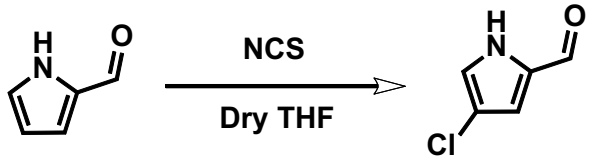
Supporting Information

EXPERIMENTAL SECTION

Materials and measurements: All chemical reagents and solvents used in this study were obtained from commercial sources and used as received. Complexes **H**, **Me** and **Br** were prepared according to the established procedure.[1-3] The NMR spectra (^{1}H and ^{13}C NMR) were recorded by using a Bruker AVANCE 400 NMR or Bruker AVANCEIII600 spectrometer. The chemical shifts (in ppm) of ^{1}H NMR and ^{13}C NMR were referenced relative to tetramethylsilane (TMD) $(CH_3)_4Si$. The coupling constants, *J* are reported in Hertz (Hz). Multiplicity is abbreviated as follows: s = singlet, d = doublet, t = triplet, and m = multiplet. The high-resolution mass spectra (HRMS, FAB-MS) were performed with a JEOL JMS-700 instrument. The gas chromatography-mass spectra (GC-MS) were obtained using a Shimadzu GCMS-QP5050A equipped with a J&W Scientific DB-1 column (length: 30m; ID: 0.25 mm, film: 0.25 mm) and helium as the carrier gas. For the measurement, the injector and detector temperatures were 250 ºC, the oven temperature was initially held at 100 °C for 2 min, then increased to 240 °C at the rate of 10 °C/min. Gel permeation chromatography (GPC) was carried out on a JAI LaboACE LC-5060 equipped with a UV-VIS 4ch 400LA detector using a single JAIGEL-2H column and chloroform as the eluent. UV–vis absorption spectra were recorded using a Hitachi U-3900H spectrophotometer. Fluorescence excitation and emission spectra were collected at room temperature on a Hitachi F-7000 and JASCO FP-8500 fluorescence spectrophotometer. Emission spectra were collected in the range between 300-800 nm, with a scan speed of 240 nm/min, and the slits were set at 5.0 nm (excitation slit) and 5.0 nm (emission slit). Circular dichroism (CD) spectra were recorded on a JASCO J-1500 spectrometer at 25 °C. Circularly polarized luminescence (CPL) and DC (nonpolarized fluorescence) spectra were measured by using a comprehensive chiroptical spectrophotometer (CCS) equipped with a Stokes–Mueller matrix analysis system. The absolute photoluminescence quantum yields (PLQYs) were determined using absolute PL quantum yields measurement system C9920-02 (Hamamatsu photonics) after excitation at maximum absorption wavelength (λ_{abs}^{max}). Time-resolved photoluminescence lifetimes (TRPL) were carried out by using time-correlated single photon counting lifetime spectroscopy system, Quantaurus-Tau C11367-05 (Hamamatsu photonics). The decay constants and fitting parameters (τ, A) for transient decays were determined using the embedded software of Quantaurus-Tau. Powder X-ray diffraction (PXRD) data were collected at room temperature using a Rigaku SmartLab system (Rigaku) diffractometer with a copper Kα source. Time-resolved photoluminescence (TR-PL) measurements were performed using a polychromator and a streak camera system (Hamamatsu C4780, time resolution: < 30 ps). The excitation light (400 nm) was generated by second harmonic generation (SHG) from the output of a Ti:sapphire regenerative amplifier (Spectra-Physics, Spitfire Ace, pulse duration: 120 fs, repetition rate: 1 kHz, pulse energy: 3.6 mJ/pulse and central wavelength: 800 nm).

X-ray crystal structure analysis: Suitable crystals were selected and measured on X-ray diffraction data were collected using a Rigaku XtaLAB Synergy equipped with Cu-Kα radiation (λ = 1.54184 Å) with HyPix diffractometer. CrysAlisPro[4] was used to integrate, correct, and scale the collected data. The structures were refined using SHELXT (Sheldrick, 2015)[5] Intrinsic Phasing and SHELXL (Sheldrick, 2015).[6] Anisotropic refinement was used for all non-hydrogen atoms. Hydrogen atoms were located at calculated positions and were included in the structure factor calculation, but they were not refined. The program Olex2-1.2 was used as a graphical interface.[7] The CCDC numbers are 2497171 for $\mathbf{L_{Cl}}$, and 2497172 for **Cl**, respectively. Crystallographic data have been deposited in the database of the Cambridge Crystallographic Data Centre. The data is available for free upon request to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44) 1223-336-033; email: deposit@ccdc.cam.ac.uk).

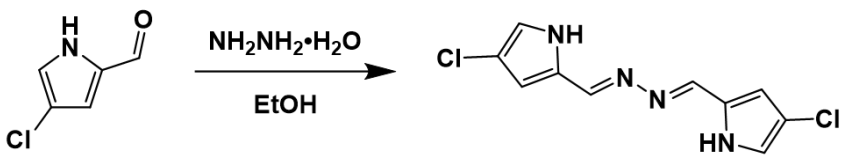
Synthesis



Synthesis of 4-Chloro-1H-pyrrole-2-carbaldehyde (1):

Pyrrole-2-carboxyaldehyde (1.95 g, 20.5 mmol, 1.0 eq) was dissolved in dry THF (40 mL) under a nitrogen atmosphere. *N*-chlorosuccinimide (3.00 g, 23.2 mmol, 1.13 eq) was then added, and the reaction mixture was stirred at room temperature for 27 hours (**Fig. S2(a)**). The resulting solution was passed through a dry silica-gel column chromatography with dichloromethane as eluent and concentrated under reduced pressure. The crude product was purified by normal-phase automated flash column chromatography (Biotage Isolera Spectra System), equipped with a column cartridge (Sfär Silica HC D High Capacity Duo 20 µm 50 g). Using an optimized ethyl acetate/hexane solvent gradient. Further purification by GPC with chloroform to give 4-chloro-1H-pyrrole-2-carbaldehyde **(1)** as a white powder (719 mg, 27%).

Identification of **4-Chloro-1H-pyrrole-2-carbaldehyde (1)**: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.98 (m, 1H, Py), 7.27 (m, 1H, Py), 9.51 (d, 1H, CHO), 11.33 (s, 1H, NH). The GC–MS spectrum of 4-chloro-1H-pyrrole-2-carbaldehyde (**1**) is shown in **Fig. S2(b)**.

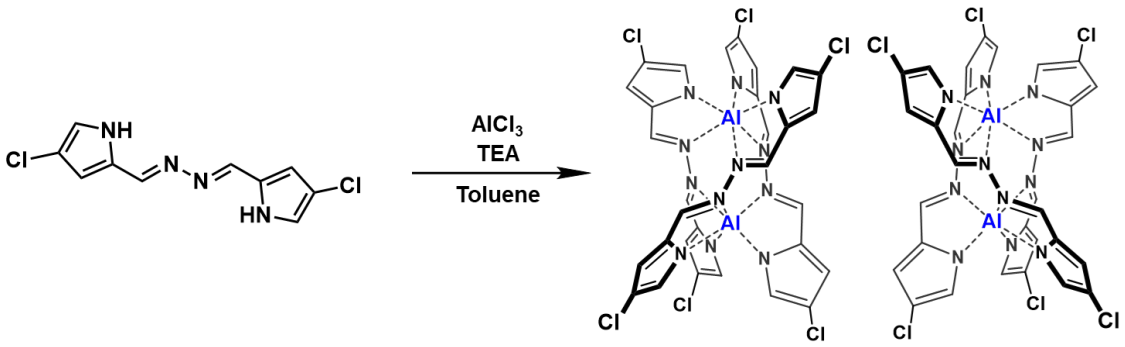


Synthesis of $\mathbf{L_{Cl}}$:

Compound **1** (516 mg, 1.5 mmol) was dissolved in ethanol (2.0 mL) at room temperature under a nitrogen atmosphere. Hydrazine monohydrate (63 µL, 1.29 mmol) and a few drops of acetic acid were added to the solution, and the reaction mixture was cooled for 15 hours. The precipitate was collected by filtration, washed

with cold ethanol to obtain $\mathbf{L_{Cl}}$. The filtrate was recrystallized repeatedly from chloroform to yield $\mathbf{L_{Cl}}$ as yellow crystals (145 mg, 30%).

Identification of $\mathbf{L_{Cl}}$: m.p.: >193 °C, ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.13 (s, 2H, NH), 8.25 (s, 2H, NH), 6.89 (s, 2H, Py), 6.51 (s, 2H, Py).
HRMS (FAB, positive): *m/z* calcd. for $C_{10}H_8Cl_2N_4$ $[M]^+$ 254.0126, found 254.0126.
Elemental analysis calcd (%) for $C_{10}H_8Cl_2N_4$: C 47.08, H 3.16, N 21.96; found: C 46.80, H 3.00, N 21.81.



Synthesis of Cl:
$\mathbf{L_{Cl}}$ (65 mg, 0.26 mmol) was dissolved in toluene (11 mL) and stirred for 10 min at room temperature under a nitrogen atmosphere. Triethylamine (TEA) (4.2 mL, 280 mmol) and aluminum chloride ($AlCl_3$) (89.8 mg, 0.66 mmol) were then added, and the reaction mixture was refluxed for 5 h. After the reaction, the mixture was passed through a dry silica-gel column chromatography with dichloromethane as eluent and concentrated under reduced pressure. The crude product was further purified by silica-gel column chromatography (dichloromethane / hexane) to yield **Cl** as a yellow powder (19.4 mg, 27.7%). **Cl** was recrystallized from THF/hexane to obtain crystals suitable for single crystal X-ray diffraction analysis.
Identification of **Cl**: m.p.: >300 °C, ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.80 (s, 6H, N=C-H), 6.70 (s, 6H, Py), 6.51 (s, 6H, Py). ^{13}C NMR (150 MHz, $CDCl_3$): δ = 151.0, 133.4, 130.1, 118.2, 117.2. HRMS (FAB, positive): *m/z* calcd. for $C_{30}H_{18}Al_2Cl_6N_{12}$ $[M]^+$ 811.9510, found 811.9513.
Elemental analysis Calcd (%) for [**Cl**] $(C_{10}H_8Cl_2N_4)\cdot 2.3$ THF $\cdot 0.1$ hexane (%): C, 47.67; H, 3.81; N, 17.02. Found: C, 47.53; H, 3.78; N, 16.70.

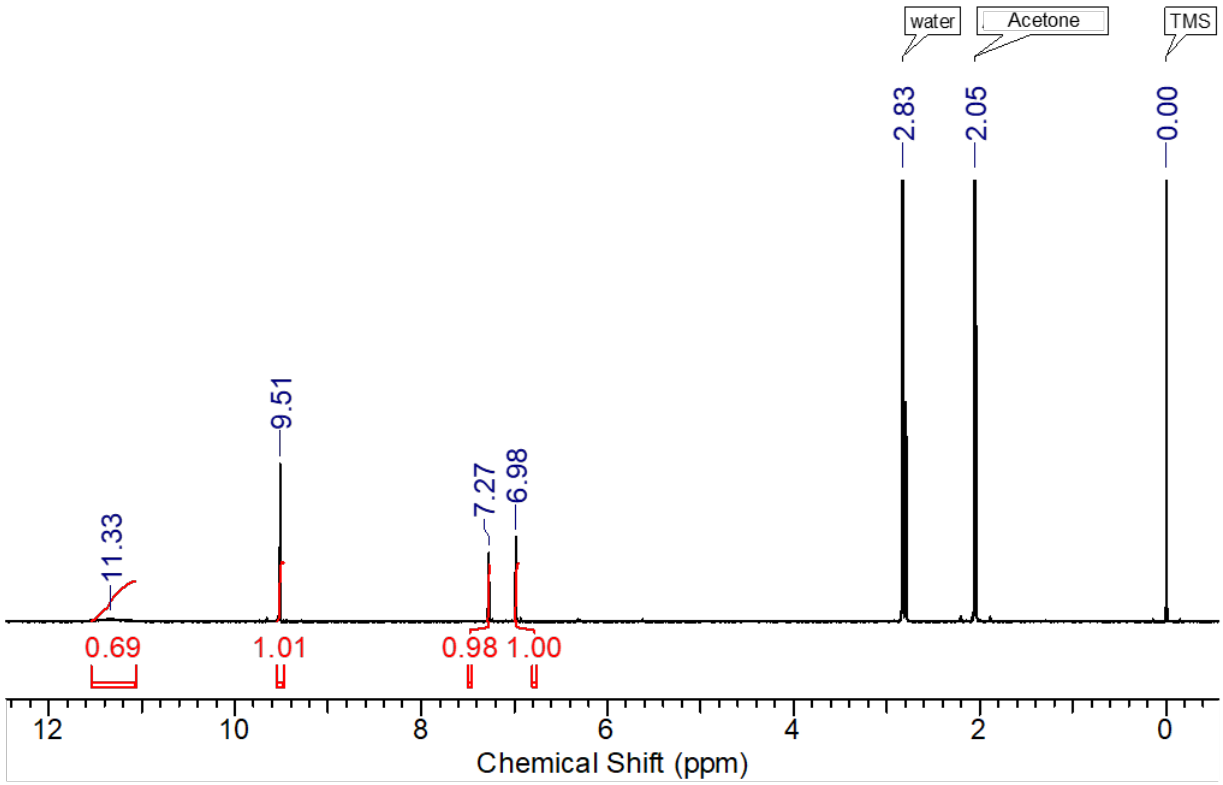


Fig. S1 ^{1}H NMR spectrum of compound **1** in $CDCl_3$ at 298 K.

