Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for:

1,3-Dipolar Cycloaddition of Azomethine Ylides and Imidoyl Halides for Synthesis of π-Extended Imidazolium Salts

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Table of Contents

1. Experimental Section

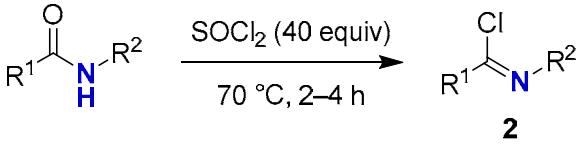
General: All reactions were carried out in a glove box or using standard Schlenk techniques under nitrogen atmosphere. Thin-layer chromatography (TLC) was performed using glass plates pre-coated with silica gel impregnated with a fluorescent indicator (Merck, #1.15685.0001). Silica gel column chromatography was performed as described by Still, et al.,[1] employing silica gel (Davisil, 60 Å, 40-63 micron) purchased from Sigma-Aldrich.

Instrumentation: NMR spectra were recorded on a Bruker AV 400 (^{1}H: 400 MHz and ^{13}C: 100 MHz) NMR spectrometer. Chemical shift values for protons are referenced to the signal of tetramethylsilane (δ 0.00) or the residual signal of chloroform-*d* (δ 7.26). Chemical shift values for carbons are referenced to the signal of tetramethylsilane (δ 0.00) or the carbon resonance of chloroform-*d* (δ 77.2). High-resolution mass (HRMS) spectra were taken on a Waters Q-Tof Premier mass spectrometer with the electron spray ionization time-of-flight (ESI-TOF) method. Infrared (IR) spectra were recorded on a Shimadzu FTIR-8400 spectrometer with an attenuated total reflection (ATR) system. Ultraviolet–visible (UV–vis) absorption spectra were recorded on Shimadzu UV-1800 and UV-3100 spectrometers. Fluorescence spectra were recorded on a Cary Eclipse Spectrofluorometer. Melting temperatures and decomposition temperatures were recorded on an OptiMelt MPA-100 apparatus.

Materials: The following reagents were purchased from the indicated suppliers and used as received: cesium fluoride (CsF; Sigma), thionyl chloride ($SOCl_2$; Sigma), cesium acetate (CsOAc; Sigma), cesium carbonate (Cs_2CO_3; Sigma), *N,N*-diisopropylethylamine (TCI), lithium fluoride (LiF; Alfa Aesar), sodium fluoride (NaF; Alfa Aesar), potassium fluoride (KF; Alfa Aesar), 15-crown-5 (Alfa), palladium(II) acetate (Sigma), di-*tert*-butyl(methyl)phosphonium tetrafluoroborate (Sigma), and 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU, Sigma).
The following reagents were pre-dried over activated 4 Å molecular sieves and heated to reflux over calcium hydride under nitrogen atmosphere, collected by distillation and stored under argon in a Schlenk flask: 1,2-dichlorodichloroethane (DCE; Sigma), chlorobenzene (TCI) and dimethylacetamide (DMA).
The following reagents were prepared according to literature procedures: 2-*t*-butyl-8-hydroisoquinolino[4,3,2-*de*]phenanthridin-9-ium chloride[2] and imidoyl chlorides **2**.[3]

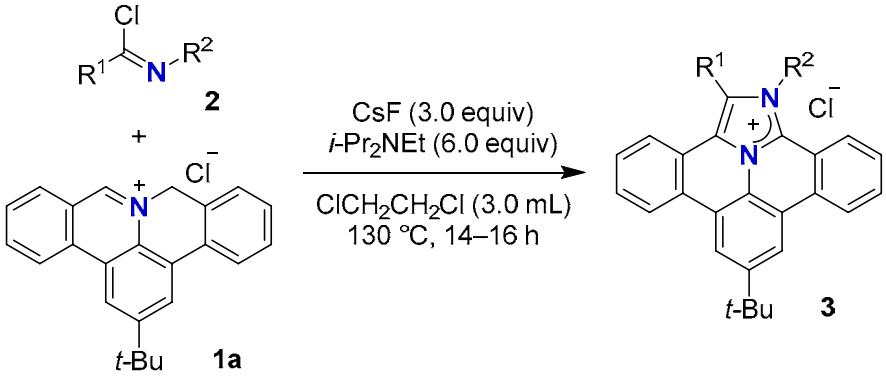
(1) W. C. Still, M. Kahn and A. Mitra, *J. Org. Chem.* 1978, **43**, 2923–2925.
(2) Y. Tokimaru, S. Ito and K. Nozaki, *Angew. Chem. Int. Ed.* 2018, **57**, 9818–9822.
(3) T. van Dijk, S. Burck, M. K. Rong, A. J. Rosenthal, M. Nieger, J. C. Slootweg and K. Lammertsma, *Angew. Chem. Int. Ed*. 2014, **53**, 9068–9071.

General Procedure for Preparation of Imidoyl Chlorides 2[3]



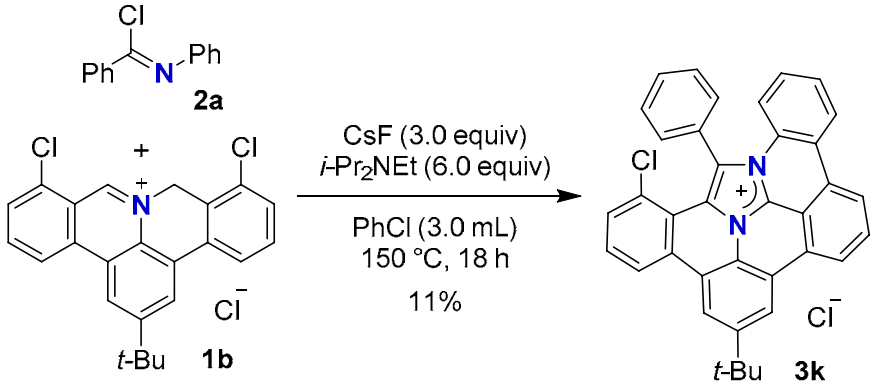
In a 25-mL Schlenk tube was added a carboxamide (0.10 mmol, 1.0 equiv). The tube was evacuated and refilled with nitrogen for three times. After adding thionyl chloride (290 μL, 4.0 mmol, 40 equiv), the reaction mixture was stirred for 2 to 4 hours at 70 °C (oil bath temperature). After cooling to room temperature, the excess thionyl chloride was removed by a vacuum pump equipped with a liquid nitrogen trap. The imidoyl chloride **2** obtained in a quantitative yield was directly used in the next step without further purification.

General Procedure for 1,3-Dipolar Cycloaddition of Polycyclic Aromatic Azomethine Ylide 1 with Imidoyl Chlorides 2



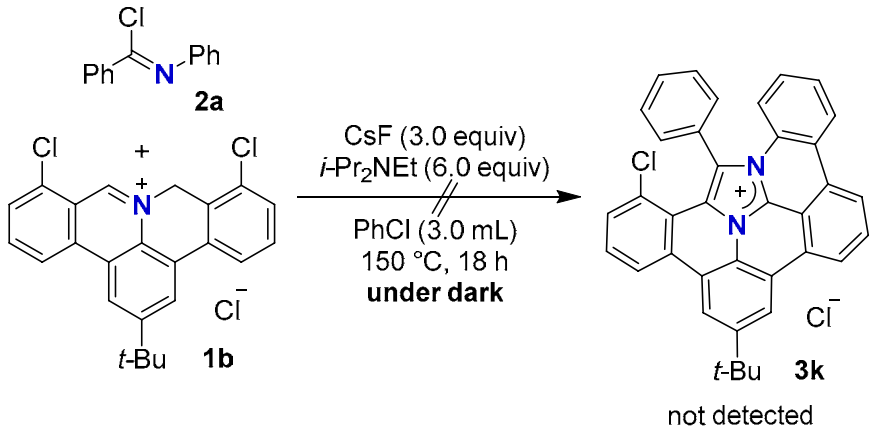
In the glovebox, imidoyl chloride **2** (0.10 mmol, 1.0 equiv) and cesium fluoride (12.6 mg, 0.30 mmol, 3.0 equiv) were placed into a 25-mL Schlenk tube. After being taken out from the glove box, the Schlenk tube was connected to a nitrogen line. To the mixture were added iminium salt **1a** (108 mg, 0.30 mmol, 3.0 equiv), 1,2-dichloroethane (3.0 mL), and *N,N*-diisopropylethylamine (105 μL, 0.60 mmol, 6.0 equiv). The reaction mixture was stirred for 14–16 hours at 130 °C (oil bath temperature). The reaction mixture was cooled to room temperature, diluted with dichloromethane (50 mL), and washed with water 1 time and brine 3 times. After evaporation, the crude mixture was purified by silica gel column chromatography with dichloromethane : methanol (10 : 1) to obtain **3** as a colorless solid.

A Procedure for Synthesizing Helicene Compounds 4

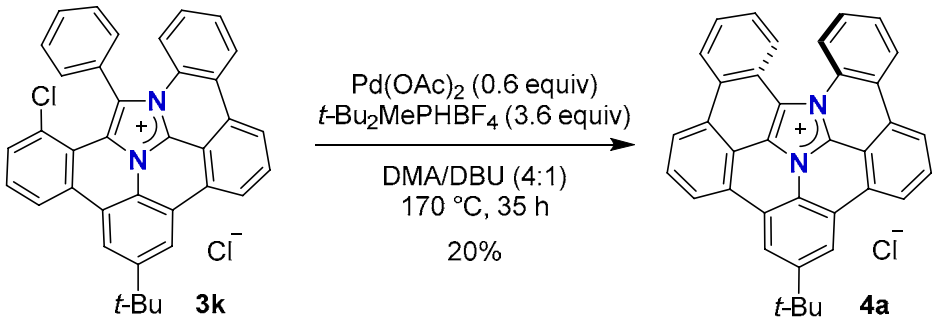


In the glovebox, imidoyl chloride **2** (0.20 mmol) and cesium fluoride (25.2 mg, 0.60 mmol) was placed in a 25-mL Schlenk tube. After being taken out from glove box, the Schlenk tube was connected to nitrogen line. To the mixture were added iminium salt **1b** (172 mg, 0.40 mmol), chlorobenzene(3.0 mL), and *N,N*-diisopropylethylamine (0.21 mL, 1.2 mmol). The reaction mixture was stirred for 18 hours at 150 °C (oil bath temperature). The reaction mixture was cooled to room temperature, diluted with dichloromethane (50 mL), washed with water 1 time and brine 3 times. After evaporation, the crude mixture was purified by silica gel column chromatography with dichloromethane : methanol (10:1) 3 times to obtain **3k** as brown solid (12.3 mg, 0.022 mmol, 11%).

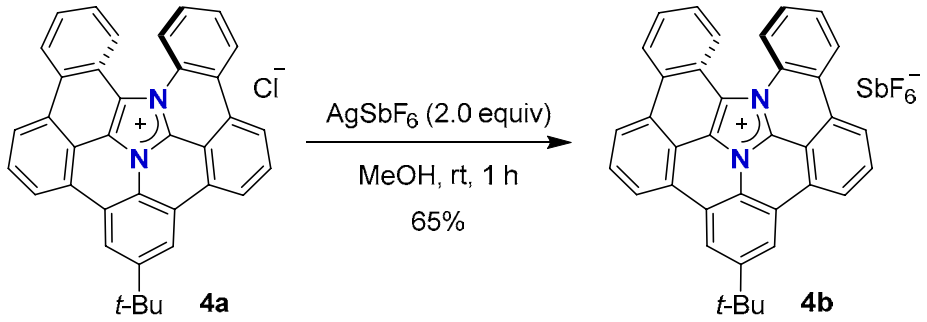
Control Experiment: Cycloaddition reaction under dark



The same cycloaddition reaction was performed in the dark with the Schlenk tube covered with aluminum foil. As a result, compound **3k** was not detected in the NMR spectrum of the crude mixture, indicating that cyclization to form **3k** is accelerated by irradiation of ambient light.

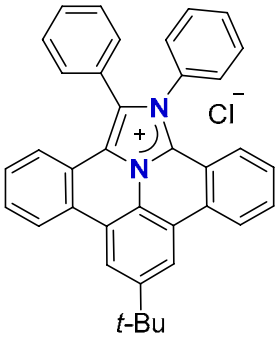


In the glovebox, imidazolium salt **3k** (9.8 mg, 17 μmol), palladium acetate (2.3 mg, 10 μmol), and di-*tert*-butyl(methyl)phosphonium tetrafluoroborate (15 mg, 62 μmol) were placed into a 25-mL Schlenk tube . After being taken out from glove box, the Schlenk tube was connected to a nitrogen line. To the mixture were added a mixture of dimethylacetamide and 1,8-diazabicyclo[5.4.0]undec-7-ene (DMA/DBU = 4/1; 2.0 mL). The reaction mixture was stirred at room temperature for 5 to 10 minutes, then stirred at 170 °C (oil bath temperature) for 35 hours. The reaction mixture was cooled to room temperature, diluted with ethyl acetate (25 mL) and toluene (25 mL), washed with water 1 time and brine 3 times. After evaporation, the crude mixture was purified by silica gel column chromatography with dichloromethane : methanol (10:1) to obtain **4a** as a colorless solid (1.8 mg, 3.4 μmol, 20%).



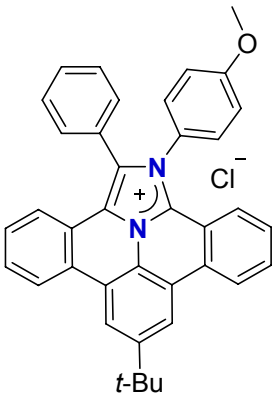
In a 25-mL Schlenk tube placed with imidazolium salt **4a** (6.0 mg, 11 μmol) and a magnetic stirring bar was added methanol (2.0 mL) to completely dissolve the solids. A solution of silver hexafluoroantimonate (7.8 mg, 22 μmol) in methanol (2.0 mL) was added dropwise into the above reaction mixture. After stirring at room temperature for 2 hour, the mixture was was evaporated under vacuum. The crude residue was purified by silica gel column chromatography to yield **4b** as a white solid (5.3 mg, 7.2 μmol, 65%).

8-*tert*-butyl-1,2-diphenyltribenzo[*b,g,ij*]imidazo[2,1,5-*de*]quinolizinium chloride (3a):



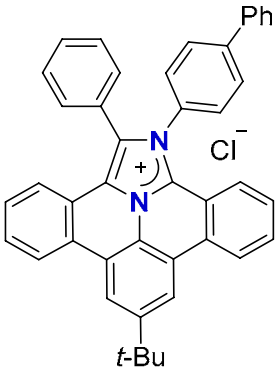
Colorless solid; R_f: 0.3 (dichloromethane : methanol = 10 : 1); mp >400 °C; IR (neat); cm^{-1} 3048, 2952, 2907, 2864, 1977, 1728, 1574, 1534, 1505, 1442, 1416, 1391, 1277, 1255, 1182, 1035, 869, 811, 767, 738, 721, 702, 691; ^{1}H NMR (400 MHz, $CDCl_3$, 300 K) δ 8.74 (d, J = 8.4 Hz, 1H), 8.68 (d, J = 10.0 Hz, 2H), 8.50 (d, J = 8.4 Hz, 1H), 7.98–7.92 (m, 2H), 7.89 (t, J = 8.0 Hz, 1H), 7.75 (d, J = 8.0 Hz, 2H), 7.68 (t, J = 8.0 Hz, 1H), 7.63–7.57 (m, 3H), 7.55–7.42 (m, 5H), 7.38 (t, J = 8.0 Hz, 1H), 7.28 (d, J = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 300 K) δ 151.6, 134.2, 132.3, 132.1 (2C), 131.6, 131.0, 130.9 (2C), 130.6 (2C), 130.3, 129.7, 129.6, 129.4 (2C),129.0 (2C), 127.5, 127.3, 125.8, 124.8, 124.5, 124.2, 123.6 (2C), 123.5, 122.5, 121.9, 121.7, 120.5, 119.3, 117.2, 35.9, 31.7 (3C); HRMS (ESI) *m*/*z* calcd for $C_{37}H_{29}ClN_2$ $[M-Cl]^+$ 501.2331, found 501.2329.

8-*tert*-butyl-1-(4-methoxyphenyl)-2-phenyltribenzo[*b,g,ij*]imidazo[2,1,5-*de*]quinolizinium chloride (3b)



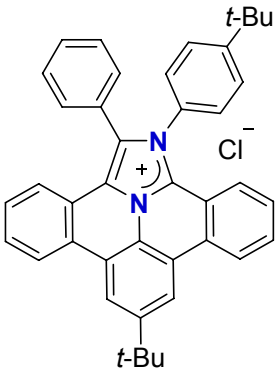
Colorless solid; R_f: 0.3 (dichloromethane:methanol = 10:1); mp 370-373 °C (decomp); IR (neat); cm^{-1} 3048, 2957, 2907, 2869, 1608, 1585, 1572, 1514, 1461, 1441, 1414, 1364, 1303, 1249, 1180, 1030, 871, 848, 767, 746, 693; ^{1}H NMR (400 MHz, $CDCl_3$, 300 K) δ 8.74 (d, J = 8.0 Hz, 1H), 8.69 (d, J = 1.6 Hz, 1H), 8.66 (d, J = 1.6 Hz, 1H), 8.50 (d, J = 8.0 Hz, 1H), 7.90 (t, J = 8.0 Hz, 1H), 7.82 (d, J = 8.8 Hz, 2H), 7.75–7.70 (m, 2H), 7.68 (t, J = 8.0 Hz, 1H), 7.55–7.47 (m, 5H), 7.41–7.34 (m, 2H), 7.09 (d, J = 9.2 Hz, 2H), 3.89 (s, 3H), 1.63 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, 300 K) δ 161.5, 151.8, 132.5, 132.3, 131.9 (2C), 131.2, 131.1, 130.9, 130.8, 130.5, 129.9 (2C), 129.8 (2C), 129.6 (2C), 127.3, 126.1, 125.7, 124.6, 124.4, 124.2, 123.7, 123.4, 123.3, 122.4, 121.7, 121.4, 120.5, 119.3, 117.0, 115.9, 55.8, 35.9, 31.7 (3C); HRMS (ESI) *m*/*z* calcd for $C_{38}H_{31}ClN_2O$ $[M-Cl]^+$ 531.2436, found 531.2433.

1-([1,1'-biphenyl]-4-yl)-8-*tert*-butyl-2-phenyltribenzo[*b,g,ij*]imidazo[2,1,5-*de*]quinolizinium chloride (3c)



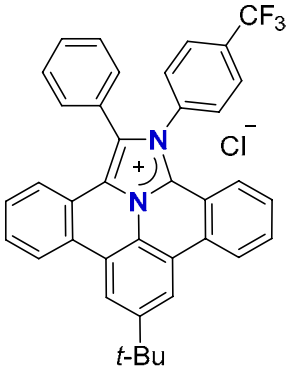
Colorless solid; R_f: 0.3 (dichloromethane:methanol = 10:1); mp >400 °C; IR (neat); cm^{-1} 3053, 3032, 2962, 2907, 2867, 1608, 1571, 1532, 1489, 1442, 1417, 1391, 1361, 1314, 1278, 1253, 1180, 1074, 1032, 1009, 977, 863, 766, 740, 692; ^{1}H NMR (400 MHz, $CDCl_3$, 300 K) δ 8.75 (d, J = 8.4 Hz, 1H), 8.70 (s, 1H), 8.68 (s, 1H), 8.51 (d, J = 8.0 Hz, 1H), 8.04 (d, J = 8.4 Hz, 2H), 7.89 (t, J = 8.4 Hz, 1H), 7.85–7.76 (m, 4H), 7.71–7.63 (m, 3H), 7.54–7.34 (m, 10H), 1.63 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, 300 K) δ 151.6, 144.0, 138.8, 133.2, 132.4, 132.3, 132.1 (2C), 131.1, 131.0 (2C), 130.3, 129.7, 129.6, 129.5 (2C), 129.4 (2C), 129.1 (2C), 128.9 (2C), 128.6, 127.5, 127.2 (2C), 125.9, 124.8, 124.6, 124.2, 123.6 (2C), 123.5, 122.5, 121.9, 121.7, 120.5, 119.3, 117.2, 35.9, 31.7 (3C); HRMS (ESI) *m*/*z* calcd for $C_{43}H_{33}ClN_2$ $[M-Cl]^+$ 577.2644, found 577.2643.

8-*tert*-butyl-1-(4-butylphenyl)-2-phenyltribenzo[*b,g,ij*]imidazo[2,1,5-*de*]quinolizinium chloride (3d)



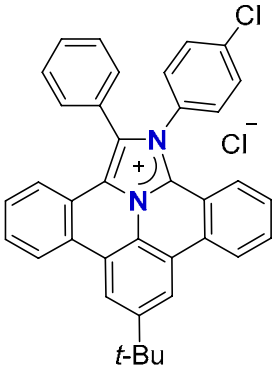
Colorless solid; R_f: 0.3 (dichloromethane:methanol = 10:1); mp 360–363 °C (decomp); IR (neat); cm^{-1} 3053, 3030, 2960, 2907, 2867, 1575, 1532, 1516, 1462, 1414, 1364, 1314, 1276, 1253, 1203, 1107, 1030, 871, 859, 781, 767, 744, 718, 691; ^{1}H NMR (400 MHz, $CDCl_3$, 300 K) δ 8.75 (d, J = 8.4 Hz, 1H), 8.71 (s, 1H), 8.67 (s, 1H), 8.51 (d, J = 8.4 Hz, 1H), 7.91 (t, J = 7.2 Hz, 1H), 7.78 (d, J = 8.4 Hz, 2H), 7.74–7.64 (m, 3H), 7.58 (d, J = 8.4 Hz, 2H), 7.55–7.42 (m, 5H), 7.39 (t, J = 7.6 Hz, 1H), 7.28 (d, J = 10.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, 300 K) δ 155.3, 151.8, 132.5, 132.2, 131.9 (2C), 131.2, 131.0 (2C), 130.9, 130.5, 129.8, 129.7, 129.5 (2C), 128.2 (2C), 127.6 (2C), 127.4 (2C), 125.7, 124.7, 124.5, 124.2, 123.7, 123.5, 123.4, 122.5, 121.7, 121.6, 120.5, 119.4, 117.0, 35.9, 35.1, 31.7 (3C), 31.2 (3C); HRMS (ESI) *m*/*z* calcd for $C_{41}H_{37}ClN_2$ $[M-Cl]^+$ 557.2957, found 557.2953.

8-*tert*-butyl-2-phenyl-1-(4-(trifluoromethyl)phenyl)tribenzo[*b,g,ij*]imidazo[2,1,5-*de*]quinolizinium chloride (3e)



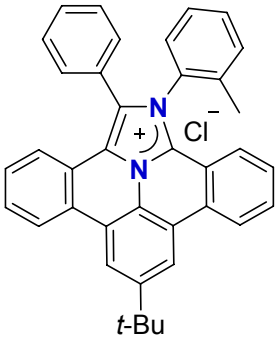
Colorless solid; R_f: 0.3 (dichloromethane:methanol = 10:1); mp >400 °C; IR (neat); cm^{-1} 3055, 2960, 2907, 2872, 1618, 1572, 1535, 1505, 1442, 1394, 1322, 1253, 1166, 1126, 1069, 1027, 979, 869, 801, 767, 690; ^{1}H NMR (400 MHz, $CDCl_3$, 300 K) δ 8.73 (d, J = 8.0 Hz, 1H), 8.68 (s, 1H), 8.66 (s, 1H), 8.48 (d, J = 8.0 Hz, 1H), 8.41 (d, J = 8.4 Hz, 2H), 7.90–7.78 (m, 5H), 7.66 (t, J = 7.6 Hz 1H), 7.54–7.43 (m, 5H), 7.36 (t, J = 7.6 Hz, 1H), 7.25 (d, J = 8.8 Hz, 1H), 1.63 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, 300 K) δ 151.5, 137.8, 133.5, 133.2, 132.5, 132.2 (2C), 132.1, 131.1 (2C), 130.8, 130.3 (2C), 130.2, 129.6, 129.5 (3C), 127.6, 127.5, 127.4, 125.8, 124.9, 124.6, 124.3, 124.2, 123.7, 123.6, 123.5, 123.1 (q, J = 103.0 Hz, 1C), 122.6, 122.0, 120.5, 119.2, 35.9, 31.7 (3C); HRMS (ESI) *m*/*z* calcd for $C_{38}H_{28}ClF_3N_2$ $[M-Cl]^+$ 569.2205, found 569.2201.

8-*tert*-butyl-1-(4-chlorophenyl)-2-phenyltribenzo[*b,g,ij*]imidazo[2,1,5-*de*]quinolizinium chloride (3f)



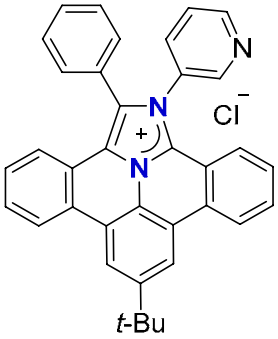
Colorless solid; R_f: 0.3 (dichloromethane:methanol = 10:1); mp >400 °C; IR (neat); cm^{-1} 3050, 3025, 3007, 2962, 2907, 2869, 1572, 1532, 1497, 1442, 1417, 1361, 1278, 1253, 1183, 1090, 1025, 977, 871, 854, 796, 766, 739, 705, 691; ^{1}H NMR (400 MHz, $CDCl_3$, 300 K) δ 8.72 (d, J = 8.4 Hz, 1H), 8.68 (s, 1H), 8.65 (s, 1H), 8.48 (d, J = 8.0 Hz, 1H), 8.11 (d, J = 8.4 Hz, 2H), 7.87 (t, J = 7.6 Hz, 1H), 7.81 (d, J = 6.0 Hz, 2H), 7.65 (t, J = 7.6 Hz, 1H), 7.60–7.46 (m, 7H), 7.36 (t, J = 7.6 Hz, 2H) 1.62 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, 300 K) δ 151.4, 137.6, 133.0, 132.5, 132.2 (3C), 131.0 (2C), 130.9, 130.7 (4C), 130.2, 129.6, 129.5 (3C), 127.5, 125.8, 124.8, 124.4, 124.2, 123.6, 123.5 (2C), 122.5, 122.0, 121.8, 120.5, 119.2, 117.3, 35.9, 31.7 (3C); HRMS (ESI) *m*/*z* calcd for $C_{37}H_{28}Cl_2N_2$ $[M-Cl]^+$ 535.1941, found 535.1937.

8-*tert*-butyl-2-phenyl-1-(2-methylphenyl)tribenzo[*b,g,ij*]imidazo[2,1,5-*de*]quinolizinium chloride (3g)



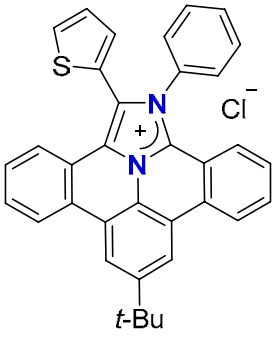
Colorless solid; R_f: 0.3 (dichloromethane:methanol = 10:1); mp 355–358 °C (decomp); IR (neat); cm^{-1} 3040, 2952, 2902, 2864, 1632, 1572, 1532, 1502, 1464, 1441, 1415, 1383, 1363, 1272, 1250, 1032, 932, 869, 781, 767, 739, 726, 693; ^1H NMR (400 MHz, $CDCl_3$, 300 K) δ 8.80 (d, J = 8.4 Hz, 1H), 8.74 (s,1H), 8.71 (s, 1H), 8.54 (d, J = 8.4 Hz, 1H), 8.11 (d, J = 7.6 Hz, 1H), 7.96 (t, J = 7.6 Hz, 1H), 7.93–7.87 (m, 1H), 7.72 (t, J = 7.6 Hz, 1H), 7.59-7.37 (m, 10H), 7.21 (d, J = 8.4 Hz, 1H), 2.06 (s, 3H), 1.64 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, 300 K) δ 152.0, 134.9, 133.0, 132.9, 132.8, 132.1, 131.8, 131.7, 131.3, 130.9, 130.6, 130.2 (2C), 130.0 (2C), 129.9 (2C), 129.3, 128.8, 127.5, 125.4, 124.7, 124.4, 123.8, 123.6, 123.5, 123.4, 122.5, 121.9, 121.7, 120.7, 119.5, 116.9, 36.0, 31.7 (3C), 17.7; HRMS (ESI) m/z calcd for $C_{38}H_{31}ClN_2$ $[M-Cl]^+$ 515.2487, found 515.2474.

