

Supporting Information

Construction of chiral through-space luminophores via symmetry breaking triggered by sequenced chlorination

Yufeng Xie^{1,2,6}, Huaying Liu^{1,6}, Zhongliang Li³, Xin Zhang⁴, Lijuan Song¹, Kang Zhou⁵, Feng Yuan¹, Hengzhi You^{1,2}, Engui Zhao¹, and Zikai He^{1,2*}

¹ School of Science, Harbin Institute of Technology, Shenzhen 518055, China. E-mail: hezikai@hit.edu.cn

² School of Chemical Engineering and Technology, Harbin Institute of Technology
Harbin, Heilongjiang 150001, China

³ Academy for Advanced Interdisciplinary Studies and Department of Chemistry,
Southern University of Science and Technology, Shenzhen 518055, China

⁴ Shenzhen Bay Laboratory, Shenzhen 518055, China

⁵ Hoffmann Institute of Advanced Materials, Shenzhen Polytechnic, Shenzhen 518055,
China

⁶ These authors contributed equally to this work.

Supporting Information

Contents

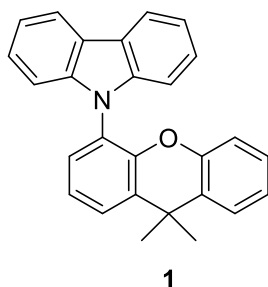
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S1-General experimental details

All reactions were carried out under nitrogen atmosphere. Starting materials and solvent were used without treatment. 2-methyltetrahydrofuran was washed with 10% aqueous NaOH, dried, distilled from sodium metal.

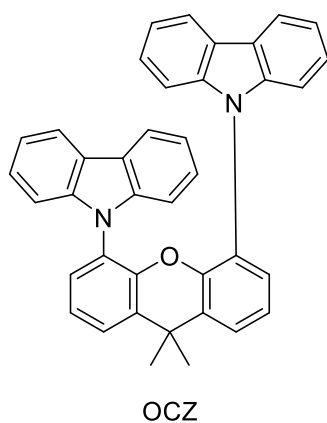
^1H and ^{13}C NMR spectra were collected on a QOne Instruments Quantum-I 400 M. UV-visible spectra were collected on Shimadzu UV-2600. High-resolution mass spectroscopy analysis was carried out on Waters ACQUITYUPLC H-Class/Xevo G2-XS QTof. Single-crystal XRD was carried out on Rigaku XtaLAB Synergy and Bruker APEX-II CCD. High performance liquid chromatography (HPLC) was carried out on Agilent 1260 LC. All photophysical measurements, including steady or delay spectra, decay curve, circularly polarized spectra, and quantum yield, were carried out on Edinburgh Instruments FLS1000 with different accessories. Thermogravimetric experiments were carried out on Netzsch STA449F5.

S2-Synthesis and characterization



9-(9,9-dimethyl-9H-xanthen-4-yl)-9H-carbazole (**1**)

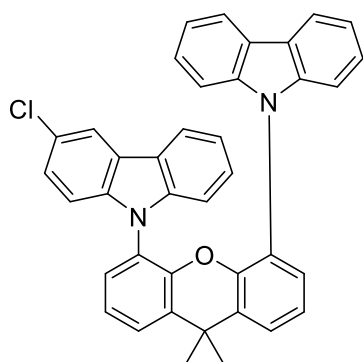
9-(5-iodo-9,9-dimethyl-9H-xanthen-4-yl)-9H-carbazole (0.501 g, 0.4 mmol) was added to a 50 ML two-mouth round-bottomed flask. The reaction system was vacuumed and heated to remove trace amounts of water, vacuumed and purged with N₂ for three times. *n*-butyllithium (2.4 M, 0.2 mL) dropwise to the flask, keep the temperature at -78 °C, and stir for 0.5 h. Saturated ammonium chloride aqueous solution was added to the system to quench the reaction, and the reaction solution was extracted three times with dichloromethane. The combined organic phase was dried with anhydrous Na₂SO₄, organic solvent was removed under reduced pressure. The residue was purified by silica-gel column chromatography by employing DCM/petroleum ether (*v:v* = 1:5) as eluent to give **2** as white solid in 65.3% yield (0.098 g). M. p. 164-165 °C. ¹H NMR (DMSO-*d*₆, 400 MHz): δ 8.27 (d, *J* = 7.6 Hz, 2H), 7.81-7.78 (dd, *J* = 8.0 Hz, 1H), 7.60-7.58 (dd, *J* = 7.6 Hz, 1H), 7.50-7.48 (m, 1H), 7.41-7.36 (m, 3H), 7.29 (t, *J* = 7.6 Hz, 2H), 7.16-7.04 (m, 4H), 6.32-6.30 (dd, *J* = 7.6 Hz, 1H), 1.70 (s, 6H) ppm. ¹³C NMR (CDCl₃, 100 MHz): δ 150.1, 147.1, 141.4, 127.5, 127.3, 125.9, 125.7, 123.7, 123.3, 120.2, 119.8, 117.1, 110.6, 34.7, 32.1 ppm. HRMS (ESI) *m/z*: [M+H]⁺ calculated for C₂₇H₂₂NO, 376.1696; found, 376.1696.



9,9'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis(9H-carbazole) (OCZ)

9-(5-iodo-9,9-dimethyl-9H-xanthen-4-yl)-9H-carbazole (0.501 g, 1 mmol), 9H-carbazole (0.201 g, 1.20 mmol), active copper powder (0.445 g, 7 mmol), 18-crown ether-6 (0.049 g, 0.2 mmol), K₂CO₃ (1.133 g, 8.2 mmol) were added to 100 mL two-necked round-bottom flask, vacuumed and purged

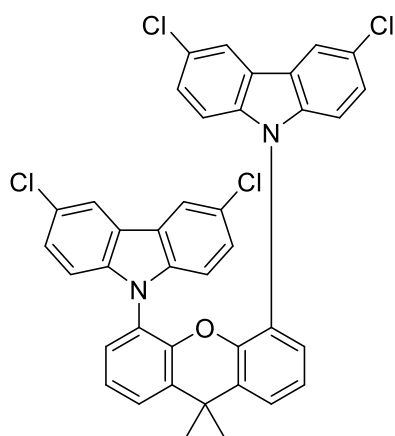
with N₂ for three times. 30 mL anhydrous and anaerobic 1,2-dichlorobenzene were injected into the reaction system. The reaction mixture was refluxed in sand bath for 72 h, followed by cooling to room temperature and filtration to remove excess copper powder and inorganic salts. Organic solvent was removed under reduced pressure. The residue was dissolved with dichloromethane (DCM), washed with saturated salt water, and extracted with DCM for three times. The organic phase was combined and dried with anhydrous Na₂SO₄. Organic solvent was removed under reduced pressure. The residue was purified by silica-gel column chromatography by employing DCM/petroleum ether (v:v = 1:20) as eluent to give OCZ as white solid in 52.0% yield (0.281 g). M. p. 277-278 °C. ¹H NMR (DMSO-*d*₆, 400 MHz): δ 7.81-7.78 (d, *J* = 7.2 Hz, 2H), 7.70 (d, *J* = 7.2 Hz, 4H), 7.34-7.28 (m, 4H), 6.78-6.74 (m, 4H), 6.72-6.68 (m, 4H), 6.63 (d, *J* = 8 Hz, 4H), 1.86 (s, 6H) ppm. ¹³C NMR (CDCl₃, 100 MHz): δ 145.2, 140.0, 131.3, 127.5, 125.7, 125.2, 124.5, 122.8, 121.8, 119.1, 109.3, 34.8, 33.5 ppm. HRMS (ESI) *m/z*: [M+H]⁺ calculated for C₃₉H₂₉N₂O, 541.2275; found, 541.2277.



OCZ-1Cl

9-(5-(9H-carbazol-9-yl)-9,9-dimethyl-9H-xanthen-4-yl)-3-chloro-9H-carbazole(OCZ-1Cl)

OCZ (0.108 g, 0.2 mmol) was firstly dissolved in 5 mL freshly distilled DMF. Afterwards, 5 mL DMF solution containing *N*-chlorosuccinimide (0.027 g, 0.2 mmol) was slowly added to the solution. The mixture was continuously stirred and heated at 60 °C for 3 h. After cooling to room temperature, the reaction was quenched by water, and extracted by DCM. After removal of solvent under reduced

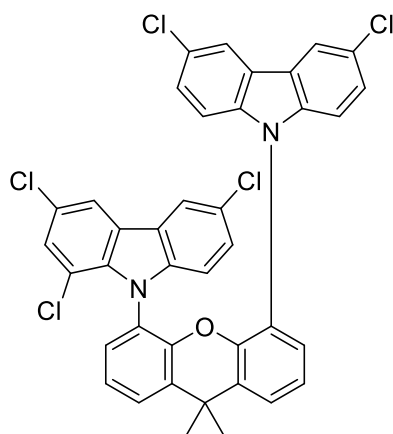


OCZ-4Cl

pressure, the residue was purified by a silica-gel column chromatography using DCM/petroleum ether ($v:v = 1:80$) as the eluent to give OCZ-1Cl as white solid in 26.1% yield (0.030g). M. p. 256-257 °C. ^1H NMR (CDCl_3 , 400 MHz): 7.80 (d, $J = 8.0$ Hz, 1H), 7.70-7.65 (m, 3H), 7.58-7.56 (m, 2H), 7.26-7.19 (m, 4H), 7.01 (t, $J = 7.2$ Hz, 1H), 6.91-6.86 (m, 3H), 6.78 (t, $J = 8$ Hz, 1H), 6.73-6.71 (m, 2H), 6.67-6.57 (m, 3H), 6.52-6.50 (m, 1H) 1.88 (d, $J = 8.8$ Hz, 6H) ppm. ^{13}C NMR (CDCl_3 , 100 MHz): δ 145.3, 140.7, 140.1, 140.0, 131.6, 131.4, 127.7, 127.4, 126.1, 125.8, 125.4, 125.2, 124.8, 124.7, 124.6, 124.5, 124.4, 123.8, 123.7, 123.6, 122.8, 122.0, 120.1, 119.7, 119.6, 119.5, 119.4, 119.1, 34.8, 33.5, 33.1 ppm. HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{39}\text{H}_{28}\text{ClN}_2\text{O}$, 575.1885; found, 575.1862.

9,9'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis(3,6-dichloro-9H-carbazole) (OCZ-4Cl).

OCZ (0.108 g, 0.2 mmol) was firstly dissolved in 5 mL freshly distilled DMF, and 5 mL DMF solution containing *N*-chlorosuccinimide (0.107 g, 0.8 mmol) was slowly added to the solution. The mixture was continuously stirred and heated at 60 °C for 3 h. After cooling to room temperature, the reaction was quenched by water, and extracted by DCM. After removal of solvent under reduced pressure, the residue was purified by a silica gel column chromatography using DCM/petroleum ether ($v:v = 1:80$) as the eluent to give OCZ-4Cl as white solid in 40.6% yield (0.055 g). M. p. 257-258 °C. ^1H NMR ($\text{DMSO}-d_6$, 400 MHz): δ 7.93 (s, 4H), 7.85-7.80 (m, 2H), 7.35-7.31 (m, 4H), 6.82-6.80 (d, $J = 8.8$ Hz, 4H), 6.65 (d, $J = 8.4$ Hz, 4H), 1.85 (s, 6H) ppm. ^{13}C NMR (CDCl_3 , 100 MHz): δ 145.1, 138.8, 131.6, 127.4, 126.5, 125.6, 125.4, 124.2, 124.0, 122.9, 120.0, 110.5, 34.9, 33.3 ppm. HRMS (ESI) m/z : $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{39}\text{H}_{25}\text{Cl}_4\text{N}_2\text{O}$, 677.0716; found, 677.0724.

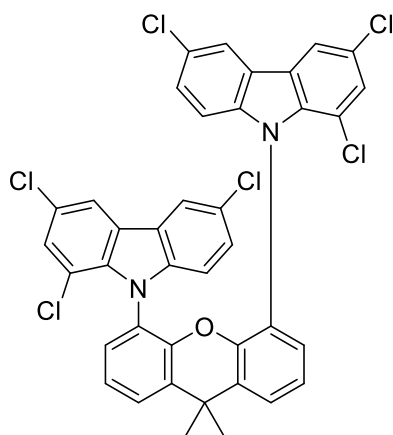


OCZ-5Cl

1,3,6-trichloro-9-(5-(3,6-dichloro-9H-carbazol-9-yl)-9,9-dimethyl-9H-xanthen-4-yl)-9H-carbazole (OCZ-5Cl).

OCZ (0.108 g, 0.2 mmol) was firstly dissolved in 5 mL freshly distilled DMF, and 5 mL DMF solution containing *N*-chlorosuccinimide (0.107 g, 1.0 mmol) was slowly added to the solution. The mixture was continuously stirred and heated at 60 °C for 3 h. After removal of solvent under reduced pressure, the residue was purified by a silica-gel column chromatography using DCM/petroleum ether ($v:v = 1:80$) as the eluent to give OCZ-5Cl as white solid in 37.6% yield (0.053 g). M. p. 239-

240 °C. ¹H NMR (CDCl₃, 400 MHz): 7.80 (s, 1H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.62-7.58 (m, 3H), 7.24-7.17 (m, 2H), 7.16-7.13 (m, 2H), 7.10 (d, *J* = 8.0 Hz, 1H), 7.05 (d, *J* = 8.0 Hz, 1H), 6.81 (d, *J* = 8.4 Hz, 1H), 6.59-6.57 (m, 3H), 6.38 (d, *J* = 8.4 Hz, 1H), 1.83 (d, *J* = 4.8 Hz, 6H) ppm. ¹³C NMR (CDCl₃, 100 MHz): 147.2, 145.6, 140.3, 139.2, 138.7, 134.2, 132.1, 128.5, 127.3, 126.8, 126.7, 126.4, 126.3, 126.0, 125.9, 125.5, 125.0, 124.7, 124.2, 124.0, 123.3, 123.0, 122.6, 122.3, 120.1, 120.0, 119.5, 118.5, 116.2, 110.7, 110.5, 110.4, 35.0, 32.6, 32.4 ppm. HRMS (ESI) *m/z*: [M+H]⁺ calculated for C₃₉H₂₄Cl₅N₂O, 711.0326; found, 711.0307.

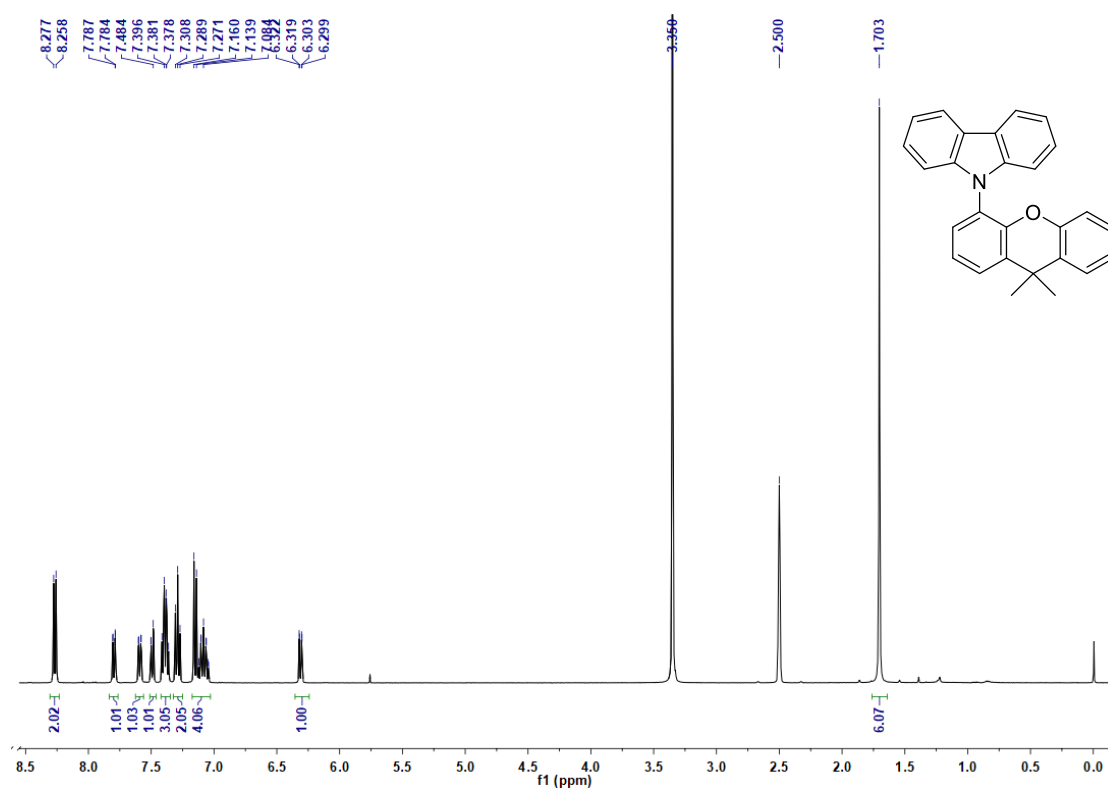


OCZ-6Cl

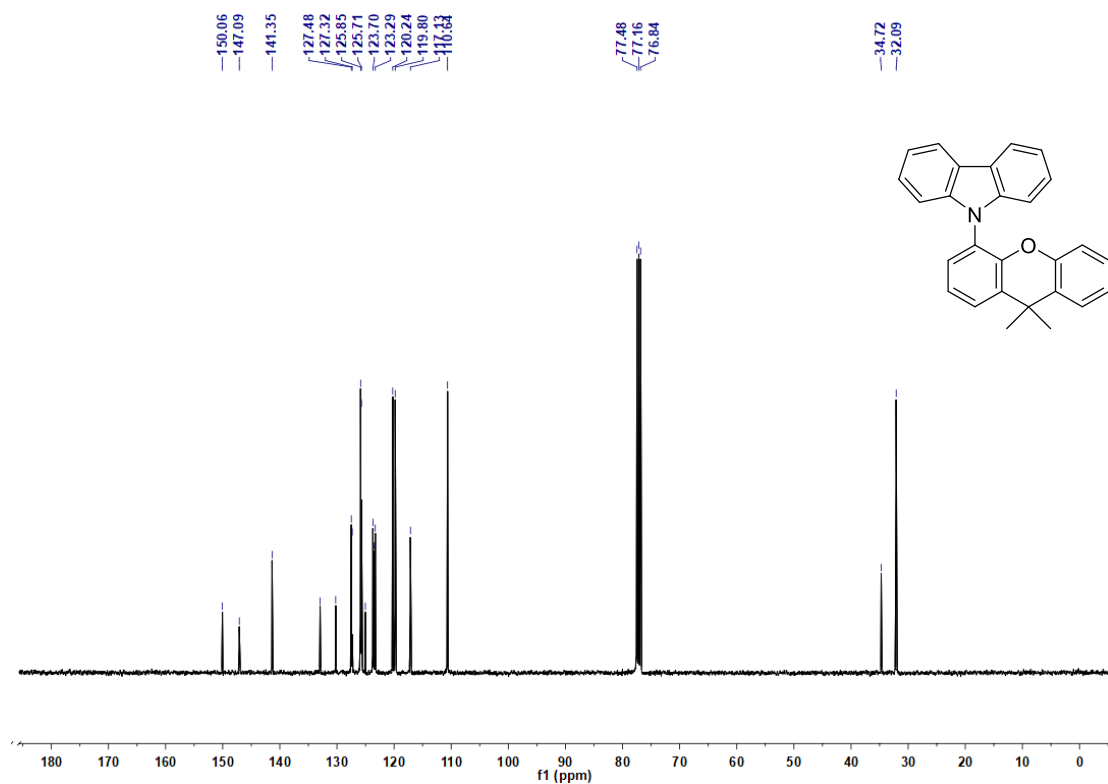
Characterization data for 9,9'-(9,9-dimethyl-9H-xanthene-4,5-diyl) bis(1,3,6-trichloro-9H-carbazole) (OCZ-6Cl).

OCZ (0.108 g, 0.2 mmol) was firstly dissolved in 5 mL freshly distilled DMF, and 5 mL DMF solution containing N-chlorosuccinimide (0.107 g, 1.2 mmol) was slowly added to the solution. The mixture was continuously stirred and heated at 60 °C for 3 h. After cooling to the room temperature, the reaction was quenched by water, and extracted by DCM. After removal of solvent under reduced pressure, the residue was purified by a silica gel column chromatography using DCM/petroleum ether (*v:v* = 1:80) as the eluent to give OCZ-6Cl as white solid in 30.3% yield (0.045 g). M. p. 242-243 °C. ¹H NMR (CDCl₃, 400 MHz): δ 7.75 (s, 2H), 7.63-7.59 (m, 4H), 7.22-7.18 (m, 4H), 7.12-7.10 (m, 2H), 6.68 (d, *J* = 8.8 Hz, 2H), 6.61 (s, 2H), 1.80 (s, 6H) ppm. ¹³C NMR (CDCl₃, 100 MHz): δ 147.1, 140.5, 134.3, 131.0, 128.3, 127.0, 126.9, 126.5, 125.9, 125.1, 125.0, 124.6, 123.3, 122.1, 120.0, 118.3, 116.4, 110.6, 34.8, 32.5 ppm. HRMS (ESI) *m/z*: [M+H]⁺ calculated for C₃₉H₂₃Cl₆N₂O, 744.9936; found, 744.9938.

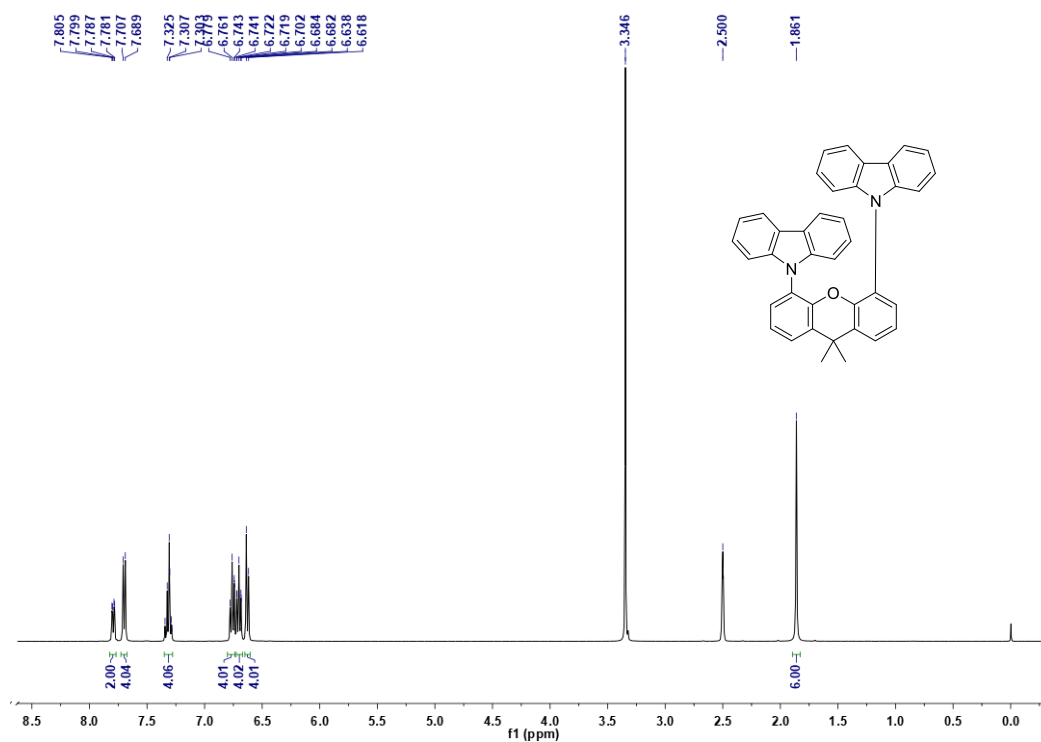
S3 – ^1H and ^{13}C spectra of new compounds



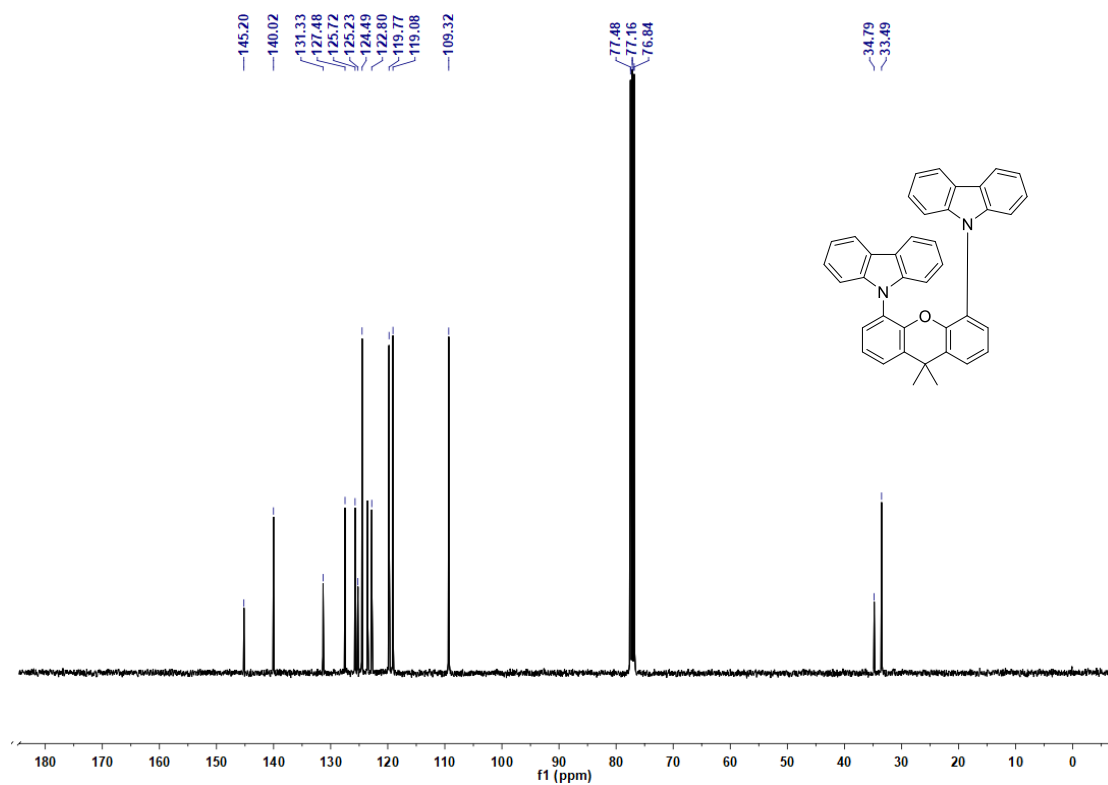
Supplementary Chart 1. ^1H NMR spectra of **1** (DMSO- d_6 , 400 MHz).



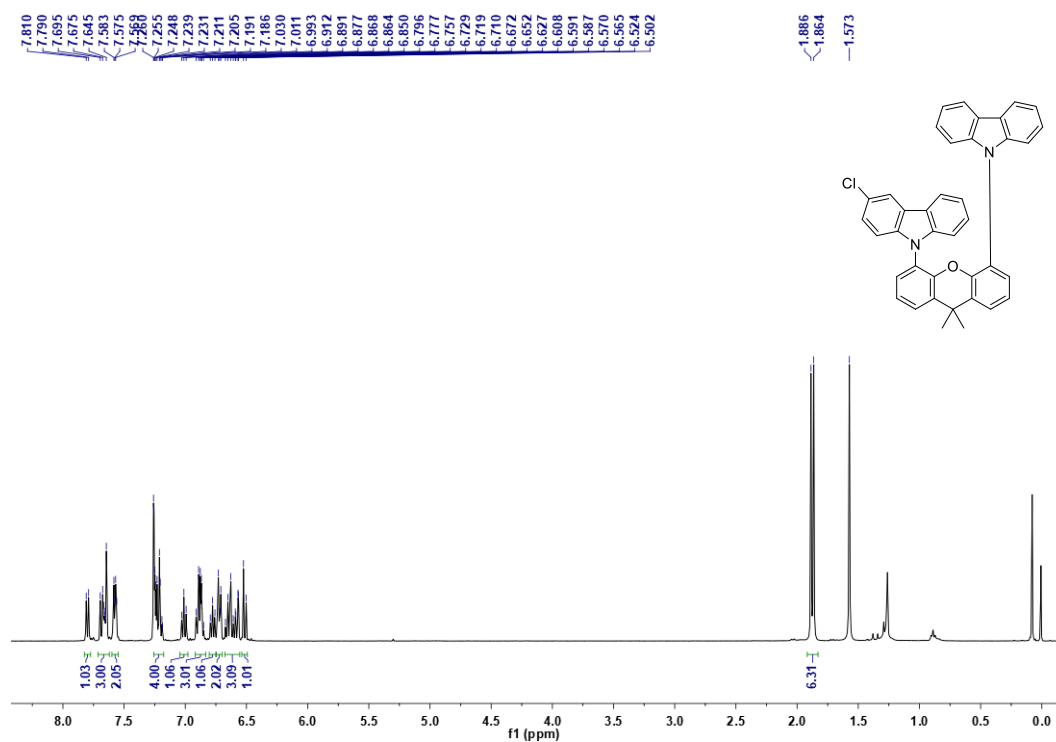
Supplementary Chart 2. ^{13}C NMR spectra of **1** (CDCl $_3$, 100 MHz).