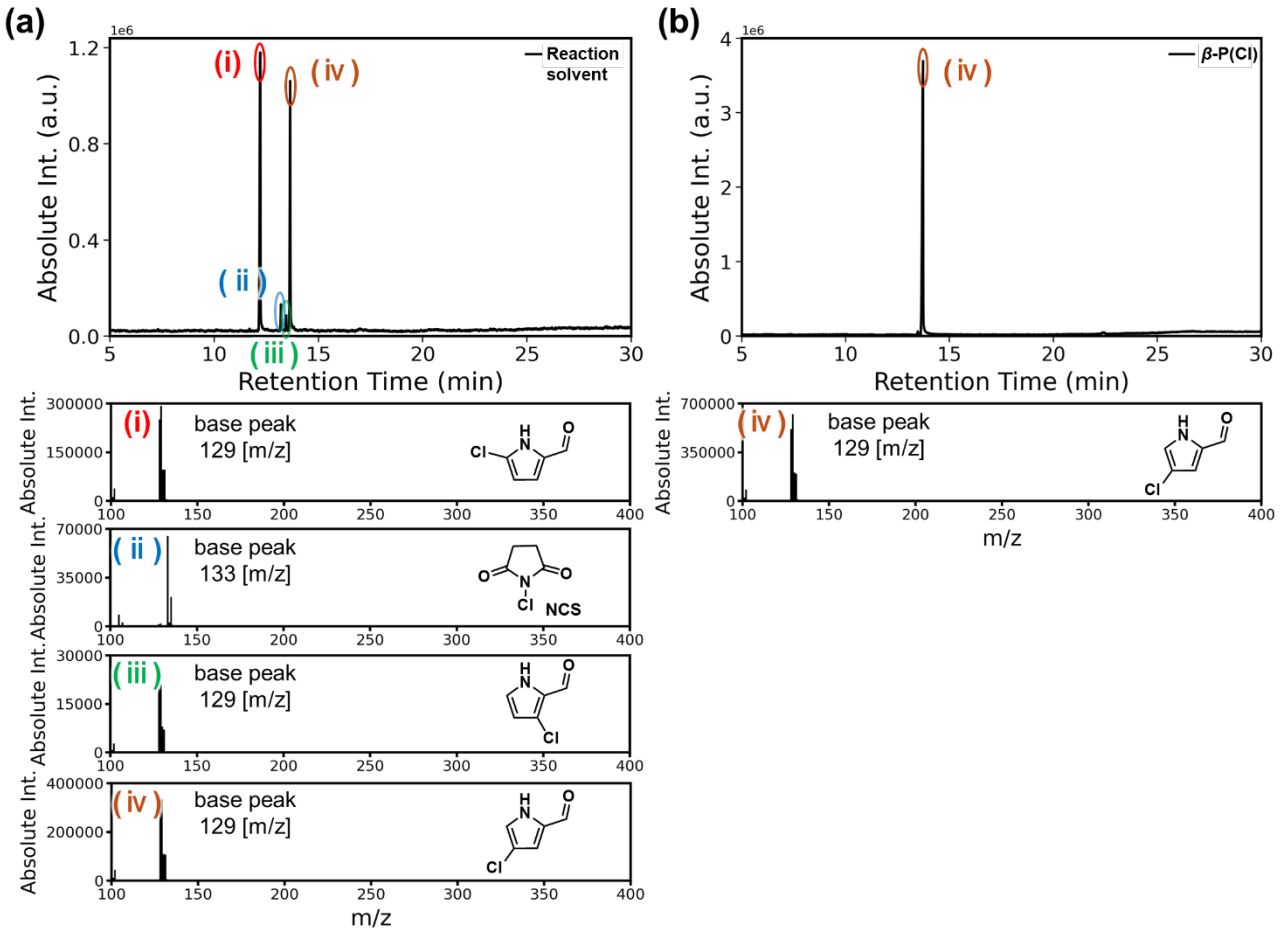


Fig. S2 GC–MS spectra of (a) the crude reaction mixture obtained after stirring pyrrole-2-carboxaldehyde with *N*-chlorosuccinimide in dry THF for 27 h under nitrogen, and (b) the purified product 4-chloro-1H-pyrrole-2-carbaldehyde (**1**).

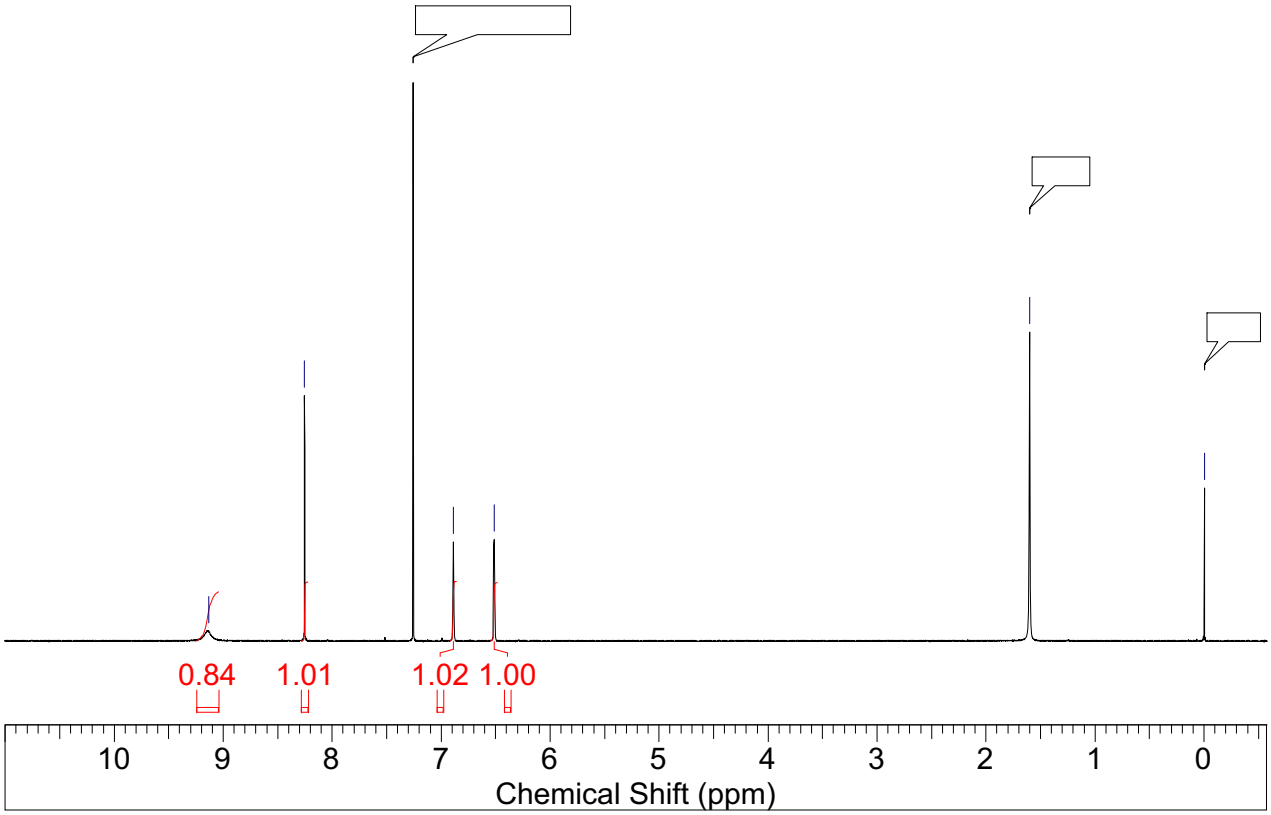


Fig. S3 ^{1}H NMR spectrum of compound $\mathbf{L_{Cl}}$ in $CDCl_3$ at 298 K.

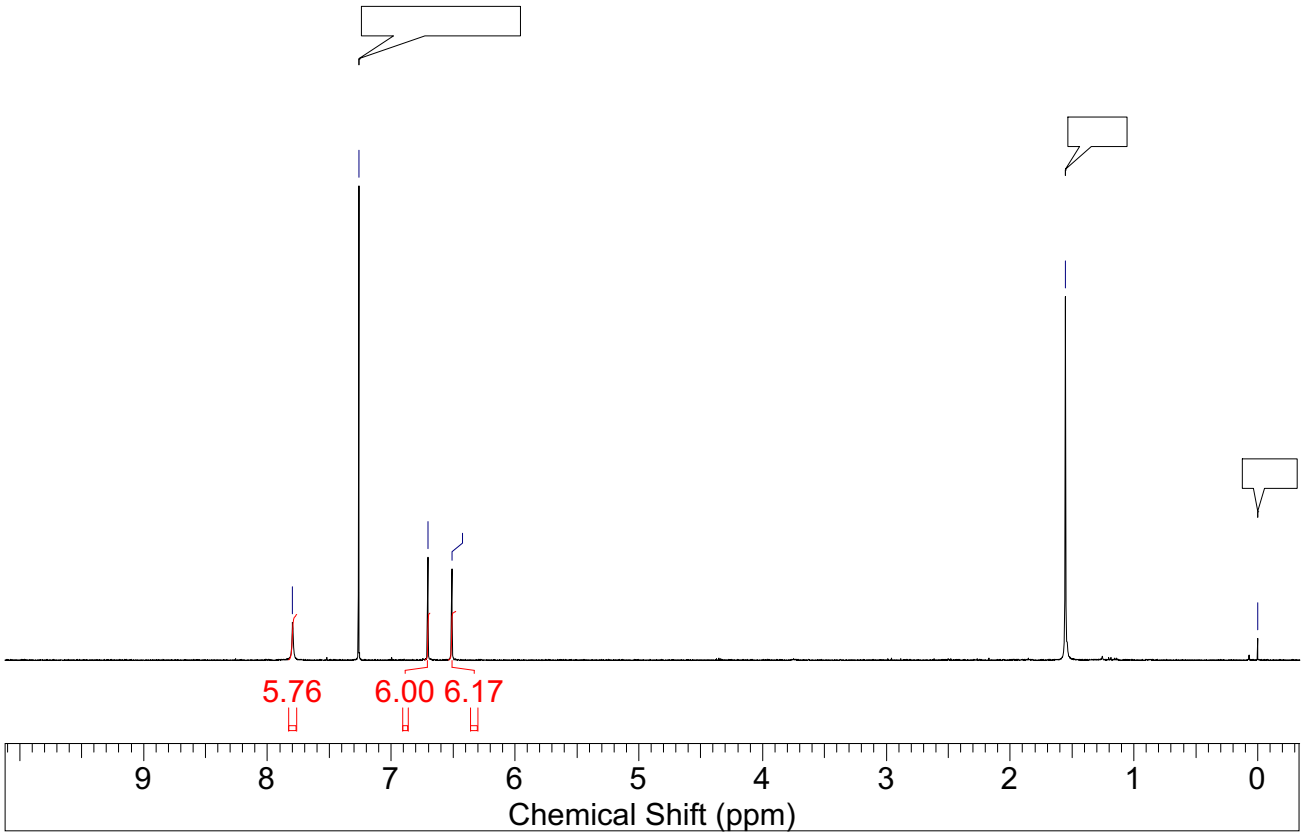


Fig. S4 ^{1}H NMR spectrum of compound **Cl** in $CDCl_3$ at 298 K.