8-*tert*-butyl-2-phenyl-1-(pyridin-3-yl)tribenzo[*b,g,ij*]imidazo[2,1,5-*de*]quinolizinium chloride (3h)



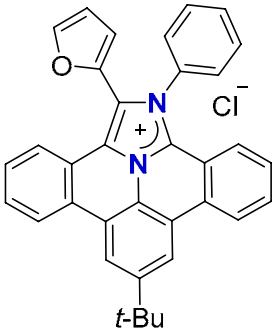
Colorless solid; R_f: 0.3 (dichloromethane:methanol = 10:1); mp >400 °C; IR (neat); cm^{-1} 3008, 2962, 2930, 2894, 2874, 1637, 1586, 1574, 1532, 1494, 1476, 1443, 1417, 1375, 1312, 1202, 1167, 1086, 1058, 1040, 1030, 978, 932, 859, 844, 830, 767, 733, 700; ^1H NMR (400 MHz, $CDCl_3$, 300 K) δ 9.45 (d, J = 7.6 Hz, 1H), 8.79 (d, J = 4.4 Hz, 1H), 8.76–8.71 (m, 2H), 8.68 (d, J = 8.4 Hz, 2H), 8.49 (d, J = 8.4 Hz, 1H), 8.30–8.18 (m, 1H), 7.88 (t, J = 7.6 Hz, 1H), 7.75–7.60 (m, 2H), 7.58–7.40 (m, 6H), 7.37 (t, J = 7.6 Hz, 1H), 7.30 (d, J = 8.4 Hz, 1H), 1.63 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, 300 K) δ 152.3, 151.5, 148.2, 139.3, 133.5, 132.9, 132.3, 132.2, 131.1 (2C), 130.9, 130.2, 130.1, 129.6 (2C), 129.1, 127.5, 125.6, 125.5, 125.0, 124.9, 124.3 (2C), 123.7, 123.5 (2C), 122.6, 122.0, 121.9, 120.5, 119.3, 117.3, 35.9, 31.7 (3C); HRMS (ESI) m/z calcd for $C_{36}H_{28}ClN_3$ $[M-Cl]^+$ 502.2283, found 502.2276.

8-(*tert*-butyl)-1-phenyl-2-(thiophen-2-yl)tribenzo[*b,g,ij*]imidazo[2,1,5-*de*]quinolizinium chloride (3i):



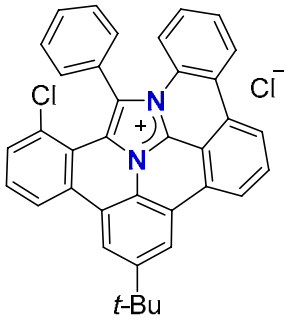
Colorless solid; R_f: 0.3 (dichloromethane:methanol = 10:1); mp >400 °C; IR (neat); cm^{-1} 3032, 3005, 2955, 2904, 2869, 1635, 1597, 1575, 1535, 1505, 1459, 1442, 1415, 1395, 1364, 1316, 1273, 1253, 1223, 1175, 1080, 1037, 949, 874, 849, 798, 768, 742, 714, 692; ^1H NMR (400 MHz, $CDCl_3$, 300 K) δ 8.76 (d, J = 8.0 Hz, 1H), 8.71 (s, 1H), 8.69 (s, 1H), 8.53 (d, J = 8.0 Hz, 1H), 8.00–7.85 (m, 3H), 7.80–7.60 (m, 7H), 7.48 (t, J = 7.6 Hz, 2H), 7.29 (d, J = 8.0 Hz, 1H), 7.18 (dd, J = 4.0, 5.2 Hz, 1H), 1.63 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, 300 K) δ 151.9, 135.3, 133.9, 132.9, 132.7, 131.8, 131.6, 131.0, 130.8, 130.7 (2C), 129.9, 129.7, 128.8 (2C), 128.6 (2C), 127.7, 125.1, 124.6, 124.3, 124.1, 123.9, 123.6, 123.5, 123.3, 122.4, 121.5, 120.6, 119.5, 116.9, 35.9, 31.7 (3C); HRMS (ESI) m/z calcd for $C_{35}H_{27}ClN_2S$ $[M-Cl]^+$ 507.1895, found 507.1890.

8-*tert*-butyl-2-(furan-2-yl)-1-phenyltribenzo[*b,g,ij*]imidazo[2,1,5-*de*]quinolizinium chloride (3j)



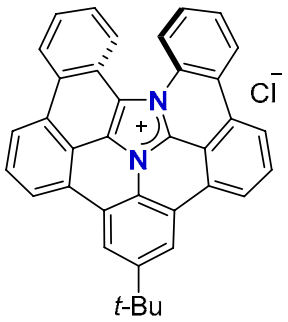
Colorless solid; R_f: 0.3 (dichloromethane:methanol = 10:1); mp 340–343 °C (decomp); IR (neat); cm^{-1} 3040, 3000, 2947, 2902, 2864, 1979, 1635, 1605, 1580, 1533, 1506, 1442, 1415, 1389, 1364, 1316, 1278, 1256, 1218, 1180, 1160, 1145, 1072, 1009, 984, 906, 889, 872, 844, 801, 767, 746, 693; ^{1}H NMR (400 MHz, $CDCl_3$, 300 K) δ 8.77 (d, J = 8.4 Hz, 1H), 8.73 (s, 1H), 8.71 (s, 1H), 8.56 (d, J = 8.0 Hz, 1H), 7.98–7.89 (m, 3H), 7.79 (t, J = 7.6 Hz, 1H), 7.76-7.62 (m, 5H), 7.56 (t, J = 7.6 Hz, 1H), 7.50 (t, J = 7.6 Hz, 1H), 7.32 (d, J = 8.4 Hz, 1H), 7.07 (d, J = 3.2 Hz, 1H), 8.56 (dd, J = 2.0, 3.6 Hz, 1H), 1.64 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, 300 K) δ 152.1, 145.9, 137.2, 134.0, 133.1, 133.0, 132.1, 131.2, 131.1, 130.9 (2C), 130.1, 129.9, 128.5 (2C), 127.8, 125.2, 124.7, 124.4 (2C), 123.7, 123.4, 123.2, 122.4, 121.1, 120.9, 120.8, 119.6, 118.8, 116.8, 112.4, 36.0, 31.7 (3C); HRMS (ESI) m/z calcd for $C_{35}H_{27}ClN_2O$ $[M-Cl]^+$ 491.2123, found 491.2117.

9-*tert*-butyl-14-chloro-15-phenyl-14b^1,15a-diazadibenzo[*fg,ij*]cyclopenta[*rst*]pentaphenium chloride (3k)



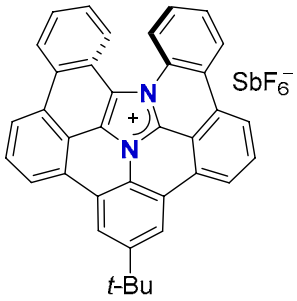
Brown solid; R_f: 0.3 (dichloromethane:methanol = 10:1); mp 360–365 °C (decomp); IR (neat); cm^{-1} 2960, 2907, 2864, 1650, 1591, 1577, 1532, 1459, 1443, 1406, 1392, 1363, 1250, 1030, 920, 877, 802, 760, 722, 696; ^{1}H NMR (400 MHz, $CDCl_3$, 300 K) δ 8.93 (d, J = 8.0 Hz, 2H), 8.89 (d, J = 7.7 Hz, 1H), 8.82 (s, 1H), 8.65 (s, 1H), 8.58 (d, J = 7.9 Hz, 1H), 8.53 (t, J = 8.0 Hz, 1H), 7.89 (d, J = 7.0 Hz, 2H), 7.84–7.69 (m, 5H), 7.56 (d, J = 7.8 Hz, 1H), 7.43 (t, J = 7.9 Hz, 1H), 7.38 (d, J = 8.2 Hz, 1H), 1.65 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, 300 K) δ 152.5, 134.7, 133.3, 132.8, 132.1 (2C), 131.9 (2C), 131.6, 131.2, 130.6, 130.5, 130.1, 129.7, 129.3, 128.8, 128.5, 128.3, 126.3, 124.1, 123.4, 123.0 (2C), 122.8, 122.7, 122.3, 122.1, 121.4, 121.3 (2C), 120.8, 119.0, 111.9, 36.1, 31.7 (3C); HRMS (ESI) m/z calcd for $C_{37}H_{26}Cl_2N_2$ $[M-Cl]^+$ 533.1785, found 533.1787.

9-*tert*-butyl-7b^2,17b-diazadibenzo[*fg,ij*]benzo[6,7]indeno[5,4,3,2,1-*pqrst*]pentaphenium chloride (4a)



Colorless solid; R_f: 0.3 (dichloromethane:methanol = 10:1); mp 320–325 °C (decomp); IR (neat); cm^{-1} 2957, 2921, 2851, 1660, 1632, 1595, 1466, 1454, 1391, 1260, 1096, 1021, 884, 815, 757, 699; ^{1}H NMR (400 MHz, CD_3OD, 300 K) δ 9.02–8.87 (m, 4H), 8.83 (s, 1H), 8.79 (d, J = 8.0 Hz, 2H), 8.74 (s, 1H), 8.64 (d, J = 8.8 Hz, 1H), 8.56 (d, J = 7.6 Hz, 1H), 8.47 (t, J = 8.0 Hz, 1H), 8.09 (t, J = 7.6 Hz, 1H), 8.05–7.95 (m, 2H), 7.85 (t, J = 7.6 Hz, 1H), 7.79 (t, J = 7.6 Hz, 1H), 1.71 (s, 9H); ^{13}C NMR (100 MHz, CD_3OD, 300 K) δ 153.4, 135.2, 134.6, 132.1, 131.0, 130.7, 130.5, 129.8, 129.7, 129.6, 129.5, 128.7, 128.5, 127.8, 126.5, 125.7, 125.5, 123.8 (2C), 123.6, 123.1, 123.0, 122.3 (2C), 122.2 (2C), 122.1, 121.8, 121.7, 121.1, 120.3, 119.7 (2C), 111.9, 36.0, 30.9 (3C); HRMS (ESI) m/z calcd for $C_{37}H_{25}ClN_2$ $[M-Cl]^+$ 497.2018, found 497.2021.

9-*tert*-butyl-7b^2,17b-diazadibenzo[*fg,ij*]benzo[6,7]indeno[5,4,3,2,1-*pqrst*]pentaphenium hexafluoroantimonate (4b)



Colorless solid; R_f: 0.3 (dichloromethane:methanol = 10:1); mp 376–380 °C (decomp); IR (neat); cm^{-1} 2958, 2917, 2871, 1661, 1607, 1595, 1576, 1543, 1454, 1390, 1366, 1325, 1248, 1164, 1119, 1056, 969, 882, 815, 756, 650; ^{1}H NMR (400 MHz, CD_3CN, 300 K) δ 8.78 (d, J = 8.2 Hz, 1H), 8.76 (d, J = 8.0 Hz, 1H), 8.71 (d, J = 8.0 Hz, 1H), 8.62 (s, 1H), 8.56 (d, J = 8.3 Hz, 1H), 8.47 (s, 1H) 8.45 (d, J = 8.4 Hz, 1H), 8.36 (t, J = 7.6 Hz, 1H), 8.35 (d, J = 7.5 Hz, 1H), 8.24 (d, J = 7.8 Hz, 1H), 8.21 (d, J = 8.3 Hz, 1H), 7.98–7.88 (m, 2H), 7.71 (t, J = 7.9 Hz, 1H) 7.59 (t, J = 7.4 Hz, 1H), 7.53 (t, J = 7.5 Hz, 1H), 1.66 (s, 9H); ^{13}C NMR (100 MHz, CD_3CN, 300 K) δ 154.3, 135.6, 132.7, 132.0, 131.4, 131.1, 130.5, 130.2, 130.1, 130.0, 129.8, 129.7, 128.9, 127.5, 126.3 (2C), 124.9 (2C), 124.4, 123.8, 123.7, 123.5 (2C), 123.4, 122.9, 122.4, 122.3, 122.2, 120.8, 120.7, 120.4, 115.3, 112.6, 37.1, 31.9 (3C); HRMS (ESI) m/z calcd for $[M-SbF_6]^+$ 497.2018, found 497.2026.

2. NMR Spectra

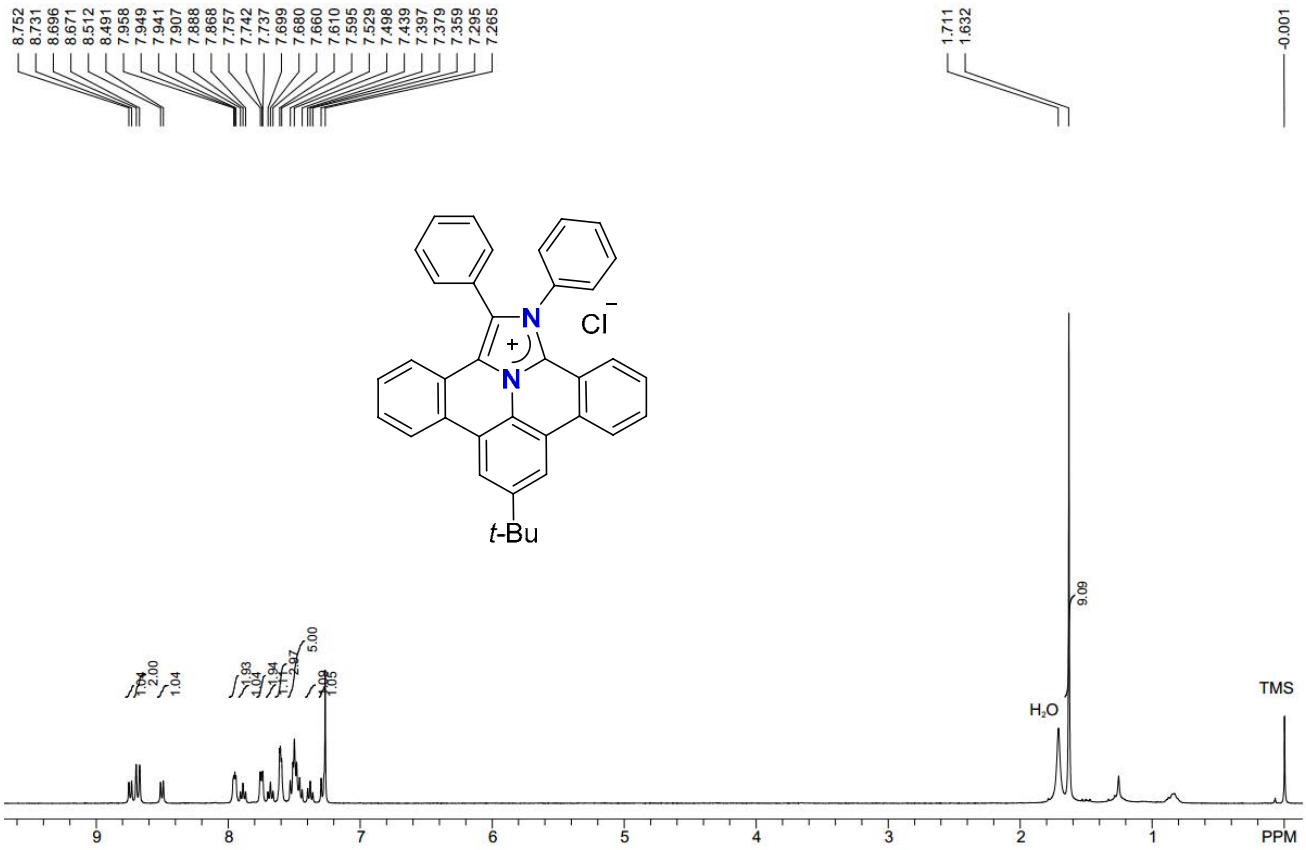


Figure S1. ^{1}H NMR spectrum of **3a** (400 MHz, $CDCl_3$, 300 K).

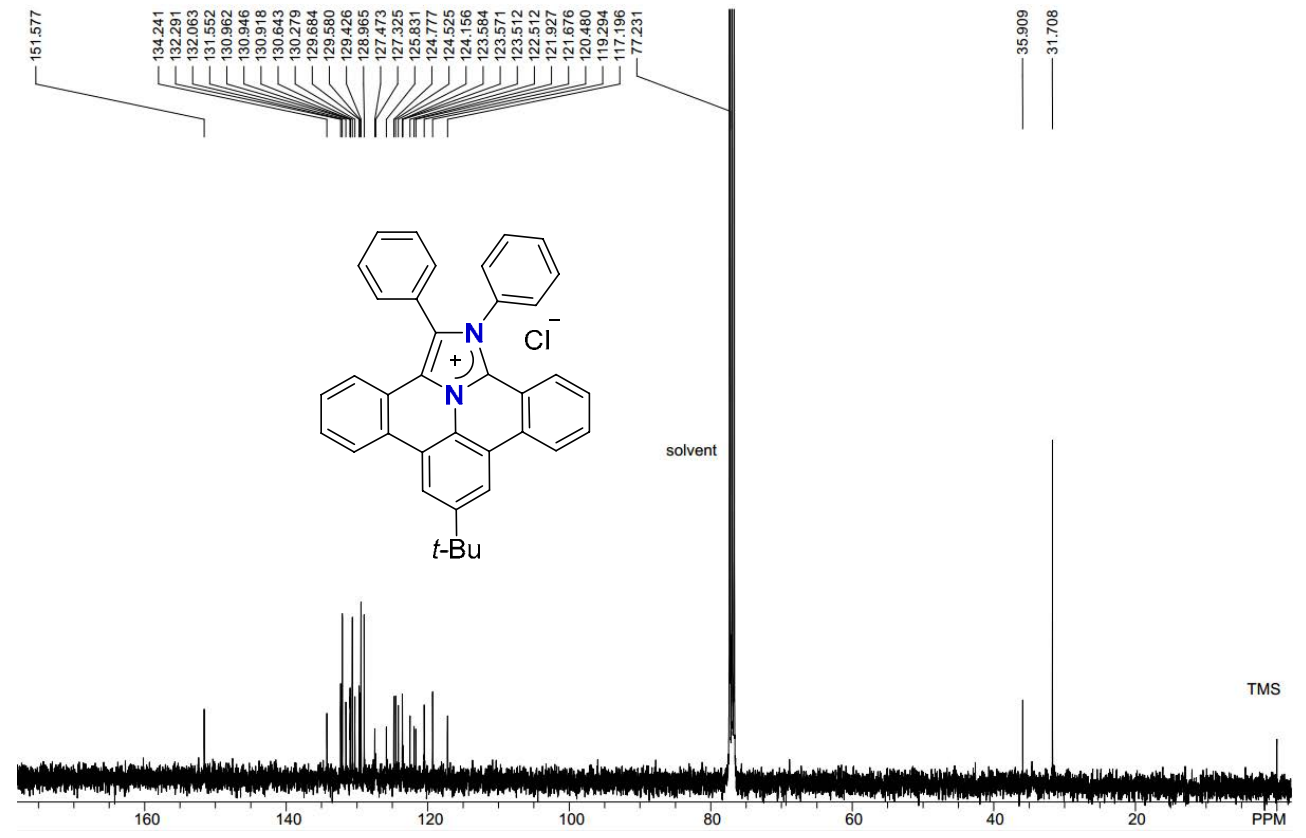


Figure S2. ^{13}C NMR spectrum of **3a** (100 MHz, $CDCl_3$, 300 K).

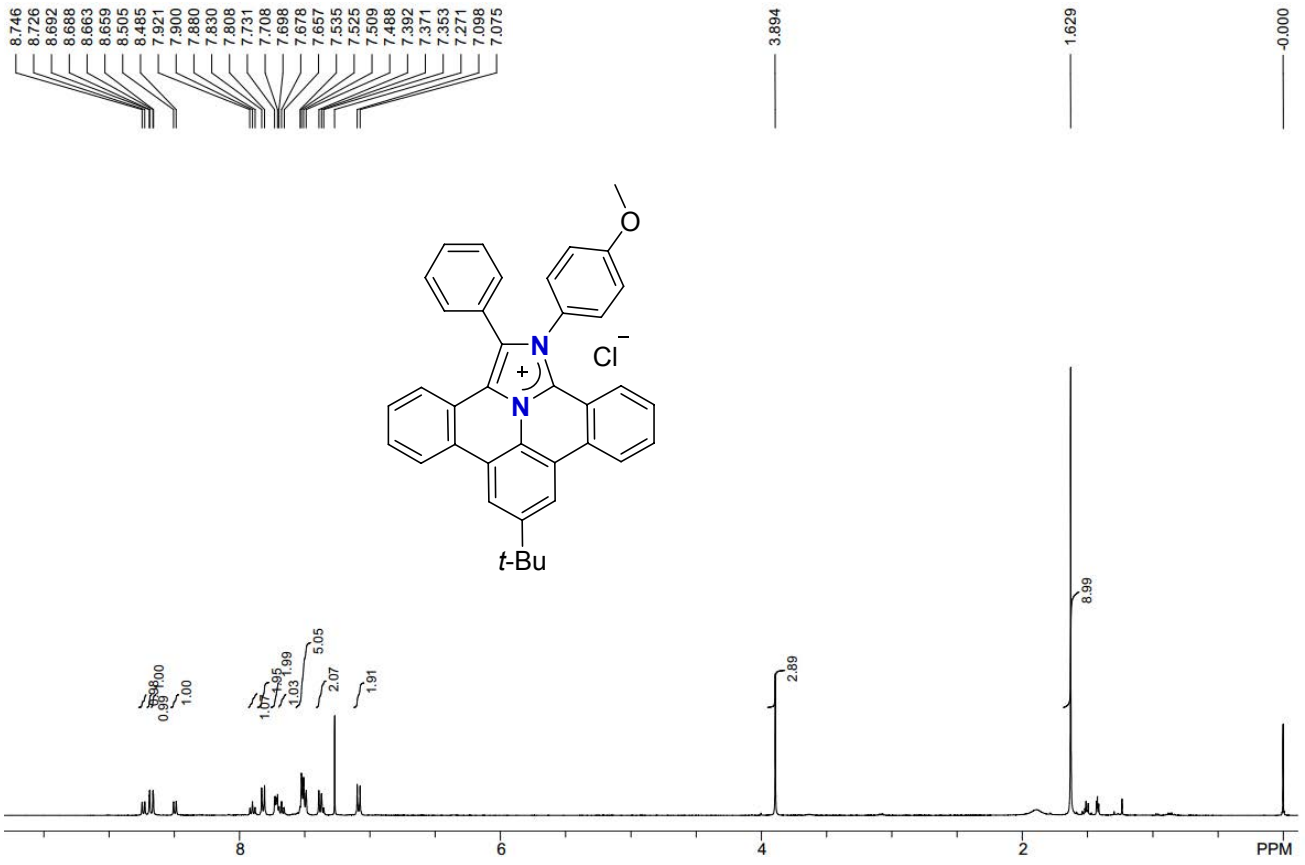


Figure S3. ^{1}H NMR spectrum of **3b** (400 MHz, $CDCl_3$, 300 K).

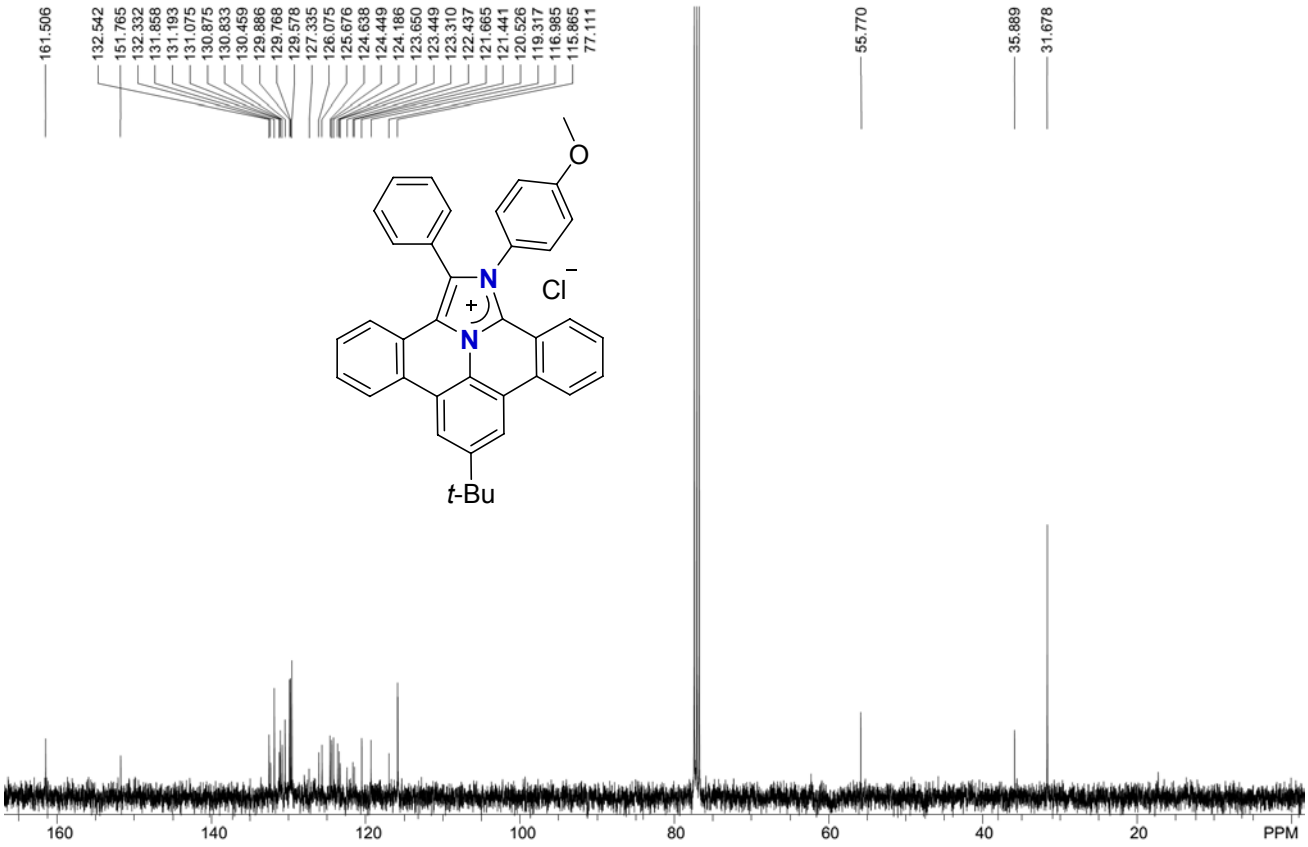


Figure S4. ^{13}C NMR spectrum of **3b** (100 MHz, $CDCl_3$, 300 K).

