Supplementary Information

Ring-fluorinated heptamethine cyanine dye: Synthesis, photophysical properties, and vaporochromic properties in response to ammonia

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[b] Department of Material Science, Graduate School of Science, University of Hyogo, 3-2-1 Koto, Kamigori-cho, Ako, Hyogo 678-1297, Japan

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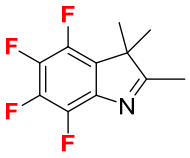
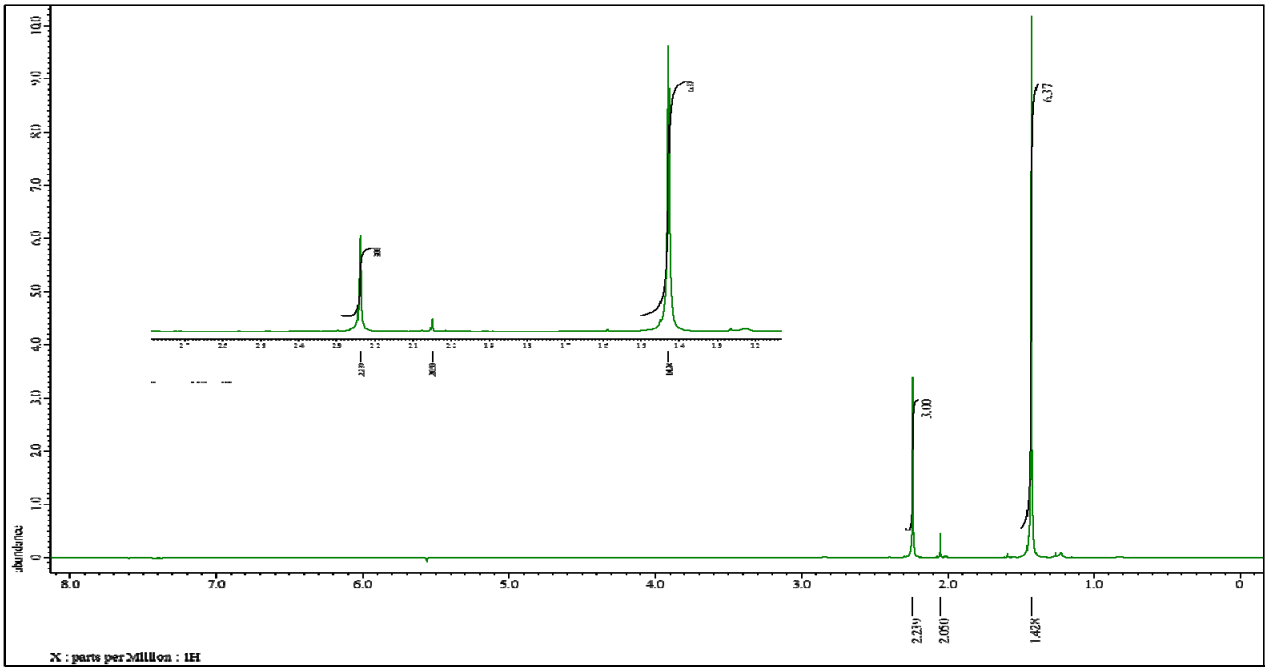
(Contents)

4,5,6,7-Tetrafluoro-2,3,3-trimethyl-3*H*-indole (1)



^{1}H NMR



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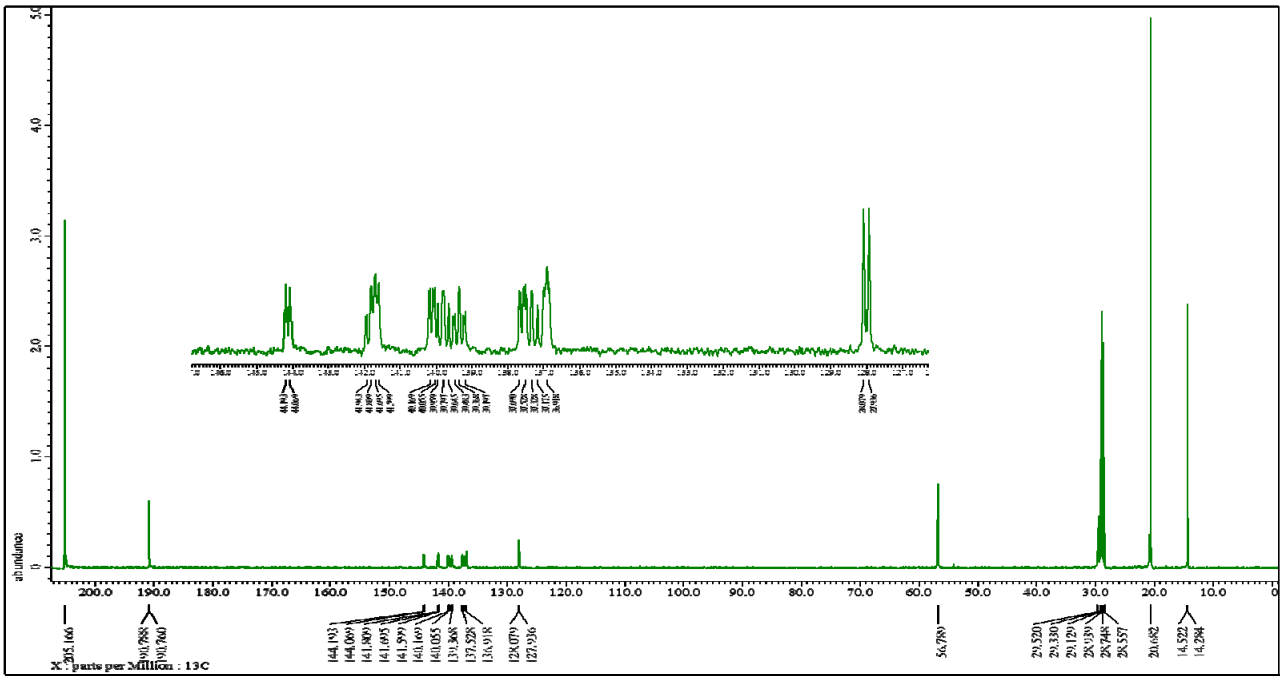
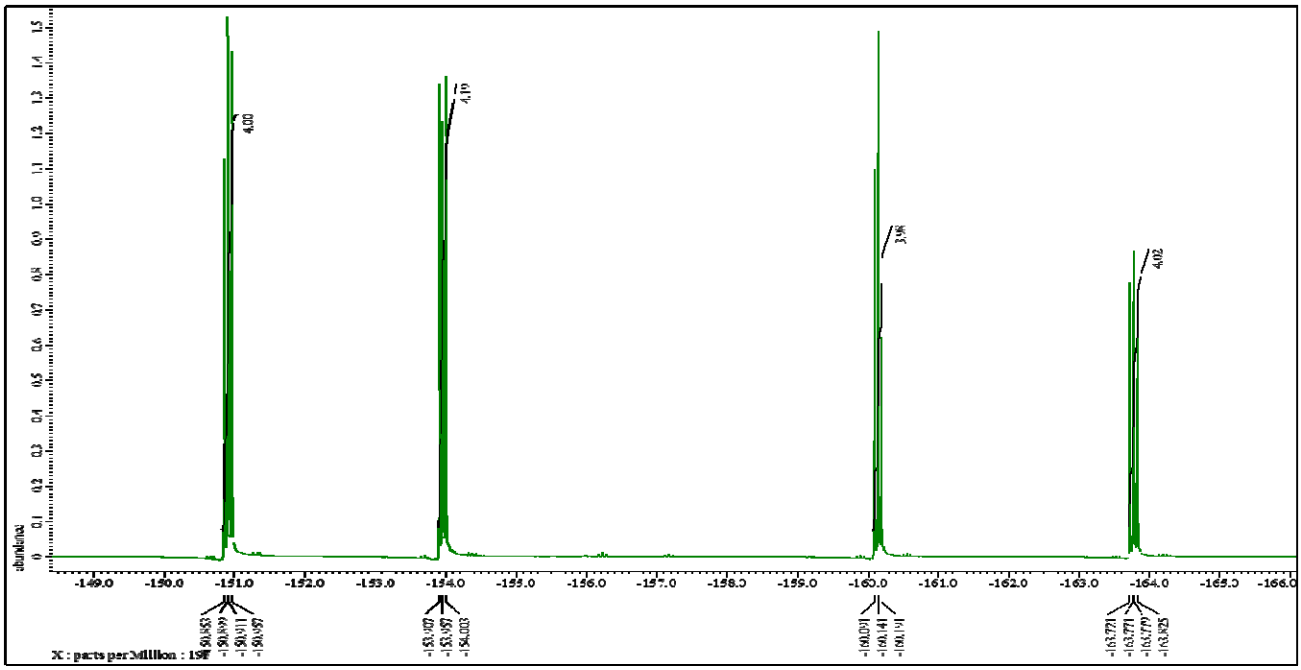


^{19}F NMR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4.19
3.98
4.02
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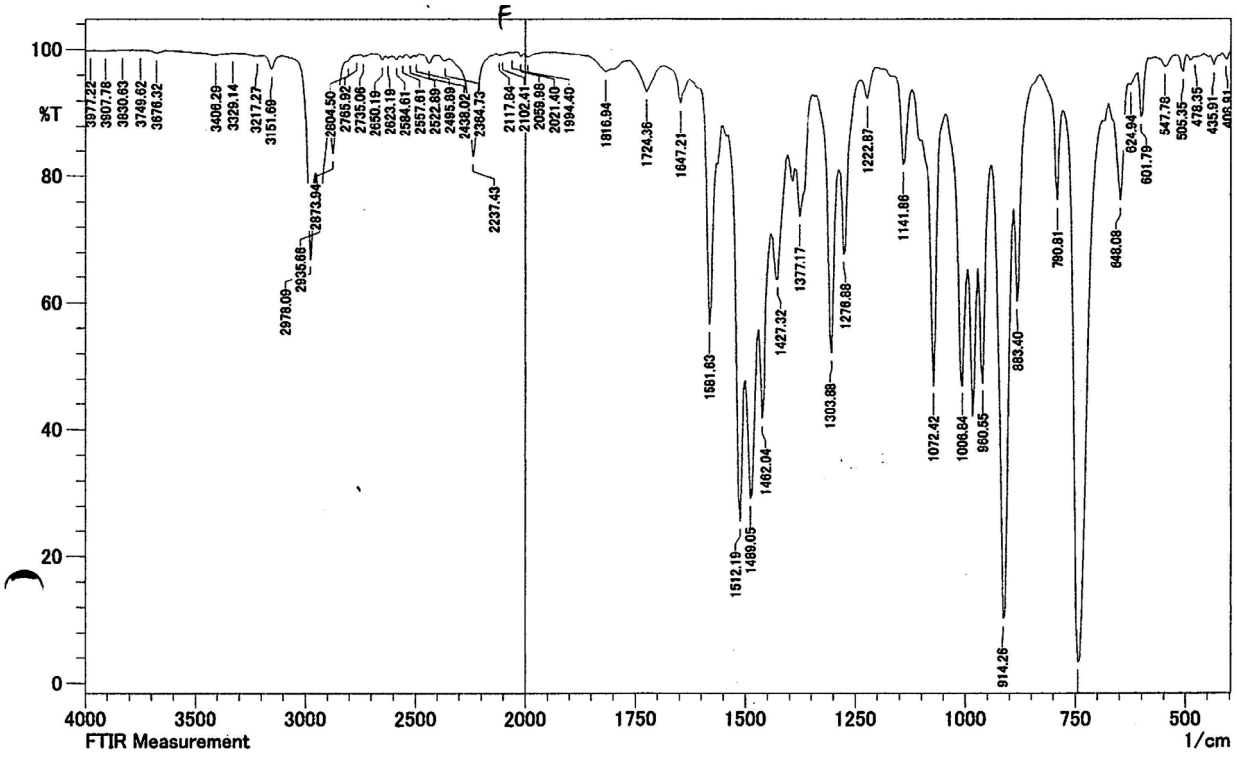
-152.0
-153.0
-154.0
-155.0
-156.0
-157.0
-158.0
-159.0
-160.0
-161.0
-162.0
-163.0
-164.0
-165.0
-166.0
X : parts per Million : 19F

IR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20
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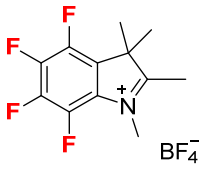
3329.14
3217.27
3151.68
2978.09
2935.68
2873.94
2804.50
2785.92
2735.06
2650.19
2623.19
2584.61
2557.61
2522.89
2495.89
2438.02
2384.73
2237.43
2117.84
2102.41
2056.98
2021.40
1994.40
1816.94
1724.36
1647.21
1581.63
1512.19
1489.05
1482.04
1427.32
1377.17
1303.88
1278.88
1222.87
1141.86
1072.42
1008.84
960.55
914.26
883.40
790.81
648.08
624.94
601.79
547.78
505.35
478.35
435.91
406.91
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
FTIR Measurement
1/cm

4,5,6,7-Tetrafluoro-1,2,3,3-tetramethyl-3*H*-indol-1-ium tetrafluoroborate (2a)



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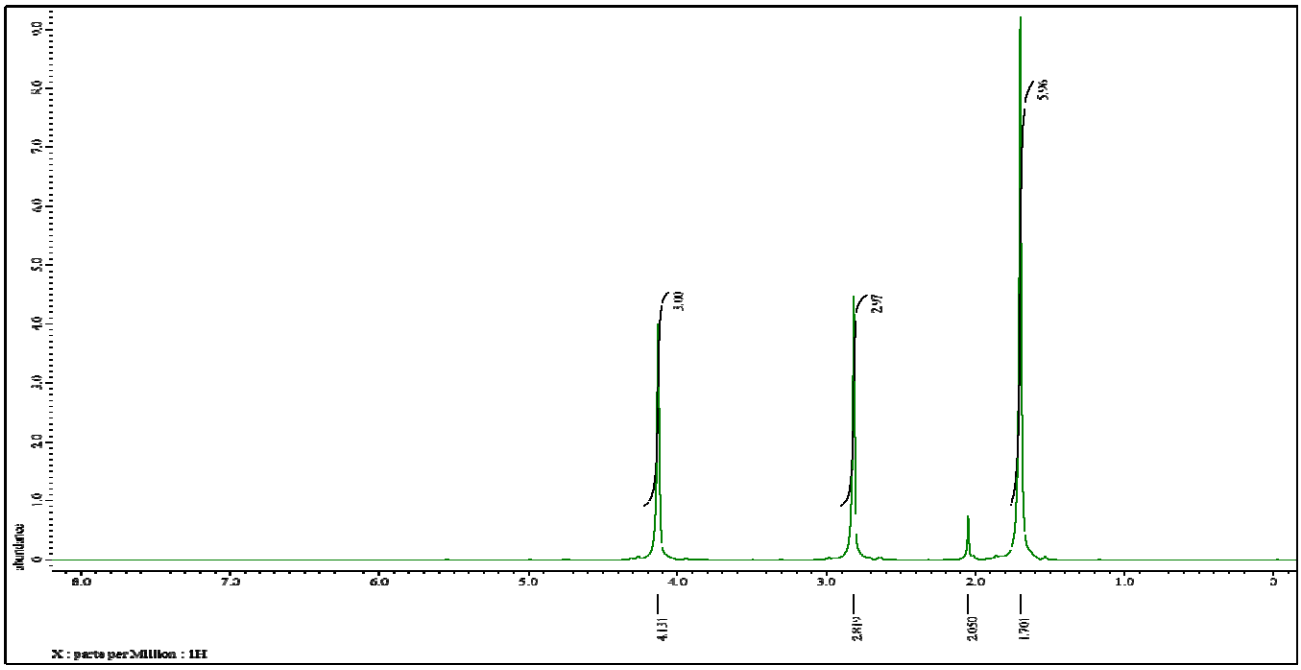