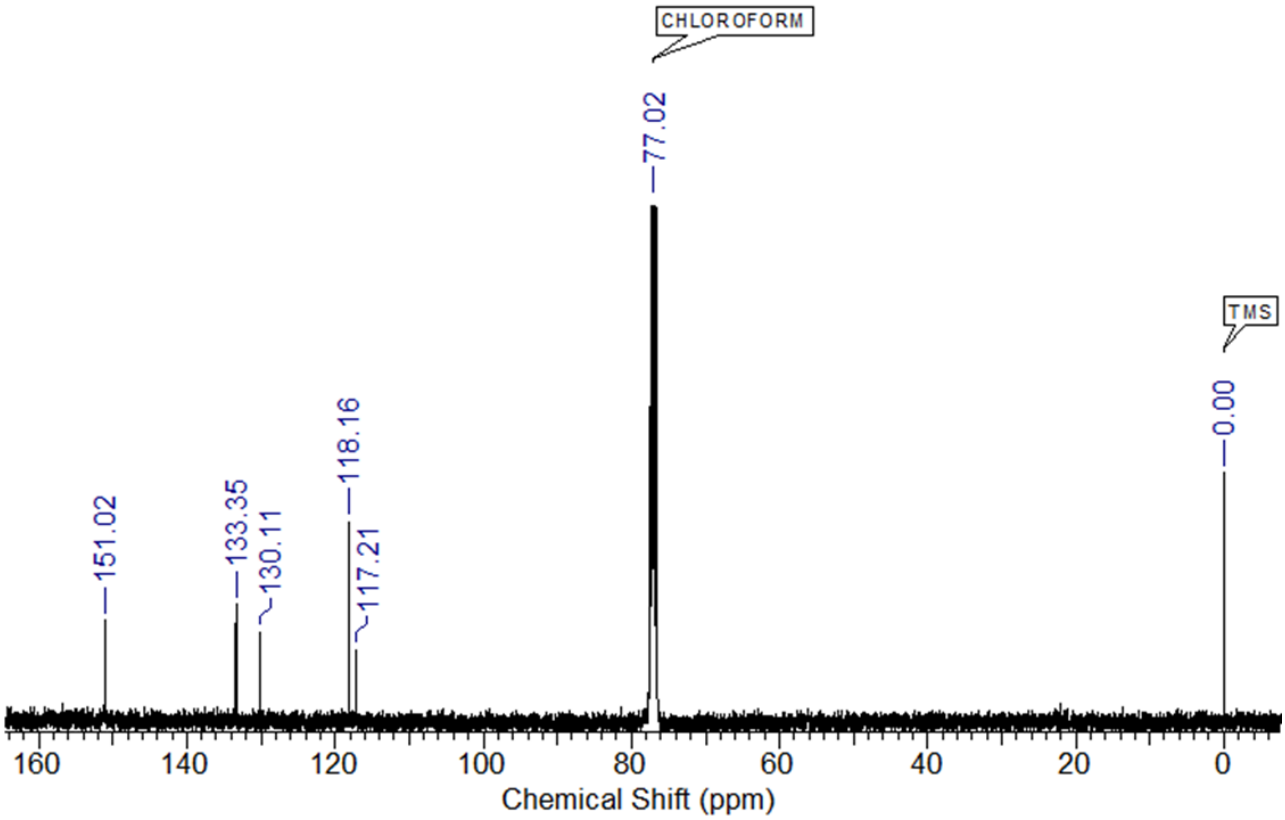


Fig. S5 ^{13}C NMR spectrum of compound **Cl** in $CDCl_3$ at 298 K.

Crystal Structures

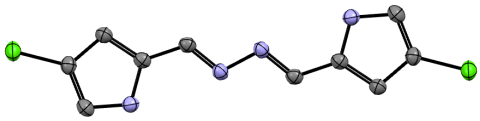


Fig. S6 Crystal structure of $\mathbf{L_{Cl}}$ at 150 K determined by X-ray diffraction. Ellipsoids are plotted at the 50% probability level. Hydrogen atoms are omitted for clarity. Color code: C, gray; N, blue; Cl, green.

Table S1 Crystallographic data for $\mathbf{L_{Cl}}$ at 150 K determined by X-ray diffraction.

Compound	$\mathbf{L_{Cl}}$
CCDC No.	2497171
Empirical formula	$C_{10}H_8N_8Cl_2$
Formula weight	255.10
Temperature [K]	150
Wavelength [Å]	1.54184
Crystal system	monoclinic
Space group	I2/a
a [Å]	17.1658(7)
b [Å]	9.8021(4)
c [Å]	14.1827(6)
α [°]	90
β [°]	103.106(4)
γ [°]	90
Volume [Å^3]	2324.25(18)
Z	8
Density (calculated) [g/cm^3]	1.458
Absorption coefficient [mm^{-1}]	4.845
F(000)	1040.0
θ [°]	5.231 to 77.439
Reflections collected	10760
Independent reflections	2359 [R_{int} = 0.0386, R_{sigma} = 0.0282]
Data / restraints / parameters	2359/0/145
Goodness-of-fit on F^2	1.034
*R*1 [$I>2\sigma(I)$]	0.0412
*wR*2 (all data)	0.1131
Largest diff. peak and hole [e.Å^{-3}]	0.55/-0.28

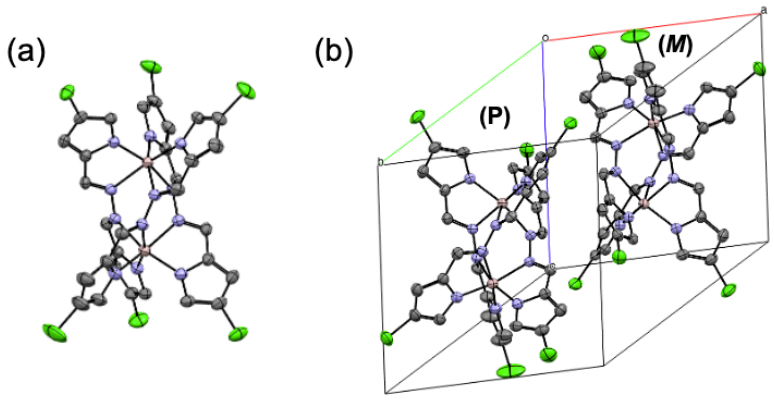


Fig. S7 (a) Crystal structure of **Cl** at 150 K determined by X-ray diffraction. Ellipsoids are plotted at the 50% probability level. Hydrogen atoms are omitted for clarity. (b) Molecular packing structure of **Cl**, illustrating the subset of unit cell. Disordered solvent molecules are omitted for clarity. An equal number of (*M*) and (*P*)-enantiomers are included in the structure. Color code: C, gray; N, blue; Al, pink; Cl, green.

Table S2 Crystallographic data for **Cl** at 150 K determined by X-ray diffraction.

Compound	**Cl**
CCDC No.	2497172
Empirical formula	$C_{36}H_{32}Al_2Cl_6N_{12}$
Formula weight	899.39
Temperature [K]	150
Wavelength [Å]	1.54184
Crystal system	triclinic
Space group	P-1
a [Å]	11.2448(3)
b [Å]	13.9951(4)
c [Å]	14.3932(4)
α [°]	99.520(2)
β [°]	107.885(2)
γ [°]	107.695(2)
Volume [Å^3]	1968.24(10)
Z	2
Density (calculated) [g/cm^3]	1.518
Absorption coefficient [mm^{-1}]	4.798
F(000)	920.0
θ [°]	3.459 to 77.697
Reflections collected	35880
Independent reflections	7977 [R_{int} = 0.0577, R_{sigma} = 0.0386]
Data / restraints / parameters	7977/0/451
Goodness-of-fit on F^2	1.063
*R*1 [$I>2\sigma(I)$]	0.0494
*wR*2 (all data)	0.1375
Largest diff. peak and hole [e.Å^{-3}]	0.68/-0.66

Optical Properties

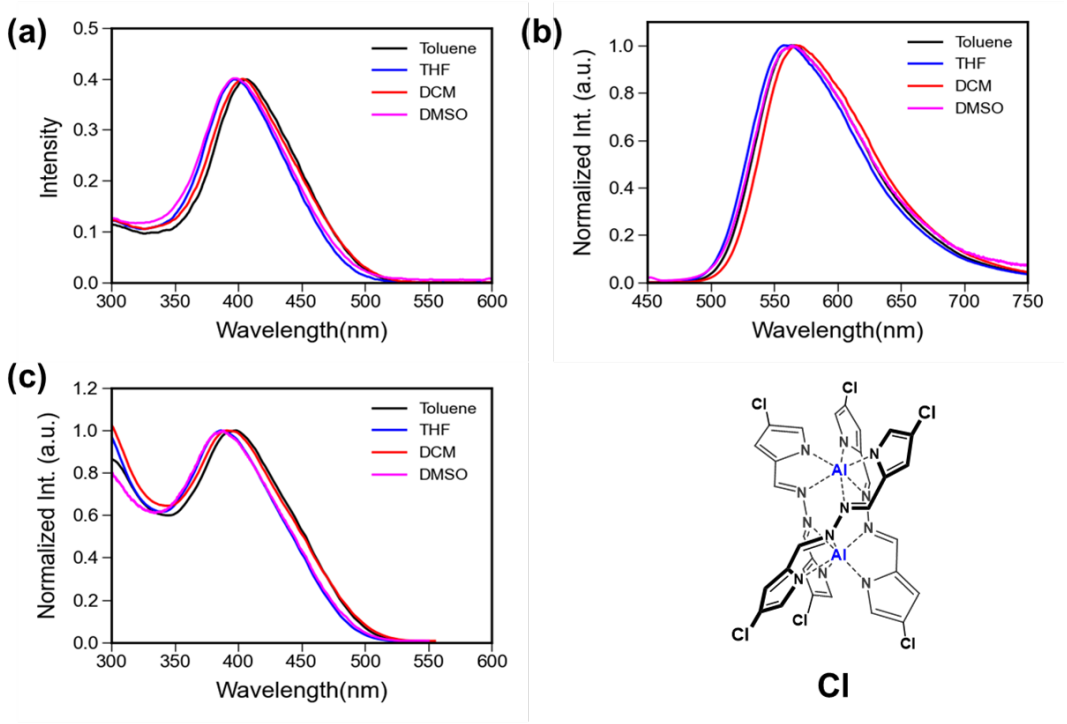


Fig. S8 (a) UV–vis absorption spectra, (b) emission spectra (excited at λ_{abs}^{max}), and (c) excitation spectra (emission wavelength at λ_{em}^{max}) of **Cl** in various solvents ($c = 10^{-6}$ M).

Table S3 Photophysical properties of **Cl** in various solvents.

Solvent	λ_{abs}^{max} / nm[a)]	λ_{em}^{max} / nm[b)]	**PLQY**[c)]	τ_{av} / ns
Toluene	405	566	0.69	3.3
THF	397	558	0.27	1.6
DCM	404	567	0.26	1.6
DMSO	398	566	0.01	0.11

[a)] Absorption maxima; [b)] Emission maxima, excited at λ_{abs}^{max}; [c)] Absolute photoluminescence quantum yields. Excited at λ_{abs}^{max}.

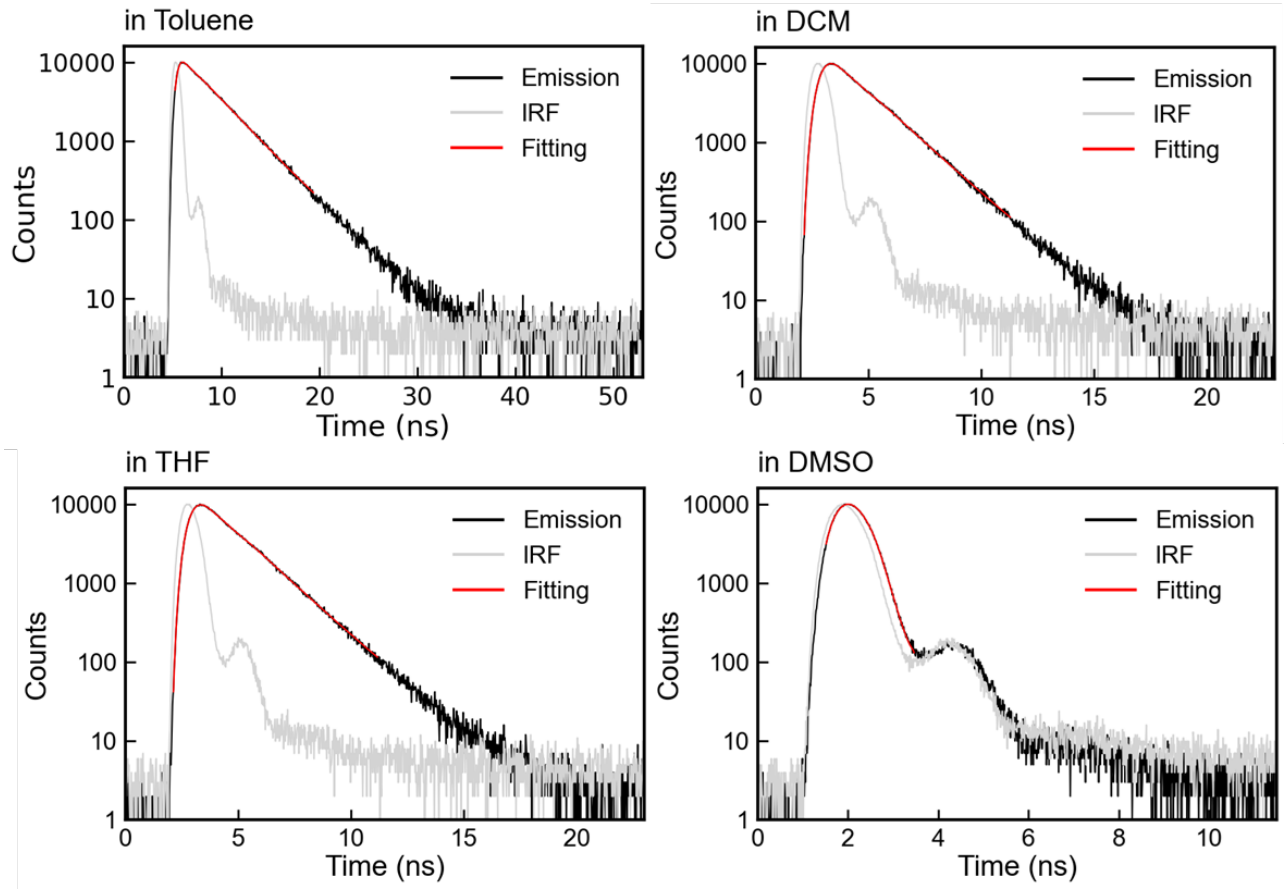


Fig. S9 Emission decay curves (black line), fits (red line), and instrument response function (IRF) (gray line) of **Cl** in various solvents.