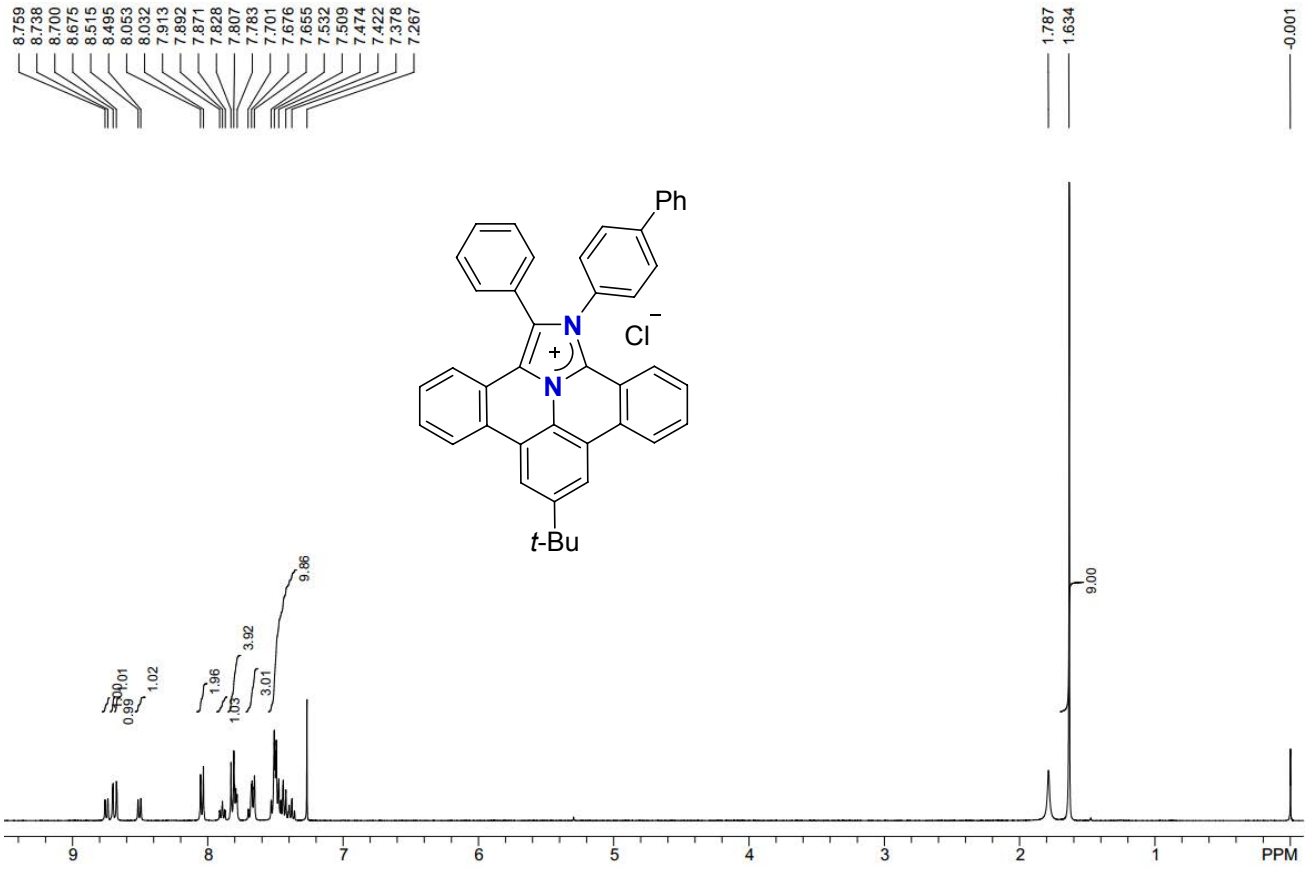


Figure S5. ^{1}H NMR spectrum of **3c** (400 MHz, $CDCl_3$, 300 K).

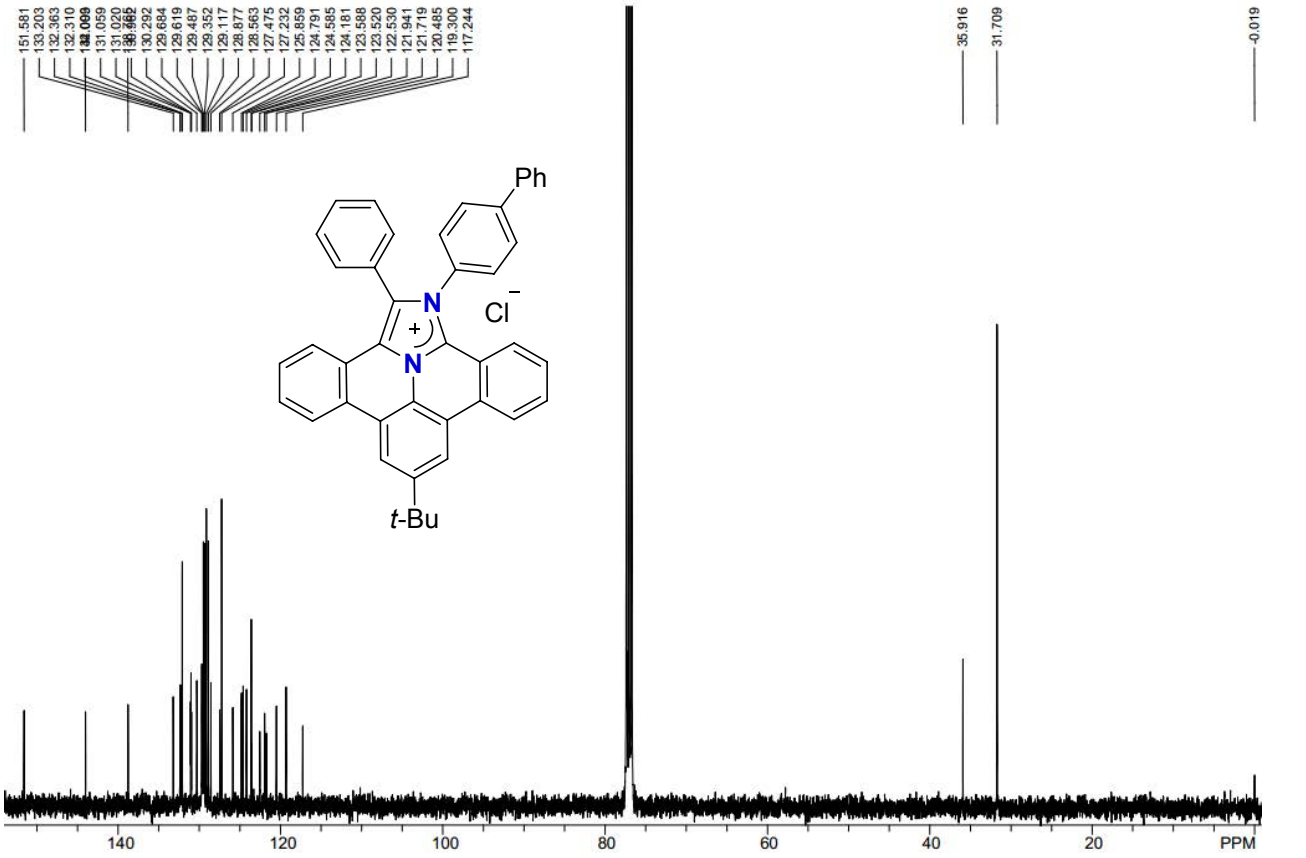


Figure S6. ^{13}C NMR spectrum of **3c** (100 MHz, $CDCl_3$, 300 K).

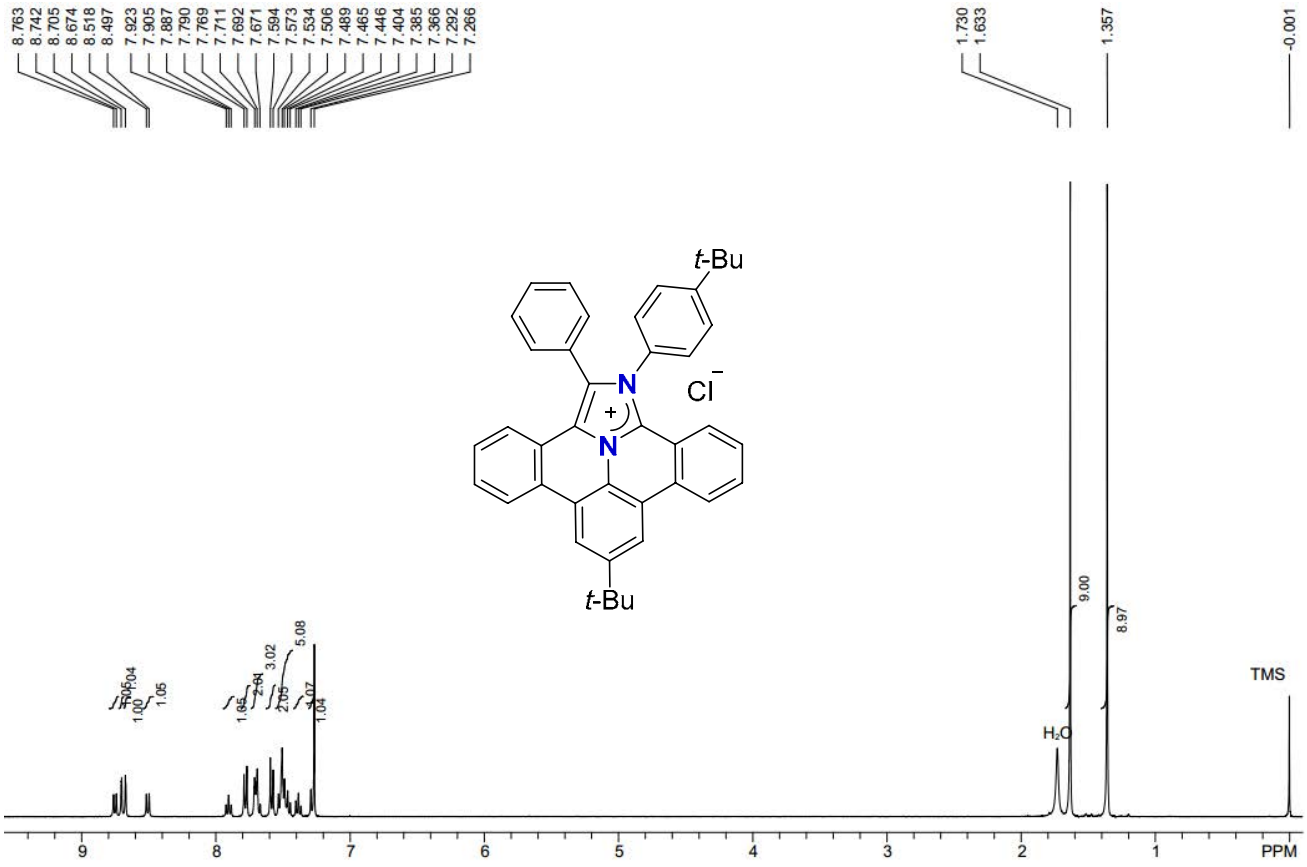


Figure S7. ^{1}H NMR spectrum of **3d** (400 MHz, $CDCl_3$, 300 K).

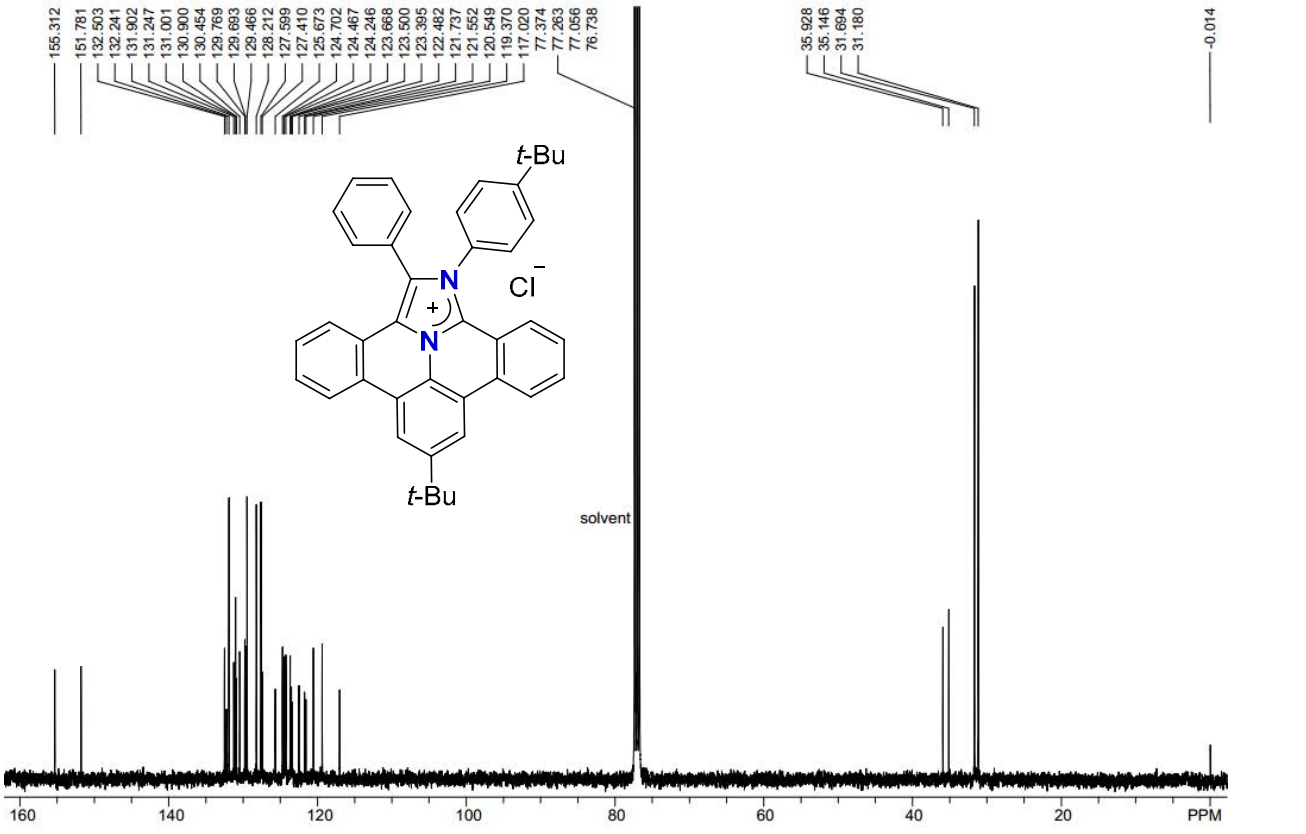


Figure S8. ^{13}C NMR spectrum of **3d** (100 MHz, $CDCl_3$, 300 K).

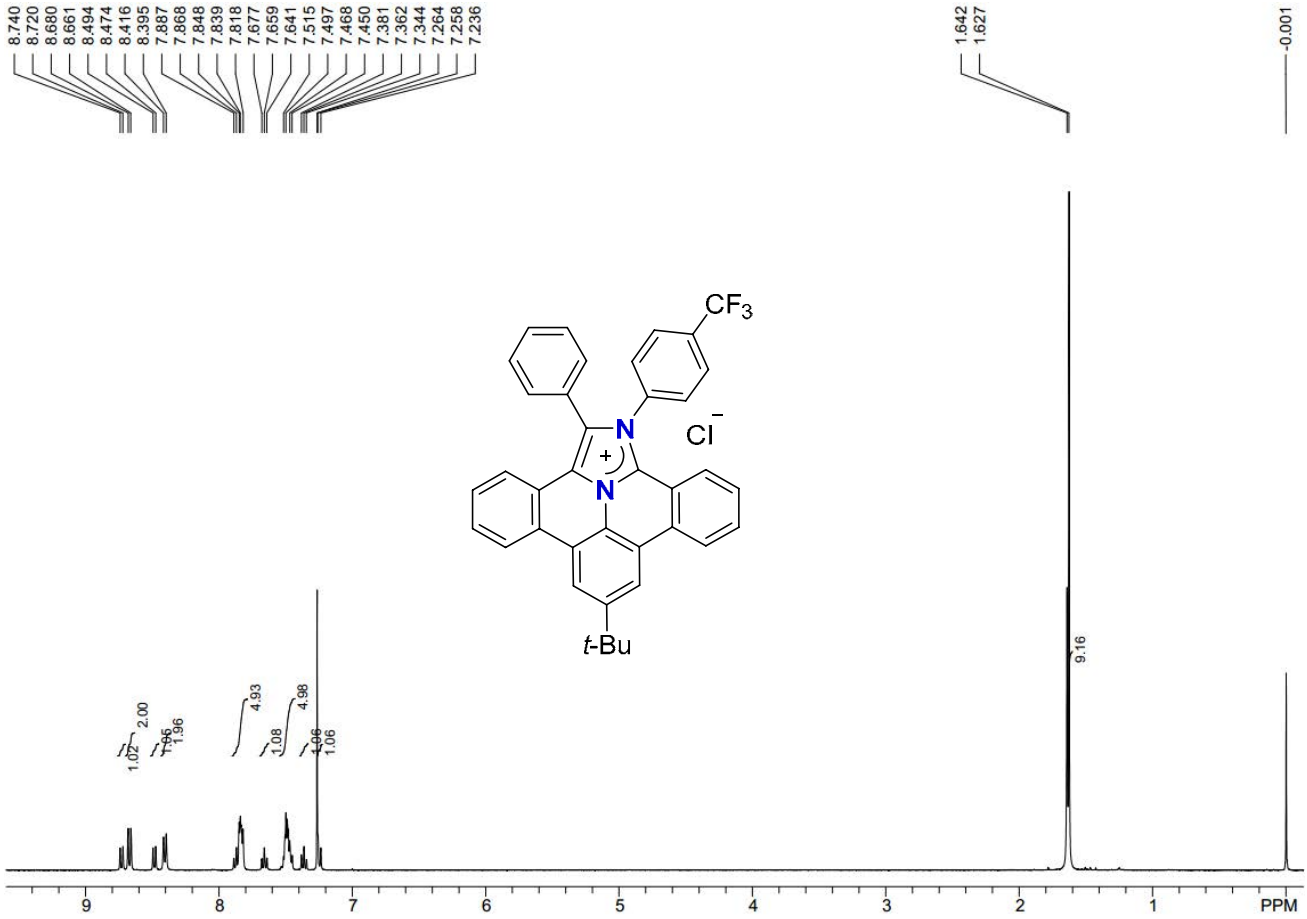


Figure S9. ^{1}H NMR spectrum of **3e** (400 MHz, $CDCl_3$, 300 K).

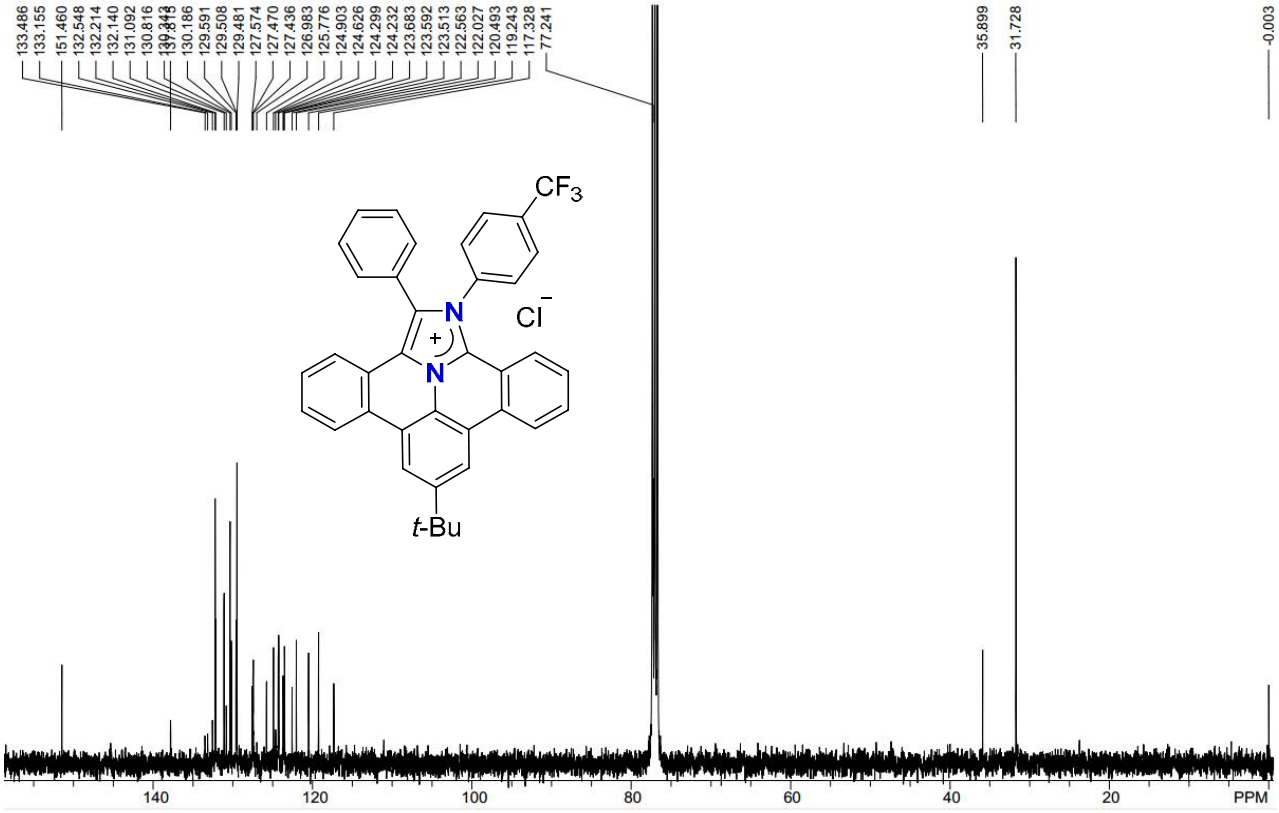


Figure S10. ^{13}C NMR spectrum of **3e** (100 MHz, $CDCl_3$, 300 K).

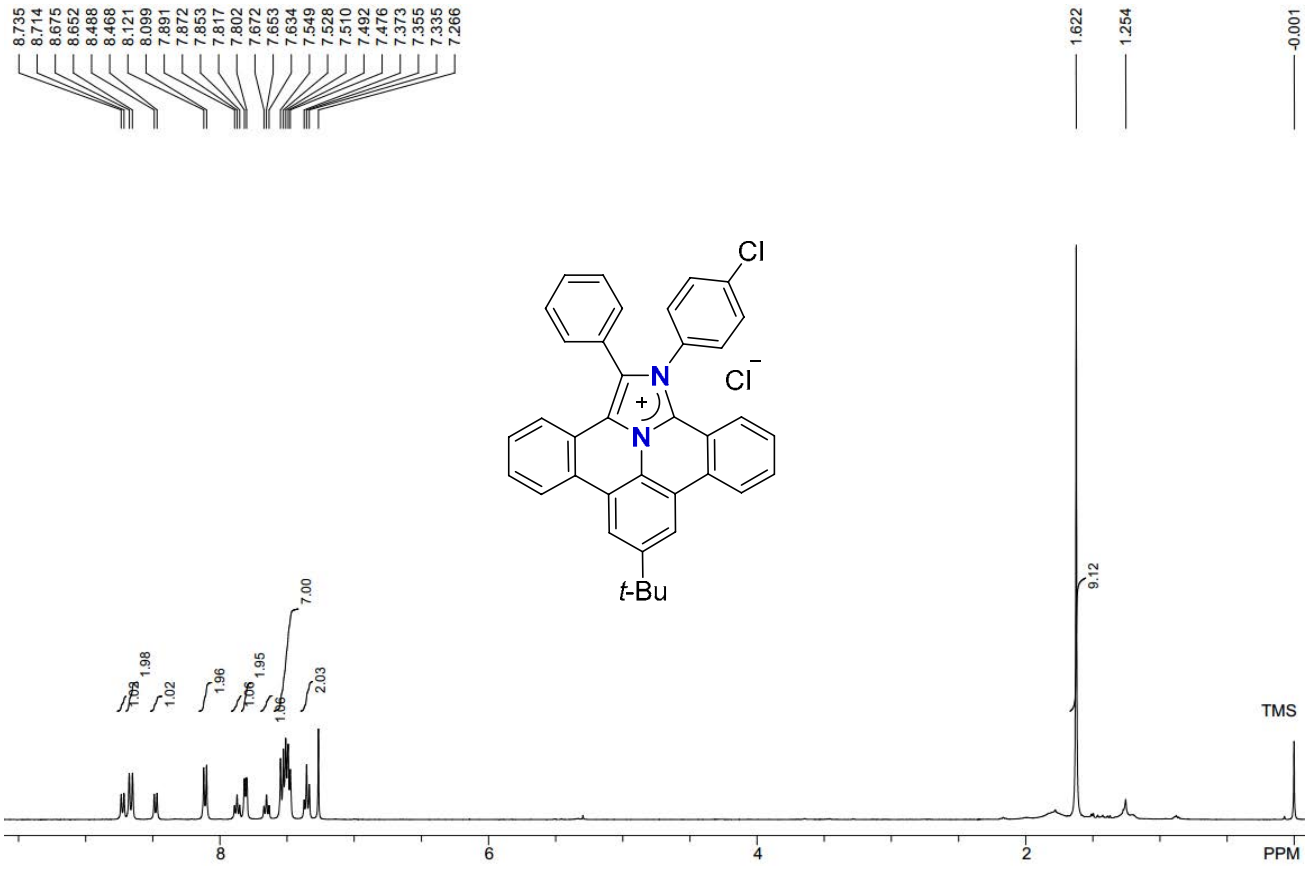


Figure S11. ^{1}H NMR spectrum of **3f** (400 MHz, $CDCl_3$, 300 K).

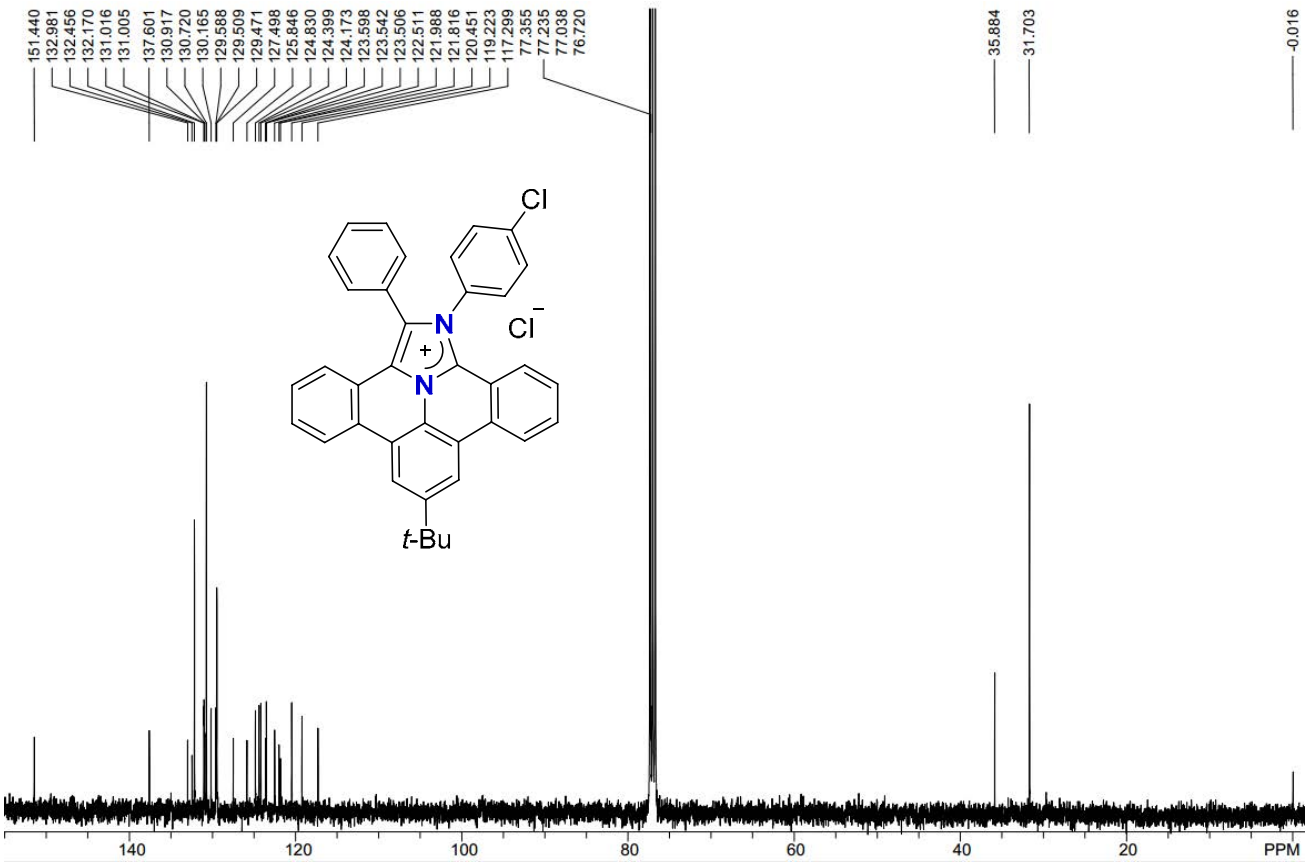


Figure S12. ^{13}C NMR spectrum of **3f** (100 MHz, $CDCl_3$, 300 K).

