautomeric form**, **S_1^T**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/6-31+g(d) level of theory **using the QM/MM method (QM region)**.

O	2.515154000000	2.057540000000	-1.384306000000
H	0.895939000000	1.120203000000	-1.061701000000
N	3.335232000000	1.090867000000	-1.093039000000
N	7.527209000000	0.362612000000	-0.945701000000
N	0.618032000000	0.166524000000	-0.815303000000
N	4.084753000000	-0.900871000000	-0.520080000000
C	4.723267000000	1.205700000000	-1.099383000000
C	5.178167000000	-0.044391000000	-0.744799000000
C	3.010022000000	-0.194688000000	-0.738516000000
C	5.376964000000	2.496644000000	-1.454205000000
H	5.952092000000	2.385002000000	-2.378354000000
H	6.087670000000	2.777818000000	-0.673126000000
H	4.614948000000	3.271864000000	-1.578370000000
C	6.556606000000	-0.519925000000	-0.640035000000
C	6.834313000000	-1.846789000000	-0.250257000000
H	6.008942000000	-2.513798000000	-0.020103000000
C	8.166198000000	-2.253860000000	-0.181206000000
H	8.422642000000	-3.269982000000	0.107796000000
C	9.175345000000	-1.336970000000	-0.496905000000
H	10.225120000000	-1.612476000000	-0.454157000000
C	8.793719000000	-0.043191000000	-0.876141000000
H	9.545857000000	0.700296000000	-1.139420000000
C	1.624040000000	-0.721116000000	-0.614978000000
C	1.345219000000	-2.032733000000	-0.296745000000
H	2.177978000000	-2.707652000000	-0.143801000000
C	-0.006317000000	-2.442140000000	-0.177462000000
H	-0.248583000000	-3.471827000000	0.068194000000
C	-1.054703000000	-1.514031000000	-0.388403000000
C	-2.440459000000	-1.833883000000	-0.297696000000
H	-2.721920000000	-2.862056000000	-0.084728000000
C	-3.410541000000	-0.858396000000	-0.482798000000
H	-4.460331000000	-1.117294000000	-0.390149000000
C	-3.052879000000	0.470007000000	-0.790052000000
H	-3.825398000000	1.223826000000	-0.913200000000
C	-1.705833000000	0.818466000000	-0.924427000000
H	-1.413614000000	1.838174000000	-1.167022000000
C	-0.717459000000	-0.158102000000	-0.719397000000

Table S68. Optimized geometry of the **first singlet excited state** of **[$Zn(HL^q)Cl_2$]** (**tautomeric form**, **S_1^T**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **using the QM/MM method (QM region)**.

Zn	-2.250408000000	-2.487278000000	0.658983000000

Cl	-2.039366000000	-2.798484000000	2.862974000000
Cl	-1.849136000000	-3.976084000000	-0.959944000000
N	-1.522869000000	-0.463384000000	0.241461000000
N	-4.063588000000	-1.418903000000	0.240276000000
O	0.118311000000	2.567164000000	0.221249000000
H	1.729174000000	1.543234000000	0.056754000000
C	-2.598375000000	0.445653000000	0.285760000000
C	-3.958167000000	-0.073226000000	0.210863000000
C	-5.254980000000	-2.000489000000	0.101482000000
H	-5.261101000000	-3.087342000000	0.100823000000
C	-6.430915000000	-1.264045000000	-0.048691000000
H	-7.386445000000	-1.764799000000	-0.140851000000
C	-6.340684000000	0.131554000000	-0.071674000000
H	-7.238399000000	0.728277000000	-0.195909000000
C	-5.095324000000	0.743293000000	0.053563000000
H	-4.997764000000	1.823629000000	0.021314000000
C	-2.101251000000	1.728531000000	0.304557000000
C	-2.708773000000	3.089221000000	0.381697000000
H	-1.915243000000	3.825700000000	0.538776000000
H	-3.413460000000	3.148761000000	1.216230000000
H	-3.240255000000	3.330480000000	-0.546378000000
N	-0.727629000000	1.579682000000	0.239724000000
C	-0.422522000000	0.228132000000	0.199207000000
C	0.949427000000	-0.344032000000	0.118038000000
C	1.207311000000	-1.698284000000	0.126822000000
H	0.387984000000	-2.408982000000	0.122053000000
C	2.545701000000	-2.145449000000	0.129257000000
H	2.766289000000	-3.206826000000	0.169046000000
C	3.612093000000	-1.212623000000	0.078786000000
C	3.295522000000	0.184179000000	-0.000995000000
C	4.301275000000	1.153634000000	-0.136708000000
H	4.032670000000	2.205391000000	-0.203860000000
C	5.632466000000	0.744594000000	-0.191557000000
H	6.403072000000	1.480189000000	-0.372085000000
C	5.976383000000	-0.616226000000	-0.053867000000
H	7.025164000000	-0.903587000000	-0.062960000000
C	4.985267000000	-1.579472000000	0.086760000000
H	5.231139000000	-2.632622000000	0.198504000000
N	1.975758000000	0.553177000000	0.051332000000

Table S69. Optimized geometry of the **ground state** of **[Zn(HL^{q})Br$_2$]** (**normal form**, **S$_0^N$**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **using the QM/MM method (QM region)**.

