Electronic Supplementary Information

# Efficient emission of Zn(II) and Cd(II) complexes with nopinaneannelated 4,5-diazaluorene and 4,5-diazaluoren-9-one ligands: how slight structural modification alters fluorescence mechanism

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# Table of Contents

Experimental part	3
Crystallographic data	3
Table S1	3
Table S2	4
Table S3	5
Figure S1	6
Figure S2	6
Figure S3	6
Figure S4	7
Figure S5	7
Figure S6	8
Figure S7	8
Figure S8	9
Figure S9	9
Figure S10	
Figure S11	
Figure \$12	
Figure \$13	
Figure \$14	
Figure S15	
Figure S16	
Figure S17	
Figure S12	13
Figure S10	13
Figure 519	13 14
Figure \$20	14 1 <i>1</i>
	14 1 /
IR Spectroscopy	14 14
	14
Figure SZZ	14
I dulle 54	15
	10
	10 17
	1/
	20
lable S11	
lable S12	
Table \$13	
Figure S23	
Table S14	25
Table S15	26
Figure S24	27
Table S16	27
Table S17	28
Figure S25	28
Table S18	29
Table S19	29
Figure S26	30
Table S20	30
Table S21	31
Table S22	31
Table S23	32
Table S24	32

## Experimental part

### Crystallographic data

**Table S1**. Crystallographic characteristics, experimental data and structure refinement for [ZnL<sup>o</sup>Cl<sub>2</sub>]·MeCN and [CdL<sup>o</sup>Cl<sub>2</sub>]<sub>n</sub>·nH<sub>2</sub>O.

Complex	[ZnL <sup>o</sup> Cl <sub>2</sub> ]·MeCN	[CdL <sup>o</sup> Cl <sub>2</sub> ] <sub>n</sub> ·nH <sub>2</sub> O
Empirical formula	C <sub>27</sub> H <sub>28</sub> Cl <sub>2</sub> N <sub>3</sub> OZn	$C_{25}H_{26}CdCl_2N_2O\cdot H_2O$
Formula weight	546.79	571.79
Crystal system	Orthorhombic	Monoclinic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	P2 <sub>1</sub>
<i>a,</i> Å	10.2980(5)	6.9333 (3)
<i>b,</i> Å	14.6532(7)	28.6315 (14)
<i>c,</i> Å	17.2961(9)	12.6065 (7)
β,°		99.520 (2)
<i>V</i> , Å <sup>3</sup>	2610.0(2)	2468.1 (2)
<i>Z</i> ; <i>d</i> <sub>calc</sub> , g/cm <sup>3</sup>	4, 1.392	4, 1.539
μ (mm⁻¹)	1.170	1.126
Crystal size, mm	0.2 x 0.15 x 0.1	0.16 x 0.05 x 0.03
Theta range for data collection (°)	3.642 - 62.19	3.572 - 60.06
Reflections collected	39080	40701
Independent reflections	7626	12477
(R <sub>int</sub> )	0.0578	0.0485
Number of reflections with <i>I</i> >2 <i>s</i> ( <i>I</i> )	5839	10189
Number of refined parameters	312	591
GOOF on F <sup>2</sup>	0.997	1.021
Final <i>R</i> indices ( $I>2\sigma_I$ )		
<i>R</i> <sub>1</sub>	0.0419	0.0342
wR <sub>2</sub>	0.0857	0.0732
<i>R</i> indices (all data)		
<i>R</i> <sub>1</sub>	0.0697	0.0514
wR <sub>2</sub>	0.0941	0.0776
Largest diff. peak and hole (e/Å <sup>3</sup> )	0.88/ -0.49	0.85/ -0.92
Flack parameter	0.013(5)	-0.013(11)

Table S2. Selected bond lengths (Å) and angles (°) for [ZnL<sup>o</sup>Cl<sub>2</sub>]·MeCN.



Bond	d (Å)
Zn(1)Cl(1)	2.180(1)
Zn(1)Cl(2)	2.190(1)
Zn(1)-N(13)	2.138(3)
Zn(1)–N(13A)	2.157(3)
N(13)-C(12)	1.335(5)
N(13)-C(3)	1.357(5)
N(13A)–C(12A)	1.330(5)
N(13)-C(3A)	1.344(5)
C(11)-C(12)	1.389(5)
C(12)–C(12a)	1.441(5)
Angle	ω (deg.)
Cl(1)-Zn(1)-Cl(2)	123.0(1)
N(13)–Zn(1)–N (13A)	84.2(1)
N(13)-Zn(1)-Cl(1)	111.6(1)
N(13) –Zn(1)–Cl(2)	111.6(1)
N(13A)-Zn(1)-Cl(1)	1114.(1)
N(13A)-Zn(1)-Cl(2)	105.5(1)

 $\label{eq:stable} \textbf{Table S3}. \ \text{Selected bond lengths (Å) and angles (°) for } [\textbf{CdL}^{o}\textbf{Cl}_2]_n \cdot \textbf{nH}_2\textbf{O}.$ 



Bond	d (Å)	Bond	d (Å)
Cd(1)Cl(1)	2.602(1)	Cd(2)Cl(1)	2.588(1)
Cd(1)Cl(2)	2.570(1)	Cd(2)Cl(2)	2.593(1)
Cd(1)Cl(3)	2.564(1)	Cd(2)-Cl(3) <sup>2</sup>	2.684(1)
Cd(1)Cl(4)1	2.675(1)	Cd(2)Cl(4)	2.571(1)
Cd(1)-N(1)	2.441(4)	Cd(2)-N(1A)	2.426(4)
Cd(1)-N(2)	2.439(4)	Cd(2)–N(2A)	2.482(4)
Angle	ω (deg.)	Angle	ω (deg.)
Cl(1)Cd(1)Cl(4) <sup>1</sup>	172.1(1)	Cl(1)Cd(2)Cl(4)	93.9(1)
Cl(2)Cd(1)Cl(4) <sup>1</sup>	96.4(1)	Cl(2)Cd(2)Cl(4)	103.2(1)
Cl(3)Cd(1)Cl(4) <sup>1</sup>	85.7(1)	Cl(3) <sup>2</sup> Cd(2)Cl(4)	85.4(1)
Cl(1)Cd(1)Cl(2)	86.0(1)	Cl(1)Cd(2)Cl(2)	85.9(1)
Cl(1)Cd(1)Cl(3)	101.8(1)	Cl(1)Cd(2)Cl(3) <sup>2</sup>	97.5(1)
Cl(2)Cd(1)Cl(3)	91.2(1)	Cl(2)Cd(2)Cl(3) <sup>2</sup>	170.7(1)
N(1)Cd(1)Cl(1)	93.8(1)	N(1A)Cd(2)Cl(1)	102.3(1)
N(1)Cd(1)Cl(2)	97.7(1)	N(1A)Cd(2)Cl(2)	94.7(1)
N(1)Cd(1)Cl(4) <sup>1</sup>	78.4(1)	N(1A)Cd(2)Cl(4)	156.7(1)
N(1)Cd(1)Cl(3)	162.6(1)	N(1A)Cd(2)Cl(3) <sup>2</sup>	76.1(1)
N(2)Cd(1)Cl(1)	88.1(1)	N(2A)Cd(2)Cl(1)	166.5(1)
N(2)Cd(1)Cl(2)	170.9(1)	N(2A)Cd(2)Cl(2)	81.2(1)
N(2)Cd(1)Cl(4) <sup>1</sup>	88.6(1)	N(2A)Cd(2)Cl(4)	93.1(1)
N(2)Cd(1)Cl(3)	96.9(1)	N(2A)Cd(2)Cl(3) <sup>2</sup>	94.7(1)
N(1)Cd(1)N(2)	75.8(1)	N(1A)Cd(2)N(2A)	74.8(1)

<sup>1</sup> -1+X,+Y,+Z, <sup>2</sup> 1+X,+Y,+Z



**Figure S1**. Packing diagram of **[ZnL<sup>o</sup>Cl<sub>2</sub>]·MeCN**, view along the *a* axis.



Figure S2. Packing diagram of [ZnL<sup>o</sup>Cl<sub>2</sub>]·MeCN, view along the *b* axis.



**Figure S3**. Packing diagram of **[ZnL<sup>o</sup>Cl<sub>2</sub>]·MeCN**, view along the *c* axis.



Figure S4. A 2D supramolecular layer in the structure of [ZnL<sup>o</sup>Cl<sub>2</sub>]·MeCN (frontal view and side view).



Figure S5. Packing of 2D supramolecular layers in the structure of [ZnL<sup>o</sup>Cl<sub>2</sub>]·MeCN (side view).



Figure S6. A 2D supramolecular layer in the structure of [ZnLCl<sub>2</sub>]·CH<sub>2</sub>Cl<sub>2</sub> (frontal view and side view).



Figure S7. Packing of 2D supramolecular layers in the structure of [ZnLCl<sub>2</sub>]·CH<sub>2</sub>Cl<sub>2</sub> (side view).



Figure S8. A 2D supramolecular layer in the structure of [ZnLCl<sub>2</sub>]-*i*PrOH (frontal view and side view)



Figure S9. Packing of 2D supramolecular layers in the structure of [ZnLCl<sub>2</sub>]·*i*PrOH (side view).



**Figure S10**. Packing diagram of **[CdL<sup>o</sup>Cl<sub>2</sub>]<sub>n</sub>·nH<sub>2</sub>O**, view along the *a* axis.



**Figure S11**. Packing diagram of  $[CdL^{o}Cl_{2}]_{n} \cdot nH_{2}O$ , view along the *b* axis.



Figure S12. Packing diagram of  $[CdL^{o}Cl_{2}]_{n} \cdot nH_{2}O$ , view along the *c* axis.



Figure S13. Hydrogen bonds between the  $H_2O$  molecules and 1D polymeric chain in the structure of  $[CdL^oCl_2]_n \cdot nH_2O$ .



Figure S14. The H<sub>2</sub>O molecules between the 1D polymeric chain in the structure of  $[CdL^{o}Cl_{2}]_{n} \cdot nH_{2}O$ .



Figure S15. The packing of supramolecular layers in the structure of  $[CdL^{o}Cl_{2}]_{n} \cdot nH_{2}O$  (two layers are shown).



Figure S16. The packing of 1D supramolecular chains in the structure of [CdLCl<sub>2</sub>]<sub>n</sub>.



Figure S17. The angle between the planes of two pyridine moieties (6.02°) in the structure of L<sup>0</sup>.



Figure S18. The angle between the planes of two pyridine moieties (8.77°) in the structure of  $[ZnL^{o}Cl_{2}]$ ·MeCN.



**Figure S19**. The angles between the planes of the pyridine moieties (3.62 and 4.17°) in the structure of  $[CdL^{o}Cl_{2}]_{n} \cdot nH_{2}O$ .

#### Thermogravimetric analysis



Figure S20. TGA data for L<sup>0</sup>, ZnL<sup>0</sup>Cl<sub>2</sub>·2.5H<sub>2</sub>O and CdL<sup>0</sup>Cl<sub>2</sub>·0.5H<sub>2</sub>O.

IR spectroscopy



Figure S21. IR spectra of L<sup>o</sup>, ZnL<sup>o</sup>Cl<sub>2</sub>·2.5H<sub>2</sub>O and CdL<sup>o</sup>Cl<sub>2</sub>·0.5H<sub>2</sub>O in KBr in the 4000 – 400 cm<sup>-1</sup> range.



Figure S22. IR spectra of L<sup>o</sup>, ZnL<sup>o</sup>Cl<sub>2</sub>·2.5H<sub>2</sub>O and CdL<sup>o</sup>Cl<sub>2</sub>·0.5H<sub>2</sub>O in KBr in the 1900 – 400 cm<sup>-1</sup> range.

Compound	aromatic	aliphatic v(C–H)	v(C=O)	v(C=N)	v(C=O)
	v(C–H)				
Lo	3031, 3002	2971, 2948, 2927, 2900,	1720	1597, 1576 <i>,</i>	1470, 1455,
		2868, 2828		1559	1446,1421
ZnL <sup>o</sup> Cl <sub>2</sub> ·2.5H <sub>2</sub> O	3037, 2996	2969, 2954, 2934, 2872	1733	1617, 1594,	1469, 1458, 1447,
				1577	1424
CdL <sup>0</sup> Cl <sub>2</sub> ·0.5H <sub>2</sub> O	3042, 2992	2973, 2950, 2928, 2868	1725	1617, 1597,	1470, 1457, 1446,
				1572	1420

Table S4. Main vibrational frequencies (cm<sup>-1</sup>) in the IR spectra of L<sup>o</sup>, ZnL<sup>o</sup>Cl<sub>2</sub>·2.5H<sub>2</sub>O and CdL<sup>o</sup>Cl<sub>2</sub>·0.5H<sub>2</sub>O.

## Theoretical part

**Table S5.** Optimized geometry of the **ground state** of **L** in Cartesian (XYZ) coordinates as calculated in Gaussian at the B3LYP/6-31+g(d) level of theory.