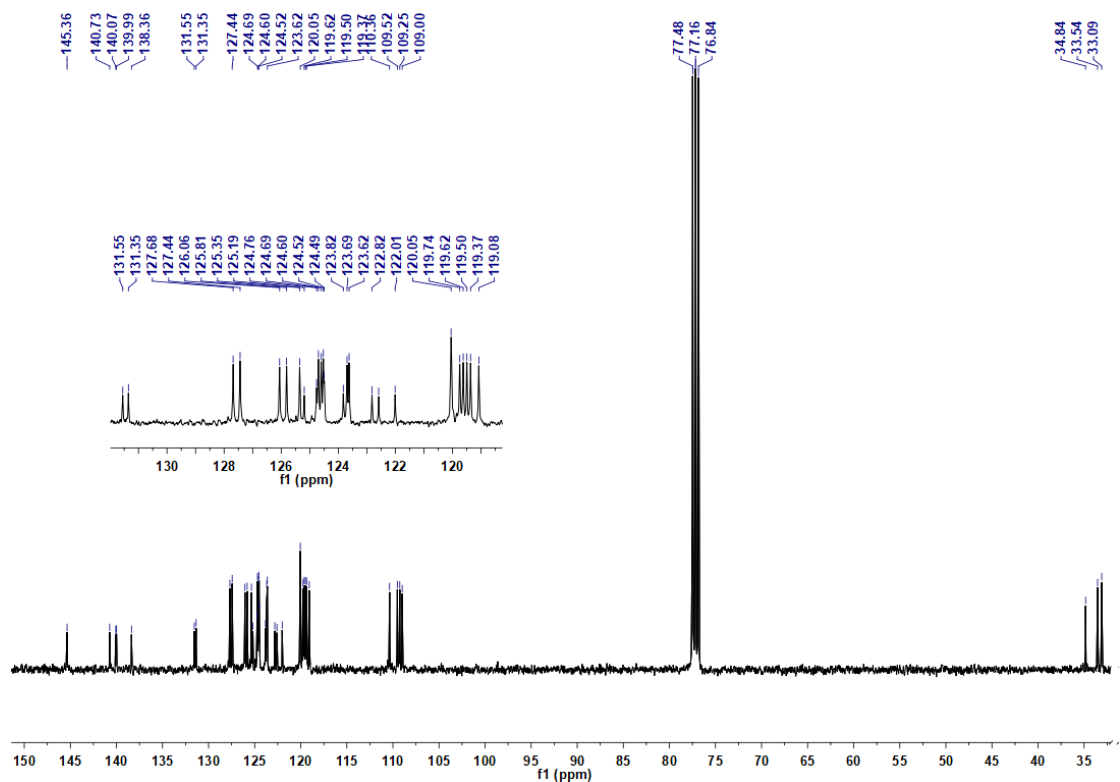
Supplementary Chart 3. ¹H NMR spectra of OCZ (DMSO-*d*₆, 400 MHz).



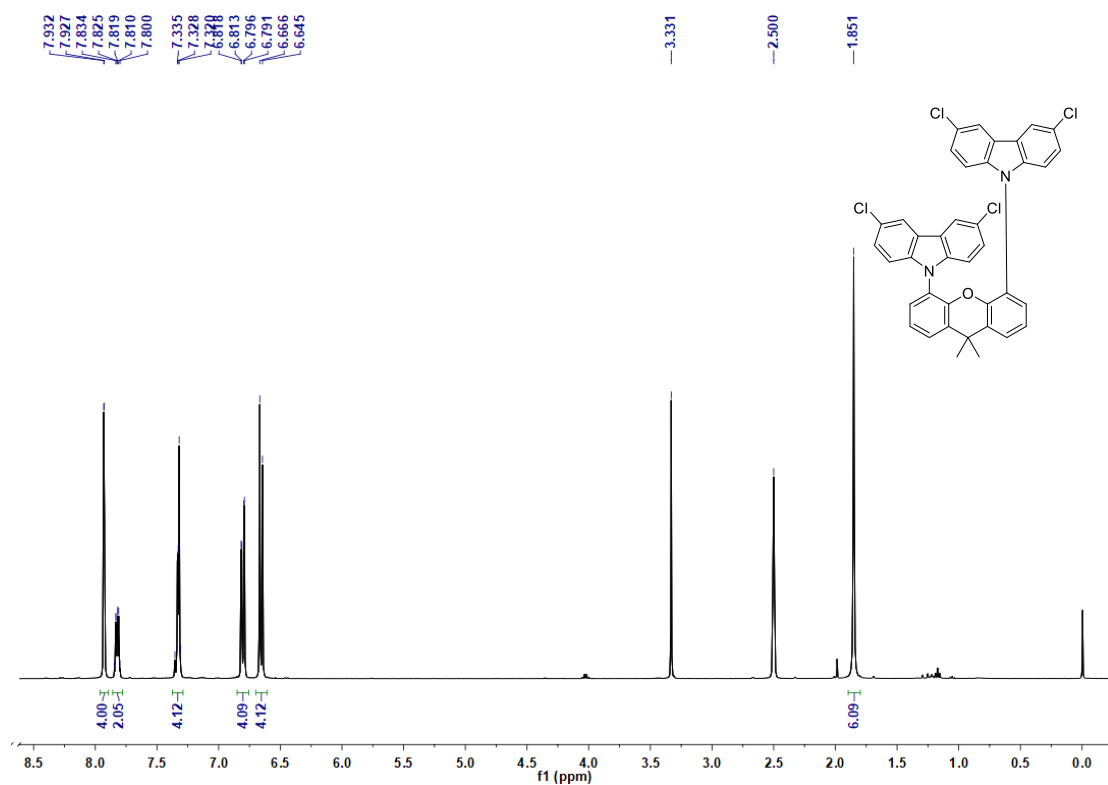
Supplementary Chart 4. ¹³C NMR spectra of OCZ (CDCl₃, 100 MHz).



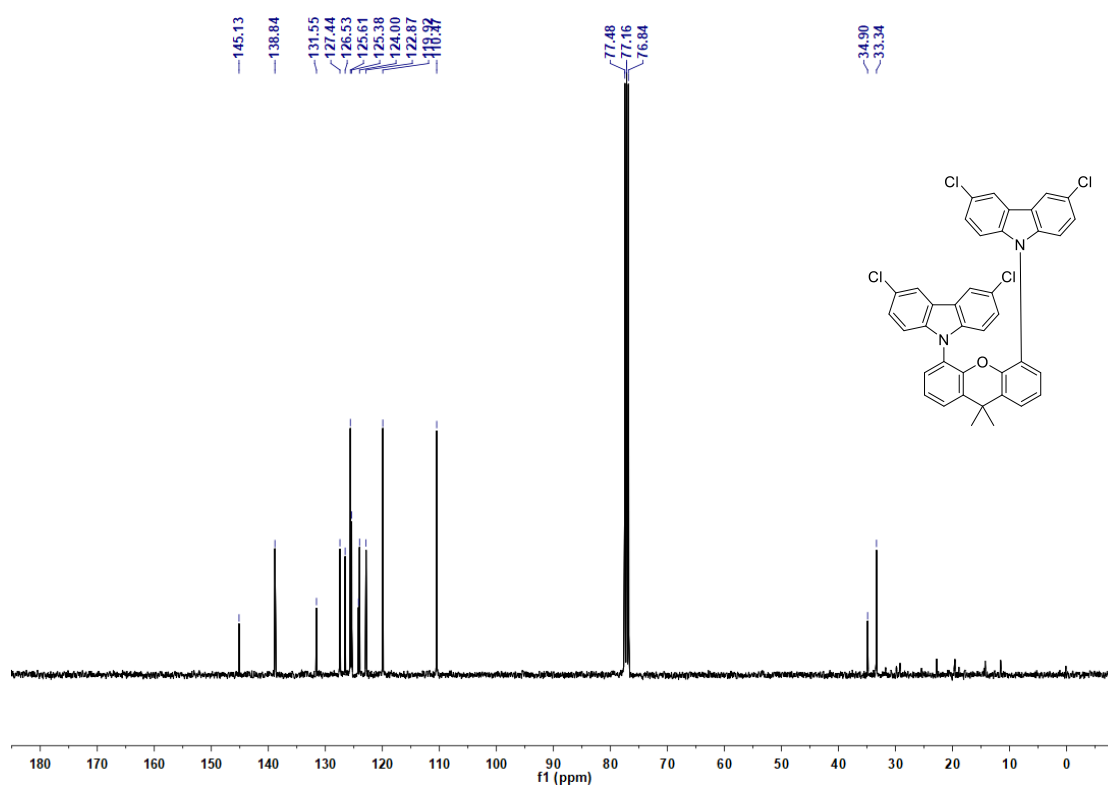
Supplementary Chart 5. ¹H NMR spectra of OCZ-1Cl (CDCl₃, 400 MHz).



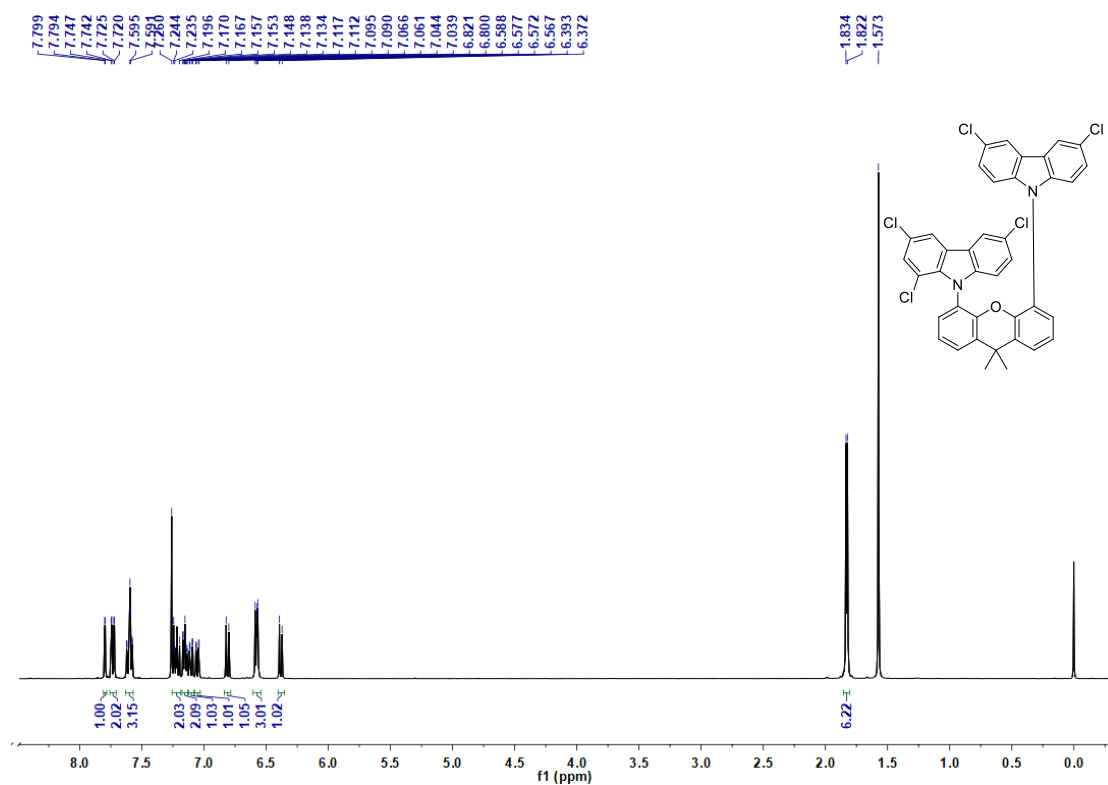
Supplementary Chart 6. ¹³C NMR spectra of OCZ-1Cl (CDCl₃, 100 MHz).



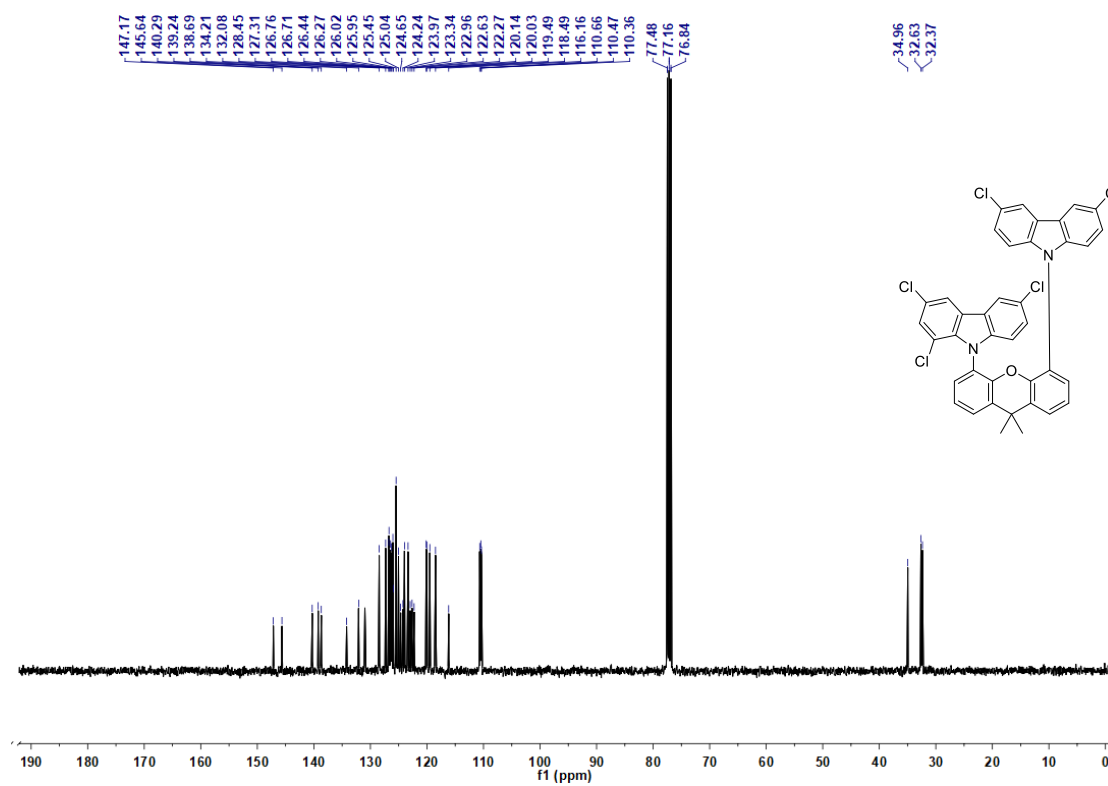
Supplementary Chart 7. ¹H NMR spectra of OCZ-4Cl (DMSO-*d*₆, 400 MHz).



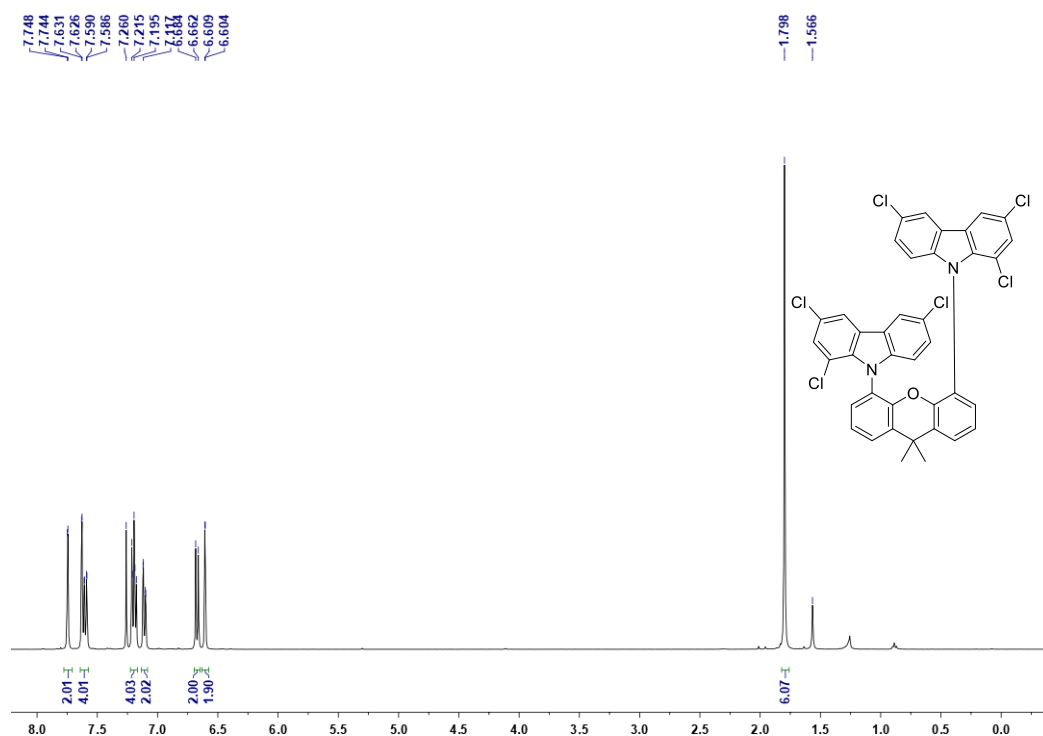
Supplementary Chart 8. ¹³C NMR spectra of OCZ-4Cl (CDCl₃, 100 MHz).



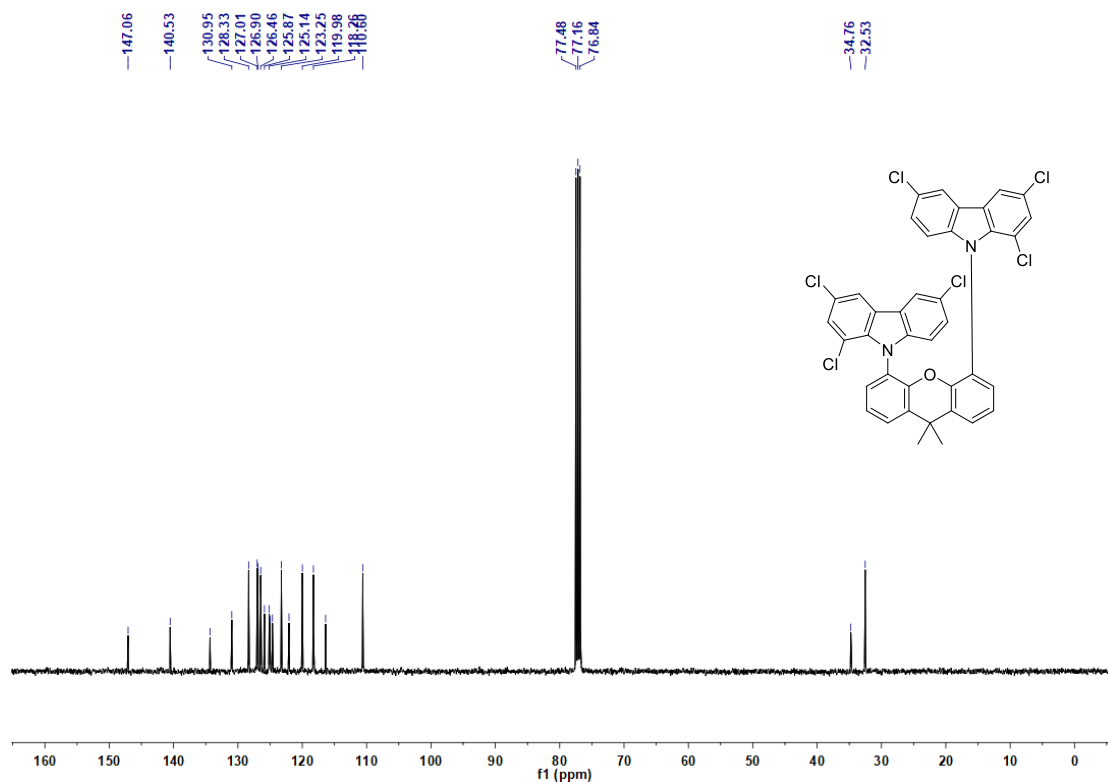
Supplementary Chart 9. ¹H NMR spectra of OCZ-5Cl (CDCl₃, 400 MHz).



Supplementary Chart 10. ¹³C NMR spectra of OCZ-5Cl (CDCl₃, 100 MHz).

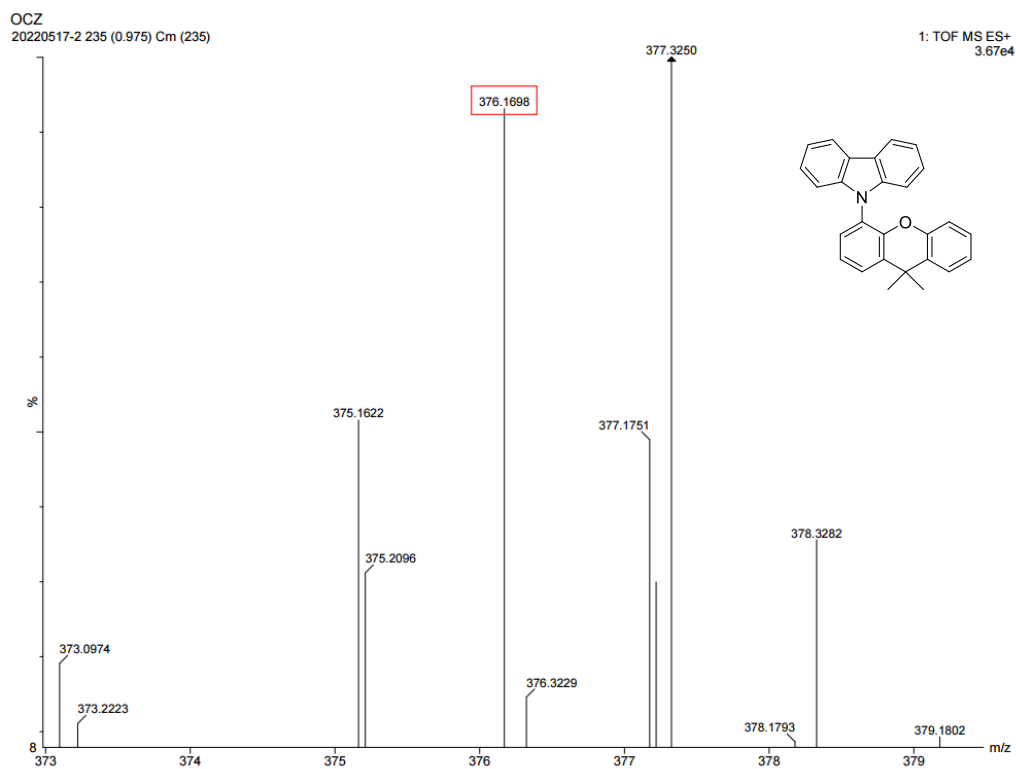


Supplementary Chart 11. ¹H NMR spectra of OCZ-6Cl (CDCl₃, 400 MHz).

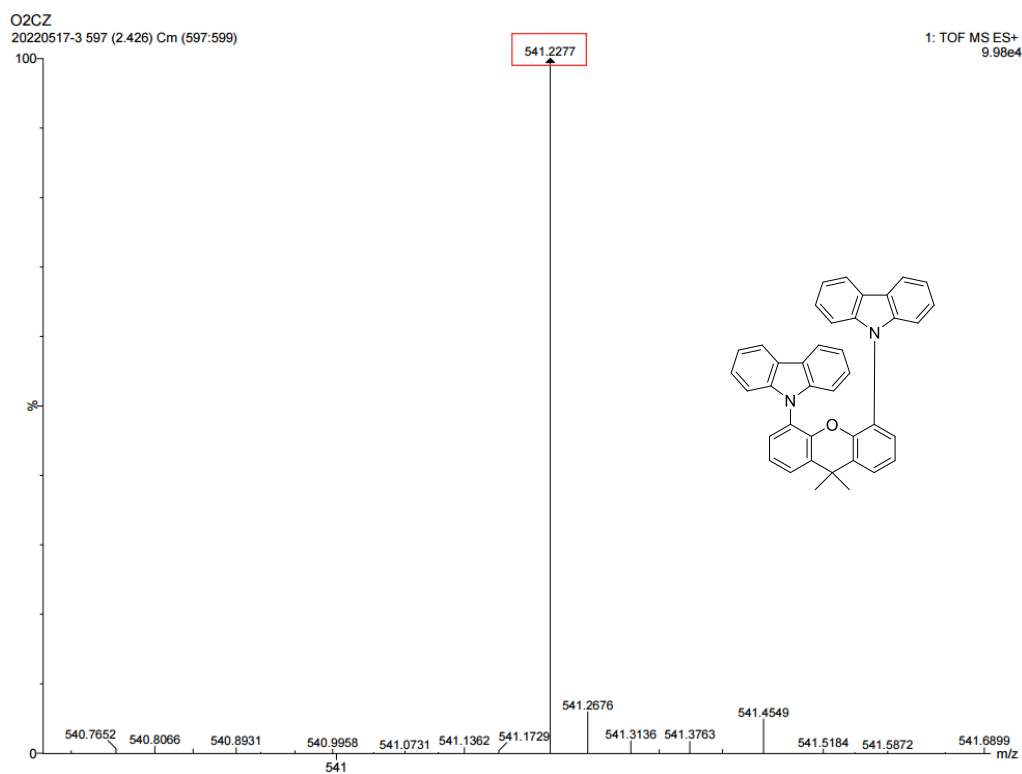


Supplementary Chart 12. ¹³C NMR spectra of OCZ-6Cl (CDCl₃, 100 MHz).

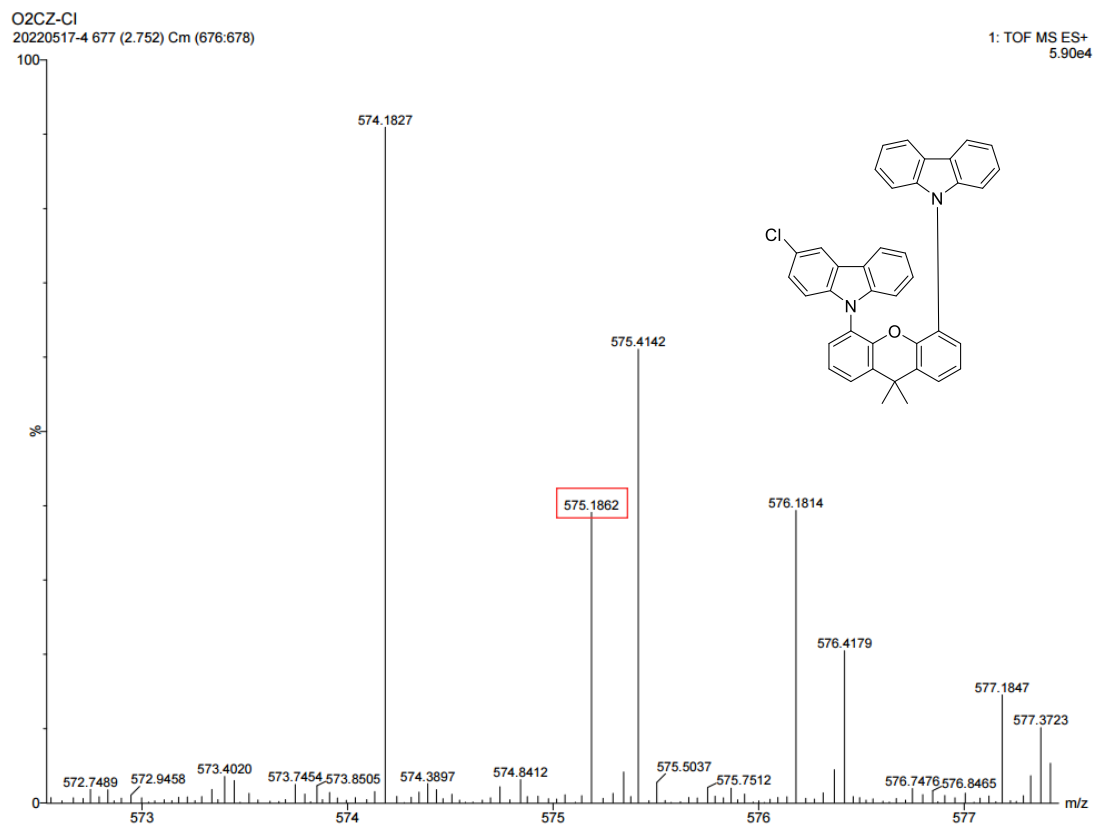
S4 –High-resolution mass spectra



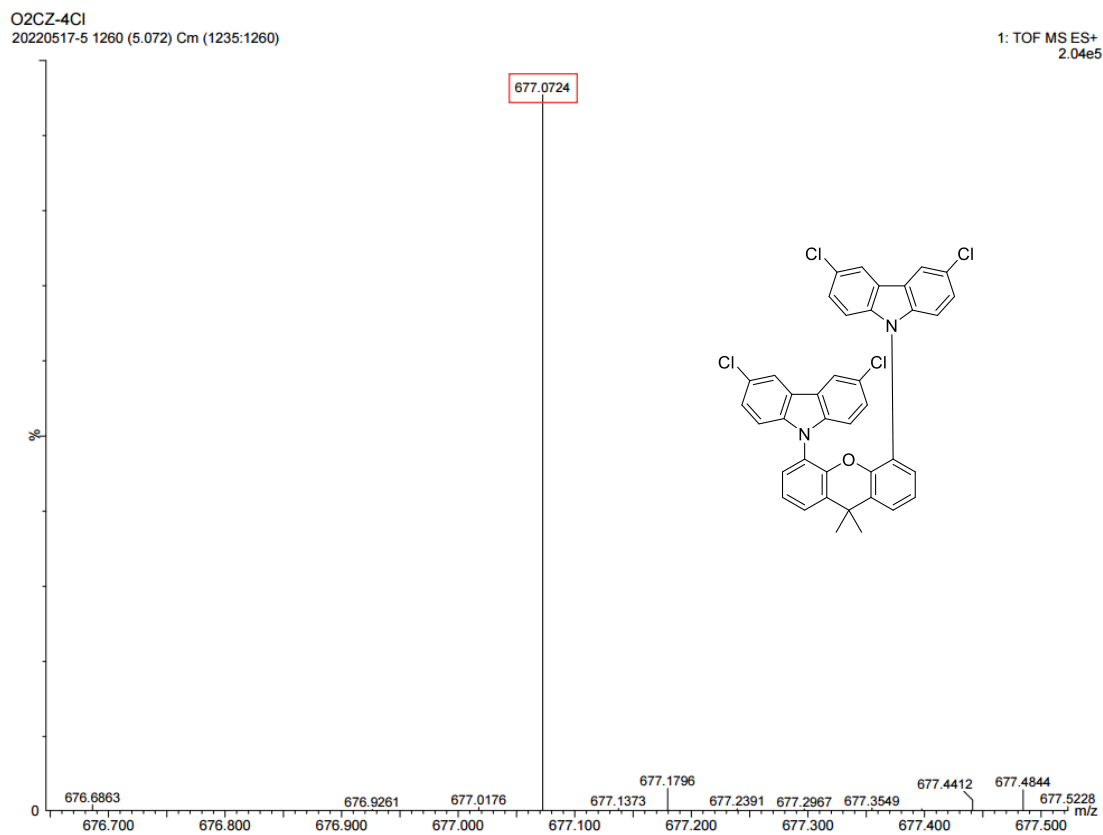
Supplementary Chart 13. High-resolution mass spectrum of 1.