Table S4 Summary of lifetime analyses for **Cl** in various solvents. Emission lifetimes (τ), pre-exponential factor (A) and intensity average lifetime (τ_{av}).

Solvent	λ_{ex} / nm[a)]	λ_{em} / nm[b)]	**CHI**	τ_{av} / ns	τ_1 / ns	A_1
Toluene	405	566	1.25	3.29	3.29	766.75
THF	405	558	1.18	1.61	1.61	386.58
DCM	405	567	1.19	1.62	1.62	389.77
DMSO	405	566	1.21	0.12	0.12	975.13

[a)] Excitation wavelength. [b)] Emission wavelength.

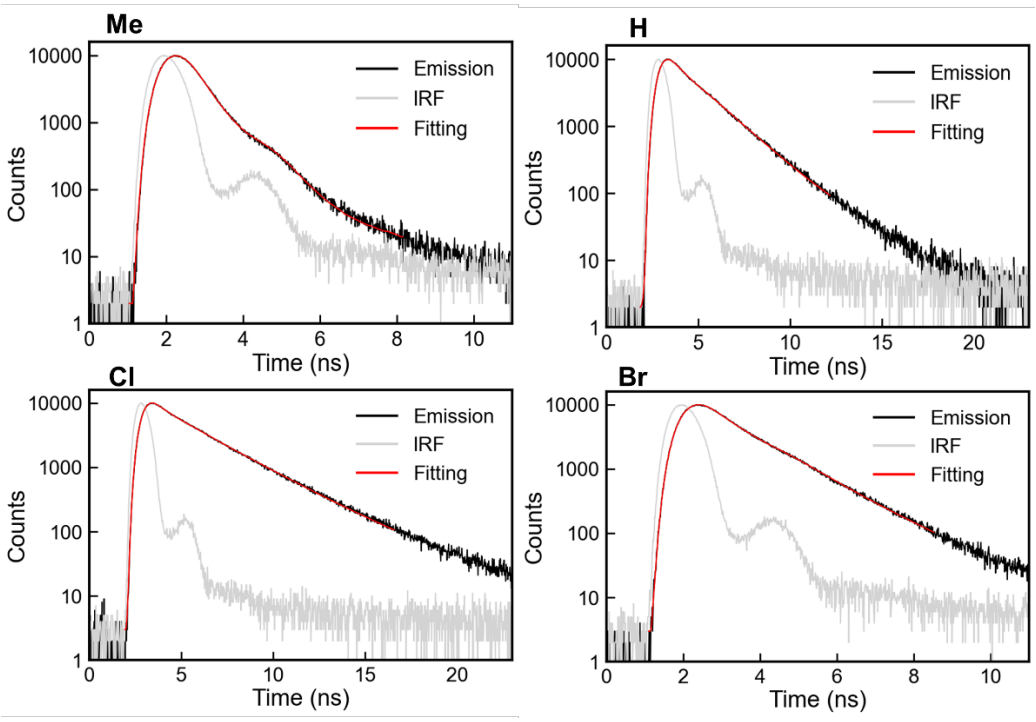


Fig. S10 Emission decay curves (black line), fits (red line), and instrument response function (IRF) (gray line) of **Me**, **H**, **Cl**, and **Br** in the solid states.

Table S5 Summary of lifetime analyses for **Me**, **H**, **Cl**, and **Br** in crystalline. Emission lifetimes (τ), pre-exponential factor (A) and intensity average lifetime (τ_{av}).

Compd.	λ_{ex} / nm[a)]	λ_{em} / nm[b)]	CHI	τ_{av} / ns	τ_1 / ns	τ_2 / ns	A_1	A_2
Me	405	466	1.26	0.51	0.33	0.74	283.65	96.03
H	405	574	1.29	1.65	0.61	1.78	110.53	323.54
Cl	405	567	1.08	2.57	0.94	2.81	118.37	269.78
Br	405	568	1.18	1.11	0.44	1.24	93.41	166.40

a) Excitation wavelength. [b)] Emission wavelength.

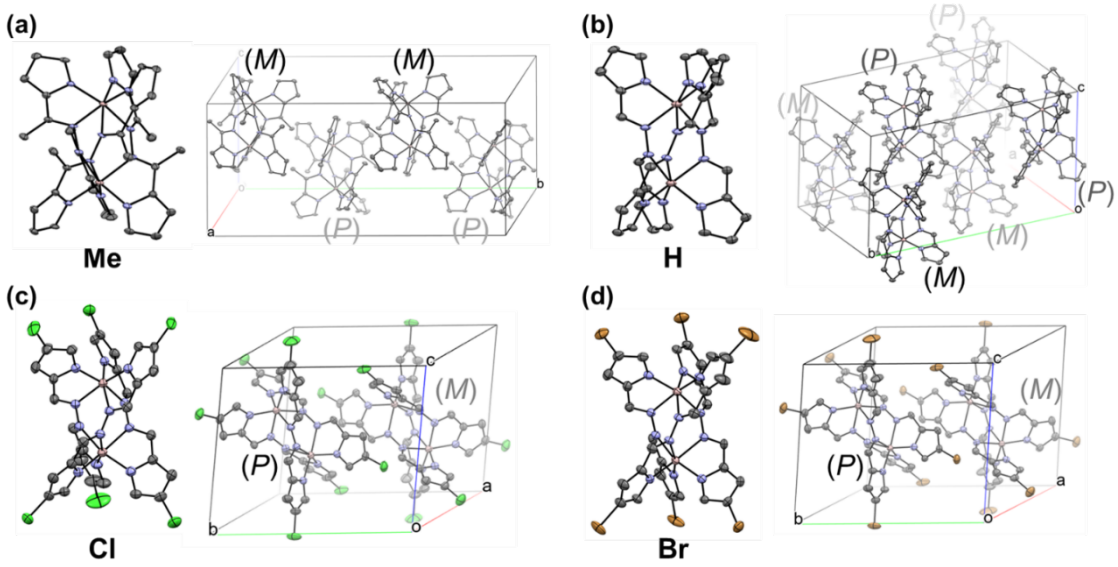


Fig. S11 Crystal structure using depth cue of (a) **Me**, (b) **H**, (c) **Cl**, and (d) **Br** by X-ray diffraction. (Right) Ellipsoids are plotted at the 50% probability level. In the structure depicted by using the ellipsoid model, carbon (C) atoms are represented in gray, nitrogen (N) atoms in blue, aluminum (Al) atoms in pink, chlorine (Cl) atoms in green, and bromine (Br) in orange. The crystal structures of **Me**, **H**, **Br** were taken from literature (refs.1 and 3; CCDC 1969992 for **Me**, 1969993 for **H**, and 2314538 for **Br**). Hydrogen atoms are omitted for clarity. (Left) Molecular packing structure, illustrating the subset of unit cell. Disordered solvent molecules are omitted for clarity. An equal number of (*M*) and (*P*)- enantiomers are included in the structure.

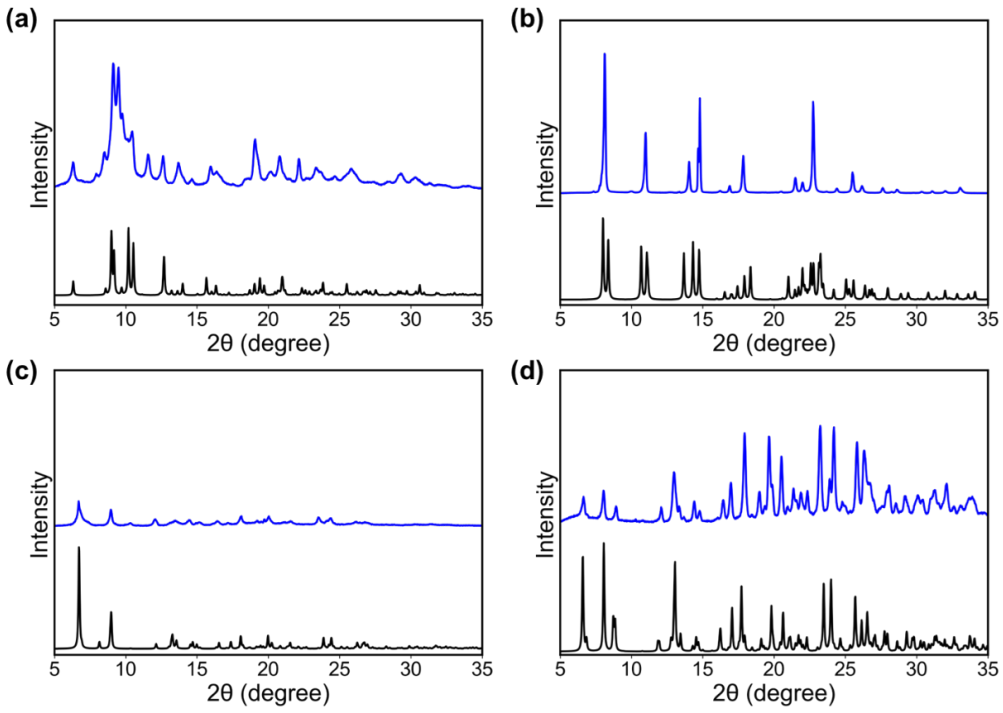


Fig. S12 Powder X-ray diffraction (PXRD) patterns of the (a) **Me**, (b) **H**, (c) **Cl**, and (d) **Br** in the solid state. The blue line represents experimental data, and the black line shows simulated PXRD patterns based on single-crystal structures.

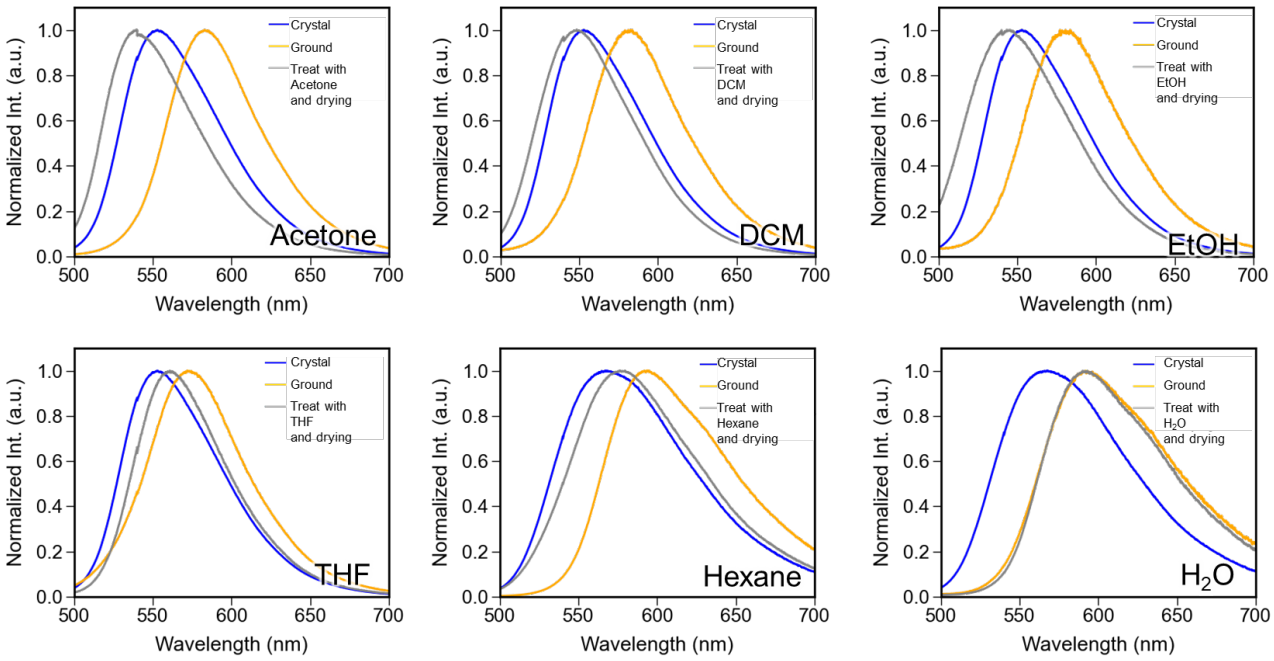


Fig. S13 Emission spectra showing the effect of various solvent treatments on the mechanochromic behavior of **Cl**.