C	1.533888000000	5.235059000000	-0.355896000000	
н	1.679093000000	4.163737000000	-0.512152000000	
Н	2.073617000000	5.509892000000	0.559560000000	
Н	2.014763000000	5.764007000000	-1.188806000000	
С	0.061896000000	5.641610000000	-0.248356000000	
C	-0.887984000000	4.836650000000	0.727168000000	
н	-0.974038000000	5.184774000000	1.762888000000	
C C	-0 597873000000	3 358095000000	0 638484000000	
C	-0 442313000000	2 510338000000	1 736995000000	
С	-0 510704000000	2 904347000000	2 749811000000	
C C		1 16203600000	1 /0200/000000	
		0.0000000000000000000000000000000000000	2 4/03/2000000	
	0.0000000000000	0.15247200000	2.440342000000	
П	0.800734000000	7 155472000000	0.00044000000	
L L	0.000000000000	7.155402000000	0.009440000000	
н	-1.019893000000	7.53899100000	0.103849000000	
н	0.482022000000	7.700212000000	-0.812195000000	
Н	0.53606/000000	7.410132000000	0.932364000000	
С	-2.045953000000	5.140292000000	-0.273706000000	
Н	-2.821112000000	4.373323000000	-0.373418000000	
Н	-2.523150000000	6.106222000000	-0.096692000000	
C	-0.945567000000	5.190094000000	-1.370318000000	
Н	-1.087782000000	5.870836000000	-2.217854000000	
С	-0.656546000000	3.755145000000	-1.845901000000	
Н	-1.472645000000	3.397087000000	-2.487532000000	
Н	0.251737000000	3.713418000000	-2.461303000000	
С	-0.502816000000	2.809693000000	-0.663488000000	
Ν	-0.271350000000	1.517065000000	-0.913217000000	
С	-0.129279000000	0.725748000000	0.155939000000	
С	-1.533888000000	-5.235059000000	-0.355896000000	
Н	-1.679093000000	-4.163737000000	-0.512152000000	
н	-2.073617000000	-5.509892000000	0.559560000000	
н	-2.014763000000	-5.764007000000	-1.188806000000	
C	-0.061896000000	-5.641610000000	-0.248356000000	
C	0.887984000000	-4.836650000000	0.727168000000	
Н	0.974038000000	-5.184774000000	1.762888000000	
C	0.597873000000	-3.358095000000	0.638484000000	
C C	0 442313000000	-2 510338000000	1 736995000000	
н	0 510704000000	-2 904347000000	2 749811000000	
C C	0.310704000000	-1 16293600000	1 /9200/000000	
Ц		-0 152/172000000	3 098786000000	
C C		-7.15540200000	0.000110000000	
	1.010802000000	7.133402000000	0.009440000000	
	1.019893000000	7.338991000000	0.103849000000	
	-0.482022000000	-7.700212000000	-0.812195000000	
H	-0.53606/000000	-7.410132000000	0.932364000000	
	2.045953000000	-5.140292000000	-0.273706000000	
н	2.821112000000	-4.3/3323000000	-0.3/3418000000	
Н	2.523150000000	-6.106222000000	-0.096692000000	
I C	0.945567000000	-5.190094000000	-1.370318000000	

Н	1.087782000000	-5.870836000000	-2.217854000000	
C	0.656546000000	-3.755145000000	-1.845901000000	
н	1.472645000000	-3.397087000000	-2.487532000000	
Н	-0.251737000000	-3.713418000000	-2.461303000000	
C	0.502816000000	-2.809693000000	-0.663488000000	
N	0.271350000000	-1.517065000000	-0.913217000000	
C	0.129279000000	-0.725748000000	0.155939000000	

**Table S6.** Optimized geometry of the first singlet excited state of L in Cartesian (XYZ) coordinates ascalculated in Gaussian at the B3LYP/6-31+g(d) level of theory.

С	1.531796000000	5.213966000000	-0.336031000000	
Н	1.670467000000	4.142282000000	-0.496738000000	
Н	2.059492000000	5.478167000000	0.589430000000	
Н	2.028077000000	5.746554000000	-1.157671000000	
С	0.061465000000	5.628454000000	-0.247190000000	
С	-0.905785000000	4.810575000000	0.722910000000	
Н	-1.002144000000	5.164009000000	1.755701000000	
С	-0.617042000000	3.345862000000	0.639369000000	
С	-0.450577000000	2.494449000000	1.763701000000	
Н	-0.524552000000	2.88987800000	2.774099000000	
С	-0.204623000000	1.163874000000	1.508230000000	
C	0.000000000000	0.000000000000	2.458338000000	
Н	0.866412000000	0.151547000000	3.117369000000	
C	0.000000000000	7.138630000000	0.024736000000	
Н	-1.019488000000	7.525439000000	0.108750000000	
Н	0.494364000000	7.688501000000	-0.786779000000	
Н	0.526190000000	7.383887000000	0.955737000000	
C	-2.050018000000	5.133534000000	-0.297672000000	
Н	-2.829110000000	4.373143000000	-0.412370000000	
Н	-2.520893000000	6.101775000000	-0.112108000000	
C	-0.936112000000	5.182281000000	-1.377138000000	
Н	-1.065424000000	5.862312000000	-2.227543000000	
C	-0.649962000000	3.746112000000	-1.846151000000	
Н	-1.463593000000	3.388351000000	-2.493005000000	
Н	0.259591000000	3.691609000000	-2.459911000000	
C	-0.505845000000	2.789515000000	-0.675417000000	
Ν	-0.260323000000	1.509459000000	-0.953542000000	
C	-0.120770000000	0.700677000000	0.144792000000	
С	-1.531796000000	-5.213966000000	-0.336031000000	
Н	-1.670467000000	-4.142282000000	-0.496738000000	
Н	-2.059492000000	-5.478167000000	0.589430000000	
Н	-2.028077000000	-5.746554000000	-1.157671000000	
C	-0.061465000000	-5.628454000000	-0.247190000000	
C	0.905785000000	-4.810575000000	0.722910000000	
Н	1.002144000000	-5.164009000000	1.755701000000	
C	0.617042000000	-3.345862000000	0.639369000000	
C	0.450577000000	-2.494449000000	1.763701000000	
Н	0.524552000000	-2.889878000000	2.774099000000	
C	0.204623000000	-1.163874000000	1.508230000000	
Н	-0.866412000000	-0.151547000000	3.117369000000	
C	0.000000000000	-7.138630000000	0.024736000000	
Н	1.019488000000	-7.525439000000	0.108750000000	

Н	-0.494364000000	-7.68850100000	-0.786779000000	
Н	-0.526190000000	-7.383887000000	0.955737000000	
C	2.050018000000	-5.133534000000	-0.297672000000	
Н	2.829110000000	-4.373143000000	-0.412370000000	
Н	2.520893000000	-6.101775000000	-0.112108000000	
C	0.936112000000	-5.182281000000	-1.377138000000	
Н	1.065424000000	-5.862312000000	-2.227543000000	
C	0.649962000000	-3.746112000000	-1.846151000000	
Н	1.463593000000	-3.388351000000	-2.493005000000	
Н	-0.259591000000	-3.691609000000	-2.459911000000	
C	0.505845000000	-2.789515000000	-0.675417000000	
N	0.260323000000	-1.509459000000	-0.953542000000	
C	0.120770000000	-0.700677000000	0.144792000000	

**Table S7.** Optimized geometry of the **ground state** of  $L^{0}$  in Cartesian (XYZ) coordinates as calculated in Gaussian at the B3LYP/6-31+g(d) level of theory.

N	1.543141000000	-1.047981000000	-0.152652000000	
C	0.741953000000	0.010781000000	-0.074156000000	
0	-0.000017000000	3.47802000000	-0.000096000000	
N	-1.543182000000	-1.047962000000	0.152951000000	
С	1.180553000000	1.346848000000	-0.118264000000	
С	-3.400293000000	0.525185000000	0.344744000000	
С	-0.741966000000	0.010798000000	0.074369000000	
С	-2.534260000000	1.618463000000	0.254545000000	
Н	-2.901685000000	2.641444000000	0.291857000000	
С	3.400258000000	0.525114000000	-0.344791000000	
С	2.534246000000	1.618422000000	-0.254597000000	
Н	2.901701000000	2.641388000000	-0.292024000000	
C	2.854499000000	-0.779772000000	-0.286079000000	
С	-4.895734000000	0.621885000000	0.524996000000	
Н	-5.241206000000	1.659402000000	0.589958000000	
C	5.264487000000	-1.473999000000	-0.546128000000	
Н	5.956508000000	-2.319417000000	-0.634134000000	
C	0.000003000000	2.259396000000	0.000026000000	
C	-2.854525000000	-0.779731000000	0.286301000000	
C	4.895694000000	0.621801000000	-0.525165000000	
Н	5.241137000000	1.659319000000	-0.590294000000	
C	-5.633677000000	-0.344953000000	-0.486322000000	
C	-1.180554000000	1.346854000000	0.118330000000	
C	3.814260000000	-1.955003000000	-0.361407000000	
Н	3.517570000000	-2.602957000000	-1.197009000000	
Н	3.703682000000	-2.564757000000	0.545007000000	
C	-5.288865000000	-0.382574000000	1.652366000000	
Н	-4.582351000000	-0.49054000000	2.481998000000	
Н	-6.285951000000	-0.201147000000	2.057488000000	
C	-5.264563000000	-1.47391000000	0.546188000000	
Н	-5.956574000000	-2.319334000000	0.634227000000	
C	5.633728000000	-0.344893000000	0.486201000000	
C	-5.120165000000	-0.449812000000	-1.924649000000	
Н	-4.042197000000	-0.614406000000	-1.993192000000	
Н	-5.346941000000	0.469813000000	-2.478889000000	
Н	-5.618412000000	-1.27670700000	-2.446677000000	

C	5.120409000000	-0.449473000000	1.924620000000	
Н	4.042504000000	-0.614375000000	1.993355000000	
н	5.346967000000	0.47041000000	2.478525000000	
Н	5.618968000000	-1.276034000000	2.446877000000	
С	7.146108000000	-0.075896000000	0.535155000000	
Н	7.605092000000	0.013502000000	-0.453537000000	
Н	7.658330000000	-0.889536000000	1.063794000000	
Н	7.352822000000	0.853041000000	1.081021000000	
C	-3.814311000000	-1.954941000000	0.361637000000	
Н	-3.703641000000	-2.564799000000	-0.544698000000	
Н	-3.517709000000	-2.602794000000	1.197346000000	
C	5.288736000000	-0.382789000000	-1.652436000000	
Н	4.582168000000	-0.490826000000	-2.482013000000	
Н	6.285814000000	-0.201438000000	-2.057625000000	
C	-7.146045000000	-0.075925000000	-0.535510000000	
Н	-7.605145000000	0.013691000000	0.453104000000	
Н	-7.658231000000	-0.889660000000	-1.064042000000	
Н	-7.352652000000	0.852903000000	-1.081599000000	

**Table S8.** Optimized geometry of the **first singlet excited state** of  $L^{0}$  in Cartesian (XYZ) coordinates as calculated in Gaussian at the B3LYP/6-31+g(d) level of theory.