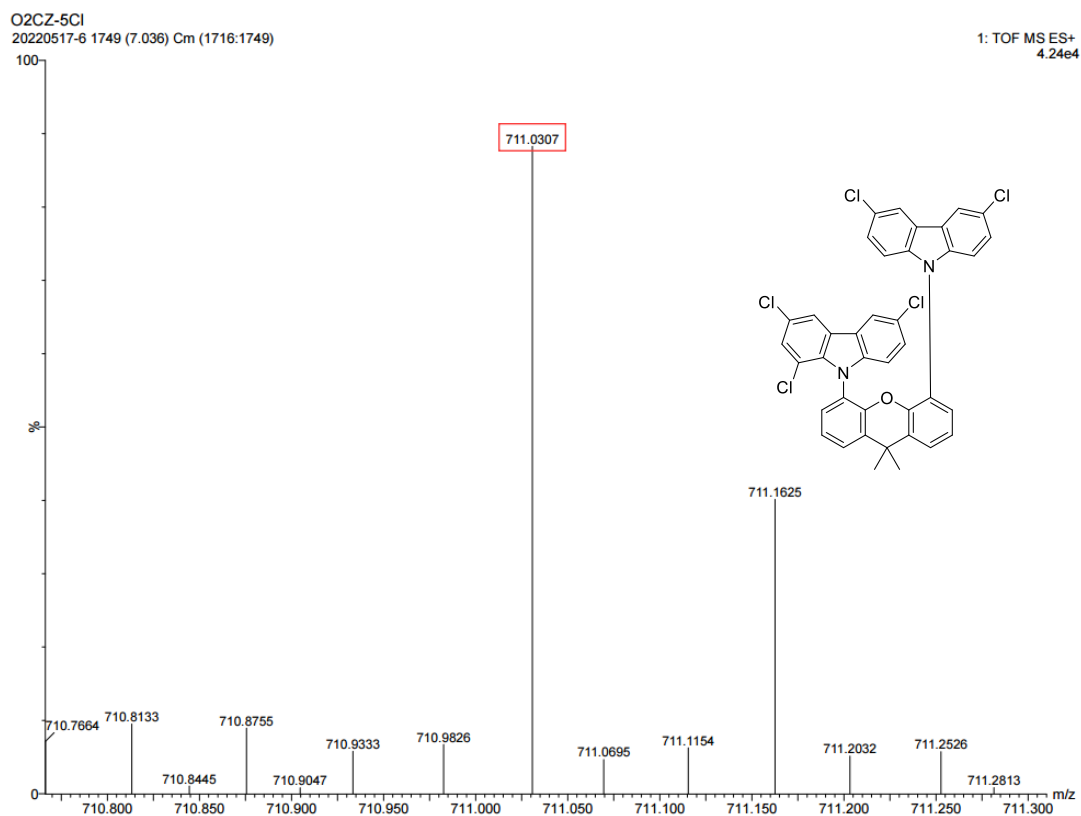
Supplementary Chart 14. High-resolution mass spectrum of OCZ.



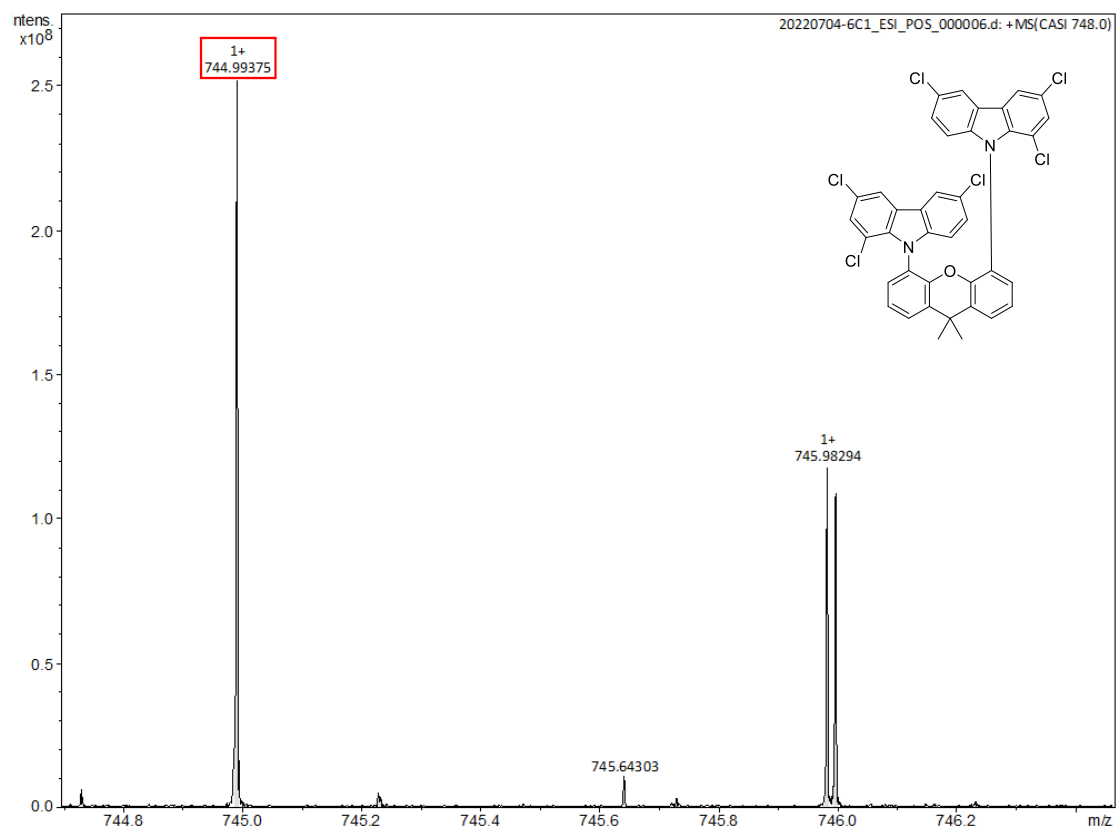
Supplementary Chart 15. High-resolution mass spectrum of OCZ-1Cl.



Supplementary Chart 16. High-resolution mass spectrum of OCZ-4Cl.

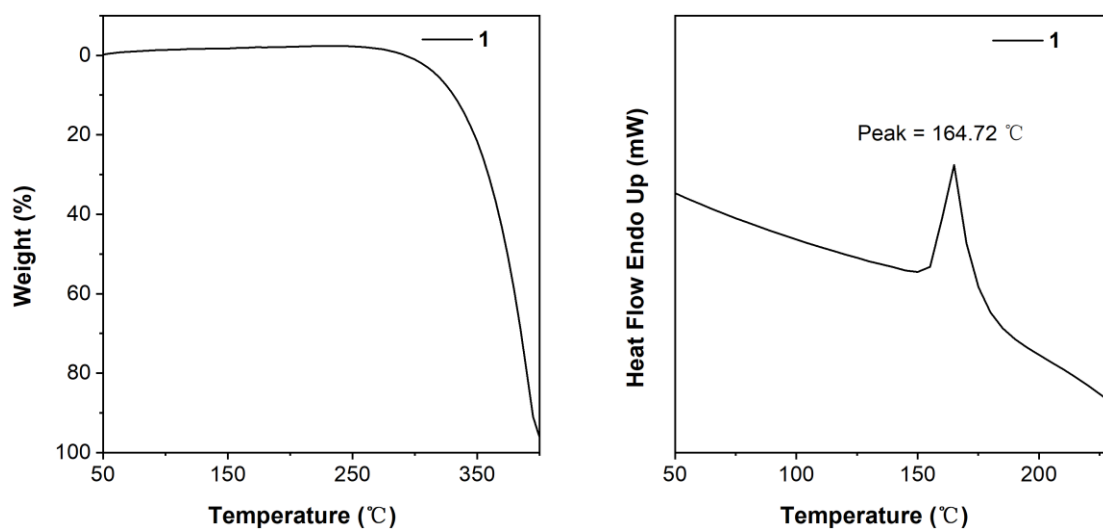


Supplementary Chart 17. High-resolution mass spectrum of OCZ-5Cl.

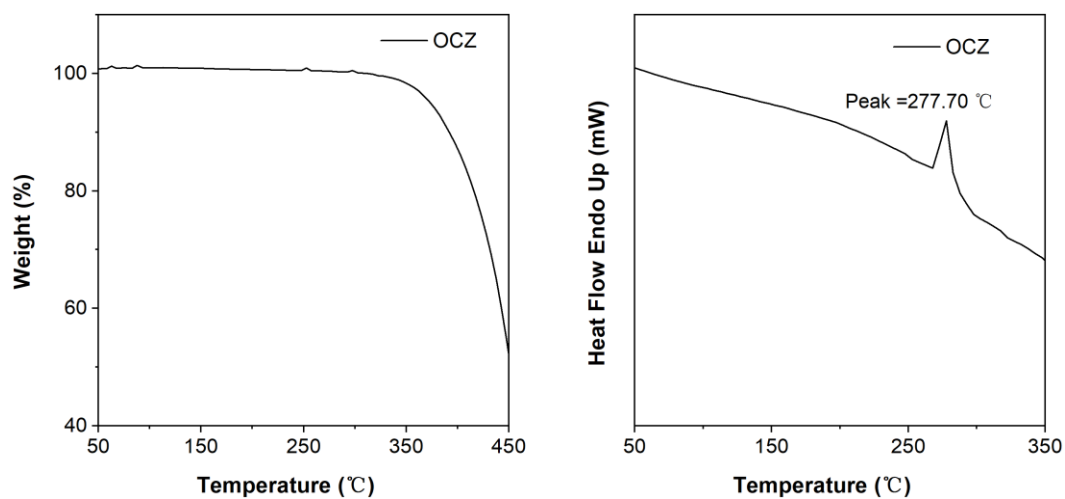


Supplementary Chart 18. High-resolution mass spectrum of OCZ-6Cl.

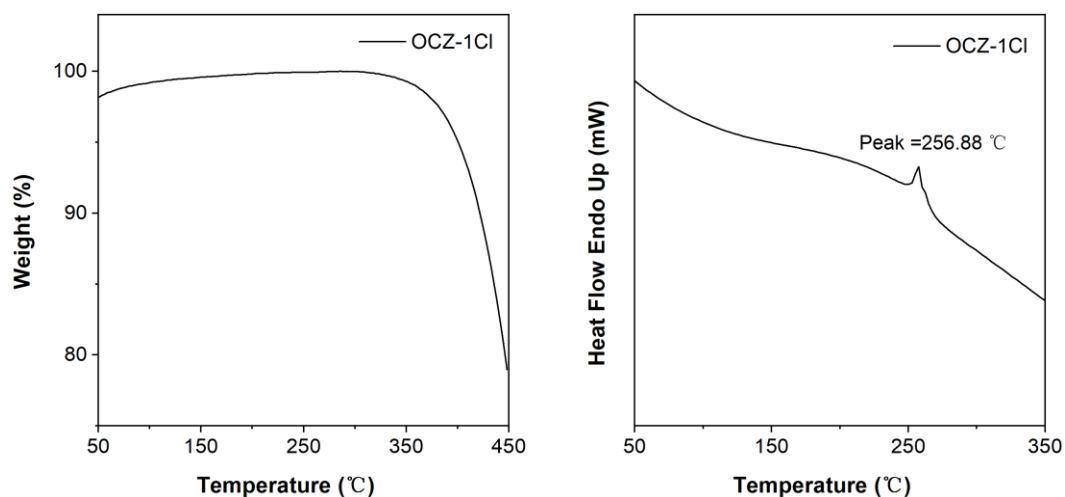
S5 – TGA and DSC curves



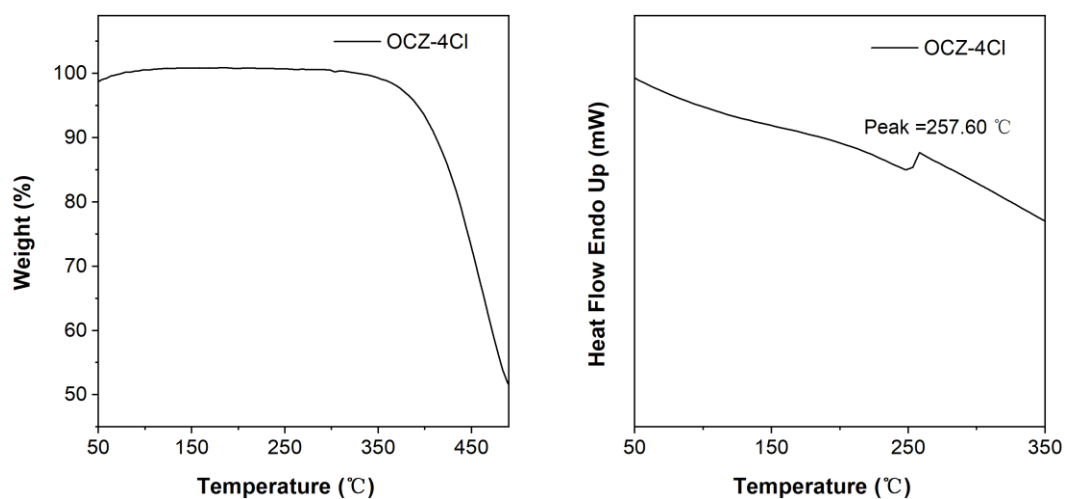
Supplementary Chart 19. TGA and DSC curves of **1** under N₂ atmosphere, the heating rate is 10 °C/min.



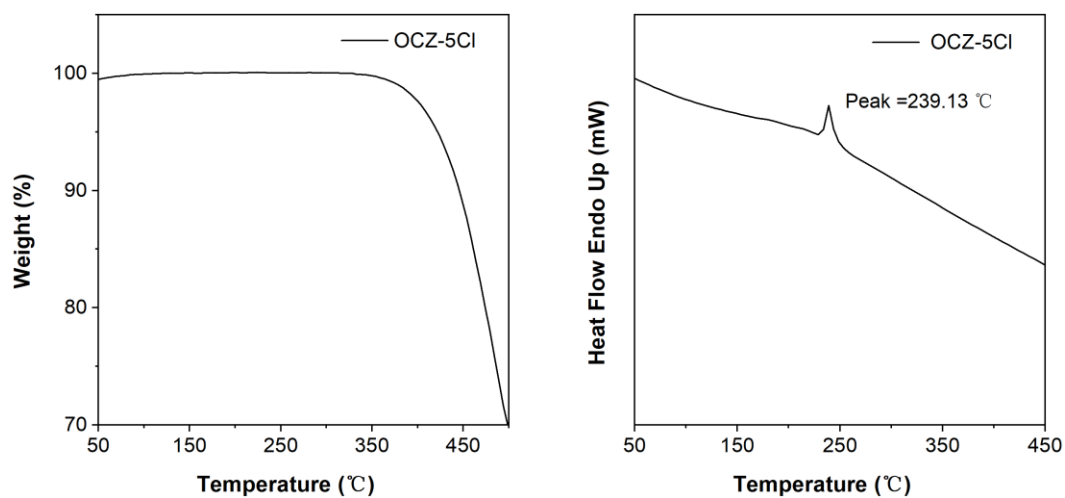
Supplementary Chart 20. TGA and DSC curves of **OCZ** under N₂ atmosphere, the heating rate is 10 °C/min.



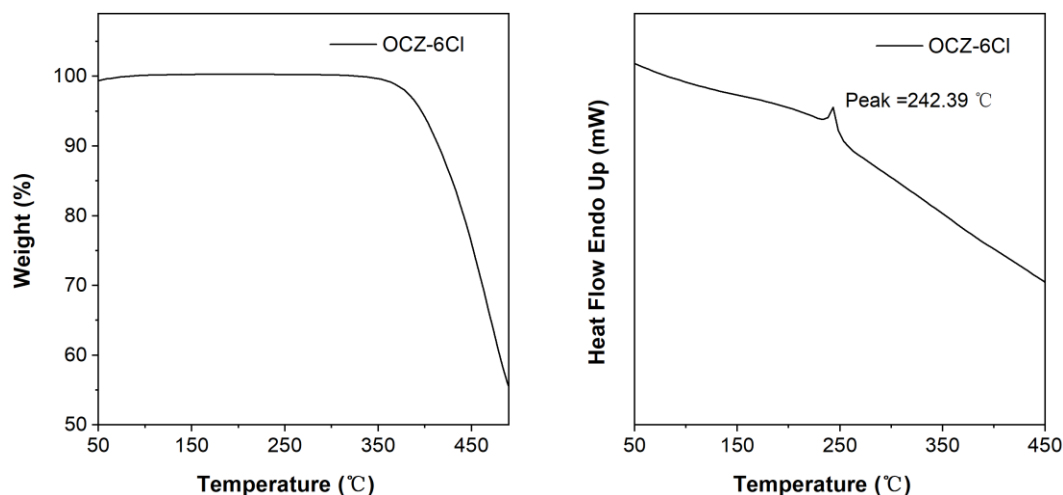
Supplementary Chart 21. TGA and DSC curves of OCZ-Cl under N₂ atmosphere, the heating rate is 10 °C/min.



Supplementary Chart 22. TGA and DSC curves of OCZ-4Cl under N₂ atmosphere, the heating rate is 10°C/min.



Supplementary Chart 23. TGA and DSC curves of OCZ-5Cl under N₂ atmosphere, the heating rate is 10 °C/min.



Supplementary Chart 24. TGA and DSC curves of OCZ-6Cl under N₂ atmosphere, the heating rate is 10 °C/min.

S6. Chiral HPLC Analysis

OCZ-5Cl and OCZ-6Cl were separated by semi-preparative HPLC.

HPLC Analysis Conditions:

Column: Chiralpak® IC 5 μm, 20 mm × 250 mm

Mobile phase: *n*-hexane: dichloromethane = 75:25

Temperature: 26.5°C

Flow rate: 5.0 mL/min

Abs. detector: 254 nm

Chiral HPLC analysis was used to investigate the enantiomeric excess of chiral molecule after separated procedures. Analysis of the optimized process as well as the enantiomer excess of (*M*)-OCZ-5Cl, (*P*)-OCZ-5Cl, (*M*)-OCZ-6Cl and (*P*)-OCZ-6Cl.

HPLC Analysis Conditions:

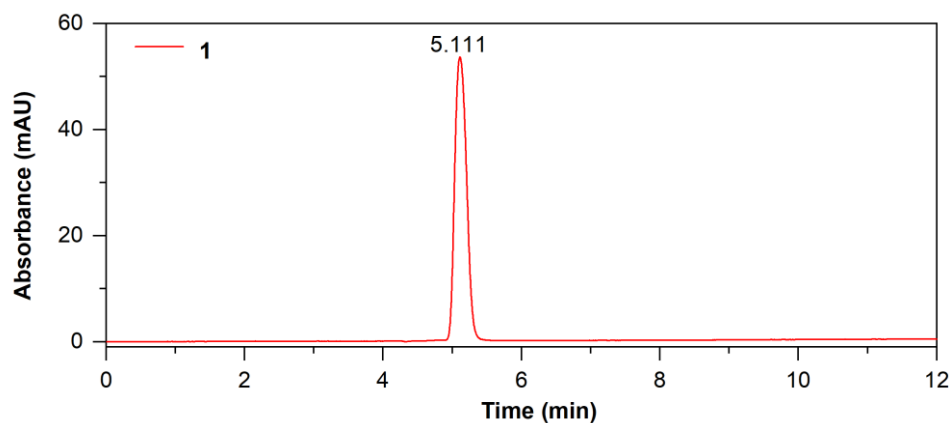
Column: Chiralpak® IC 5 μm, 4.6 mm × 250 mm

Mobile phase: *n*-hexane: isopropanol

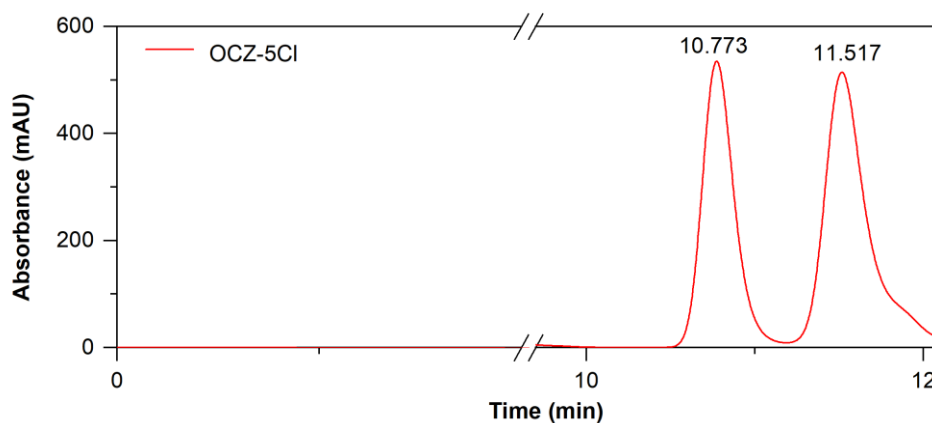
Temperature: 26.5°C

Flow rate: 1.0 mL/min

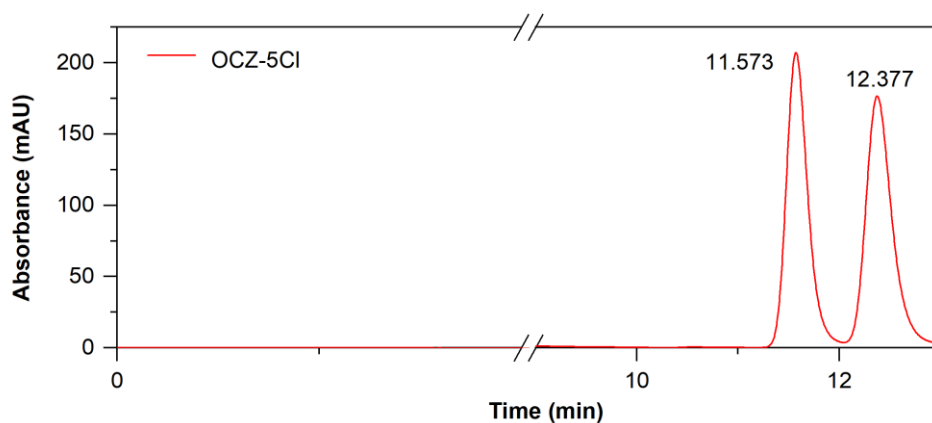
Abs. detector: 225 nm



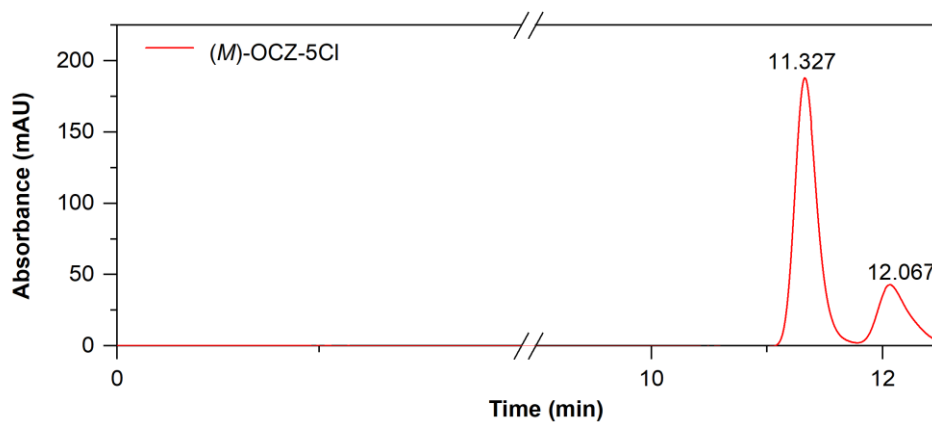
Supplementary Figure 1. HPLC profile of **1** (eluent: 75% *n*-hexane and 25% dichloromethane).



Supplementary Figure 2. HPLC profile of OCZ-5Cl (eluent: 98% *n*-hexane and 2% isopropanol).

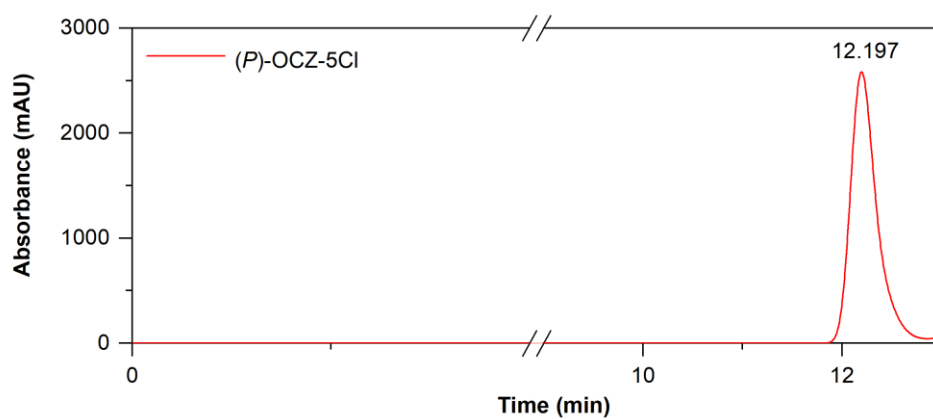


Supplementary Figure 3. HPLC profile of OCZ-5Cl (eluent: 99% *n*-hexane and 1% isopropanol).



Supplementary Figure 4. HPLC profile of (*M*)-OCZ-5Cl (eluent: 99% *n*-hexane and 1%

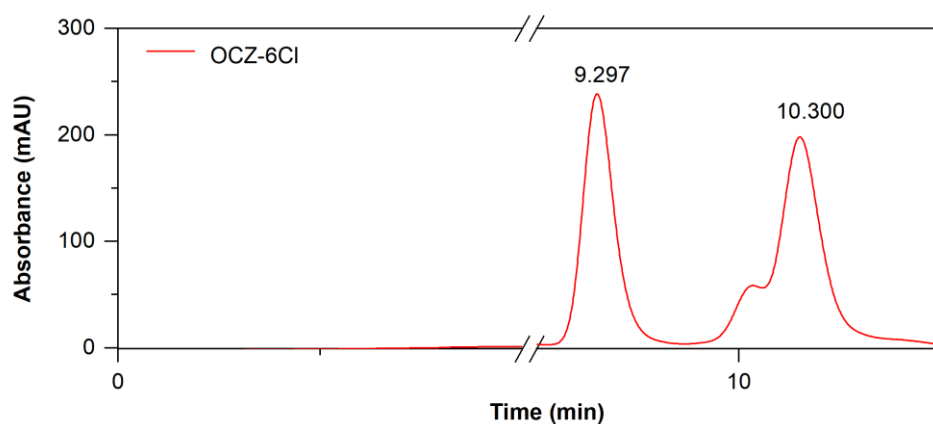
isopropanol).