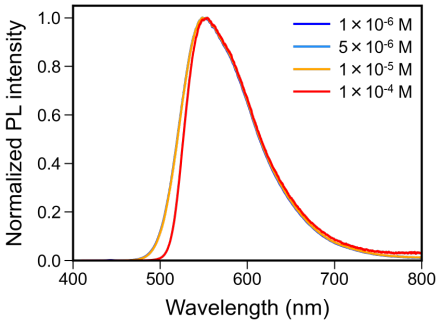


Fig. S14 Emission spectra of **H** in toluene at various concentrations.

Table S6 Summary of average lifetime (τ_{av}) for **H** in toluene at various concentrations.

Concentration	**λ_{ex} / nm[a)]**	**λ_{em} / nm[b)]**	**τ_{av} / ns**
1×10^{-6} M	405	551	3.28
5×10^{-6} M	405	551	3.28
1×10^{-5} M	405	551	3.28
1×10^{-4} M	405	551	3.59

[a)] Excitation wavelength. [b)] Emission wavelength

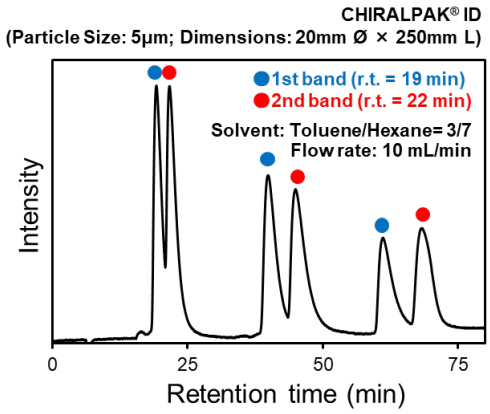


Fig. S15 Chiral HPLC profile (UV detection: l = 400 nm) for the separation of enantiomers of **Cl** (column: CHIRALPAK ID, solvent: toluene:hexane = 3:7, Flow rate: 10 mL/min). Frac. 1 (blue) = (*P*)-**Cl** , Frac. 2 (red) = (*M*)-**Cl**.

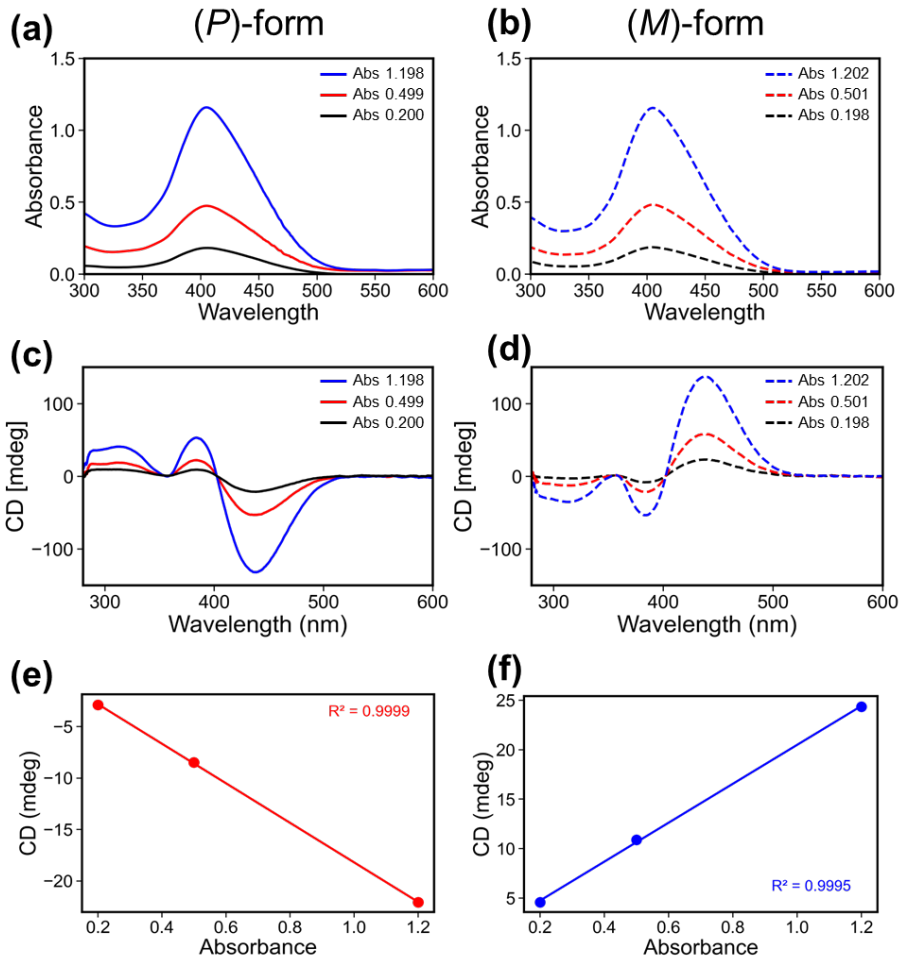


Fig. S16 Concentration-dependent UV–vis absorption and CD spectra of (*P*)-**Cl** and (*M*)-**Cl** in toluene measured at 298 K. (a, b) UV–vis absorption spectra at maximum absorbance of 0.2, 0.5, 1.2, and their (c, d) CD spectra. (e, f) A linear correlation between absorbance and ellipticity at 406 nm in toluene.

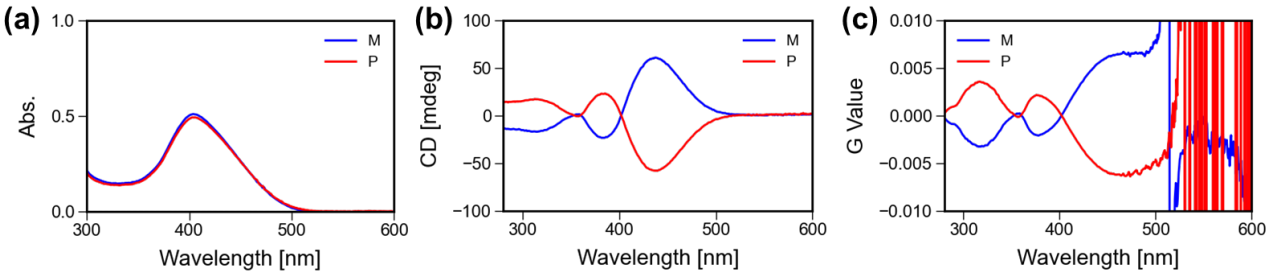


Fig. S17 (a) UV-vis absorption, (b) CD and (c) g_{abs} spectra of (*P*)-**Cl** and (*M*)-**Cl** in toluene. The concentration is 3.1×10^{-5} M.

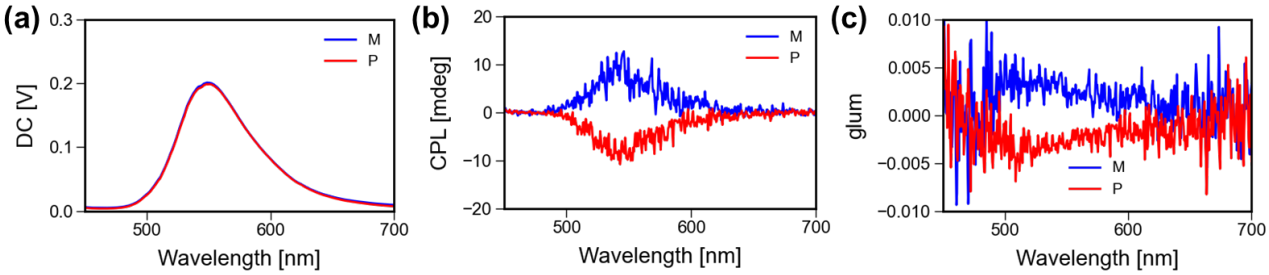


Fig. S18 (a) DC (nonpolarized fluorescence), (b) CPL and (c) g_{lum} spectra of (*P*)-**Cl** and (*M*)-**Cl** in toluene. The concentration is 3.1×10^{-5} M. Excited at 399 nm.

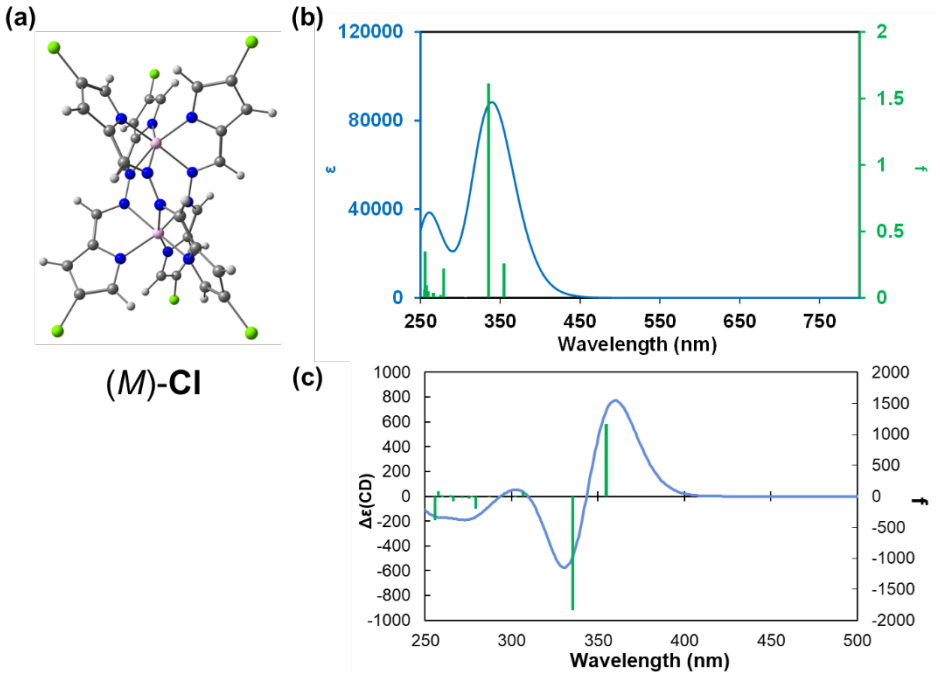


Fig. S19 Calculated (a) optimized structure, (b) UV-vis absorption and (c) CD spectra of (*M*)-**Cl** by TD-DFT method.

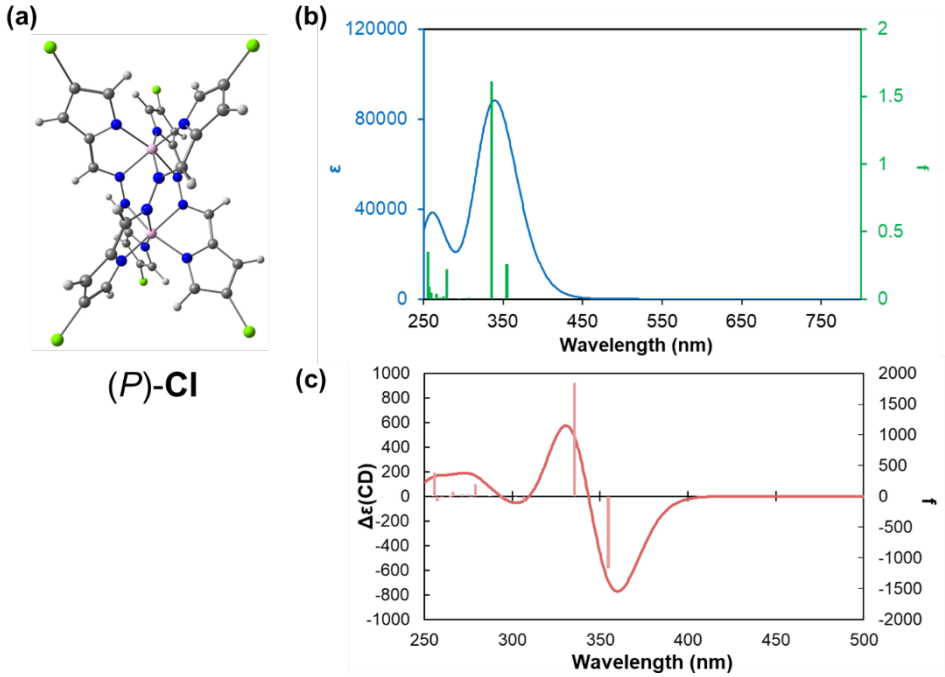


Fig. S20 Calculated (a) optimized structure, (b) UV-vis absorption and (c) CD spectra of (*P*)-**Cl** by TD-DFT method.