Br	-2.102796000000	2.924662000000	-2.893366000000
Br	-2.007819000000	3.758215000000	1.204976000000
Zn	-2.541708000000	2.359463000000	-0.638421000000
O	-0.789297000000	-2.979490000000	-0.238218000000
H	0.150916000000	-2.624174000000	-0.259624000000
N	-2.107444000000	0.271075000000	-0.243342000000
N	-4.508570000000	1.509804000000	-0.325381000000

N	-1.538903000000	-1.832879000000	-0.246220000000
N	1.189950000000	-1.247827000000	-0.235071000000
C	-3.239941000000	-0.494076000000	-0.231023000000
C	-4.549274000000	0.174312000000	-0.158880000000
C	-5.623354000000	2.234013000000	-0.217239000000
H	-5.514008000000	3.307940000000	-0.357665000000
C	-6.861512000000	1.658645000000	0.070572000000
H	-7.741485000000	2.286099000000	0.150889000000
C	-6.920386000000	0.274195000000	0.257128000000
H	-7.861179000000	-0.203950000000	0.517768000000
C	-5.755530000000	-0.485746000000	0.131450000000
H	-5.771242000000	-1.559364000000	0.292841000000
C	-2.895761000000	-1.847344000000	-0.241215000000
C	-3.666063000000	-3.129092000000	-0.261078000000
H	-3.019234000000	-3.928468000000	-0.626482000000
H	-4.533346000000	-3.045879000000	-0.922073000000
H	-4.011426000000	-3.412166000000	0.740678000000
C	-1.070746000000	-0.556614000000	-0.240530000000
C	0.356223000000	-0.218700000000	-0.181988000000
C	2.530375000000	-1.021692000000	-0.202323000000
C	3.055784000000	0.307145000000	-0.151348000000
C	2.132185000000	1.386067000000	-0.054708000000
H	2.504728000000	2.405030000000	0.033469000000
C	0.781086000000	1.135699000000	-0.055033000000
H	0.058760000000	1.938791000000	0.064428000000
C	4.464677000000	0.498032000000	-0.177030000000
H	4.843670000000	1.517484000000	-0.186868000000
C	5.315814000000	-0.586842000000	-0.190766000000
H	6.393167000000	-0.437058000000	-0.200986000000
C	4.787849000000	-1.910025000000	-0.187121000000
H	5.467890000000	-2.757645000000	-0.158317000000
C	3.426198000000	-2.127978000000	-0.215850000000
H	3.012060000000	-3.132542000000	-0.246019000000

Table S70. Optimized geometry of the **ground state** of **[Zn(HL^{q})Br$_2$]** (**tautomeric form**, **S$_0^T$**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **using the QM/MM method (QM region)**.

Br	-2.085364000000	2.933039000000	-2.889797000000
Br	-1.979943000000	3.755989000000	1.199054000000
Zn	-2.558744000000	2.362127000000	-0.640096000000
O	-0.756708000000	-2.927666000000	-0.272769000000
H	0.738378000000	-2.162664000000	-0.270008000000
N	-2.123088000000	0.290062000000	-0.241214000000
N	-4.520776000000	1.517873000000	-0.321484000000
N	-1.529456000000	-1.854149000000	-0.259986000000
N	1.192203000000	-1.217027000000	-0.226904000000
C	-3.234625000000	-0.477558000000	-0.226211000000
C	-4.548796000000	0.180881000000	-0.154174000000
C	-5.640629000000	2.232016000000	-0.209876000000
H	-5.542243000000	3.306741000000	-0.352480000000

C	-6.872526000000	1.645602000000	0.083843000000
H	-7.756845000000	2.266045000000	0.167769000000
C	-6.919173000000	0.260562000000	0.269346000000
H	-7.854998000000	-0.225130000000	0.533589000000
C	-5.748656000000	-0.489873000000	0.136849000000
H	-5.752329000000	-1.564667000000	0.292091000000
C	-2.882517000000	-1.844348000000	-0.242812000000
C	-3.647795000000	-3.126584000000	-0.270209000000
H	-2.966368000000	-3.909819000000	-0.611398000000
H	-4.502429000000	-3.062142000000	-0.950430000000
H	-4.009793000000	-3.410484000000	0.726040000000
C	-1.082683000000	-0.556029000000	-0.252226000000
C	0.307177000000	-0.208474000000	-0.188504000000
C	2.548410000000	-1.040862000000	-0.196845000000
C	3.059293000000	0.284383000000	-0.151092000000
C	2.125023000000	1.365487000000	-0.063394000000
H	2.502184000000	2.382854000000	0.023097000000
C	0.773767000000	1.134975000000	-0.069366000000
H	0.060464000000	1.947323000000	0.041262000000
C	4.464240000000	0.472880000000	-0.173026000000
H	4.844770000000	1.491348000000	-0.182413000000
C	5.316356000000	-0.615707000000	-0.184135000000
H	6.393441000000	-0.466868000000	-0.191211000000
C	4.786860000000	-1.932780000000	-0.179298000000
H	5.462570000000	-2.783466000000	-0.147335000000
C	3.420654000000	-2.153325000000	-0.207906000000
H	3.009398000000	-3.159186000000	-0.236989000000

Table S71. Optimized geometry of the **first singlet excited state** of **[Zn(HL^{q})Br$_2$]** (**tautomeric form**, **S$_1^T$**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **using the QM/MM method (QM region)**.