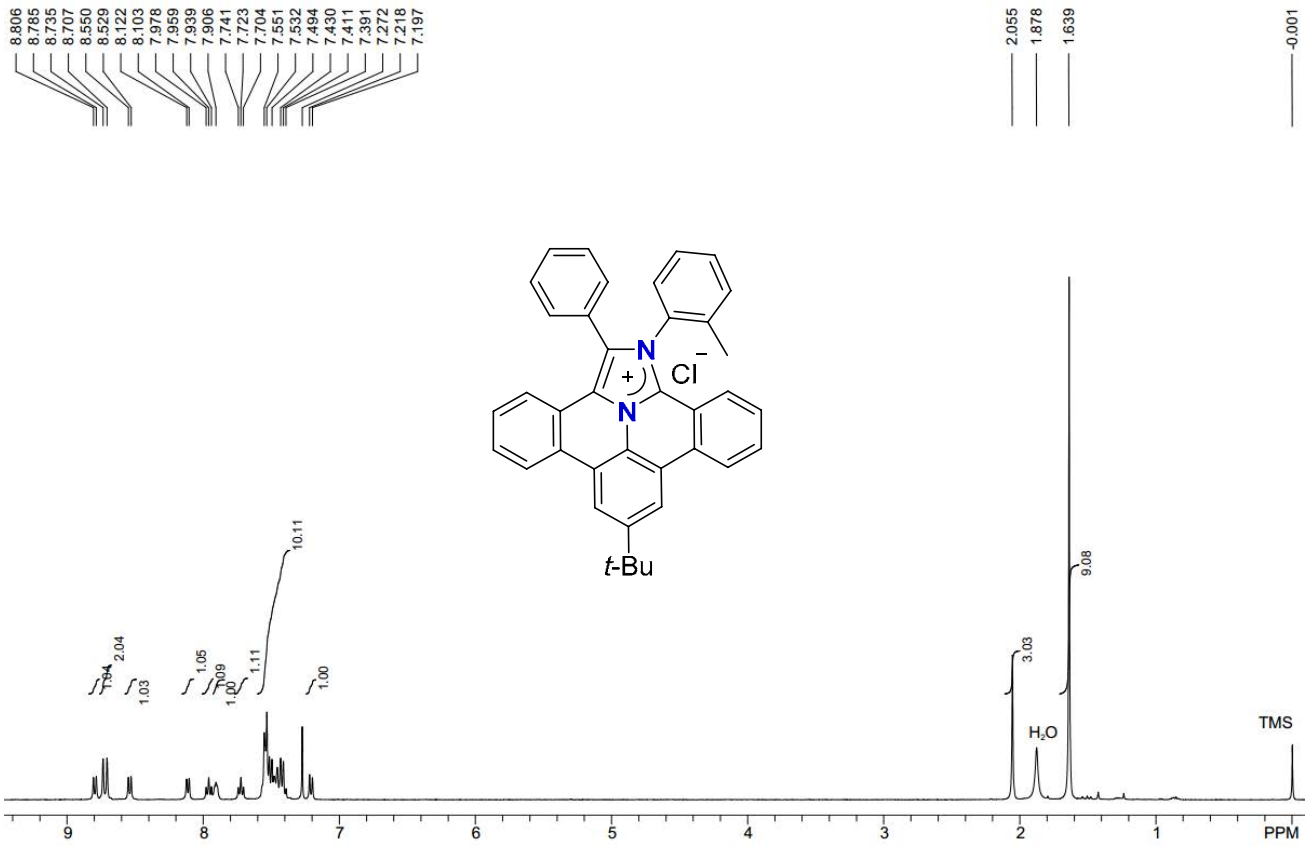


Figure S13. ^{1}H NMR spectrum of **3g** (400 MHz, $CDCl_3$, 300 K).

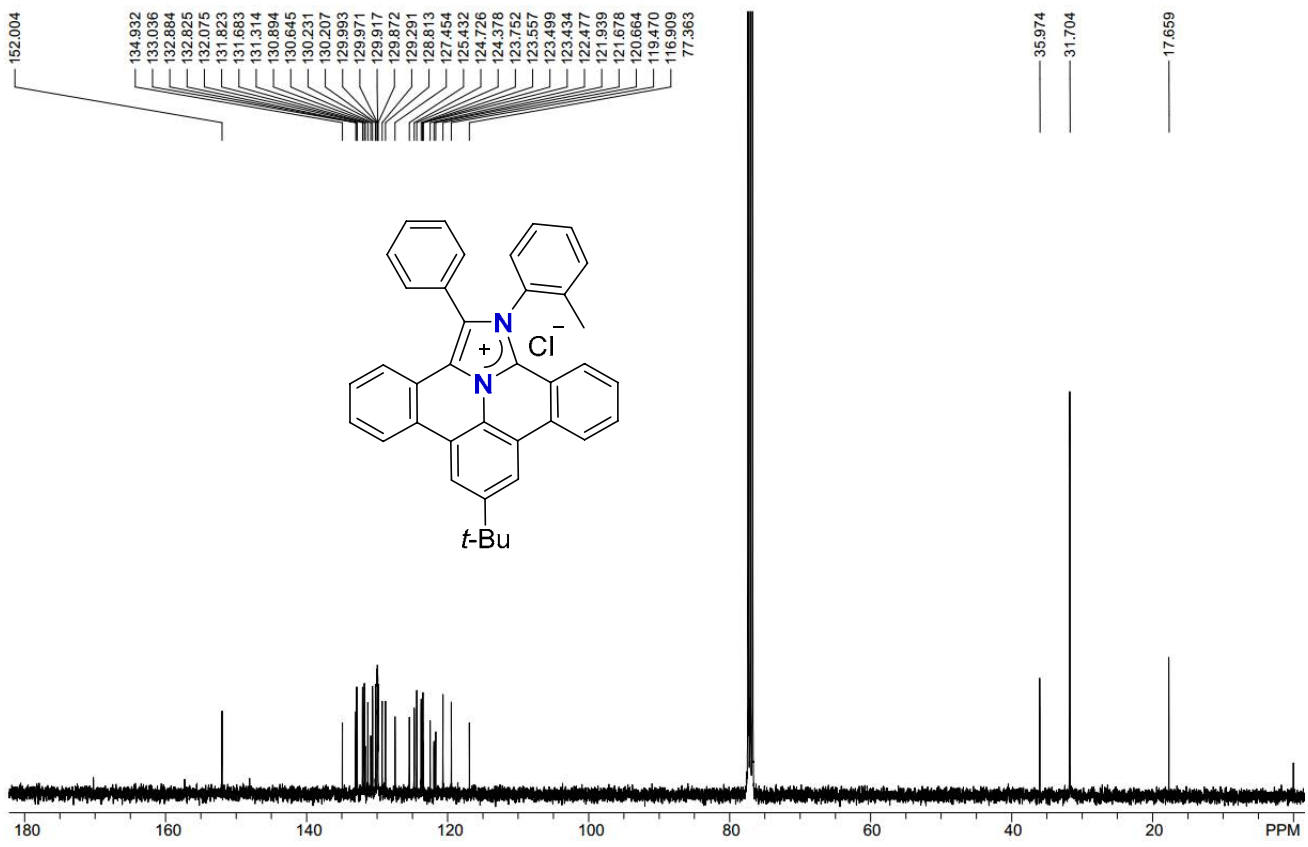


Figure S14. ^{13}C NMR spectrum of **3g** (100 MHz, $CDCl_3$, 300 K).

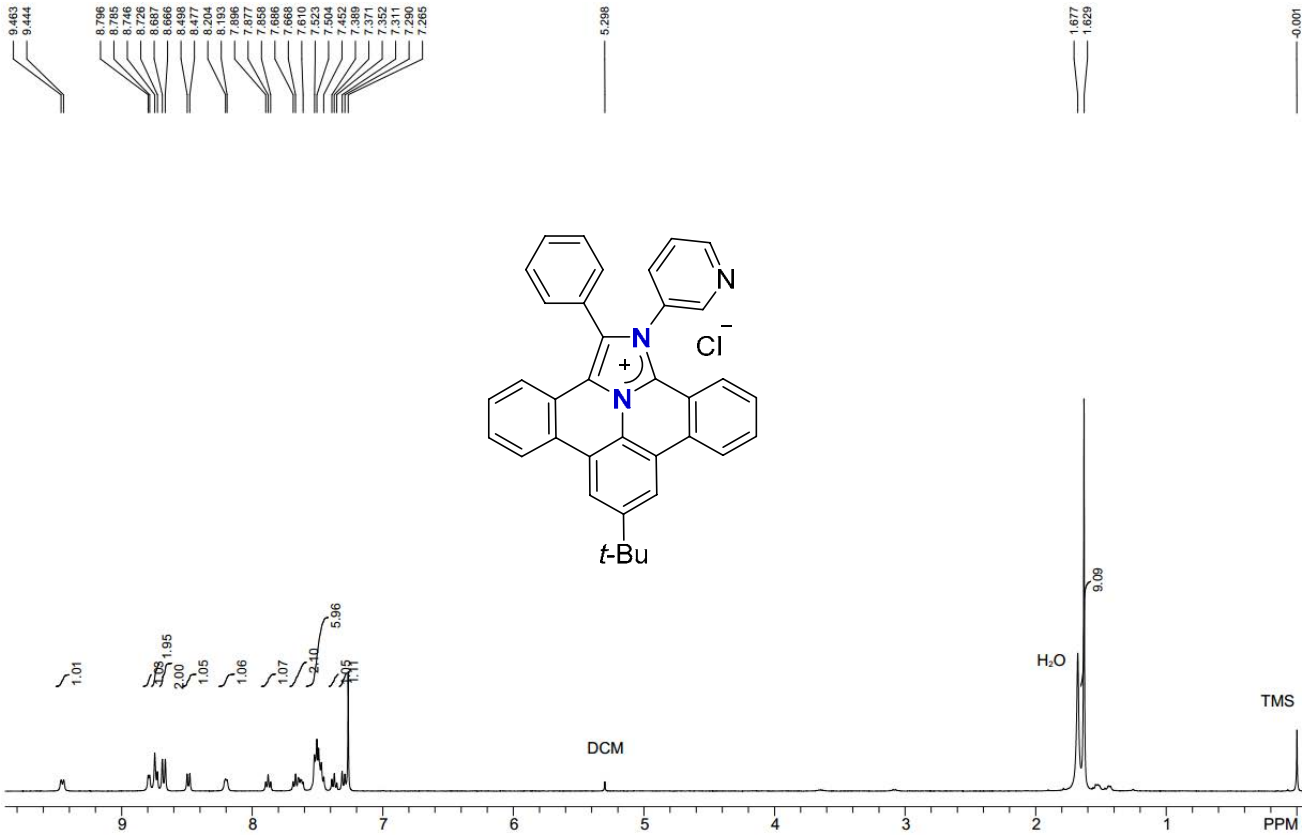


Figure S15. ^{1}H NMR spectrum of **3h** (400 MHz, $CDCl_3$, 300 K).

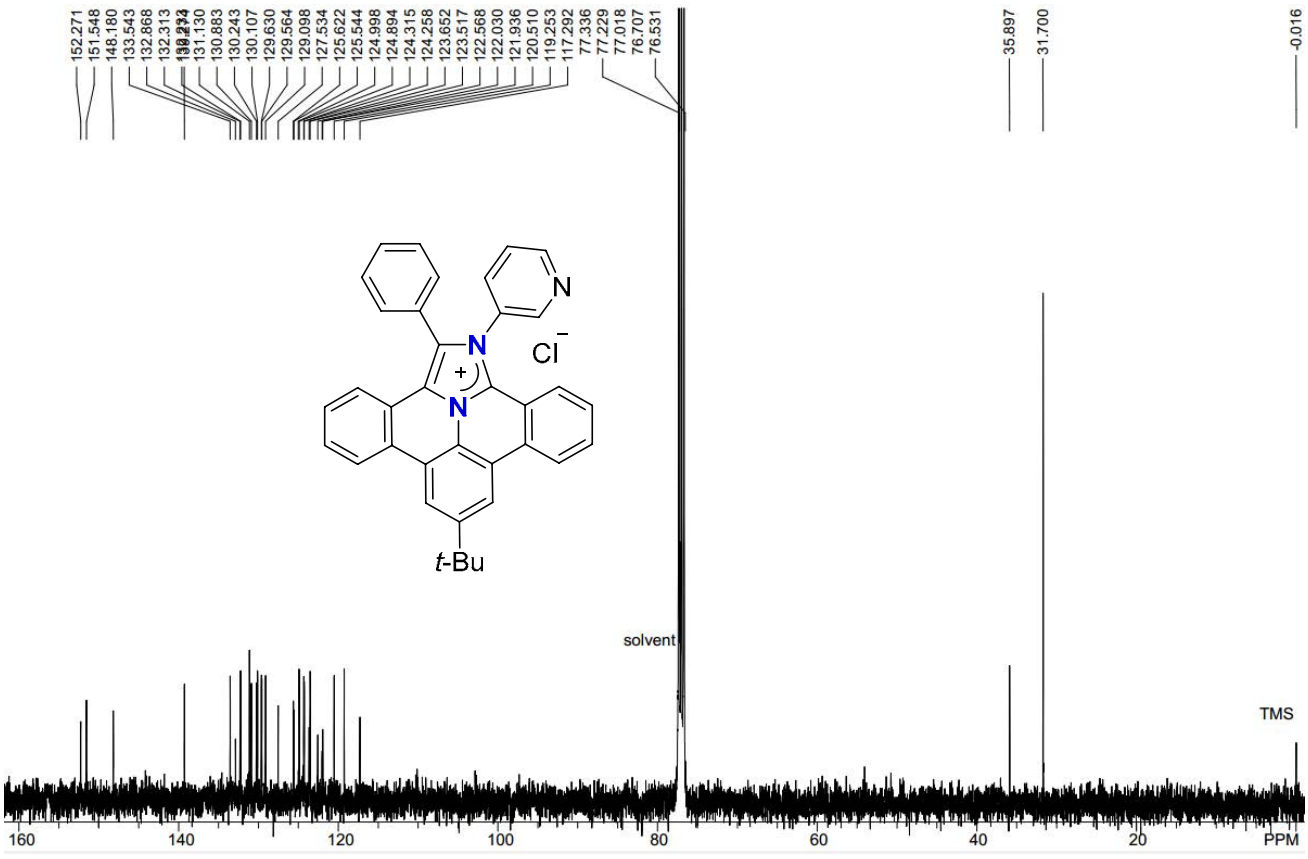


Figure S16. ^{13}C NMR spectrum of **3h** (100 MHz, $CDCl_3$, 300 K).

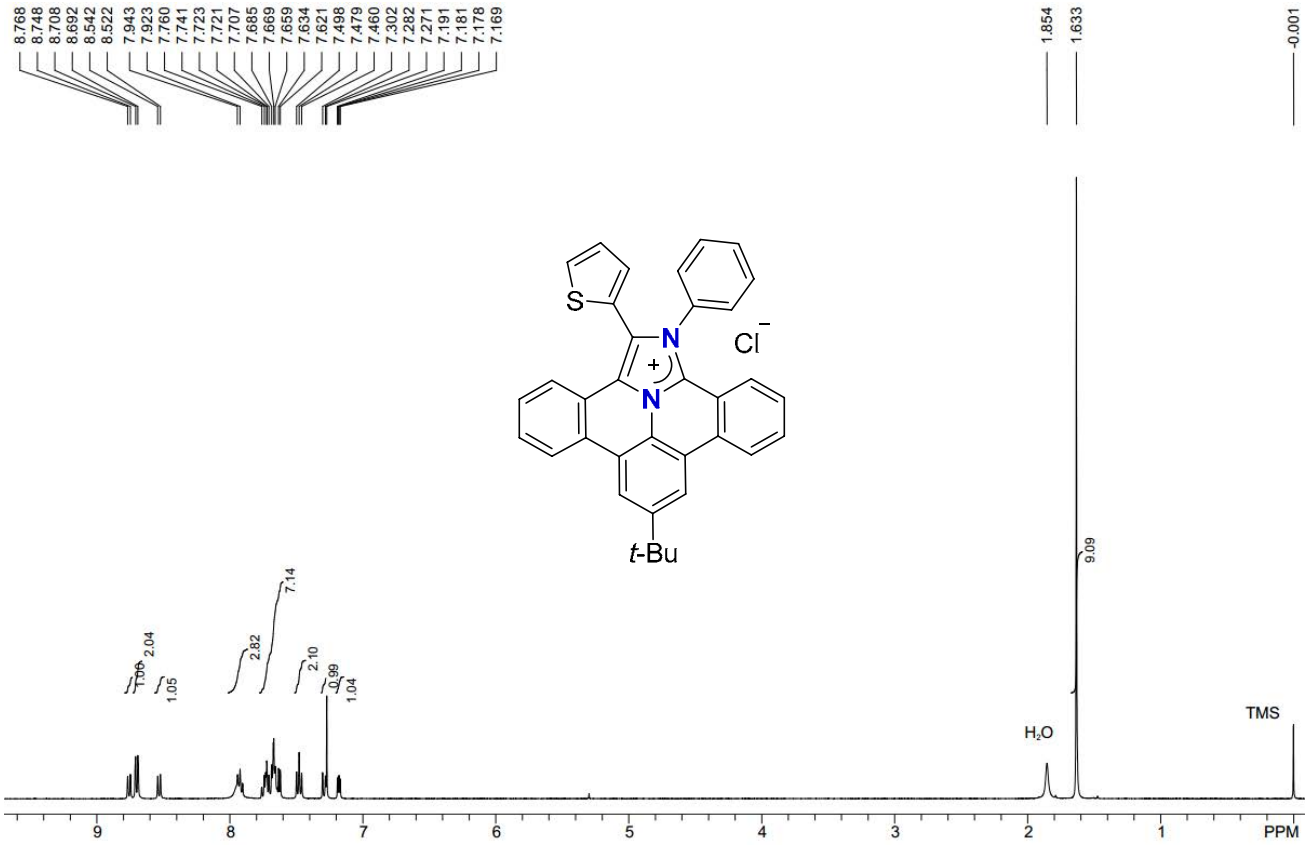


Figure S17. ^{1}H NMR spectrum of **3i** (400 MHz, $CDCl_3$, 300 K).

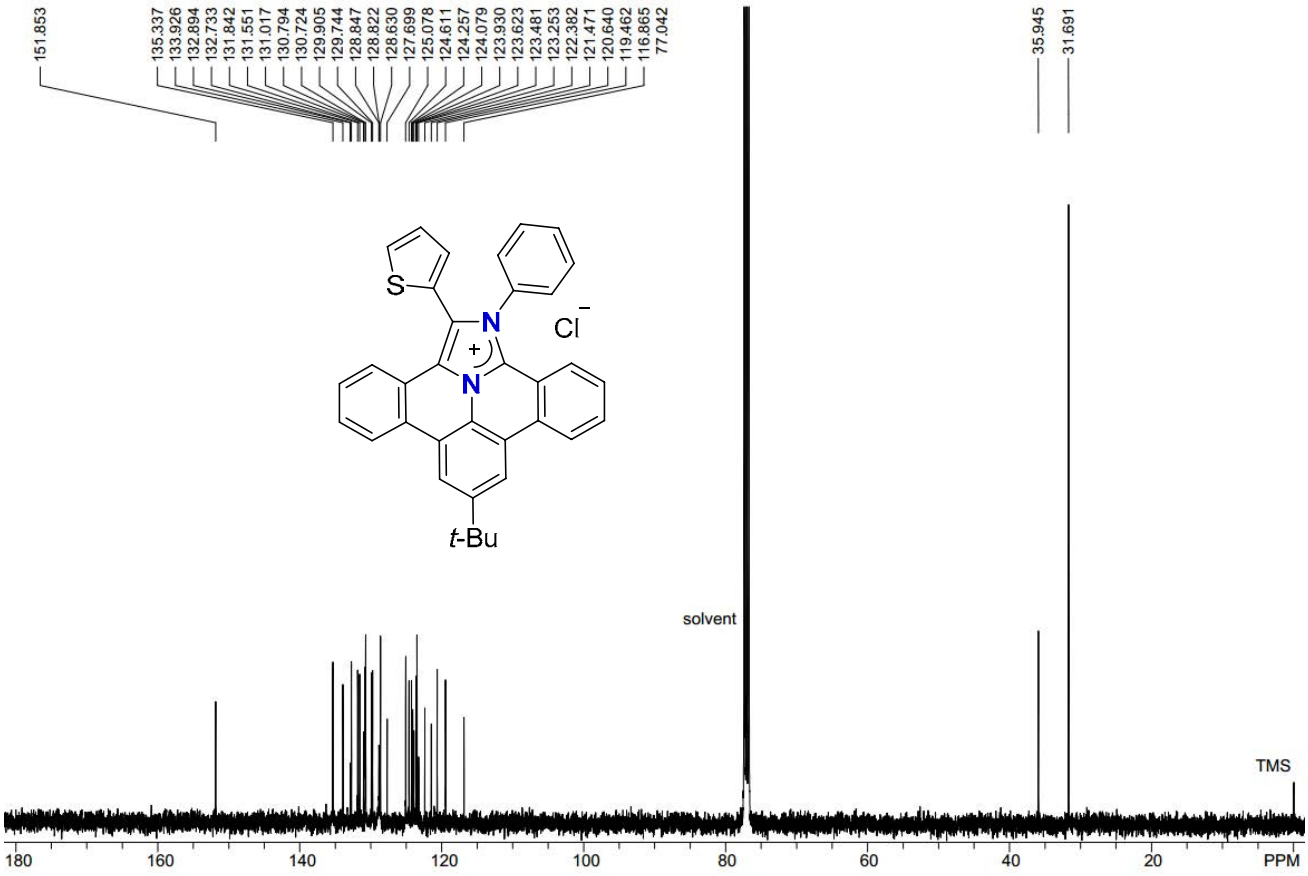


Figure S18. ^{13}C NMR spectrum of **3i** (100 MHz, $CDCl_3$, 300 K).

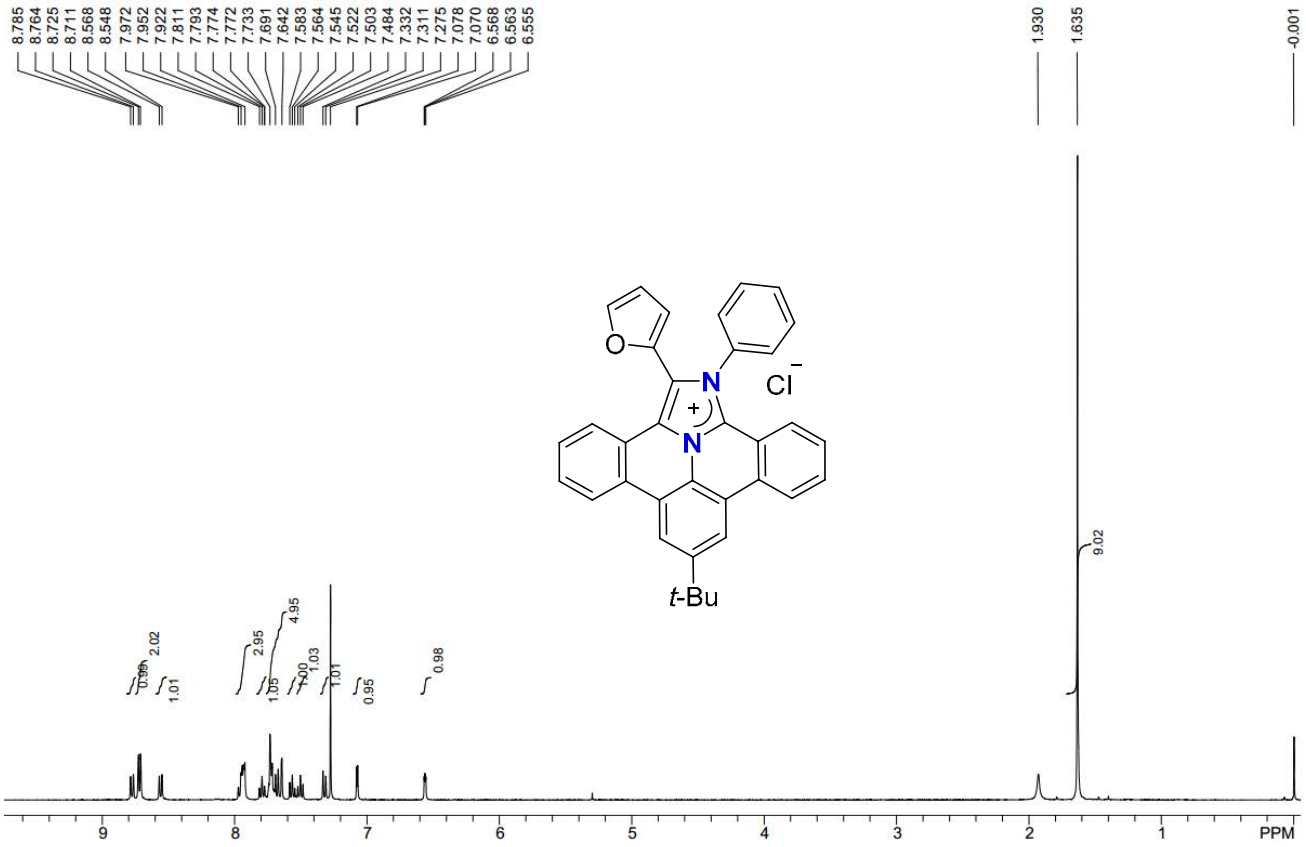


Figure S19. ^{1}H NMR spectrum of **3j** (400 MHz, $CDCl_3$, 300 K).