N 1.53629300000 -0.09552300000 -0.07111900000   C 0.70369500000 3.52434900000 0.0004000000   N -1.53629100000 1.09552700000 0.15259500000   C 1.34261900000 1.36281500000 0.11567300000   C -3.36204400000 0.53263400000 0.34834000000   C -3.36204400000 0.62850100000 0.07100000000   C -3.36204400000 1.61994100000 0.25622000000   C -2.50688100000 1.61994700000 0.25622000000   C 3.36205300000 1.61994700000 0.25622500000   C 3.36205300000 1.61994700000 0.25622500000   C 2.50688700000 1.61994700000 0.2862300000   C 2.87492200000 2.6420300000 0.2862300000   C 2.8172800000 0.62928400000 0.52934000000   C 3.84305500000 1.46914100000 0.54353800000   C 5.24373600000 2.3022900000 0.52928300000   C -2.8172800000 1.66562500000 0.52928300000   C -2.8172800000					
C 0.703695000000 -0.02849900000 -0.07111900000   O 0.000005000000 3.52434900000 0.0004000000   N -1.53629100000 -1.09552700000 0.15259500000   C 1.14261900000 1.36281500000 0.34834000000   C -3.36204400000 0.53263400000 0.07100000000   C -0.70369600000 -0.02850100000 0.25622000000   C -2.50688100000 1.61994100000 0.25622000000   C 3.36205300000 0.53264200000 -0.34834100000   C 2.50688700000 1.61994700000 -0.25622500000   C 2.87492200000 2.6420300000 -0.28662300000   C 2.81728500000 -0.82138400000 0.52934000000   C 5.48370200000 1.6656900000 0.5938300000   C 5.24373600000 1.46914100000 -0.54353800000   C -2.81727800000 -0.328594000000 0.52928300000   C -2.81727800000 0.62929800000 -0.5928300000   C -2.81727800000 -0.33583900000 -0.59283000000   C -5.991630000	Ν	1.536293000000	-1.095523000000	-0.152702000000	
O 0.00000500000 3.52434900000 0.00004000000   N -1.53629100000 -1.095527000000 0.15259500000   C 1.14261900000 1.36281500000 0.34834000000   C -3.362044000000 -0.3265100000 0.71000000000   C -0.70369600000 0.02850100000 0.25622000000   H -2.50688100000 1.61994100000 0.25622000000   C 3.36205300000 0.53264200000 -0.34834100000   C 2.50688700000 1.6194700000 -0.26522500000   H -2.87491500000 2.64200300000 -0.28663300000   C 2.81728500000 0.62928400000 0.5293400000   H -5.18870200000 1.66560900000 0.59383200000   C 5.24373600000 -2.3022900000 0.62955400000   C -2.81727800000 -2.8173800000 0.2866800000   C -2.81727800000 0.62929800000 0.52928300000   C -2.81727800000 0.62929800000 0.52928300000   C -5.9106300000 -0.33583900000 0.4825100000   C -5.9106300000	C	0.703695000000	-0.028499000000	-0.071119000000	
N -1.536291000000 -1.095527000000 0.152595000000   C 1.14261900000 1.362815000000 -0.11567300000   C -3.36204400000 0.53263400000 0.07100000000   C -0.70369600000 -0.02850100000 0.07100000000   C -2.506881000000 1.61994100000 0.25622000000   H -2.874915000000 2.64199600000 0.29614200000   C 3.36205300000 1.61994700000 -0.25622500000   H 2.87492200000 2.64200300000 -0.29611300000   C 2.87492200000 2.64200300000 -0.2862300000   C -4.84305500000 1.6656900000 0.5938300000   C -4.843055000000 1.6656900000 0.59383800000   H 5.188702000000 -2.30229000000 -0.2865800000   C -2.81727800000 -0.82139100000 0.2828300000   C -3.84307100000 1.66562000000 -0.59828300000   C -5.19472000000 1.6625500000 -0.59828300000   C -5.5916300000 -0.35838900000 -0.59828300000   C -1.462	0	0.000005000000	3.524349000000	0.000040000000	
C 1.142619000000 1.362815000000 -0.115673000000   C -3.362044000000 0.532634000000 0.348340000000   C -0.70369600000 -0.02850100000 0.275622000000   C -2.50688100000 2.64199600000 0.296142000000   H -2.87491500000 2.64199600000 -0.34834100000   C 3.36205300000 0.532642000000 -0.34834100000   C 2.50688700000 1.61994700000 -0.29611300000   H 2.87492200000 2.64200300000 -0.2961300000   C 2.81728500000 -0.82138400000 -0.296300000   C 2.81728500000 -0.6292400000 0.59348200000   C 5.48373600000 1.46914100000 -0.54353800000   C 5.24373600000 -2.8679600000 -0.82856800000   C -2.81727800000 -2.82979600000 -0.52928300000   C -2.81727800000 -6.2354500000 -0.52928300000   C -3.83359600000 -1.6652500000 -0.52928300000   C -5.9106300000 -1.362811000000 -0.48241000000   C	Ν	-1.536291000000	-1.095527000000	0.152595000000	
C -3.362044000000 0.532634000000 0.348340000000   C -0.703696000000 -0.028501000000 0.07100000000   C -2.50688100000 1.619941000000 0.25622000000   C 3.362053000000 0.532642000000 -0.348341000000   C 2.506887000000 1.619947000000 -0.25622500000   H 2.87492200000 2.64200300000 -0.29611300000   C 2.50688700000 1.61994700000 -0.28662300000   H 2.87492200000 2.64200300000 -0.29611300000   C 2.81728500000 -0.82138400000 -0.28662300000   C 2.81728500000 1.66560900000 0.59348200000   H -5.18870200000 1.46914100000 -0.62955400000   C -0.0000300000 -2.30229000000 -0.52928300000   C -2.817278000000 -0.82139100000 -0.28668000000   C -2.817278000000 -0.62929800000 -0.52928300000   C -3.80359600000 -0.3583900000 -0.52928300000   C -5.9106300000 -0.35283000000 -0.362560000000   H	C	1.142619000000	1.362815000000	-0.115673000000	
C -0.70369600000 -0.02850100000 0.07100000000   C -2.50688100000 1.61994100000 0.25622000000   H -2.87491500000 2.64199600000 -0.34834100000   C 3.36205300000 0.53264200000 -0.34834100000   C 2.50688700000 1.61994700000 -0.25622500000   H 2.87492200000 2.64200300000 -0.2866300000   C 2.81728500000 -0.82138400000 0.5293400000   C -4.84305500000 1.6650900000 0.5293400000   H -5.18870200000 1.46914100000 -0.5433800000   C -2.81727800000 -2.802900000 -0.62955400000   C -0.0000300000 2.26979600000 -0.59828300000   C -2.81727800000 -0.82139100000 0.52928300000   C -2.81727800000 -0.33583900000 -0.59828300000   C -2.81727800000 -0.33583900000 -0.59828300000   C -5.916300000 -1.97431800000 -0.32656000000   C -1.4261800000 -1.97431800000 -1.20249800000   H 3.52321200	C	-3.362044000000	0.532634000000	0.348340000000	
C -2.506881000000 1.619941000000 0.25622000000   H -2.874915000000 2.64199600000 0.29614200000   C 3.36205300000 0.53264200000 -0.34834100000   C 2.50688700000 1.61994700000 -0.25622500000   H 2.87492200000 2.6420030000 -0.28662300000   C 2.81728500000 0.62928400000 0.5293400000   C -4.84305500000 1.66560900000 0.5938200000   H -5.18870200000 -1.46914100000 -0.54353800000   C 5.24373600000 -2.3022900000 -0.62955400000   C -0.0000300000 2.26979600000 -0.5928300000   C -2.81727800000 -0.82139100000 0.28656800000   C -2.81727800000 -0.82139100000 0.52928300000   C -2.81727800000 -0.33583900000 -0.52928300000   C -3.80359600000 -1.97431800000 -0.59828300000   C -1.14261800000 -1.97431800000 -3.625600000   C -5.24651000000 -2.62439300000 -1.20249800000   H 3.5232	C	-0.703696000000	-0.028501000000	0.071000000000	
H-2.8749150000002.6419960000000.296142000000C3.3620530000000.532642000000-0.348341000000C2.5068870000001.619947000000-0.256225000000H2.8749220000002.642003000000-0.296113000000C2.817285000000-0.821384000000-0.286623000000H-5.1887020000001.6656090000000.598382000000H-5.188702000000-1.469141000000-0.54353800000C5.243736000000-2.30229000000-0.629554000000H5.950400000002.269796000000-0.000049000000C-2.817278000000-0.821391000000-0.28283000000C-2.817278000000-0.629298000000-0.529283000000C-2.8172780000001.665625000000-0.598283000000H5.188720000001.65625000000-0.598283000000C-2.8172780000001.652794000000-0.32526000000C-3.80359600000-1.97431800000-1.202498000000H3.70188800000-2.591371000000.539842000000H-4.54182100000-0.507979000002.48163900000H-6.23765000000-0.175978000002.05969000000H-6.23765000000-1.4691550000000.543551000000H-5.950381000000-2.302306000000.629571000000	C	-2.506881000000	1.619941000000	0.256220000000	
C3.362053000000.53264200000-0.34834100000C2.506887000001.61994700000-0.25622500000H2.874922000002.64200300000-0.29611300000C2.81728500000-0.821384000000.28662300000C-4.843055000000.629284000000.52934000000H-5.188702000001.665609000000.59838200000C5.24373600000-1.46914100000-0.54353800000H5.95040000000-2.30229000000-0.629554000000C-0.00003000002.26979600000-0.00049000000C-2.81727800000-0.821391000000.28656800000C-2.817278000000.6292800000-0.52928300000C-5.5916300000-0.33583900000-0.5828300000C-5.59166300000-1.362811000000.11561200000C-1.142618000001.362811000000.11561200000C3.8035960000-1.97431800000-0.36256000000H3.70188800000-2.591371000001.65279400000H-4.54182100000-0.507979000002.48163900000H-6.23765000000-0.175978000002.05969000000H-6.23765000000-1.469155000000.543551000000H-5.95038100000-2.302366000000.629571000000	Н	-2.874915000000	2.641996000000	0.296142000000	
C 2.50688700000 1.61994700000 -0.25622500000   H 2.87492200000 2.64200300000 -0.29611300000   C 2.81728500000 -0.82138400000 -0.28662300000   C -4.84305500000 0.62928400000 0.52934000000   H -5.18870200000 1.66560900000 0.59838200000   C 5.24373600000 -1.46914100000 -0.54353800000   H 5.950400000000 2.26979600000 -0.62955400000   C -0.0000300000 2.26979600000 -0.62958800000   C -2.81727800000 -0.82139100000 0.28656800000   C -2.81727800000 1.66562500000 -0.59828300000   C 4.84307100000 1.66562500000 -0.59828300000   C -5.95916300000 -0.33583900000 -0.488241000000   C -1.14261800000 1.36281100000 0.115612000000   C 3.80359600000 -1.97431800000 -0.36256000000   H 3.70188800000 -2.59137100000 0.53984200000   H 3.70188800000 -2.50797900000 2.48163900000  H -5.2465100000	C	3.362053000000	0.532642000000	-0.348341000000	
H2.874922000002.64200300000-0.29611300000C2.81728500000-0.82138400000-0.28662300000C-4.843055000000.629284000000.52934000000H-5.188702000001.665609000000.59838200000C5.24373600000-1.46914100000-0.54353800000H5.950400000002.26979600000-0.62955400000C-0.00003000002.26979600000-0.0004900000C-2.81727800000-0.821391000000.28656800000C-2.817278000001.66562500000-0.59828300000H5.188720000001.66562500000-0.59828300000C-5.59106300000-0.33583900000-0.488241000000C-1.142618000001.362811000000.11561200000C3.80359600000-1.97431800000-0.36256000000H3.70188800000-2.591371000000.53984200000H-5.24651000000-0.507979000002.48163900000H-4.54182100000-0.507979000002.48163900000H-6.23765000000-1.75978000002.05969000000H-5.95038100000-2.302366000000.629571000000	C	2.506887000000	1.619947000000	-0.256225000000	
C2.81728500000-0.82138400000-0.28662300000C-4.843055000000.629284000000.52934000000H-5.188702000001.665609000000.59838200000C5.24373600000-1.46914100000-0.54353800000H5.95040000000-2.30229000000-0.629554000000C-0.00003000002.26979600000-0.00004900000C-2.81727800000-0.821391000000.28656800000C-2.817278000000.62929800000-0.52928300000H5.188720000001.66562500000-0.5928300000C-5.59106300000-0.33583900000-0.488241000000C-1.142618000001.362811000000.115612000000C3.80359600000-1.97431800000-0.36256000000H3.70188800000-2.591371000000.53984200000H-5.24651000000-0.507979000002.48163900000H-6.23765000000-0.175978000002.05969000000H-5.95038100000-2.302306000000.629571000000	Н	2.874922000000	2.642003000000	-0.296113000000	
C-4.843055000000.629284000000.52934000000H-5.188702000001.665609000000.59838200000C5.24373600000-1.46914100000-0.54353800000H5.950400000002.202900000-0.62955400000C-0.00003000002.26979600000-0.0004900000C-2.817278000000.821391000000.28656800000C4.843071000000.62929800000-0.52928300000H5.188720000001.66562500000-0.59828300000C-5.59106300000-0.33583900000-0.48824100000C-1.142618000001.362811000000.11561200000C3.80359600000-1.97431800000-1.20249800000H3.70188800000-2.591371000000.53984200000H-4.54182100000-0.507979000002.48163900000H-6.23765000000-0.175978000002.05969000000H-5.95038100000-2.302306000000.629571000000	C	2.817285000000	-0.821384000000	-0.286623000000	
H-5.188702000001.665609000000.59838200000C5.24373600000-1.46914100000-0.54353800000H5.950400000002.26979600000-0.62955400000C-0.00003000002.26979600000-0.00004900000C-2.81727800000-0.821391000000.28656800000C4.843071000000.62929800000-0.52928300000H5.188720000001.66562500000-0.59828300000C-5.59106300000-0.33583900000-0.48824100000C-1.42618000001.362811000000.11561200000C3.80359600000-1.97431800000-0.36256000000H3.52321200000-2.591371000000.53984200000H3.70188800000-2.591371000001.65279400000H-4.54182100000-0.507979000002.48163900000H-6.23765000000-0.175978000002.05969000000H-5.95038100000-2.302366000000.62957100000	C	-4.843055000000	0.629284000000	0.529340000000	
C5.243736000000-1.469141000000-0.543538000000H5.950400000000-2.302290000000-0.629554000000C-0.000030000002.269796000000-0.000049000000C-2.817278000000-0.8213910000000.286568000000C4.8430710000000.629298000000-0.529283000000H5.188720000001.665625000000-0.598283000000C-5.591063000000-0.335839000000-0.488241000000C-1.1426180000001.3628110000000.115612000000C3.803596000000-1.974318000000-0.362560000000H3.523212000000-2.5913710000000.539842000000H3.701888000000-2.5913710000000.539842000000H-4.541821000000-0.362794000000H-6.23765000000-0.1759780000002.05969000000H-5.950381000000-2.3023060000000.629571000000	Н	-5.188702000000	1.665609000000	0.598382000000	
H5.95040000000-2.30229000000-0.629554000000C-0.00003000002.26979600000-0.00004900000C-2.81727800000-0.821391000000.28656800000C4.843071000000.62929800000-0.52928300000H5.188720000001.66562500000-0.59828300000C-5.59106300000-0.33583900000-0.488241000000C-5.591063000001.362811000000.115612000000C-1.142618000001.36281100000-0.36256000000H3.52321200000-2.62439300000-1.20249800000H3.70188800000-2.591371000000.53984200000H-4.54182100000-0.507979000002.48163900000H-6.23765000000-0.175978000002.05969000000H-6.23765000000-1.469155000000.543551000000H-5.95038100000-2.302306000000.629571000000	C	5.243736000000	-1.469141000000	-0.543538000000	
C-0.00003000002.26979600000-0.00004900000C-2.81727800000-0.821391000000.28656800000C4.843071000000.62929800000-0.52928300000H5.188720000001.66562500000-0.59828300000C-5.59106300000-0.33583900000-0.48824100000C-1.142618000001.362811000000.115612000000C3.80359600000-1.97431800000-0.36256000000H3.52321200000-2.62439300000-1.20249800000H3.70188800000-2.591371000000.53984200000C-5.24651000000-0.367979000002.48163900000H-6.23765000000-0.175978000002.05969000000H-5.95038100000-2.302306000000.629571000000	Н	5.95040000000	-2.302290000000	-0.629554000000	
C-2.817278000000-0.8213910000000.286568000000C4.8430710000000.629298000000-0.529283000000H5.188720000001.665625000000-0.598283000000C-5.591063000000-0.33583900000-0.488241000000C-1.1426180000001.3628110000000.115612000000C3.803596000000-1.974318000000-0.362560000000H3.523212000000-2.624393000000-1.202498000000H3.701888000000-2.5913710000000.539842000000C-5.246510000000-0.362794000000H-4.541821000000-0.1759780000002.059690000000H-6.237650000000-1.4691550000000.543551000000H-5.950381000000-2.3023060000000.629571000000	C	-0.000003000000	2.269796000000	-0.000049000000	
C4.843071000000.62929800000-0.52928300000H5.188720000001.66562500000-0.59828300000C-5.59106300000-0.33583900000-0.488241000000C-1.142618000001.362811000000.115612000000C3.80359600000-1.97431800000-0.36256000000H3.52321200000-2.62439300000-1.20249800000H3.70188800000-2.591371000000.53984200000C-5.24651000000-0.384125000001.65279400000H-4.54182100000-0.507979000002.48163900000H-6.23765000000-0.175978000002.05969000000H-5.95038100000-2.302306000000.629571000000	C	-2.817278000000	-0.821391000000	0.286568000000	
H5.188720000001.66562500000-0.59828300000C-5.59106300000-0.33583900000-0.48824100000C-1.142618000001.362811000000.11561200000C3.80359600000-1.97431800000-0.36256000000H3.52321200000-2.62439300000-1.20249800000H3.70188800000-2.591371000000.53984200000C-5.24651000000-0.384125000001.65279400000H-4.54182100000-0.507979000002.48163900000H-6.23765000000-0.175978000002.05969000000C-5.24372000000-1.469155000000.543551000000H-5.95038100000-2.302306000000.629571000000	C	4.843071000000	0.629298000000	-0.529283000000	
C-5.59106300000-0.33583900000-0.488241000000C-1.142618000001.362811000000.115612000000C3.80359600000-1.97431800000-0.36256000000H3.52321200000-2.62439300000-1.202498000000H3.70188800000-2.591371000000.539842000000C-5.24651000000-0.384125000001.65279400000H-4.54182100000-0.507979000002.48163900000H-6.23765000000-0.175978000002.05969000000H-5.95038100000-2.302306000000.629571000000	Н	5.188720000000	1.665625000000	-0.598283000000	
C-1.142618000001.362811000000.11561200000C3.80359600000-1.97431800000-0.36256000000H3.52321200000-2.62439300000-1.20249800000H3.70188800000-2.591371000000.53984200000C-5.24651000000-0.384125000001.65279400000H-4.54182100000-0.507979000002.48163900000H-6.23765000000-0.175978000002.05969000000C-5.24372000000-1.469155000000.543551000000H-5.95038100000-2.302306000000.629571000000	C	-5.591063000000	-0.335839000000	-0.488241000000	
C3.803596000000-1.974318000000-0.362560000000H3.523212000000-2.624393000000-1.202498000000H3.701888000000-2.5913710000000.539842000000C-5.246510000000-0.3841250000001.652794000000H-4.541821000000-0.5079790000002.481639000000H-6.237650000000-0.1759780000002.059690000000C-5.243720000000-1.4691550000000.543551000000H-5.950381000000-2.3023060000000.629571000000	C	-1.142618000000	1.362811000000	0.115612000000	
H3.523212000000-2.624393000000-1.202498000000H3.701888000000-2.5913710000000.539842000000C-5.246510000000-0.3841250000001.652794000000H-4.541821000000-0.5079790000002.481639000000H-6.237650000000-0.1759780000002.059690000000C-5.243720000000-1.4691550000000.543551000000H-5.950381000000-2.3023060000000.629571000000	C	3.803596000000	-1.974318000000	-0.362560000000	
H3.701888000000-2.5913710000000.539842000000C-5.246510000000-0.3841250000001.652794000000H-4.541821000000-0.5079790000002.481639000000H-6.237650000000-0.1759780000002.0596900000000C-5.243720000000-1.4691550000000.543551000000H-5.950381000000-2.30230600000000.629571000000	Н	3.523212000000	-2.624393000000	-1.202498000000	
C-5.24651000000-0.384125000001.652794000000H-4.54182100000-0.507979000002.48163900000H-6.23765000000-0.175978000002.059690000000C-5.24372000000-1.469155000000.543551000000H-5.95038100000-2.3023060000000.629571000000	Н	3.701888000000	-2.591371000000	0.539842000000	
H-4.541821000000-0.5079790000002.481639000000H-6.237650000000-0.1759780000002.059690000000C-5.243720000000-1.4691550000000.543551000000H-5.950381000000-2.3023060000000.629571000000	C	-5.246510000000	-0.384125000000	1.652794000000	
H-6.23765000000-0.1759780000002.059690000000C-5.24372000000-1.4691550000000.543551000000H-5.950381000000-2.3023060000000.629571000000	Н	-4.541821000000	-0.507979000000	2.481639000000	
C -5.24372000000 -1.469155000000 0.543551000000 H -5.950381000000 -2.302306000000 0.629571000000	Н	-6.237650000000	-0.175978000000	2.059690000000	
H -5.950381000000 -2.302306000000 0.629571000000	C	-5.24372000000	-1.469155000000	0.543551000000	
	Н	-5.950381000000	-2.302306000000	0.629571000000	