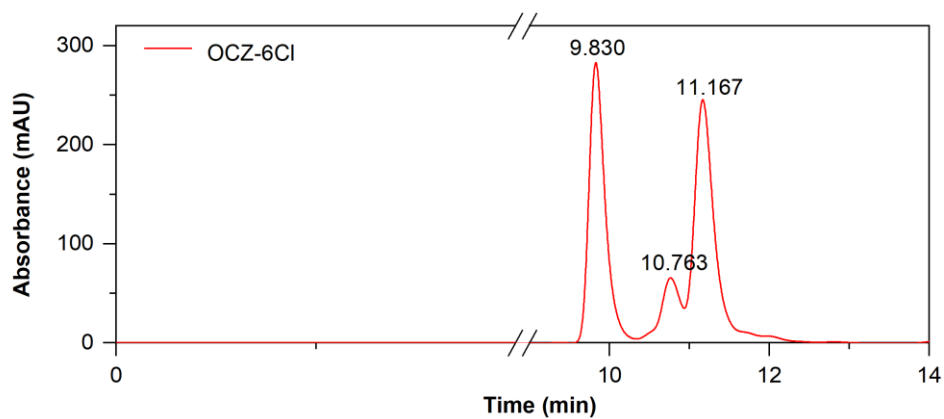


Supplementary Figure 5. HPLC profile of (*P*)-OCZ-5Cl (eluent: 99% *n*-hexane and 1% isopropanol).

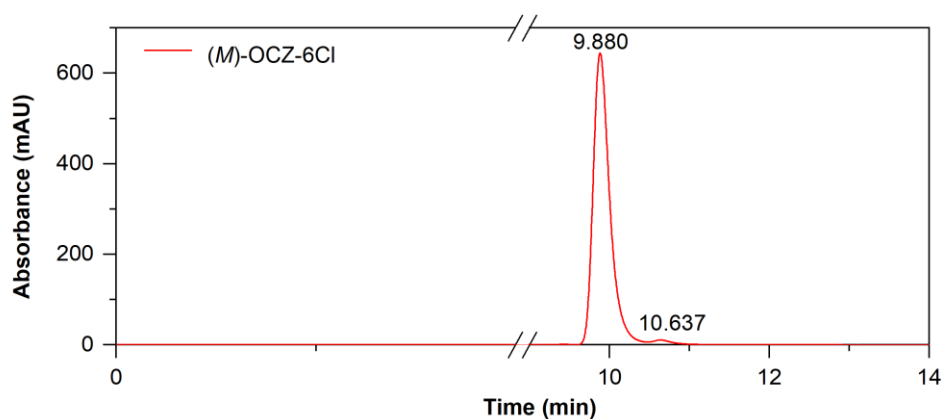
Supplementary Table 1 The summary of HPLC profiles of (*M*)-OCZ-5Cl and (*P*)-OCZ-5Cl.

Figure	Compound	Time (min)	Height (mAU)	Area (mAU*min)	Area (%)	ee value
Supplementary Figure 1	(<i>M</i>)-OCZ- 5Cl	10.773	311.14	68.41	49.27	--
	(<i>P</i>)-OCZ- 5Cl	11.517	295.11	70.41	50.73	--
Supplementary Figure 2	(<i>M</i>)-OCZ- 5Cl	11.573	206.33	50.92	49.57	--
	(<i>P</i>)-OCZ- 5Cl	12.377	174.32	51.80	50.43	--
Supplementary Figure 3	(<i>M</i>)-OCZ- 5Cl	11.327	187.19	42.29	79.18	58.36
	(<i>P</i>)-OCZ- 5Cl	12.067	38.25	11.12	20.82	
Supplementary Figure 4	(<i>M</i>)-OCZ- 5Cl	--	--	--	--	--
	(<i>P</i>)-OCZ- 5Cl	12.197	2557.69	770.82	100	>99%

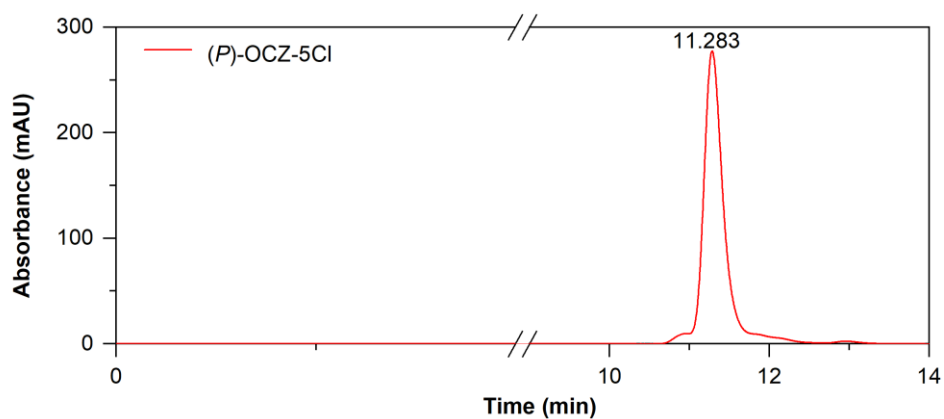
**Supplementary Figure 6.** HPLC profile of OCZ-6Cl (eluent: 98% *n*-hexane and 2% isopropanol).



Supplementary Figure 7. HPLC profile of OCZ-6Cl (eluent: 99% *n*-hexane and 1% isopropanol).



Supplementary Figure 8. HPLC profile of (*M*)-OCZ-6Cl (eluent: 99% *n*-hexane and 1% isopropanol).



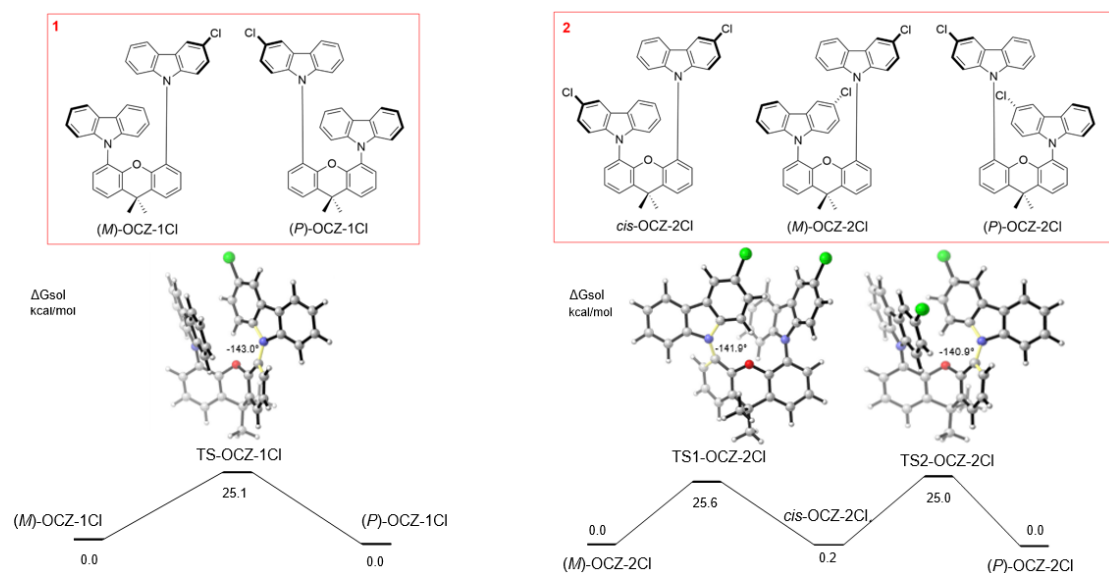
Supplementary Figure 9. HPLC profile of (*P*)-OCZ-6Cl (eluent: 99% *n*-hexane and 1% isopropanol).

Supplementary Table 2 The summary of HPLC profiles of (*M*)-OCZ-6Cl, *cis*-OCZ-6Cl and (*P*)-OCZ-6Cl.

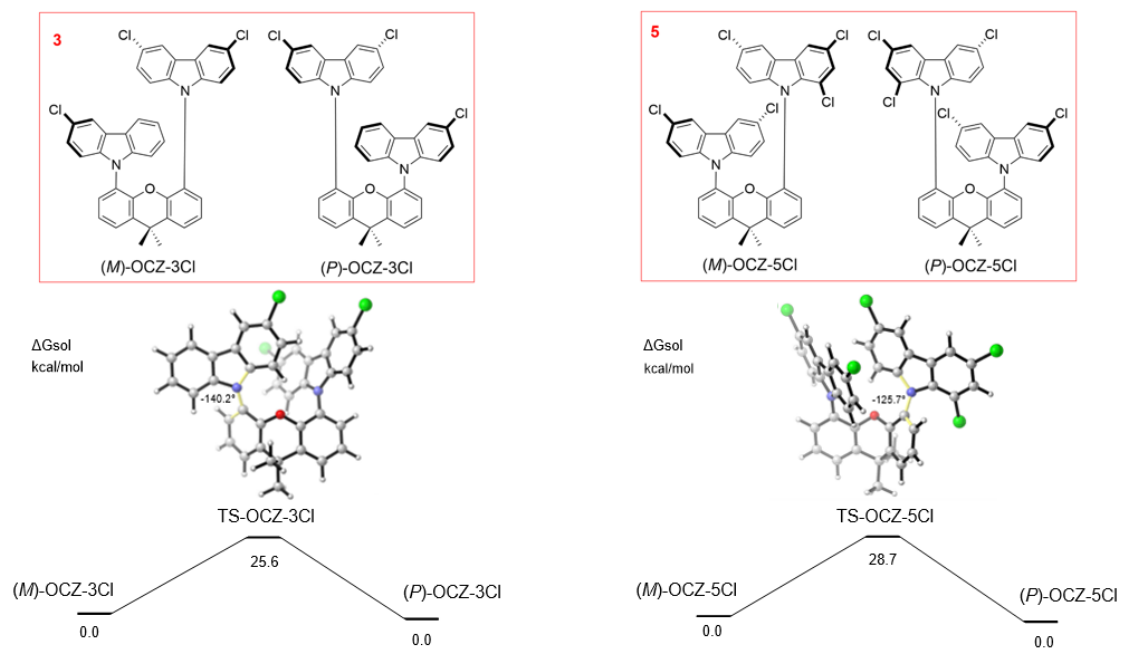
Figure	Compound	Time (min)	Height (mAU)	Area (mAU*min)	Area (%)	ee value
Supplementary Figure 5	(<i>M</i>)-OCZ-6Cl	9.297	139.81	--	--	--
	<i>cis</i> -OCZ-6Cl	--	--	--	--	--
	(<i>P</i>)-OCZ-6Cl	10.300	115.29	--	--	--
Supplementary Figure 6	(<i>M</i>)-OCZ-6Cl	9.830	281.17	65.07	45.04	--
	<i>cis</i> -OCZ-6Cl	10.763	58.49	15.04	10.41	--
	(<i>P</i>)-OCZ-6Cl	11.167	237.01	64.38	44.55	--
Supplementary Figure 7	(<i>M</i>)-OCZ-6Cl	9.880	640.41	150.98	98.18	>99%
	<i>cis</i> -OCZ-6Cl	10.637	6.02	1.26	0.82	--
	(<i>P</i>)-OCZ-6Cl	--	--	--	--	--
Supplementary Figure 8	(<i>M</i>)-OCZ-6Cl	--	--	--	--	--
	<i>cis</i> -OCZ-6Cl	11.017	9.35	1.92	5.85	--
	(<i>P</i>)-OCZ-6Cl	11.283	276.68	76.06	94.15	>99%

S7 – Computational Section

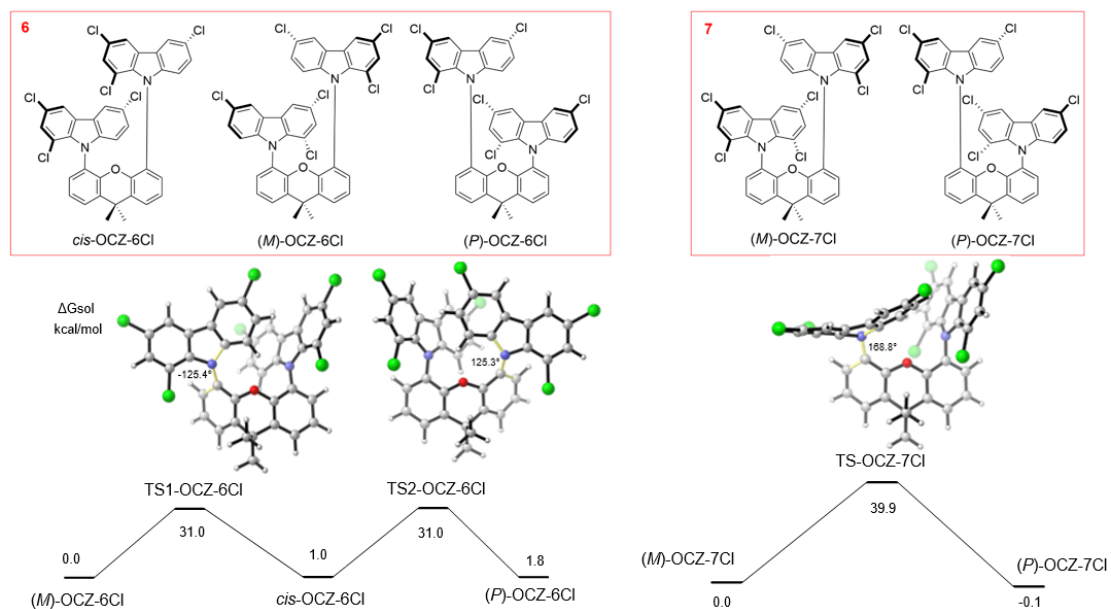
All calculations were implemented in Gaussian 16.¹ Unrestrained geometry were optimized using the B3LYP functional including dispersion corrections²⁻⁴ with the standard 6-31G(d) basis set. Single point calculations were performed at the same B3LYP level of theory with the 6-311+G(d) basis set. Solvation energies were evaluated by a self-consistent reaction field (SCRF) using an SMD^{5,6} implicit solvation model with solvent parameters chosen to represent toluene. Vibrational frequency analyses were used to ensure the identities of the local minimas (zero imaginary frequencies) and transition structures (one imaginary frequency). Intrinsic reaction coordinate (IRC) calculations⁷⁻⁹ were carried out to confirm that the stationary points were smoothly connected to each other. The Gibbs energies were calculated at 298.15 K and 1 atm. Images of the optimized structures were prepared using CYLview.¹⁰



Supplementary Figure 10. Calculated energy profile of OCZ-1Cl and OCZ-2Cl.



Supplementary Figure 11. Calculated energy profile of OCZ-3Cl and OCZ-5Cl.



Supplementary Figure 12. Calculated energy profile of OCZ-6Cl and OCZ-7Cl.

Supplementary Table 3. Energetics of Computed Intermediates and TSs.

Complex	SCF-Done Energy	Single Point Energy in Solvent	Free Energy with Corrections in Solvent	Imaginary Frequency
(<i>M</i>)-OCZ-1Cl	-2147.045528	-2148.020739	-2147.529394	
(<i>P</i>)-OCZ-1Cl	-2147.045565	-2148.020734	-2147.529481	
TS-OCZ-1Cl	-2147.008219	-2147.985277	-2147.489422	-16.90
(<i>M</i>)-OCZ-2Cl	-2606.655951	-2607.651444	-2607.171871	
(<i>P</i>)-OCZ-2Cl	-2606.655956	-2607.651450	-2607.171940	
<i>cis</i> -OCZ-2Cl	-2606.655930	-2607.651777	-2607.171577	
TS1- OCZ-2Cl	-2606.617276	-2607.614885	-2607.131093	-18.64
TS2- OCZ-2Cl	-2606.618077	-2607.615915	-2607.131965	-15.75
(<i>M</i>)-OCZ-3Cl	-3066.265726	-3067.281951	-3066.813811	
(<i>P</i>)-OCZ-3Cl	-3066.265713	-3067.281940	-3066.813651	
TS-OCZ-3Cl	-3066.226596	-3067.244893	-3066.772953	-15.81
(<i>M</i>)-OCZ-5Cl	-3985.480920	-3986.537525	-3986.092443	
(<i>P</i>)-OCZ-5Cl	-3985.480598	-3986.537171	-3986.092126	
TS-OCZ-5Cl	-3985.437328	-3986.494954	-3986.046672	-16.03
(<i>M</i>)-OCZ-6Cl	-4445.089229	-4446.165868	-4445.731698	
(<i>P</i>)-OCZ-6Cl	-4445.085147	-4446.161652	-4445.728851	
<i>cis</i> - OCZ-6Cl	-4445.087152	-4446.163706	-4445.730112	
TS1-OCZ-6Cl	-4445.041766	-4446.119046	-4445.682353	-15.55
TS2-OCZ-6Cl	-4445.041717	-4446.119061	-4445.682271	-15.12
(<i>M</i>)-OCZ-7Cl	-4904.691303	-4905.786979	-4905.364572	
(<i>P</i>)-OCZ-7Cl	-4904.691293	-4905.787023	-4905.364673	
TS- OCZ-7Cl	-4904.626095	-4905.787023	-4905.300950	-22.81

Cartesian Coordinates

(M)-OCZ-1Cl

C	0.61748900	4.55232900	1.45638400
C	-0.73050900	4.55853900	1.10702400
C	-1.38257100	3.39957000	0.66424500
C	-0.62122000	2.23375000	0.57792600
C	0.73227900	2.19616500	0.95751900
C	1.34911200	3.36588800	1.39370500
C	-2.42917700	0.95376800	-0.23927500
C	-3.31906300	2.02624100	-0.16799000
C	-4.65088300	1.77904400	-0.52677400
H	-5.37097300	2.58992700	-0.47965200
C	-5.07341500	0.51897600	-0.94231200
C	-4.15849000	-0.52982200	-1.03194800
C	-2.82545800	-0.31985700	-0.68411500
H	1.09445400	5.46640500	1.79528000
H	-1.29077700	5.48559400	1.17839000
H	2.39296200	3.32912400	1.68733500
H	-6.11157100	0.35725400	-1.21453500
H	-4.45976800	-1.51335700	-1.37651700
O	-1.11587700	1.04964100	0.11866300
C	-2.86437200	3.41598200	0.28383200
C	1.11561300	-0.21680600	1.51946200
C	2.51050000	0.73424100	-0.00047500
C	0.09933600	-0.47288500	2.43871900
C	2.01163500	-1.22934400	1.09577800
C	3.12544300	1.59251900	-0.90978600
C	2.89972700	-0.62373600	0.12591300
C	-0.01539100	-1.77187800	2.92732500
C	1.88309400	-2.52251400	1.61118600
C	4.15288600	1.08080900	-1.69974900
H	2.80789800	2.62458600	-1.01293800
C	3.93708100	-1.12245800	-0.66355700
C	0.86768800	-2.78735700	2.52337500
H	-0.81270200	-2.00722900	3.62553400
H	2.55615300	-3.31118900	1.28700000
C	4.54472800	-0.25867600	-1.56604000
H	4.65255700	1.71380900	-2.42440800
H	4.24490900	-2.15994400	-0.59964500
C	-0.71662500	-1.38137600	-1.53626000
C	-1.97242500	-2.58122000	-0.06762900
C	-0.19700700	-0.39580100	-2.37441500
C	-0.07353900	-2.63372000	-1.36987700
C	-2.91746300	-2.99560500	0.86995100
C	-0.87177300	-3.39729700	-0.43280800
C	0.99148900	-0.67752800	-3.04471000
C	1.11306400	-2.89476800	-2.06147800
C	-2.75487600	-4.25966300	1.43504400
H	-3.74373300	-2.35285400	1.15503500
C	-0.73619800	-4.66264600	0.14331900
C	1.64109300	-1.91380300	-2.89521900
H	1.43030500	0.08005300	-3.68664000
H	1.61861100	-3.84907800	-1.94106700
C	-1.68025300	-5.08937800	1.07394500
H	-3.47602700	-4.60763000	2.16931300
H	0.10397300	-5.29806800	-0.12291200
N	1.44457600	0.97868300	0.86824200

N	-1.87917700	-1.36596400	-0.75398400
Cl	5.83059600	-0.87367900	-2.60606000
H	2.57226600	-2.09475000	-3.42246700
H	-0.69510400	0.55969700	-2.49474100
H	-1.58436100	-6.07063500	1.52946100
H	0.73542500	-3.79281200	2.90818300
H	-0.58530100	0.30836400	2.75054700
C	-3.69422900	3.85269500	1.51466500
H	-3.39332100	4.84878000	1.85394800
H	-4.76129800	3.88956000	1.27440600
H	-3.55308900	3.15137400	2.34260800
C	-3.08403300	4.41765800	-0.87514900
H	-4.13979500	4.45518400	-1.16168300
H	-2.77865100	5.42725400	-0.58226800
H	-2.50106100	4.12421100	-1.75341600

(P)-OCZ-1CI

C	1.49499000	4.47572100	0.59217400
C	0.13164800	4.66768200	0.38318900
C	-0.73861400	3.59176100	0.16091700
C	-0.18360300	2.31186600	0.16601900
C	1.19494700	2.09648200	0.34116800
C	2.03153000	3.18815500	0.55913800
C	-2.26519400	1.26238100	-0.20840900
C	-2.95009300	2.47607400	-0.27885000
C	-4.32361600	2.42197000	-0.55118300
H	-4.88712300	3.34741800	-0.61675000
C	-4.98357200	1.21036700	-0.73952300
C	-4.28193400	0.00948100	-0.63572500
C	-2.91502300	0.02535600	-0.36506100
H	2.14336800	5.32929000	0.76220300
H	-0.26787800	5.67697800	0.39390500
H	3.09447300	3.01509900	0.69092400
H	-6.04853900	1.19940100	-0.94869600
H	-4.78001800	-0.94694100	-0.75404000
O	-0.92105600	1.17632300	0.01007600
C	-2.23504100	3.81281600	-0.06870700
C	1.58272700	-0.12844100	-0.74791900
C	2.27774500	0.11627400	1.40095300
C	1.03256900	0.06059600	-2.01482700
C	2.13267800	-1.37242500	-0.35092900
C	2.51876200	0.58065300	2.69243700
C	2.57402400	-1.21716300	1.01916900
C	1.03180500	-1.02595400	-2.88582600
C	2.13118600	-2.44409800	-1.24873800
C	3.07308200	-0.30608400	3.61328400
H	2.27110600	1.59662400	2.98064800
C	3.13820600	-2.09356800	1.94741200
C	1.57805000	-2.26525600	-2.51180400
H	0.58754000	-0.91602900	-3.87026700
H	2.53961300	-3.40663700	-0.95406600
C	3.37603500	-1.62077000	3.23185100
H	3.26986300	0.01391400	4.63032500
H	3.36023900	-3.12248900	1.68804900
C	-2.06790900	-2.13737300	-1.27410500
C	-1.45855900	-1.61556500	0.85428100
C	-2.55747200	-2.10821600	-2.57923200
C	-1.29481200	-3.22223500	-0.78815300
C	-1.26364600	-0.99290400	2.08643800
C	-0.90873200	-2.89046600	0.56802900
C	-2.27387500	-3.19918800	-3.39956300
C	-1.03091300	-4.30621400	-1.62882600
C	-0.49613100	-1.66401600	3.03604900
H	-1.68686700	-0.01700600	2.29631000
C	-0.15045700	-3.54697900	1.54193900
C	-1.52388600	-4.29087900	-2.93119100
H	-2.64217400	-3.20244100	-4.42163800
H	-0.43645700	-5.14303800	-1.27265200
C	0.05371600	-2.92915800	2.77189800
H	-0.30976300	-1.19262700	3.99605800
H	0.27978700	-4.52314300	1.33515500
N	1.70025100	0.77682200	0.31427600
N	-2.17609400	-1.17412100	-0.26559000

Cl	4.05042500	-2.71910300	4.43685700
H	-1.32394400	-5.12750400	-3.59424200
H	-3.13041300	-1.26234200	-2.94439500
H	0.65733800	-3.41773200	3.53001100
H	1.54113200	-3.09592300	-3.20833300
H	0.60815500	1.01535200	-2.30565500
C	-2.84343700	4.51882100	1.16671300
H	-2.36146700	5.48614200	1.34090000
H	-3.91405600	4.69694100	1.02461200
H	-2.71445300	3.90495500	2.06329800
C	-2.42533500	4.69973900	-1.32230500
H	-3.48658900	4.89067600	-1.50937200
H	-1.92905400	5.66680700	-1.19433400
H	-2.00348400	4.21229600	-2.20644600

TS-OCZ-1CI

C	-4.64199900	2.96094300	-0.95033400
C	-3.81583300	3.88524000	-0.30809900
C	-2.60099500	3.48402900	0.24988600
C	-2.24469900	2.13531200	0.17090300
C	-2.99559300	1.22510900	-0.58711000
C	-4.22013700	1.64566600	-1.11770300
C	0.01826600	2.50264800	0.65048900
C	-0.20287100	3.88142700	0.49433100
C	0.82239800	4.68489500	0.00036200
H	0.66900300	5.74699100	-0.14632900
C	2.03710300	4.09680600	-0.34444300
C	2.26923300	2.75747900	-0.06280500
C	1.30832500	1.93376600	0.55837900
H	-5.59121100	3.28134300	-1.36847800
H	-4.12094700	4.92384800	-0.24958000
H	-4.80335700	0.93851300	-1.69823800
H	2.81926900	4.68498700	-0.81440700
H	3.22351000	2.32195100	-0.32430200
O	-1.09837300	1.69853000	0.81598600
C	-1.58424200	4.40390400	0.91712500
C	-1.30717000	-0.26867700	-1.63739900
C	-3.11400200	-1.28163100	-0.69675600
C	-0.35926200	0.65276500	-2.07758700
C	-1.17052100	-1.65845100	-1.87683800
C	-4.27558200	-1.56581800	0.02022400
C	-2.32620800	-2.30373500	-1.28787100
C	0.77160300	0.15407500	-2.72078800
C	-0.02674600	-2.13355500	-2.52380800
C	-4.64810800	-2.90462600	0.13706200
C	-2.72053800	-3.63754100	-1.15252700
C	0.94431500	-1.22368500	-2.93354400
H	1.53641000	0.84944100	-3.05403400
H	0.10652100	-3.19854900	-2.69035200
C	-3.88146200	-3.93071800	-0.44102300
H	-5.54618800	-3.15715500	0.69335400
H	-2.11620700	-4.43405300	-1.57625500
C	1.12827200	-0.61112600	1.10925300
C	3.12051500	0.47792900	1.38184200
C	-0.20963100	-1.00219500	1.17221400
C	2.14010000	-1.59273000	1.26848600
C	4.11186800	1.40448500	1.72782800
C	3.39647800	-0.90533700	1.44479600
C	-0.52001900	-2.35378700	1.29842300
C	1.83048500	-2.95165400	1.35339600
C	5.38180200	0.92983600	2.04936400
C	4.67869700	-1.36555500	1.75802700
C	0.49216800	-3.31497200	1.34522500
H	-1.55632200	-2.66179100	1.35178200
H	2.61038500	-3.69797200	1.45702100
C	5.67701700	-0.44179800	2.04397900
H	6.15390400	1.64436900	2.31969900
H	4.87924800	-2.43231700	1.80161100
N	-2.48274700	-0.05165700	-0.90431700
N	1.74579500	0.67569500	1.06476000
H	-1.00632200	-0.28360400	1.14688600
C	-1.79501800	5.86990900	0.52292600

H	-2.77228600	6.22088100	0.86700100
H	-1.04245000	6.50535000	0.99886100
H	-1.73808600	6.01299200	-0.56080000
C	-1.71425600	4.28222100	2.45846900
H	-0.95190500	4.89618700	2.94985700
H	-2.70324100	4.62752200	2.77907300
H	-1.58875600	3.24793100	2.78786200
Cl	0.05204500	-5.01881200	1.43540200
H	-0.48508000	1.71708700	-1.91718500
H	-4.85817500	-0.77461200	0.48083700
H	3.90615300	2.46620500	1.76882300
H	6.67835200	-0.78075500	2.29166800
H	-4.19401300	-4.96362600	-0.32271300
H	1.84432900	-1.58087600	-3.42475700