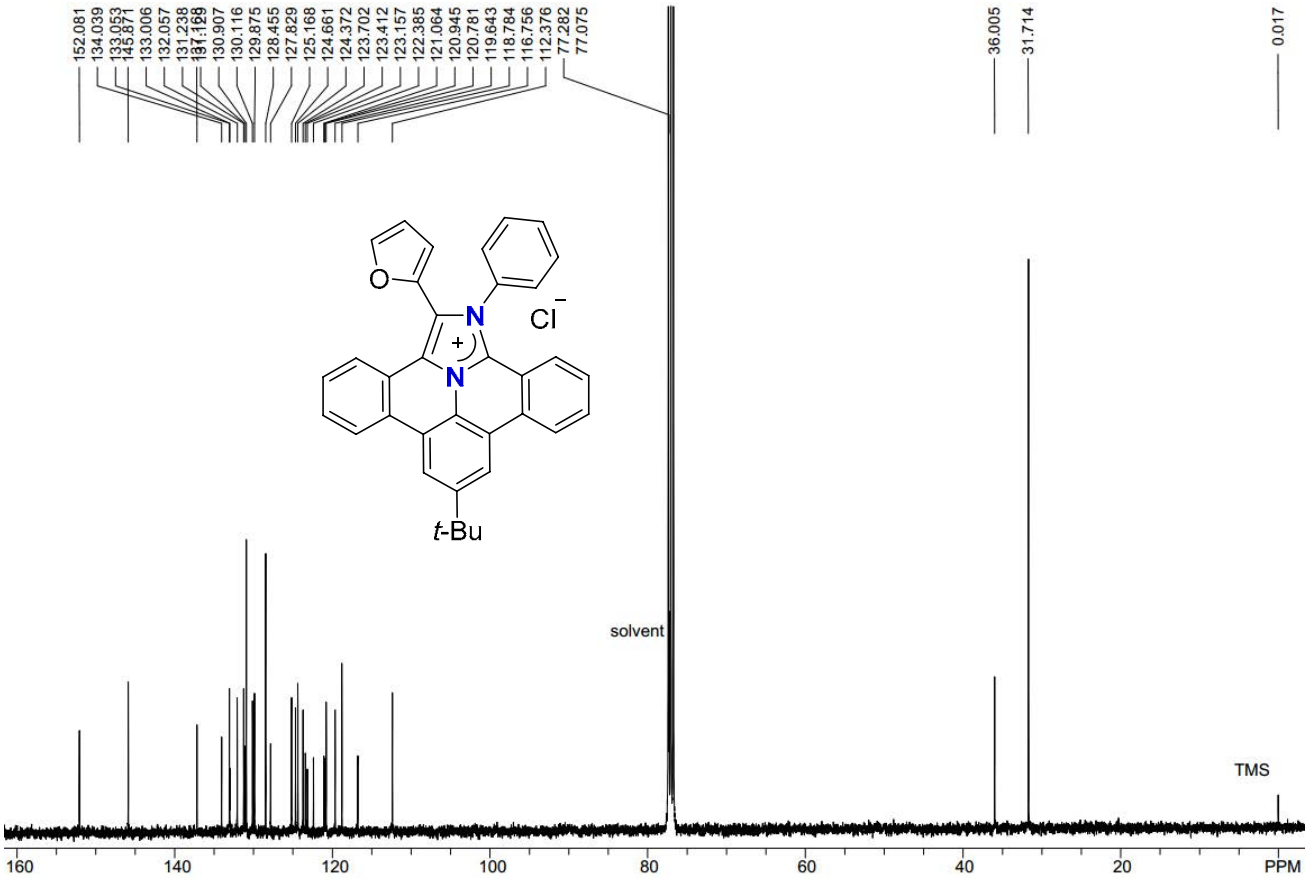


Figure S20. ^{13}C NMR spectrum of **3j** (100 MHz, $CDCl_3$, 300 K).

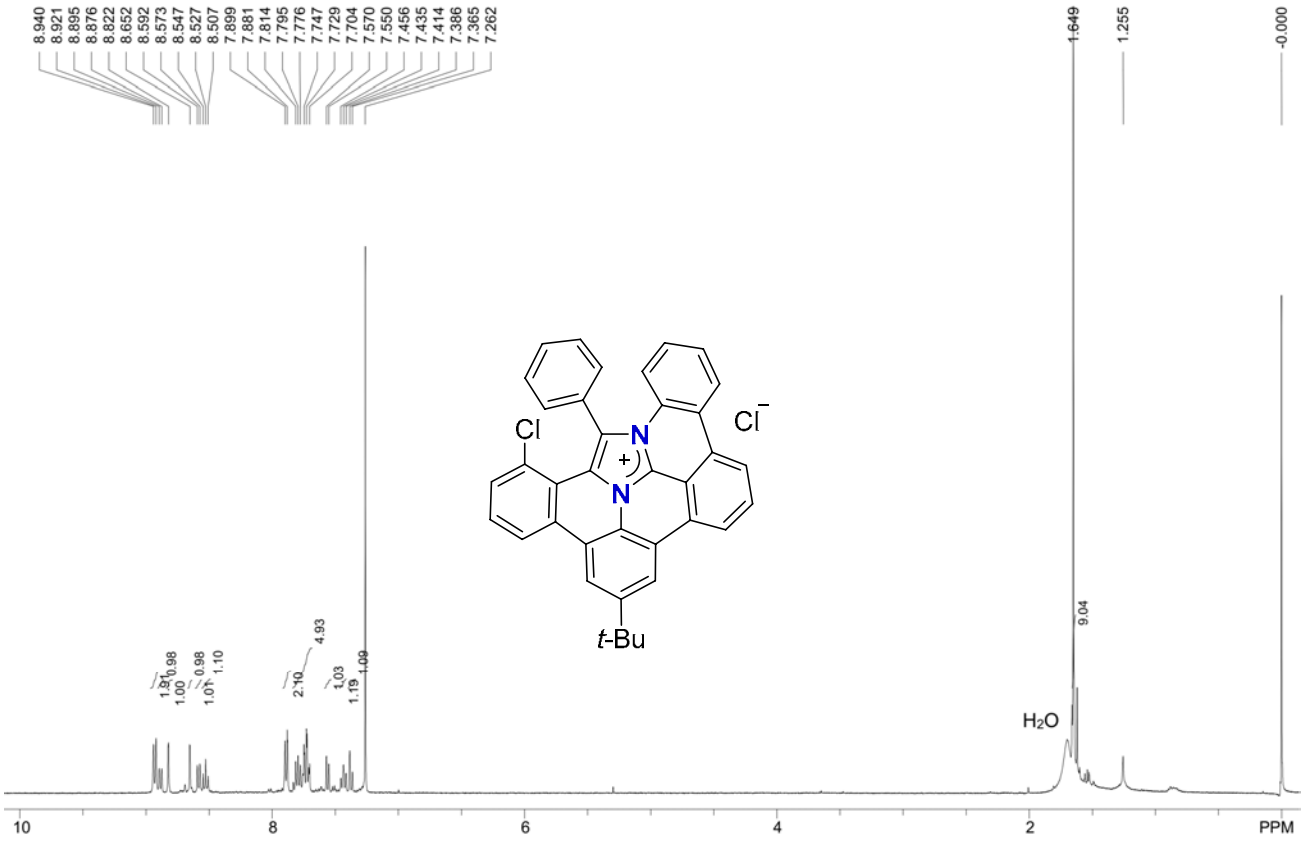


Figure S21. ^{1}H NMR spectrum of **3k** (400 MHz, $CDCl_3$, 300 K).

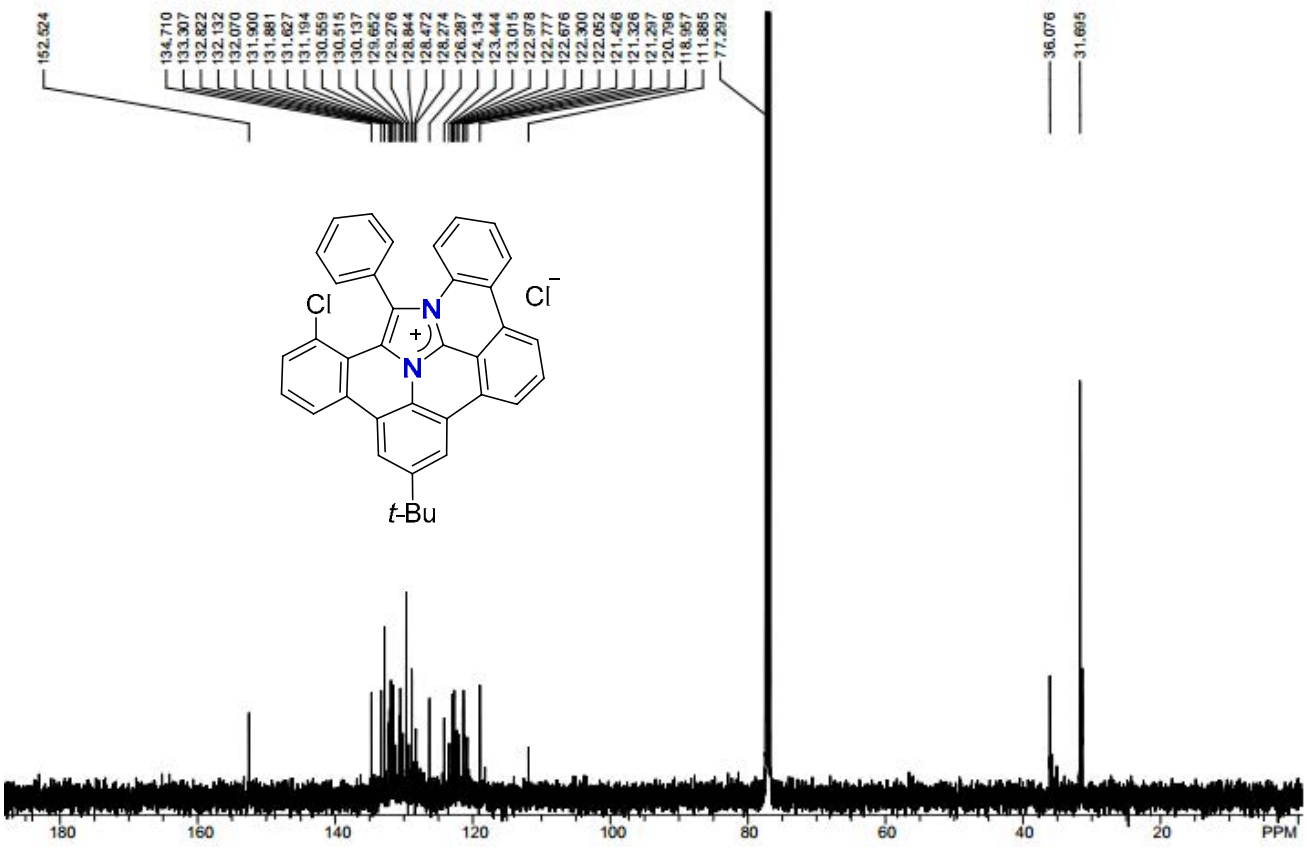


Figure S22. ^{13}C NMR spectrum of **3k** (100 MHz, $CDCl_3$, 300 K).

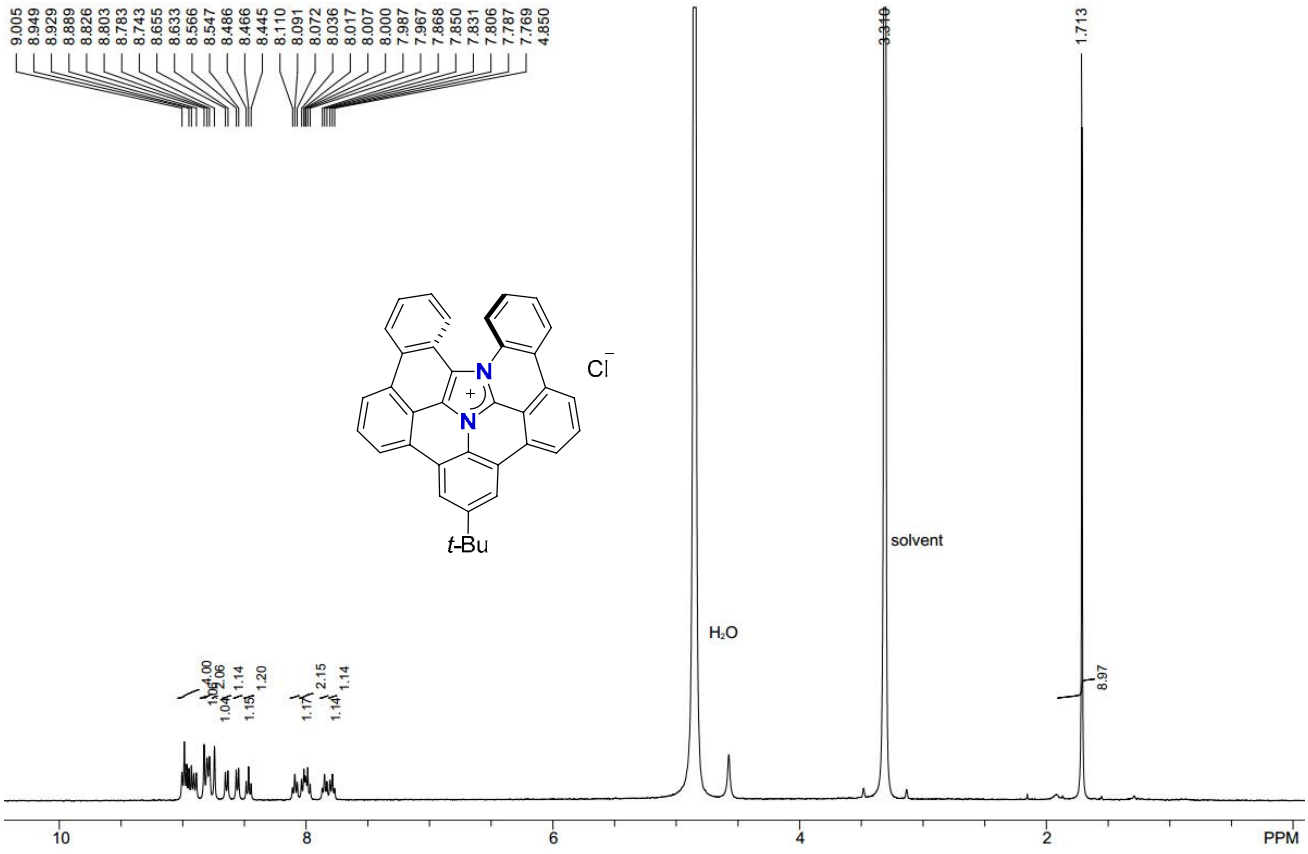


Figure S23. ^{1}H NMR spectrum of **4a** (400 MHz, CD_3OD, 300 K).

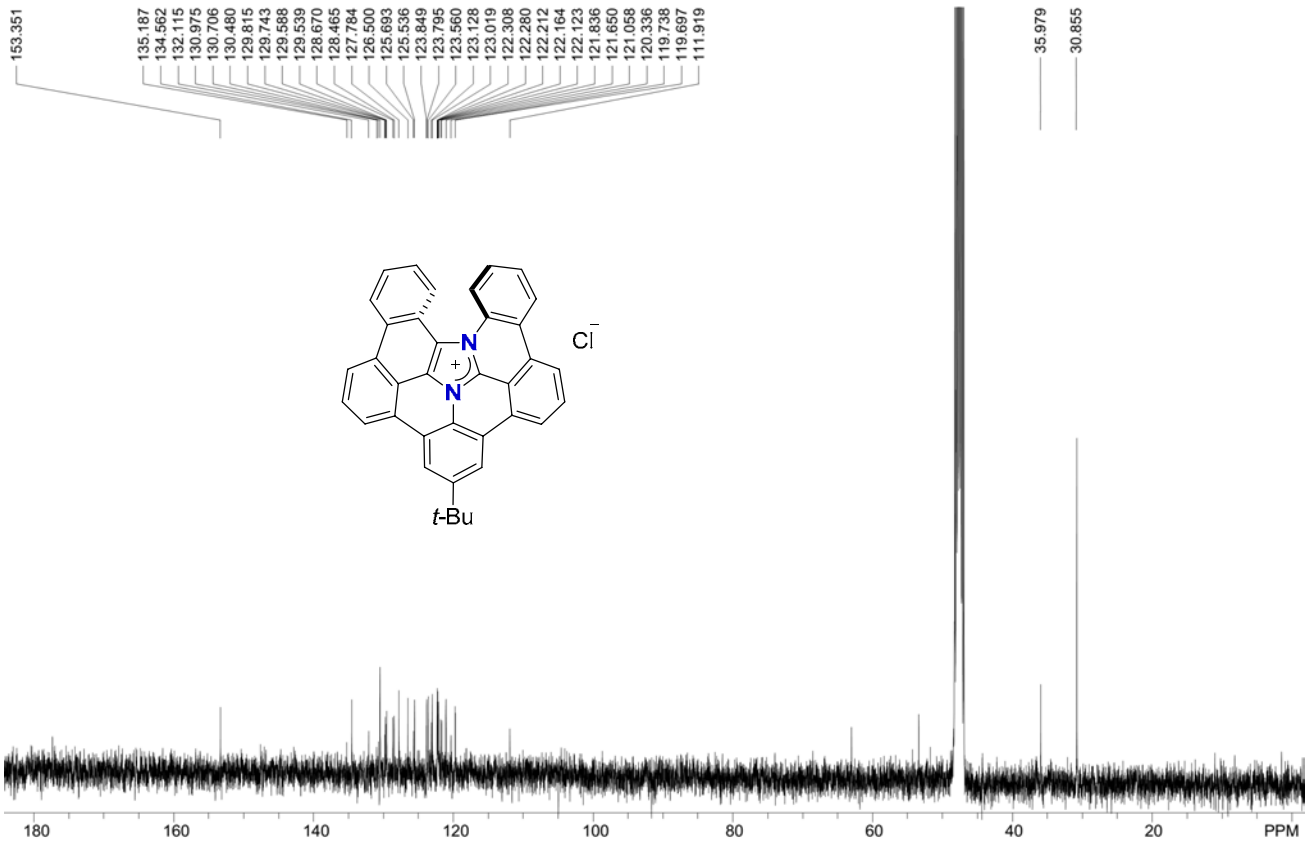


Figure S24. ^{13}C NMR spectrum of **4a** (100 MHz, CD_3OD, 300 K).

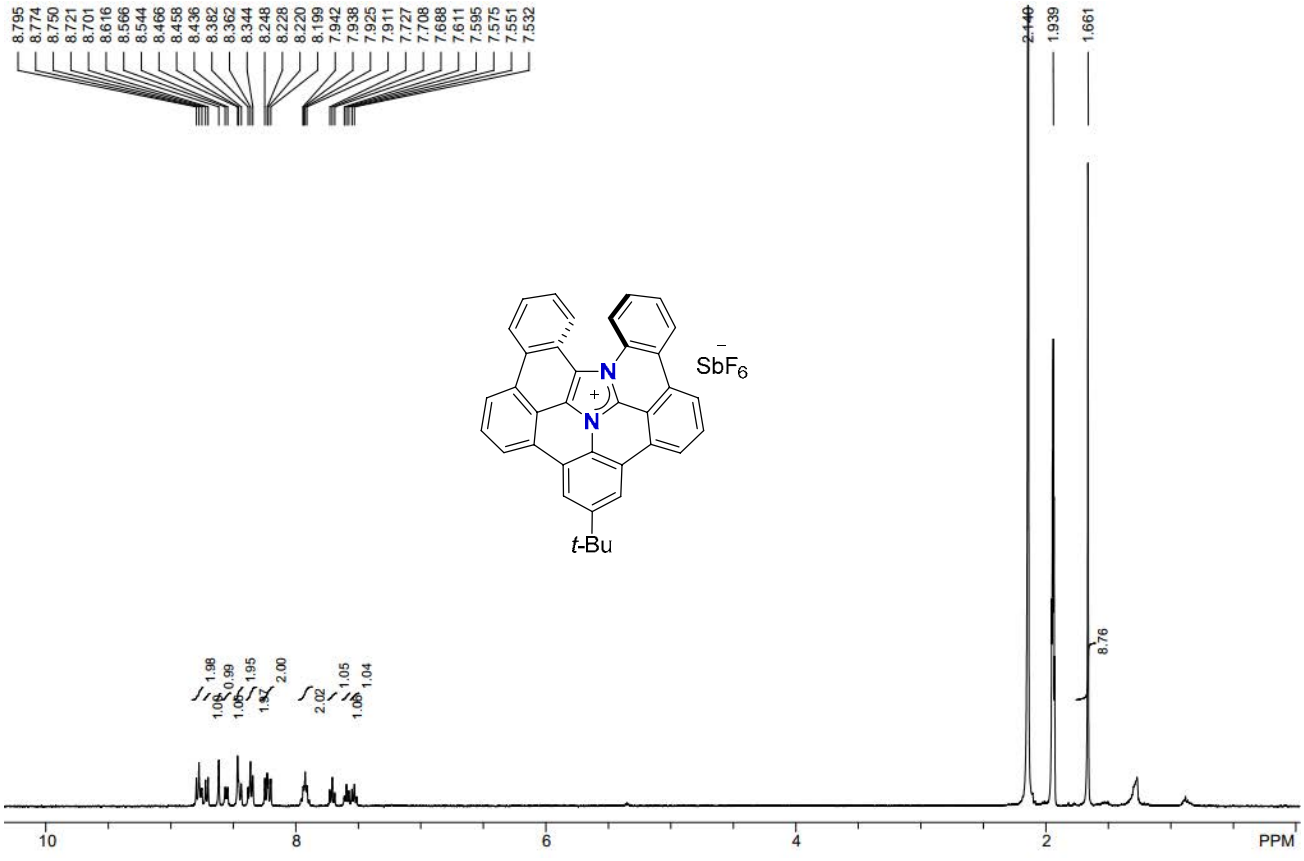


Figure S25. ^{1}H NMR spectrum of **4b** (400 MHz, CD_3CN, 300 K).

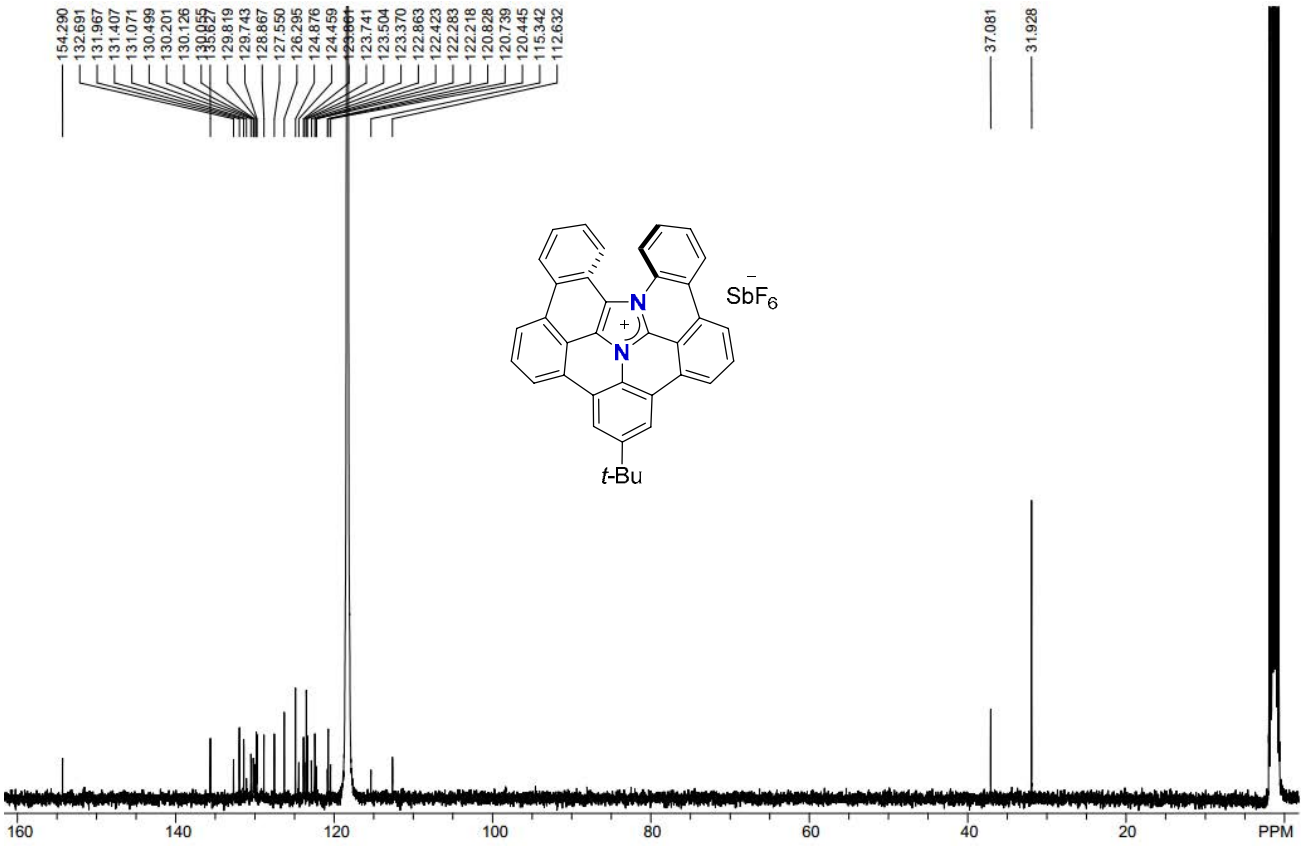


Figure S26. ^{13}C NMR spectrum of **4b** (100 MHz, CD_3CN, 300 K).

3. Optical Properties

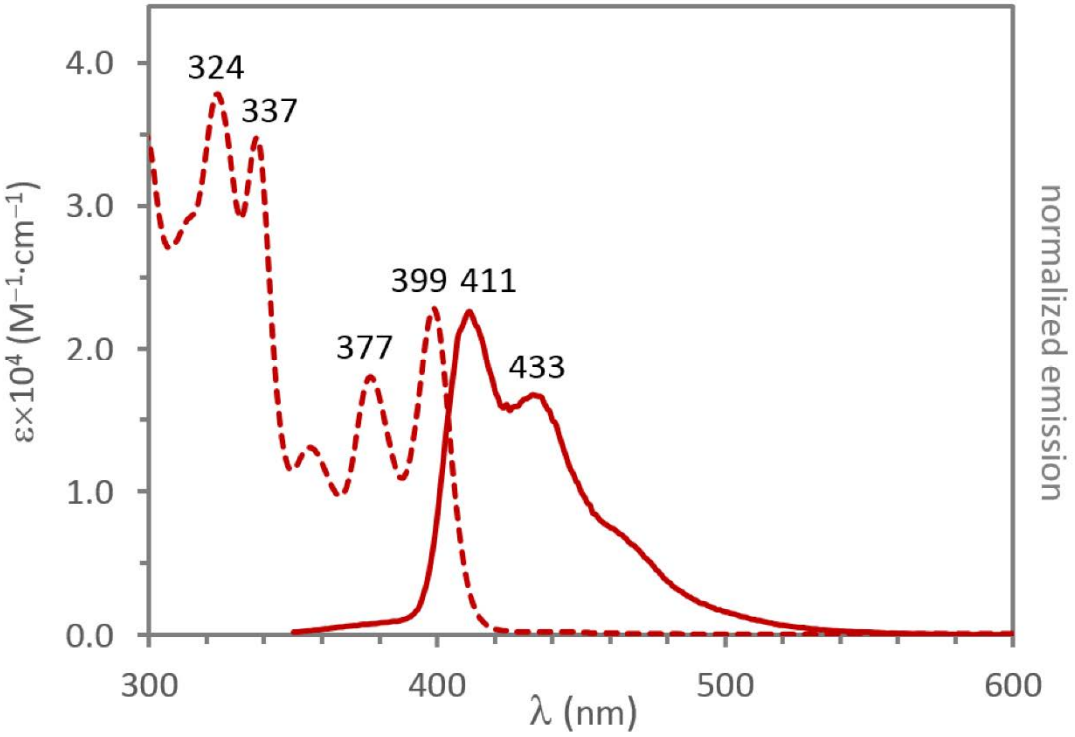


Figure S27. UV–vis absorption (2.5×10^{-5} M) and emission (2.5×10^{-6} M; excited at 340 nm) spectra of **4b** in dichloromethane.