C	5.591042000000	-0.335853000000	0.488297000000	
C	-5.067348000000	-0.439014000000	-1.923112000000	
Н	-3.993367000000	-0.632717000000	-1.983969000000	
Н	-5.262816000000	0.492532000000	-2.468555000000	
Н	-5.583270000000	-1.246197000000	-2.458341000000	
С	5.067278000000	-0.439063000000	1.923148000000	
Н	3.993296000000	-0.632777000000	1.983964000000	
Н	5.262719000000	0.492474000000	2.468616000000	
Н	5.583188000000	-1.246251000000	2.458380000000	
C	7.096506000000	-0.037171000000	0.542005000000	
Н	7.557895000000	0.054610000000	-0.445396000000	
Н	7.619362000000	-0.840216000000	1.076481000000	
Н	7.284099000000	0.897221000000	1.084818000000	
C	-3.803588000000	-1.974327000000	0.362504000000	
Н	-3.701913000000	-2.591354000000	-0.539920000000	
Н	-3.523173000000	-2.624428000000	1.202413000000	
C	5.246571000000	-0.38408000000	-1.652750000000	
Н	4.541915000000	-0.507911000000	-2.481627000000	
Н	6.237727000000	-0.175922000000	-2.059600000000	
C	-7.096529000000	-0.037155000000	-0.541889000000	
Н	-7.557886000000	0.054593000000	0.445528000000	
Н	-7.619401000000	-0.840181000000	-1.076377000000	
Н	-7.284137000000	0.897256000000	-1.084665000000	

**Table S9.** Optimized geometry of the **ground state** of **[ZnLCl<sub>2</sub>]** in Cartesian (XYZ) coordinates as calculated in Gaussian at the B3LYP/LANL2DZ/6-31+g(d) level of theory.

Zn	-0.000076000000	-1.766385000000	-0.000146000000	
Cl	-0.250426000000	-2.688284000000	-2.050337000000	
Cl	0.250148000000	-2.692427000000	2.048079000000	
N	-1.455688000000	-0.053557000000	0.161257000000	
С	-3.365605000000	1.403054000000	0.367378000000	
N	1.455732000000	-0.053569000000	-0.160273000000	
С	2.778354000000	0.113231000000	-0.303326000000	
С	4.862792000000	1.429265000000	-0.553550000000	
Н	5.254213000000	2.449947000000	-0.622295000000	
С	-1.185531000000	2.372191000000	0.128784000000	
С	3.673909000000	-1.105449000000	-0.381644000000	
н	3.345395000000	-1.735998000000	-1.218862000000	
Н	3.538139000000	-1.707774000000	0.526342000000	
С	-0.718423000000	1.058431000000	0.079451000000	
С	3.365614000000	1.403022000000	-0.366847000000	
С	0.718470000000	1.058426000000	-0.078570000000	
С	2.559829000000	2.545902000000	-0.276372000000	
Н	3.014095000000	3.533216000000	-0.324952000000	
С	-2.778329000000	0.113258000000	0.304096000000	
С	0.000012000000	3.324066000000	0.000280000000	
Н	-0.094597000000	3.979828000000	-0.875305000000	
Н	0.094611000000	3.979940000000	0.875780000000	
C	5.141796000000	-0.682882000000	-0.571887000000	
Н	5.795071000000	-1.557142000000	-0.661154000000	
С	-5.141838000000	-0.682865000000	0.572218000000	
Н	-5.795102000000	-1.557143000000	0.661397000000	

C	1.185560000000	2.372187000000	-0.128142000000
C	-2.559815000000	2.545922000000	0.276857000000
Н	-3.014085000000	3.533243000000	0.325248000000
C	5.559919000000	0.431027000000	0.458186000000
C	-5.205634000000	0.404580000000	1.680485000000
Н	-4.492722000000	0.323486000000	2.507598000000
Н	-6.207435000000	0.544878000000	2.08925000000
C	5.205350000000	0.404494000000	-1.680244000000
Н	6.207070000000	0.544743000000	-2.089227000000
Н	4.492255000000	0.323378000000	-2.507191000000
C	-3.673887000000	-1.105420000000	0.382366000000
Н	-3.345592000000	-1.735863000000	1.219757000000
Н	-3.537858000000	-1.707861000000	-0.52550000000
C	5.048100000000	0.350532000000	1.899071000000
Н	5.515399000000	-0.494321000000	2.419847000000
Н	3.965295000000	0.225408000000	1.978388000000
Н	5.314732000000	1.261589000000	2.449827000000
C	-4.86280300000	1.429283000000	0.553815000000
Н	-5.254293000000	2.449949000000	0.622389000000
C	-5.047538000000	0.350413000000	-1.898773000000
Н	-3.964749000000	0.225022000000	-1.97782000000
Н	-5.313806000000	1.261568000000	-2.449550000000
Н	-5.514903000000	-0.494296000000	-2.419719000000
C	-5.559718000000	0.430961000000	-0.458027000000
C	-7.082257000000	0.637641000000	-0.50120900000
Н	-7.32880300000	1.557447000000	-1.045975000000
Н	-7.542166000000	0.706342000000	0.488746000000
Н	-7.560174000000	-0.196451000000	-1.029427000000
C	7.082485000000	0.637604000000	0.501015000000
Н	7.329239000000	1.557225000000	1.045993000000
Н	7.542115000000	0.706596000000	-0.489047000000
Н	7.560493000000	-0.196685000000	1.028842000000

**Table S10.** Optimized geometry of the **first singlet excited state** of **[ZnLCl<sub>2</sub>]** in Cartesian (XYZ) coordinates as calculated in Gaussian at the B3LYP/LANL2DZ/6-31+g(d) level of theory.

Zn	-0.000005000000	-1.750898000000	0.000002000000	
CI	-0.279438000000	-2.777380000000	-2.017232000000	
Cl	0.279417000000	-2.777441000000	2.017204000000	
N	-1.433498000000	-0.074232000000	0.166678000000	
C	-3.349858000000	1.412442000000	0.382847000000	
N	1.433488000000	-0.074233000000	-0.166654000000	
C	2.759759000000	0.117798000000	-0.315443000000	
C	4.834025000000	1.438757000000	-0.565582000000	
Н	5.230938000000	2.456726000000	-0.635774000000	
C	-1.186968000000	2.403852000000	0.133342000000	
C	3.660387000000	-1.091259000000	-0.386458000000	
н	3.336210000000	-1.724848000000	-1.225464000000	
Н	3.510781000000	-1.698901000000	0.517256000000	
C	-0.697065000000	1.071481000000	0.081022000000	
C	3.349850000000	1.412437000000	-0.382831000000	
C	0.697056000000	1.071480000000	-0.080996000000	
С	2.546277000000	2.589120000000	-0.284478000000	

Н	3.007342000000	3.571161000000	-0.335679000000	
C	-2.75977000000	0.117800000000	0.315459000000	
C	-0.000003000000	3.354263000000	0.000012000000	
Н	-0.097795000000	4.010077000000	-0.875018000000	
Н	0.097790000000	4.010077000000	0.875042000000	
C	5.130068000000	-0.676868000000	-0.567318000000	
Н	5.781459000000	-1.553568000000	-0.647413000000	
C	-5.130078000000	-0.676863000000	0.567320000000	
Н	-5.781476000000	-1.553558000000	0.647407000000	
C	1.186961000000	2.403850000000	-0.133317000000	
C	-2.546284000000	2.589124000000	0.284498000000	
Н	-3.007348000000	3.571165000000	0.335697000000	
C	5.542022000000	0.438088000000	0.461245000000	
C	-5.198624000000	0.400390000000	1.681357000000	
Н	-4.494867000000	0.309712000000	2.514609000000	
Н	-6.203752000000	0.554147000000	2.078427000000	
C	5.198620000000	0.400388000000	-1.681352000000	
Н	6.203752000000	0.554145000000	-2.078415000000	
Н	4.494866000000	0.309713000000	-2.514608000000	
C	-3.660399000000	-1.091258000000	0.386471000000	
Н	-3.336230000000	-1.724847000000	1.225481000000	
Н	-3.510789000000	-1.698901000000	-0.517241000000	
C	5.020414000000	0.368936000000	1.898207000000	
Н	5.495072000000	-0.463879000000	2.431786000000	
Н	3.938292000000	0.232661000000	1.966988000000	
Н	5.271408000000	1.289514000000	2.440235000000	
C	-4.83403200000	1.438761000000	0.565588000000	
Н	-5.230951000000	2.456729000000	0.635776000000	
C	-5.020333000000	0.368935000000	-1.898195000000	
Н	-3.938206000000	0.232661000000	-1.966926000000	
Н	-5.27130400000	1.289510000000	-2.440239000000	
Н	-5.494966000000	-0.463884000000	-2.431791000000	
C	-5.54200000000	0.438092000000	-0.461257000000	
C	-7.060326000000	0.661700000000	-0.507635000000	
H	-7.296600000000	1.585797000000	-1.049364000000	
H	-7.525178000000	0.727066000000	0.480096000000	
Н	-7.542258000000	-0.165999000000	-1.043417000000	
C	7.060349000000	0.661695000000	0.507558000000	
H	/.296647000000	1.58579600000	1.049269000000	
H	7.525155000000	0.727051000000	-0.480196000000	
Н	/.542303000000	-0.166001000000	1.043325000000	

**Table S11.** Optimized geometry of the **ground state** of **[ZnL<sup>o</sup>Cl<sub>2</sub>]** in Cartesian (XYZ) coordinates as calculated in Gaussian at the B3LYP/LANL2DZ/6-31+g(d) level of theory.