(M)-OCZ-2Cl

C	-3.05176800	3.57376200	-4.85337500
C	-1.85463600	4.23710300	-4.59612400
C	-0.69289300	3.54475600	-4.22839700
C	-0.78564900	2.15673800	-4.12253600
C	-1.97403100	1.46291700	-4.40954800
C	-3.11025600	2.18223600	-4.77180900
C	1.46199100	1.92704700	-3.44029500
C	1.71447100	3.29523600	-3.54395300
C	3.01669300	3.72854900	-3.25991400
H	3.25042700	4.78582900	-3.33640100
C	4.01866900	2.83811000	-2.88246700
C	3.73227700	1.47875100	-2.75389500
C	2.44824100	1.01419700	-3.02784500
H	-3.93479700	4.13795300	-5.13582200
H	-1.82048800	5.31865100	-4.68233000
H	-4.02389700	1.64100300	-4.99414700
H	5.01786700	3.20425500	-2.66946900
H	4.48853900	0.76959300	-2.43408200
O	0.25384900	1.36543700	-3.73148300
C	0.61903700	4.28254300	-3.95250700
C	-1.20574300	-0.84202300	-5.03524000
C	-2.77456300	-0.67271100	-3.40087200
C	-0.25401500	-0.58342900	-6.02055800
C	-1.50925600	-2.16270900	-4.61965500
C	-3.65315500	-0.21357800	-2.42147300
C	-2.50642400	-2.05448200	-3.57546000
C	0.40000600	-1.67466700	-6.58786100
C	-0.84738500	-3.24139100	-5.21387700
C	-4.27729800	-1.15736000	-1.60860000
H	-3.83830100	0.84628900	-2.28372300
C	-3.14492500	-2.99142400	-2.76124700
C	0.10592600	-2.99136500	-6.19528900
H	1.16041500	-1.50260500	-7.34333200
H	-1.06684700	-4.25878600	-4.90227800
C	-4.01951500	-2.52382200	-1.78833000
H	-4.96262800	-0.84097800	-0.83034500
H	-2.94901300	-4.05297200	-2.86274200
C	1.14842800	-0.90909200	-2.07673700
C	2.67933300	-1.37978400	-3.68782300
C	0.30810500	-0.27819100	-1.16060600
C	1.10899400	-2.31086800	-2.28287500
C	3.62501400	-1.30411200	-4.70858200
C	2.08194700	-2.61025400	-3.31256300
C	-0.58461700	-1.07597400	-0.44856100
C	0.21250800	-3.09065900	-1.54594800
C	3.98079500	-2.48368700	-5.35898200
H	4.06343700	-0.35583600	-5.00039100
C	2.45347900	-3.78704500	-3.96495700
C	-0.63159500	-2.46819000	-0.63244400
H	-1.26526600	-0.60982900	0.25712100
H	0.16833000	-4.16573400	-1.69636900
C	3.39711900	-3.70121100	-4.98096600
H	4.70768700	-2.46680100	-6.16322100
H	2.00341800	-4.73966400	-3.70900200
N	-1.99880300	0.05346000	-4.30663700
N	2.12395200	-0.35701400	-2.91644100

Cl	-4.80909200	-3.68303400	-0.71845700
H	-1.34827300	-3.05728400	-0.06975200
H	0.34218200	0.79596600	-1.01486100
H	0.64395000	-3.81683900	-6.64961300
H	-0.02529600	0.43125000	-6.32760500
C	1.05439800	5.02987400	-5.23566800
H	0.29001900	5.74962600	-5.54494800
H	1.98602700	5.58017800	-5.07066100
H	1.21342500	4.32470700	-6.05708200
C	0.40490200	5.29811400	-2.80481200
H	1.32838400	5.84598700	-2.59278000
H	-0.36577300	6.02927500	-3.06834200
H	0.09290100	4.78551800	-1.88983300
Cl	3.85471400	-5.16639400	-5.85030300

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C	-0.07322600	-4.63587300	1.66692300
C	-1.39138400	-4.52651600	1.23114900
C	-1.90832400	-3.31868300	0.74320900
C	-1.04247600	-2.22544500	0.70414900
C	0.28134900	-2.30311900	1.17050600
C	0.76305300	-3.51928100	1.64856700
C	-2.66695600	-0.80608500	-0.25330500
C	-3.65257100	-1.79330600	-0.23516200
C	-4.92518300	-1.43496100	-0.70018300
H	-5.71802900	-2.17639100	-0.69486300
C	-5.19920600	-0.15246300	-1.16864100
C	-4.18761000	0.80754900	-1.20725300
C	-2.91111700	0.48483000	-0.75337200
H	0.29806000	-5.58532100	2.03911000
H	-2.03517900	-5.39964300	1.27025200
H	1.78494100	-3.57253300	2.00914200
H	-6.19516300	0.09480300	-1.52185200
H	-4.36933100	1.80481600	-1.59397800
O	-1.40056300	-1.00525800	0.21173200
C	-3.36002000	-3.20703600	0.27216800
C	0.85678300	0.06047000	1.78455700
C	2.25992100	-1.01903900	0.36093700
C	-0.19478800	0.41508000	2.62829300
C	1.89582200	0.96990300	1.46464800
C	2.85098200	-1.92826700	-0.51423500
C	2.78804700	0.28303600	0.55435400
C	-0.19577400	1.70675800	3.14981900
C	1.87793800	2.25655200	2.01140200
C	3.99414300	-1.52583000	-1.20142600
H	2.42968300	-2.91575900	-0.66895900
C	3.93938400	0.67171500	-0.13256800
C	0.83014500	2.61918900	2.85111100
H	-1.01250700	2.01754400	3.79396600
H	2.66542900	2.96557900	1.77161700
C	4.52146900	-0.24201000	-1.00225300
H	4.48031300	-2.20098400	-1.89659600
H	4.35762400	1.66510000	-0.01503300
C	-1.84485200	2.62270000	-0.03704200
C	-0.64875800	1.31111300	-1.45479200
C	-2.79216000	3.13083900	0.84973800
C	-0.61897700	3.29173600	-0.28476700
C	-0.19665400	0.28164900	-2.27895200
C	0.14187400	2.45766000	-1.19136500
C	-2.50653000	4.33291100	1.49350000
C	-0.34797400	4.50031100	0.35895600
C	1.07206500	0.41359000	-2.83877700
H	-0.80729300	-0.59412800	-2.46958800
C	1.40678400	2.57157600	-1.77598500
C	-1.29878700	4.99880500	1.24074700
H	-3.21412000	4.75843400	2.19614200
H	0.58652300	5.02655400	0.19978000
C	1.86643400	1.54698800	-2.59662700
H	1.45861800	-0.38162900	-3.46868100
H	2.02554100	3.44273300	-1.57954300
N	1.10172300	-1.15283500	1.12929000
N	-1.86395200	1.43406700	-0.76936100

Cl	5.95354300	0.23676100	-1.91429100
H	-3.71921100	2.60302500	1.04613800
H	0.79069800	3.62140800	3.26497000
H	-0.98780200	-0.28672800	2.86235300
C	-3.60519000	-4.21367300	-0.87723700
H	-3.41635100	-5.23949100	-0.54554500
H	-4.64076900	-4.15977600	-1.22742700
H	-2.94567900	-3.99999500	-1.72379600
C	-4.29926200	-3.53118900	1.45842300
H	-5.34882300	-3.47213700	1.15359200
H	-4.11579600	-4.54241200	1.83490800
H	-4.14044300	-2.82576600	2.27966300
H	2.85511700	1.61065000	-3.03904900
Cl	-0.96469100	6.50312200	2.09935500

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C	-3.80656900	2.99931100	-4.13180200
C	-2.72794400	3.85973900	-3.94671600
C	-1.42491900	3.37728100	-3.76525000
C	-1.24625900	1.99346300	-3.78035400
C	-2.32210200	1.10472200	-3.95476500
C	-3.60545600	1.61953800	-4.12874300
C	1.08802500	2.16095400	-3.44821900
C	1.05878500	3.55590700	-3.41042400
C	2.27299700	4.21963400	-3.19091400
H	2.28362400	5.30438700	-3.15498500
C	3.46549900	3.52277400	-3.01671300
C	3.47149100	2.12962900	-3.06773500
C	2.28139100	1.43611800	-3.28126600
H	-4.80551800	3.40148500	-4.26679500
H	-2.89988100	4.93144900	-3.94534400
H	-4.43217700	0.92892600	-4.25680200
H	4.39204500	4.06348300	-2.85235400
H	4.38979100	1.56521800	-2.94577900
O	-0.02635500	1.39623000	-3.64020800
C	-0.24622500	4.33499600	-3.58380400
C	-1.50933500	-1.07583500	-2.99495000
C	-2.39359700	-1.10766300	-5.08898100
C	-1.02586700	-0.70349900	-1.74047300
C	-1.47024700	-2.42109100	-3.43833100
C	-2.91592400	-0.76596200	-6.33505600
C	-2.02956900	-2.44149600	-4.77370100
C	-0.48875300	-1.70253600	-0.93336200
C	-0.93616700	-3.40817400	-2.60417200
C	-3.08943300	-1.78260900	-7.27223300
H	-3.17352100	0.25943000	-6.57691100
C	-2.21649500	-3.45335600	-5.71739800
C	-0.44626300	-3.04244600	-1.35550600
H	-0.07701800	-1.43701700	0.03536200
H	-0.89596000	-4.44176300	-2.93603700
C	-2.74601300	-3.10442000	-6.95394200
H	-3.49066700	-1.55760500	-8.25397900
H	-1.93471100	-4.47880100	-5.50947000
C	2.70856800	-0.77861700	-2.22893600
C	1.84844500	-0.80961000	-4.33231100
C	3.14388300	-0.40273800	-0.95833800
C	2.60596600	-2.13961100	-2.61045000
C	1.30830700	-0.48182800	-5.57559700
C	2.06417200	-2.15790000	-3.95202400
C	3.48980700	-1.41830400	-0.06855200
C	2.96536600	-3.13882600	-1.70242600
C	0.98296800	-1.52015200	-6.44395300
H	1.13394000	0.54853400	-5.86173200
C	1.74468600	-3.19173500	-4.83542700
C	3.40709000	-2.77284500	-0.43416800
H	3.83001300	-1.15396900	0.92866800
H	2.88493900	-4.18596700	-1.98003800
C	1.21161900	-2.85338200	-6.07194100
H	0.54025100	-1.30596900	-7.40971300
H	1.90396600	-4.23043000	-4.56807400
N	-2.08903800	-0.28791700	-3.99776200
N	2.26245500	0.02274100	-3.28639700

Cl	-2.98187600	-4.35567400	-8.17010100
H	3.68697100	-3.53917000	0.28244900
H	3.20097600	0.64155100	-0.67054200
H	-0.00726700	-3.79137100	-0.70459400
H	-1.05442900	0.32876300	-1.41080300
C	-0.13024300	5.24177700	-4.83263300
H	-1.04511500	5.82458900	-4.97864400
H	0.70264400	5.94412900	-4.72736200
H	0.04009000	4.64052500	-5.73084100
C	-0.49097400	5.20560300	-2.32803000
H	0.32924400	5.91416500	-2.17691200
H	-1.41617200	5.78162300	-2.42765600
H	-0.57188100	4.57893800	-1.43473400
Cl	0.80832900	-4.13330100	-7.21114500

TS1-OCZ-2Cl

C	-4.65184700	2.96467600	-0.90919200
C	-3.81338000	3.88505800	-0.27754600
C	-2.59249100	3.47973700	0.26404400
C	-2.24230700	2.12940500	0.18199900
C	-3.00637900	1.22435500	-0.56893700
C	-4.23592400	1.64858000	-1.08429400
C	0.02777300	2.48765700	0.63526400
C	-0.18940100	3.86642600	0.47407700
C	0.83537400	4.66323400	-0.03188200
H	0.68444700	5.72503000	-0.18321800
C	2.04704500	4.07023600	-0.37952900
C	2.27760200	2.73264700	-0.08825600
C	1.31638800	1.91615200	0.54137600
H	-5.60529900	3.28880900	-1.31441100
H	-4.11346500	4.92485500	-0.21504700
H	-4.82770500	0.94490600	-1.66049300
H	2.82842300	4.65402200	-0.85613700
H	3.23202100	2.29303900	-0.34355300
O	-1.09034300	1.68683700	0.81245300
C	-1.56245900	4.39756900	0.91290200
C	-1.33962600	-0.26420800	-1.66171400
C	-3.12755000	-1.28101300	-0.69477900
C	-0.39751100	0.65964100	-2.10968300
C	-1.21087200	-1.65122500	-1.91988600
C	-4.27477200	-1.57433200	0.04067300
C	-2.35525300	-2.29888900	-1.31325100
C	0.71610500	0.16477100	-2.78429500
C	-0.08409300	-2.12312200	-2.59867300
C	-4.65459700	-2.91029300	0.15211700
C	-2.74367500	-3.63501900	-1.19084600
C	0.87930000	-1.21100800	-3.01929300
H	1.47589800	0.86149400	-3.12580600
H	0.04164100	-3.18627900	-2.78146500
C	-3.89182300	-3.91731500	-0.45929300
H	-5.53883900	-3.18116500	0.71773800
H	-2.15961500	-4.43545500	-1.63061500
C	1.15103900	-0.62586400	1.10433200
C	3.12450400	0.48605800	1.41476200
C	-0.18445300	-1.02821900	1.12420200
C	2.16665300	-1.59567700	1.30702500
C	4.09937900	1.42861700	1.76372000
C	3.41113900	-0.89341900	1.50768400
C	-0.48568200	-2.38121400	1.25538800
C	1.86652300	-2.95660200	1.39691000
C	5.36552700	0.97166100	2.12318000
C	4.68983100	-1.33564800	1.85935300
C	0.53250900	-3.33310300	1.34764400
H	-1.51990400	-2.69917600	1.28201700
H	2.64923200	-3.69464000	1.53344900
C	5.67248700	-0.39725800	2.15156900
H	6.12541600	1.69809500	2.39632200
H	4.89940300	-2.39943600	1.92632200
N	-2.49854900	-0.05184900	-0.90116100
N	1.75618000	0.66527500	1.06259800
Cl	-4.40576100	-5.59145500	-0.28198100
H	-0.98528200	-0.31611300	1.06725600

C	-1.77151800	5.86280100	0.51481400
H	-2.74189900	6.22054700	0.87108900
H	-1.00918300	6.49643100	0.97731600
H	-1.72901700	6.00077700	-0.57024000
C	-1.67138500	4.28331300	2.45649900
H	-0.89877700	4.89514300	2.93421400
H	-2.65376400	4.63563100	2.78946700
H	-1.54692000	3.24983700	2.78892400
Cl	0.10125100	-5.03769500	1.43991000
H	-0.51540900	1.72210300	-1.93236600
H	-4.84964400	-0.79120900	0.52351300
H	3.88370800	2.48912300	1.77708400
H	6.67070500	-0.72210800	2.42885000
H	1.76627000	-1.56420100	-3.53603600

TS2- OCZ-2Cl

C	-4.66193600	2.97412500	-0.87550300
C	-3.81279400	3.88871100	-0.24991200
C	-2.58774000	3.47663000	0.27687100
C	-2.24380100	2.12486900	0.18808700
C	-3.01918800	1.22666700	-0.56000700
C	-4.25254900	1.65751300	-1.06055000
C	0.03237300	2.47348000	0.61918200
C	-0.18138700	3.85266600	0.45666700
C	0.84093500	4.64443200	-0.06238000
H	0.69144500	5.70617100	-0.21564000
C	2.04817200	4.04745900	-0.41908500
C	2.27850200	2.71104900	-0.12201900
C	1.31983500	1.90049800	0.51877600
H	-5.61847900	3.30345000	-1.26908500
H	-4.10741400	4.92964600	-0.18101700
H	-4.85267600	0.95805800	-1.63311800
H	2.82655300	4.62755900	-0.90491200
H	3.23137200	2.26760900	-0.37762200
O	-1.08672500	1.67509700	0.80561700
C	-1.54615900	4.39000000	0.91290200
C	-1.36508800	-0.25997000	-1.66818600
C	-3.15338300	-1.27992200	-0.70516800
C	-0.41780000	0.66067000	-2.11035600
C	-1.23954600	-1.64619800	-1.93250500
C	-4.30248600	-1.57035900	0.02955900
C	-2.38580400	-2.29618800	-1.33136100
C	0.70159700	0.17365800	-2.77915800
C	-0.11237000	-2.12485800	-2.60417400
C	-4.68108800	-2.90834900	0.12768400
C	-2.78546700	-3.63041300	-1.21423000
C	0.84712600	-1.20301700	-3.00551100
H	1.47162300	0.85718000	-3.11781800
H	0.02541800	-3.18350100	-2.79313400
C	-3.93355800	-3.92886300	-0.48540100
H	-5.56933300	-3.16595800	0.69708100
H	-2.19647200	-4.42217000	-1.66742500
C	1.17249900	-0.63963700	1.09152000
C	3.12881600	0.49531700	1.42599100
C	-0.15890800	-1.05483600	1.07800800
C	2.19348900	-1.59667700	1.32679700
C	4.08919500	1.45283200	1.77372200
C	3.42697200	-0.87974800	1.54208800
C	-0.45003700	-2.40986600	1.21547100
C	1.90457500	-2.95919100	1.42512200
C	5.35388700	1.01337600	2.15886700
C	4.70433800	-1.30432900	1.91934700
C	0.57572400	-3.34878000	1.34768100
H	-1.48124400	-2.73852800	1.21516900
H	2.69098200	-3.68795700	1.58716000
C	5.67303000	-0.35207700	2.21290300
H	6.10336100	1.75100700	2.43078100
H	4.92386000	-2.36491400	2.00245800
N	-2.52030900	-0.04942000	-0.90534800
N	1.76471500	0.65611100	1.04998800
H	-0.96465500	-0.35060400	0.99421400
C	-1.75353700	5.85622000	0.51756200

H	-2.71713600	6.21880400	0.88708700
H	-0.98176700	6.48598100	0.96957000
H	-1.72519600	5.99406600	-0.56796800
C	-1.63557300	4.27618000	2.45777600
H	-0.85374300	4.88402000	2.92546500
H	-2.61178000	4.63347800	2.80337100
H	-1.51214600	3.24204900	2.78857300
Cl	0.16132500	-5.05792900	1.45668700
H	-0.52950600	1.72350600	-1.93289500
H	-4.87024400	-0.78445700	0.51669000
H	3.86379200	2.51140100	1.76485400
H	6.67028100	-0.66300000	2.50892800
H	-4.25178300	-4.96141400	-0.38106400
Cl	2.29690300	-1.77532200	-3.82566300

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C	1.59003400	4.37883200	0.39978400
C	0.22818600	4.61121100	0.22633900
C	-0.68433100	3.55854600	0.07446400
C	-0.17308500	2.26090700	0.10920600
C	1.20010900	2.00211600	0.26165100
C	2.07954000	3.07295400	0.40831100
C	-2.30184500	1.27619400	-0.16732600
C	-2.94897200	2.51043600	-0.23930300
C	-4.33435800	2.49661300	-0.44944700
H	-4.86846800	3.43941500	-0.51294300
C	-5.04368100	1.30545300	-0.57969900
C	-4.37728900	0.08378200	-0.48664800
C	-3.00004400	0.06135700	-0.27920100
H	2.27308800	5.21451200	0.51331900
H	-0.13611300	5.63357000	0.21009100
H	3.13880800	2.86813500	0.52165900
H	-6.11679600	1.32711800	-0.73985900
H	-4.91017600	-0.85778100	-0.56755300
O	-0.95576200	1.14634500	0.00849300
C	-2.18001000	3.82620600	-0.10513800
C	1.53217800	-0.28937200	-0.71721600
C	2.33844600	0.08716000	1.37434200
C	0.92447000	-0.18026300	-1.96779700
C	2.15553400	-1.49004600	-0.29407900
C	2.64859000	0.62900900	2.62017200
C	2.66559200	-1.25188000	1.04059300
C	0.94612100	-1.29947700	-2.79628900
C	2.17082000	-2.59731100	-1.14806000
C	3.31534600	-0.18084900	3.53721800
H	2.37706600	1.64761600	2.87538600
C	3.33898700	-2.05197300	1.96600300
C	1.56532500	-2.49587600	-2.39619500
H	0.46251700	-1.25000300	-3.76688300
H	2.64456000	-3.52363000	-0.83521900
C	3.65736800	-1.49838200	3.20041100
H	3.57464600	0.20291400	4.51745900
H	3.59289300	-3.08197200	1.74365600
C	-2.21712900	-2.09091400	-1.25773800
C	-1.52785900	-1.63125200	0.85529000
C	-2.74608900	-2.02214500	-2.54566200
C	-1.42401800	-3.18752400	-0.83621600
C	-1.27173800	-1.04198400	2.09287500
C	-0.99002200	-2.89693700	0.51284100
C	-2.47740300	-3.07333600	-3.41884100
C	-1.16886100	-4.24057100	-1.71650000
C	-0.47375800	-1.73756100	2.99625000
H	-1.67342700	-0.06804800	2.34759600
C	-0.19877500	-3.59164100	1.43114100
C	-1.70008800	-4.16278700	-2.99743500
H	-2.86502600	-3.05504600	-4.43118900
H	-0.55403200	-5.08416200	-1.42377100
C	0.04188700	-3.00016800	2.66382500
H	-0.23870400	-1.30600100	3.96217400
H	0.21971300	-4.56334600	1.19373700
N	1.66328400	0.66786600	0.29700900
N	-2.29311700	-1.16215100	-0.21719900

Cl	4.50743100	-2.48033400	4.38834100
H	-3.33778300	-1.17185900	-2.86677800
H	1.55464400	-3.35069500	-3.06454500
H	0.44681800	0.74112800	-2.28167200
C	-2.71252600	4.59697200	1.12660900
H	-2.19084000	5.55176900	1.24518700
H	-3.78118200	4.80883700	1.02085300
H	-2.56789500	4.01171100	2.03976400
C	-2.39092200	4.67393700	-1.38240500
H	-3.45179500	4.89574600	-1.53438800
H	-1.85729500	5.62660700	-1.30970000
H	-2.02202500	4.14098400	-2.26394100
Cl	-1.36759800	-5.45994200	-4.14327000
Cl	1.01920600	-3.85498500	3.84906800

(P)-OCZ-3Cl

C	0.49066300	4.45577700	1.69029000
C	-0.84378500	4.47926900	1.29364700
C	-1.47140000	3.34773600	0.75553600
C	-0.70142400	2.19144100	0.62679300
C	0.64133000	2.13764700	1.03922100
C	1.23309000	3.28113100	1.57202200
C	-2.47710400	0.95986200	-0.32611600
C	-3.36757900	2.03098700	-0.24236700
C	-4.68023600	1.80910900	-0.67982800
H	-5.39922500	2.62047800	-0.62615100
C	-5.08675700	0.57508300	-1.18066600
C	-4.17389800	-0.47554100	-1.27047300
C	-2.86114800	-0.28947100	-0.84333400
H	0.94937700	5.34745700	2.10538100
H	-1.41202200	5.39765500	1.40241500
H	2.26836200	3.23331900	1.89259200
H	-6.10998300	0.43452200	-1.51375700
H	-4.46192700	-1.44106400	-1.67277200
O	-1.17947500	1.03154600	0.08722000
C	-2.93559600	3.38917700	0.31362600
C	1.08880900	-0.30195700	1.45065400
C	2.53566800	0.82009500	0.10374300
C	0.03376800	-0.67195500	2.28445600
C	2.08899800	-1.22712600	1.05968100
C	3.17194800	1.76926500	-0.69381100
C	3.00886500	-0.51356900	0.19779000
C	-0.00981300	-1.99287800	2.72349800
C	2.02699300	-2.54587900	1.52078800
C	4.31238400	1.37742800	-1.39191000
H	2.79261300	2.78203100	-0.77640500
C	4.15617600	-0.89283400	-0.50205800
C	0.97654100	-2.92211600	2.35124600
H	-0.83122200	-2.31437700	3.35620400
H	2.78688700	-3.26481700	1.22743700
C	4.79245400	0.06439100	-1.28338500
H	4.83651200	2.08586400	-2.02341600
H	4.53533800	-1.90728700	-0.45844600
C	-0.71369400	-1.36303900	-1.58886700
C	-2.05101000	-2.55307300	-0.19355100
C	-0.13568200	-0.38006200	-2.39144300
C	-0.07761600	-2.61105100	-1.37371700
C	-3.04331800	-2.96130400	0.69638400
C	-0.92649400	-3.36738200	-0.47927700
C	1.08958500	-0.66007500	-2.98891000
C	1.14725700	-2.88612000	-1.98687200
C	-2.90422900	-4.20742000	1.30263400
H	-3.89239400	-2.32589200	0.92338700
C	-0.80176600	-4.61886200	0.12662500
C	1.70905300	-1.90420000	-2.79152500
H	1.57864100	0.08402600	-3.60668200
H	1.65041800	-3.83548300	-1.84118500
C	-1.79535000	-5.01649600	1.01190600
H	-3.65094300	-4.55911200	2.00559900
H	0.05515900	-5.25502000	-0.06402100
N	1.37836000	0.94315600	0.87789400
N	-1.92416100	-1.34802800	-0.88850800

Cl	6.24148200	-0.38183500	-2.17738900
H	-0.61781800	0.57852800	-2.54439200
H	0.90496300	-3.94547000	2.70502200
H	-0.72888300	0.04163200	2.57560700
C	-3.82013900	3.74759000	1.53171700
H	-3.53731200	4.72058200	1.94518100
H	-4.87572700	3.79921500	1.24740000
H	-3.71336700	2.99626200	2.31996500
C	-3.10643800	4.46180600	-0.78873900
H	-4.14867800	4.51820800	-1.11837200
H	-2.81686400	5.45064000	-0.41964000
H	-2.48464300	4.22459400	-1.65729500
Cl	3.24128600	-2.22413500	-3.59194700
Cl	-1.64989600	-6.57642400	1.81907600

TS-OCZ-3Cl

C	-4.66711500	2.97426900	-0.84624800
C	-3.80985000	3.88649400	-0.22850100
C	-2.58055800	3.47231100	0.28665100
C	-2.24027100	2.11956500	0.19643200
C	-3.02471900	1.22465900	-0.54602800
C	-4.26140600	1.65728700	-1.03630500
C	0.04020200	2.46326100	0.60964200
C	-0.17157900	3.84224200	0.44323100
C	0.85029900	4.62984700	-0.08321600
H	0.70193700	5.69116900	-0.24030700
C	2.05617400	4.03022200	-0.44036400
C	2.28614500	2.69534900	-0.13609200
C	1.32709700	1.88918700	0.50929600
H	-5.62656900	3.30566600	-1.23070100
H	-4.10129600	4.92811700	-0.15704800
H	-4.86712600	0.96004100	-1.60578600
H	2.83410500	4.60771800	-0.92992400
H	3.23963300	2.24987500	-0.38654100
O	-1.07950100	1.66634100	0.80363800
C	-1.53081500	4.38513200	0.90934700
C	-1.38738300	-0.25838400	-1.68537100
C	-3.16074600	-1.28023700	-0.70222200
C	-0.44473400	0.66396000	-2.13455000
C	-1.26835200	-1.64225600	-1.96361300
C	-4.29878100	-1.57803000	0.04610400
C	-2.40599500	-2.29350000	-1.34857800
C	0.65975100	0.17973200	-2.82866300
C	-0.15584000	-2.11855000	-2.66127800
C	-4.68555500	-2.91257000	0.14060100
C	-2.80105500	-3.62937100	-1.24290800
C	0.79760300	-1.19540400	-3.07262200
H	1.42547200	0.86423400	-3.17499900
H	-0.02503800	-3.17563600	-2.86340100
C	-3.93993300	-3.91573900	-0.49917500
H	-5.56286100	-3.18689300	0.71524600
H	-2.23052300	-4.42597800	-1.70682500
C	1.18996000	-0.64826000	1.09023100
C	3.13226500	0.50194400	1.45039600
C	-0.13805000	-1.07136400	1.04693000
C	2.21165400	-1.59693500	1.35464400
C	4.08170000	1.46957900	1.79966600
C	3.43632200	-0.87005600	1.58648700
C	-0.42320300	-2.42730500	1.18646900
C	1.92863900	-2.96056900	1.45615700
C	5.34256900	1.04212100	2.20989300
C	4.70996100	-1.28240700	1.98931200
C	0.60440900	-3.35962400	1.35013400
H	-1.45185000	-2.76320000	1.16808700
H	2.71548400	-3.68349400	1.64072700
C	5.66815700	-0.32079900	2.28667400
H	6.08396300	1.78726300	2.48340400
H	4.93455200	-2.34054800	2.08830300
N	-2.52925200	-0.05102300	-0.90176800
N	1.77358300	0.65029700	1.05124300
Cl	-4.46494900	-5.58709300	-0.34319000
H	-0.94505200	-0.37135300	0.94244100