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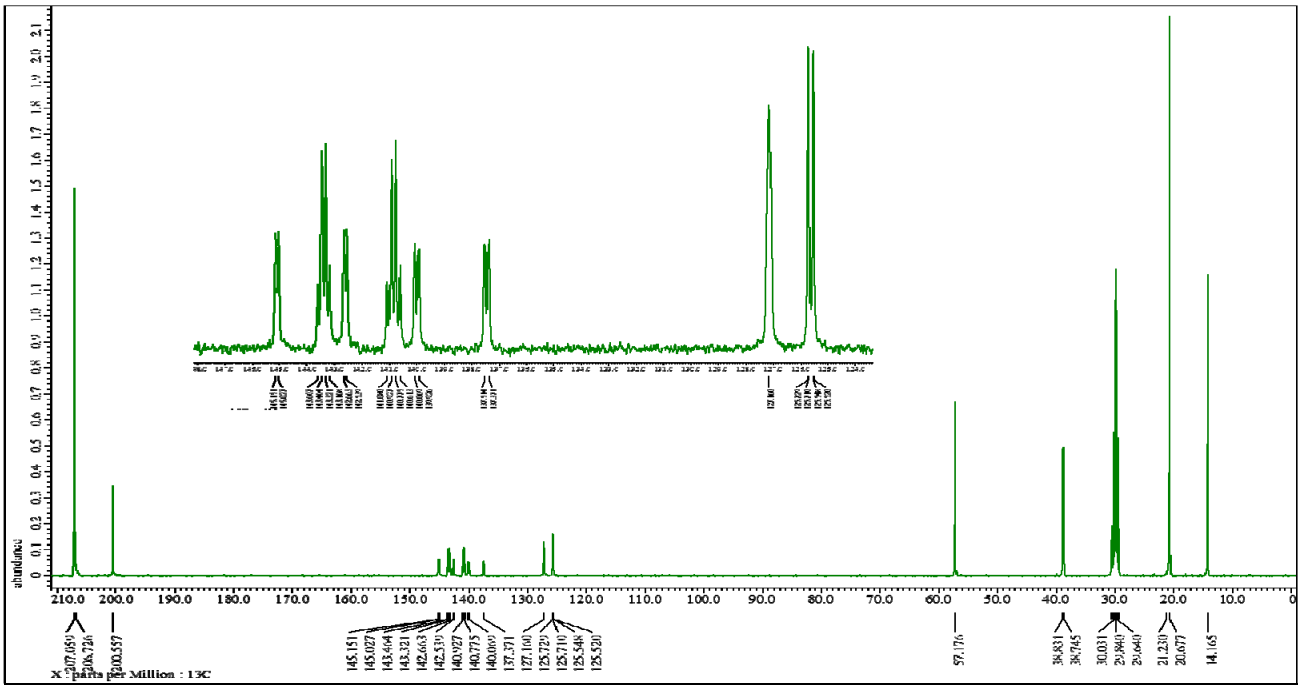

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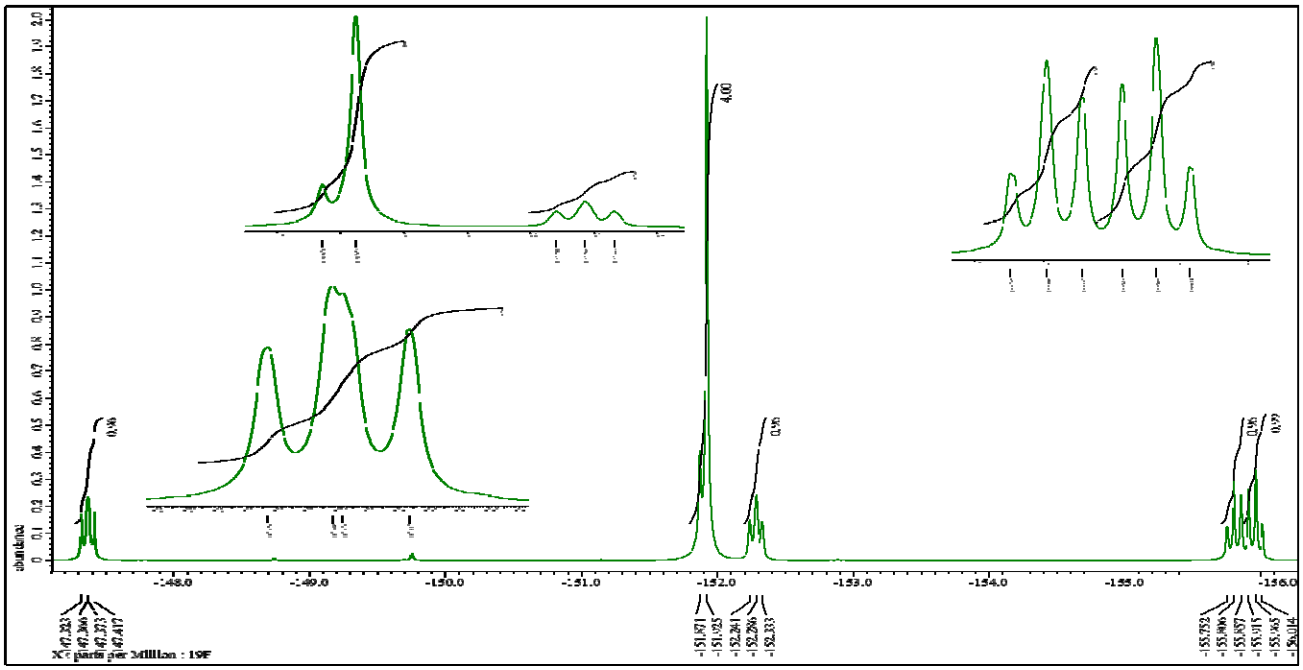
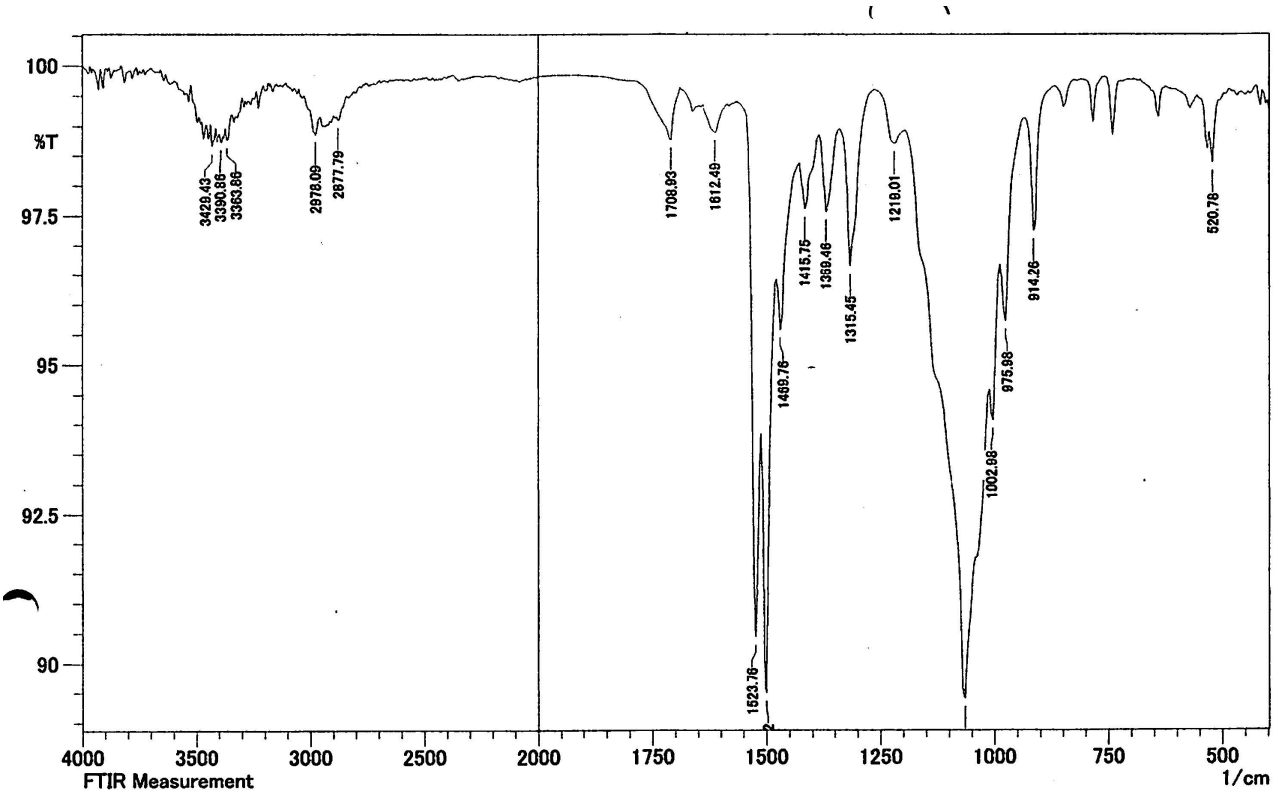


IR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92.5
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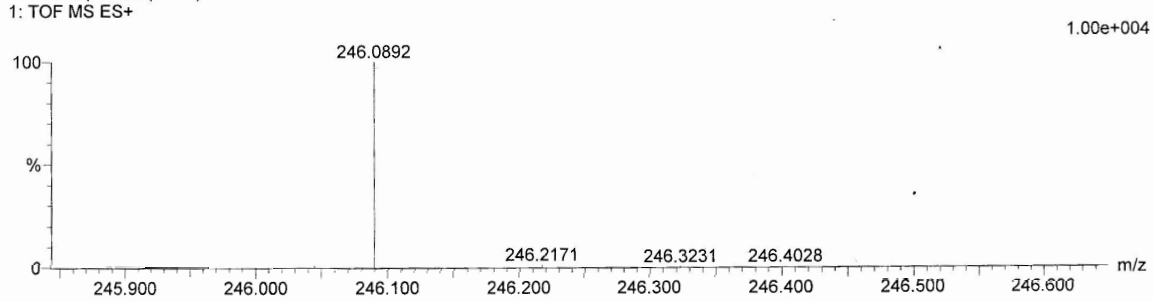
1612.49
1523.76
1469.76
1415.75
1369.49
1315.45
1218.01
1002.88
975.88
914.26
520.78
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
FTIR Measurement

HRMS

Elemental Composition Report **Page 1**

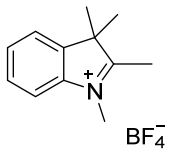
Single Mass Analysis
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 200.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 12-12 H: 12-13 N: 1-1 19F: 4-4 Na: 0-1
20190830p-2-2 8 (0.284)
1: TOF MS ES+

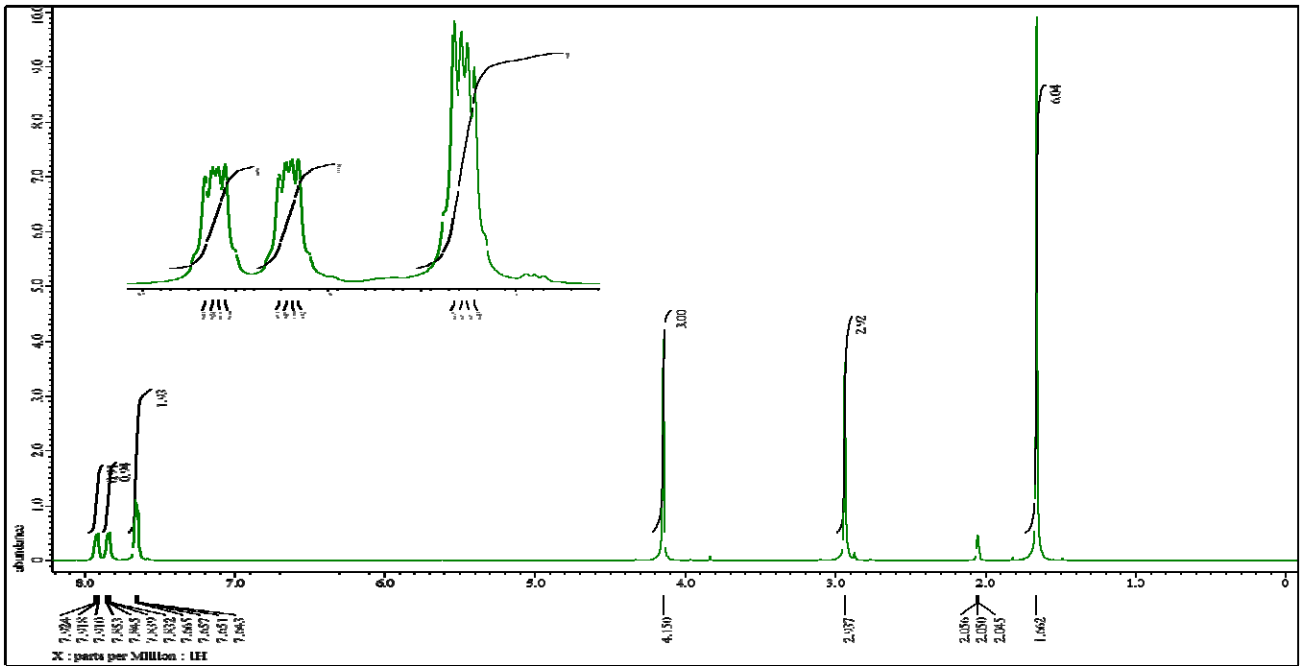


Minimum:				-1.5						
Maximum:		10.0	1000.0	200.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula			
246.0892	246.0906	-1.4	-5.7	5.5	53.4	0.0	C12	H12	N	19F4