Zn	0.000052000000	-1.895996000000	0.000201000000	
Cl	-0.254841000000	-2.787935000000	-2.055622000000	
Cl	0.254748000000	-2.789366000000	2.055299000000	
N	-1.460583000000	-0.167356000000	0.161642000000	
Ν	1.460537000000	-0.167296000000	-0.161248000000	
С	-4.871431000000	1.330790000000	0.553621000000	
Н	-5.259701000000	2.352207000000	0.621874000000	
C	4.871282000000	1.331035000000	-0.553692000000	

H   5.25947100000   2.35249300000   0.36796500000     C   3.374328000000   1.301847000000   0.36796500000     C   2.7833800000   0.01155000000   0.34476600000     C   2.78338300000   0.115500000   0.34476600000     C   3.68542600000   1.20413700000   0.38320600000     H   -3.35619200000   1.3809500000   0.5222100000     H   -3.356467300000   1.2398500000   0.52382200000     H   3.354667300000   1.38383700000   0.5721400000     H   5.86613000000   0.66289000000   0.66289000000     C   5.5591200000   0.327630000   0.66289000000     C   5.56914900000   0.33274000000   0.4580600000     C   5.56914900000   0.322541000000   2.08741900000     C   5.215464000000   0.22451000000   2.0883900000     C   5.215464000000   0.22451000000   2.0881900000     C   5.215464000000   0.22451000000   2.0883900000     C   5.215464000000   0.224561000				
C -3.37442000000 1.301845000000 -0.367513000000   C 2.789338000000 0.011153500000 0.30476600000   C 2.78933700000 0.11165000000 0.3320600000   H 3.35519200000 -1.83409900000 1.22061200000   H 3.35519200000 -1.83409900000 0.52422100000   H 3.35476400000 -1.8383700000 0.52422100000   H 3.5476400000 -1.8383700000 0.5282200000   H 3.54667300000 -1.8358700000 0.5282200000   H 3.54647300000 -1.85581800000 0.660889000000   C 5.15319200000 -0.78137100000 0.57289300000   C 5.15319200000 0.33276300000 -0.45872500000   C 5.56914900000 0.3225200000 1.68050700000   C 5.556914900000 0.24256100000 2.50822500000   C 5.556914900000 0.24827000000 2.5082500000   C 5.15464000000 0.248517000000 2.5082500000   C 5.1546000000 0.24821600000 -5.50817000000   C 7.01731000000	Н	5.259471000000	2.352493000000	-0.621794000000
C 3.37432800000 1.03198700000 -0.36751300000   C 2.78939800000 0.01165000000 -0.30453500000   C 3.68542600000 -1.20413700000 0.3842600000   H 3.35466200000 -1.83699500000 -0.52422100000   H 3.35466200000 -1.20398500000 -0.52422100000   H 3.54647300000 -1.20398500000 0.52382200000   H 3.54647300000 -1.855800000 0.57201400000   H 5.56914900000 -0.878137100000 0.57201400000   C 5.15319200000 -0.8550600000 -0.66228800000   C 5.56914900000 0.33270400000 -0.45872500000   C 5.56914900000 0.3225200000 1.65995100000   C 5.56914900000 0.22451000000 2.08471900000   C 5.21546400000 0.22451000000 -2.083090000   C 5.21546400000 0.22451000000 -2.0830900000   C 5.25454700000 0.22451000000 -2.0830900000   C 7.09099900000 0.42432300000 -0.502415000000   C 7.9125900000	С	-3.374420000000	1.301845000000	0.367965000000
C   -2.789338000000   0.011535000000   -0.30476600000     C   2.789337000000   -1.204137000000   0.383206000000     H   -3.35519200000   -1.80699500000   -0.524221000000     H   -3.54606200000   -1.8089500000   -0.3836000000     H   -3.5476400000   -1.833837000000   -0.32382000000     H   3.5476400000   -1.808900000   0.57214000000     C   5.153346000000   -0.78137100000   0.57289300000     C   5.153346000000   -0.7811600000   -0.7829300000     C   5.153346000000   -0.78117000000   -0.45872500000     C   5.153346000000   -0.323763000000   -0.6229800000     C   5.51919000000   -0.323763000000   -0.45872500000     C   5.569149000000   0.322451000000   2.50822500000     H   -6.217785000000   0.32874000000   2.50822500000     H   -4.503577000000   0.424827000000   -2.508317000000     H   -7.559715000000   0.42483000000   -0.502471000000     C	С	3.374328000000	1.301987000000	-0.367513000000
C 2.789337000000 -0.1165000000 -0.30453500000   H 3.55192000000 -1.83409900000 0.38220600000   H -3.5460200000 -1.80699500000 0.52422100000   C 3.685373000000 -1.203985000000 0.52422100000   H 3.54674000000 -1.833837000000 0.52382200000   H 3.54647300000 -1.85588000000 0.52382200000   C -5.15334600000 -0.78137100000 0.57283900000   H 5.80613900000 -1.65551600000 0.45872500000   C 5.56914900000 0.33276400000 0.45872500000   C 5.56914900000 0.2456100000 2.50822500000   C 5.56914900000 0.24586100000 2.5082100000   C 5.56914900000 0.22546100000 2.50821700000   C 5.56914900000 0.225461000000 2.508517000000   C 5.51454000000 0.225461000000 -2.508517000000   C 5.215464000000 0.2254000000 -2.508517000000   C 7.5097500000 0.231743000000 -1.60923000000   C 7.509750000	С	-2.789398000000	0.011535000000	0.304766000000
C -3.68542600000 -1.204137000000 0.38320600000   H -3.355192000000 -1.80699500000 0.524221000000   C 3.68537300000 -1.20398500000 0.52422100000   H 3.5454647300000 -1.80698000000 0.52382200000   C -5.15334600000 -1.85581800000 0.57201400000   H -5.86473300000 -0.78113700000 0.57201400000   C -5.15334600000 -0.7811360000 0.57201400000   H -5.80613300000 -0.7811360000 0.6628900000   C -5.568912000000 0.33276400000 -0.6827800000   C -5.56914900000 0.33276400000 2.6872500000   C -5.21606600000 0.3025200000 1.67995100000   H -6.21778500000 0.24851000000 2.08741900000   C 5.21546400000 0.30685200000 -1.68050700000   H -6.21778500000 0.48277000000 -2.08830900000   C 7.09099900000 0.4823800000 -0.50241500000   H -7.531637000000 0.48277000000 -1.03129900000  H 7.35163900000<	С	2.789337000000	0.011650000000	-0.304535000000
H -3.35512000000 -1.834099000000 -1.220412000000   H -3.354606200000 -1.2398500000 -0.38360000000   C 3.685373000000 -1.838337000000 -0.23836000000   H 3.354764000000 -1.838337000000 .0523822000000   C 5.153346000000 -0.78111600000 .057214000000   H -5.80613000000 -1.65551600000 .06623800000   C 5.15319200000 -0.78111600000 .05238200000   H 5.80515000000 .06622800000 .06622800000   C 5.568149000000 .033276300000 .045872500000   C 5.568149000000 .0322451000000 .2082500000   C 5.216666000000 .04682700000 .16805700000   H -6.21778500000 .044827000000 .20831900000   H -6.21778000000 .044827000000 .20831900000   H 4.503577000000 .04483200000 .2083900000   H -3.215454000000 .052415000000 .20883900000   H -3.35145000000 .044952000000 .052415000000   H -3.3514500000	С	-3.685426000000	-1.204137000000	0.38320600000
H -3.54605200000 -1.80695500000 -0.524221000000   H -3.5476400000 -1.20398500000 -0.3836000000   H -3.5476400000 -1.80698000000 0.52382200000   H -5.50610300000 -0.78137100000 0.57289300000   H -5.80610300000 -1.6555800000 -0.66229800000   C 5.55914900000 -3.3274600000 -0.45872500000   C -5.56914900000 0.33270400000 -0.45872500000   C -5.56914900000 0.33270400000 -0.45872500000   C -5.21606600000 0.32252000000 -1.6559100000   H -4.504514000000 0.22456100000 -2.0831900000   H -4.504514000000 0.22546100000 -2.0831900000   H -5.21546400000 0.482500000 -2.0831900000   H -5.21545700000 0.44952600000 -2.0833900000   H -7.56971500000 0.22917900000 -1.3292900000   H -7.56971500000 0.29217900000 -1.04692300000   H -7.551457000000 0.52124000000 -1.046923000000   H -7.	Н	-3.355192000000	-1.834099000000	1.220612000000
C 3.68537300000 -1.20398500000 -0.38360000000   H 3.35476400000 -1.83383700000 0.52382200000   C -5.153346000000 -0.78137100000 0.572014000000   H -5.806103000000 -1.655818000000 0.66088900000   C 5.15319200000 -1.65550600000 -0.66229800000   C 5.568912000000 0.33276300000 -0.45872500000   C 5.568912000000 0.32276300000 -0.45872500000   C 5.216066000000 0.3282500000 1.6955100000   H -6.21778500000 0.44882700000 2.5082500000   H -6.2177800000 0.44827000000 2.508517000000   H 4.50357700000 0.44925600000 -2.0830900000   H 6.21703100000 0.44925000000 -0.48217000000   H 7.551457000000 0.45123800000 -0.5021500000   H 7.551457000000 0.45221400000 -0.50241500000   H 7.551457000000 0.4521400000 -0.50241500000   H 7.551457000000 0.51237000000 -0.48497000000   H 7.5514	Н	-3.546062000000	-1.806995000000	-0.524221000000
H 3.35476400000 -1.833837000000 .02202700000   H 3.54647300000 -0.5238200000   C 5.15334600000 -0.78137100000 .052038200000   H -5.80610300000 -1.65581800000 .05608900000   C 5.15319200000 -0.78111600000 .052289300000   C 5.5681200000 .033276300000 -0.4652500000   C -5.5681900000 .033276300000 .045872500000   C -5.21066600000 .03065200000 .168050700000   H -4.50451400000 .228741900000 .208741900000   H -6.217785000000 .2483200000 .2087100000   H -6.21785000000 .24833000000 .2087100000   H -6.21785000000 .61438300000 .208830900000   H -7.50375000000 .6138300000 .4627000000   H -7.551457000000 .6138200000 .103129900000   H -7.551457000000 .61302200000 .10312900000   H -7.551457000000 .12632500000 .128912400000   H -7.551457000000 .146275000000 .	С	3.685373000000	-1.203985000000	-0.38360000000
H 3.54647300000 -1.80598000000 0.523822000000   C -5.15334600000 -0.78137100000 0.57281300000   H 5.80510300000 -1.65550600000 0.65628900000   C -5.56891200000 0.33276300000 0.45872500000   C -5.56914900000 0.332704000000 0.45806000000   C -5.21606600000 0.30625200000 1.67995100000   H -4.50451400000 0.24256100000 2.08741900000   H -6.21778500000 0.4482700000 2.0883090000   H -6.21703500000 0.242546100000 2.0883090000   H 4.50357700000 0.24238300000 0.50241500000   H -7.55145700000 0.61153800000 0.488717000000   H -7.55145700000 0.61327000000 1.042811000000   H -7.351030000 0.4277000000 1.04841000000   H -7.35163700000 0.52137900000 0.488497000000   H -7.35163700000 0.25152900000 0.488497000000   H -5.3255800000 0.59187000000 2.44965000000   H -5.32512700000	Н	3.354764000000	-1.833837000000	-1.220927000000
C -5.15334600000 -0.781371000000 0.572014000000   H -5.80610300000 -1.655518100000 0.66088900000   C 5.15319200000 -0.781116000000 -0.57289300000   H 5.80955500000 -1.65550600000 -0.66229800000   C -5.56914900000 0.33276300000 -0.45872500000   C -5.21606600000 0.30252200000 1.67995100000   H -6.21778500000 0.24456100000 2.50822500000   H -6.21778500000 0.24545100000 2.50851700000   H -5.21546400000 0.264500000 -2.60851700000   H -6.21703100000 0.4485200000 -2.60830900000   H -5.251457000000 0.5133800000 0.48717000000   H -7.551457000000 0.51338000000 1.04192300000   H -7.35103000000 1.46277000000 1.03129900000   H -7.50275000000 0.52132900000 1.028411000000   H 7.551457000000 0.5139200000 2.44965500000   H -5.255317000000 0.213552900000 2.42029700000   H -5.	Н	3.546473000000	-1.806980000000	0.523822000000
H -5.80610300000 -1.655818000000 0.66088900000   C 5.15319200000 -0.78111600000 0.6622800000   C -5.56891200000 0.33276400000 0.45872500000   C -5.26891200000 0.33276400000 0.4580600000   C -5.21606600000 0.32276400000 2.5822500000   H -6.21778500000 0.224561000000 2.50822500000   H -6.21778500000 0.44882700000 2.50851700000   H 4.50357700000 0.2246100000 -2.0839900000   H 4.50357700000 0.248925000000 -2.0839900000   H -5.56911500000 0.29070000000 -2.0839900000   H -7.5547500000 0.29070000000 -1.0312900000   H -7.5547500000 0.29070000000 1.032411000000   H -7.55127000000 0.4633900000 0.48849700000   H 7.55127000000 0.25122900000 -2.42057000000   H -5.32517800000 0.53198700000 -2.42057000000   H -5.35637000000 0.25182900000 -2.42057000000  H -5.3551800000	С	-5.153346000000	-0.781371000000	0.572014000000