C	-1.73795600	5.85034900	0.51001000
H	-2.69524100	6.21831600	0.89042400
H	-0.95823000	6.47919000	0.94931000
H	-1.72301000	5.98335200	-0.57639700
C	-1.60619400	4.27745800	2.45546300
H	-0.81849900	4.88506700	2.91339900
H	-2.57817700	4.63866800	2.80872200
H	-1.48223100	3.24434100	2.78930900
Cl	0.19547700	-5.06859600	1.46003200
Cl	2.22776100	-1.76164200	-3.92779800
H	-0.54965100	1.72517300	-1.94400600
H	-4.86069900	-0.79914400	0.55031500
H	3.85076300	2.52668000	1.77254400
H	6.66225600	-0.62215200	2.60244400

(M)-OCZ-5Cl

C	2.05936700	-4.22007100	-2.22306100
C	0.94321500	-4.82840200	-1.65245100
C	-0.02330500	-4.09390700	-0.95149700
C	0.20228700	-2.72439200	-0.81902800
C	1.28689600	-2.08462500	-1.43618600
C	2.21900100	-2.83598700	-2.14010700
C	-1.78557800	-2.37547000	0.39320000
C	-2.19639800	-3.70045300	0.24660800
C	-3.46134200	-4.02984600	0.75336100
H	-3.81989900	-5.04973800	0.65559500
C	-4.26834400	-3.08836100	1.38863300
C	-3.80418200	-1.78534400	1.57940700
C	-2.55231800	-1.42789400	1.09092400
H	2.78927700	-4.81976900	-2.75688000
H	0.81554300	-5.90115700	-1.75983000
H	3.05160200	-2.33003600	-2.61672600
H	-5.24404500	-3.37764800	1.76527100
H	-4.38774400	-1.04794700	2.12064100
O	-0.61179000	-1.89433500	-0.10614200
C	-1.28183700	-4.75429800	-0.38360100
C	0.41818100	0.06804300	-2.22808100
C	1.96297200	0.22608000	-0.57940500
C	-0.49335900	-0.40066900	-3.17258500
C	0.54745800	1.44417100	-1.93295300
C	2.88149500	0.01959500	0.45377900
C	1.54421200	1.55180500	-0.88974100
C	-1.28669500	0.53646700	-3.82719900
C	-0.24391600	2.38006800	-2.60515000
C	3.41061400	1.11430100	1.13029200
C	2.07252500	2.65033500	-0.21177300
C	-1.15366300	1.90404300	-3.54010700
H	-2.01519200	0.21645000	-4.56362600
H	-0.17509100	3.44051900	-2.39429400
C	3.00840100	2.41040700	0.78435000
H	4.10788800	0.95863400	1.94324000
H	1.75607500	3.66001200	-0.44673700
C	-0.88505100	0.03559600	2.19059500
C	-2.23789300	1.03921400	0.67300300
C	-0.22973500	-0.88897800	3.00115900
C	-0.47645300	1.39029000	2.11744200
C	-3.17571800	1.31342600	-0.32059100
C	-1.33868200	2.03121800	1.14613700
C	0.84911900	-0.44093200	3.75727800
C	0.59483100	1.83459800	2.89722200
C	-3.22087900	2.60581000	-0.83681000
H	-3.84185000	0.54203800	-0.69226800
C	-1.39795600	3.32590100	0.62615500
C	1.24087300	0.90515700	3.70258200
H	1.39637500	-1.12944800	4.39071300
H	0.93215600	2.86380800	2.86586600
C	-2.34183300	3.58957900	-0.35881600
H	-3.91924500	2.85568700	-1.62661400
H	-0.72160400	4.10190600	0.96724300
N	1.30908300	-0.66149200	-1.43370000
N	-1.97950100	-0.15623400	1.34441700
Cl	3.67611100	3.76731800	1.67994400

H	-0.54215900	-1.92698900	3.03794600
H	-0.58746800	-1.45950600	-3.38738900
C	-2.03101500	-5.47799700	-1.52669600
H	-1.39888900	-6.24463600	-1.98451000
H	-2.93210200	-5.97361200	-1.15298900
H	-2.32708100	-4.76773400	-2.30460300
C	-0.87857500	-5.77648100	0.70618300
H	-1.76326900	-6.26885700	1.12297300
H	-0.22394700	-6.54912900	0.28977000
H	-0.34532700	-5.27975000	1.52245400
Cl	2.62161000	1.41890100	4.66721200
Cl	-2.20043900	3.04449800	-4.37674600
Cl	-2.41050700	5.20339100	-1.06075200
Cl	3.36342800	-1.59171100	0.95016100

(P)-OCZ-5Cl

C	1.47138400	4.43351600	0.06134300
C	0.09855500	4.62456700	-0.07609300
C	-0.79947500	3.54881300	-0.08874000
C	-0.25886400	2.27116600	0.05226900
C	1.11720300	2.05884200	0.21525500
C	1.98506100	3.14536700	0.20265500
C	-2.35882400	1.21623200	-0.15686700
C	-3.04166900	2.42719900	-0.27551700
C	-4.42669200	2.36251600	-0.47889100
H	-4.99143000	3.28504100	-0.56808200
C	-5.09763700	1.14566500	-0.57092700
C	-4.39038600	-0.05141700	-0.46017500
C	-3.01267400	-0.02322400	-0.25669400
H	2.14056100	5.28765400	0.06240200
H	-0.28599500	5.63487800	-0.17399100
H	3.04846800	2.97060500	0.32598000
H	-6.17179400	1.12847700	-0.72436000
H	-4.89043600	-1.01163400	-0.53013400
O	-1.01313200	1.13338600	0.05192100
C	-2.30910800	3.76913600	-0.20369200
C	1.61121200	-0.24690200	-0.59175400
C	2.22482200	0.22397900	1.54055000
C	1.05452200	-0.21965900	-1.87021600
C	2.31133100	-1.37757900	-0.11249000
C	2.36388100	0.72744200	2.83819800
C	2.71402200	-1.08043200	1.24467800
C	1.20766300	-1.34658300	-2.67156400
C	2.47029100	-2.50129500	-0.92796200
C	3.04666000	-0.02146200	3.79362100
C	3.39696900	-1.83093000	2.20070100
C	1.91592500	-2.46387200	-2.20004800
H	0.76920900	-1.37594700	-3.66218500
H	3.00372900	-3.37975700	-0.58230400
C	3.56786500	-1.27754200	3.46201400
H	3.15862500	0.36755300	4.79793800
H	3.76203900	-2.82676300	1.98020500
C	-2.15291400	-2.11917300	-1.27974500
C	-1.46436700	-1.68233500	0.83903900
C	-2.70537600	-2.04525100	-2.55740800
C	-1.30960500	-3.19150400	-0.89401800
C	-1.22558400	-1.11641900	2.09145800
C	-0.87767700	-2.91635600	0.45993100
C	-2.41724100	-3.07247000	-3.45271400
C	-1.03517800	-4.22108900	-1.79698000
C	-0.40359500	-1.80821900	2.97631900
H	-1.65863700	-0.16340000	2.37224800
C	-0.06194400	-3.60731200	1.35960600
C	-1.59757900	-4.14360000	-3.06515800
H	-2.82634100	-3.05200800	-4.45654000
H	-0.38549500	-5.04723500	-1.53300800
C	0.15460000	-3.04311800	2.60957800
H	-0.18514200	-1.39492200	3.95409800
H	0.38908500	-4.55745800	1.09582800
N	1.59125800	0.73396700	0.40603500
N	-2.25786300	-1.21960000	-0.21478500
Cl	4.42401800	-2.18362900	4.69756700

H	-3.33564000	-1.21322300	-2.85173300
H	0.50809900	0.64473400	-2.22915900
C	-2.79931500	4.54698400	1.04142800
H	-2.29966400	5.51842700	1.11349500
H	-3.87868400	4.72317700	0.98880000
H	-2.58691900	3.98455200	1.95562800
C	-2.61234700	4.58531600	-1.48222300
H	-3.68520800	4.77496600	-1.58188600
H	-2.10704400	5.55531900	-1.45516500
H	-2.27462000	4.04716300	-2.37303200
Cl	-1.27031500	-5.42029400	-4.23007500
Cl	1.15357700	-3.90221600	3.77549000
Cl	1.64267000	2.24675300	3.34393100
Cl	2.09648100	-3.85857000	-3.25472600

TS-OCZ-5CI

C	0.69779700	3.81122700	-1.36820000
C	-0.59446900	4.09963700	-0.93795700
C	-1.26648700	3.19059200	-0.12065300
C	-0.62568900	1.99562100	0.23918300
C	0.75731200	1.81297300	0.03857800
C	1.36423300	2.70161400	-0.86394800
C	-2.72093700	0.94919800	0.28970400
C	-3.44516000	2.14432200	0.22598400
C	-4.79801300	2.08872800	-0.11226900
H	-5.38133100	3.00141400	-0.15142000
C	-5.40800100	0.87053800	-0.41477100
C	-4.64518700	-0.29044400	-0.47543800
C	-3.28271600	-0.25565400	-0.15854200
H	1.21147100	4.47780700	-2.05327700
H	-1.07915800	5.01620600	-1.25161900
H	2.39702600	2.52702700	-1.13995600
H	-6.46404700	0.83836400	-0.66352600
H	-5.07524900	-1.22638100	-0.81637900
O	-1.40864900	0.96569300	0.74214100
C	-2.65825100	3.42392200	0.48280000
C	1.49983700	-0.53408000	0.81519700
C	2.97879000	1.19277300	0.86720300
C	0.40225800	-1.34525300	1.08944300
C	2.79947100	-1.09308100	0.77887800
C	3.62901400	2.39341800	1.18453500
C	3.74531700	0.00322300	0.80037000
C	0.60410000	-2.71548400	1.23322700
C	2.99609800	-2.47222700	0.87404800
C	5.02056000	2.42234300	1.26675700
C	5.13623000	0.01929500	0.89650000
C	1.87821900	-3.26947800	1.07790600
H	-0.23252500	-3.36098200	1.46532600
H	3.98872700	-2.90610200	0.82895600
C	5.75710700	1.24578400	1.09471300
H	5.52280800	3.35238900	1.50143100
H	5.71623700	-0.89480100	0.84400900
C	-1.45067700	-1.41083800	-1.37530100
C	-2.71327000	-2.69529800	0.00725400
C	-0.87337500	-0.35626900	-2.07955300
C	-1.00123000	-2.74481700	-1.53189200
C	-3.60997800	-3.16305800	0.96736500
C	-1.81651000	-3.56750700	-0.66283200
C	0.21514500	-0.63958300	-2.89863300
C	0.09335500	-3.01951300	-2.35526300
C	-3.60625200	-4.52574000	1.25405600
H	-4.28355500	-2.48833500	1.48465900
C	-1.81577700	-4.93186500	-0.36107100
C	0.69363700	-1.95397500	-3.01435100
H	0.70633500	0.15906600	-3.44247000
H	0.48114000	-4.02615900	-2.46341500
C	-2.71691700	-5.38869600	0.59372600
H	-4.28674800	-4.92901100	1.99529000
H	-1.12499000	-5.61620400	-0.84049900
N	1.60063500	0.88866300	0.73837800
N	-2.47271600	-1.38637700	-0.41671400
Cl	7.50783500	1.32405500	1.20333300

H	-1.23934700	0.65902500	-1.98981900
H	-0.58086500	-0.92759700	1.22218900
C	-2.50304200	3.63760400	2.01194600
H	-1.88546700	4.52045700	2.20756400
H	-3.48658100	3.78734500	2.47055400
H	-2.02980500	2.77533600	2.48826500
C	-3.35063900	4.65320500	-0.11636400
H	-4.32016400	4.81842400	0.36224400
H	-2.75159800	5.55096900	0.06116600
H	-3.51000200	4.54704900	-1.19412600
Cl	2.10125300	-2.25423400	-4.02661200
Cl	-2.74454200	-7.10021200	0.99763000
Cl	2.76023300	3.85583900	1.60150100
Cl	2.06290900	-5.01509900	1.18843100

(M)-OCZ-6Cl

C	-3.66813400	3.14001700	-3.58868700
C	-2.52810200	3.93638900	-3.52188800
C	-1.24032500	3.38457100	-3.47747400
C	-1.14376900	1.99424900	-3.50414800
C	-2.27913600	1.17558100	-3.56495100
C	-3.54397000	1.75039700	-3.61112800
C	1.20527500	2.02199900	-3.38839900
C	1.26705600	3.41451800	-3.37659100
C	2.54062900	3.99694500	-3.31632600
H	2.62472100	5.07914600	-3.30402000
C	3.70024800	3.22780100	-3.27103200
C	3.61087600	1.83542700	-3.28734200
C	2.36081700	1.23064200	-3.35005200
H	-4.65093900	3.59886800	-3.61967300
H	-2.63928000	5.01606800	-3.50431400
H	-4.41352100	1.10361200	-3.66198600
H	4.67127600	3.71005000	-3.22688300
H	4.49635800	1.20943400	-3.25425200
O	0.03935100	1.31928800	-3.45575200
C	0.00246900	4.27284600	-3.41546200
C	-1.68385200	-1.14674100	-2.70728700
C	-2.31617700	-0.91467900	-4.87223700
C	-1.30131100	-0.99474400	-1.36891600
C	-1.66769600	-2.44607200	-3.29146300
C	-2.66628400	-0.40446700	-6.12183700
C	-2.06852700	-2.29201700	-4.67215400
C	-0.92735000	-2.11372100	-0.63060500
C	-1.30640200	-3.56965800	-2.54757900
C	-2.78439900	-1.30279300	-7.17783600
C	-2.20841500	-3.18953800	-5.73427900
C	-0.94580900	-3.38345500	-1.22145500
H	-0.61783600	-1.99686700	0.40003900
H	-1.30474100	-4.55868400	-2.99092800
C	-2.56412000	-2.67523000	-6.97410300
H	-3.04953400	-0.94873200	-8.16761200
H	-2.02283900	-4.24957700	-5.61046800
C	2.45149000	-0.89494400	-2.10345700
C	1.82496200	-1.08030900	-4.27458700
C	2.78873800	-0.41243500	-0.83939800
C	2.23966200	-2.27185800	-2.34365500
C	1.43869500	-0.89944200	-5.60827700
C	1.84253900	-2.39603300	-3.72842700
C	2.93060600	-1.33778400	0.19001600
C	2.40329800	-3.19600000	-1.30809700
C	1.09350700	-2.00574000	-6.37897500
C	1.51004400	-3.50646800	-4.50479000
C	2.74602700	-2.70896700	-0.05368900
H	3.18688300	-1.00591400	1.18976700
H	2.24526000	-4.25643800	-1.46281900
C	1.14448000	-3.29118100	-5.82514600
H	0.78108600	-1.86703600	-7.40602600
H	1.53393300	-4.50764000	-4.09029600
N	-2.11700200	-0.23260600	-3.66846700
N	2.23415900	-0.18355600	-3.28688300
Cl	-2.73738000	-3.76787300	-8.34150700
H	2.92751700	0.64764600	-0.66004500

C	0.04243500	5.17862900	-4.66926100
H	-0.84957000	5.81073300	-4.72249200
H	0.91764800	5.83557500	-4.64818600
H	0.08977800	4.57311600	-5.57934900
C	-0.05967200	5.14432000	-2.13852800
H	0.81622400	5.79698800	-2.06862600
H	-0.95105000	5.77948100	-2.14274000
H	-0.09148500	4.51438100	-1.24449200
Cl	0.72917400	-4.66303100	-6.84079800
Cl	-0.49519100	-4.77314400	-0.24588600
Cl	1.38739200	0.68245000	-6.36590800
Cl	2.94828900	-3.83613000	1.28133100
Cl	-1.28952100	0.56542100	-0.56599600
H	-2.83262500	0.65642500	-6.27024800

(P)-OCZ-6Cl

C	-3.65486000	3.15609700	-3.64019700
C	-2.51710400	3.95431900	-3.54399300
C	-1.22955300	3.40359200	-3.48805400
C	-1.13657600	2.01326600	-3.53232800
C	-2.26544300	1.19405800	-3.66853300
C	-3.53076200	1.76851900	-3.70319000
C	1.21396700	2.03244900	-3.36702500
C	1.28178100	3.42490400	-3.37581600
C	2.55917900	3.99723900	-3.30577700
H	2.65365600	5.07868800	-3.31048900
C	3.71122300	3.21752700	-3.22994900
C	3.61225700	1.82676900	-3.20245900
C	2.35752700	1.23058400	-3.25177000
H	-4.63750000	3.61493500	-3.67509000
H	-2.63115900	5.03340100	-3.51163000
H	-4.39891300	1.12605500	-3.80388000
H	4.68542400	3.69301300	-3.18329800
H	4.49193800	1.19776200	-3.11822300
O	0.04490700	1.33635700	-3.45830500
C	0.01820400	4.28714200	-3.42061800
C	-1.67028500	-1.04627300	-2.75134700
C	-2.29696400	-0.98976000	-4.92982600
C	-1.28106300	-0.71524400	-1.45360600
C	-1.68818200	-2.38639400	-3.20237700
C	-2.59434800	-0.65182500	-6.25458400
C	-2.09642700	-2.35858400	-4.58986300
C	-0.91915400	-1.75150300	-0.59856800
C	-1.33366900	-3.42187500	-2.33331500
C	-2.76989000	-1.66284100	-7.19592900
C	-2.27064900	-3.37122300	-5.53301500
C	-0.96044000	-3.08453700	-1.03945500
H	-0.59562300	-1.53634000	0.41309300
H	-1.34567000	-4.45788700	-2.65320600
C	-2.62714700	-3.00485500	-6.82340100
H	-3.00820900	-1.40398800	-8.22001800
H	-2.11642000	-4.41265600	-5.27713400
C	2.42886000	-0.98394700	-2.04690400
C	1.80251800	-0.99587800	-4.22618500
C	2.72058400	-0.67481300	-0.71389200
C	2.25278800	-2.34699100	-2.42182500
C	1.40652600	-0.63876000	-5.51493800
C	1.84468100	-2.34658000	-3.80962500
C	2.91430700	-1.70629500	0.20131800
C	2.44529100	-3.38019100	-1.50489100
C	1.06276400	-1.65913000	-6.39617900
C	1.50836700	-3.36566800	-4.70489900
C	2.79541200	-3.04067400	-0.20544300
H	3.14819900	-1.46950900	1.23174700
H	2.30960900	-4.41731000	-1.78741000
C	1.12842800	-3.00206500	-5.98965300
H	0.73466100	-1.42396200	-7.40189600
H	1.53911200	-4.40914600	-4.41164700
N	-2.07775000	-0.20884300	-3.79403900
N	2.19531300	-0.17824600	-3.16235100
Cl	-2.88620400	-4.24376100	-8.03933300
C	0.06110500	5.19359200	-4.67375900

H	-0.82538300	5.83365300	-4.72251400
H	0.94244000	5.84246700	-4.65503500
H	0.09780200	4.58950300	-5.58527400
C	-0.04080700	5.15987700	-2.14442700
H	0.83392500	5.81445900	-2.07896000
H	-0.93380100	5.79287900	-2.14651400
H	-0.06624800	4.53182400	-1.24886300
Cl	0.71416100	-4.25863000	-7.14669100
Cl	-0.52355800	-4.36264400	0.08520100
Cl	3.07665300	-4.30545600	0.97848700
Cl	2.79185200	0.97646300	-0.12011500
Cl	-2.69512900	1.01257600	-6.80592100
H	1.35706000	0.39951700	-5.82245800
H	-1.25057600	0.31551900	-1.11948500

cis-OCZ-6Cl

C	-3.64721200	3.10230000	-3.55160800
C	-2.51804100	3.90890400	-3.43238600
C	-1.22422500	3.37156800	-3.40163600
C	-1.11151600	1.98458700	-3.49411600
C	-2.23264700	1.16015200	-3.65628500
C	-3.50506800	1.72032500	-3.66571900
C	1.23932700	2.03536800	-3.36378500
C	1.28499000	3.42736100	-3.31234700
C	2.55287600	4.02185100	-3.24462200
H	2.62581200	5.10412700	-3.20307300
C	3.72054800	3.26383600	-3.22838500
C	3.64660900	1.87104100	-3.27967000
C	2.40312500	1.25391300	-3.34959300
H	-4.63541200	3.55014300	-3.56638000
H	-2.64352900	4.98489400	-3.36232500
H	-4.36489200	1.07037600	-3.78811300
H	4.68674100	3.75519100	-3.17875400
H	4.53932600	1.25465400	-3.26778000
O	0.08049700	1.32182700	-3.44397200
C	0.00948700	4.27119200	-3.31400500
C	-1.67105300	-1.12144500	-2.82351200
C	-2.28477100	-0.96859700	-5.00086300
C	-1.27212800	-0.84789100	-1.51521900
C	-1.73806200	-2.44413400	-3.31897600
C	-2.55906100	-0.57154300	-6.31458100
C	-2.13775400	-2.35427900	-4.70627600
C	-0.94187800	-1.92353000	-0.69743500
C	-1.41407600	-3.51976200	-2.48732300
C	-2.74804300	-1.54289600	-7.29453600
C	-2.33478900	-3.32669200	-5.68642000
C	-1.02350400	-3.23825800	-1.18535000
H	-0.60524200	-1.75456800	0.31870500
H	-1.45850000	-4.54306100	-2.84324500
C	-2.65010800	-2.90152100	-6.96926200
H	-2.96307700	-1.24000500	-8.31169000
H	-2.22077700	-4.38091600	-5.46583700
C	2.50640900	-0.88476500	-2.12986600
C	1.82245600	-1.04246900	-4.28611900
C	2.89814200	-0.42015800	-0.87486500
C	2.23062000	-2.25127600	-2.36474500
C	1.42255300	-0.84573000	-5.61324300
C	1.80210400	-2.35841900	-3.74164100
C	3.02609800	-1.35237100	0.15070000
C	2.37467000	-3.18222500	-1.33264400
C	1.03365100	-1.93975300	-6.38160700
C	1.42754100	-3.45666600	-4.51600700
C	2.77106500	-2.71296600	-0.08702500
H	3.32717500	-1.03410500	1.14243500
H	2.16251000	-4.23398600	-1.48264300
C	1.05590100	-3.22804100	-5.83246200
H	0.71525500	-1.78872400	-7.40515000
H	1.42744800	-4.45913900	-4.10411800
N	-2.03869700	-0.23529700	-3.83928500
N	2.28965600	-0.16242800	-3.30787300
Cl	-2.90872200	-4.08769500	-8.23771800
H	3.09388800	0.63181300	-0.69964500

H	-1.20835900	0.16976600	-1.14738200
C	0.02906700	5.21492500	-4.54046100
H	-0.86909400	5.83985700	-4.56592600
H	0.89874200	5.87877900	-4.50776600
H	0.07177100	4.63675500	-5.46820100
C	-0.05223800	5.10377700	-2.01174500
H	0.81497600	5.76665300	-1.93081500
H	-0.95236800	5.72608900	-1.98939800
H	-0.06628900	4.44909900	-1.13498700
Cl	0.60827200	-4.58664000	-6.85161300
Cl	-2.62290300	1.11285200	-6.79971500
Cl	-0.60314000	-4.56681600	-0.11198100
Cl	1.41280200	0.73790100	-6.36570900
Cl	2.95733200	-3.84939500	1.24198200

TS1-OCZ-6Cl

C	-2.71803600	2.94880800	-2.27460800
C	-1.68530500	3.79702500	-2.66505600
C	-0.63651100	3.29509400	-3.43560100
C	-0.64076600	1.93753400	-3.79055500
C	-1.78950200	1.13769600	-3.62826900
C	-2.77599800	1.65305900	-2.77172400
C	1.69671500	1.96434500	-3.72221000
C	1.79086400	3.35788900	-3.64120800
C	2.98835100	3.92083700	-3.19889200
H	3.08768300	4.99866700	-3.14131300
C	4.05743600	3.11129100	-2.81063500
C	3.90479000	1.73041500	-2.77841100
C	2.71140600	1.14618500	-3.21131200
H	-3.51021500	3.30854900	-1.62606600
H	-1.68954900	4.83538400	-2.35639600
H	-3.62266500	1.02366500	-2.52608000
H	4.98798900	3.56132400	-2.47983300
H	4.68735200	1.08746700	-2.38984400
O	0.54829300	1.38453300	-4.24603700
C	0.52565900	4.13649100	-3.98117000
C	-1.32578800	-1.29591700	-4.34800300
C	-3.43238500	-0.45575000	-4.50778800
C	0.03411600	-1.50679500	-4.55948300
C	-2.21739800	-2.39471900	-4.33595000
C	-4.55117900	0.30071300	-4.88374400
C	-3.56181200	-1.86431700	-4.42631200
C	0.49855900	-2.81531600	-4.66389900
C	-1.74601600	-3.70835300	-4.39068900
C	-5.79192200	-0.32207300	-5.01235800
C	-4.79565800	-2.49813400	-4.56827800
C	-0.37799300	-3.89682500	-4.53114500
H	1.54585200	-3.00202200	-4.85966400
H	-2.42452000	-4.55373100	-4.36506200
C	-5.90524400	-1.70383600	-4.82675400
H	-6.65761300	0.26453000	-5.29307200
H	-4.88710200	-3.57626200	-4.50475900
C	1.57046900	-0.64390500	-1.96896700
C	3.24178200	-1.33216000	-3.33958800
C	0.59949300	0.09784500	-1.29814200
C	1.75611400	-2.02180400	-1.71851200
C	4.19531500	-1.49221600	-4.35058900
C	2.83477700	-2.46341100	-2.57558800
C	-0.23176100	-0.57527300	-0.40872200
C	0.91640900	-2.69186600	-0.82481900
C	4.76692300	-2.74518400	-4.55879500
C	3.39838600	-3.72116200	-2.79101300
C	-0.07492000	-1.95351700	-0.19155100
H	-1.01385300	-0.03714400	0.11429300
H	1.01945800	-3.75491700	-0.63867000
C	4.36902200	-3.83824300	-3.77740400
H	5.50674500	-2.87297700	-5.33908000
H	3.07336100	-4.58819900	-2.22815700
N	-2.07794700	-0.08247900	-4.32442500
N	2.46682200	-0.23232000	-2.96856600
Cl	-7.48556200	-2.45004000	-4.99551500
H	0.47572000	1.16079100	-1.46366000

H	0.71300100	-0.68051200	-4.67922100
C	0.37972300	4.24441600	-5.52212900
H	-0.56017000	4.74541400	-5.77661300
H	1.21127800	4.82481300	-5.93633300
H	0.38210400	3.25823500	-5.99271500
C	0.54484300	5.55036100	-3.39023100
H	1.36009200	6.13560800	-3.82533700
H	-0.38550400	6.07439100	-3.62758200
H	0.67044400	5.53707000	-2.30285700
Cl	5.10624800	-5.40109800	-4.08433100
Cl	-4.44326000	1.99397300	-5.31680300
Cl	0.27502700	-5.52859400	-4.59419900
Cl	4.65024500	-0.17640900	-5.41484100
Cl	-1.17304500	-2.76422300	0.91762900

TS2-OCZ-6Cl

C	0.30000700	-3.86304600	-1.28220500
C	-1.02969600	-4.06883000	-0.92438500
C	-1.67009600	-3.14760700	-0.09556400
C	-0.95923000	-2.02284900	0.34999000
C	0.44053600	-1.93515600	0.21364200
C	1.02223000	-2.82920300	-0.69993300
C	-2.96258700	-0.81612500	0.34085900
C	-3.77269800	-1.94385400	0.16968700
C	-5.08228700	-1.76259500	-0.27605500
H	-5.73170300	-2.62118200	-0.40252300
C	-5.56310400	-0.48766300	-0.58009600
C	-4.70815800	0.60653000	-0.52517600
C	-3.39082300	0.44611700	-0.08734500
H	0.79474700	-4.53800200	-1.97302300
H	-1.56648300	-4.93035800	-1.30265800
H	2.07693600	-2.72221300	-0.92243500
H	-6.58757300	-0.35844800	-0.91424300
H	-5.03232100	1.58981700	-0.84896200
O	-1.68736100	-0.96238000	0.87157200
C	-3.10802100	-3.29186300	0.42202500
C	1.31429900	0.32206000	1.10593000
C	2.66131000	-1.50867900	1.16129100
C	0.26501100	1.20104500	1.36063800
C	2.65052300	0.78592100	1.14847300
C	3.20884300	-2.76441800	1.45896400
C	3.51341100	-0.37672700	1.17274000
C	0.55623800	2.54754600	1.56297000
C	2.93937000	2.14382700	1.30191800
C	4.58933800	-2.89744800	1.60160600
C	4.89361600	-0.49774200	1.32983100
C	1.87262100	3.01300400	1.48446700
H	-0.23944300	3.24290700	1.79394900
H	3.96131000	2.50583800	1.31846000
C	5.41530100	-1.77242200	1.50844400
H	5.01249600	-3.86947100	1.82167400
H	5.53936000	0.37272500	1.33774400
C	-2.54166500	2.81834900	0.21602500
C	-1.46580100	1.45244600	-1.24083400
C	-3.27974900	3.38418800	1.26100200
C	-1.59306200	3.61770900	-0.48411800
C	-1.02149300	0.36006700	-1.98398400
C	-0.89771500	2.73648300	-1.39684400
C	-3.11042200	4.73279500	1.56528500
C	-1.41459300	4.96574200	-0.17267500
C	0.04852000	0.55698800	-2.85084600
H	-1.47579000	-0.61841800	-1.89050500
C	0.17798400	2.92663800	-2.26832000
C	-2.18958600	5.50581700	0.84542500
H	-3.68112200	5.17518000	2.37219700
H	-0.67679400	5.57012900	-0.68705900
C	0.64066900	1.82399700	-2.97473600
H	0.43720200	-0.27366800	-3.42855300
H	0.65011500	3.89579900	-2.38306500
N	1.31625200	-1.10046400	0.98381500
N	-2.45583900	1.50426100	-0.24618700
Cl	7.14881300	-1.98209000	1.69217400