Br	-2.114305000000	2.909845000000	-2.918798000000
Br	-2.012065000000	3.720506000000	1.200727000000
Zn	-2.537692000000	2.358800000000	-0.665326000000
O	-0.865648000000	-2.982671000000	-0.140865000000
H	0.864196000000	-2.175713000000	-0.330703000000
N	-2.102660000000	0.229512000000	-0.288825000000
N	-4.499088000000	1.504949000000	-0.332489000000
N	-1.578969000000	-1.896886000000	-0.203860000000
N	1.239548000000	-1.226578000000	-0.295242000000
C	-3.287549000000	-0.532771000000	-0.262948000000
C	-4.565172000000	0.165055000000	-0.180556000000
C	-5.602811000000	2.243936000000	-0.213835000000
H	-5.477579000000	3.317712000000	-0.341537000000
C	-6.851032000000	1.686622000000	0.070132000000
H	-7.719533000000	2.328879000000	0.158907000000
C	-6.935475000000	0.299769000000	0.242960000000
H	-7.884560000000	-0.164033000000	0.499509000000
C	-5.786201000000	-0.477423000000	0.108001000000

H	-5.818594000000	-1.552450000000	0.257760000000
C	-2.960876000000	-1.869436000000	-0.239841000000
C	-3.725869000000	-3.149697000000	-0.250528000000
H	-3.061662000000	-3.940988000000	-0.604629000000
H	-4.592295000000	-3.074097000000	-0.912327000000
H	-4.066444000000	-3.427963000000	0.753718000000
C	-1.099778000000	-0.596755000000	-0.231087000000
C	0.335201000000	-0.210480000000	-0.161396000000
C	2.597021000000	-1.033144000000	-0.231634000000
C	3.081766000000	0.314410000000	-0.145649000000
C	2.143010000000	1.371187000000	-0.016182000000
H	2.493329000000	2.394299000000	0.087310000000
C	0.760929000000	1.091237000000	0.005806000000
H	0.040329000000	1.889069000000	0.162191000000
C	4.488810000000	0.507483000000	-0.171822000000
H	4.858225000000	1.529524000000	-0.166230000000
C	5.358171000000	-0.575522000000	-0.194560000000
H	6.432829000000	-0.406844000000	-0.195899000000
C	4.855892000000	-1.894826000000	-0.205971000000
H	5.536147000000	-2.740775000000	-0.174306000000
C	3.480384000000	-2.125962000000	-0.251152000000
H	3.084696000000	-3.138335000000	-0.295658000000

Table S72. Optimized geometry of the **ground state** of **[Zn(HL^{q})I$_2$]** (**normal form**, **S$_0^N$**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **using the QM/MM method (QM region)**.

I	1.035469000000	3.922776000000	2.322231000000
I	1.304651000000	3.752057000000	-2.317629000000
Zn	0.608902000000	2.830060000000	0.010576000000
O	1.875961000000	-2.645210000000	0.605972000000
H	2.843031000000	-2.404720000000	0.455239000000
N	-1.431228000000	2.115637000000	-0.062133000000
N	0.877221000000	0.681870000000	0.092222000000
N	1.247443000000	-1.439176000000	0.446975000000
N	3.987158000000	-1.198581000000	0.113431000000
C	1.833157000000	-0.235248000000	0.197490000000
C	-0.100111000000	-1.313269000000	0.503932000000
C	-0.320179000000	0.042167000000	0.261858000000
C	3.281417000000	-0.082437000000	-0.003266000000
C	3.863185000000	1.176540000000	-0.327996000000
H	3.239537000000	2.053475000000	-0.472564000000
C	5.228620000000	1.236270000000	-0.482981000000
H	5.713010000000	2.179294000000	-0.730914000000
C	6.018364000000	0.060238000000	-0.333763000000
C	7.437107000000	0.048390000000	-0.456982000000
H	7.957314000000	0.986381000000	-0.647720000000
C	8.132993000000	-1.138380000000	-0.343031000000
H	9.215176000000	-1.152586000000	-0.441008000000
C	7.441099000000	-2.361868000000	-0.113723000000
H	8.001826000000	-3.292662000000	-0.070590000000

C	6.071248000000	-2.379570000000	0.037844000000
H	5.526659000000	-3.304188000000	0.216818000000
C	5.334513000000	-1.165264000000	-0.056412000000
C	-0.991437000000	-2.475169000000	0.797917000000
H	-1.532828000000	-2.808438000000	-0.096101000000
H	-1.714352000000	-2.200590000000	1.571654000000
H	-0.386856000000	-3.306605000000	1.162687000000
C	-1.576716000000	0.786582000000	0.088549000000
C	-2.845761000000	0.183228000000	0.023884000000
H	-2.953597000000	-0.892656000000	0.114479000000
C	-3.963975000000	0.993492000000	-0.181163000000
H	-4.955190000000	0.549720000000	-0.238414000000
C	-3.794854000000	2.375218000000	-0.320280000000
H	-4.635155000000	3.042600000000	-0.471220000000
C	-2.499285000000	2.889920000000	-0.261333000000
H	-2.302006000000	3.952574000000	-0.378278000000

Table S73. Optimized geometry of the **ground state** of **[Zn(HL^{q})I$_2$]** (**tautomeric form**, **S$_0^T$**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **using the QM/MM method (QM region)**.