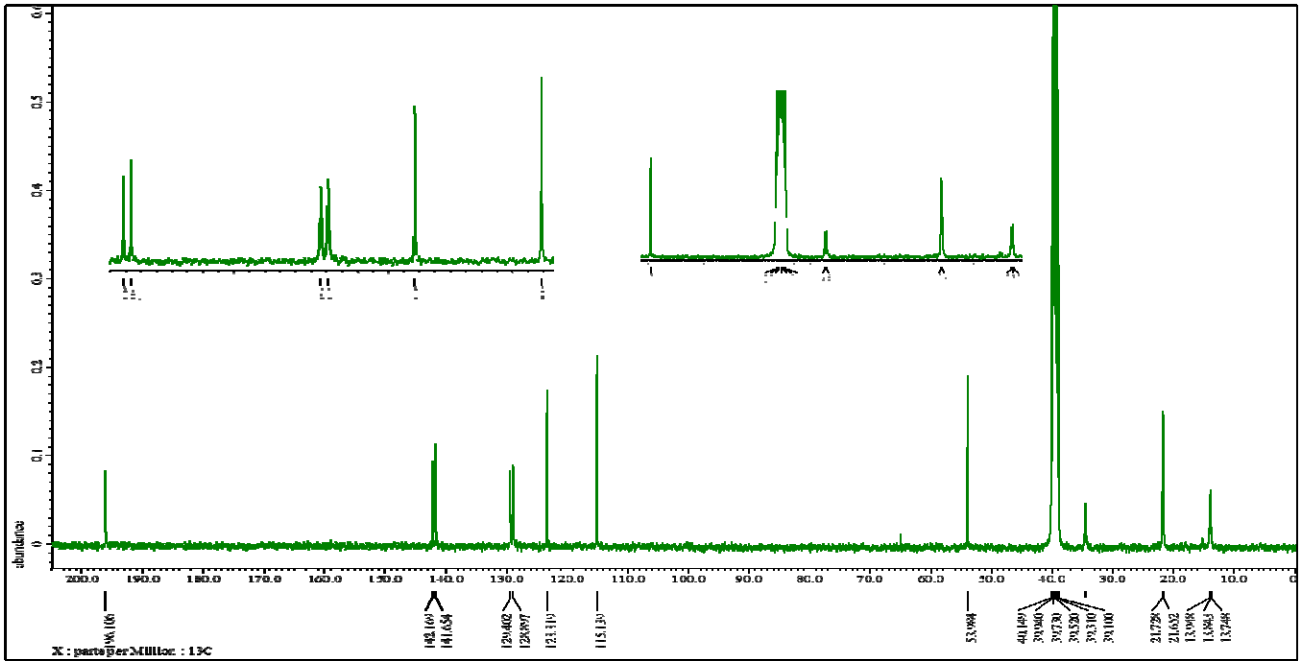
1,2,3,3-Tetramethyl-3*H*-indol-1-ium tetrafluoroborate (2b)[1]



^{1}H NMR

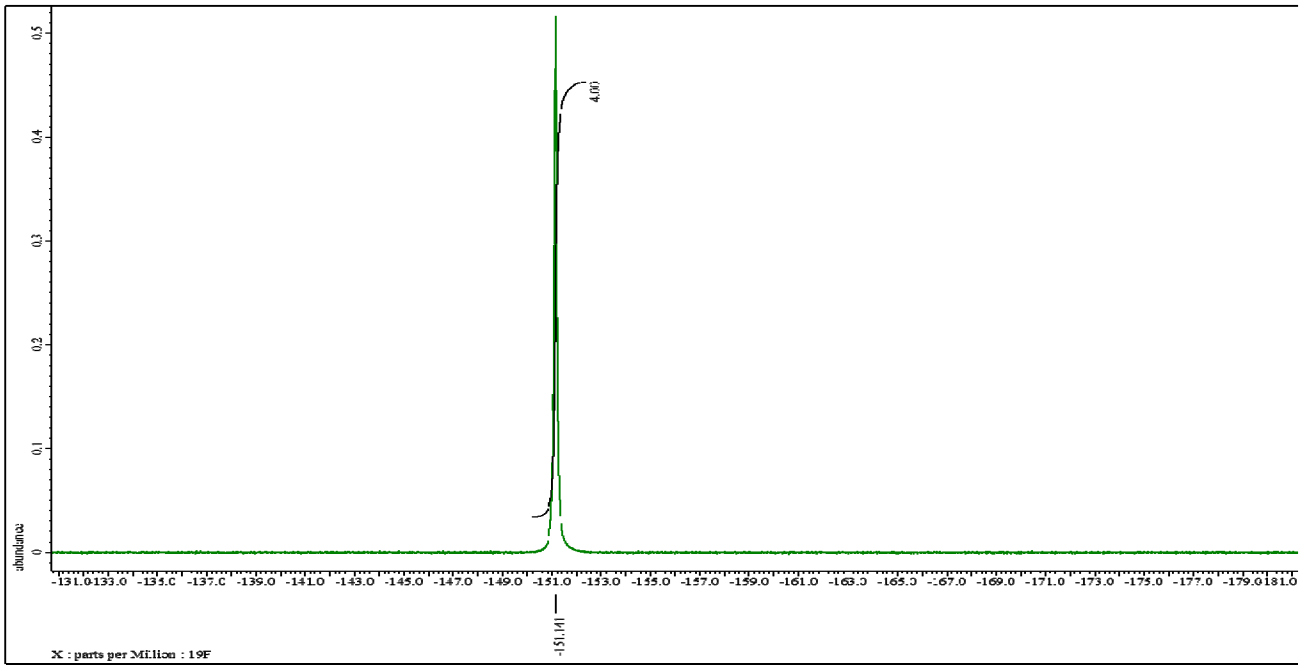


^{13}C NMR

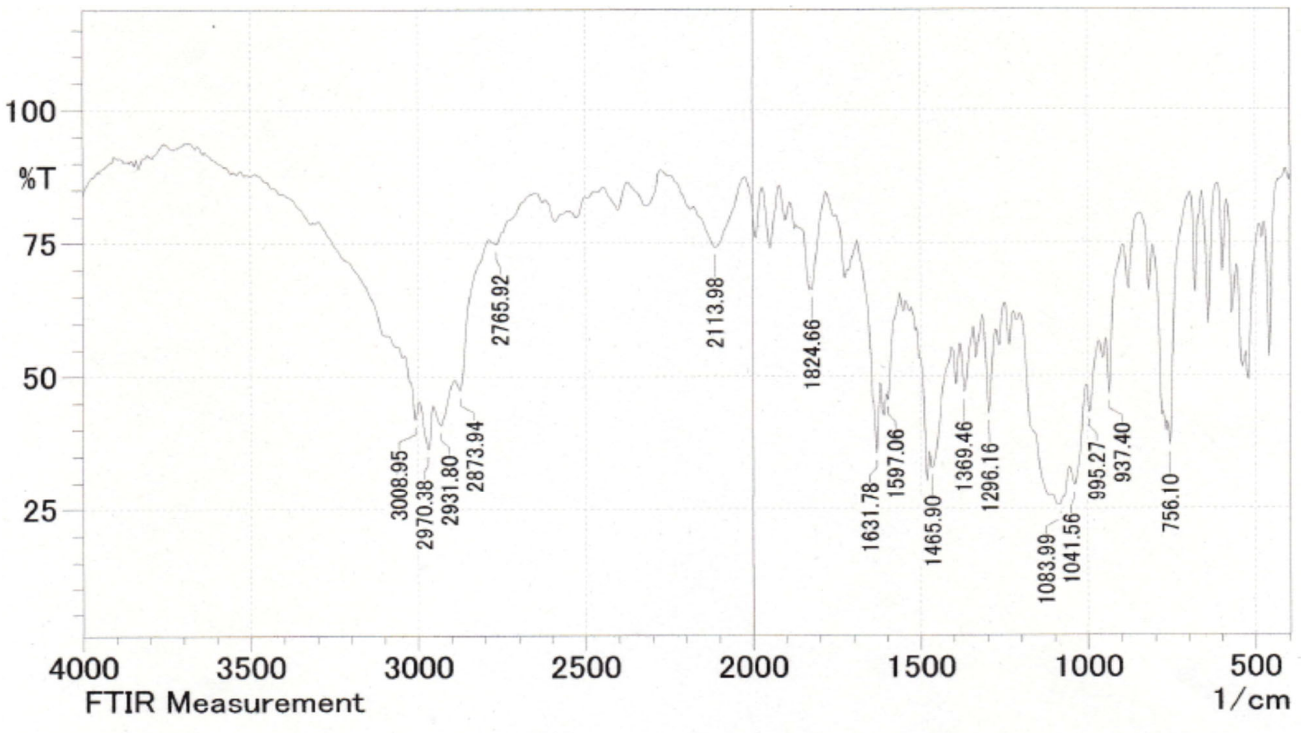


[1] C. Reichardt, H. -D. Engel, *Chem. Ber*. **1998**, 121, 1009-1011.

^{19}F NMR


4.00
abundance
-131.0 -133.0 -135.0 -137.0 -139.0 -141.0 -143.0 -145.0 -147.0 -149.0 -151.0 -153.0 -155.0 -157.0 -159.0 -161.0 -163.0 -165.0 -167.0 -169.0 -171.0 -173.0 -175.0 -177.0 -179.0 -181.0
-151.141
X : parts per Million : 19F

IR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50
25
3008.95
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2873.94
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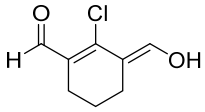
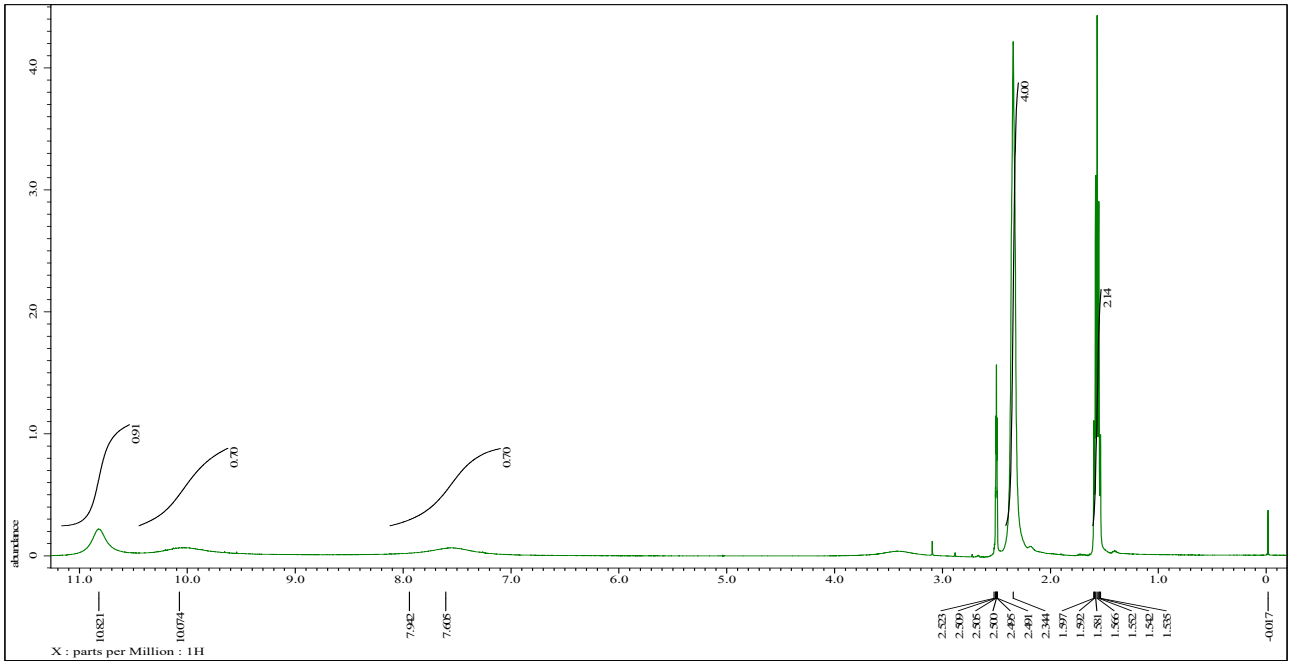
2113.98
1824.66
1631.78
1597.06
1465.90
1369.46
1296.16
1083.99
1041.56
995.27
937.40
756.10
4000
3500
3000
2500
2000
1500
1000
500
FTIR Measurement
1/cm

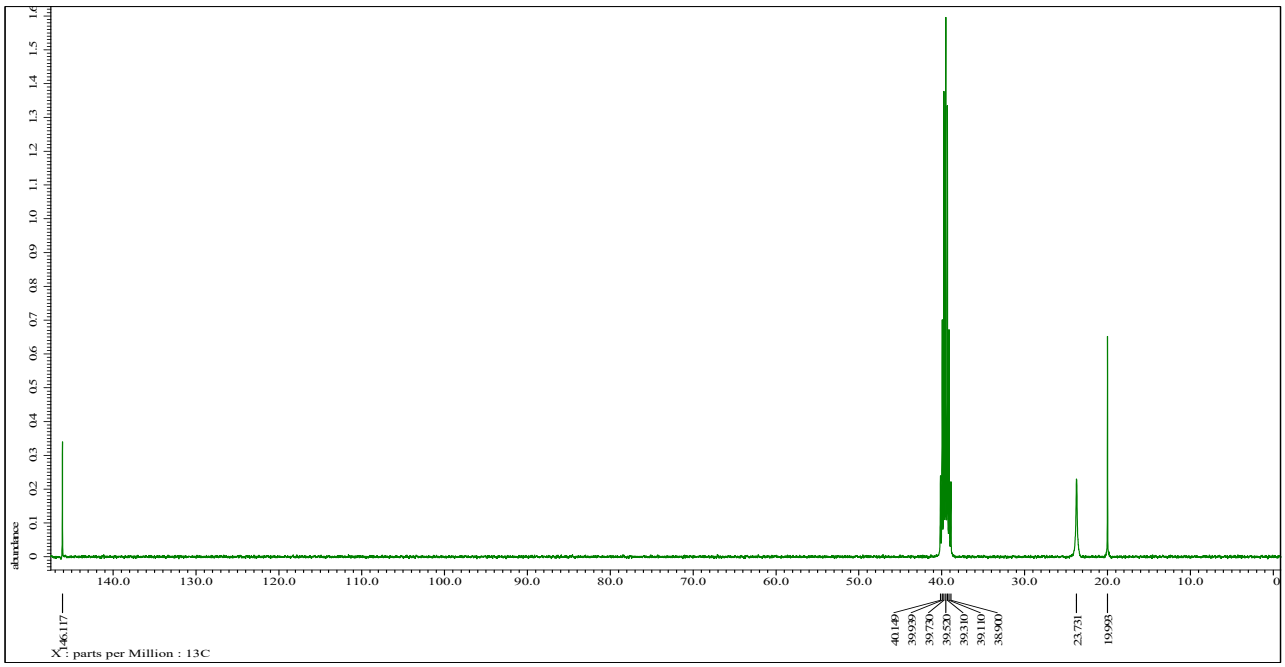
(E)-2-Chloro-3-(hydroxymethylene)cyclohex-1-enecarbaldehyde (3)[2]