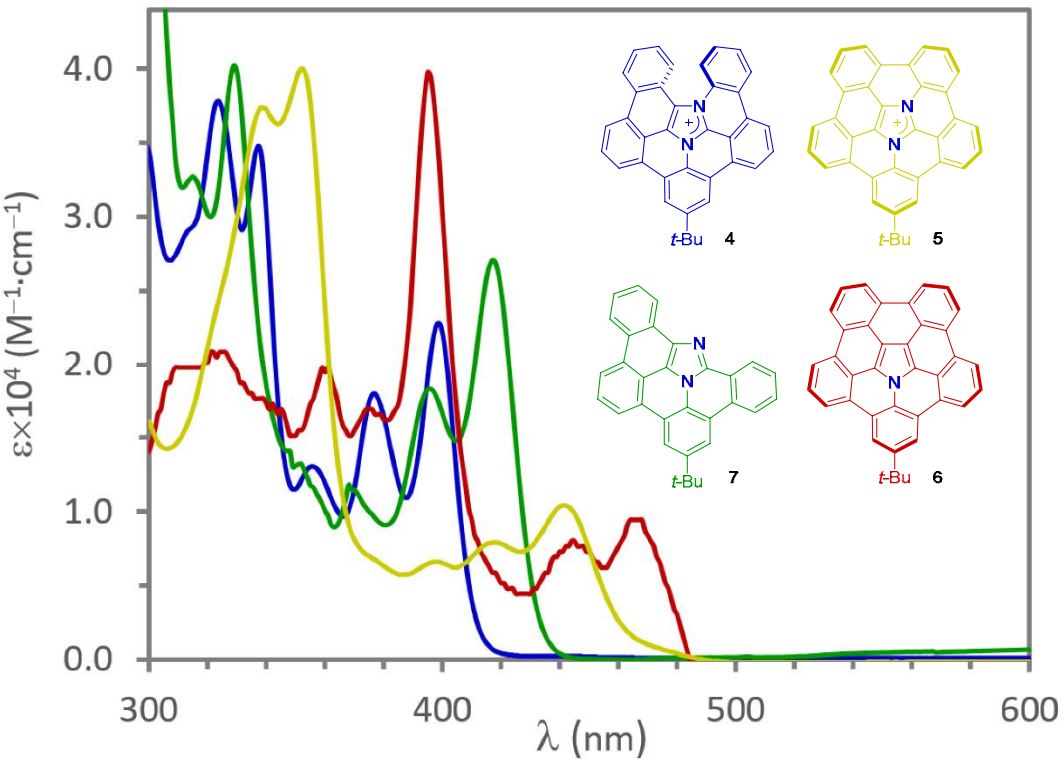


Figure S28. UV–vis absorption spectra of **4b** (2.5×10^{-5} M), **5** (2.0×10^{-5} M), **6** (2.8×10^{-5} M), and **7** (2.0×10^{-5} M) in dichloromethane.

4. X-Ray Crystallographic Data

Single crystals suitable for X-ray analysis for **3a** and **3k** were obtained by slow evaporation of sample solution in dichloromethane at room temperature. A single crystal was mounted with mineral oil on a loop-type mount and transferred to the goniometer of a Bruker D8 Quest diffractometer. The radiation was performed with Multilayer Mirror-monochromated Incoatec microfocus source (Mo-Kα, λ = 0.71073 Å).

On the other hand, needle-like single crystals of **4b** were obtained by slow vapor diffusion of hexane into a solution with a saturated concentration of **4b** in 1,2-dichlorobenzene. Data collection for X-ray analysis was conducted by Rigaku XtaLAB Synergy-Custom diffractometer (Cu-Kα, λ = 1.54184 Å) equipped with a Rigaku HyPix-Arc 150°.

The structures were solved by direct method with SHELXT[4] and refined by full-matrix least-squares techniques against F^2 with SHELXL-2018/3.[4] The intensities were corrected for Lorentz and polarization effects. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed using AFIX instructions. In the **4b** crystal packing structure, the heavily disordered solvent molecules which could not be modelled were removed by applying the SQUEEZE protocol in PLATON[5] software.

(4) Sheldrick, G. M. *Acta Cryst.* **2015**, *A71*, 3-8.
(5) Spek, A. L. *J. Appl. Cryst.* **2003**, *36*, 7–13.

Table S1. Crystal data and structure refinement for **3a**, **3k**, and **4b**.

compound	**3a**	**3k**	**4b**
CCDC number	**2160757**	**2160758**	**2160759**
Molecular formula	$C_{37}H_{29}ClN_2$	$C_{37}H_{32}Cl_2N_2O_3$	$C_{37}H_{25}N_2F_6Sb$
Formula weight	537.07	623.54	770.09
Temperature (K)	100	100	100
Wavelength (Å)	0.71073	0.71073	1.54184
Crystal system	monoclinic	Triclinic	Monoclinic
Space group	*C*2/*m*	*P*-1	$P2_1/c$
Unit cell dimensions a (Å)	30.678(3)	11.6921(13)	6.83820(10)
b (Å)	6.7193(5)	11.7421(12)	31.9395(3)
c (Å)	13.7302(14)	12.1976(12)	29.5549(3)
α (°)	90	85.354(3)	90
β (°)	102.728(4)	62.684(3)	91.5790(10)
γ (°)	90	88.515(3)	90
Volume ($Å^3$)	2760.7(4)	1482.9(3)	6452.60(13)
Z	4	2	8
Density (calculated) ($mg·m^{-3}$)	1.292	1.397	1.585
Absorption cosfficient (mm^{-1})	0.168	0.261	7.740
F(000)	1128	652	3076
Crystal size (mm^3)	0.020 x 0.200 x 0.220	0.100 x 0.140 x0.200	0.023 x 0.034 x 0.457
Theta range (°)	2.25 to 28.70	1.96 to 26.51	2.037 to 68.248
Index ranges	–41<=h<=40	–14<=h<=14	–5<=h<=8
	0<=k<=9	–14<=k<=14	-38<=k<=38
	0<=l<=18	–12<=l<=15	-35<=l<=35
Reflections collected	3825	34882	72021
Min. and max. transmission	0.9640, 0.9970	0.9500, 0.9740	---
Data / restraints / parameters	3825 / 274 / 298	6096 / 163 / 440	11746 / 204 / 938
Goodness-of-fit on F^2	1.069	1.068	1.167
Final *R* indices [$I > 2\sigma(I)$]	R_1 = 0.0727	R_1 = 0.0827	R_1 = 0.0893
	wR_2 = 0.1582	wR_2 = 0.1856	wR_2 = 0.2234
R indices (all data)	R_1 = 0.1474	R_1 = 0.1293	R_1 = 0.0920
	wR_2 = 0.1965	wR_2 = 0.2155	wR_2 = 0.2250
Largest diff. peak and hole ($e.Å^{-3}$)	0.391, –0.396	1.063, –0.932	1.930, –2.394

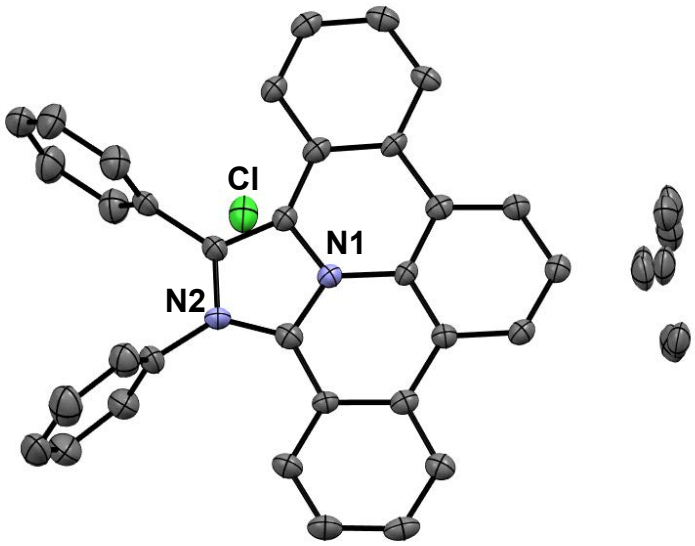


Figure S29. X-ray structures of **3a** with thermal ellipsoids of 50% probability. Hydrogen atoms were omitted for clarity.

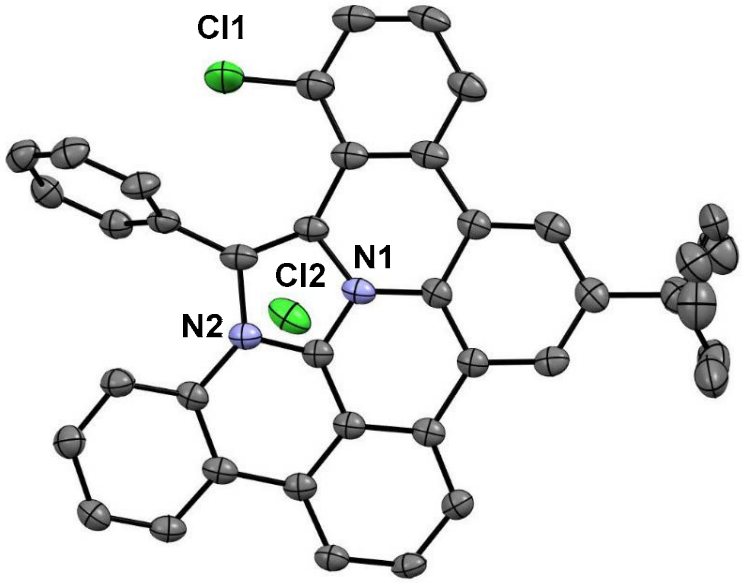


Figure S30. X-ray structures of **3k** with thermal ellipsoids of 50% probability. Hydrogen atoms and solvent molecules were omitted for clarity.

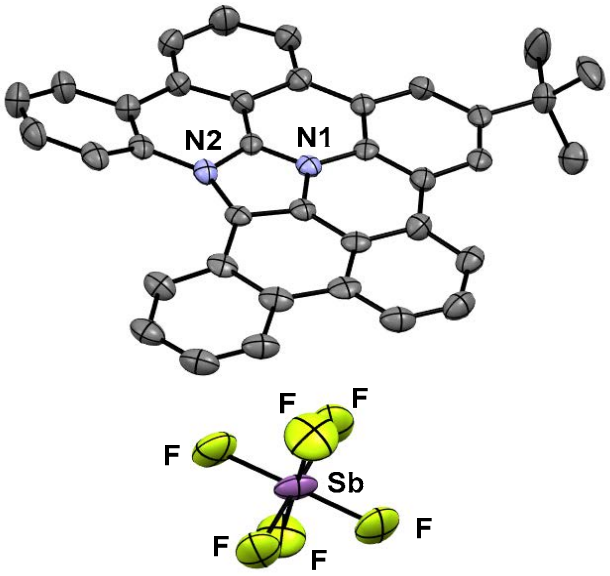


Figure S31. X-ray structures of **4b** with thermal ellipsoids of 50% probability. Hydrogen atoms and 1,2-dichlorobenzene molecules were omitted for clarity.

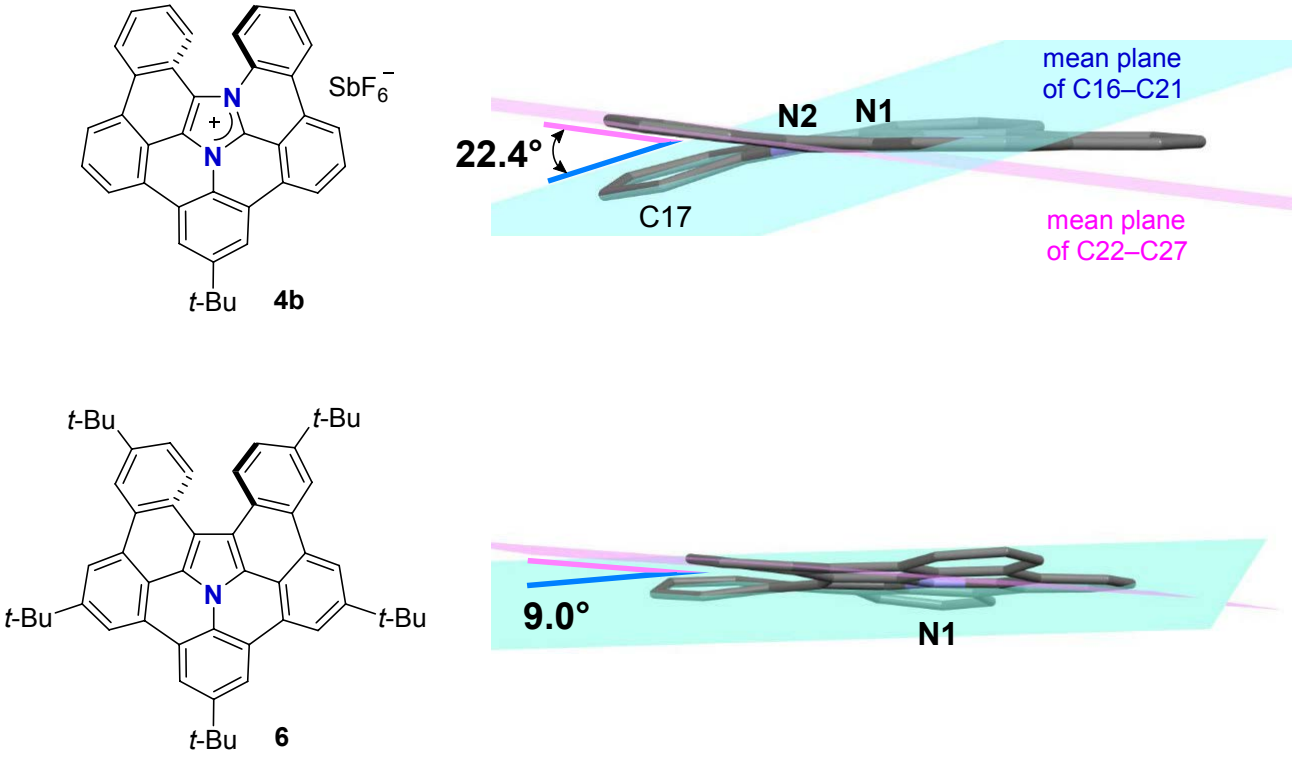


Figure S32. Dihedral angles between the terminal benzene rings of **4b** and monoaza analogue **6**.[6]

(6) H. Yokoi, S. Hiroto and H. Shinokubo, *J. Am. Chem. Soc.* 2018, **140**, 4649–4655.

5. Theoretical Calculations

The computations were performed using workstation at High-Performance Center for Computational Science, Nanyang Technological University, Singapore. All the calculations were performed by using Gaussian 16 (revision A.03) program[7] by the B3LYP method[8] with the 6-31G(d) basis set[9] for structure optimization, vibrational frequency, time-dependent density functional theory (TD-DFT). Grimme' D3 dispersion correction[10] and SMD solvation model (with dichloroethane)[11] were used to investigate the reaction mechanism of 1,3-dipolar cycloaddition (Figure S36 and S37). The geometry of azahelicene **4** was optimized under C_1 symmetry constraint. Each transition state structure was optimized without any symmetry assumptions and IRC calculations were also performed to check the transition states. The *tert*-butyl substituent is replaced by a hydrogen atom.

(7) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, *Gaussian 16, Revision A.03*, Gaussian, Inc., Wallingford CT, 2016.
(8) (a) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648–5652. (b) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B* 1998, **37**, 785–789.
(9) (a) W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.* 1972, **56**, 2257–2261. (b) R. Ditchfield, W. J. Hehre and J. A. Pople, *J. Chem. Phys.* 1971, **54**, 724–728.
(10) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.* 2010, **132**, 154104.
(11) A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B* 2009, **113**, 6378−6396.

5-1. Reaction Mechanism for Cycloaddition

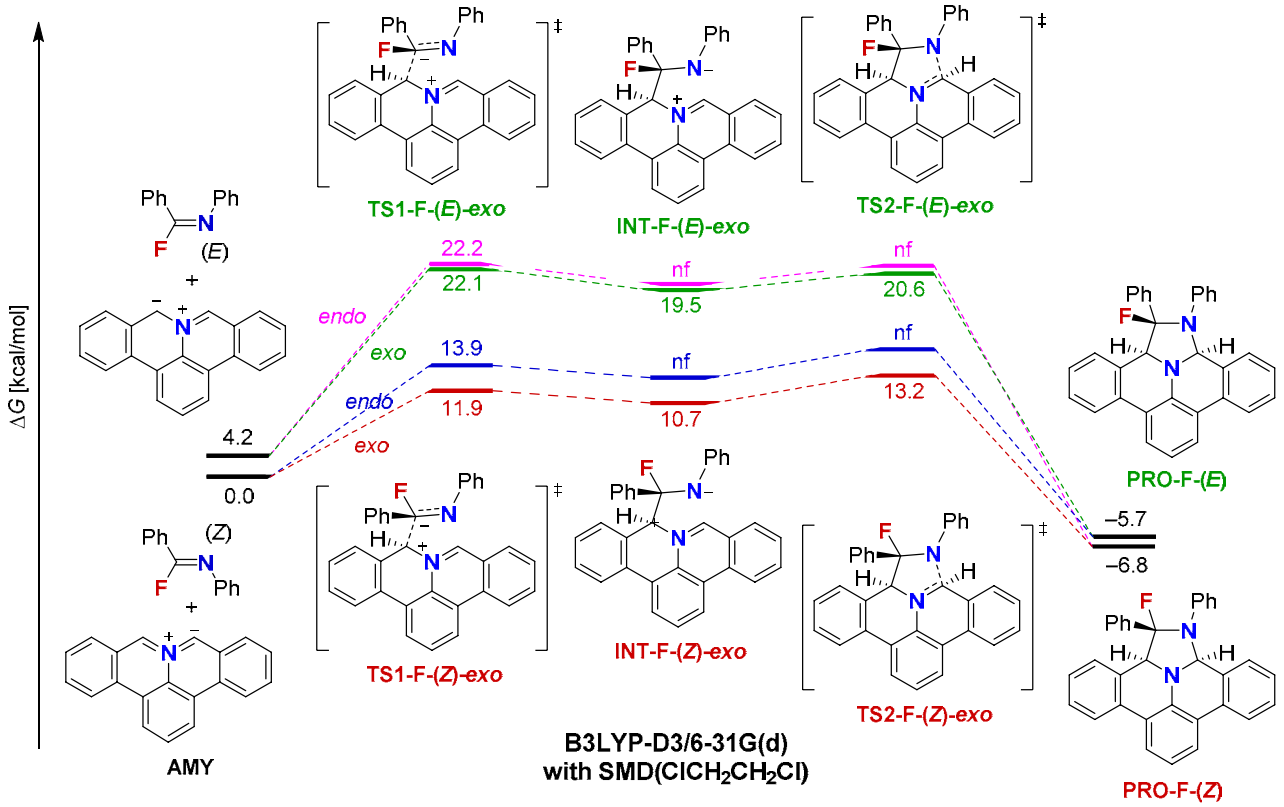


Figure S33. Energy diagram of cycloaddition of imidolyl fluoride **2-F** and an azomethine ylide formed from of iminium salt **1**. The term "nf" represents "not found".

Note) **TS1-F** was successfully determined for all the isomers. In the cases of (*Z*)-*endo* and (*E*)-*endo*, however, all subsequent calculations to determine **INT-F** did not give any intermediate presumably due to the small activation barrier of **TS2-F**, resulting in the direct formation of **PRO-F**.

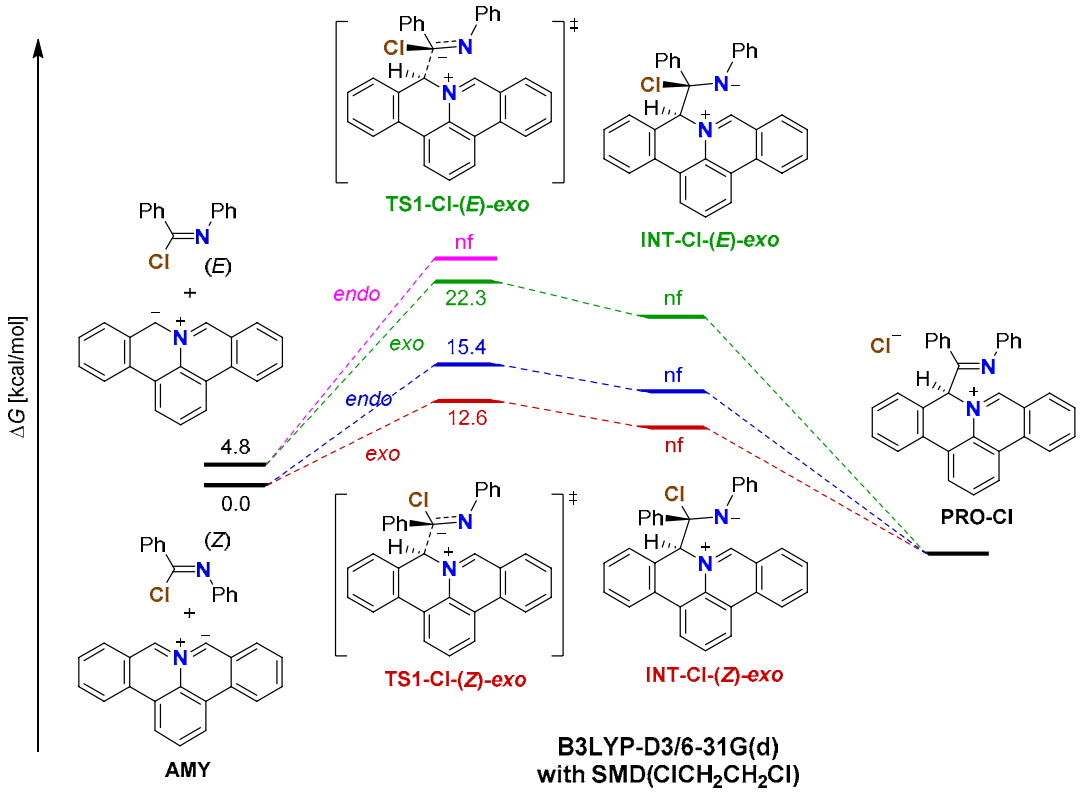


Figure S34. Energy diagram of cycloaddition of imidolyl chloride **2-Cl** and an azomethine ylide formed from of iminium salt **1**. The term "nf" represents "not found".

Note) **TS1-Cl** was successfully determined for the (*Z*)-*exo*, (*Z*)-*endo*, and (*E*)-*exo* isomers. However, all subsequent calculations to determine **INT-Cl** did not converge and resulted in the dissociation of the chlorine atom to give **PRO-Cl**.

5-2. Reaction Mechanism for Helicene Flipping

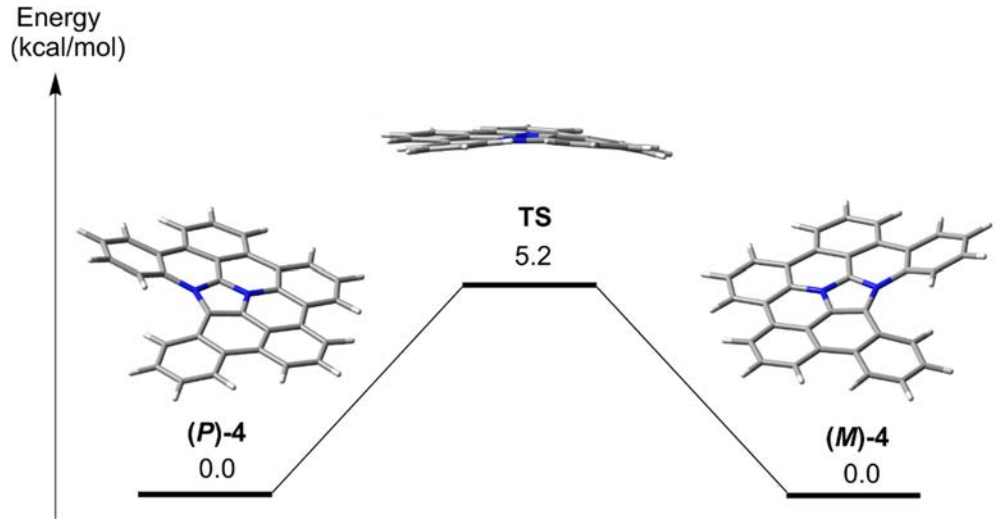


Figure S35. Energy diagram of bowl inversion of **4**. Values (kcal/mol) are relative Gibbs free energies (ΔG) at 298.15 K and 1 atm.

5-3. Molecular Orbitals of 4

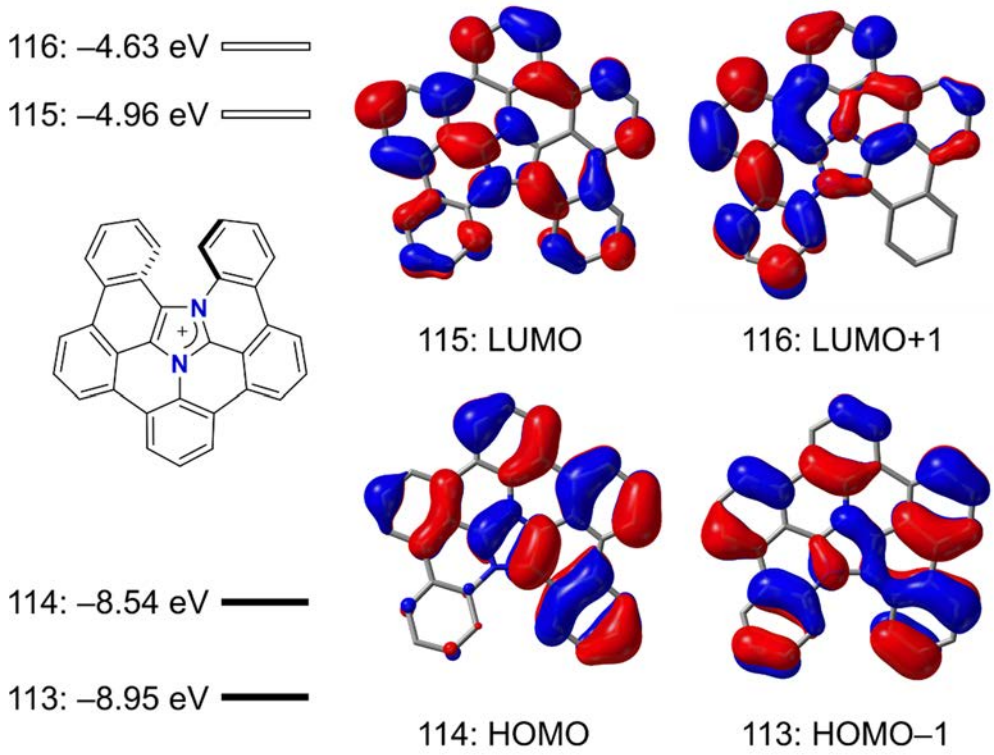


Figure S36. Kohn-Sham molecular orbitals of **4**. For each MO, the view from the convex surface of the molecule.

5-4. TD-DFT Calculations

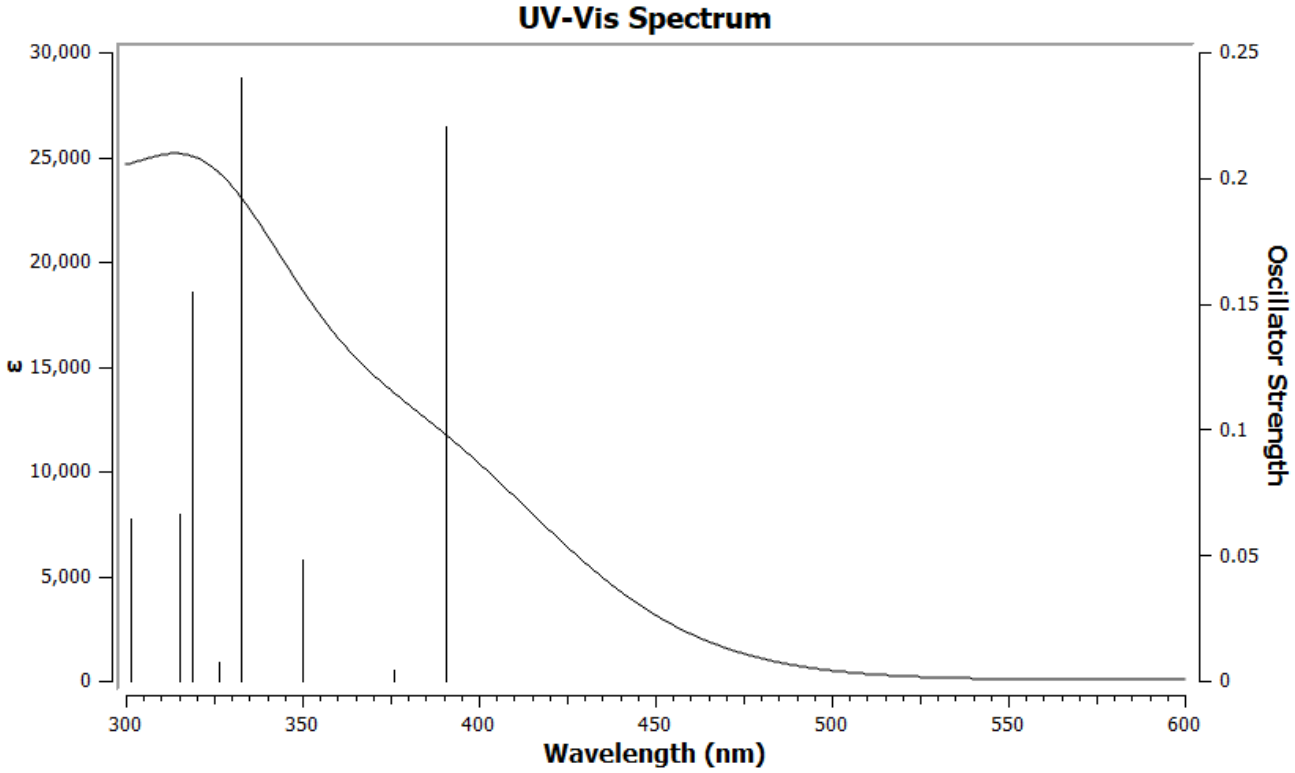


Figure S37. A simulated absorption spectrum of **4** by TD-DFT calculations.