I	1.049551000000	3.941821000000	2.319024000000
I	1.327260000000	3.750610000000	-2.309023000000
Zn	0.597983000000	2.835107000000	0.017296000000
O	1.917943000000	-2.600969000000	0.607215000000
H	3.446913000000	-2.037014000000	0.325840000000
N	-1.437708000000	2.122543000000	-0.061063000000
N	0.870682000000	0.699487000000	0.095051000000
N	1.260203000000	-1.462610000000	0.456086000000
N	4.001095000000	-1.170967000000	0.107781000000
C	1.828758000000	-0.235305000000	0.209521000000
C	-0.082502000000	-1.313980000000	0.503212000000
C	-0.307363000000	0.055013000000	0.258387000000
C	3.241712000000	-0.069844000000	0.002867000000
C	3.860776000000	1.173417000000	-0.324375000000
H	3.245535000000	2.055766000000	-0.470442000000
C	5.223783000000	1.217433000000	-0.478080000000
H	5.710306000000	2.159066000000	-0.726943000000
C	6.025346000000	0.039404000000	-0.331827000000
C	7.439703000000	0.026711000000	-0.457554000000
H	7.959782000000	0.964072000000	-0.649374000000
C	8.136945000000	-1.163521000000	-0.345971000000
H	9.218455000000	-1.178309000000	-0.447760000000
C	7.445075000000	-2.381743000000	-0.117971000000
H	8.001411000000	-3.314989000000	-0.077287000000
C	6.070805000000	-2.402282000000	0.036212000000
H	5.528987000000	-3.329003000000	0.214073000000
C	5.357222000000	-1.185315000000	-0.057935000000
C	-0.971788000000	-2.474177000000	0.800050000000
H	-1.517321000000	-2.813628000000	-0.089697000000

H	-1.691376000000	-2.211063000000	1.581596000000
H	-0.341717000000	-3.293628000000	1.151516000000
C	-1.569474000000	0.790647000000	0.086141000000
C	-2.831926000000	0.174661000000	0.019017000000
H	-2.926458000000	-0.902297000000	0.110029000000
C	-3.958117000000	0.973503000000	-0.188127000000
H	-4.944584000000	0.519673000000	-0.248198000000
C	-3.803108000000	2.357238000000	-0.324723000000
H	-4.649642000000	3.016342000000	-0.476641000000
C	-2.512809000000	2.885859000000	-0.260858000000
H	-2.327216000000	3.951049000000	-0.373692000000

Table S74. Optimized geometry of the **ground state** of **[Zn(HL^{q})Br$_2$]** (**normal form**, **S$_0^N$**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.

Zn	-1.584488000000	-1.520653000000	0.093658000000
Br	-1.103436000000	-2.094368000000	2.402099000000
Br	-1.344501000000	-3.051961000000	-1.771602000000
N	-0.707320000000	0.384641000000	-0.269559000000
N	-3.323408000000	-0.288600000000	-0.073729000000
O	1.314334000000	3.236262000000	-0.048657000000
H	2.141344000000	2.676266000000	0.059424000000
C	-1.642013000000	1.384535000000	-0.201163000000
C	-3.068077000000	1.029611000000	-0.199908000000
C	-4.584291000000	-0.733558000000	-0.068245000000
H	-4.712945000000	-1.809411000000	0.031915000000
C	-5.677954000000	0.127342000000	-0.181347000000
H	-6.689012000000	-0.269651000000	-0.169326000000
C	-5.428203000000	1.499256000000	-0.314540000000
H	-6.251051000000	2.203683000000	-0.413723000000
C	-4.109432000000	1.961117000000	-0.329320000000
H	-3.892963000000	3.017281000000	-0.453723000000
C	-1.000555000000	2.621321000000	-0.099375000000
C	-1.478104000000	4.035688000000	0.028129000000
H	-0.648938000000	4.680642000000	0.335341000000
H	-2.272007000000	4.104109000000	0.781237000000
H	-1.869536000000	4.408009000000	-0.928079000000
N	0.320359000000	2.296677000000	-0.115332000000
C	0.492450000000	0.952401000000	-0.222952000000
C	1.805729000000	0.299016000000	-0.260208000000
C	1.928960000000	-1.085998000000	-0.572717000000
H	1.055157000000	-1.675629000000	-0.837601000000
C	3.189533000000	-1.637883000000	-0.567430000000
H	3.331140000000	-2.691743000000	-0.801664000000
C	4.322085000000	-0.827352000000	-0.265106000000
C	4.094801000000	0.559131000000	0.011503000000
C	5.199960000000	1.409948000000	0.303059000000
H	5.007536000000	2.460223000000	0.512099000000
C	6.479301000000	0.891392000000	0.320249000000
H	7.323441000000	1.540113000000	0.545301000000
C	6.710615000000	-0.489047000000	0.047294000000
H	7.727192000000	-0.875939000000	0.067156000000

C	5.654606000000	-1.331217000000	-0.240516000000
H	5.821959000000	-2.386355000000	-0.451291000000
N	2.839731000000	1.083099000000	0.006155000000

Table S75. Optimized geometry of the **ground state** of **[Zn(HL^{q})Br$_2$]** (**tautomeric form**, **S$_0^T$**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.