C 5.15319200000 -0.78111600000 -0.57289300000   H 5.80595500000 -1.6555060000 -0.66229800000   C -5.56891200000 0.33276300000 -0.4587500000   C -5.56914900000 0.33274600000 0.4587600000   C -5.21606600000 0.30625200000 1.67995100000   H -4.50451400000 0.22456100000 2.5082500000   C 5.21546400000 0.30685200000 -1.68050700000   H 4.50357700000 0.44822700000 -2.08830900000   C -7.09099900000 0.54238300000 -0.50241500000   H -7.55145700000 0.61153800000 -1.68050700000   H -7.55971500000 0.62907000000 -1.04692300000   H -7.35130300000 1.46277000000 1.028411000000   H 7.51457000000 0.5123900000 -0.488497000000   H 7.531457000000 0.25152900000 -0.488497000000   H 7.551457000000 0.25152900000 -1.48928400000   H 7.551457000000 0.25152900000 -2.44965600000   H 7.55145	Н	-5.806103000000	-1.655818000000	0.660889000000
H 5.80595500000 -1.65550600000 -0.66229800000   C -5.56891200000 0.33276300000 -0.45872500000   C 5.21606600000 0.30625200000 1.67995100000   H -4.504514000000 0.22456100000 2.50822500000   H -6.21778500000 0.44882700000 2.08741900000   C 5.215464000000 0.20545100000 -2.08830900000   H 4.50357700000 0.24546100000 -2.08830900000   H 4.50357700000 0.44952600000 -2.08830900000   H 7.55971500000 0.61153800000 -0.502415000000   H -7.55971500000 0.61253800000 -1.04692300000   H -7.55971500000 0.29179400000 1.028411000000   H 7.55127000000 0.25152900000 1.48928400000   H 7.55071500000 0.25152900000 -2.44955600000   H 7.552558000000 0.25152900000 -2.42027000000   H -5.52558000000 0.12355400000 -1.39797400000   C 5.05710500000 0.25085000000 -1.499797900000  H 5.32134100000 </td <td>С</td> <td>5.153192000000</td> <td>-0.781116000000</td> <td>-0.572893000000</td>	С	5.153192000000	-0.781116000000	-0.572893000000
C -5.568912000000 0.332763000000 -0.458725000000   C 5.59149000000 0.33270400000 0.45806000000   H -4.504514000000 0.224561000000 2.50822500000   H -6.21778500000 0.24882700000 2.08741900000   H -6.21778500000 0.44882700000 -2.085300000   H -6.21738500000 0.22456100000 -2.085300000   H -6.21703100000 0.44952600000 -2.08530900000   C -7.09099900000 0.54238300000 -0.50241500000   C -7.09099900000 0.54227000000 -1.04692300000   H -7.5591500000 0.52177000000 -1.04592300000   H -7.33510300000 1.46277000000 1.028411000000   H 7.355127000000 0.5139200000 -1.44895000000   C 5.056317000000 0.25152900000 -1.4297000000   H 7.3510300000 0.25152900000 -1.4297000000   H 7.555127000000 0.25152900000 -4.20297000000   H -5.5255800000 0.259383000000 -2.420297000000  H 5.52634500000 </td <td>Н</td> <td>5.805955000000</td> <td>-1.655506000000</td> <td>-0.662298000000</td>	Н	5.805955000000	-1.655506000000	-0.662298000000
C 5.56914900000 0.33270400000 0.45806000000   C -5.21606600000 0.30625200000 1.67995100000   H -4.50451400000 0.22456100000 2.50822500000   C 5.21546400000 0.30685200000 -1.68050700000   C 5.21546400000 0.30685200000 -2.50851700000   H 4.50357700000 0.22546100000 -2.083300000   C -7.09099900000 0.54238300000 -0.50241500000   H -7.556971500000 0.61153800000 -0.48717000000   H -7.33510300000 1.46277000000 1.04692300000   H 7.57027500000 0.5421400000 1.028411000000   H 7.5512700000 0.29179400000 1.04718000000   H 7.55112700000 0.61309200000 -1.48928400000   H -5.5255800000 0.25198700000 -2.44965600000   H -5.52558000000 0.25085000000 -2.44965600000   H -5.52558000000 0.25085000000 2.44209700000   H -5.256372900000 2.44319300000 2.44955900000  H 5.32634500000	С	-5.568912000000	0.332763000000	-0.458725000000
C -5.21606600000 0.30625200000 1.67995100000   H -4.50451400000 0.22456100000 2.5082500000   C 5.21546400000 0.30685200000 -1.68050700000   H 4.50357700000 0.22546100000 -2.50851700000   H 6.21703100000 0.44952600000 -2.0883090000   C -7.09099900000 0.54238300000 -0.50241500000   H -7.5545700000 0.29070000000 -1.03129900000   H -7.355145700000 0.29179400000 1.04692300000   H -7.576971500000 0.54221400000 0.50123700000   H 7.57027500000 0.29179400000 1.04692300000   H 7.55127000000 0.51532900000 -1.04892300000   H 7.5527500000 0.25152900000 -1.8928400000   H 7.552755800000 0.25152900000 -1.8928400000   H -5.5255800000 0.25185900000 -1.97979200000   H -5.5255800000 0.12355400000 -1.97979200000   H -5.5255800000 0.12311700000 1.97963600000   H 5.32134100000 <td>С</td> <td>5.569149000000</td> <td>0.332704000000</td> <td>0.45806000000</td>	С	5.569149000000	0.332704000000	0.45806000000
H -4.504514000000 0.224561000000 2.508225000000   H -6.217785000000 0.306852000000 -1.680507000000   C 5.215464000000 0.225461000000 -2.508517000000   H 4.503577000000 0.44952600000 -2.08330900000   C -7.09099900000 0.54238300000 -0.502415000000   H -7.55145700000 0.61153800000 -1.04692300000   H -7.55145700000 0.54221400000 -1.04692300000   C 7.09126900000 0.54221400000 0.501237000000   H 7.57027500000 -0.29179400000 1.028411000000   H 7.551127000000 0.61392000000 -2.4895600000   H 7.33569900000 1.46165300000 -2.42029700000   H 7.551127000000 0.25152900000 -1.899284000000   H -5.5255800000 -0.59198700000 -2.420297000000   H -5.5255800000 0.123154000000 1.979792000000   H -5.5255800000 0.12317000000 1.979636000000   H -5.326315000000 0.12317000000 1.979636000000   H	С	-5.216066000000	0.306252000000	1.679951000000
H -6.21778500000 0.44882700000 2.08741900000   C 5.21546400000 0.30685200000 -1.68050700000   H 4.50357700000 0.22546100000 -2.508517000000   C -7.0909900000 0.54238300000 -0.50241500000   H -7.55145700000 0.61153800000 -0.8717000000   H -7.55145700000 0.61153800000 -1.04692300000   H -7.3510300000 1.4627000000 1.02841100000   H -7.3569900000 0.54221400000 0.50123700000   H 7.57027500000 -0.29179400000 1.02841100000   H 7.55112700000 0.61309200000 -1.89928400000   H 7.55255800000 0.25152900000 -1.8928400000   H -5.32011000000 1.1633900000 -2.44965600000   H -5.3715500000 0.2593800000 -1.97979200000   H -5.32134100000 1.16232500000 2.44955900000   H 5.32134100000 1.16232500000 2.44955900000   H 5.32134100000 1.27598800000 0.27598800000   H 2.99497900000	н	-4.504514000000	0.224561000000	2.508225000000
C 5.215464000000 0.306852000000 -1.680507000000   H 4.503577000000 0.225461000000 -2.508517000000   H 6.217031000000 0.449526000000 -2.08830900000   H -7.50999900000 0.542383000000 -0.502415000000   H -7.55457000000 0.61153800000 -1.0479200000   H -7.55457000000 0.29070000000 -1.014923000000   H -7.33510300000 1.46277000000 0.50123700000   H 7.3569900000 0.54221400000 0.50123700000   H 7.551127000000 0.61309200000 -0.48849700000   H 7.551127000000 0.6139200000 -2.4485600000   H -5.32011000000 1.16339000000 -2.42029700000   H -5.397374600000 0.123554000000 -1.97979200000   H -5.9710500000 0.5938300000 2.44965600000   H 5.321341000000 1.16232500000 2.44955900000   H 5.32134100000 1.16232500000 2.44955900000   H 5.32134100000 1.2311700000 0.275988000000   C 2.5	н	-6.217785000000	0.448827000000	2.087419000000
H4.503577000000.22546100000-2.50851700000H6.217031000000.44952600000-2.08830900000C-7.090999000000.54238300000-0.50241500000H-7.551457000000.611538000000.48717000000H-7.535103000001.46277000000-1.04692300000C7.091269000000.542214000000.50123700000H7.557027500000-0.291794000001.02841100000H7.335699000001.46165300000-0.4894700000H7.35511270000000.61309200000-0.48894700000H7.5551127000000.25152900000-2.420297000000H-5.5255800000-0.5918700000-2.420297000000H-5.52558000000.59198700000-2.42029700000H-5.526345000000.123554000001.97979200000H3.974528000000.123117000001.9769600000H3.974528000003.43936000000.32213400000H-2.94979000003.43936000000.32213400000H2.994866000003.44065000000.32102900000H2.994866000002.44858000000.32102900000C1.194580000002.24862000000.12969400000C0.725743000002.48622000000.12969400000C0.72570000002.48622000000.12969400000C0.72570000003.4393746000000.0061300000C0.72570000003.4393746000000.00063300000C0.72570000003.4393746000000.0063300000	С	5.215464000000	0.306852000000	-1.680507000000
H6.217031000000.44952600000-2.08830900000C-7.090999000000.54238300000-0.50241500000H-7.551457000000.611538000000.48717000000H-7.351145700000-0.29070000000-1.0312900000H-7.335103000001.462770000000.50123700000H7.57027500000-0.291794000001.02841100000H7.53127000000.61309200000-0.48849700000H7.551127000000.61309200000-0.48849700000H-5.52558000000.25152900000-2.44965600000H-5.52558000000.25198700000-2.42029700000H-5.52558000000.25085000000-1.97979200000H-5.52538000000.12317000001.97979200000H3.974528000000.12317000002.44955900000H5.321341000001.162325000002.44955900000H-3.974528000000.12317000000.27598800000H3.974528000002.443193000000.27690800000H2.994979000003.439936000000.32213400000C2.563629000002.443193000000.27598800000H2.994866000003.44065000000.123600000C1.194550000002.24858000000.1226900000C1.194580000002.248622000000.12860100000C0.725743000000.937496000000.0063300000C0.725700000003.170321000000.0061900000C0.000076000003.170321000000.0061900000	н	4.503577000000	0.225461000000	-2.508517000000
C -7.09099900000 0.54238300000 -0.50241500000   H -7.55145700000 0.61153800000 0.48717000000   H -7.56971500000 -0.2907000000 -1.03129900000   C 7.09126900000 0.54221400000 0.50123700000   H 7.57027500000 -0.29179400000 1.02841100000   H 7.3569900000 0.46165300000 1.04718000000   H 7.355112700000 0.25152900000 -1.89928400000   H -5.32011000000 1.16339000000 -2.44965600000   H -5.5255800000 -0.59198700000 -2.42029700000   H -5.5255800000 0.12355400000 -1.9797200000   H -5.52634500000 0.2508500000 2.44965600000   H 5.52634500000 0.2508500000 2.44955900000   H 5.52634500000 0.25182900000 2.44955900000   H 5.321341000000 1.46325500000 2.44955900000   H 3.974528000000 2.44319300000 0.27598800000   H 2.99496600000 3.44005500000 0.32102900000   C 1.19451800000	н	6.217031000000	0.449526000000	-2.08830900000
H-7.551457000000.611538000000.48717000000H-7.56971500000-0.29070000000-1.03129900000C7.091269000001.46277000000-1.04692300000H7.57027500000-0.291794000001.02841100000H7.535699000001.461653000001.04718000000H7.551127000000.61309200000-0.48849700000C-5.056317000000.25152900000-1.89928400000H-5.320110000001.16339000000-2.44965600000H-5.2555800000-0.591987000000-2.42027000000H-5.25538000000.12354000000-1.97972000000H-5.26345000000.123554000001.9963600000H3.974528000000.123117000001.97963600000H5.321341000001.162325000000.3213400000H-2.994979000003.43936000000.3211400000H-2.994979000002.4430800000-0.27598800000C1.194618000002.24862200000-0.12860100000C1.194550000002.42862200000-0.12860100000C0.725743000000.93743600000-0.07938300000C0.725700000003.4393600000-0.07938300000C0.725700000000.93743600000-0.07938300000C0.000076000003.17032100000-0.0006300000C0.000076000003.17032100000-0.0006300000	С	-7.090999000000	0.542383000000	-0.502415000000
H-7.569715000000-0.290700000000-1.031299000000H-7.3351030000001.462770000000-1.046923000000C7.0912690000000.5422140000000.501237000000H7.570275000000-0.2917940000001.028411000000H7.3356990000001.4616530000001.047180000000C-5.0563170000000.251529000000-2.449656000000H-5.3201100000001.16339000000-2.449656000000H-5.255580000000.591987000000-2.420297000000H-5.3257105000000.250850000001.898779000000H5.52634500000-0.5930830000002.419141000000H3.974528000000.123117000001.979636000000H5.3213410000002.443193000000.322134000000H-2.994979000003.43993600000-0.32102900000C2.563629000002.44868000000.126601000000H2.994866000003.44006500000-0.32102900000C-1.194618000002.24862200000-0.128601000000C0.725743000000.93743600000-0.079383000000C0.725700000003.43093600000-0.079383000000C0.725703000000.93743600000-0.079383000000C0.725700000003.170321000000.00663000000	н	-7.551457000000	0.611538000000	0.487170000000