Table S2. Selected wavelengths, oscillator strengths, major electronic transition of **4**.

Wavelength (λ)	Oscillator Strengths (*f*)	Transitions
390.80	0.2208	113→116 (–0.14519) 114→115 (0.67581)
375.67	0.0041	112→115 (–0.15689) 113→115 (0.40710) 114→116 (0.54008)
349.94	0.0483	112→115 (0.39200) 113→115 (0.43556) 114→116 (–0.25165) 114→117 (–0.21287) 114→118 (0.17582)
332.45	0.2402	112→115 (0.48965) 113→115 (–0.26833) 113→116 (0.14656) 114→116 (0.35467)
326.47	0.0073	113→116 (0.21925) 114→117 (0.53580) 114→118 (0.34078) 114→119 (–0.13033)
318.74	0.1548	112→115 (–0.19242) 112→116 (0.24334) 113→116 (0.53079) 114→115 (0.10818) 114→117 (–0.26908)
315.25	0.0667	111→115 (–0.16745) 112→116 (0.28428) 112→117 (–0.12432) 113→115 (–0.15079) 113→116 (–0.23079) 113→117 (–0.12561) 114→117 (–0.14390) 114→118 (0.43031) 114→119 (0.19201)
301.50	0.0644	111→115 (–0.24906) 112→115 (0.13816) 112→116 (0.46464) 113→115 (0.12031) 113→117 (0.17424) 113→118 (0.10602) 114→117 (0.16409) 114→118 (–0.27266) 114→119 (0.11808)
297.64	0.0761	109→115 (0.15557) 112→116 (–0.15503) 112→117 (0.11031) 113→116 (0.15881) 113→117 (–0.22192) 113→118 (0.15075) 114→119 (0.54475)
291.71	0.0436	111→115 (0.59271) 111→116 (–0.10502) 112→116 (0.22568) 114→119 (0.14584)

Cartesian Coordinates

AMY

C	0.00000000	1.20693100	-2.44988700
C	0.00000000	1.24613400	-1.04291400
C	0.00000000	0.00000000	-0.34646900
C	0.00000000	-1.24613400	-1.04291400
C	0.00000000	-1.20693100	-2.44988700
C	0.00000000	0.00000000	-3.13588300
C	0.00000000	2.50433200	-0.30460400
C	0.00000000	2.42973700	1.11943700
C	0.00000000	1.18283600	1.75842900
N	0.00000000	0.00000000	1.07626900
C	0.00000000	-1.18283600	1.75842900
C	0.00000000	-2.42973700	1.11943700
C	0.00000000	-2.50433200	-0.30460400
C	0.00000000	3.77439300	-0.91509800
C	0.00000000	4.93809300	-0.15903500
C	0.00000000	4.86157200	1.24944600
C	0.00000000	3.63383500	1.87931100
C	0.00000000	-3.63383500	1.87931100
C	0.00000000	-4.86157200	1.24944600
C	0.00000000	-4.93809300	-0.15903500
C	0.00000000	-3.77439300	-0.91509800
H	0.00000000	2.13260400	-3.01234000
H	0.00000000	-2.13260400	-3.01234000
H	0.00000000	0.00000000	-4.22261000
H	0.00000000	1.09543700	2.83704400
H	0.00000000	-1.09543700	2.83704400
H	0.00000000	3.85781600	-1.99672000
H	0.00000000	5.90534500	-0.65306400
H	0.00000000	5.77325400	1.84146300
H	0.00000000	3.56790500	2.96451600
H	0.00000000	-3.56790500	2.96451600
H	0.00000000	-5.77325400	1.84146300
H	0.00000000	-5.90534500	-0.65306400
H	0.00000000	-3.85781600	-1.99672000

(*Z*)-2-F

C	3.69366400	1.48207500	0.27778700
C	2.32912400	1.21614100	0.22245400
C	1.87611700	-0.09198900	-0.02534000
C	2.80849800	-1.12484000	-0.21539800
C	4.17449400	-0.85043800	-0.15799800
C	4.62020200	0.45021300	0.08805800
H	4.03717700	2.49489200	0.46861900
H	1.60368700	2.00965300	0.36802600
H	2.46471700	-2.13510600	-0.40648600
H	4.89040100	-1.65406900	-0.30550900
H	5.68518800	0.66129200	0.13197900
C	0.43381500	-0.36505200	-0.08134900
N	-0.47491900	0.49647100	0.08364800
C	-1.86095000	0.26260800	0.05593800
C	-2.66338600	1.35350200	-0.32260100
C	-2.48356400	-0.94280500	0.43570300
C	-4.05142700	1.23631700	-0.35755700
H	-2.17655500	2.28623500	-0.59278200
C	-3.87423300	-1.04392700	0.41850400
H	-1.88351700	-1.78589600	0.75547100
C	-4.66415800	0.03646800	0.01483300
H	-4.65507800	2.08641400	-0.66420300
H	-4.34291100	-1.97671100	0.72141300
H	-5.74680900	-0.05398900	-0.00141500
F	0.15766200	-1.67973800	-0.35320600

(*E*)-2-F

C	-2.75779700	0.40051800	0.46035100
C	-1.47239500	0.35934300	-0.10547400
C	-1.02584900	-0.81857300	-0.72804200
C	-1.85175200	-1.93973300	-0.76883400
C	-3.12154600	-1.90113800	-0.18508400
C	-3.57259400	-0.72951800	0.42837100
H	-3.10976800	1.31312400	0.92896600
H	-0.04616100	-0.85311600	-1.18997700
H	-1.50369700	-2.84403100	-1.25968400
H	-3.75950000	-2.78025700	-0.21354800
H	-4.56089800	-0.69331400	0.87769000
C	-0.62123400	1.56621900	-0.05280900
F	-1.37394000	2.70006300	-0.01287500
N	0.62560100	1.75178300	-0.05132900
C	1.57697800	0.71687400	0.05344200
C	1.63248500	-0.11154700	1.18630600
C	2.54101900	0.57522400	-0.95559200
C	2.62769500	-1.08285000	1.29097100
H	0.89576300	0.01591600	1.97400300
C	3.52324600	-0.41018200	-0.84833200
H	2.50298400	1.23226900	-1.81979400
C	3.57250100	-1.24311500	0.27316100
H	2.66169100	-1.71851700	2.17204200
H	4.25706000	-0.52107500	-1.64245900
H	4.34423100	-2.00319200	0.35732500

TS1-F-(*Z*)-*exo*

C	-0.26711700	-1.04045500	-0.97620700
C	1.38765200	0.63160900	-1.05046300
C	-0.89330400	1.31906400	-0.81378700
C	-2.26779000	0.95521100	-0.86383200
C	-0.47785100	2.65042500	-0.53550500
C	-3.20881600	1.94431800	-0.56124200
C	-1.47800700	3.60306300	-0.25952700
C	-2.81730000	3.24901500	-0.26002700
H	-4.26357000	1.69659900	-0.54554900
H	-1.20198800	4.62518600	-0.03032200
H	-3.57174600	3.99409000	-0.02532400
C	-2.65242400	-0.41624800	-1.22142700
C	-3.97951900	-0.79872200	-1.48995600
C	-1.63368700	-1.39127400	-1.30678100
C	-4.29300200	-2.11579400	-1.80470500
H	-4.77588900	-0.06279100	-1.46134600
C	-1.96095100	-2.72155200	-1.62919600
C	-3.27901100	-3.08326800	-1.87104800
H	-5.32446600	-2.39090700	-2.00599900
H	-3.52219800	-4.11260300	-2.12006900
C	0.94198700	2.97919500	-0.52319600
C	1.45630200	4.26322100	-0.25156600
C	1.86594900	1.93601100	-0.80712900
C	2.82392400	4.49700800	-0.26087400
H	0.78755800	5.08769800	-0.03175700
C	3.25970500	2.18967500	-0.81805900
C	3.73238500	3.45789400	-0.54302700

H	3.19627600	5.49516600	-0.04881600
H	4.80029000	3.65558200	-0.54480400
N	0.08308400	0.32804800	-1.03568700
H	2.06603400	-0.17361200	-1.29095100
H	0.49972200	-1.66491000	-1.42459400
H	3.94109500	1.37119600	-1.03182300
H	-1.16891600	-3.46250100	-1.67703500
C	0.20558500	-1.53778300	0.90314100
C	-0.86485700	-0.88797700	1.71924500
C	-2.12299600	-1.48823600	1.87372300
C	-0.64201600	0.38144200	2.27575700
C	-3.14092800	-0.82480600	2.56051500
H	-2.30520900	-2.46759600	1.44722600
C	-1.66168300	1.04315000	2.95731200
H	0.33327400	0.84079700	2.16045900
C	-2.91819600	0.44536800	3.09720400
H	-4.11219500	-1.30059000	2.66867300
H	-1.47686200	2.02993800	3.37370800
H	-3.71525000	0.96425800	3.62332300
F	-0.08953800	-2.91378800	0.73509800
C	2.58207000	-1.81069400	0.63561000
C	2.63077300	-3.01339100	-0.11707300
C	3.82150700	-1.17707400	0.91562000
C	3.85085500	-3.53233300	-0.55653300
H	1.71599300	-3.54256500	-0.34731300
C	5.02967300	-1.70457700	0.47547600
H	3.79652600	-0.25144000	1.48475200
C	5.05783500	-2.89166300	-0.26904900
H	3.85204600	-4.45587800	-1.13181500
H	5.95707200	-1.18771600	0.71237200
H	6.00095500	-3.30635400	-0.61442500
N	1.45646200	-1.15888900	1.10785700

INT-F-(*Z*)-*exo*

C	-0.19886300	-1.10164000	-0.77986800
C	1.37562500	0.64824100	-0.97188100
C	-0.92409400	1.27533400	-0.82274100
C	-2.28117900	0.86340300	-0.89492200
C	-0.56175400	2.63065100	-0.59722300
C	-3.26147600	1.82690700	-0.65382100
C	-1.59889600	3.56019700	-0.38459400
C	-2.92377900	3.15814700	-0.39575000
H	-4.30705900	1.54168400	-0.65532300
H	-1.36304700	4.60092000	-0.19766000
H	-3.70976800	3.88360200	-0.20910000
C	-2.60284400	-0.53266200	-1.23225600
C	-3.89613100	-0.94306800	-1.60426600
C	-1.56987900	-1.48843900	-1.21169200
C	-4.15802300	-2.27103900	-1.92308000
H	-4.70255800	-0.21974400	-1.65980500
C	-1.83818000	-2.82139500	-1.54751400
C	-3.12593600	-3.21660400	-1.89527400
H	-5.16416900	-2.56802000	-2.20553300
H	-3.32498400	-4.25317300	-2.15234900
C	0.84641400	3.00307600	-0.57499100
C	1.31729800	4.31328200	-0.35637800
C	1.81018900	1.98079500	-0.79593200
C	2.67803000	4.58464000	-0.35892400
H	0.62187800	5.12653500	-0.18449600
C	3.19519800	2.27197600	-0.80168100
C	3.62496500	3.56542900	-0.58025000
H	3.01653700	5.60266700	-0.18850100
H	4.68535500	3.79828200	-0.57668900
N	0.08522400	0.31489800	-0.97776600
H	2.08591300	-0.13957400	-1.17432500
H	0.54918600	-1.67110500	-1.33334100
H	3.90163900	1.46345600	-0.96555200
H	-1.03134800	-3.54643400	-1.52026200
C	0.17715400	-1.44584800	0.80746000
C	-0.84104300	-0.79871500	1.73158300
C	-2.08642700	-1.39735400	1.96400700
C	-0.57201200	0.45235400	2.30232200
C	-3.04830600	-0.75060400	2.74259100
H	-2.30208200	-2.36777300	1.53234100
C	-1.53538800	1.10164500	3.07506800
H	0.39695900	0.90731000	2.13127100
C	-2.77977800	0.50427700	3.29435900
H	-4.00975400	-1.22809600	2.91398900
H	-1.31393900	2.07594500	3.50331100
H	-3.53218400	1.01069400	3.89360700
F	-0.10916400	-2.86944900	0.80777600
C	2.56556600	-1.76100400	0.62926600
C	2.59782500	-2.97091600	-0.12400600
C	3.82987200	-1.15237000	0.88868100
C	3.80488400	-3.50824100	-0.57814400
H	1.67613800	-3.49994300	-0.32690200
C	5.02209500	-1.69808700	0.43183200
H	3.83022500	-0.22743300	1.46071600
C	5.02706000	-2.88732100	-0.31293800
H	3.78270500	-4.43580300	-1.14765500
H	5.95992700	-1.19369200	0.65694600
H	5.95935100	-3.31667400	-0.66969400
N	1.46741000	-1.09902200	1.11930300

TS2-F-(*Z*)-*exo*

C	-0.48401700	-1.01567400	-1.01408900
C	1.32229400	0.42044800	-1.09561900
C	-0.85747000	1.41233200	-0.81542800
C	-2.26205300	1.21167900	-0.80626700
C	-0.27736200	2.65423500	-0.45480400
C	-3.06920700	2.27970200	-0.40437200
C	-1.14187000	3.69739300	-0.07672700
C	-2.51636600	3.50991800	-0.04634700
H	-4.14389300	2.14862400	-0.34584300
H	-0.73423300	4.65852200	0.21470200
H	-3.16610200	4.32195700	0.26603300
C	-2.81291300	-0.10308800	-1.18211800
C	-4.18011400	-0.31401500	-1.43726400
C	-1.93625500	-1.19948000	-1.28923300
C	-4.66013400	-1.58113500	-1.75433800
H	-4.87594500	0.51749700	-1.39803800
C	-2.42236600	-2.47005800	-1.61539500
C	-3.78210100	-2.66767300	-1.83937300
H	-5.72074700	-1.72091700	-1.94436900
H	-4.15522400	-3.65691700	-2.08888100
C	1.18125800	2.79342100	-0.45855400
C	1.85312300	3.98961200	-0.14330000
C	1.96637800	1.66534000	-0.81052400
C	3.24113800	4.05654800	-0.17367100
H	1.29360100	4.87832700	0.12594300

C	3.37299800	1.74866400	-0.85441800
C	4.00892800	2.93657100	-0.53067100
H	3.73458700	4.99199000	0.07509700
H	5.09243900	3.00290700	-0.55885300
N	-0.02805500	0.34693600	-1.19215400
H	1.87617900	-0.35359800	-1.61168500
H	0.10887500	-1.65996200	-1.66856400
H	3.94425300	0.86917900	-1.13443700
H	-1.72648100	-3.30167200	-1.67749100
C	0.05047700	-1.43701300	0.47620000
C	-0.89187200	-0.93595900	1.56210300
C	-2.07097100	-1.63214400	1.86135400
C	-0.62725800	0.26885400	2.22526700
C	-2.97437400	-1.12380200	2.79631300
H	-2.28238700	-2.56926900	1.35942100
C	-1.53423300	0.78116800	3.15366200
H	0.29200300	0.79797500	2.00284200
C	-2.71351500	0.08837900	3.43999800
H	-3.88421500	-1.67553400	3.01875500
H	-1.31813600	1.72240100	3.65262300
H	-3.42126300	0.48727800	4.16222200
F	-0.09101100	-2.85637900	0.43216700
C	2.48772900	-1.71818600	0.39299800
C	2.57604800	-2.89050100	-0.40366600
C	3.70447200	-1.20500500	0.91387900
C	3.80674200	-3.50712200	-0.63678800
H	1.68039800	-3.32168300	-0.83089300
C	4.92633500	-1.82271800	0.66766900
H	3.65265900	-0.30578200	1.52132500
C	4.99095300	-2.98572200	-0.10979900
H	3.83658900	-4.40720000	-1.24756900
H	5.83454100	-1.39787700	1.08971400
H	5.94321400	-3.47413000	-0.29837700
N	1.35832000	-0.95758200	0.65025700

PRO-F-(*Z*)

C	1.07566900	-0.15790600	-1.57754300
C	-1.17036300	-0.41490100	-1.39497000
C	0.23420200	-1.92270300	-0.10103700
C	1.53681400	-2.16674100	0.40072400
C	-0.90017200	-2.45988700	0.55536800
C	1.67436800	-2.93210200	1.56658800
C	-0.70963600	-3.21985000	1.71976500
C	0.56445800	-3.45704900	2.22383100
H	2.66066200	-3.09155400	1.98888100
H	-1.57141200	-3.60457100	2.25494000
H	0.69274800	-4.03299300	3.13551200
C	2.70081200	-1.56947100	-0.28511800
C	4.02929000	-1.94662200	-0.01694300
C	2.47670700	-0.56776500	-1.24502700
C	5.09543500	-1.31749100	-0.65518600
H	4.23729400	-2.74429700	0.68868500
C	3.54785200	0.05903100	-1.88647900
C	4.85998400	-0.30398100	-1.58924000
H	6.11280300	-1.62486700	-0.42854800
H	5.68952300	0.18772100	-2.08941700
C	-2.24257800	-2.18822700	0.00846500
C	-3.39316700	-2.89839800	0.39639500
C	-2.38366600	-1.17282900	-0.95378000
C	-4.64124900	-2.58098000	-0.13462000
H	-3.31581700	-3.71535400	1.10635100
C	-3.63404000	-0.86570300	-1.49416300
C	-4.76978200	-1.55956300	-1.08108900
H	-5.51611900	-3.14200500	0.18291200
H	-5.74207200	-1.31541200	-1.49921100
N	0.06644100	-1.17826400	-1.28878000
H	-1.29053500	-0.12454000	-2.44713600
H	1.01034600	0.05912300	-2.64825100
H	-3.71263900	-0.07468000	-2.23561700
H	3.34410200	0.83430900	-2.62080400
C	0.51013400	1.16925000	-0.89916600
C	1.28399800	1.73733800	0.26951000
C	1.10447900	1.18742300	1.54550200
C	2.22968700	2.75294600	0.08826200
C	1.85875500	1.64820900	2.62440500
H	0.37619200	0.39610300	1.68663800
C	2.98289300	3.21425100	1.16976800
H	2.37183600	3.18320100	-0.89621200
C	2.80108600	2.66377400	2.44028700
H	1.70876400	1.21334100	3.60908200
H	3.71179300	4.00596700	1.01729200
H	3.38904800	3.02288900	3.28087700
F	0.59215700	2.14245700	-1.97080400
C	-1.78825600	1.73816500	-0.11982200
C	-1.89985300	3.03378300	-0.64904100
C	-2.64733300	1.34890400	0.92097000
C	-2.85047800	3.91989400	-0.13797100
H	-1.23735300	3.34189700	-1.44777200
C	-3.61237800	2.22984400	1.40714200
H	-2.54505500	0.35709800	1.34735100
C	-3.71637800	3.52142000	0.88261800
H	-2.91917500	4.92333800	-0.55034400
H	-4.27191600	1.91109200	2.21011000
H	-4.46108400	4.21150700	1.27006500
N	-0.82288700	0.80800800	-0.59244600

TS1-F-(*Z*)-*endo*

C	1.15013500	-1.13459600	0.43537500
C	-0.99181300	-0.30779600	-1.71096700
C	1.20306500	0.20108500	-1.04546500
C	-0.64411700	1.66026600	-0.38567900
C	-2.04713100	1.81173600	-0.21818100
C	0.28297600	2.58163700	0.17412900
C	-2.50217600	2.89956400	0.54879000
C	-0.23349300	3.62660400	0.94977200
C	-1.60644600	3.78235300	1.13296100
H	-3.56469800	3.04747700	0.69934200
H	0.44173300	4.33085500	1.42141500
H	-1.97699200	4.60537600	1.73709900
C	-2.95562900	0.83658500	-0.81035700
C	-4.35420200	0.86403300	-0.64895000
C	-2.39322400	-0.20441900	-1.59803500
C	-5.15810300	-0.09365600	-1.25067300
H	-4.82091900	1.63043600	-0.04084900
C	-3.22602100	-1.17171500	-2.21007300
C	-4.59563600	-1.11364000	-2.04118100
H	-6.23406200	-0.05419300	-1.10704200
H	-5.23596200	-1.85801800	-2.50513500
C	1.71878400	2.43103900	-0.09453200
C	2.67164500	3.41332500	0.23359900

C	2.15269700	1.26075400	-0.75672200
C	4.01659800	3.23459800	-0.07119500
H	2.36388600	4.33327100	0.71908500
C	3.51365300	1.09636600	-1.07367800
C	4.44017600	2.07234400	-0.73103800
H	4.73503300	4.00565800	0.19252300
H	5.48885500	1.93578100	-0.98033400
N	-0.15628800	0.56904200	-1.13220200
H	1.47931100	-0.47310200	-1.84940900
H	-0.53308200	-1.08995900	-2.29895000
C	-1.13394200	-1.78239600	0.95731700
C	-1.50533000	-0.82173200	1.93480700
C	-2.76151300	-0.86622400	2.53996700
H	-0.81565100	-0.03654500	2.20850300
C	-3.69739700	-1.84884400	2.20715000
H	-3.01172500	-0.10816400	3.27945100
H	-4.67384000	-1.87010400	2.68342800
C	2.48491200	-1.79679700	0.25770800
C	4.99029600	-2.99849300	-0.16048500
C	4.84611400	-1.98354900	0.78659400
H	5.70346000	-1.65302000	1.36732600
C	3.60286500	-1.37922600	0.99116000
H	3.49992600	-0.58296100	1.71862300
H	5.95926500	-3.46321000	-0.32286400
H	3.83056400	0.19430300	-1.58808600
H	-2.76916100	-1.96068700	-2.80079400
N	0.06816100	-1.87995200	0.27915000
F	1.21743500	-0.23034100	1.52200300
C	-3.35062800	-2.80272800	1.24271800
H	-4.06188400	-3.57537300	0.95910000
C	3.87683700	-3.41521600	-0.89892400
H	3.97711800	-4.20815100	-1.63577600
C	2.63308400	-2.82242600	-0.68871700
H	1.76369100	-3.15223400	-1.24855300
C	-2.10189600	-2.76876600	0.63325300
H	-1.83573900	-3.50843500	-0.11744300

TS1-F-(*E*)-*exo*

C	0.79752800	0.72465700	-0.85021100
C	-1.69372100	0.27639800	0.85959600
C	0.59286200	-0.26740800	0.92365000
C	-1.05336400	-1.93701500	0.21408700
C	-2.36634400	-2.19215300	-0.26616200
C	-0.03376400	-2.92745600	0.17136800
C	-2.62611800	-3.45917900	-0.82427700
C	-0.35271400	-4.16021200	-0.40731800
C	-1.63158200	-4.42061200	-0.90018400
H	-3.61310400	-3.68717100	-1.20894300
H	0.40458900	-4.93188800	-0.48300600
H	-1.84823800	-5.38710300	-1.34586900
C	-3.38648800	-1.15325700	-0.17801200
C	-4.71058500	-1.30259100	-0.63609500
C	-3.02152900	0.08327500	0.41817100
C	-5.62726600	-0.26839200	-0.50819500
H	-5.03039900	-2.23076300	-1.09593300
C	-3.96707000	1.12877100	0.54776400
C	-5.25709100	0.95419700	0.08427500
H	-6.64235800	-0.40667900	-0.86944500
H	-5.98414400	1.75576800	0.17664500
C	1.28792500	-2.64217400	0.74788600
C	2.27812200	-3.62500900	0.92984700
C	1.56157800	-1.31931300	1.16408300
C	3.50722100	-3.30726900	1.49882500
H	2.08771800	-4.65241900	0.63873400
C	2.80330700	-1.01225200	1.75001200
C	3.77021000	-1.99485100	1.91519100
H	4.25681100	-4.08276800	1.62870000
H	4.72624400	-1.74524600	2.36707700
N	-0.75402100	-0.67359200	0.75937900
H	0.66492200	0.58836700	1.58557300
H	-1.40748800	1.18149500	1.37429900
C	-0.26616200	2.80508200	-0.18664200
C	0.50649900	3.18856600	0.94061000
C	0.24788400	4.38067400	1.61933200
H	1.32431200	2.56025800	1.27555000
C	-0.77907600	5.23452000	1.21043000
H	0.86229600	4.64228300	2.47807900
H	-0.97228700	6.16198900	1.74236700
C	2.27226100	0.96957000	-1.03402100
C	5.03153000	1.34899800	-1.46945500
C	4.48715000	0.06278700	-1.48470400
H	5.12398700	-0.79992800	-1.66166500
C	3.12175300	-0.12440800	-1.27527000
H	2.70788400	-1.12452900	-1.30326400
H	6.09632100	1.49625500	-1.63015500
H	3.00041200	0.00969700	2.06223600
H	-3.65653400	2.06580100	1.00122400
N	-0.17971200	1.61882700	-0.89113600
F	0.45444400	-0.37150800	-1.67085800
C	-1.55601200	4.87188100	0.10229800
H	-2.36277500	5.52028800	-0.23204500
C	4.19167800	2.44552400	-1.26337600
H	4.59617400	3.45424300	-1.27744000
C	2.82371900	2.25958200	-1.05622000
H	2.18856200	3.12677600	-0.93038800
C	-1.31100600	3.68254400	-0.57540800
H	-1.92478300	3.39135100	-1.42356700

INT-F-(*E*)-*exo*

C	0.81442700	0.58692900	-0.66834000
C	-1.66562200	0.35303500	0.77809500
C	0.62057900	-0.19651800	0.77408900
C	-1.09174100	-1.89714400	0.20256800
C	-2.40201700	-2.13122800	-0.28771900
C	-0.09444700	-2.90641900	0.18221100
C	-2.68225400	-3.39908000	-0.83503000
C	-0.42477800	-4.13525400	-0.39133300
C	-1.70495700	-4.37893700	-0.89579600
H	-3.66987300	-3.61145200	-1.22749500
H	0.32457900	-4.91608800	-0.45817900
H	-1.93345700	-5.34400600	-1.33805400
C	-3.39553000	-1.06358900	-0.22223300
C	-4.72292800	-1.19017700	-0.67545400
C	-3.00468100	0.17793600	0.34689600
C	-5.61283700	-0.12981000	-0.56689700
H	-5.06721000	-2.11952100	-1.11433400
C	-3.92221800	1.24706000	0.46142500
C	-5.21722800	1.09497000	0.00163100
H	-6.63142800	-0.25206500	-0.92424000
H	-5.92675900	1.91310000	0.08068400