Zn	-1.636554000000	1.496806000000	-0.134902000000
Br	-1.340901000000	2.222645000000	-2.434525000000
Br	-1.132500000000	3.009048000000	1.708813000000
N	-0.706450000000	-0.393284000000	0.175334000000
N	-3.344431000000	0.239135000000	0.071942000000
O	1.366669000000	-3.195570000000	-0.062491000000
H	2.680584000000	-2.070554000000	-0.138803000000
C	-1.617106000000	-1.399276000000	0.139413000000
C	-3.051074000000	-1.075072000000	0.161480000000
C	-4.616546000000	0.650052000000	0.083505000000
H	-4.775117000000	1.723688000000	0.006628000000
C	-5.686107000000	-0.242572000000	0.183470000000
H	-6.707558000000	0.127019000000	0.186519000000
C	-5.398493000000	-1.610044000000	0.279379000000
H	-6.201280000000	-2.339264000000	0.363102000000
C	-4.067812000000	-2.036448000000	0.271039000000
H	-3.821775000000	-3.089658000000	0.356158000000
C	-0.958365000000	-2.641570000000	0.048280000000
C	-1.426857000000	-4.060681000000	-0.039587000000
H	-0.559655000000	-4.702483000000	-0.225879000000
H	-2.145839000000	-4.188910000000	-0.858621000000
H	-1.902993000000	-4.382975000000	0.896294000000
N	0.364597000000	-2.331431000000	0.026625000000
C	0.505440000000	-0.970256000000	0.113027000000
C	1.784308000000	-0.304566000000	0.158563000000
C	1.929960000000	1.090670000000	0.396945000000
H	1.056522000000	1.696355000000	0.612035000000
C	3.189926000000	1.639305000000	0.404532000000
H	3.314897000000	2.704690000000	0.590048000000
C	4.347888000000	0.831657000000	0.185782000000
C	4.157369000000	-0.563538000000	-0.020985000000
C	5.260604000000	-1.426866000000	-0.221956000000
H	5.095347000000	-2.490788000000	-0.377359000000
C	6.536635000000	-0.889440000000	-0.218977000000
H	7.391959000000	-1.543272000000	-0.374136000000
C	6.746982000000	0.502289000000	-0.017205000000
H	7.759889000000	0.897787000000	-0.020229000000
C	5.671747000000	1.348725000000	0.182984000000
H	5.818810000000	2.415437000000	0.340988000000
N	2.880281000000	-1.055232000000	-0.022868000000

Table S76. Optimized geometry of the **ground state** of **[Zn(HL^q)I$_2$]** (**normal form**, **S$_0^N$**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.

Zn	-1.586477000000	-1.519767000000	0.070206000000
I	-1.114066000000	-2.165367000000	2.582109000000
I	-1.482707000000	-3.204392000000	-1.943145000000
N	-0.705353000000	0.385468000000	-0.281444000000
N	-3.325819000000	-0.284875000000	-0.084382000000
O	1.316318000000	3.234980000000	-0.036072000000
H	2.144315000000	2.673458000000	0.063147000000
C	-1.640039000000	1.385650000000	-0.209065000000
C	-3.066654000000	1.032837000000	-0.209575000000
C	-4.588147000000	-0.725042000000	-0.077609000000
H	-4.721091000000	-1.800594000000	0.020109000000
C	-5.679150000000	0.139493000000	-0.187596000000
H	-6.691342000000	-0.254488000000	-0.173686000000
C	-5.425404000000	1.510632000000	-0.321283000000
H	-6.246045000000	2.217814000000	-0.419321000000
C	-4.105130000000	1.967817000000	-0.338299000000
H	-3.884585000000	3.022921000000	-0.464588000000
C	-0.997543000000	2.620980000000	-0.096657000000
C	-1.473201000000	4.034816000000	0.042055000000
H	-0.648767000000	4.671689000000	0.377568000000
H	-2.282971000000	4.094049000000	0.778712000000
H	-1.841977000000	4.423790000000	-0.916573000000
N	0.323056000000	2.295666000000	-0.111259000000
C	0.495473000000	0.951977000000	-0.225411000000
C	1.809749000000	0.300185000000	-0.256519000000
C	1.936858000000	-1.087649000000	-0.553175000000
H	1.064960000000	-1.682524000000	-0.808688000000
C	3.198265000000	-1.636952000000	-0.544317000000
H	3.341466000000	-2.693056000000	-0.766725000000
C	4.329333000000	-0.820322000000	-0.254686000000
C	4.099580000000	0.568366000000	0.008018000000
C	5.203869000000	1.425079000000	0.285104000000
H	5.010187000000	2.477388000000	0.482623000000
C	6.484545000000	0.909622000000	0.301376000000
H	7.328151000000	1.563025000000	0.514513000000
C	6.718252000000	-0.473120000000	0.042446000000
H	7.735997000000	-0.857002000000	0.060954000000
C	5.663077000000	-1.320999000000	-0.230781000000
H	5.832046000000	-2.377856000000	-0.431387000000
N	2.842968000000	1.088697000000	0.000806000000

Table S77. Optimized geometry of the **ground state** of **[Zn(HL^q)I$_2$]** (**tautomeric form**, **S$_0^T$**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.