H-7.3351030000001.462770000000-1.046923000000C7.0912690000000.5422140000000.501237000000H7.570275000000-0.2917940000001.028411000000H7.335699000001.4616530000001.047180000000H7.5511270000000.613092000000-0.488497000000C-5.0563170000000.251529000000-1.899284000000H-5.3201100000001.163390000000-2.449656000000H-5.52558000000-0.591987000000-2.420297000000C5.057105000000.250850000001.898779000000H5.526345000000-0.593083000002.419141000000H3.974528000000.1231170000001.979636000000H3.974528000002.443193000000.276998000000H-2.994979000003.43993600000-0.27598800000H2.994866000003.44006500000-0.27598800000H2.994866000003.44006500000-0.12860100000C-1.194618000002.248568000000.12860100000C0.725743000000.93749000000.08017600000C0.725743000000.93743600000-0.07938300000C0.72570000003.170321000000.0063300000C0.000076000003.170321000000.00061900000	н	-7.569715000000	-0.29070000000	-1.031299000000
C7.091269000000.542214000000.501237000000H7.57027500000-0.291794000001.02841100000H7.335699000001.46165300000-0.48849700000C-5.056317000000.61309200000-0.48849700000C-5.056317000000.25152900000-1.89928400000H-5.320110000001.16339000000-2.44965600000H-5.5255800000-0.59198700000-2.42029700000H-3.973746000000.12355400000-1.97979200000C5.057105000000.250850000001.89877900000H5.52634500000-0.593083000002.41914100000H3.974528000000.123117000001.97963600000H5.321341000001.162325000000.27690800000C-2.563729000002.443193000000.32213400000H-2.994866000003.44006500000-0.27598800000H2.994866000002.248568000000.12860100000C-1.194618000002.24862200000-0.12860100000C0.725743000000.937409000000.08017600000C0.725743000000.93743600000-0.07938300000C-0.00049000003.170321000000.0063300000O-0.000076000004.383378000000.00061900000	н	-7.335103000000	1.462770000000	-1.046923000000
H7.57027500000-0.291794000001.02841100000H7.335699000001.46165300000-0.48849700000H7.551127000000.61309200000-0.48849700000C-5.056317000000.25152900000-1.89928400000H-5.320110000001.16339000000-2.44965600000H-5.5255800000-0.59198700000-2.42029700000H-3.973746000000.123554000001.97979200000C5.057105000000.250850000001.89877900000H5.52634500000-0.593083000002.41914100000H3.974528000000.123117000001.97963600000H5.321341000001.162325000000.27690800000H-2.994979000003.439936000000.32213400000C-2.563629000002.44330800000-0.27598800000H2.994866000003.44006500000-0.32102900000C-1.194618000002.248568000000.12860100000C-0.725743000000.93740900000-0.7938300000C-0.725700000003.170321000000.0063300000C-0.000049000003.170321000000.00061900000	С	7.091269000000	0.542214000000	0.501237000000
H7.335699000001.461653000001.04718000000H7.551127000000.61309200000-0.48849700000C-5.056317000000.25152900000-1.89928400000H-5.320110000001.16339000000-2.44965600000H-5.5255800000-0.59198700000-2.42029700000H-3.973746000000.12355400000-1.97979200000C5.057105000000.250850000001.89877900000H5.52634500000-0.593083000002.41914100000H3.974528000000.123117000001.97963600000H5.321341000001.162325000002.44955900000C-2.563729000002.443193000000.27690800000H-2.994979000003.43993600000-0.27598800000H2.994866000002.24856800000-0.32102900000C-1.194618000002.24862200000-0.12860100000C-0.725743000000.93740900000-0.07938300000C-0.725743000003.43037800000-0.07938300000C-0.00049000003.170321000000.00063300000	н	7.570275000000	-0.291794000000	1.028411000000
H7.551127000000.61309200000-0.488497000000C-5.056317000000.25152900000-1.899284000000H-5.320110000001.16339000000-2.449656000000H-5.5255800000-0.59198700000-2.420297000000C5.057105000000.123554000001.979792000000C5.057105000000.250850000002.419141000000H3.974528000000.123117000001.979636000000H5.321341000001.162325000002.44955900000C-2.563729000002.443193000000.32213400000H-2.994979000003.439936000000.32213400000H2.994866000003.44006500000-0.27598800000C-1.194618000002.248568000000.12860100000C-0.725743000000.937409000000.08017600000C0.725700000003.170321000000.0063300000C-0.000076000004.383378000000.00061900000	Н	7.335699000000	1.461653000000	1.04718000000
C-5.0563170000000.251529000000-1.899284000000H-5.3201100000001.163390000000-2.449656000000H-5.52558000000-0.591987000000-2.420297000000H-3.9737460000000.1235540000001.979792000000C5.0571050000000.2508500000001.898779000000H5.5263450000000.1231170000001.979636000000H3.974528000000.123117000001.979636000000H5.3213410000001.1623250000002.449559000000C-2.563729000002.443193000000.32213400000H-2.994979000003.439936000000.32213400000H2.994866000003.44006500000-0.27598800000H2.994866000002.248568000000.128601000000C-1.194618000002.24862200000-0.128601000000C0.725743000000.937409000000.080176000000C0.725700000003.17032100000-0.0063300000C-0.000076000004.383378000000.0061900000	н	7.551127000000	0.613092000000	-0.488497000000
H-5.3201100000001.16339000000-2.449656000000H-5.52555800000-0.59198700000-2.42029700000H-3.9737460000000.12355400000-1.97979200000C5.057105000000.250850000001.89877900000H5.52634500000-0.593083000002.41914100000H3.974528000000.123117000001.97963600000H5.321341000001.162325000002.44955900000C-2.563729000002.443193000000.27690800000H-2.994979000003.439936000000.32213400000H2.994866000003.4406500000-0.27598800000C1.194518000002.248568000000.12860100000C0.725743000000.937409000000.08017600000C0.725700000003.170321000000.00063300000C-0.00076000004.383378000000.00061900000	С	-5.056317000000	0.251529000000	-1.899284000000
H-5.525558000000-0.591987000000-2.420297000000H-3.973746000000.12355400000-1.979792000000C5.057105000000.250850000001.898779000000H5.52634500000-0.593083000002.419141000000H3.974528000000.123117000001.979636000000H5.321341000001.162325000002.449559000000C-2.563729000002.443193000000.27690800000H-2.994979000003.439936000000.322134000000H2.994866000003.4406500000-0.27598800000H2.994866000002.248568000000.12860100000C-1.194618000002.24862200000-0.12860100000C0.725743000000.937409000000.08017600000C0.725700000003.170321000000.0063300000O-0.000076000004.383378000000.00061900000	н	-5.320110000000	1.163390000000	-2.449656000000
H-3.9737460000000.123554000000-1.979792000000C5.0571050000000.2508500000001.898779000000H5.526345000000-0.5930830000002.419141000000H3.9745280000000.1231170000001.979636000000H5.3213410000001.1623250000002.449559000000C-2.5637290000002.4431930000000.276908000000H-2.994979000003.4399360000000.322134000000C2.5636290000002.443308000000-0.275988000000H2.9948660000003.440065000000-0.321029000000C-1.1946180000002.2485680000000.128601000000C-1.1945500000002.248622000000-0.128601000000C-0.7257430000000.937409000000-0.079383000000C-0.0000490000003.1703210000000.000633000000O-0.0000760000004.3833780000000.000619000000	н	-5.525558000000	-0.591987000000	-2.420297000000
C5.057105000000.250850000001.898779000000H5.52634500000-0.593083000002.419141000000H3.974528000000.123117000001.979636000000H5.321341000001.162325000002.449559000000C-2.563729000002.443193000000.276908000000H-2.994979000003.439936000000.322134000000C2.563629000002.44330800000-0.27598800000H2.994866000003.44006500000-0.32102900000C-1.194618000002.248568000000.12969400000C1.194550000002.24862200000-0.128601000000C0.725743000000.93740900000-0.07938300000C-0.00049000003.170321000000.0063300000O-0.000076000004.383378000000.00061900000	н	-3.973746000000	0.123554000000	-1.979792000000
H5.526345000000-0.5930830000002.419141000000H3.9745280000000.1231170000001.979636000000H5.3213410000001.1623250000002.449559000000C-2.5637290000002.4431930000000.276908000000H-2.9949790000003.4399360000000.322134000000C2.5636290000002.443308000000-0.275988000000H2.9948660000003.440065000000-0.321029000000C-1.1946180000002.2485680000000.128601000000C1.1945500000002.248622000000-0.128601000000C0.7257430000000.937436000000-0.079383000000C-0.0000490000003.1703210000000.000633000000O-0.0000760000004.3833780000000.000619000000	С	5.057105000000	0.250850000000	1.898779000000
H3.974528000000.123117000001.979636000000H5.321341000001.162325000002.44955900000C-2.563729000002.443193000000.27690800000H-2.994979000003.439936000000.322134000000C2.563629000002.44330800000-0.27598800000H2.994866000003.44006500000-0.321029000000H2.994866000002.248568000000.12969400000C-1.194618000002.24862200000-0.128601000000C1.194550000000.937409000000.080176000000C0.725743000000.93743600000-0.07938300000C-0.000049000003.170321000000.000633000000O-0.000076000004.383378000000.00061900000	н	5.526345000000	-0.593083000000	2.419141000000
H5.3213410000001.1623250000002.449559000000C-2.5637290000002.4431930000000.276908000000H-2.9949790000003.4399360000000.322134000000C2.5636290000002.443308000000-0.275988000000H2.9948660000003.440065000000-0.321029000000C-1.1946180000002.2485680000000.129694000000C1.194550000002.248622000000-0.128601000000C0.7257430000000.9374090000000.080176000000C0.7257000000003.1703210000000.000633000000O-0.0000760000004.3833780000000.000619000000	Н	3.974528000000	0.123117000000	1.979636000000
C-2.5637290000002.4431930000000.276908000000H-2.9949790000003.4399360000000.322134000000C2.5636290000002.443308000000-0.275988000000H2.9948660000003.440065000000-0.321029000000C-1.1946180000002.2485680000000.129694000000C1.1945500000002.248622000000-0.128601000000C0.7257430000000.9374090000000.080176000000C0.7257000000003.1703210000000.000633000000O-0.0000760000004.3833780000000.000619000000	Н	5.321341000000	1.162325000000	2.449559000000
H-2.9949790000003.4399360000000.322134000000C2.5636290000002.443308000000-0.275988000000H2.9948660000003.440065000000-0.321029000000C-1.1946180000002.2485680000000.129694000000C1.1945500000002.248622000000-0.128601000000C-0.7257430000000.9374090000000.080176000000C0.7257000000000.937436000000-0.079383000000C-0.0000490000003.1703210000000.000633000000O-0.0000760000004.3833780000000.000619000000	С	-2.563729000000	2.443193000000	0.276908000000
C2.563629000002.44330800000-0.275988000000H2.994866000003.44006500000-0.32102900000C-1.194618000002.248568000000.129694000000C1.194550000002.24862200000-0.128601000000C-0.725743000000.937409000000.080176000000C0.725700000000.93743600000-0.079383000000C-0.00049000003.170321000000.000633000000O-0.000076000004.383378000000.000619000000	н	-2.994979000000	3.439936000000	0.322134000000
H2.994866000003.44006500000-0.32102900000C-1.194618000002.248568000000.12969400000C1.194550000002.24862200000-0.128601000000C-0.725743000000.937409000000.080176000000C0.725700000000.93743600000-0.079383000000C-0.000049000003.170321000000.000633000000O-0.000076000004.383378000000.000619000000	С	2.563629000000	2.443308000000	-0.275988000000
C-1.1946180000002.2485680000000.129694000000C1.1945500000002.248622000000-0.128601000000C-0.7257430000000.9374090000000.080176000000C0.7257000000000.937436000000-0.079383000000C-0.0000490000003.1703210000000.000633000000O-0.0000760000004.3833780000000.000619000000	н	2.994866000000	3.440065000000	-0.32102900000
C1.194550000002.24862200000-0.128601000000C-0.725743000000.937409000000.080176000000C0.7257000000000.937436000000-0.079383000000C-0.0000490000003.170321000000.000633000000O-0.0000760000004.383378000000.000619000000	С	-1.194618000000	2.248568000000	0.129694000000
C-0.7257430000000.9374090000000.080176000000C0.7257000000000.937436000000-0.079383000000C-0.0000490000003.1703210000000.000633000000O-0.0000760000004.3833780000000.000619000000	С	1.194550000000	2.248622000000	-0.128601000000
C0.725700000000.937436000000-0.079383000000C-0.0000490000003.1703210000000.000633000000O-0.0000760000004.3833780000000.000619000000	С	-0.725743000000	0.937409000000	0.080176000000
C -0.000049000000 3.170321000000 0.000633000000 O -0.000076000000 4.383378000000 0.000619000000	С	0.725700000000	0.937436000000	-0.079383000000
O -0.000076000000 4.383378000000 0.000619000000	С	-0.000049000000	3.170321000000	0.000633000000
	 0	-0.000076000000	4.383378000000	0.000619000000