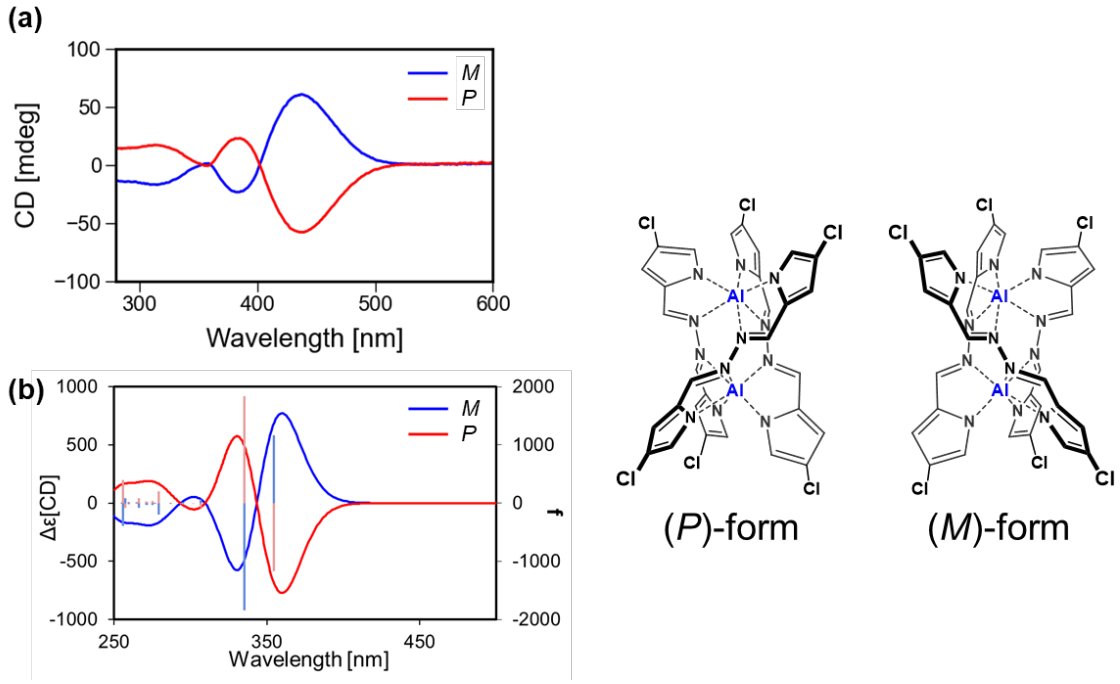


Fig. S21 (a) Experimental and (b) calculated CD spectra for **Cl**.

Table S7 Calculated photophysical property data of the ground state for (*P*)-**Cl** at the CAM-B3LYP/6-31G(d,p) level.

	Electronic Transition	TD//CAM-B3LYP/6-31G(d,p)			
		Energy/eV[a]		f[b]	Major contributions
Cl	$S_0 \rightarrow S_1$	3.4944 eV	354.81 nm	0.2592	H-2->LUMO (24%), H-1->LUMO (21%), HOMO->L+1 (21%), HOMO->L+2 (21%)
	$S_0 \rightarrow S_2$	3.4960 eV	354.65 nm	0.2593	H-2->L+1 (24%), H-1->L+1 (20%), H-1->L+2 (21%), HOMO->LUMO (21%)
	$S_0 \rightarrow S_3$	3.6974 eV	335.33 nm	1.612	H-1->L+1 (41%), HOMO->LUMO (41%)
	$S_0 \rightarrow S_4$	4.0416 eV	306.77 nm	0.008	H-5->L+1 (17%), H-2->L+3 (12%), H-1->L+3 (12%), H-1->L+5 (10%), HOMO->L+4 (12%)
[a]Only the selected low-lying excited states are presented. [b]Oscillator strength.					

Table S8 Calculated photophysical property data of the ground state for (*M*)-**Cl** at the CAM-B3LYP/6-31G(d,p) level.

	Electronic Transition	TD//CAM-B3LYP/6-31G(d,p)			
		Energy/eV[a]		f[b]	Major contributions
Cl	$S_0 \rightarrow S_1$	3.4944 eV	354.81 nm	0.2592	H-2->LUMO (24%), H-1->LUMO (21%), HOMO->L+1 (21%), HOMO->L+2 (21%)
	$S_0 \rightarrow S_2$	3.4960 eV	354.65 nm	0.2593	H-2->L+1 (24%), H-1->L+1 (20%), H-1->L+2 (21%), HOMO->LUMO (21%)
	$S_0 \rightarrow S_3$	3.6974 eV	335.33 nm	1.612	H-1->L+1 (41%), HOMO->LUMO (41%)
	$S_0 \rightarrow S_4$	4.0416 eV	306.77 nm	0.008	H-5->L+1 (17%), H-2->L+3 (12%), H-1->L+3 (12%), H-1->L+5 (10%), HOMO->L+4 (12%)
[a]Only the selected low-lying excited states are presented. [b]Oscillator strength.					

Table S9 Coordinates of electric transition dipole moment (μ) and magnetic transition dipole moments (m) of the ground state of (*P*)-**Cl** at the CAM-B3LYP/6-31G(d,p) level.

	Electronic Transition	μ [a.u.]			m [a.u.]		
		x	y	z	x	y	z
Cl	$S_0 \rightarrow S_1$	0.0021	-0.0349	1.7397	-0.0012	-0.0569	2.8472
	$S_0 \rightarrow S_2$	0.0224	-1.7396	-0.0346	-0.0091	-2.8475	-0.0566
	$S_0 \rightarrow S_3$	-4.2184	-0.0081	0.0004	1.8511	-0.0151	0.0009
	$S_0 \rightarrow S_4$	0.0004	0.043	-0.281	-0.0002	0.1524	-0.9938

Table S10 Calculated transition dipole moments (μ, m, and θ) and g_{abs} values of (*P*)-**Cl**.

	Electronic Transition	Energy [nm]	$\lvert\mu\rvert$ [10^{-20} esu cm]	$\lvert m\rvert$ [10^{-20} erg G^{-1}]	θ [º]	$cos\theta$	g_{abs}^{cal}
Cl	$S_0 \rightarrow S_1$	354.81	442.28	2.64	0.09	1.00	2.39×10^{-2}
	$S_0 \rightarrow S_2$	354.65	442.29	2.64	0.92	1.00	2.39×10^{-2}
	$S_0 \rightarrow S_3$	335.33	1072.21	1.72	179.4	-1.00	-6.40×10^{-3}
	$S_0 \rightarrow S_4$	306.76	72.25	0.93	0.1	1.00	5.16×10^{-2}

Table S11 Coordinates of electric transition dipole moment (μ) and magnetic transition dipole moments (m) of the excited state of (*P*)-**Cl** at the CAM-B3LYP/6-31G(d,p) level.

	Electronic Transition	μ [a.u.]			m [a.u.]		
		x	y	z	x	y	z
Cl	$S_1 \rightarrow S_0$	-2.4686	0.0044	1.6412	0.6701	0.0055	2.2712

Table S12 Calculated transition dipole moments (μ, m, and θ) and g_{lum} values of (*P*)-**Cl**.

	Electronic Transition	Energy [nm]	$\lvert\mu\rvert$ [10^{-20} esu cm]	$\lvert m\rvert$ [10^{-20} erg G^{-1}]	θ [º]	$cos\theta$	g_{lum}^{cal}
Cl	$S_1 \rightarrow S_0$	466.33	753.47	2.1961	72.82	0.30	3.44×10^{-3}

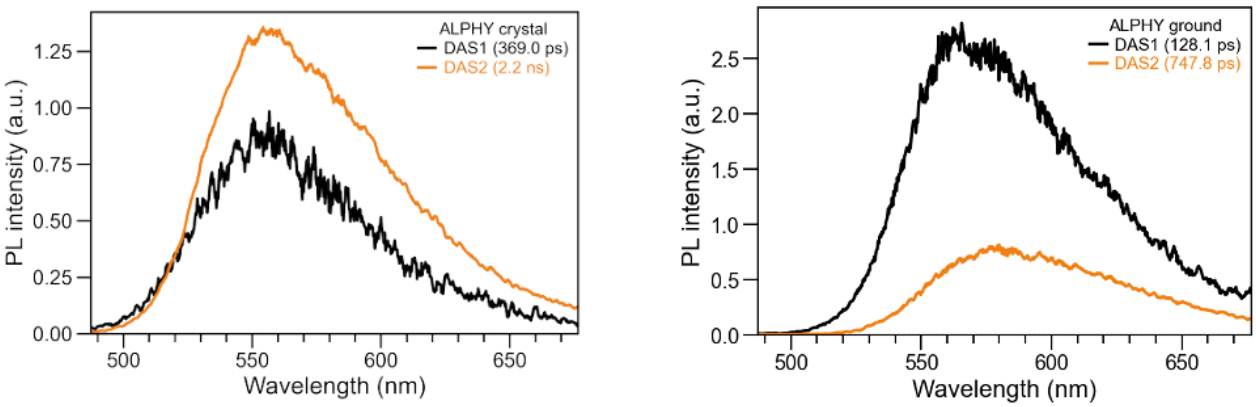


Fig. S22 The decay-associated spectra (DASs) with time constants obtained from the global analysis of TRPL data for the (a) crystalline powder and (b) ground states of **Cl.**

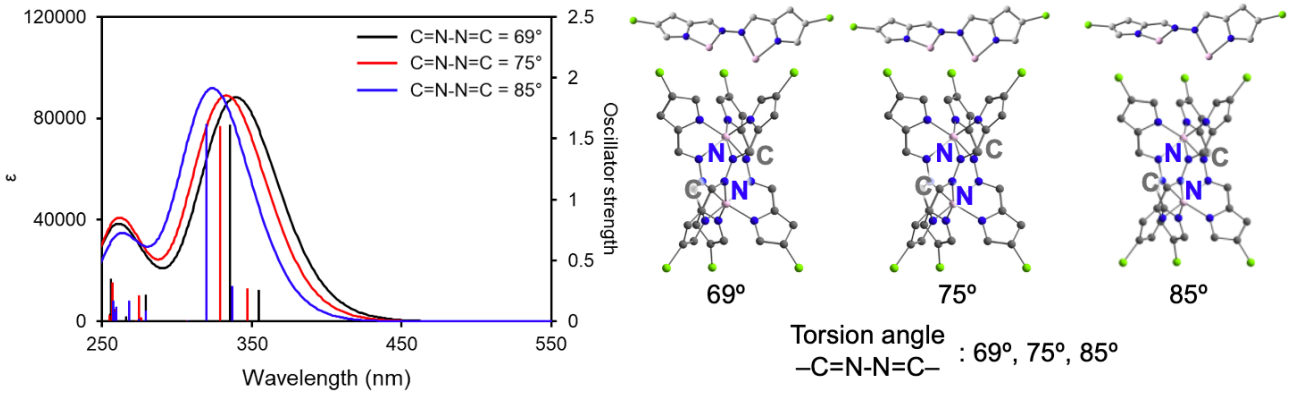


Fig. S23 Simulated UV-vis absorption spectra of **Cl** with fixed ligand torsion angles (–C=N–N=C–) by TD-DFT method.

The ground state (S_0) of (*P*)-**Cl** optimized at CAM-B3LYP/6-31G(d,p) level.