^{1}H NMR

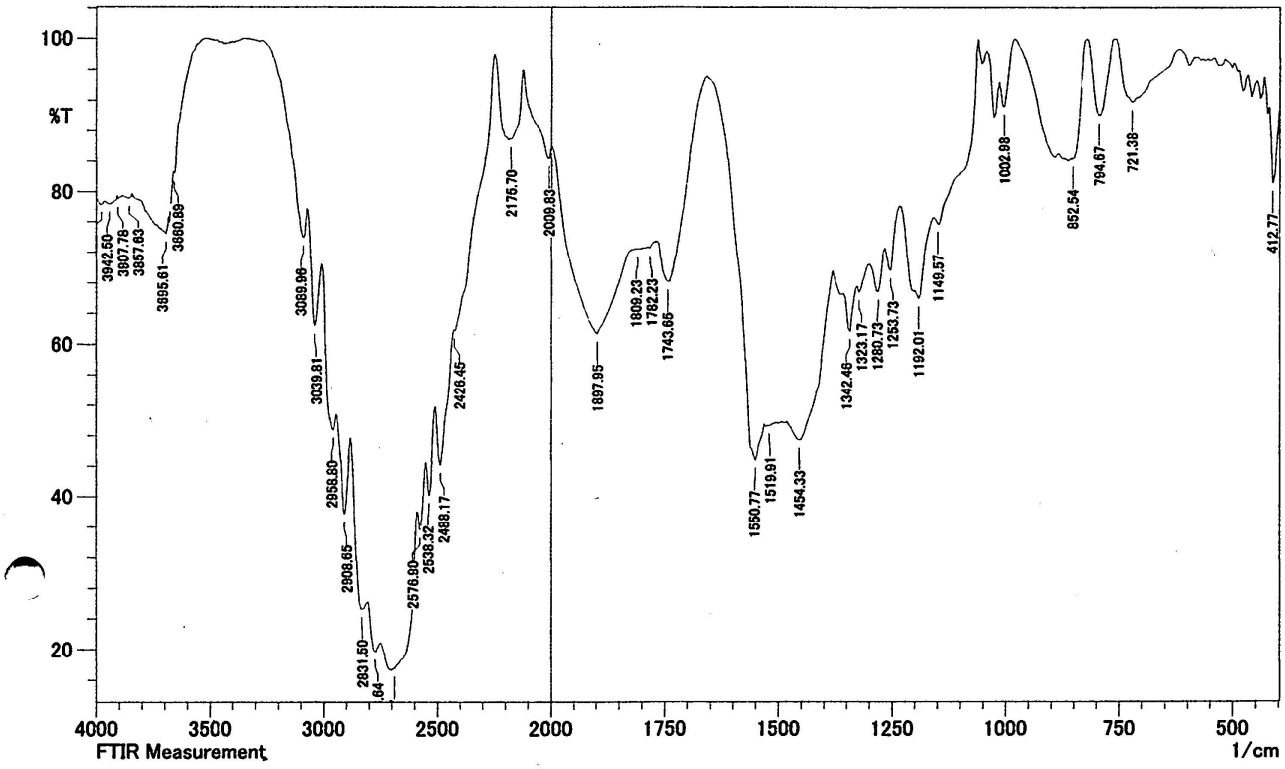


^{13}C NMR



[2] N. Y. Kang, S. J. Park, X. W. E. Ang, A. Samanta, W. H. P. Driessen, V. Ntziachristos, K. O. Vasquez, J. D. Peterson, S. W. Yun, Y. T. Chang, *Chem Commun*. **2014**, 50, 6589-6591.

IR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%T
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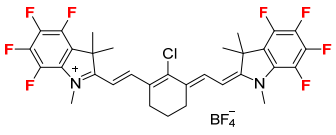
60
40
20
3942.50
3907.78
3857.83
3695.61
3660.89
3099.96
3039.81
2958.80
2908.65
2831.50
2576.90
2538.32
2488.17
2426.45
2176.70
2009.83
1897.95
1809.23
1782.23
1743.66
1550.77
1519.91
1454.33
1342.46
1323.17
1280.73
1253.73
1192.01
1149.57
1002.98
852.54
794.67
721.38
412.77
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
FTIR Measurement

2-((*E*)-2-((*E*)-2-Chloro-3-(2-((*E*)-4,5,6,7-tetrafluoro-1,3,3-trimethylindolin-2-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-4,5,6,7-tetrafluoro-1,3,3-trimethyl-3*H*-indol-1-ium tetrafluoroborate (4a)



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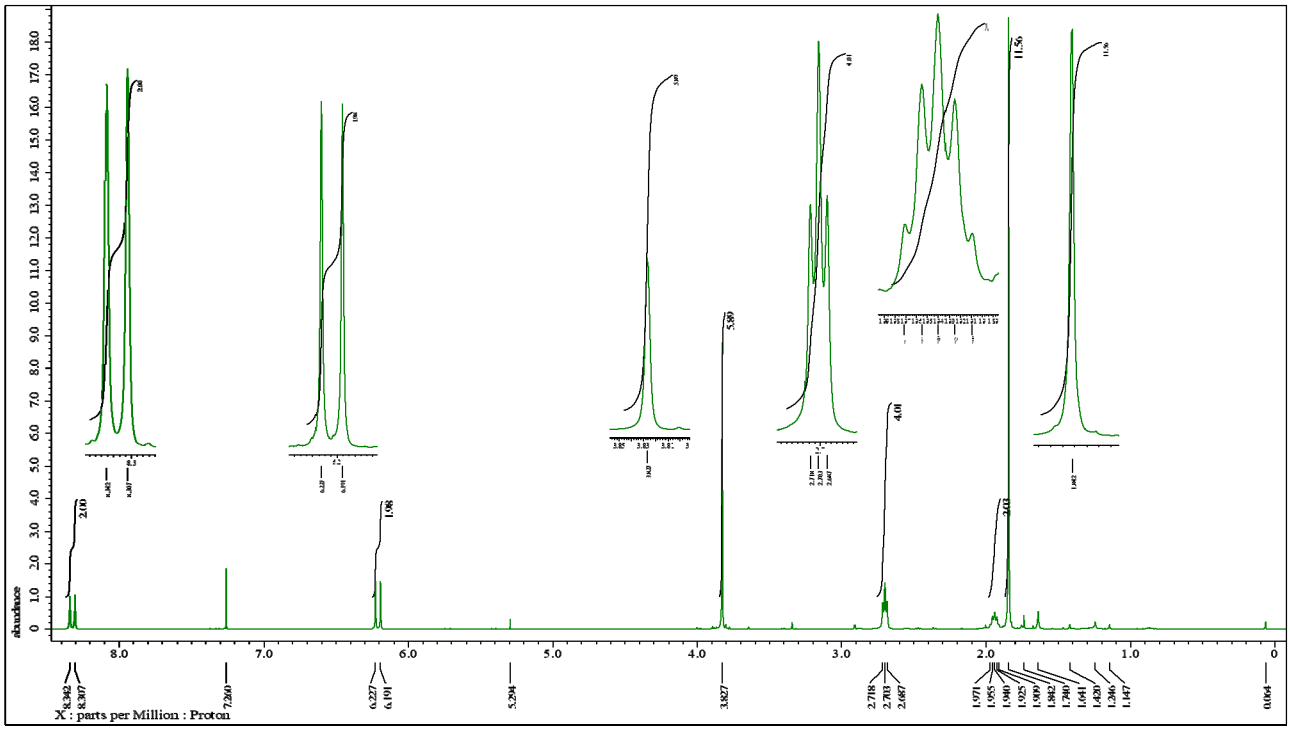

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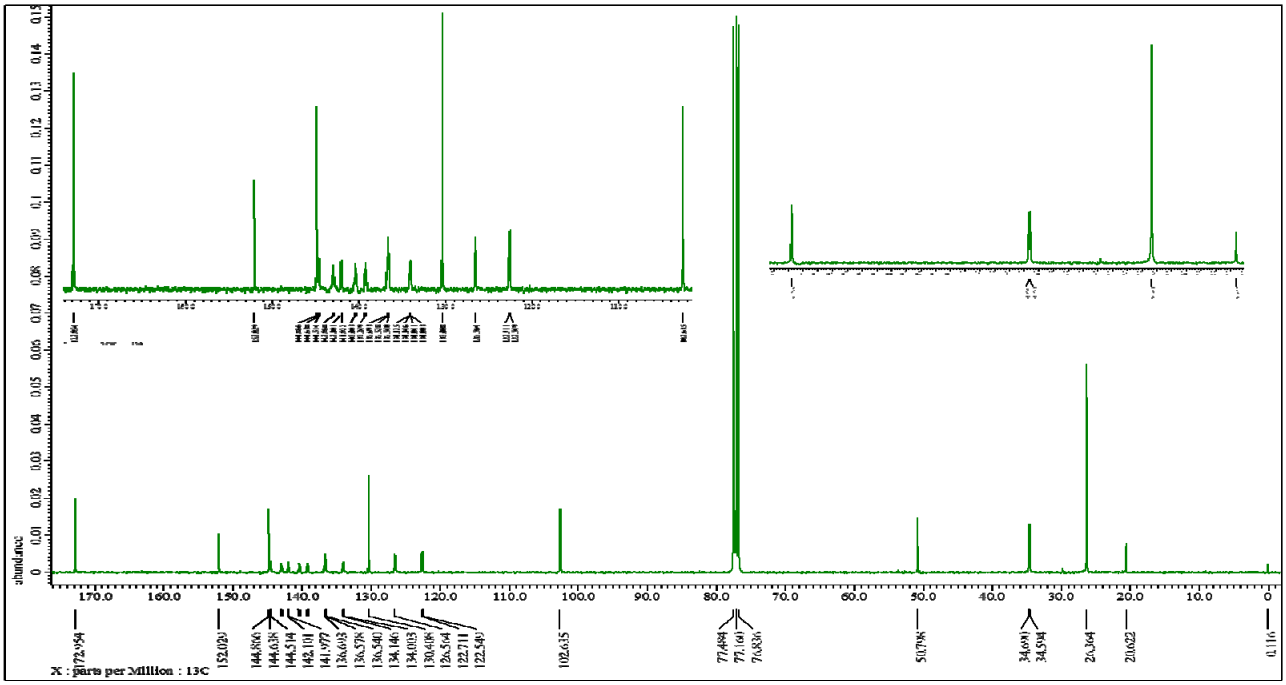
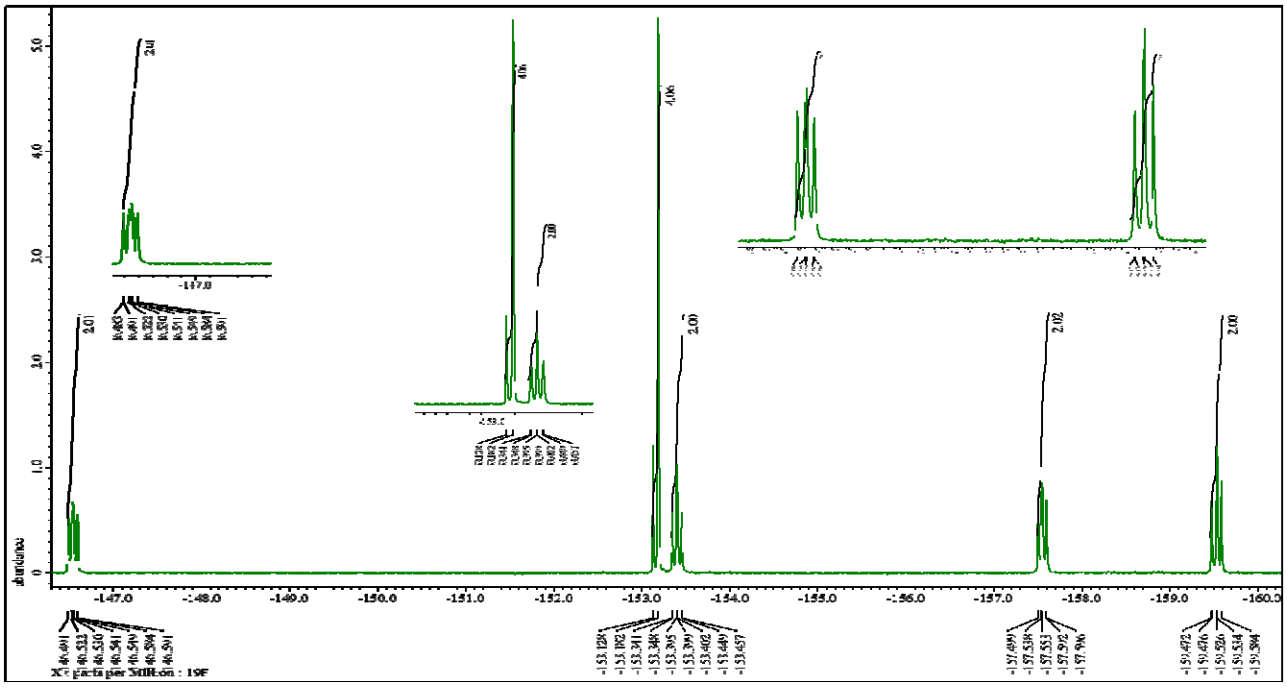