**Table S12.** Optimized geometry of the **first singlet excited state** of **[ZnL<sup>o</sup>Cl<sub>2</sub>]** in Cartesian (XYZ) coordinates as calculated in Gaussian at the B3LYP/LANL2DZ/6-31+g(d) level of theory.

Z	'n	-0.000005000000	-1.931224000000	-0.000063000000	
C	CI	-0.265916000000	-2.834038000000	-2.050521000000	
C	CI	0.265829000000	-2.834541000000	2.050158000000	
Ν	N	-1.459436000000	-0.209884000000	0.166491000000	
Ν	N	1.459459000000	-0.209921000000	-0.166593000000	
C	С	-4.818907000000	1.358391000000	0.556829000000	
F	Н	-5.205836000000	2.379335000000	0.624485000000	
C	С	4.818992000000	1.358267000000	-0.556752000000	
F	Н	5.205935000000	2.379197000000	-0.624547000000	
C	С	-3.338320000000	1.322927000000	0.372846000000	
C	С	3.338373000000	1.322844000000	-0.373013000000	
C	С	-2.759015000000	-0.018105000000	0.310432000000	
C	С	2.759055000000	-0.018174000000	-0.310422000000	
C	С	-3.684858000000	-1.208801000000	0.39406900000	
H	H	-3.373008000000	-1.837986000000	1.240024000000	
Н	ł	-3.550972000000	-1.826007000000	-0.50479300000	
C	С	3.684909000000	-1.208889000000	-0.393676000000	
H	-	3.373192000000	-1.838236000000	-1.239559000000	
F	H	3.550881000000	-1.825921000000	0.505284000000	
C	2	-5.142846000000	-0.757731000000	0.574125000000	
F	-	-5.813045000000	-1.618729000000	0.662714000000	
Ċ	C	5.142926000000	-0.757858000000	-0.573589000000	
H	4	5.813137000000	-1.618876000000	-0.66190400000	
C		-5.531273000000	0.358312000000	-0 461356000000	
(	C	5,531191000000	0.358384000000	0.461739000000	
(	r	-5 182516000000	0 327684000000	1 681178000000	
F	H	-4 475144000000	0 229857000000	2 51104300000	
F	H	-6 179772000000	0 504582000000	2 086437000000	
- -	r r	5 182774000000	0 327342000000	-1 680845000000	
L L L L L L L L L L L L L L L L L L L	н	4 475532000000	0.229355000000	-2 510803000000	
, F	H	6 180093000000	0.223333000000	-2 08598000000	
, C	- -	-7 045790000000	0.605856000000	-0 512283000000	
L L	H	-7 509918000000	0.683803000000	0 47494100000	
н	4	-7 538820000000		-1 04395000000	
		-7 265865000000	1 530768000000	-1 05864400000	
	r r	7 045701000000	0.605929000000	0 512862000000	
F	H	7.538644000000	-0.217140000000	1 044775000000	
F	н	7.265693000000	1.530952000000	1.05907100000	
F	н	7.509989000000	0.683675000000	-0 47430300000	
C		-5.005895000000	0.273136000000	-1 89690200000	
H	H	-5.231093000000	1.198678000000	-2.440763000000	
H		-5.498502000000	-0.548730000000	-2 43056900000	
H	4	-3.927113000000	0.108889000000	-1.96676000000	
	r r	5 005583000000	0 273493000000	1 89721700000	
F	H	5 498093000000	-0 548274000000	2 431125000000	
F	н	3 926787000000	0 109275000000	1 966932000000	
F	н	5 230705000000	1 199140000000	2 440933000000	
۱ ۲	C	-2.53017000000	2.454231000000	0.277027000000	
L L	H	-2.958174000000	3,451924000000	0.32190300000	
r r	r.	2 53020800000	2 45416900000	-0 277575000000	
L L	H	2.958211000000	3 451852000000	-0 322671000000	
r r	r.	-1 15396300000	2 26856600000	0 12705500000	
c c	r r	1 15397000000	2 268537000000	-0 12783700000	
( )	r r	-0 602022000000	0 90216000000	0.078438000000	
(		0.052552000000	0.002100000000	0.070-0000000	

С	0.692934000000	0.902143000000	-0.078967000000
С	-0.000021000000	3.180438000000	-0.000716000000
0	0.000144000000	4.430432000000	0.000633000000

**Table S13.** Excited state properties of L at the relaxed ground state geometry  $(S_0)$  as calculated in Gaussian at the B3LYP/6-31+g(d) level of theory. Transitions with contribution >10% are shown.

State	Energy	Energy	Contributions (%)	Oscillator	Character
	(eV)	(nm)		strength	
S1	4.1800	297	HOMO -> LUMO (91.5)	0.7010	$\pi - \pi^*$
S2	4.3715	284	HOMO-1 -> LUMO (97.2)	0.0032	$\sigma - \pi^*, n - \pi^*$
S3	4.4654	278	HOMO-2 -> LUMO (94.5)	0.0000	$\sigma - \pi^*, n - \pi^*$
S4	4.5770	271	HOMO -> LUMO+1 (91.0)	0.1071	$\pi - \pi^*$
S5	4.8167	257	HOMO-3 -> LUMO (21.8)	0.0113	$\pi - \pi^*$
			HOMO -> LUMO+3 (67.0)		



Figure S23. Calculated absorption spectrum of L.

**Table S14.** Isosurface contour plots of the molecular orbitals of L at the relaxed ground state geometry  $(S_0)$  as calculated in Gaussian at the B3LYP/6-31+g(d) level of theory.





**Table S15.** Excited state properties of  $L^0$  at the relaxed ground state geometry ( $S_0$ ) as calculated in Gaussian at the B3LYP/6-31+g(d) level of theory. Transitions with contribution >10% are shown.

State	Energy (eV)	Energy (nm)	Contributions (%)	Oscillator strength	Character
S1	2.9420	421	HOMO -> LUMO (99.1)	0.0001	$\pi - \pi^*$ , ILCT
S2	2.9776	416	HOMO-1 -> LUMO (93.5)	0.0000	$\sigma - \pi^*, n - \pi^*$
S3	3.6193	343	HOMO-2 -> LUMO (97.9)	0.0000	$\sigma - \pi^*, n - \pi^*$
S4	4.0013	310	HOMO-4 -> LUMO (86.1)	0.0000	$\sigma - \pi^*, n - \pi^*$
S5	4.0678	305	HOMO-5 -> LUMO (20.6)	0.2702	$\pi - \pi^*$ , ILCT
			HOMO -> LUMO+1 (76.8)		
S6	4.2474	292	HOMO-1 -> LUMO+1 (90.1)	0.0000	$\sigma - \pi^*, n - \pi^*$
S7	4.4757	277	HOMO-3 -> LUMO (84.3)	0.0396	$\pi - \pi^*$ , ILCT
S8	4.4983	276	HOMO-2 -> LUMO+1 (92.0)	0.0039	$\sigma - \pi^*, n - \pi^*$
S9	4.6798	265	HOMO-6 -> LUMO (46.1)	0.0015	$\pi - \pi^*$ , ILCT
			HOMO -> LUMO+2 (42.3)		
S10	4.8468	256	HOMO-5 -> LUMO (77.4)	1.0717	$\pi - \pi^*$ , ILCT
			HOMO -> LUMO+1 (20.5)		



Figure S24. Calculated absorption spectrum of L<sup>o</sup>.

**Table S16.** Isosurface contour plots of the molecular orbitals of  $L^0$  at the relaxed ground state geometry ( $S_0$ ) as calculated in Gaussian at the B3LYP/6-31+g(d) level of theory.





**Table S17.** Excited state properties of  $[ZnLCl_2]$  at the relaxed ground state geometry ( $S_0$ ) as calculated in Gaussian at the B3LYP/LANL2DZ/6-31+g(d) level of theory. Transitions with contribution >10% are shown.

State	Energy	Energy	Contributions (%)	Oscillator	Character
	(eV)	(nm)		strength	
S1	3.6555	339	HOMO -> LUMO (99.9)	0.0030	XLCT
S2	3.7116	334	HOMO-2 -> LUMO (29.9)	0.0378	XLCT, $\pi - \pi^*$
			HOMO-1 -> LUMO (69.7)		
S3	3.7712	329	HOMO-3 -> LUMO (99.4)	0.0026	XLCT
S4	3.8398	323	HOMO-4 -> LUMO (99.4)	0.0000	XLCT
S5	3.9099	317	HOMO-2 -> LUMO (67.9)	0.5545	XLCT, $\pi - \pi^*$
			HOMO-1 -> LUMO (27.6)		
S6	4.4501	279	HOMO -> LUMO+1 (94.9)	0.0002	XLCT
S7	4.4914	276	HOMO-1 -> LUMO+1 (94.5)	0.0982	XLCT, $\pi - \pi^*$



Figure S25. Calculated absorption spectrum of [ZnLCl<sub>2</sub>].



**Table S18.** Isosurface contour plots of the molecular orbitals of  $[ZnLCl_2]$  at the relaxed ground state geometry  $(S_0)$  as calculated in Gaussian at the B3LYP/LANL2DZ/6-31+g(d) level of theory.

**Table S19.** Excited state properties of  $[ZnL^oCl_2]$  at the relaxed ground state geometry ( $S_0$ ) as calculated in Gaussian at the B3LYP/LANL2DZ/6-31+g(d) level of theory. Transitions with contribution >10% are shown.

State	Energy	Energy	Contributions (%)	Oscillator	Character
	(eV)	(nm)		strength	
S1	2.9260	424	HOMO-3 -> LUMO (51.5)	0.0025	XLCT, $\pi - \pi^*$ , ILCT
			HOMO-1 -> LUMO (47.7)		
S2	2.9829	416	HOMO -> LUMO (99.8)	0.0000	XLCT
S3	3.0525	406	HOMO-6 -> LUMO (47.6)	0.0000	$\pi - \pi^*$ , ILCT

			HOMO-4 -> LUMO (49.5)		
S4	3.0763	403	HOMO-3 -> LUMO (47.6)	0.0000	XLCT, $\pi - \pi^*$ , ILCT
			HOMO-1 -> LUMO (52.0)		
S5	3.1013	400	HOMO-2 -> LUMO (99.4)	0.0000	XLCT
S6	3.2734	379	HOMO-6 -> LUMO (46.8)	0.0000	$\pi - \pi^*$ , ILCT
			HOMO-4 -> LUMO (50.2)		
S7	3.6055	344	HOMO -> LUMO+1 (99.7)	0.0032	XLCT
S8	3.6603	339	HOMO-1 -> LUMO+1 (96.4)	0.0191	XLCT
S12	3.8669	321	HOMO-3 -> LUMO+1 (87.7)	0.3829	XLCT, $\pi - \pi^*$
S23	4.7015	264	HOMO-11 -> LUMO (84.7)	0.4227	$\pi - \pi^*$ , ILCT



Figure S26. Calculated absorption spectrum of [ZnL<sup>o</sup>Cl<sub>2</sub>].

**Table S20.** Isosurface contour plots of the molecular orbitals of  $[ZnL^{o}Cl_{2}]$  at the relaxed ground state geometry ( $S_{0}$ ) as calculated in Gaussian at the B3LYP/LANL2DZ/6-31+g(d) level of theory.





Table S21. Comparison of the most relevant bond lengths for L.



Table S22. Comparison of the most relevant bond lengths for  ${\bf L}^{\rm o}.$ 





Table S23. Comparison of the most relevant bond lengths for [ZnLCl<sub>2</sub>].

Table S24. Comparison of the most relevant bond lengths for [ZnL<sup>o</sup>Cl<sub>2</sub>].