Zn	-1.640769000000	1.496303000000	-0.109971000000
I	-1.192323000000	2.288814000000	-2.588978000000
I	-1.274591000000	3.057793000000	1.988525000000

N	-0.708312000000	-0.391044000000	0.203944000000
N	-3.350189000000	0.232763000000	0.046873000000
O	1.368906000000	-3.190511000000	-0.037452000000
H	2.674679000000	-2.069112000000	-0.119857000000
C	-1.617053000000	-1.398708000000	0.159718000000
C	-3.051946000000	-1.078450000000	0.165080000000
C	-4.624238000000	0.636782000000	0.039009000000
H	-4.788904000000	1.707670000000	-0.058376000000
C	-5.690779000000	-0.258423000000	0.145844000000
H	-6.713598000000	0.107069000000	0.132008000000
C	-5.398239000000	-1.622220000000	0.272584000000
H	-6.198400000000	-2.353276000000	0.364995000000
C	-4.065651000000	-2.041929000000	0.285393000000
H	-3.816630000000	-3.091881000000	0.397163000000
C	-0.955915000000	-2.639397000000	0.066923000000
C	-1.426070000000	-4.057194000000	-0.031160000000
H	-0.564720000000	-4.699292000000	-0.240953000000
H	-2.159702000000	-4.172701000000	-0.838951000000
H	-1.886947000000	-4.391070000000	0.908448000000
N	0.366429000000	-2.326739000000	0.051516000000
C	0.505232000000	-0.964990000000	0.142255000000
C	1.784694000000	-0.299457000000	0.176651000000
C	1.936994000000	1.096909000000	0.403900000000
H	1.067654000000	1.706303000000	0.622166000000
C	3.198118000000	1.642776000000	0.396111000000
H	3.327069000000	2.709065000000	0.572847000000
C	4.351961000000	0.830712000000	0.172784000000
C	4.155894000000	-0.565378000000	-0.021812000000
C	5.254691000000	-1.433709000000	-0.225549000000
H	5.084177000000	-2.498257000000	-0.370734000000
C	6.532217000000	-0.899954000000	-0.237857000000
H	7.384282000000	-1.557458000000	-0.395405000000
C	6.748199000000	0.492781000000	-0.048667000000
H	7.762254000000	0.885088000000	-0.063465000000
C	5.677337000000	1.343986000000	0.154455000000
H	5.829396000000	2.411306000000	0.303325000000
N	2.877797000000	-1.053413000000	-0.008965000000

Table S78. Optimized geometry of the **first singlet excited state** of **[Zn(HL^{q})Br$_2$]** (**normal form**, **S$_1^N$**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.

Zn	-1.666417000000	-1.531711000000	0.100686000000
Br	-1.220270000000	-2.189062000000	2.397199000000
Br	-1.344456000000	-3.033047000000	-1.788336000000
N	-0.712922000000	0.344673000000	-0.219999000000
N	-3.342158000000	-0.224877000000	-0.073639000000
O	1.411989000000	3.155028000000	-0.024030000000
H	2.237890000000	2.512140000000	0.027773000000

C	-1.606812000000	1.374363000000	-0.163569000000
C	-3.022439000000	1.101210000000	-0.149093000000
C	-4.622646000000	-0.594177000000	-0.064076000000
H	-4.814927000000	-1.663279000000	-0.000448000000
C	-5.676037000000	0.328122000000	-0.129819000000
H	-6.704351000000	-0.022063000000	-0.121492000000
C	-5.364638000000	1.696846000000	-0.207547000000
H	-6.153177000000	2.443386000000	-0.263816000000
C	-4.028256000000	2.091239000000	-0.218229000000
H	-3.764164000000	3.140977000000	-0.291920000000
C	-0.898695000000	2.624938000000	-0.073181000000
C	-1.341400000000	4.046227000000	0.028240000000
H	-0.472660000000	4.690479000000	0.190405000000
H	-2.040281000000	4.169487000000	0.864886000000
H	-1.844455000000	4.358805000000	-0.896666000000
N	0.381944000000	2.272326000000	-0.076603000000
C	0.528074000000	0.874607000000	-0.178080000000
C	1.794825000000	0.248061000000	-0.217414000000
C	1.956170000000	-1.157631000000	-0.445111000000
H	1.093663000000	-1.781425000000	-0.666075000000
C	3.218367000000	-1.691757000000	-0.422747000000
H	3.375576000000	-2.753836000000	-0.599325000000
C	4.356197000000	-0.840835000000	-0.171523000000
C	4.109544000000	0.577914000000	0.018834000000
C	5.228255000000	1.447429000000	0.247827000000
H	5.035210000000	2.509069000000	0.388755000000
C	6.513182000000	0.934801000000	0.291181000000
H	7.354401000000	1.602467000000	0.468084000000
C	6.748836000000	-0.453937000000	0.108762000000
H	7.764798000000	-0.841187000000	0.147135000000
C	5.677373000000	-1.322146000000	-0.120985000000
H	5.853883000000	-2.387334000000	-0.264836000000
N	2.871442000000	1.087749000000	-0.012308000000

Table S79. Optimized geometry of the **first singlet excited state** of **[Zn(HL^{q})Br$_2$]** (**tautomeric form**, **S$_1^T$**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **in CH$_2$Cl$_2$ continuum solvation model**.