C	1.22060200	-2.63547700	0.78822400
C	2.14003000	-3.65510900	1.09633700
C	1.55267300	-1.30867800	1.11947500
C	3.35744400	-3.35967300	1.70239700
H	1.89745900	-4.69062400	0.88184200
C	2.76737000	-1.02226100	1.75267600
C	3.67398800	-2.03870400	2.03817600
H	4.05305100	-4.16277300	1.92931300
H	4.61719400	-1.80612800	2.52421600
N	-0.77031300	-0.64100900	0.73456400
H	0.69482800	0.58657200	1.52942300
H	-1.38119500	1.24092900	1.32353200
C	-0.17788700	2.75394900	-0.10487500
C	0.63446300	3.13432800	1.00350900
C	0.41928700	4.33393000	1.68648000
H	1.46315700	2.50513600	1.31008800
C	-0.60599100	5.20562800	1.31638100
H	1.07060600	4.58595400	2.52115800
H	-0.76571300	6.13678700	1.85290600
C	2.28425100	0.86857600	-1.00616600
C	4.97734500	1.28089500	-1.73863600
C	4.46060900	-0.01460600	-1.65602800
H	5.09232900	-0.87168800	-1.87466100
C	3.12747700	-0.21642500	-1.30204300
H	2.73406100	-1.22476100	-1.26684300
H	6.01691400	1.44092800	-2.01278800
H	3.00345700	0.00772300	2.00565900
H	-3.58800400	2.18312100	0.89914700
N	-0.13746200	1.58583600	-0.82238700
F	0.44330400	-0.44093800	-1.60423400
C	-1.42266300	4.85311400	0.23065600
H	-2.22783000	5.51576700	-0.08037300
C	4.13937100	2.36726200	-1.48552800
H	4.51778800	3.38240100	-1.57353100
C	2.80225200	2.16314700	-1.13305400
H	2.16753600	3.02379800	-0.97049800
C	-1.21754900	3.66493500	-0.45738200
H	-1.85783500	3.39190000	-1.29238500

TS2-F-(*E*)-*exo*

C	0.73054400	0.62759800	-0.57920300
C	-1.58461200	0.17958600	0.79549900
C	0.70500900	-0.21598400	0.82492700
C	-0.85460800	-2.03880800	0.21706100
C	-2.13689400	-2.35837000	-0.29374000
C	0.22029100	-2.96236100	0.16085900
C	-2.31926800	-3.63078300	-0.86757800
C	-0.01444800	-4.20297800	-0.43721400
C	-1.27228500	-4.53677200	-0.94283500
H	-3.28572200	-3.90610100	-1.27362500
H	0.79495300	-4.91899500	-0.52662500
H	-1.42777400	-5.50758000	-1.40391900
C	-3.20765700	-1.36178000	-0.22536100
C	-4.52022800	-1.58799700	-0.68204400
C	-2.91462400	-0.09968400	0.34942900
C	-5.49184700	-0.60050900	-0.57273100
H	-4.79074000	-2.54000900	-1.12460100
C	-3.91183800	0.88950700	0.47167000
C	-5.19321500	0.64392300	0.00603700
H	-6.49697100	-0.80030700	-0.93361500
H	-5.96324400	1.40460800	0.09409700
C	1.52521400	-2.58900700	0.73647600
C	2.54508600	-3.52711100	0.98251500
C	1.75204700	-1.24602500	1.09255700
C	3.75420500	-3.13762100	1.55112300
H	2.39034100	-4.57446800	0.74570300
C	2.95954700	-0.86641200	1.68913400
C	3.96510100	-1.80250400	1.91216700
H	4.52752200	-3.87996600	1.72836300
H	4.90225800	-1.49747100	2.36893000
N	-0.63761800	-0.78656300	0.80985800
H	0.73502600	0.54215100	1.61010900
H	-1.42335300	1.00752300	1.47365100
C	-0.54890900	2.66274300	-0.01065000
C	0.20426100	3.15210400	1.08944900
C	-0.11867400	4.36272800	1.70554500
H	1.06965200	2.60187200	1.44324200
C	-1.20560400	5.12434000	1.27116700
H	0.48987000	4.70959300	2.53789900
H	-1.45169300	6.06466500	1.75670900
C	2.11320300	1.17156700	-0.95493800
C	4.68402000	2.01658300	-1.76205200
C	4.38663900	0.65464600	-1.67102900
H	5.14197600	-0.08904700	-1.91110900
C	3.11431700	0.23922800	-1.28228300
H	2.89071200	-0.81948800	-1.24759200
H	5.67543600	2.34371600	-2.06446700
H	3.11024700	0.17393000	1.96420000
H	-3.65582000	1.84247200	0.92455200
N	-0.40436300	1.44352800	-0.65266000
F	0.50144800	-0.41015000	-1.54852300
C	-1.96934100	4.65497400	0.19448500
H	-2.81872200	5.23298600	-0.16279100
C	3.68713300	2.95101600	-1.48205400
H	3.89129000	4.01432800	-1.57728100
C	2.41156700	2.53306600	-1.09173500
H	1.65451600	3.28256800	-0.90943800
C	-1.64997000	3.45398100	-0.43015200
H	-2.24390100	3.08831700	-1.26306500

PRO-F-(*E*)

C	-0.73524000	0.72922200	0.07537100
C	1.07662600	-0.20716500	-1.19897800
C	-1.18672400	-0.30853100	-1.00699100
C	0.09606500	-2.18139700	-0.12722300
C	1.36565400	-2.60911100	0.32436600
C	-1.08507300	-2.78521800	0.37387200
C	1.43139800	-3.63345700	1.28260400
C	-0.96689900	-3.80687400	1.32414100
C	0.27947700	-4.23181700	1.77851800
H	2.39637100	-3.94855600	1.66448800
H	-1.86241600	-4.25325900	1.74340600
H	0.34940900	-5.01351500	2.52919400
C	2.57558700	-1.98441700	-0.24015900
C	3.86115500	-2.53607700	-0.08855700
C	2.43806000	-0.82026300	-1.01845200
C	4.97120000	-1.94441400	-0.68534800
H	3.99832600	-3.44983100	0.47990800
C	3.54989400	-0.25742400	-1.65130900

C	4.81983200	-0.80462100	-1.47948300
H	5.95343500	-2.38923100	-0.54990700
H	5.67860000	-0.35531100	-1.96989000
C	-2.40105800	-2.28582900	-0.07294000
C	-3.60389200	-2.98121800	0.14252400
C	-2.45989500	-1.04746100	-0.73647400
C	-4.82486300	-2.43876100	-0.25322100
H	-3.59125800	-3.95818600	0.61473500
C	-3.68429000	-0.50754400	-1.13667000
C	-4.87218700	-1.19426200	-0.88811200
H	-5.74146600	-2.99395000	-0.07262400
H	-5.82278500	-0.77069700	-1.19963600
N	-0.00846400	-1.17755100	-1.12047100
H	-1.27344300	0.24704400	-1.94689700
H	1.02590700	0.26371200	-2.18926500
C	1.46573800	1.83794800	0.35566900
C	2.32127900	2.58699700	-0.46595600
C	3.10189700	3.60849700	0.07754200
H	2.35620300	2.38596500	-1.53071900
C	3.01585800	3.91952100	1.43665300
H	3.76422500	4.17597300	-0.57129400
H	3.61786300	4.72153000	1.85489400
C	-1.49968500	2.03328800	0.01817700
C	-2.99352600	4.39472800	-0.22049500
C	-3.24872700	3.50414600	0.82392100
H	-4.02712900	3.72321500	1.55000200
C	-2.50779700	2.32559300	0.94262000
H	-2.70980600	1.63253200	1.75062900
H	-3.57077300	5.31103300	-0.31088800
H	-3.70090000	0.45230500	-1.64607000
H	3.41781300	0.60880300	-2.29186500
N	0.66277600	0.80219400	-0.16229200
F	-0.98979700	0.13984900	1.35957800
C	2.14345000	3.19236800	2.25226500
H	2.06410800	3.42606400	3.31092100
C	-1.99034300	4.10252900	-1.14985400
H	-1.78280800	4.79107700	-1.96459500
C	-1.24786500	2.92841100	-1.03082200
H	-0.46303900	2.70678700	-1.74826600
C	1.38353900	2.15032200	1.72327600
H	0.71967900	1.56910300	2.35404000

TS1-F-(*E*)-*endo*

C	1.06503600	-0.40579700	-1.61311500
C	-1.26914300	-0.56034600	-1.79434700
C	-0.18722700	-1.84548900	-0.07691400
C	1.03017600	-2.36640300	0.44456000
C	-1.44745200	-2.17101700	0.49295700
C	0.94627200	-3.20404100	1.56458300
C	-1.46262600	-3.03098700	1.60619200
C	-0.28243800	-3.53319400	2.13360300
H	1.85130100	-3.60379100	2.00639600
H	-2.40649700	-3.30725200	2.06081700
H	-0.31419400	-4.18899300	2.99880500
C	2.31279200	-2.00390100	-0.17482100
C	3.54612500	-2.56031100	0.21523900
C	2.30475900	-1.02773600	-1.19612500
C	4.73571200	-2.14287100	-0.36931500
H	3.58217700	-3.32903700	0.97968800
C	3.51621700	-0.60412000	-1.77502200
C	4.72175900	-1.15320600	-1.36439300
H	5.67593300	-2.58456400	-0.05156600
H	5.65219600	-0.81890300	-1.81512700
C	-2.66563400	-1.60312300	-0.07464800
C	-3.94715100	-1.78003900	0.48229900
C	-2.54923000	-0.83088700	-1.26138700
C	-5.06544000	-1.21830800	-0.11654900
H	-4.07213400	-2.34697600	1.39803200
C	-3.70006100	-0.27347000	-1.86771000
C	-4.94501000	-0.46606800	-1.30034100
H	-6.04287200	-1.36039200	0.33552500
H	-5.82717900	-0.02884000	-1.75871700
N	-0.14238800	-0.99864500	-1.20348200
H	-1.14767900	-0.01942400	-2.72039800
H	1.02231300	-0.10537300	-2.65253300
H	-3.58359800	0.32102500	-2.76940100
H	3.48825100	0.17388500	-2.53246100
C	0.85245600	1.57483100	-1.06972500
C	1.76012600	1.89081800	0.09076600
C	2.47195600	3.10176400	0.04638800
C	1.91165600	1.06700300	1.21215400
C	3.29545200	3.48376800	1.10483300
H	2.37493400	3.74299300	-0.82325000
C	2.74076900	1.44586100	2.26959400
H	1.39830000	0.11642200	1.26259400
C	3.43444600	2.65609400	2.22240300
H	3.83228300	4.42758600	1.05378600
H	2.84673300	0.78604700	3.12666300
H	4.08083500	2.94993600	3.04520700
F	1.52951700	2.00679000	-2.24870700
C	-1.35367800	2.01271200	-0.13299500
C	-1.35888600	1.34413500	1.11126200
C	-2.45136700	2.85968400	-0.41676600
C	-2.39332300	1.53801600	2.02674800
H	-0.57458000	0.63861800	1.34378600
C	-3.47705500	3.05445800	0.50371800
H	-2.47035100	3.36184100	-1.38044100
C	-3.45735300	2.39551200	1.73829500
H	-2.37112100	0.99587000	2.96953300
H	-4.30177700	3.71780000	0.25317200
H	-4.26191300	2.53848800	2.45455000
N	-0.42801500	1.85605500	-1.15577900

(*Z*)-2-Cl

C	-3.61758900	-1.72572500	0.19765300
C	-2.27285800	-1.38234600	0.10649900
C	-1.88820500	-0.03066000	0.00125200
C	-2.88040500	0.96204100	-0.00594400
C	-4.22683200	0.61069900	0.09203200
C	-4.60056400	-0.73034800	0.19192400
H	-3.89987400	-2.77217400	0.27140400
H	-1.50849900	-2.15164400	0.10948300
H	-2.60789900	2.00807500	-0.07981300
H	-4.98316700	1.39038500	0.09001800
H	-5.65053800	-1.00033800	0.26387200
C	-0.44083100	0.26897800	-0.08060900
N	0.45261700	-0.58778400	0.13202000
C	1.84633000	-0.43640500	0.11672100
C	2.59833800	-1.32971600	-0.66203400
C	2.50087500	0.51262800	0.91863200

C	3.98957400	-1.24199900	-0.67206400
H	2.08087200	-2.07422000	-1.25994000
C	3.89408900	0.57554000	0.91822200
H	1.91678800	1.17997700	1.54354400
C	4.64329400	-0.29207500	0.11861600
H	4.56424300	-1.92581100	-1.29097300
H	4.39442500	1.30881200	1.54513200
H	5.72819300	-0.23450400	0.11829400
Cl	-0.02789200	1.98954500	-0.56944400

(*E*)-2-Cl

C	-2.45265400	-0.37512000	0.69406700
C	-1.34829000	-0.05040200	-0.10795500
C	-0.82920000	-1.00603700	-0.99747900
C	-1.40971300	-2.27018100	-1.07784100
C	-2.49888700	-2.59611900	-0.26487100
C	-3.01624000	-1.64810000	0.62201200
H	-2.86086700	0.36238400	1.37770400
H	0.01809100	-0.75498700	-1.62667100
H	-1.01072000	-3.00009400	-1.77637600
H	-2.94583100	-3.58454000	-0.32571300
H	-3.86318500	-1.89699500	1.25498400
C	-0.70093500	1.28238400	-0.03142100
N	0.51423600	1.61321700	-0.02583600
C	1.58334800	0.69523100	0.08583800
C	1.65538200	-0.23626700	1.13389400
C	2.63624600	0.79119200	-0.83533500
C	2.76407800	-1.07526200	1.24009300
H	0.84734100	-0.29069700	1.85684500
C	3.72970000	-0.06895900	-0.73299900
H	2.57933200	1.53069100	-1.62884000
C	3.80039400	-1.00301900	0.30463000
H	2.81508600	-1.79039800	2.05692500
H	4.53406700	0.00035500	-1.46051500
H	4.65933900	-1.66290000	0.38852200
Cl	-1.87362800	2.65639000	-0.00775300

TS1-Cl-(*Z*)-*exo*

C	-0.45689900	-0.96567300	-1.07288000
C	1.39864000	0.49096600	-1.20344000
C	-0.75317300	1.44778000	-0.79701700
C	-2.16345300	1.26903300	-0.79765600
C	-0.15397600	2.69740800	-0.48037700
C	-2.95151500	2.34928400	-0.39062400
C	-1.00646700	3.75470800	-0.10567200
C	-2.37819000	3.57444700	-0.04643100
H	-4.02749900	2.23643800	-0.33028600
H	-0.58745900	4.71996400	0.15200800
H	-3.01655500	4.39509100	0.26734000
C	-2.73718500	-0.01230700	-1.22575300
C	-4.10686600	-0.18771800	-1.49319200
C	-1.86287900	-1.11093700	-1.39117700
C	-4.60272000	-1.42406400	-1.89014800
H	-4.79129100	0.64905600	-1.40267900
C	-2.37406800	-2.35403100	-1.80849000
C	-3.73211200	-2.51263000	-2.04822600
H	-5.66427500	-1.54041200	-2.08948600
H	-4.11667600	-3.47691700	-2.36883300
C	1.29406800	2.84002900	-0.53127600
C	1.98632600	4.02591000	-0.21412100
C	2.05622400	1.70686100	-0.92820100
C	3.37047000	4.08049500	-0.29114200
H	1.44392400	4.91216100	0.09494600
C	3.46938700	1.77695900	-1.00419200
C	4.11836900	2.95369900	-0.68624500
H	3.88268400	5.00548900	-0.04217200
H	5.20155300	3.01158500	-0.73782200
N	0.07158000	0.34848400	-1.11193500
H	1.95558800	-0.38404500	-1.50667500
H	0.21572300	-1.67784400	-1.53632500
H	4.02524500	0.89233100	-1.30065600
H	-1.69217200	-3.18891000	-1.93122700
C	0.04624900	-1.46252300	0.88196700
C	-0.97799600	-0.72352300	1.68836100
C	-2.33063900	-1.09182000	1.74703900
C	-0.57670600	0.46293900	2.33090900
C	-3.25555700	-0.29188800	2.41847000
H	-2.66361900	-1.99791300	1.25728000
C	-1.50307100	1.25970900	2.99984300
H	0.46687800	0.75236500	2.28757400
C	-2.85044300	0.89036500	3.04103800
H	-4.29936900	-0.59332500	2.44419000
H	-1.17118200	2.17460100	3.48366900
H	-3.57510500	1.51525100	3.55636200
C	2.46170500	-1.78546100	0.60403100
C	2.55410900	-2.83994700	-0.33503900
C	3.66969400	-1.23533100	1.09519600
C	3.80096100	-3.31326900	-0.74813300
H	1.65413900	-3.28520700	-0.73816700
C	4.90642100	-1.71669000	0.67757200
H	3.60439900	-0.41651200	1.80625600
C	4.98433700	-2.76293200	-0.24967600
H	3.84300700	-4.12362800	-1.47255400
H	5.81523200	-1.27175100	1.07586900
H	5.94929500	-3.13954300	-0.57772100
N	1.29750200	-1.19675000	1.06244000
Cl	-0.47613600	-3.40997300	0.79315700

TS1-Cl-(*Z*)-*endo*

C	1.09113700	-1.18329400	0.42303100
C	-1.01240400	-0.20633900	-1.67177500
C	1.19435200	0.24441400	-0.99459100
C	-0.61162300	1.78122700	-0.39303200
C	-2.00973300	1.98076400	-0.23845500
C	0.34057300	2.69739400	0.13070400
C	-2.43414500	3.10417500	0.49571900
C	-0.14511500	3.78223900	0.86791100
C	-1.51368800	3.97943100	1.05044100
H	-3.49215000	3.28762400	0.63853900
H	0.55004200	4.48426600	1.31304700
H	-1.86015800	4.83136800	1.62810200
C	-2.94472100	1.02363300	-0.81612900
C	-4.34345200	1.10231900	-0.67002900
C	-2.41042300	-0.05455900	-1.57345600
C	-5.17131400	0.15238300	-1.24961400
H	-4.79036100	1.90099900	-0.08923600
C	-3.26853000	-1.01251300	-2.16551200
C	-4.63586200	-0.90845600	-2.00540300
H	-6.24660700	0.22939300	-1.11665300
H	-5.29658300	-1.64642000	-2.45034800

C	1.76978700	2.50275100	-0.14444500
C	2.74427100	3.48063800	0.12415900
C	2.17189300	1.29344300	-0.75346900
C	4.08092500	3.26238500	-0.19251800
H	2.46056700	4.42774700	0.57044900
C	3.52108700	1.09455400	-1.09590700
C	4.47139700	2.06707400	-0.81106500
H	4.81757700	4.03056100	0.02532900
H	5.51187000	1.90291900	-1.07735300
N	-0.15425800	0.64970600	-1.09645200
H	1.45104400	-0.44614800	-1.79143000
H	-0.57532200	-1.01494500	-2.24040600
C	-1.26268100	-1.88434000	0.84393900
C	-1.83287900	-0.90355800	1.69051800
C	-3.12076700	-1.06794700	2.19924400
H	-1.27456100	-0.00937900	1.92762800
C	-3.88894100	-2.19167900	1.88369700
H	-3.53302100	-0.29178000	2.84036000
H	-4.89289700	-2.30605600	2.28314600
C	2.39269700	-1.91105700	0.17535500
C	4.75789200	-3.29111000	-0.50668500
C	4.80009000	-2.20016900	0.36208200
H	5.74696300	-1.87438400	0.78477700
C	3.63127700	-1.51152900	0.69641300
H	3.68676100	-0.66326400	1.36563900
H	5.66916600	-3.82351300	-0.76609900
H	3.81155100	0.17070600	-1.58542700
H	-2.83267400	-1.83141900	-2.73047200
N	-0.01165900	-1.84492500	0.26723200
C	-3.34414000	-3.16155400	1.03470200
H	-3.92507100	-4.04129800	0.76728100
C	3.52859600	-3.69386700	-1.03647800
H	3.47639400	-4.54509200	-1.71069600
C	2.35997600	-3.01321400	-0.69921100
H	1.40589400	-3.33135100	-1.10475300
C	-2.05983400	-3.01039100	0.52209500
H	-1.63635300	-3.76352200	-0.13713400
Cl	1.28559800	-0.08058600	2.09216700

TS1-Cl-(*E*)-*exo*

C	0.96940800	0.63163600	-0.84545000
C	-1.60753100	0.61083700	0.83613800
C	0.51942000	-0.39840600	0.88299800
C	-1.46123100	-1.71416700	0.28095900
C	-2.80741100	-1.70648800	-0.17177800
C	-0.67930800	-2.90106600	0.28601000
C	-3.34459100	-2.91610400	-0.65350500
C	-1.26482700	-4.06499700	-0.22070600
C	-2.57983000	-4.07066800	-0.68736200
H	-4.36748100	-2.94694300	-1.00946600
H	-0.68934500	-4.98250600	-0.26177400
H	-3.00728700	-4.99010500	-1.07647000
C	-3.57880100	-0.47003400	-0.13209000
C	-4.90793600	-0.35212700	-0.58487100
C	-2.95446200	0.68288000	0.41442400
C	-5.58519500	0.85538700	-0.49006000
H	-5.41759200	-1.20651300	-1.01577800
C	-3.66027100	1.90557500	0.51752800
C	-4.96287500	1.99046600	0.06449300
H	-6.60913200	0.92257000	-0.84648100
H	-5.50605000	2.92828600	0.13453700
C	0.68028500	-2.87652100	0.84265600
C	1.42835900	-4.04042500	1.09813400
C	1.23769600	-1.62422100	1.18493500
C	2.69231900	-3.96683300	1.67436000
H	1.01604800	-5.01631000	0.86494600
C	2.50548200	-1.56363800	1.79316000
C	3.23083100	-2.72296400	2.03222500
H	3.25179700	-4.87891100	1.86211300
H	4.21055600	-2.66418500	2.49804700
N	-0.88466900	-0.51441000	0.74391600
H	0.77638900	0.43921300	1.52291300
H	-1.14042600	1.44586000	1.33484100
C	0.33717300	2.83071000	-0.04575800
C	1.22881600	3.00360900	1.04283300
C	1.21304200	4.17498400	1.80166400
H	1.94992300	2.22959500	1.28028000
C	0.32155300	5.20964000	1.50881300
H	1.91119400	4.27699500	2.62944500
H	0.31710400	6.11925600	2.10291200
C	2.46823600	0.61852300	-1.00932100
C	5.26652900	0.64062200	-1.35804200
C	4.58233400	-0.56986800	-1.21838700
H	5.12422900	-1.51148800	-1.24357900
C	3.19843100	-0.58105800	-1.05580100
H	2.67810500	-1.52723100	-0.98854800
H	6.34562000	0.64888700	-1.48697800
H	2.91559200	-0.59456300	2.06275000
H	-3.15589900	2.76983100	0.94011400
N	0.19939400	1.69190100	-0.82393500
C	-0.56590100	5.05539500	0.43573100
H	-1.26738900	5.84971200	0.19151200
C	4.54785900	1.83720800	-1.35503900
H	5.06120600	2.78500500	-1.49426100
C	3.16161200	1.82660900	-1.19103100
H	2.61952200	2.76357200	-1.21746700
C	-0.56341400	3.88927600	-0.32233800
H	-1.26093400	3.75916200	-1.14501000
Cl	0.27331600	-0.60025000	-2.18891700

4

C	4.70691400	0.55587400	0.23285300
C	4.81013500	1.94281900	0.30778400
C	3.69017700	2.78848600	0.26519600
C	2.41032100	2.24549600	0.16031100
C	2.33990100	0.82308000	0.10420100
C	3.44338600	-0.05729100	0.11729600
C	1.14813500	3.03010500	0.09718300
C	-0.09310000	2.35154100	0.02947900
N	-0.04936000	0.97168400	0.04206600
C	1.08279500	0.21520100	0.05138100
C	-1.37195100	2.94862100	-0.05685500
C	-2.56558300	2.07934200	-0.14337300
C	-2.40384100	0.66112900	-0.08593600
C	-1.10587100	0.15886700	0.00558600
C	-3.88101800	2.52978000	-0.29715700
C	-4.93420400	1.61324100	-0.39204900
C	-4.74023400	0.23033400	-0.32569700
C	-3.44898500	-0.28572500	-0.15904700
C	1.05879400	4.42770600	0.08751400

C	-0.18487200	5.06543200	0.01077500
C	-1.38146200	4.35351100	-0.06334700
C	0.74932400	-1.12215400	-0.00343300
N	-0.68706800	-1.13894800	0.01953900
C	1.84853900	-2.05364400	-0.17117900
C	3.18445400	-1.50085300	-0.04642100
C	-1.71706400	-2.11588700	0.17901500
C	-3.07761800	-1.70096500	0.01576400
C	1.70794000	-3.41020300	-0.53155000
C	2.80707900	-4.24107600	-0.66802800
C	4.09555500	-3.73700000	-0.45414500
C	4.26907900	-2.39327100	-0.16831100
C	-4.06544000	-2.69729200	0.13530700
C	-3.75350500	-4.01112200	0.45070100
C	-2.42544800	-4.36679600	0.70287500
C	-1.41544300	-3.42148600	0.57619600
H	5.61631200	-0.03297400	0.26351700
H	5.79588600	2.38918400	0.39663500
H	3.83947300	3.86175400	0.31917600
H	-4.09952400	3.59055800	-0.35393400
H	-5.94369000	1.99182800	-0.52036800
H	-5.60142600	-0.42340300	-0.40273700
H	1.95796600	5.03238700	0.13543700
H	-0.21756600	6.15036400	0.00581300
H	-2.31865800	4.89587900	-0.12391400
H	0.72570200	-3.80491800	-0.75358300
H	2.66416500	-5.27893900	-0.95265800
H	4.96057200	-4.38646100	-0.54460800
H	5.27913200	-2.01500300	-0.06107100
H	-5.10634300	-2.42322200	0.00588000
H	-4.54481000	-4.74856900	0.53796200
H	-2.17562900	-5.37624600	1.01357600
H	-0.39788800	-3.68616000	0.82631700

4-TS

C	-3.47439200	1.12347500	1.03577400
C	-3.65057900	2.30032600	0.31010600
C	-2.66690700	2.79018400	-0.55735400
C	-1.46518900	2.09794700	-0.71345800
C	-1.31808700	0.89226900	0.03107600
C	-2.29017300	0.37181000	0.89935900
C	-0.33487800	2.57354500	-1.53781300
C	0.89669500	1.88875900	-1.48325400
N	0.95014900	0.73419700	-0.71332800
C	-0.09503400	0.20179200	-0.01077700
C	2.08801800	2.29006600	-2.13691100
C	3.31895300	1.50250700	-1.91299000
C	3.27439000	0.37154100	-1.03885100
C	2.04391900	0.01554100	-0.46401200
C	-0.36850100	3.70342800	-2.36346500
C	0.78129000	4.12611500	-3.05358300
C	1.99712700	3.44581700	-2.93572500
C	4.55994900	1.79660400	-2.48553500
C	5.68051500	1.01196400	-2.18665500
C	5.61099000	-0.07803000	-1.31291000
C	4.39232200	-0.41878600	-0.71554300
C	0.32970500	-0.90494800	0.70841700
N	1.74955000	-1.00936400	0.38786200
C	2.86209200	-1.86530900	0.70568200
C	-0.69285300	-1.53897500	1.54387500
C	-0.58190300	-2.75313200	2.25155300
C	-1.61596300	-3.30979600	2.97549600
C	-2.85795400	-2.68172100	3.01994900
C	-3.02796700	-1.49694100	2.33499900
C	-1.98926800	-0.88071500	1.59774200
C	4.16312900	-1.53654000	0.20028500
C	5.24437000	-2.34958100	0.58293300
C	5.09130300	-3.46294700	1.39077700
C	3.81332400	-3.80428000	1.82969700
C	2.72615700	-3.01249500	1.48877100
H	-4.25712700	0.81816900	1.71928600
H	-4.57033400	2.86339800	0.43543800
H	-2.84274500	3.72346900	-1.08117400
H	-1.28777900	4.26692300	-2.47885500
H	0.72459000	5.00640800	-3.68609600
H	2.86770800	3.81812500	-3.46379200
H	4.66976700	2.63483500	-3.16422400
H	6.63279400	1.25798100	-2.64648700
H	6.51046900	-0.65075500	-1.12207100
H	0.33363400	-3.31009500	2.24211700
H	-1.45395100	-4.25065500	3.49214200
H	-3.68534600	-3.12022000	3.56858500
H	-4.00640700	-1.03326800	2.34666300
H	6.23670700	-2.09515900	0.23072900
H	5.95280300	-4.06272500	1.66540500
H	3.65306800	-4.68773900	2.43928700
H	1.75881300	-3.31302400	1.83085300