H	-0.74862400	0.84865800	1.44033900
C	-3.85794600	-4.43944100	-0.26307000
H	-3.34401100	-5.38870700	-0.08629700
H	-4.86480900	-4.54019100	0.15229500
H	-3.94312100	-4.28440500	-1.34336400
C	-3.06052700	-3.57064800	1.94765800
H	-4.07827800	-3.65677900	2.34349900
H	-2.52686800	-4.50683300	2.14238700
H	-2.55104600	-2.76646800	2.48409000
Cl	-1.99963500	7.19747200	1.27253300
Cl	-4.36887500	2.43222500	2.25017900
Cl	2.01209400	2.01307300	-4.05952700
Cl	2.21960900	-4.17381200	1.77727800
Cl	2.17401000	4.73553500	1.67182800

(M)-OCZ-7Cl

C	-3.45264300	3.07214600	-2.33695300
C	-3.02254400	3.92405000	-1.32118300
C	-2.07574400	3.52448400	-0.36845400
C	-1.55430400	2.24055400	-0.50359000
C	-2.03363400	1.34598900	-1.46614400
C	-2.97572500	1.76285000	-2.39535400
C	-0.17598400	2.45435700	1.39032200
C	-0.70042100	3.70088100	1.72481600
C	-0.21977900	4.29266400	2.90082400
H	-0.60786500	5.26151300	3.19960800
C	0.75257700	3.68224800	3.69076000
C	1.31777400	2.47147100	3.28753400
C	0.86522800	1.86786800	2.12152700
H	-4.18421600	3.41731700	-3.06006200
H	-3.44069200	4.92415100	-1.26093400
H	-3.33820900	1.05715000	-3.13493900
H	1.09756300	4.16807900	4.59757700
H	2.12665000	2.00813200	3.84255000
O	-0.58307500	1.73154400	0.30822100
C	-1.68274800	4.42639700	0.80286500
C	-0.54973000	-0.62566500	-2.03383900
C	-2.13740400	-0.92109800	-0.44095000
C	0.35925500	-0.14264100	-2.98371900
C	-0.43373300	-1.96552600	-1.57889000
C	-3.15909700	-0.80550300	0.51237600
C	-1.43388800	-2.15017500	-0.55326200
C	1.31736300	-1.00393200	-3.50913300
C	0.52821900	-2.83071100	-2.10143200
C	-3.45313400	-1.89403600	1.32852100
C	-1.73805000	-3.24673000	0.25458500
C	1.38260800	-2.33432600	-3.07398800
H	2.03099000	-0.63355900	-4.23395000
H	0.61093900	-3.85483300	-1.75647400
C	-2.74694900	-3.09496800	1.19312400
H	-4.23661800	-1.80504300	2.07063500
H	-1.19248600	-4.17884500	0.17359900
C	1.16076900	-0.60757200	1.94381500
C	2.32065500	0.66580100	0.46991500
C	0.29090900	-1.06380300	2.93386600
C	1.85735400	-1.50095200	1.09571200
C	2.87758400	1.68098200	-0.31702700
C	2.59844700	-0.69410700	0.15162300
C	0.14291200	-2.43951400	3.08541900
C	1.71233100	-2.88019800	1.26278000
C	3.68941500	1.34087200	-1.39532000
C	3.43411100	-1.03397800	-0.91262600
C	0.85724600	-3.32516500	2.26193800
H	-0.53500900	-2.83841900	3.83097500
H	2.23879300	-3.58473700	0.62865900
C	3.96193400	-0.00273900	-1.67587000
H	4.10988400	2.12344500	-2.01406200
H	3.64849800	-2.06751100	-1.15549100
N	-1.61960400	-0.01639800	-1.37568200
N	1.48586600	0.70327600	1.58978200
Cl	-3.14867100	-4.42544900	2.26559000
H	-0.26005600	-0.37015300	3.55976700

C	-0.99768600	5.70361500	0.26122500
H	-1.66849300	6.24705800	-0.41236700
H	-0.72341800	6.37569100	1.08080400
H	-0.08904800	5.44570100	-0.29106700
C	-2.95740300	4.80174000	1.59396400
H	-2.71379700	5.44544500	2.44494700
H	-3.66583400	5.34401000	0.96043800
H	-3.45285200	3.90229000	1.97182000
Cl	0.63626100	-5.05745400	2.48157200
Cl	2.61972100	-3.38369500	-3.74785900
Cl	4.98053100	-0.37823900	-3.05758200
Cl	-4.11019000	0.65252500	0.74645400
Cl	0.36510600	1.52833100	-3.50924000
Cl	2.60574600	3.38788600	-0.00772900

(P)-OCZ-7Cl

C	-4.34666100	3.16007100	0.41237900
C	-3.29085400	4.06063200	0.54149600
C	-1.95258300	3.64855600	0.48509400
C	-1.72314400	2.28436200	0.32739200
C	-2.76814700	1.37911200	0.11559100
C	-4.08519700	1.81160800	0.17060100
C	0.61501400	2.53934100	0.32720500
C	0.53901300	3.93012100	0.35578900
C	1.75255300	4.62935200	0.30564400
H	1.73617100	5.71472400	0.32044300
C	2.98115100	3.97366100	0.25296600
C	3.02927600	2.57984100	0.30657200
C	1.84125300	1.86297500	0.36538900
H	-5.37074500	3.51452300	0.46572400
H	-3.51219100	5.11423300	0.68141900
H	-4.88435300	1.09753400	0.00367300
H	3.90060600	4.54824400	0.21027300
H	3.97182200	2.04362800	0.33991700
O	-0.47872200	1.72525300	0.31586900
C	-0.79886200	4.65189200	0.53027800
C	-2.03542200	-0.29901700	-1.57295800
C	-2.26477400	-1.06380200	0.55018100
C	-1.94152900	0.44441900	-2.75806300
C	-1.68003000	-1.67437800	-1.59065200
C	-2.42398000	-1.23314900	1.93141500
C	-1.84095800	-2.16369600	-0.24116500
C	-1.49847400	-0.18178100	-3.91954000
C	-1.24964200	-2.30638900	-2.75808000
C	-2.22515300	-2.49155000	2.49058700
C	-1.63714700	-3.42603900	0.31737100
C	-1.16065000	-1.54014200	-3.90993300
H	-1.41818200	0.39169300	-4.83451700
H	-0.96950300	-3.35257900	-2.76572000
C	-1.84842300	-3.57071800	1.67998200
H	-2.33403600	-2.62645500	3.55911800
H	-1.31855000	-4.26540700	-0.28978000
C	1.89219200	-0.48902100	-0.47860800
C	1.48584900	-0.20854300	1.73388000
C	2.10694000	-0.29117000	-1.84236400
C	1.67726800	-1.77925900	0.06142800
C	1.22838500	0.26082000	3.02749100
C	1.41592000	-1.60677300	1.47329500
C	2.13067000	-1.41295300	-2.66607300
C	1.71513800	-2.90071300	-0.77053900
C	0.90800600	-0.64794400	4.03195100
C	1.12174000	-2.51976100	2.48641700
C	1.94675700	-2.69555700	-2.12392700
H	2.27814600	-1.30475900	-3.73431500
H	1.55826100	-3.89984000	-0.37967500
C	0.86463000	-2.01883100	3.75432600
H	0.69450600	-0.28651400	5.02987500
H	1.06991400	-3.58385700	2.29102900
N	-2.43050400	0.04934200	-0.27580600
N	1.82444700	0.45238800	0.55028400
Cl	-1.58755900	-5.13840600	2.42836200
H	2.24160100	0.70471100	-2.25045500

C	-0.98661700	5.68231100	-0.60720100
H	-1.92751200	6.22826500	-0.48960200
H	-0.17547800	6.41703700	-0.60697500
H	-0.99895300	5.18153500	-1.57997900
C	-0.79520200	5.36833600	1.90181900
H	0.01194200	6.10629300	1.95331400
H	-1.74325200	5.89035400	2.06857400
H	-0.65258500	4.64528600	2.71057100
Cl	1.97866000	-4.08740700	-3.20078100
Cl	-0.58879700	-2.26889500	-5.40111700
Cl	0.44083800	-3.12202000	5.05469400
Cl	-2.82395100	0.09763000	2.99792700
Cl	-2.35390100	2.14793800	-2.87214300
Cl	1.29326000	1.96197400	3.45751900

TS-OCZ-7Cl

C	-4.34780900	2.89787500	-0.91957100
C	-3.54176200	3.69113100	-0.10581100
C	-2.29935000	3.23830100	0.34201900
C	-1.85544600	1.97106200	-0.04934700
C	-2.65508500	1.17730300	-0.87613500
C	-3.89958400	1.63945700	-1.30163100
C	0.39542800	2.42569100	0.49379000
C	0.04262300	3.76308800	0.76108200
C	0.99813500	4.76910800	0.65629100
H	0.72837000	5.80234400	0.83467500
C	2.30374000	4.43424800	0.32230700
C	2.66778200	3.10123800	0.20962800
C	1.75479300	2.04711300	0.35948600
H	-5.31462600	3.25997400	-1.25374100
H	-3.88883300	4.67506700	0.18716100
H	-4.49723300	0.99753300	-1.94099500
H	3.05845500	5.20372100	0.19385900
H	3.69575800	2.87257700	-0.00013600
O	-0.62914700	1.49253100	0.36438500
C	-1.37899500	4.01714700	1.26337100
C	-1.64058500	-0.36478400	-2.56229700
C	-2.80690900	-1.30513600	-0.86431400
C	-0.90877800	0.46522000	-3.42159000
C	-1.82013600	-1.73333400	-2.89697700
C	-3.43947600	-1.61233800	0.34701800
C	-2.56495400	-2.33384900	-1.81103300
C	-0.39357200	-0.06636900	-4.60082600
C	-1.29534900	-2.26929700	-4.07454400
C	-3.84103200	-2.92246500	0.58691200
C	-2.96242900	-3.65113200	-1.56872600
C	-0.59348900	-1.41717900	-4.91511900
H	0.17444400	0.56950900	-5.26829900
H	-1.42712000	-3.31486300	-4.32800100
C	-3.60365700	-3.92143400	-0.36781500
H	-4.31241900	-3.17227100	1.52884700
H	-2.76546200	-4.44256900	-2.28261400
C	1.42591500	-0.37527500	0.88854900
C	3.40917800	0.58948100	1.40749900
C	0.47731500	-1.03643100	0.12253000
C	1.79331900	-0.86700800	2.15585700
C	4.74923600	0.96867100	1.29170300
C	3.04851400	-0.22210000	2.51367400
C	-0.16331400	-2.14495200	0.67514600
C	1.12356200	-1.94571100	2.73436600
C	5.62414600	0.77170900	2.36650600
C	3.91053200	-0.44843500	3.58139400
C	0.12896900	-2.55672700	1.97937500
H	-0.87085500	-2.71536000	0.09229100
H	1.39866100	-2.33251700	3.70920200
C	5.18384500	0.10967100	3.51140200
H	6.65627200	1.08673800	2.27972000
H	3.62101300	-1.06795100	4.42236500
N	-2.23455400	-0.11462000	-1.31999500
N	2.29562200	0.70018600	0.49214400
Cl	-4.11263700	-5.56111900	-0.00905900
H	0.26448700	-0.72038200	-0.88818600

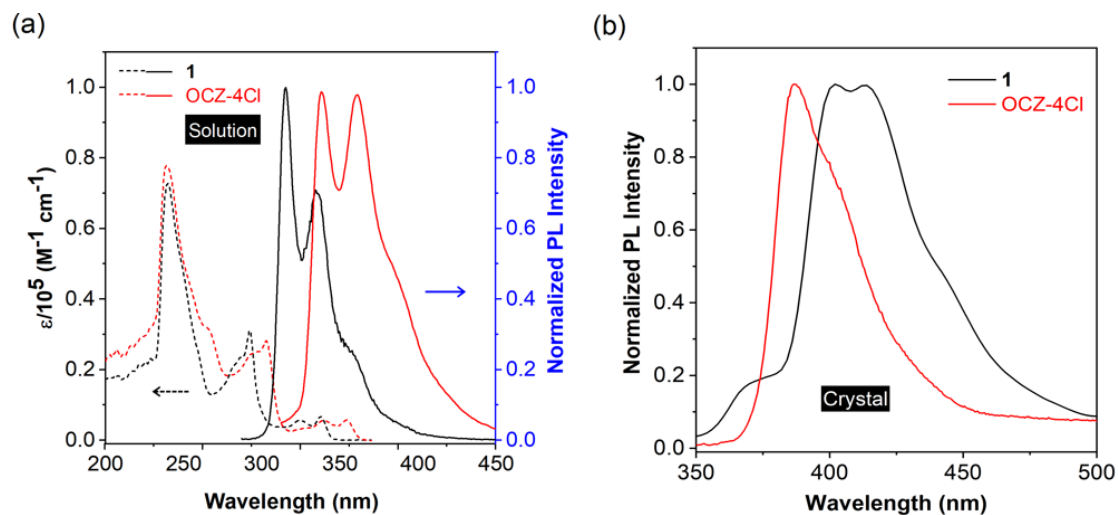
C	-1.72904200	5.50825000	1.31590200
H	-2.74096600	5.64812000	1.70677100
H	-1.05315800	6.03645900	1.99396400
H	-1.67006700	5.97740100	0.32851700
C	-1.50364400	3.43248600	2.69732900
H	-0.80256900	3.93737900	3.37052400
H	-2.52200200	3.57780500	3.07433900
H	-1.28348000	2.36180700	2.71020000
Cl	-0.74315000	-3.93028100	2.64432300
Cl	0.08272600	-2.04005900	-6.41029900
Cl	6.30221500	-0.11748900	4.84352900
Cl	-3.66753700	-0.42924300	1.61401800
Cl	-0.57594900	2.14411200	-3.05644900
Cl	5.48366900	1.48424000	-0.22039500

S8 – Supplementary photophysical data

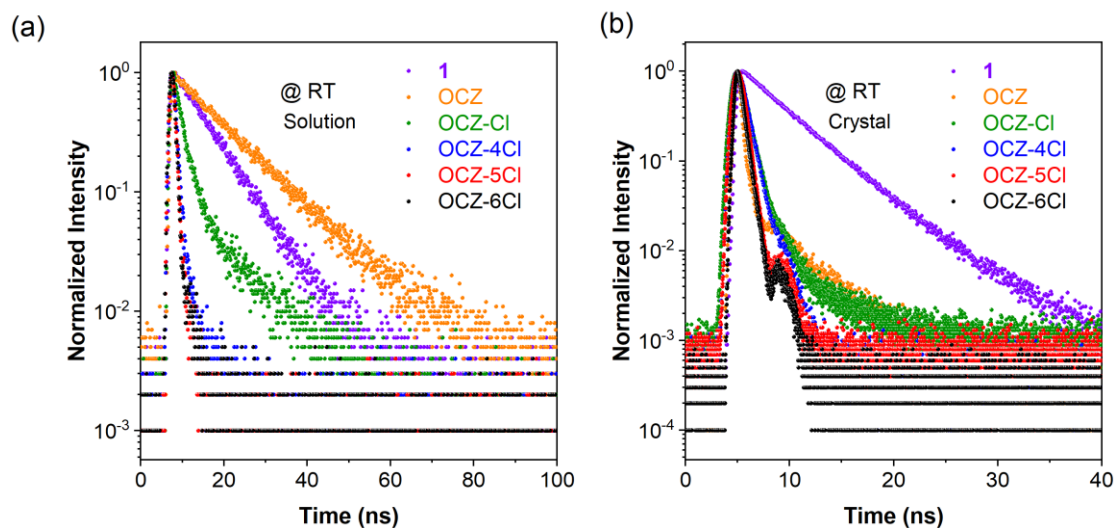
Supplementary Table 4. Photophysical Properties of **1**, OCZ, OCZ-1Cl, OCZ-4Cl, OCZ-5Cl and OCZ-6Cl

Compound	Type	λ_{abs} (nm)	λ_{em} (nm)	Half- width	Φ_{F} (%)	$\langle\tau\rangle$ (ns)	k_{f}^a (s ⁻¹)	k_{nr}^b (s ⁻¹)
1	Solution	337	358	25	40.88	7.45	5.49×10^7	7.93×10^7
	Crystal	-	414	50	18.28	4.32	4.23×10^7	1.89×10^8
OCZ	Solution	337	360	48	14.76	11.94	1.24×10^7	7.14×10^7
	Crystal	-	376	32	16.86	0.97	1.74×10^8	8.57×10^8
OCZ-1Cl	Solution	337	370	46	2.40	4.53	5.30×10^6	2.15×10^8
	Crystal	-	386	24	1.48	0.89	1.66×10^7	1.11×10^9
OCZ-4Cl	Solution	354	379	42	0.72	0.91	7.91×10^6	1.09×10^9
	Crystal	-	387	34	0.46	0.71	6.48×10^6	1.42×10^9
OCZ-5Cl	Solution	356	383	44	0.34	0.50	6.80×10^6	2.00×10^9
	Crystal	-	394	28	0.23	0.43	5.35×10^6	2.32×10^9
OCZ-6Cl	Solution	357	383	46	0.31	0.48	6.46×10^6	2.08×10^9
	Crystal	-	399	28	0.22	0.35	6.29×10^6	2.85×10^9

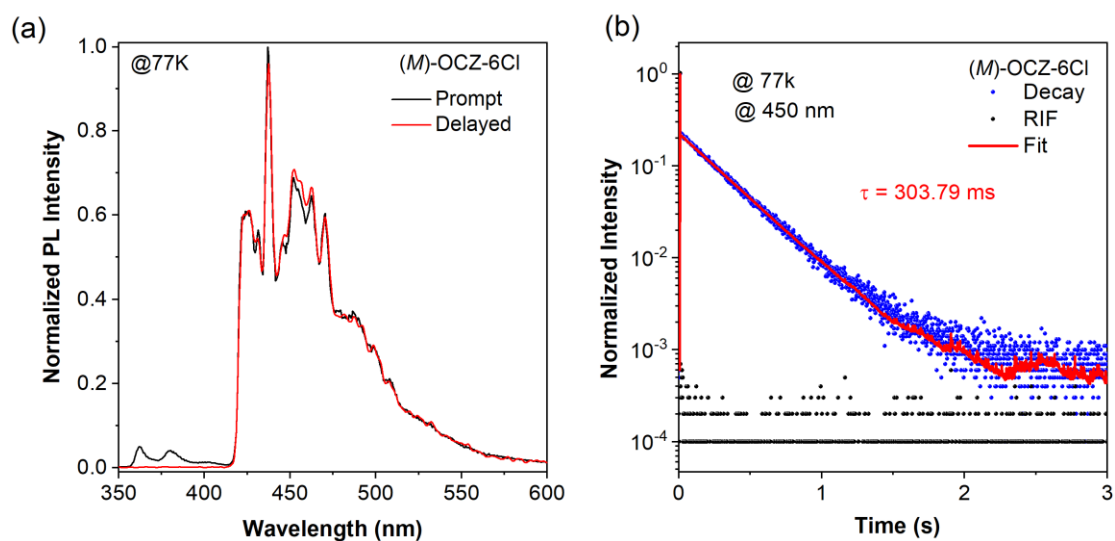
^a Radiative rate constant k_{f} obtained from the equation: $k_{\text{f}} = \Phi_{\text{F}}/\langle\tau\rangle$. ^b Non-radiative rate constant k_{nr} obtained from the equation: $k_{\text{nr}} = (1-\Phi_{\text{F}})/\langle\tau\rangle$.



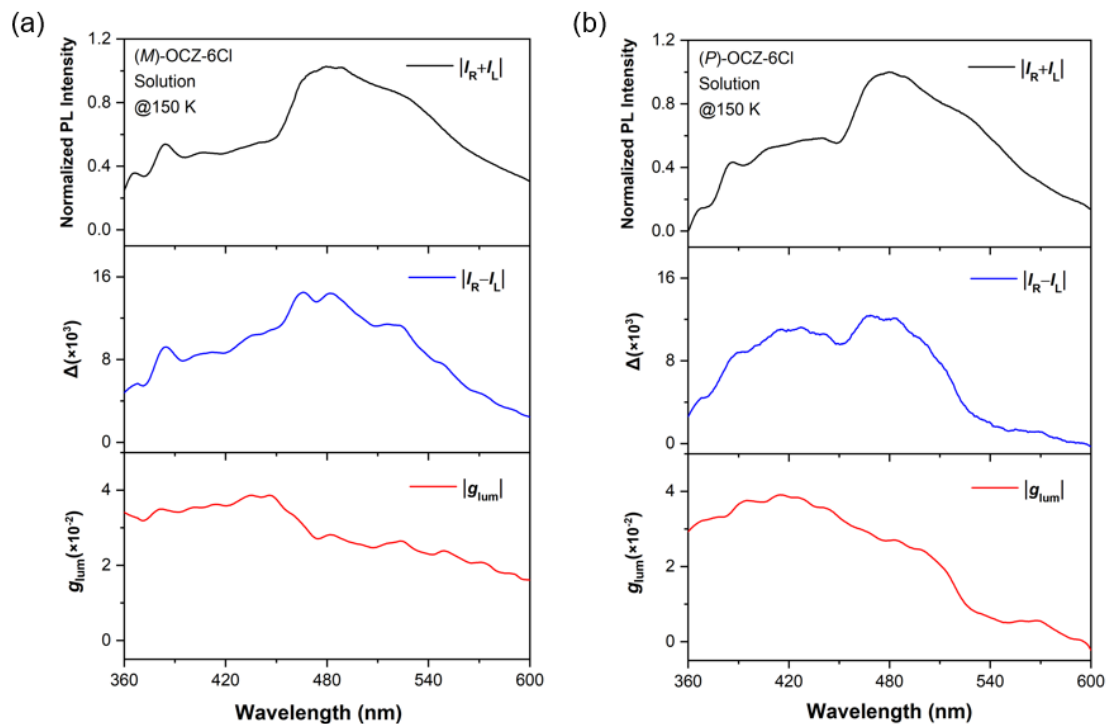
Supplementary Figure 13. (a) UV-Vis absorption spectra of **1** and OCZ-4Cl in 2-MeTHF solution (10^{-5} M) at room temperature. (b) Normalized PL spectra of **1** and OCZ-4Cl crystals at room temperature.



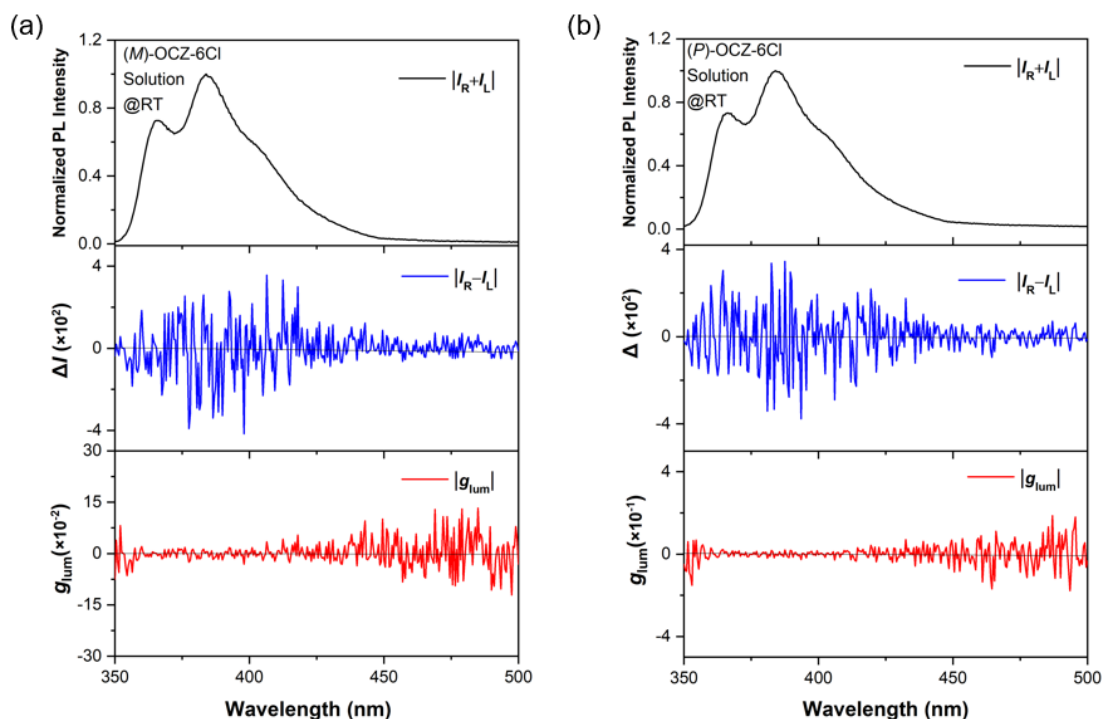
Supplementary Figure 14. (a) Decay curves of 1, OCZ, OCZ-1Cl, OCZ-4Cl, OCZ-5Cl and OCZ-6Cl in 2-Me-THF solution (10^{-5} M) at room temperature. (b) Decay curves of 2, OCZ, OCZ-1Cl, OCZ-4Cl, OCZ-5Cl and OCZ-6Cl crystals at room temperature.



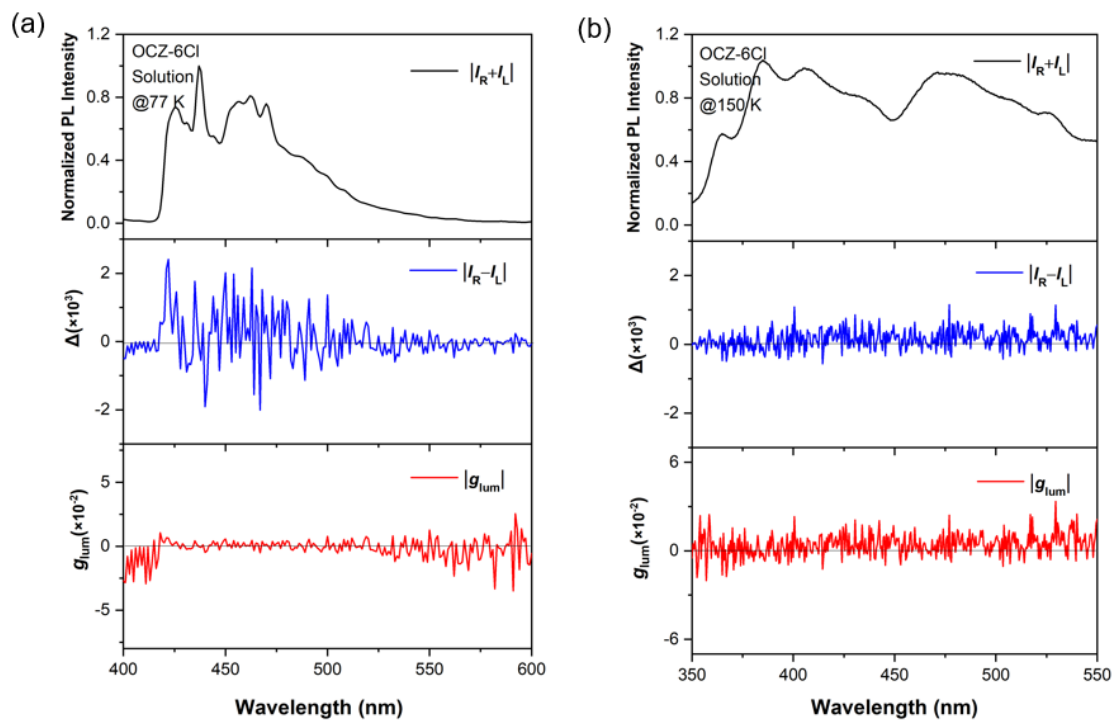
Supplementary Figure 15. (a) Normalized prompt and delayed PL spectra of (M)-OCZ-6Cl in 2-Me-THF (1×10^{-5} M) at 77 K with 300 nm excitation. (b) Decay curve of (M)-OCZ-6Cl in 2-Me-THF solution (10^{-5} M) at 77 K.