Zn	-1.440084000000	-1.437060000000	0.271660000000
Br	-0.979994000000	-1.929586000000	2.599886000000
Br	-1.337487000000	-2.872859000000	-1.694245000000
N	-0.652236000000	0.493511000000	-0.179327000000
N	-3.216421000000	-0.206448000000	0.184059000000
O	1.292954000000	3.235090000000	-0.799409000000
H	2.707468000000	1.950255000000	0.558703000000
C	-1.626301000000	1.505485000000	-0.211251000000
C	-3.017831000000	1.115729000000	-0.022390000000
C	-4.453807000000	-0.673408000000	0.362007000000
H	-4.544436000000	-1.745936000000	0.521991000000
C	-5.578395000000	0.158652000000	0.347496000000

H	-6.568713000000	-0.262350000000	0.496057000000
C	-5.387099000000	1.530895000000	0.138732000000
H	-6.234965000000	2.211749000000	0.120454000000
C	-4.093479000000	2.021278000000	-0.049874000000
H	-3.918189000000	3.079113000000	-0.218352000000
C	-1.017377000000	2.731416000000	-0.431094000000
C	-1.514329000000	4.137441000000	-0.557699000000
H	-0.660273000000	4.808915000000	-0.693609000000
H	-2.059300000000	4.440228000000	0.345037000000
H	-2.181264000000	4.240944000000	-1.423119000000
N	0.317851000000	2.427449000000	-0.563613000000
C	0.502923000000	1.047717000000	-0.403917000000
C	1.815926000000	0.408338000000	-0.485485000000
C	2.020994000000	-0.808613000000	-1.134726000000
H	1.182765000000	-1.274000000000	-1.649185000000
C	3.275139000000	-1.414382000000	-1.099573000000
H	3.443934000000	-2.367116000000	-1.594269000000
C	4.356569000000	-0.779056000000	-0.395689000000
C	4.114706000000	0.470599000000	0.260171000000
C	5.143216000000	1.131799000000	0.957634000000
H	4.936342000000	2.081358000000	1.448376000000
C	6.417790000000	0.563709000000	1.008781000000
H	7.212246000000	1.078857000000	1.544217000000
C	6.676449000000	-0.668066000000	0.372620000000
H	7.671821000000	-1.104427000000	0.419101000000
C	5.659625000000	-1.326711000000	-0.317261000000
H	5.853549000000	-2.276783000000	-0.812437000000
N	2.848687000000	1.012820000000	0.198669000000

Table S80. Optimized geometry of the **first singlet excited state** of **[Zn(HL^{q})I$_2$]** (**normal form**, **S$_1^N$**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.

Zn	-1.652730000000	-1.528471000000	0.106483000000
I	-1.195993000000	-2.153506000000	2.630657000000
I	-1.550149000000	-3.186052000000	-1.925279000000
N	-0.705817000000	0.351703000000	-0.227028000000
N	-3.330862000000	-0.220102000000	-0.097265000000
O	1.414994000000	3.165562000000	-0.009480000000
H	2.240399000000	2.529110000000	0.045560000000
C	-1.600883000000	1.380960000000	-0.167906000000
C	-3.016168000000	1.106382000000	-0.161054000000
C	-4.608440000000	-0.597187000000	-0.099988000000
H	-4.793662000000	-1.668489000000	-0.047680000000
C	-5.666213000000	0.319999000000	-0.163763000000
H	-6.692892000000	-0.035031000000	-0.164847000000
C	-5.360572000000	1.690827000000	-0.226712000000
H	-6.152557000000	2.433922000000	-0.280070000000
C	-4.026379000000	2.092277000000	-0.227254000000
H	-3.768950000000	3.143965000000	-0.290607000000
C	-0.894924000000	2.631156000000	-0.064803000000

C	-1.343849000000	4.049725000000	0.046009000000
H	-0.482792000000	4.696190000000	0.236810000000
H	-2.062212000000	4.157728000000	0.868104000000
H	-1.827687000000	4.373054000000	-0.885751000000
N	0.386521000000	2.279980000000	-0.065610000000
C	0.534697000000	0.883889000000	-0.172958000000
C	1.800416000000	0.256971000000	-0.201454000000
C	1.958525000000	-1.149545000000	-0.425795000000
H	1.092810000000	-1.770406000000	-0.639804000000
C	3.218610000000	-1.687093000000	-0.408551000000
H	3.373082000000	-2.749922000000	-0.582366000000
C	4.359086000000	-0.836309000000	-0.167683000000
C	4.115462000000	0.582651000000	0.024868000000
C	5.237476000000	1.450398000000	0.245609000000
H	5.047137000000	2.512137000000	0.389169000000
C	6.522092000000	0.936289000000	0.276832000000
H	7.365496000000	1.602915000000	0.447070000000
C	6.754586000000	-0.452439000000	0.090787000000
H	7.770538000000	-0.840618000000	0.118523000000
C	5.679935000000	-1.319295000000	-0.129370000000
H	5.854052000000	-2.384502000000	-0.275886000000
N	2.878275000000	1.095217000000	0.001386000000

Table S81. Optimized geometry of the **first singlet excited state** of **[Zn(HL^{q})I$_2$]** (**tautomeric form**, **S$_1^T$**) in Cartesian (XYZ) coordinates as calculated in Gaussian at the BMK/LANL2DZ/6-31+g(d) level of theory **in CH_2Cl_2 continuum solvation model**.