Al	1.929516000	-0.000351000	0.000010000
Al	-1.929634000	0.000570000	-0.000112000
N	0.650090000	0.205899000	-1.614106000
N	0.650184000	1.295009000	0.985263000
N	2.923018000	1.287656000	-1.101271000
N	0.649260000	-1.500910000	0.628653000
N	-0.649950000	-0.273083000	-1.604069000
N	2.922552000	0.309118000	1.666196000
N	-0.649517000	1.526315000	0.565075000
N	-0.650294000	-1.251940000	1.038916000
N	2.921782000	-1.598627000	-0.565068000
N	-2.922846000	-0.238742000	1.677621000
N	-2.922741000	-1.332716000	-1.046349000
N	-2.921959000	1.573540000	-0.631977000
C	-2.345863000	2.792617000	-0.331722000
C	2.346508000	1.587526000	-2.320270000
C	2.347079000	1.216440000	2.534404000
C	-2.345843000	-1.683846000	-2.251395000
C	-1.072404000	2.721643000	0.281742000
H	-0.457436000	3.601017000	0.467665000
C	-2.347043000	-1.108336000	2.583436000
C	2.345416000	-2.803955000	-0.214196000
C	1.072968000	1.011348000	-2.541697000
H	0.457875000	1.254616000	-3.406859000
C	4.095504000	-1.881398000	-1.151322000
C	4.096596000	1.936961000	-1.052521000
C	-1.073622000	-1.604333000	2.215584000
H	-0.459083000	-2.205466000	2.884178000
C	-4.096707000	0.149976000	2.199373000
C	1.071949000	-2.707130000	0.395686000
H	0.456794000	-3.577821000	0.618244000
C	1.073727000	1.696749000	2.145947000
H	0.459295000	2.325576000	2.788669000
C	4.096210000	-0.057733000	2.203969000
C	-3.172478000	-1.268119000	3.697451000
C	3.170279000	-3.865599000	-0.588979000
C	3.172508000	1.422685000	3.640790000

C	4.282471000	0.610545000	3.417354000
Cl	5.654921000	0.432645000	4.456178000
C	3.171295000	2.443568000	-3.051635000
C	-1.072282000	-1.117427000	-2.496629000
H	-0.456797000	-1.397165000	-3.350416000
C	-3.170343000	-2.570131000	-2.946132000
C	4.280897000	-3.266452000	-1.179827000
C	-4.282807000	-0.466706000	3.439806000
C	-4.096335000	-1.979396000	-0.970563000
C	-4.281189000	-2.747117000	-2.123830000
Cl	-5.653135000	-3.750897000	-2.447261000
C	-4.095583000	1.831337000	-1.229826000
C	4.281854000	2.655199000	-2.237183000
Cl	5.653935000	3.644387000	-2.602332000
C	-3.170859000	3.837494000	-0.750704000
C	-4.281204000	3.213962000	-1.316268000
Cl	-5.653358000	3.996138000	-2.023237000
H	2.992025000	-4.921860000	-0.451092000
H	4.746960000	-1.109268000	-1.536060000
H	2.992927000	2.853175000	-4.034941000
H	4.748147000	1.883588000	-0.191561000
H	4.747006000	-0.777682000	1.727795000
H	2.994956000	2.070651000	4.486421000
H	-4.748116000	-1.889632000	-0.112816000
H	-2.991644000	-3.020974000	-3.911164000
H	-4.746730000	1.043672000	-1.582233000
H	-2.992806000	4.898637000	-0.657174000
H	-4.747897000	0.848770000	1.693151000
H	-2.994875000	-1.879937000	4.569590000
Cl	5.652963000	-4.077808000	-1.853334000
Cl	-5.655343000	-0.245383000	4.470143000

The ground state (S_0) of (*M*)-**Cl** optimized at CAM-B3LYP/6-31G(d,p) level.

Al	-1.929516000	-0.000351000	0.000010000
Al	1.929634000	0.000570000	-0.000112000
N	-0.650090000	0.205902000	-1.614106000
N	-0.650184000	1.295007000	0.985265000
N	-2.923018000	1.287658000	-1.101269000

N	-0.649260000	-1.500911000	0.628650000
N	0.649950000	-0.273080000	-1.604070000
N	-2.922552000	0.309115000	1.666196000
N	0.649517000	1.526314000	0.565077000
N	0.650294000	-1.251941000	1.038914000
N	-2.921782000	-1.598626000	-0.565070000
N	2.922846000	-0.238745000	1.677620000
N	2.922741000	-1.332714000	-1.046351000
N	2.921959000	1.573541000	-0.631975000
C	2.345863000	2.792617000	-0.331717000
C	-2.346508000	1.587530000	-2.320267000
C	-2.347079000	1.216436000	2.534406000
C	2.345843000	-1.683843000	-2.251398000
C	1.072404000	2.721643000	0.281746000
H	0.457436000	3.601016000	0.467671000
C	2.347043000	-1.108340000	2.583434000
C	-2.345416000	-2.803954000	-0.214200000
C	-1.072968000	1.011352000	-2.541695000
H	-0.457875000	1.254621000	-3.406857000
C	-4.095504000	-1.881396000	-1.151325000
C	-4.096596000	1.936962000	-1.052518000
C	1.073622000	-1.604337000	2.215581000
H	0.459083000	-2.205471000	2.884175000
C	4.096707000	0.149973000	2.199373000
C	-1.071949000	-2.707131000	0.395682000
H	-0.456794000	-3.577822000	0.618238000
C	-1.073727000	1.696746000	2.145950000
H	-0.459295000	2.325572000	2.788673000
C	-4.096210000	-0.057736000	2.203969000
C	3.172478000	-1.268125000	3.697449000
C	-3.170279000	-3.865598000	-0.588985000
C	-3.172508000	1.422679000	3.640792000
C	-4.282471000	0.610540000	3.417355000
Cl	-5.654921000	0.432638000	4.456179000
C	-3.171295000	2.443573000	-3.051631000
C	1.072282000	-1.117424000	-2.496631000
H	0.456797000	-1.397160000	-3.350418000
C	3.170343000	-2.570127000	-2.946136000

C	-4.280897000	-3.266451000	-1.179832000
C	4.282807000	-0.466711000	3.439805000
C	4.096335000	-1.979394000	-0.970566000
C	4.281189000	-2.747113000	-2.123835000
Cl	5.653135000	-3.750893000	-2.447267000
C	4.095583000	1.831339000	-1.229823000
C	-4.281854000	2.655202000	-2.237179000
Cl	-5.653935000	3.644391000	-2.602326000
C	3.170859000	3.837495000	-0.750698000
C	4.281204000	3.213964000	-1.316263000
Cl	5.653358000	3.996141000	-2.023231000
H	-2.992025000	-4.921860000	-0.451099000
H	-4.746960000	-1.109266000	-1.536061000
H	-2.992927000	2.853181000	-4.034937000
H	-4.748147000	1.883589000	-0.191558000
H	-4.747006000	-0.777685000	1.727794000
H	-2.994956000	2.070644000	4.486425000
H	4.748116000	-1.889632000	-0.112819000
H	2.991644000	-3.020968000	-3.911169000
H	4.746730000	1.043675000	-1.582232000
H	2.992806000	4.898638000	-0.657167000
H	4.747897000	0.848767000	1.693153000
H	2.994875000	-1.879944000	4.569587000
Cl	-5.652963000	-4.077805000	-1.853340000
Cl	5.655343000	-0.245390000	4.470143000

The ground state (S_1) of (*P*)-**Cl** optimized at CAM-B3LYP/6-31G(d,p) level.

Al	1.895875000	0.059383000	-0.051852000
Al	-1.895714000	0.060179000	0.050945000
N	0.624735000	1.087343000	-1.296236000
N	0.678625000	0.685164000	1.497077000
N	2.937358000	1.697676000	-0.393241000
N	0.614351000	-1.560258000	-0.249437000
N	-0.678512000	0.676983000	-1.501183000
N	2.941600000	-0.508236000	1.525759000
N	-0.624459000	1.094586000	1.289979000
N	-0.614223000	-1.558740000	0.257469000
N	2.910352000	-1.093156000	-1.269168000

N	-2.910207000	-1.085667000	1.274487000
N	-2.941562000	-0.516447000	-1.523471000
N	-2.936914000	1.700312000	0.383463000
C	-2.366583000	2.588872000	1.273415000
C	2.366380000	2.582234000	-1.286760000
C	2.414253000	-0.149515000	2.749795000
C	-2.413609000	-0.165356000	-2.749469000
C	-1.068923000	2.238215000	1.717497000
H	-0.458334000	2.891514000	2.338848000
C	-2.463187000	-2.407034000	1.333700000
C	2.463109000	-2.414762000	-1.321095000
C	1.068738000	2.229218000	-1.728886000
H	0.457744000	2.879510000	-2.352984000
C	4.090253000	-1.050083000	-1.896253000
C	4.138154000	2.197163000	-0.060751000
C	-1.213407000	-2.662230000	0.735425000
H	-0.717613000	-3.623663000	0.784445000
C	-4.090103000	-1.038937000	1.901341000
C	1.213331000	-2.666466000	-0.721384000
H	0.717361000	-3.628064000	-0.765123000
C	1.141240000	0.461276000	2.691962000
H	0.553284000	0.687826000	3.579932000
C	4.119383000	-1.103663000	1.766383000
C	-3.395403000	-3.196744000	2.026776000
C	3.395241000	-3.208425000	-2.009780000
C	3.274528000	-0.527849000	3.782873000
C	4.356429000	-1.129254000	3.144835000
Cl	5.752966000	-1.811547000	3.905686000
C	3.221583000	3.659995000	-1.520778000
C	-1.140581000	0.445639000	-2.694849000
H	-0.552186000	0.666707000	-3.583906000
C	-3.273528000	-0.549851000	-3.780574000
C	4.416302000	-2.336877000	-2.370395000
C	-4.416404000	-2.323106000	2.382430000
C	-4.119302000	-1.113166000	-1.760958000
C	-4.355781000	-1.147163000	-3.139329000
Cl	-5.752103000	-1.833897000	-3.896582000
C	-4.138121000	2.197567000	0.049003000

C	4.345915000	3.401804000	-0.738712000
Cl	5.756992000	4.394714000	-0.604027000
C	-3.222489000	3.667011000	1.502991000
C	-4.346669000	3.404846000	0.721984000
Cl	-5.758379000	4.396285000	0.583189000
H	3.328472000	-4.265282000	-2.219460000
H	4.662237000	-0.136985000	-1.989928000
H	3.054087000	4.509437000	-2.166427000
H	4.792137000	1.701552000	0.642979000
H	4.739184000	-1.497231000	0.972496000
H	3.135908000	-0.386440000	4.844547000
H	-4.739494000	-1.501766000	-0.964931000
H	-3.134449000	-0.414995000	-4.843043000
H	-4.791734000	1.698658000	-0.652733000
H	-3.055567000	4.519198000	2.145157000
H	-4.662002000	-0.125272000	1.989887000
H	-3.328892000	-4.252464000	2.242199000
Cl	5.845251000	-2.726827000	-3.250954000
Cl	-5.845594000	-2.707764000	3.264966000

Table S13 Calculated photophysical property data of the ground state for (*P*)-**Cl** at the CAM-B3LYP/6-31G(d,p) level fixed 69 degree of –C=N–N=C– dihedral angle (**Cl 69**).

	Electronic Transition	TD//CAM-B3LYP/6-31G(d,p)			
		Energy/eV[a]		f[b]	Major contributions
Cl 69	$S_0 \rightarrow S_1$	3.4946 eV	354.79 nm	0.2591	H-2->LUMO (24%), H-1->LUMO (17%), H-1->L+2 (12%), HOMO->L+1 (17%)
	$S_0 \rightarrow S_2$	3.4948 eV	354.77 nm	0.2590	H-2->L+1 (24%), H-1->L+1 (17%), HOMO->LUMO (17%), HOMO->L+2 (12%)
	$S_0 \rightarrow S_3$	3.6971 eV	335.36 nm	1.6123	H-1->LUMO (27%), H-1->L+1 (14%), HOMO->LUMO (14%), HOMO->L+1 (28%)
	$S_0 \rightarrow S_4$	4.0416 eV	306.77 nm	0.008	H-5->L+1 (17%), H-2->L+3 (12%), H-1->L+3 (10%), HOMO->L+4 (10%)
[a]Only the selected low-lying excited states are presented. [b]Oscillator strength.					

Table S14 Calculated photophysical property data of the ground state for (*P*)-**Cl** at the CAM-B3LYP/6-31G(d,p) level fixed 75 degree of –C=N–N=C– dihedral angle (**Cl 75**).

	Electronic Transition	TD//CAM-B3LYP/6-31G(d,p)			
		Energy/eV[a]		f[b]	Major contributions
Cl 75	$S_0 \rightarrow S_1$	3.5737 eV	346.94 nm	0.2688	H-2->L+1 (14%), H-1->L+1 (10%), H-1->L+2 (21%), HOMO->LUMO (10%)
	$S_0 \rightarrow S_2$	3.5737 eV	346.94 nm	0.2688	H-2->LUMO (14%), H-1->LUMO (10%), HOMO->L+1 (10%), HOMO->L+2 (21%)
	$S_0 \rightarrow S_3$	3.7702 eV	328.85 nm	1.6025	H-1->LUMO (16%), H-1->L+1 (23%), HOMO->LUMO (23%), HOMO->L+1 (16%)
	$S_0 \rightarrow S_4$	4.0433 eV	306.64 nm	0.009	H-5->L+1 (10%), H-2->L+3 (11%), H-1->L+4 (14%), H-1->L+5 (14%), HOMO->L+3 (14%)
[a]Only the selected low-lying excited states are presented. [b]Oscillator strength.					