^{19}F NMR



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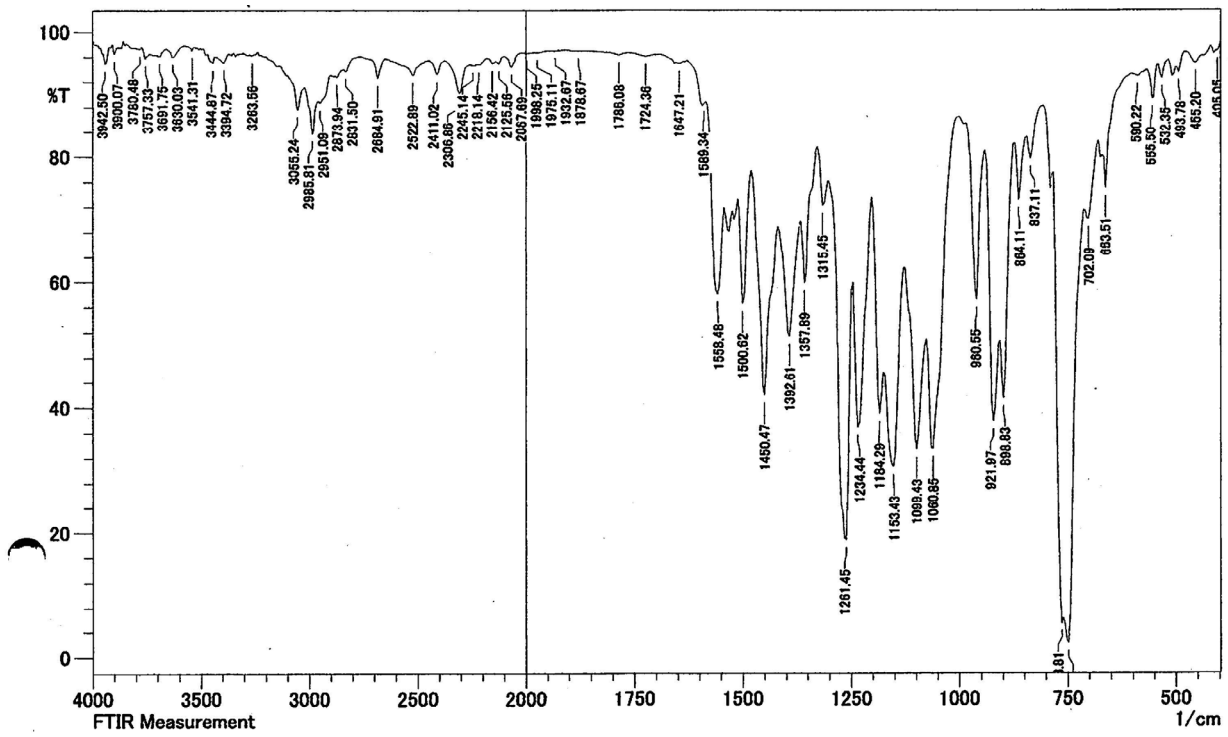
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0
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
FTIR Measurement
3942.50
3900.07
3780.48
3757.33
3691.75
3630.03
3541.31
3444.87
3394.72
3263.56
3055.24
2985.81
2951.09
2873.94
2831.50
2684.91
2922.89
2411.02
2306.86
2245.14
2218.14
2156.42
2125.56
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1569.34
1558.48
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1357.89
1315.45
1261.45
1234.44
1184.29
1153.43
1098.43
1060.85
980.55
921.97
898.83
864.11
837.11
781
702.09
683.51
590.22
555.50
532.35
493.78
465.20
405.05

HRMS

データ:20181113 ajioka F8
試料名:
説明:
イオン化モード:ESI+
処理履歴:m/z軸決定[ピーク検出[重心,30,面積];ベース補正[1.0%];平滑化[3]...

測定日時:2018/11/13 16:44:08
測定者:AccuTOF
質量校正データ:PEGMIX_ESI+_1000...
作成日時:2018/11/13 16:58:16
作成者:AccuTOF

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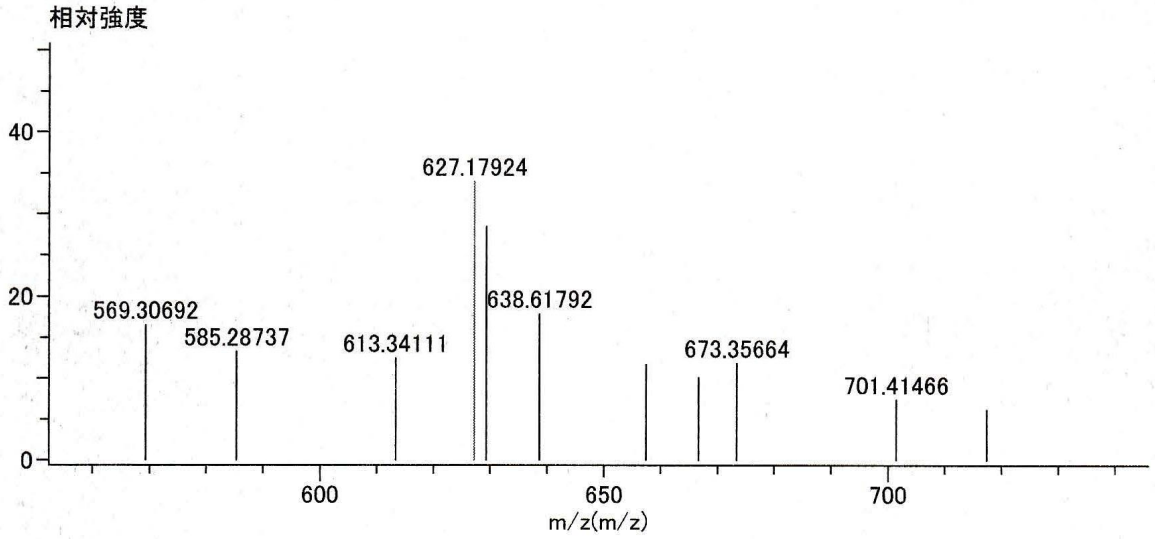
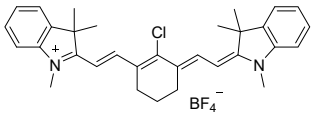
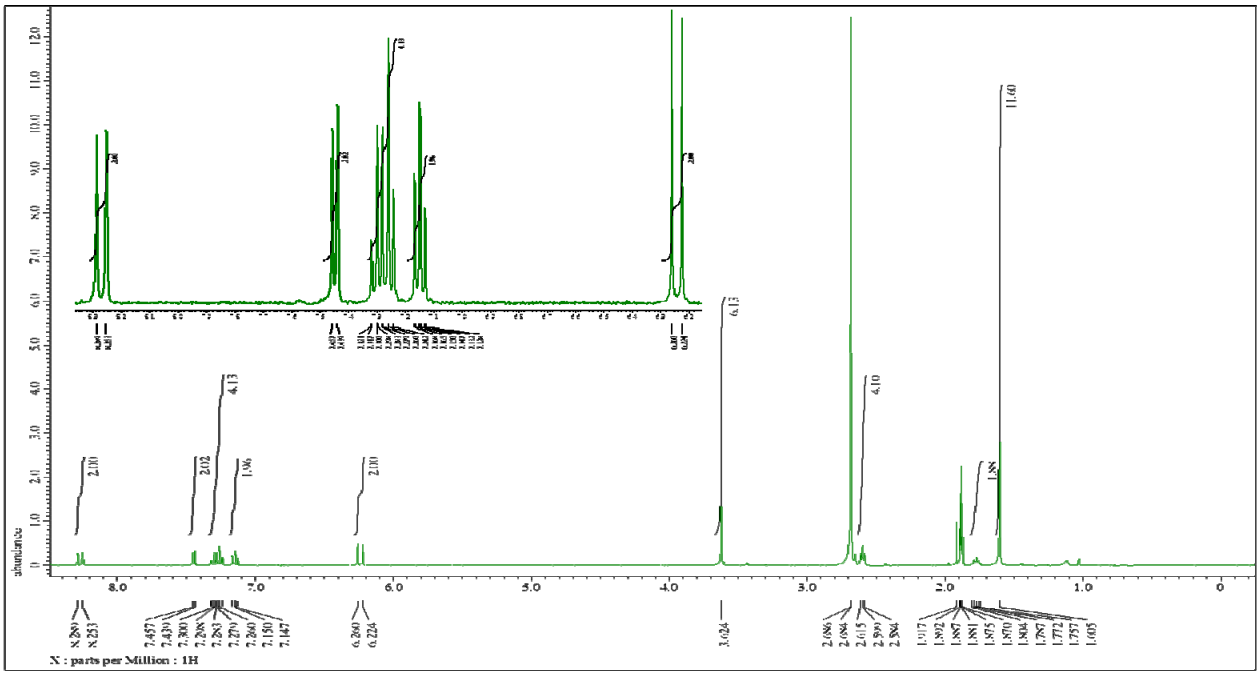


Mass	強度	Calc. Mass	質量差 mmu	質量差 ppm	Formula	不飽和数
627.17924	9503.12	627.18133	-2.08	-3.32	$^{12}C_{32}{}^{1}H_{28}{}^{35}Cl_{1}{}^{19}F_{8}{}^{14}N_{2}$	15.5

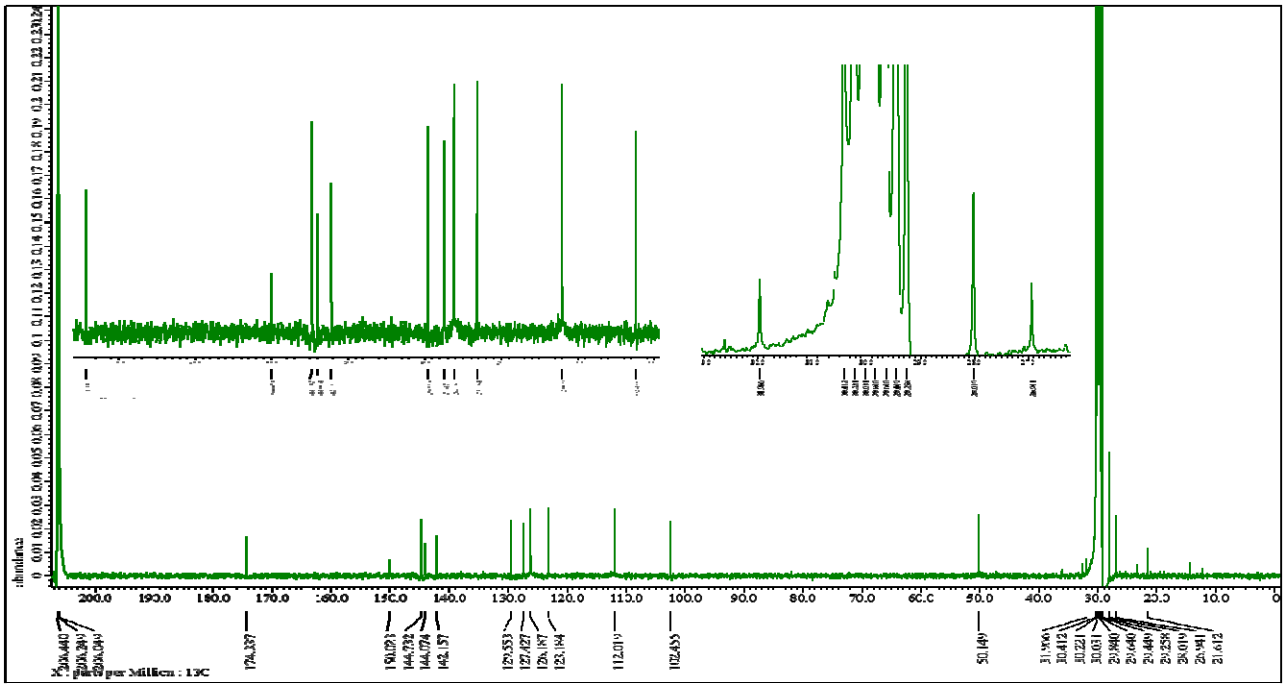
2-((*E*)-2-((*E*)-2-Chloro-3-(2-((*E*)-1,3,3-trimethylindolin-2-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-1,3,3-trimethyl-3*H*-indol-1-ium tetrafluoroborate (4b)