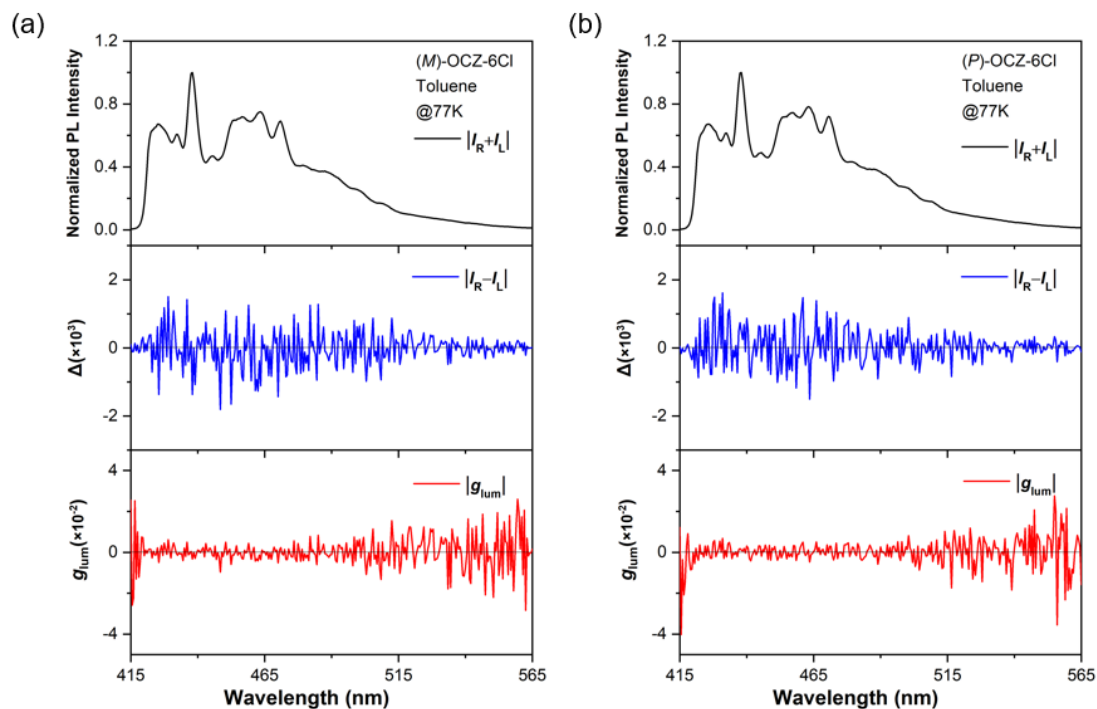
Supplementary Figure 16. Normalized PL spectra (top), CPL spectra (middle), and g_{lum} (bottom) of (M)-OCZ-6Cl (a) and (P)-OCZ-6Cl (b) in 2-Me-THF solution (10^{-5} M) at 150 K with 300 nm excitation.



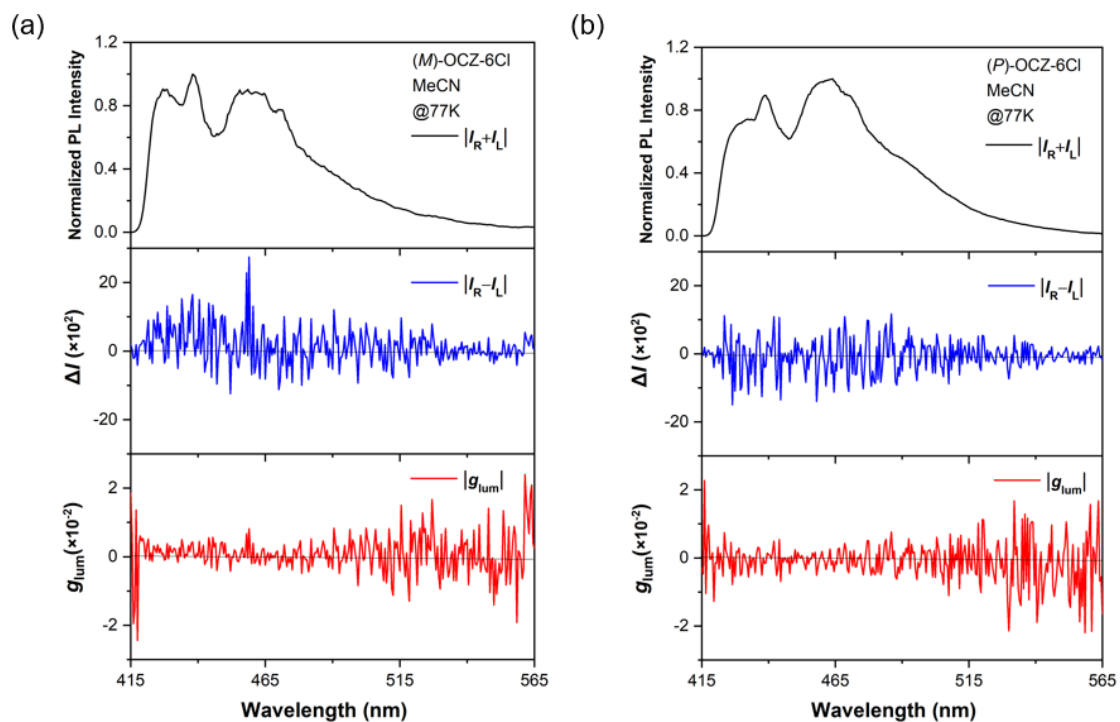
Supplementary Figure 17. Normalized PL spectra (top), CPL spectra (middle), and g_{lum} (bottom) of (M)-OCZ-6Cl (a) and (P)-OCZ-6Cl (b) in 2-Me-THF solution (10^{-5} M) at room temperature with 300 nm excitation.



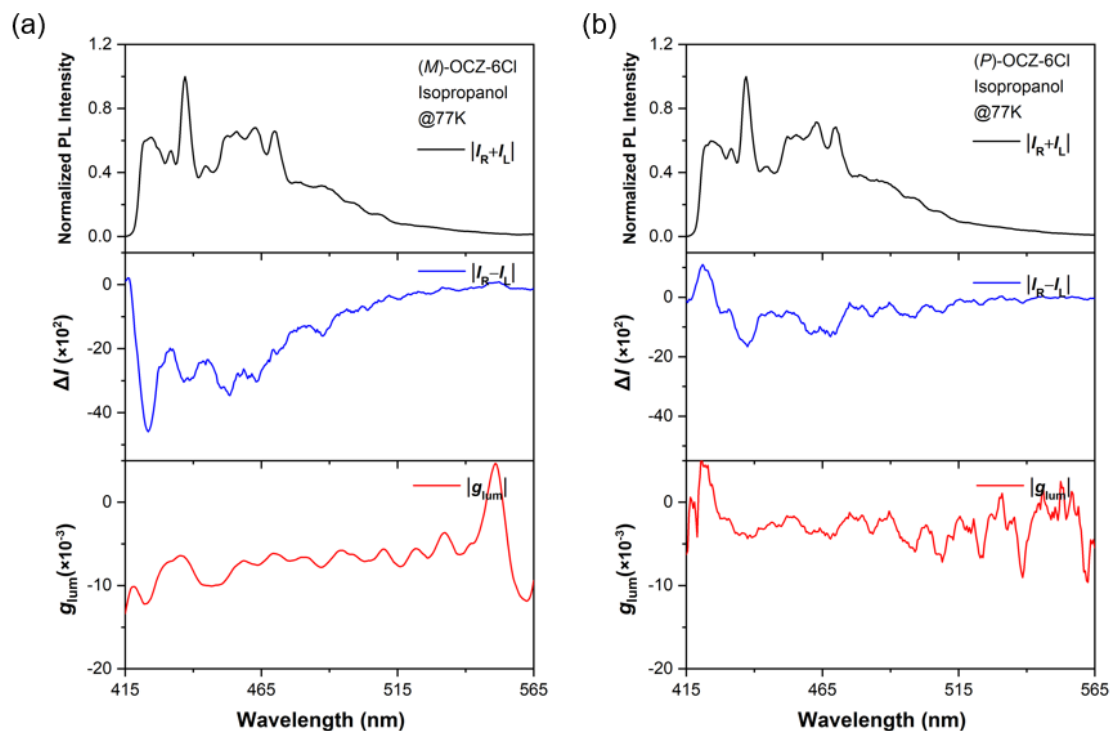
Supplementary Figure 18. Normalized PL spectra (top), CPL spectra (middle), and g_{lum} (bottom) of OCZ-6Cl in 2-Me-THF solution (10^{-5} M) at 77 K (a) and 150 K (b).



Supplementary Figure 19. Normalized PL spectra (top), CPL spectra (middle), and g_{lum} (bottom) of (M)-OCZ-6Cl (a) and (P)-OCZ-6Cl (b) in toluene solution (10^{-5} M) at 77 K with 300 nm excitation.

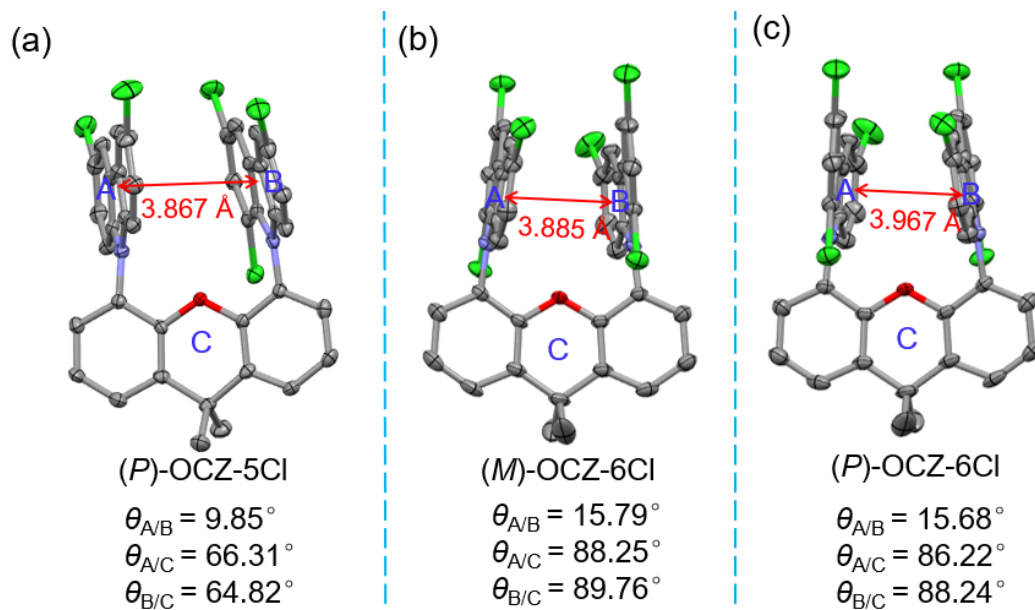


Supplementary Figure 20. Normalized PL spectra (top), CPL spectra (middle), and g_{lum} (bottom) of (M)-OCZ-6Cl (a) and (P)-OCZ-6Cl (b) in MeCN solution (10^{-5} M) at 77 K with 300 nm excitation.



Supplementary Figure 21. Normalized PL spectra (top), CPL spectra (middle), and g_{lum} (bottom) of (M)-OCZ-6Cl (a) and (P)-OCZ-6Cl (b) in isopropanol solution (10^{-5} M) at 77 K with 300 nm excitation.

S9 – Crystal data and structure refinement



Supplementary Figure 22. Single-crystal structures of (*P*)-OCZ-5Cl, (*M*)-OCZ-6Cl and (*P*)-OCZ-6Cl, together with the shortest π - π distances and torsion angle (carbon, oxygen, nitrogen, and chlorine atoms shown as grey, red, blue, and green ellipsoids at the 20% probability level).

Supplementary Table 5 Crystal Data and Structure Refinement for **1**.

CCDC (No.)	2175568	
Empirical formula	C ₂₇ H ₂₁ NO	
Formula weight	375.45	
Wavelength	0.71073 Å	
Temperature (K)	300.00(10) K	
Crystal system	orthorhombic	
Space group	P2 ₁ 2 ₁ 2 ₁	
Unit cell dimensions	a = 11.2170(7) Å	$\alpha = 90^\circ$
	b = 11.6286(8) Å	$\beta = 90^\circ$
	c = 15.4571(9) Å	$\gamma = 90^\circ$
Volume	2016.2(2) Å ³	
Z	4	
Density (calculated)	1.237 Mg/m ³	
Absorption coefficient	0.075 mm ⁻¹	
<i>F</i> (000)	792	
Crystal size	1.00×1.00×1.00 mm ³	
θ range [°]	2.192–30.750	
Index ranges	-15 ≤ <i>h</i> ≤ 14, -13 ≤ <i>k</i> ≤ 14, -17 ≤ <i>l</i> ≤ 20	
Reflections collected	11393	
Independent reflections	4712 [R(int) = 0.0239]	

Absorption correction	Multi-scan
Max. and min. transmission	0.784 and 1.000
Refinement metho	Full-matrix least-squares on F2
Data / restraints / parameter	4712/ 0 / 266
Goodness-of-fit on F2	1.036
Final R indices [I>2sigma(I)]	R ₁ = 0.0377, wR ₂ = 0.0858
R indices (all data)	R ₁ = 0.0590, wR ₂ = 0.0935
Largest diff. peak and hole	0.137 and - 0.131 e. Å ⁻³

Supplementary Table 6. Crystal Data and Structure Refinement for OCZ.

CCDC (No.)	2175756
Empirical formula	C ₃₉ H ₂₈ N ₂ O
Formula weight	540.63
Wavelength	0.71073 Å
Temperature (K)	259 K
Crystal system	monoclinic
Space group	P 2(1)/n
Unit cell dimensions	a = 12.6063(6) Å α = 90 deg. b = 16.7260(6) Å β = 107.567(6) deg. c = 14.1967(8) Å γ = 90 deg.
Volume	2853.8(3) Å ³
Z	4
Density (calculated)	1.258 Mg/m ³
Absorption coefficient	0.075 mm ⁻¹
<i>F</i> (000)	1136.0
Crystal size	1.50×0.10×0.10 mm ³
θ range [°]	1.936 - 30.687
Index ranges	-14≤ <i>h</i> ≤16, -23≤ <i>k</i> ≤20, -17≤ <i>l</i> ≤19
Reflections collected	24319
Independent reflections	7025 [R(int) = 0.0408]
Absorption correction	Multi-scan
Max. and min. transmission	0.138 and 1.000
Refinement metho	Full-matrix least-squares on F ²
Data / restraints / parameter	7025 / 0 / 382
Goodness-of-fit on F ²	1.026
Final R indices [I>2sigma(I)]	R ₁ = 0.0531, wR ₂ = 0.1360
R indices (all data)	R ₁ = 0.0774, wR ₂ = 0.1485
Largest diff. peak and hole	0.187 and - 0.243 e. Å ⁻³

Supplementary Table 7. Crystal Data and Structure Refinement for OCZ-4Cl.

CCDC (No.)	2175569
Empirical formula	C ₃₉ H ₂₄ Cl ₄ N ₂ O
Formula weight	678.40
Wavelength	1.54184 Å
Temperature (K)	299.99(10) K
Crystal system	monoclinic
Space group	P 2 ₁ /c
Unit cell dimensions	a = 12.9740(2) Å α= 90 deg. b = 11.1554(10) Å β= 102.293(10) deg. c = 26.5704(3) Å γ= 90 deg.
Volume	3757.37(8) Å ³
Z	4
Density (calculated)	1.199 Mg/m ³
Absorption coefficient	3.101 mm ⁻¹
F (000)	1392.0
Crystal size	1.00×1.00×0.10 mm ³
θ range [°]	3.401- 75.576
Index ranges	-16<=h<=13, -14<=k<=14, -32<=l<=32
Reflections collected	51847
Independent reflections	7698 [R(int) = 0.0460]
Absorption correction	Multi-scan
Max. and min. transmission	0.693and 1.000
Refinement metho	Full-matrix least-squares on F ²
Data / restraints / parameter	7698 / 0 / 417
Goodness-of-fit on F ²	1.074
Final R indices [I>2sigma(I)]	R ₁ = 0.0442, wR ₂ = 0.1258
R indices (all data)	R ₁ = 0.0524, wR ₂ = 0.1323
Largest diff. peak and hole	0.245 and - 0.390 e. Å ⁻³

Supplementary Table 8. Crystal Data and Structure Refinement for OCZ-5Cl.

CCDC (No.)	2175570
Empirical formula	C ₃₉ H ₂₃ Cl ₅ N ₂ O
Formula weight	712.84
Wavelength	1.54178 Å
Temperature (K)	298.0 K
Crystal system	monoclinic
Space group	P12 ₁ /c ₁
Unit cell dimensions	a = 18.3467(3) Å α = 90 deg. b = 18.1735(3) Å β = 92.9930(10) deg. c = 9.8494(2) Å γ = 90 deg.
Volume	3279.54(10) Å ³
Z	4
Density (calculated)	1.444 Mg/m ³
Absorption coefficient	4.314 mm ⁻¹
F (000)	1456
Crystal size	0.50×0.35×0.09 mm ³
θ range [°]	2.412 - 68.084
Index ranges	-22≤h≤22, -21≤k≤21, -11≤l≤11
Reflections collected	43168
Independent reflections	5998 [R(int) = 0.0604]
Absorption correction	Multi-scan
Max. and min. transmission	0.019 and 0.121
Refinement metho	Full-matrix least-squares on F ²
Data / restraints / parameter	5998 / 4 / 436
Goodness-of-fit on F ²	1.059
Final R indices [I>2sigma(I)]	R ₁ = 0.0701, wR ₂ = 0.2040
R indices (all data)	R ₁ = 0.0754, wR ₂ = 0.2097
Largest diff. peak and hole	0.986 and - 0.731 e. Å ⁻³

Supplementary Table 9. Crystal Data and Structure Refinement for OCZ-6Cl.

CCDC (No.)	2175571
Empirical formula	C ₃₉ H ₂₂ Cl ₆ N ₂ O
Formula weight	678.40
Wavelength	1.54178 Å
Temperature (K)	300 K
Crystal system	triclinic
Space group	P12 ₁ /c ₁
Unit cell dimensions	a = 10.2590(3) Å α = 77.3970(10) deg. b = 13.1075(3) Å β = 70.0820(10) deg. c = 13.7924(3) Å γ = 87.1270(10) deg.
Volume	1701.11(7) Å ³
Z	2
Density (calculated)	1.199 Mg/m ³
Absorption coefficient	3.101 mm ⁻¹
F (000)	760
Crystal size	0.35×0.15×0.13 mm ³
θ range [°]	3.457 -68.255
Index ranges	-12≤h≤12, -15≤k≤15, -16≤l≤16
Reflections collected	23895
Independent reflections	6217 [R(int) = 0.0499]
Absorption correction	Multi-scan
Max. and min. transmission	0.450 and 0.753
Refinement metho	Full-matrix least-squares on F ²
Data / restraints / parameter	6217 / 0 / 435
Goodness-of-fit on F ²	1.087
Final R indices [I>2σ(I)]	R ₁ = 0.0751, wR ₂ = 0.2225
R indices (all data)	R ₁ = 0.0865, wR ₂ = 0.2363
Largest diff. peak and hole	1.115 and - 0.599 e. Å ⁻³

Supplementary Table 10. Crystal Data and Structure Refinement for (*P*)-OCZ-5Cl.

CCDC (No.)	2180397
Empirical formula	C ₃₉ H ₂₃ Cl ₅ N ₂ O
Formula weight	712.84
Wavelength	1.54184 Å
Temperature (K)	304.12(10) K
Crystal system	monoclinic
Space group	P121 ₁
Unit cell dimensions	a = 9.8640(3) Å α = 90 deg. b = 18.0319(4) Å β = 94.458(2) deg. c = 18.5133(5) Å γ = 90 deg.
Volume	3282.94(15) Å ³
Z	4
Density (calculated)	1.442 Mg/m ³
Absorption coefficient	4.310 mm ⁻¹
<i>F</i> (000)	1456
Crystal size	1.00×1.00×0.10 mm ³
θ range [°]	2.379 - 66.071
Index ranges	-11≤ <i>h</i> ≤10, -21≤ <i>k</i> ≤19, -22≤ <i>l</i> ≤23
Reflections collected	22938
Independent reflections	10853 [R(int) = 0.0401]
Absorption correction	Multi-scan
Max. and min. transmission	0.730 and 1.000
Refinement metho	Full-matrix least-squares on F ²
Data / restraints / parameter	10853 / 1 / 851
Goodness-of-fit on F ²	1.041
Final R indices [I>2σ(I)]	R ₁ = 0.0557, wR ₂ = 0.1415
R indices (all data)	R ₁ = 0.0848, wR ₂ = 0.1585
Largest diff. peak and hole	0.488 and - 0.302 e. Å ⁻³

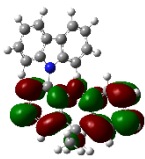
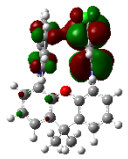
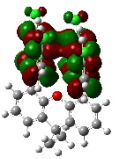
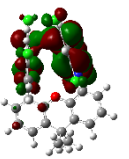
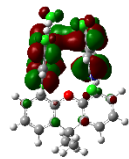
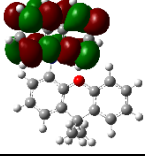
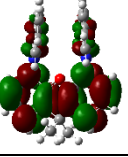
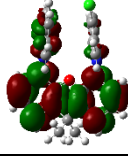
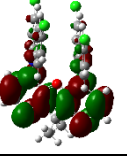
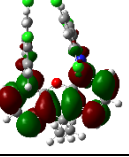
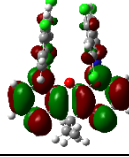
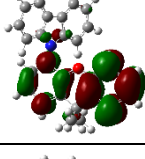
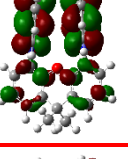
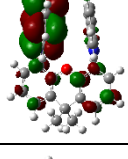
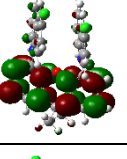
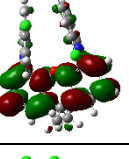
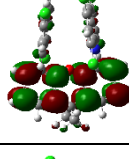
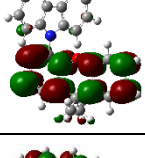
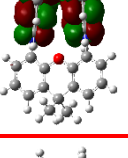
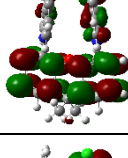
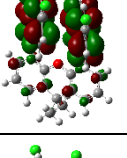
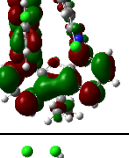
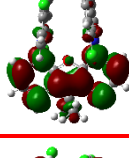
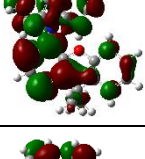
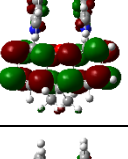
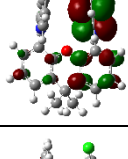
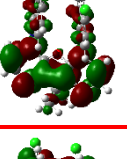
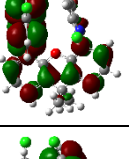
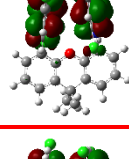
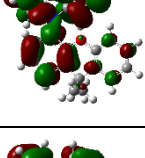
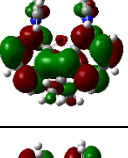
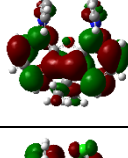
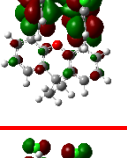
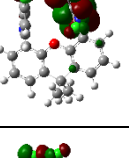
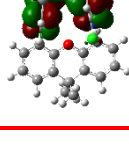
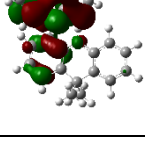
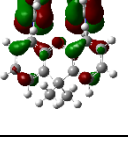
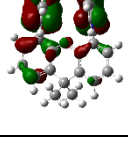
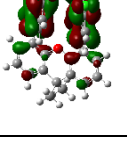
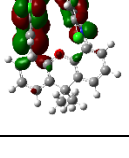
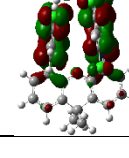
Supplementary Table 11. Crystal Data and Structure Refinement for (*M*)-OCZ-6Cl.

CCDC (No.)	2177012
Empirical formula	C ₃₉ H ₂₂ Cl ₆ N ₂ O
Formula weight	747.28
Wavelength	1.54184 Å
Temperature (K)	304.1(6) K
Crystal system	monoclinic
Space group	P21
Unit cell dimensions	a = 11.2664(2) Å α = 90 deg. b = 13.9686(2) Å β = 113.405(2) deg. c = 11.9220(2) Å γ = 90 deg.
Volume	1721.86(5) Å ³
<i>Z</i>	2
Density (calculated)	1.441 Mg/m ³
Absorption coefficient	4.833 mm ⁻¹
<i>F</i> (000)	728
Crystal size	0.50×0.50×0.50 mm ³
θ range [°]	4.033-76.045
Index ranges	-13≤ <i>h</i> ≤14, -12≤ <i>k</i> ≤17, -14≤ <i>l</i> ≤14
Reflections collected	20434
Independent reflections	5473 [R(int) = 0.0324]
Absorption correction	Multi-scan
Max. and min. transmission	0.643 and 1.000
Refinement metho	Full-matrix least-squares on F ²
Data / restraints / parameter	5473 / 1 / 435
Goodness-of-fit on F ²	1.036
Final R indices [I>2sigma(I)]	R ₁ = 0.0359, wR ₂ = 0.0979
R indices (all data)	R ₁ = 0.0405, wR ₂ = 0.1021
Largest diff. peak and hole	0.342 and - 0.336 e. Å ⁻³

Supplementary Table 12. Crystal Data and Structure Refinement for (*P*)-OCZ-6Cl.

CCDC (No.)	2177013
Empirical formula	C ₃₉ H ₂₂ Cl ₆ N ₂ O
Formula weight	747.28
Wavelength	1.54184 Å
Temperature (K)	304.56(10) K
Crystal system	monoclinic
Space group	P121 ₁
Unit cell dimensions	a = 11.27550(10) Å α = 90 deg. b = 13.98460(10) Å β = 113.4660(10) deg. c = 11.93170(10) Å γ = 90 deg.
Volume	1725.83(3) Å ³
Z	2
Density (calculated)	1.438 Mg/m ³
Absorption coefficient	4.822 mm ⁻¹
<i>F</i> (000)	760
Crystal size	1.00×1.00×0.10 mm ³
θ range [°]	4.039- 76.784
Index ranges	-13≤ <i>h</i> ≤14, -17≤ <i>k</i> ≤17, -14≤ <i>l</i> ≤14
Reflections collected	50480
Independent reflections	6832 [R(int) = 0.0464]
Absorption correction	Multi-scan
Max. and min. transmission	0.331 and 1.000
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameter	6832 / 1 / 435
Goodness-of-fit on <i>F</i> ²	1.072
Final R indices [I>2σ(I)]	R ₁ = 0.0424, wR ₂ = 0.1232
R indices (all data)	R ₁ = 0.0458, wR ₂ = 0.1273
Largest diff. peak and hole	0.417 and - 0.386 e. Å ⁻³

Supplementary Table 13. Electron cloud distributions **1**, OCZ, OCZ-1Cl, OCZ-4Cl, OCZ-5Cl and OCZ-6Cl in the ground state calculated by TD-DFT B3LYP/6-31G(d), Gaussian 16 program.

	1	OCZ	OCZ-1Cl	OCZ-4Cl	OCZ-5Cl	OCZ-6Cl
LUMO+5						
LUMO+4						
LUMO+3						
LUMO+2						
LUMO+1						
LUMO						
HOMO						

References

1. Frisch, M. J. T.; G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J.

- B.; Fox, D. J. , Gaussian, Inc., Wallingford CT, 2016.
2. Grimme, S., Antony, J., Ehrlich, S. & Krieg, H. A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* **132**, doi:10.1063/1.3382344 (2010).
 3. Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **98**, 5648-5652, doi:10.1063/1.464913 (1993).
 4. Lee, C. T., Yang, W. T. & Parr, R. G. Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B* **37**, 785-789, doi:10.1103/PhysRevB.37.785 (1988).
 5. Marenich, A. V., Cramer, C. J. & Truhlar, D. G. Performance of SM6, SM8, and SMD on the SAMPL1 Test Set for the Prediction of Small-Molecule Solvation Free Energies. *J. Phys. Chem. B* **113**, 4538-4543, doi:10.1021/jp809094y (2009).
 6. Marenich, A. V., Cramer, C. J. & Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B* **113**, 6378-6396, doi:10.1021/jp810292n (2009).
 7. Fukui, K. The Path of Chemical Reactions - the IRC Approach. *Acc. Chem. Res.* **14**, 363-368, doi:10.1021/ar00072a001 (1981).
 8. Hratchian, H. P. & Schlegel, H. B. Accurate reaction paths using a Hessian based predictor-corrector integrator. *J. Chem. Phys.* **120**, 9918-9924, doi:10.1063/1.1724823 (2004).
 9. Hratchian, H. P. & Schlegel, H. B. Using Hessian updating to increase the efficiency of a Hessian based predictor-corrector reaction path following method. *J. Chem. Theory Comput.* **1**, 61-69, doi:10.1021/ct0499783 (2005).
 10. Legault, C. Y. CYLview; Université de Sherbrooke, Sherbrooke, Canada, 2009; <http://www.cylview.org>.