Table S15 Calculated photophysical property data of the ground state for (*P*)-**Cl** at the CAM-B3LYP/6-31G(d,p) level fixed 85 degree of –C=N–N=C– dihedral angle (**Cl 85**).

	Electronic Transition	TD//CAM-B3LYP/6-31G(d,p)			
		Energy/eV[a]		f[b]	Major contributions
Cl 85	$S_0 \rightarrow S_1$	3.6818 eV	336.75 nm	0.2879	H-2->L+1 (15%), H-1->LUMO (12%), H-1->L+4 (20%), HOMO->L+1 (12%)
	$S_0 \rightarrow S_2$	3.6818 eV	336.75 nm	0.2876	H-2->LUMO (15%), H-1->L+1 (12%), HOMO->LUMO (12%), HOMO->L+4 (21%)
	$S_0 \rightarrow S_3$	3.8755 eV	319.92 nm	1.6205	H-1->L+1 (29%), HOMO->LUMO (29%)
	$S_0 \rightarrow S_4$	4.0302 eV	307.64 nm	0.009	H-2->L+3 (10%), H-1->L+2 (11%), HOMO->L+3 (12%), HOMO->L+5 (22%)
[a]Only the selected low-lying excited states are presented. [b]Oscillator strength.					

The ground state (S_0) of (*P*)-**Cl 69** (fixed 69 degree of –C=N–N=C– dihedral angle) optimized at CAM-B3LYP/6-31G(d,p) level.

Al	1.930059000	0.000612000	0.000086000
Al	-1.929766000	0.000207000	-0.000554000
N	0.650317000	-0.752425000	-1.442728000
N	0.649823000	1.626271000	0.068909000
N	2.923289000	0.427819000	-1.639804000
N	0.649832000	-0.872026000	1.373301000
N	-0.649383000	-1.140405000	-1.160750000
N	2.922430000	1.206996000	1.190644000
N	-0.649921000	1.575742000	-0.408039000
N	-0.650057000	-0.433957000	1.567754000
N	2.922833000	-1.633506000	0.449992000
N	-2.923363000	0.761056000	1.513555000
N	-2.922106000	-1.692044000	-0.098281000
N	-2.922583000	0.930827000	-1.416839000
C	-2.346715000	2.102990000	-1.866910000
C	2.347250000	-0.023115000	-2.811547000
C	2.346181000	2.447187000	1.385680000
C	-2.345562000	-2.668081000	-0.887628000
C	-1.073201000	2.395263000	-1.322996000
H	-0.458461000	3.223449000	-1.672629000
C	-2.347463000	0.564831000	2.753727000
C	2.346025000	-2.422986000	1.425804000
C	1.073562000	-0.622293000	-2.664125000
H	0.458759000	-0.917549000	-3.513169000
C	4.096518000	-2.200552000	0.130251000
C	4.097331000	0.987859000	-1.970502000
C	-1.073729000	-0.051780000	2.734981000
H	-0.459170000	-0.163225000	3.627126000
C	-4.097145000	1.378330000	1.719812000
C	1.072333000	-1.995469000	1.870637000
H	0.456859000	-2.583353000	2.550054000
C	1.072673000	2.618952000	0.792578000
H	0.457619000	3.501707000	0.961379000
C	4.095913000	1.213281000	1.841983000
C	-3.172821000	1.070133000	3.759397000

C	3.170666000	-3.508726000	1.724227000
C	3.170939000	3.248405000	2.176700000
C	4.281290000	2.454605000	2.457017000
C	3.172613000	0.260687000	-3.900638000
C	-1.071989000	-2.342913000	-1.412359000
H	-0.456648000	-3.059814000	-1.954068000
C	-3.170222000	-3.792212000	-0.952157000
C	4.281538000	-3.354148000	0.897422000
C	-4.283124000	1.580935000	3.090185000
C	-4.095722000	-2.179620000	0.333273000
C	-4.280852000	-3.468148000	-0.175583000
C	-4.096343000	0.800737000	-2.054558000
C	4.283181000	0.899624000	-3.352961000
C	-3.171903000	2.721052000	-2.807640000
C	-4.282167000	1.886031000	-2.915455000
H	2.992110000	-4.297377000	2.440208000
H	4.748183000	-1.786259000	-0.626254000
H	2.994634000	0.034518000	-4.941624000
H	4.748619000	1.436167000	-1.233311000
H	4.747106000	0.350643000	1.862038000
H	2.992734000	4.262983000	2.501273000
H	-4.747170000	-1.616236000	0.986586000
H	-2.991794000	-4.713178000	-1.487380000
H	-4.747439000	-0.047053000	-1.893529000
H	-2.993997000	3.645398000	-3.337180000
H	-4.748282000	1.662893000	0.905156000
H	-2.995030000	1.066366000	4.824696000
Cl	-5.655624000	2.350973000	3.809747000
Cl	5.653612000	-4.404807000	0.808059000
Cl	5.653197000	2.902262000	3.411979000
Cl	5.655857000	1.501839000	-4.217580000
Cl	-5.652796000	-4.476951000	0.131990000
Cl	-5.654514000	2.123958000	-3.942368000

The ground state (S_0) of (*P*)-**Cl 75** (fixed 75 degree of –C=N–N=C– dihedral angle) optimized at CAM-B3LYP/6-31G(d,p) level.

Al	1.932367000	-0.000041000	-0.000010000
Al	-1.932408000	0.000014000	0.000151000

N	0.651228000	1.024511000	-1.264033000
N	0.651475000	0.582597000	1.519307000
N	2.914765000	1.683183000	-0.234330000
N	0.651243000	-1.607022000	-0.255045000
N	-0.651475000	0.612882000	-1.507119000
N	2.914998000	-0.638723000	1.574727000
N	-0.651256000	0.998949000	1.284566000
N	-0.651394000	-1.611740000	0.223124000
N	2.914651000	-1.044525000	-1.340610000
N	-2.914827000	-1.071008000	1.319575000
N	-2.914973000	-0.607163000	-1.587100000
N	-2.914633000	1.678295000	0.267893000
C	-2.320045000	2.575162000	1.134282000
C	2.320107000	2.597310000	-1.082415000
C	2.320622000	-0.360745000	2.790460000
C	-2.320463000	-0.305078000	-2.797006000
C	-1.050954000	2.187161000	1.625933000
H	-0.421267000	2.848164000	2.219713000
C	-2.320424000	-2.269921000	1.662880000
C	2.320068000	-2.236177000	-1.708017000
C	1.050929000	2.219296000	-1.581619000
H	0.421168000	2.892036000	-2.161982000
C	4.082679000	-0.970452000	-1.997122000
C	4.082893000	2.214570000	0.158006000
C	-1.051251000	-2.501674000	1.081162000
H	-0.421533000	-3.346380000	1.356699000
C	-4.082837000	-1.009996000	1.977462000
C	1.050906000	-2.479429000	-1.131024000
H	0.421123000	-3.318370000	-1.423493000
C	1.051529000	0.260673000	2.712807000
H	0.422194000	0.427388000	3.585815000
C	4.082962000	-1.244487000	1.838844000
C	-3.128584000	-2.975780000	2.555518000
C	3.128116000	-2.924026000	-2.614705000
C	3.128621000	-0.802108000	3.839502000
C	4.247205000	-1.357976000	3.222267000
C	3.128289000	3.726338000	-1.224892000
C	-1.051427000	0.314796000	-2.706849000

H	-0.421944000	0.498883000	-3.576250000
C	-3.128431000	-0.725309000	-3.854713000
C	4.246896000	-2.111762000	-2.787174000
C	-4.247229000	-2.166976000	2.744349000
C	-4.082893000	-1.207582000	-1.863342000
C	-4.247070000	-1.293356000	-3.248774000
C	-4.082633000	2.217630000	-0.113896000
C	4.247147000	3.469422000	-0.435348000
C	-3.128082000	3.701222000	1.299236000
C	-4.246803000	3.460366000	0.504476000
H	2.934097000	-3.878818000	-3.080759000
H	4.744563000	-0.121343000	-1.899550000
H	2.934346000	4.607350000	-1.818756000
H	4.744753000	1.705461000	0.844543000
H	4.744789000	-1.584754000	1.054757000
H	2.934719000	-0.728134000	4.899413000
H	-4.744805000	-1.563445000	-1.086278000
H	-2.934501000	-0.630095000	-4.912922000
H	-4.744484000	1.722545000	-0.810628000
H	-2.934124000	4.570134000	1.910675000
H	-4.744589000	-0.158988000	1.897086000
H	-2.934740000	-3.939827000	3.002187000
Cl	-5.606141000	-2.508311000	3.759846000
Cl	5.605705000	-2.432715000	-3.809422000
Cl	5.605843000	-2.083114000	4.011366000
Cl	5.606075000	4.515088000	-0.202303000
Cl	-5.605810000	-2.002276000	-4.052297000
Cl	-5.605490000	4.510753000	0.292191000

The ground state (S_0) of (*P*)-**Cl 85** (fixed 85 degree of –C=N–N=C– dihedral angle) optimized at CAM-B3LYP/6-31G(d,p) level.

Al	1.937082000	0.000416000	0.000243000
Al	-1.937066000	0.000406000	-0.000260000
N	0.652963000	0.954948000	-1.318152000
N	0.653142000	0.663859000	1.486271000
N	2.900839000	1.684044000	-0.284198000
N	0.652961000	-1.618180000	-0.167983000

N	-0.653089000	0.529478000	-1.539205000
N	2.901591000	-0.595040000	1.600200000
N	-0.652929000	1.068015000	1.228385000
N	-0.653066000	-1.596882000	0.310904000
N	2.901716000	-1.087887000	-1.315158000
N	-2.901835000	-0.966893000	1.406431000
N	-2.901527000	-0.734572000	-1.541159000
N	-2.900766000	1.702653000	0.133751000
C	-2.272686000	2.670685000	0.893756000
C	2.272727000	2.580950000	-1.126943000
C	2.273273000	-0.314647000	2.798440000
C	-2.273150000	-0.561543000	-2.759511000
C	-1.011910000	2.302345000	1.420079000
H	-0.356756000	3.008316000	1.928266000
C	-2.273324000	-2.108556000	1.865560000
C	2.273159000	-2.265754000	-1.671191000
C	1.011927000	2.167430000	-1.618500000
H	0.356745000	2.825579000	-2.187228000
C	4.059101000	-1.040931000	-1.991923000
C	4.058060000	2.246786000	0.095178000
C	-1.012167000	-2.379849000	1.284107000
H	-0.356921000	-3.172671000	1.641833000
C	-4.059255000	-0.860084000	2.076299000
C	1.012035000	-2.484399000	-1.067898000
H	0.356798000	-3.305841000	-1.353873000
C	1.012229000	0.317405000	2.686353000
H	0.356921000	0.480276000	3.540705000
C	4.058651000	-1.205411000	1.897512000
C	-3.050000000	-2.730907000	2.844497000
C	3.049749000	-2.972467000	-2.591153000
C	3.049681000	-0.758987000	3.870183000
C	4.183438000	-1.318377000	3.285297000
C	3.049330000	3.731011000	-1.278958000
C	-1.012131000	0.077996000	-2.703861000
H	-0.356800000	0.164493000	-3.569269000
C	-3.049489000	-1.099202000	-3.787665000
C	4.183771000	-2.186657000	-2.783138000
C	-4.184013000	-1.931145000	2.965971000

C	-4.058576000	-1.368904000	-1.783232000
C	-4.183279000	-1.604520000	-3.155535000
C	-4.057953000	2.229575000	-0.294068000
C	4.183051000	3.504622000	-0.501894000
C	-3.049293000	3.829694000	0.943244000
C	-4.182968000	3.535362000	0.189221000
H	2.826560000	-3.923663000	-3.051482000
H	4.740763000	-0.205991000	-1.909569000
H	2.826416000	4.605045000	-1.872976000
H	4.739310000	1.758176000	0.777608000
H	4.739929000	-1.551577000	1.132931000
H	2.826623000	-0.682438000	4.924159000
H	-4.739908000	-1.645891000	-0.991008000
H	-2.826372000	-1.116434000	-4.844265000
H	-4.739152000	1.682429000	-0.930585000
H	-2.826413000	4.752914000	1.457514000
H	-4.740874000	-0.035702000	1.920220000
H	-2.826869000	-3.637548000	3.387363000
Cl	-5.518148000	-2.190067000	4.037028000
Cl	5.517833000	-2.539563000	-3.827099000
Cl	5.517156000	-2.047121000	4.112476000
Cl	5.516945000	4.585308000	-0.285247000
Cl	-5.516950000	-2.403761000	-3.914898000
Cl	-5.516844000	4.592610000	-0.122383000

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