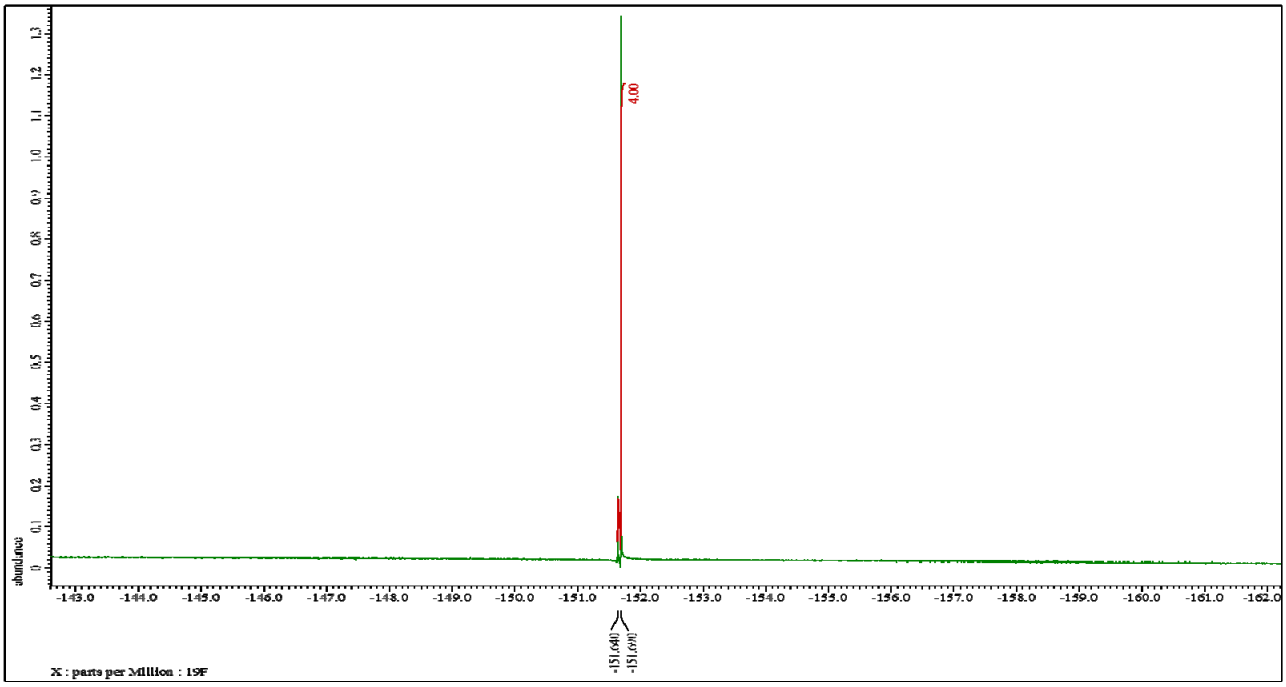
^{1}H NMR



^{13}C NMR



^{19}F NMR


4.00
abundance
-143.0
-144.0
-145.0
-146.0
-147.0
-148.0
-149.0
-150.0
-151.0
-152.0
-153.0
-154.0
-155.0
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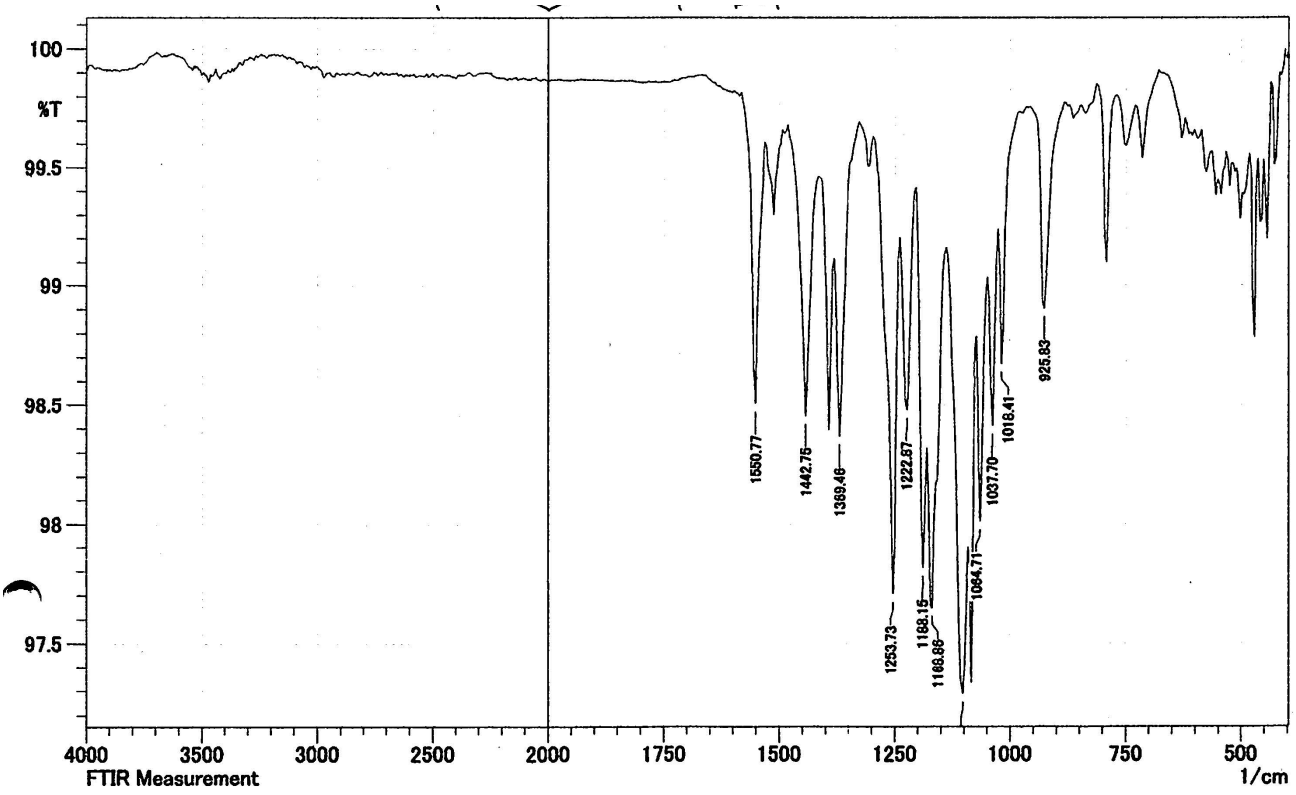
-151.640
-151.691
X : parts per Million : 19F

IR


100
%T
99.5
99
98.5
98
97.5
1550.77
1442.76
1369.46
1253.73
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1188.15
1168.86
1084.71
1037.70
1016.41
925.83
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
FTIR Measurement
1/cm

HRMS

データ:ajioka BF4 F0 20190219
試料名:
説明:
イオン化モード:ESI+
処理履歴:m/z軸決定[ピーク検出[重心,30,面積];ベース補正[1.0%];平滑化[3]...

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測定者:AccuTOF
質量校正データ:PEGMIX_ESI+_1000...
作成日時:2019/02/19 13:59:37
作成者:AccuTOF

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不飽和数:-30.0 .. 30.0 (端数:両方)
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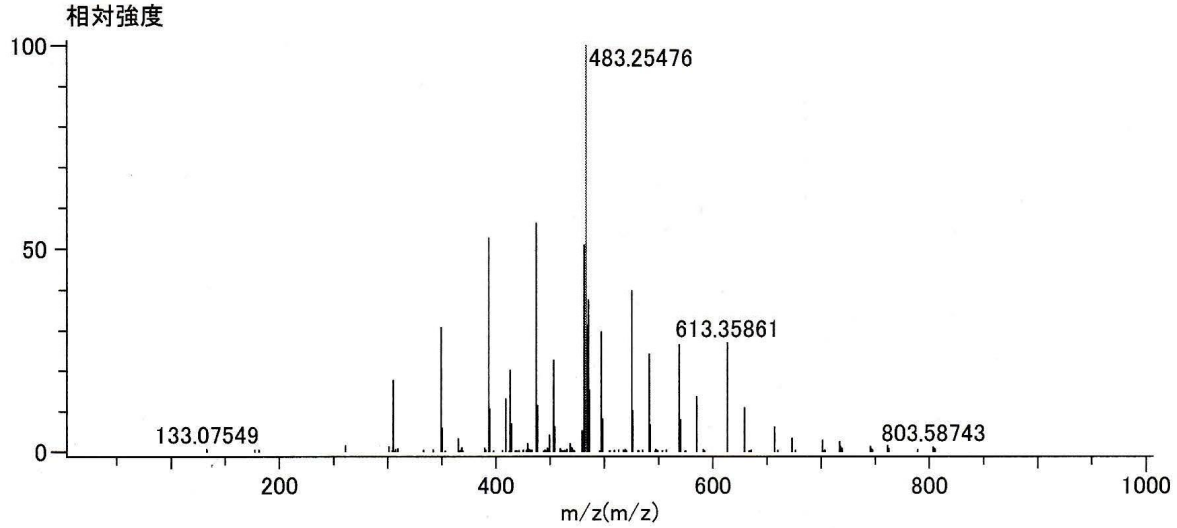
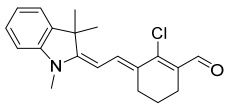
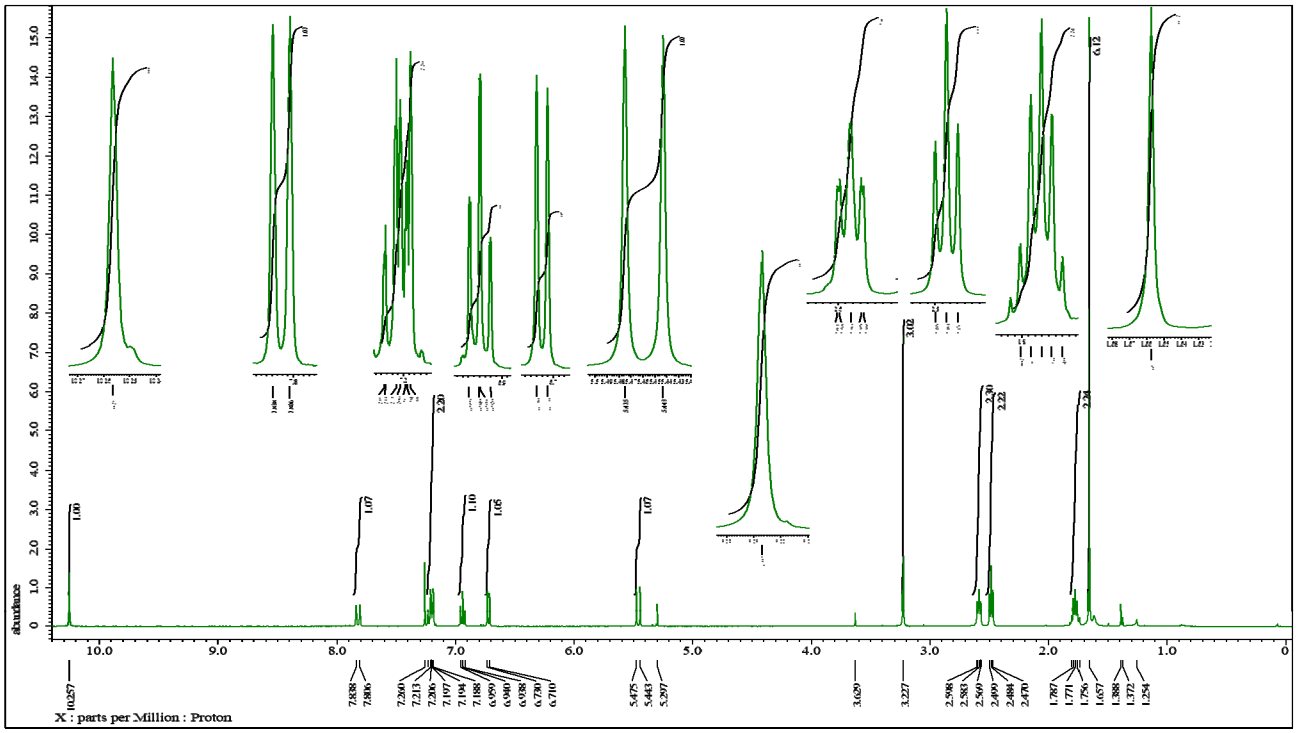


Mass	強度	Calc. Mass	質量差 mmu	質量差 ppm	Formula	不飽和数
483.25476	70742.11	483.25670	−1.94	−4.02	$^{12}C_{32}{}^{1}H_{36}{}^{35}Cl_{1}{}^{14}N_{2}$	15.5

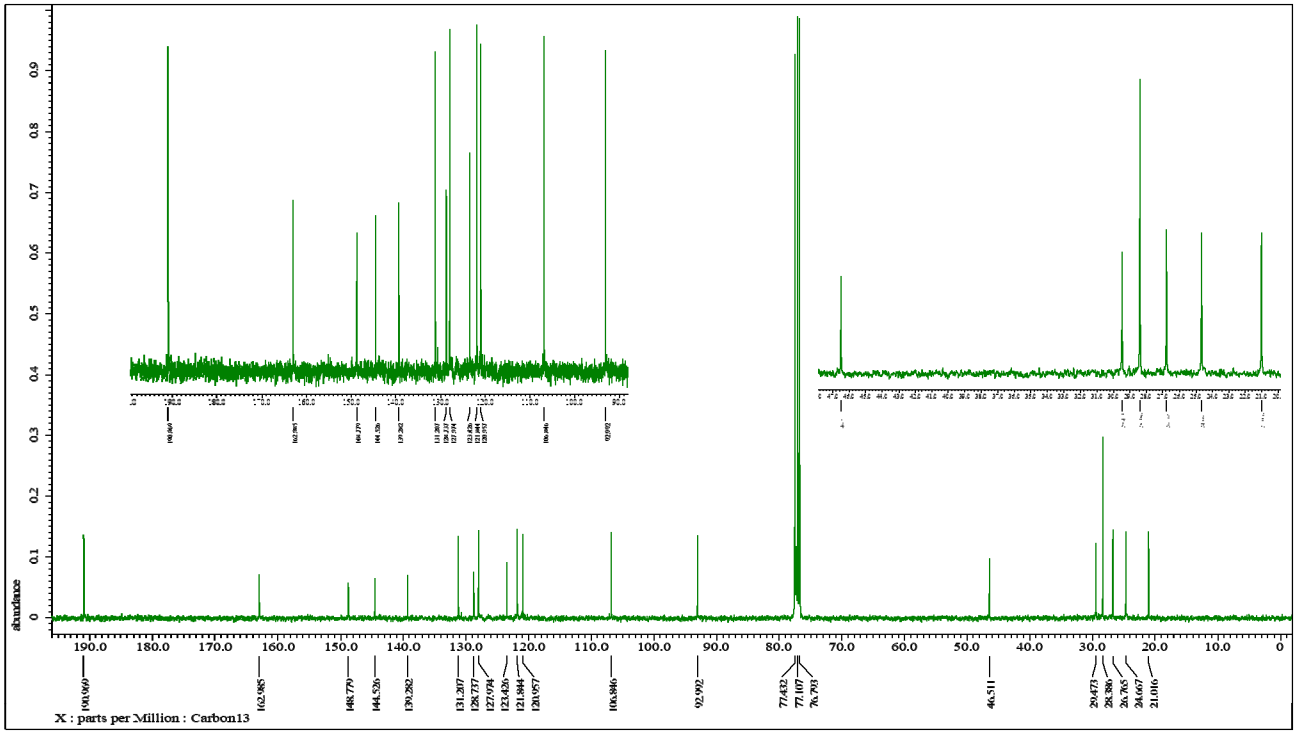
(*E*)-2-chloro-3-(2-((*E*)-1,3,3-trimethylindolin-2-ylidene)ethylidene)cyclohex-1-ene-1-carbaldehyde (5b)[3]