Zn	-1.477676000000	-1.451829000000	0.080353000000
I	-0.834747000000	-2.278485000000	2.497323000000
I	-1.459035000000	-2.818651000000	-2.173359000000
N	-0.656194000000	0.488673000000	-0.242999000000
N	-3.221779000000	-0.203774000000	0.162194000000
O	1.293913000000	3.240104000000	-0.819283000000
H	2.715379000000	2.008811000000	0.422388000000
C	-1.627720000000	1.503227000000	-0.254660000000
C	-3.015854000000	1.119928000000	-0.035821000000
C	-4.455567000000	-0.661183000000	0.385059000000
H	-4.549641000000	-1.734985000000	0.535802000000
C	-5.570740000000	0.182308000000	0.426722000000
H	-6.558274000000	-0.229954000000	0.613191000000
C	-5.373818000000	1.554757000000	0.221849000000
H	-6.214783000000	2.243967000000	0.243519000000
C	-4.084221000000	2.034645000000	-0.013226000000
H	-3.905876000000	3.092519000000	-0.177398000000
C	-1.014281000000	2.731771000000	-0.453894000000
C	-1.507205000000	4.141423000000	-0.553923000000
H	-0.654404000000	4.808698000000	-0.715085000000
H	-2.017893000000	4.441863000000	0.369707000000
H	-2.203475000000	4.254697000000	-1.394469000000
N	0.319021000000	2.428202000000	-0.589993000000

C	0.503079000000	1.044184000000	-0.452126000000
C	1.816122000000	0.403503000000	-0.508698000000
C	2.018401000000	-0.856843000000	-1.073005000000
H	1.184584000000	-1.346840000000	-1.570997000000
C	3.266159000000	-1.468206000000	-0.988674000000
H	3.429749000000	-2.452114000000	-1.420216000000
C	4.348310000000	-0.795892000000	-0.322804000000
C	4.111956000000	0.498733000000	0.242800000000
C	5.144112000000	1.200648000000	0.894688000000
H	4.943641000000	2.184659000000	1.315159000000
C	6.413607000000	0.627678000000	0.990434000000
H	7.210794000000	1.174015000000	1.489649000000
C	6.665258000000	-0.649008000000	0.445513000000
H	7.657002000000	-1.088402000000	0.527492000000
C	5.646211000000	-1.347401000000	-0.199947000000
H	5.834318000000	-2.331658000000	-0.625724000000
N	2.850539000000	1.042759000000	0.141584000000

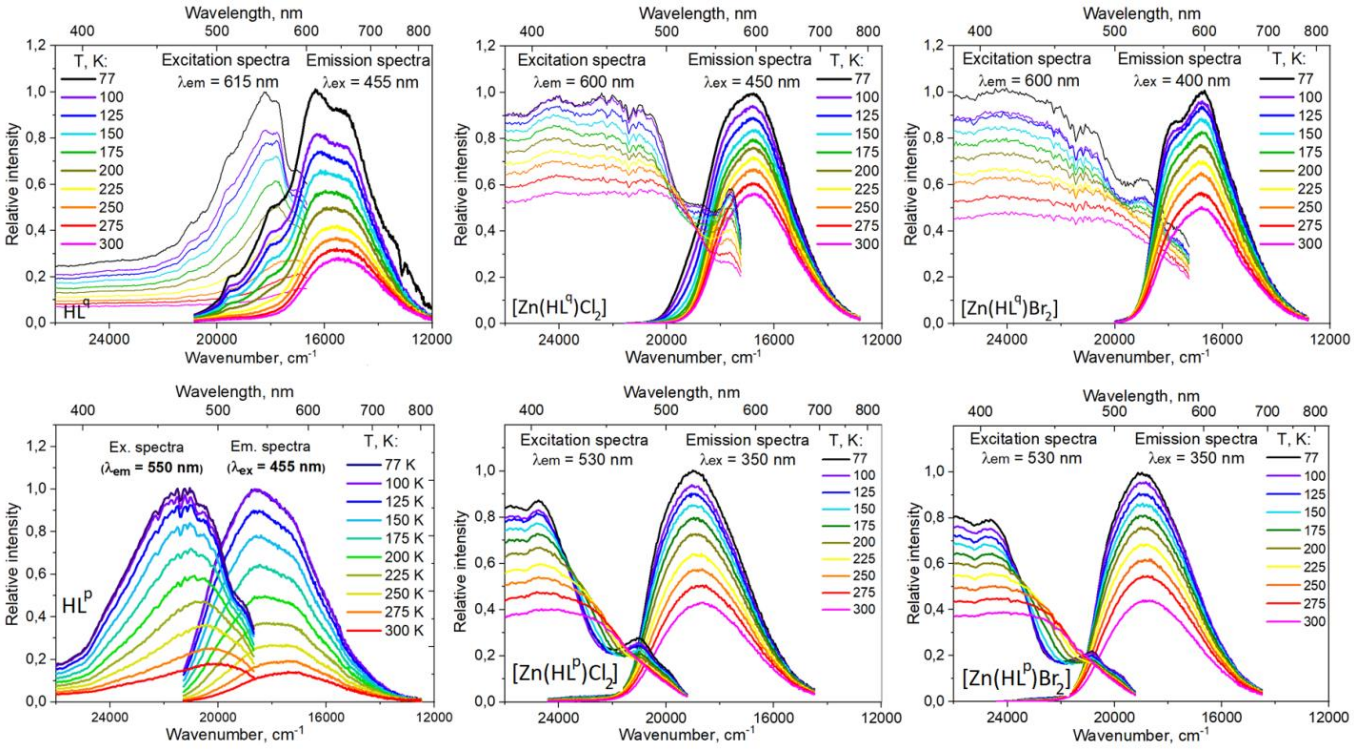


Figure S26. Comparison between the emission properties of HL^q / $[Zn(HL^q)Hal_2]$ and HL^p / $[Zn(HL^p)Hal_2]$ in the solid state.