^{1}H NMR

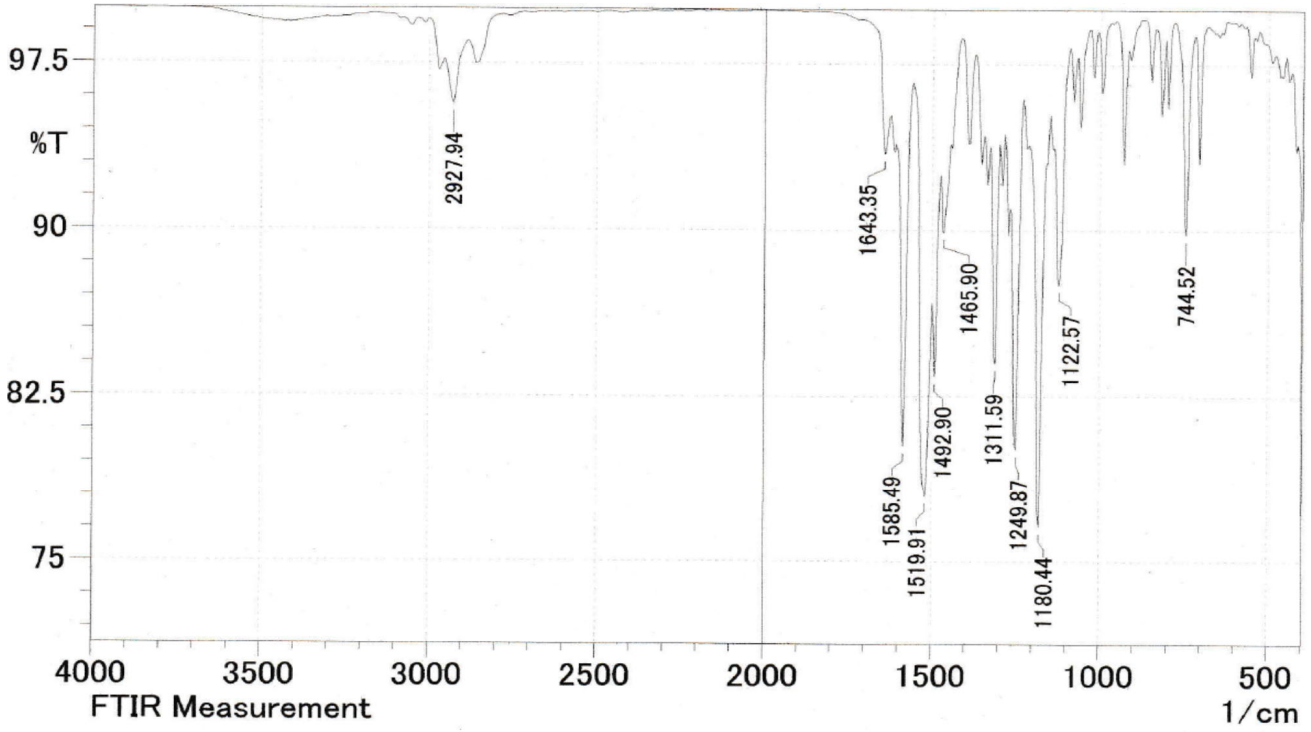


^{13}C NMR



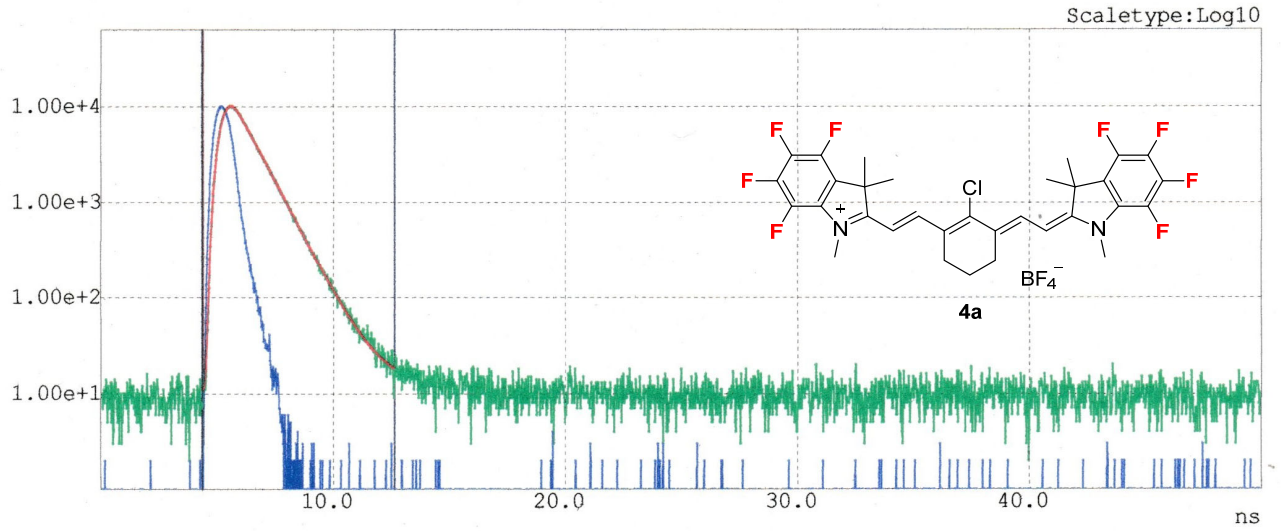
[3] J. W. Yan, J. Y. Zhu, K. X. Zhou, J. S. Wang, H. Y. Tan, Z. Y. Xu, S. B. Chen, Y. T. Lu, M. C. Cui, L. Zhang, *Chem. Commun.* **2017**, *53*, 9910-9913.

IR

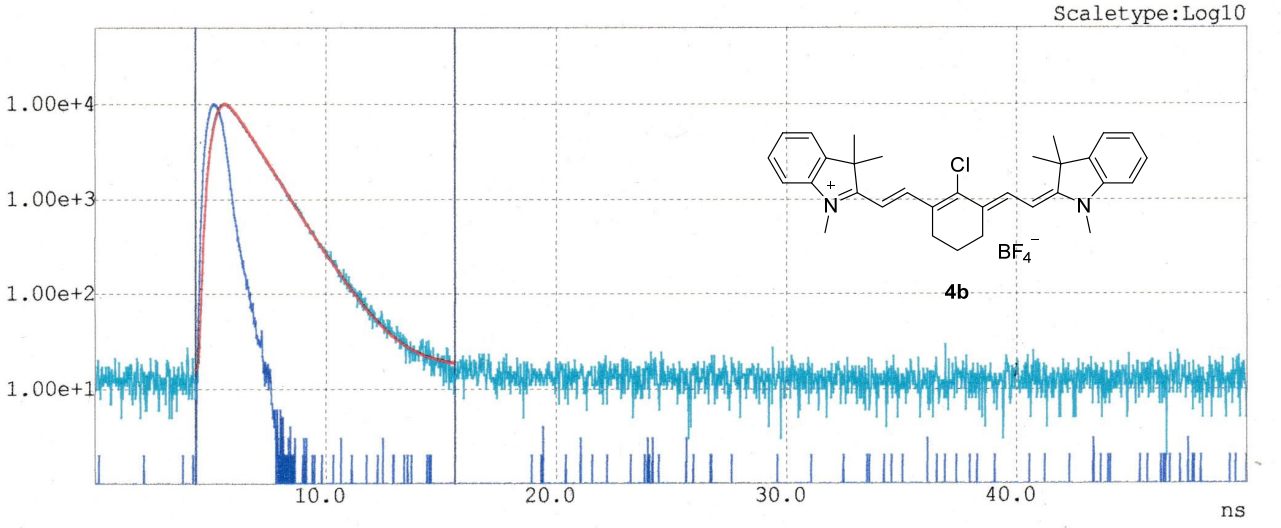

97.5
%T
90
82.5
75
2927.94
1643.35
1585.49
1519.91
1492.90
1465.90
1311.59
1249.87
1180.44
1122.57
744.52
4000
3500
3000
2500
2000
1500
1000
500
FTIR Measurement
1/cm

Fluorescence decay curves

4a: CH_2Cl_2 solution (3×10^{-6} M)



4b: CH_2Cl_2 solution (3×10^{-6} M)



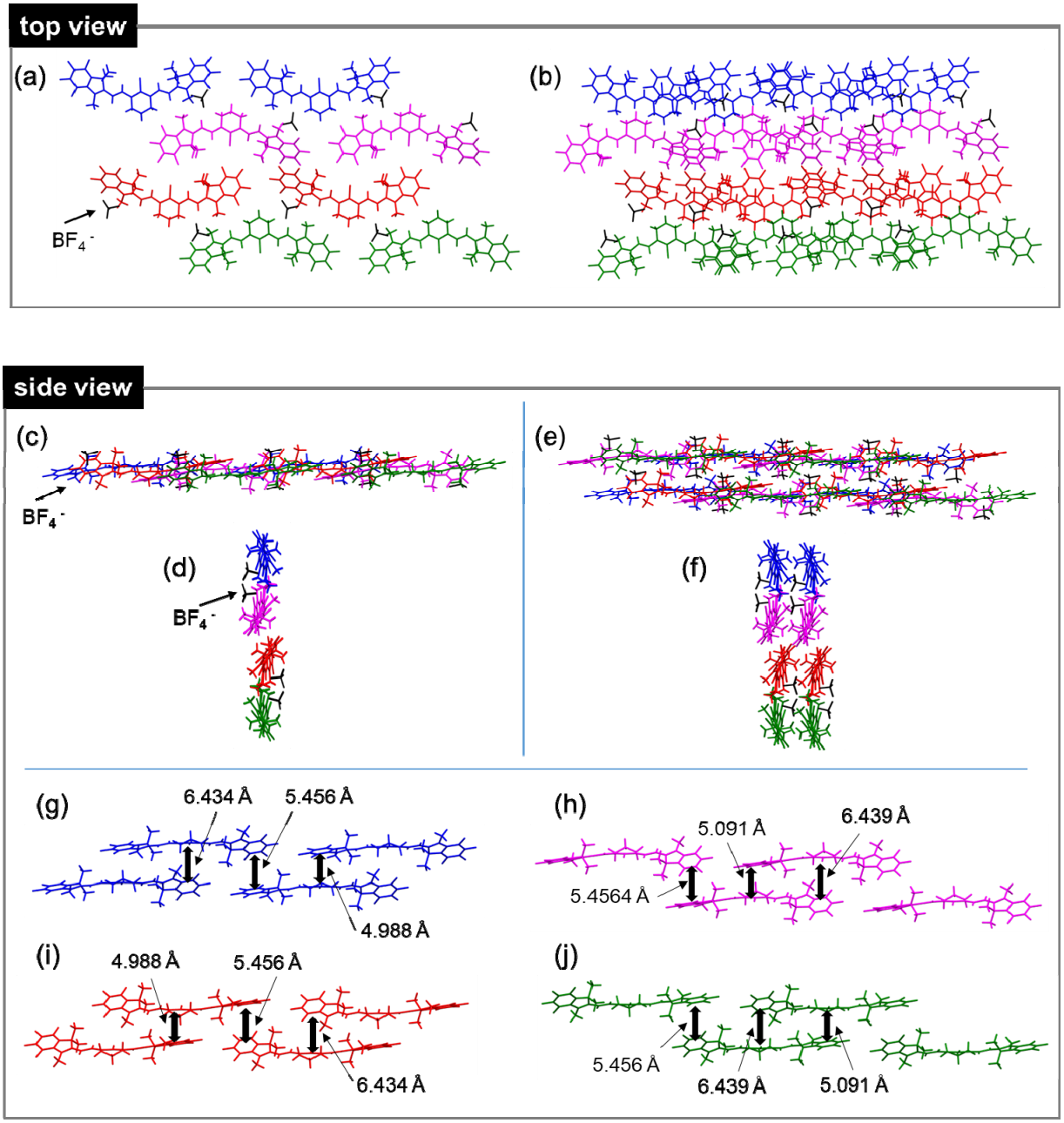


Figure S1 Packing of the molecules in X-ray diffraction structure of the ring-fluorinated HMCD **4a**: Top view of a single layer (a), top view of double layer (b), side view of a single layer (c), another side view of a single layer (d), side view of double layer (e), another side view of double layer (f), side view of the extracted blue molecules from (e) and the distances between the indolium and the methine double bond (g), side view of the extracted magenta molecules from (e) and the distances between the indolium and the methine double bond (h), side view of the extracted red molecules from (e) and the distances between the indolium and the methine double bond (h), side view of the extracted green molecules from (e) and the distances between the indolium and the methine double bond (h).

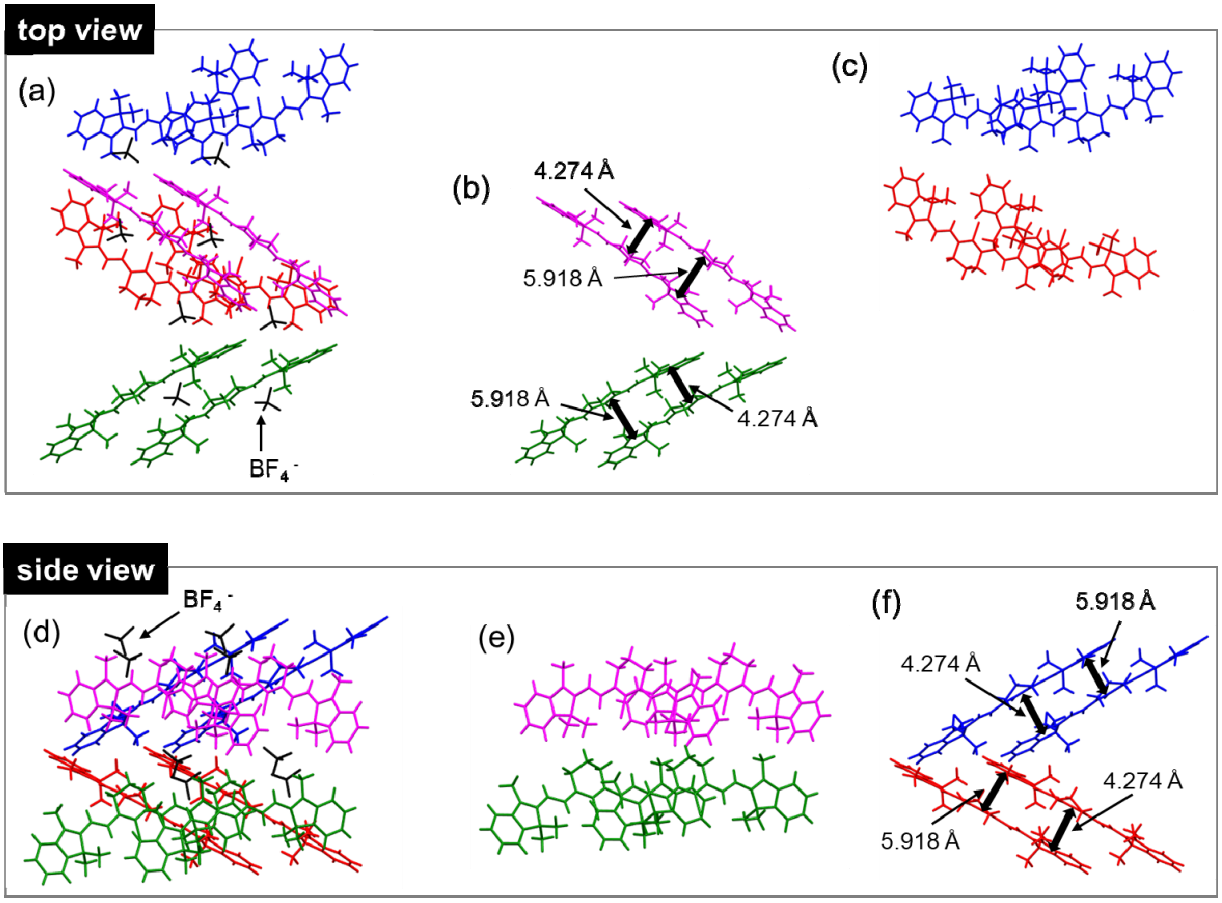
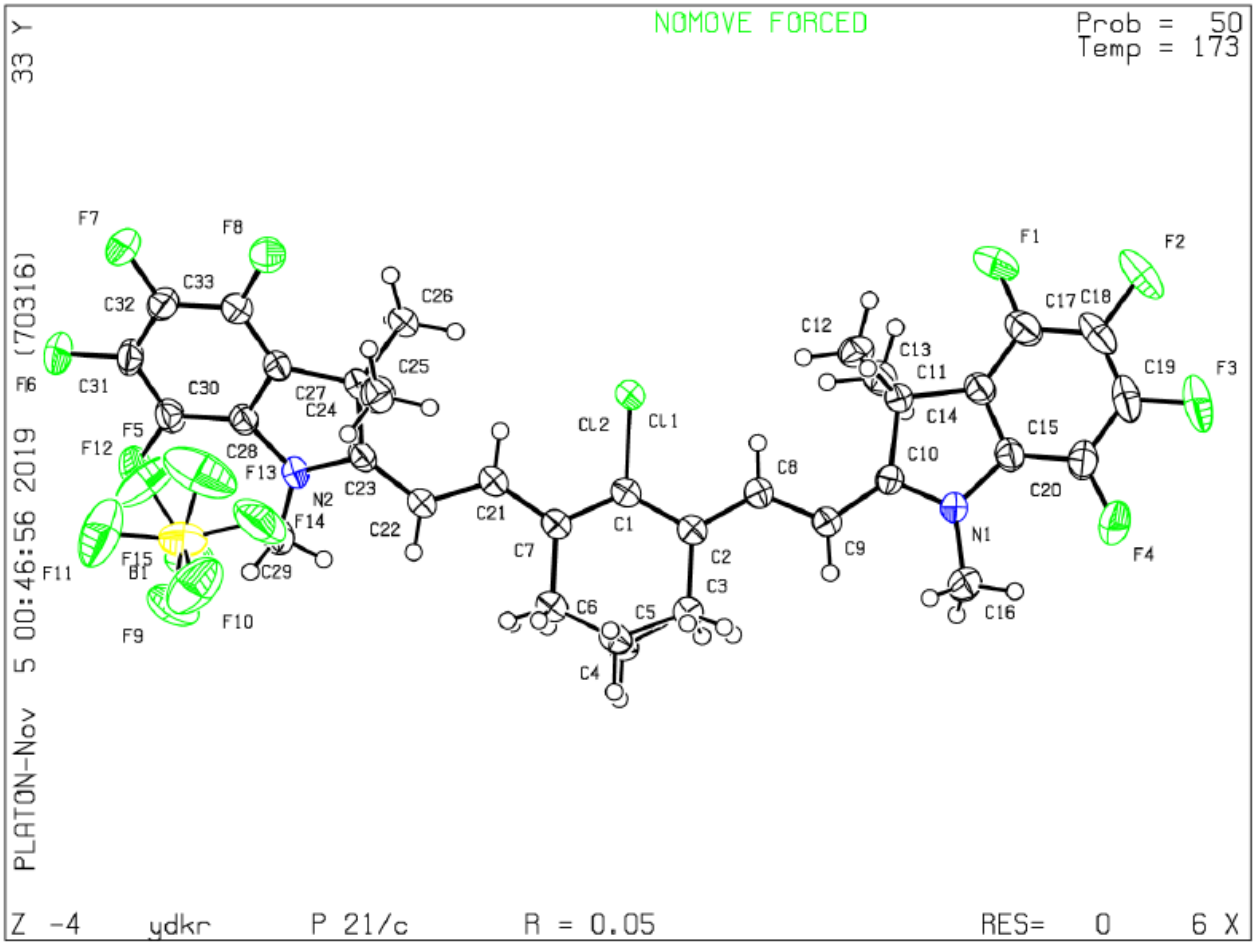


Figure S2. Packing of the molecules in X-ray diffraction structure of the HMCD **4b**: Top view (a), the extracted magenta and green molecules from (a) and the distances between indoline and methine double bond (b), extracted blue and red molecules from (a) (c), side view (d), the extracted magenta and green molecules from (d) and the distances between the indolium and the methine double bond (e), the extracted blue and red molecules from (a) and the distances between the indolium and the methine double bond (f).



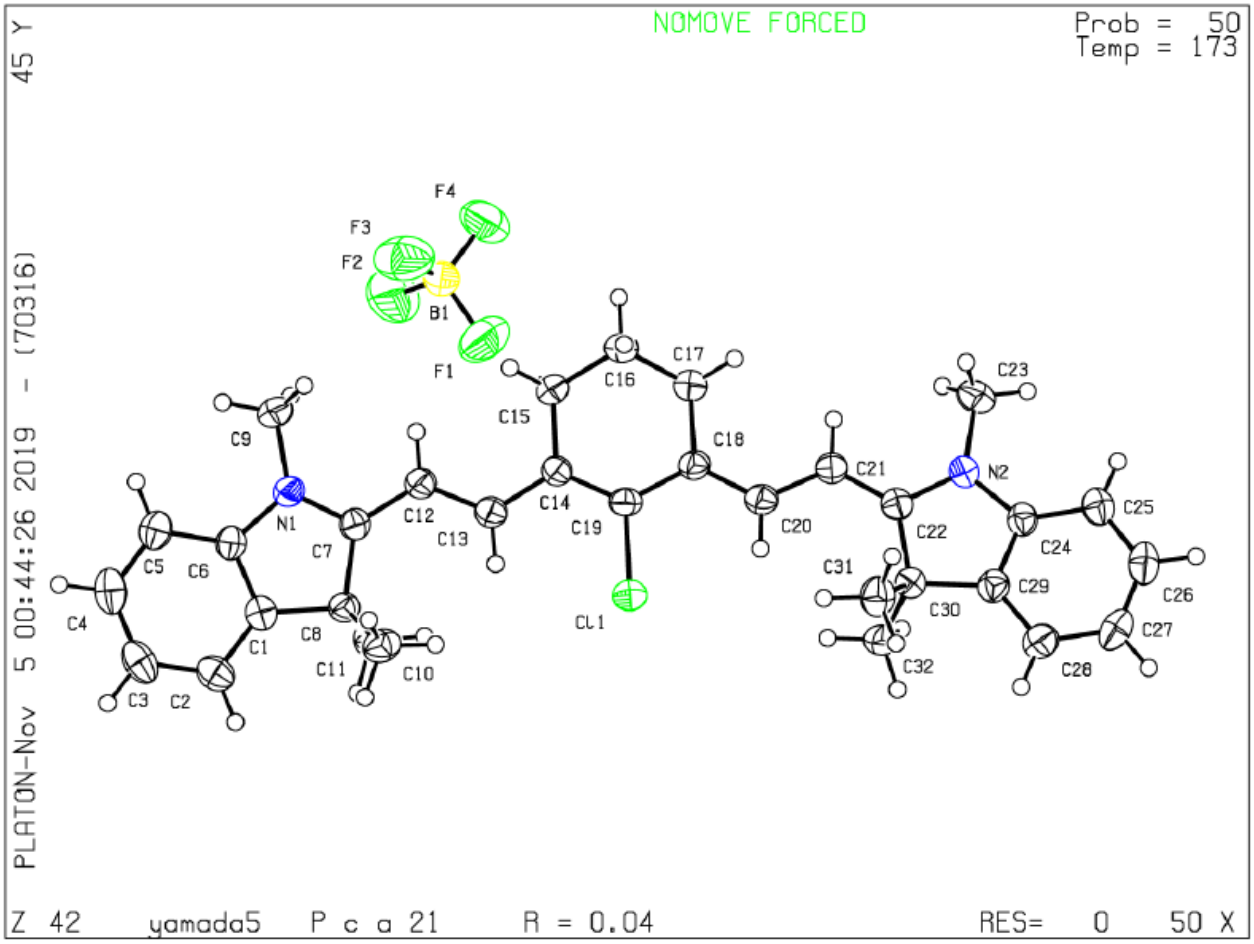
Crystals of ring-fluorinated dye **4a** prepared by the vapor diffusion method with hexane and dichloromethane.

The X-ray Crystal Structure was collected on Rigaku Saturn 724+ CCD diffractometer with a VariMax Mo optic system.

Figure S3. ORTEP Diagram of **4a**.

Table S3. Crystal Data and Structure Refinement for **4a**.

Identification code	**4a**	
Empirical formula	$C_{32}H_{28}BClF_{12}N_2$	
Formula weight	714.82	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 9.2949(3) Å	α= 90°.
	b = 27.7483(8) Å	β= 96.464(3)°.
	c = 12.3186(4) Å	γ = 90°.
Volume	3156.99(17) $Å^3$	
Z	4	
Density (calculated)	1.504 Mg/m^3	
Absorption coefficient	0.219 mm^{-1}	
F(000)	1456	
Crystal size	0.180 x 0.090 x 0.080 mm^3	
Theta range for data collection	1.818 to 25.497°	
Index ranges	-10<=h<=11, -33<=k<=33, -14<=l<=14	
Reflections collected	33500	
Independent reflections	5855 [R(int) = 0.0514]	
Completeness to theta = 25.242°	99.6%	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	5855 / 96 / 489	
Goodness-of-fit on F^2	1.011	
Final R indexes [I>=2sigma(I)]	R_1 = 0.0456, wR_2 = 0.1306	
Final R indexes (all data)	R_1 = 0.0583, wR_2 = 0.1401	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.498 and -0.441 e.$Å^{-3}$	



Crystals of non-fluorinated **4b** prepared by the vapor diffusion method with hexane and dicloromethane.

The X-ray Crystal Structure was collected on Rigaku AFC 10 (CCD: Saturn 724+) + VariMax Mo Optic.

Figure S4. ORTEP Diagram of **4b**.

Table S4. Crystal Data and Structure Refinement for **4b**.

Identification code	**4b**	
Empirical formula	C_{32} H_{36} B Cl F_4 N_2	
Formula weight	570.89	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$Pca2_1$	
Unit cell dimensions	a = 31.542(4) Å	α= 90°.
	b = 7.8263(8) Å	β= 90°.
	c = 11.5946(12) Å	γ = 90°.
Volume	2862.2(6) $Å^3$	
Z	4	
Density (calculated)	1.325	
Absorption coefficient	0.185 mm^{-1}	
Absorption coefficient	0.185 mm^{-1}	
F(000)	1200	
Crystal size	0.150 x 0.100 x 0.090 mm^3	
Theta range for data collection	2.180 to 25.496°.	
Index ranges	-38<=h<=37, -9<=k<=9, -11<=l<=14	
Reflections collected	16438	
Independent reflections	3973 [R(int) = 0.0524]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.89283	
Refinement method	Full-matrix least-squares on F^2	
Final R indexes [I>=2sigma(I)]	R_1 = 0.0428, wR_2 = 0.0993	
R indexes (all data)	R_1 = 0.0621, wR_2 = 0.1114	
Absolute structure parameter	0.49(9)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.198 and -0.179 e.Å-3	

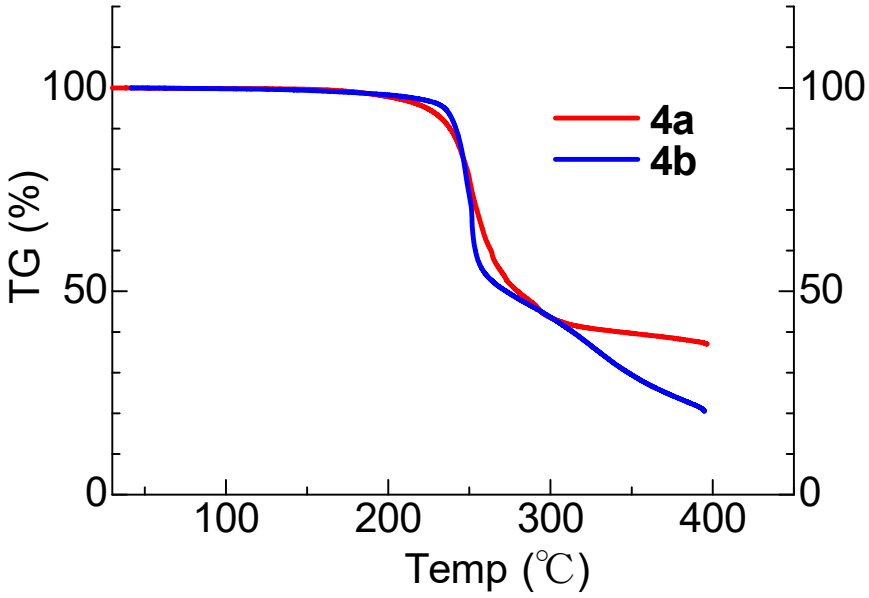


Figure S5. TG-DTA of the NIR dyes **4a,b.**

Electrochemical measurements of the dyes.

Electrochemical measurements of the dyes were performed in MeCN solutions (1.0×10^{-3} M) containing Bu_4NClO_4 (0.1 M). The E_{ox} values were measured using three small electrodes. A silver quasi-reference electrode, a platinum wire, and a carbon electrode were used as the reference, counter, and working electrodes, respectively. All the electrode potentials were calibrated concerning the Fc/ferrocenium redox couple. Electrochemical measurements were performed at a scan rate of 100 mV s^{-1}. The E_{ox} value of Fc *vs.* SCE was 0.380 V.[4] The E_{ox} values *vs.* SCE were determined using the observed E_{ox} (V *vs*. Ag) values of the dyes in MeCN solutions as follows:

E_{ox} (V *vs.* SCE) = E (V *vs.* Ag, observed value) + 0.380 – (measured E_{ox} value of Fc for Ag in the MeCN solution).

The energy of the HOMO (eV) was obtained using the E_{ox} (V vs. SCE) values, as follows:

HOMO (eV) = –(E_{ox} (V *vs.* SCE) + 4.4)

The band gap ($E_{0\text{-}0}$) and energy of the LUMO (eV) were calculated using the λ_{onset}^{abs} value as follows:

$E_{0\text{-}0}$ (eV) = $1240/\lambda_{onset}^{abs}$ (nm)

LUMO (eV) = HOMO (eV) – $E_{0\text{-}0}$ (eV)

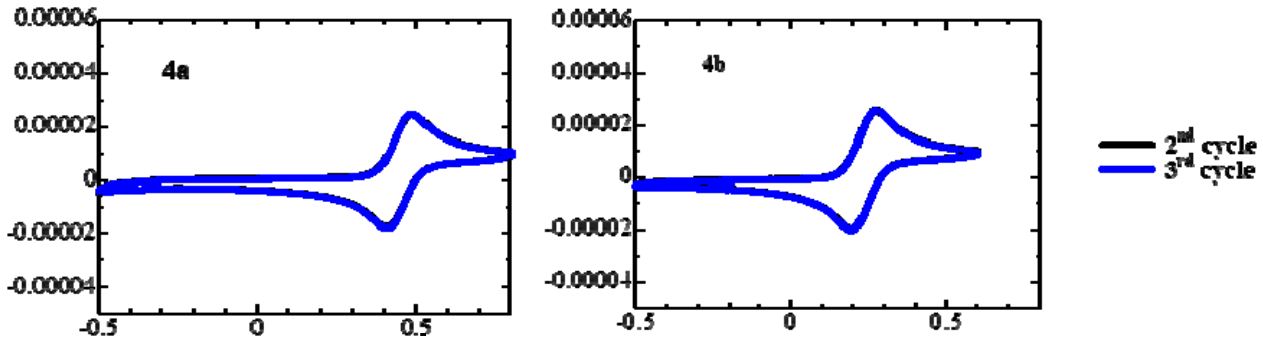


Figure S6. Cyclic voltammograms of the NIR dyes **4a,b** (1.0×10^{-3} M) in dehydrated acetonitrile containing Bu_4NClO_4 (0.1 M) as a supporting electrolyte with the scan rate of 100 mV s^{-1}.

[4] a) N. G. Connelly, W. E. Geiger, *Chem. Rev.* **1996**, *96*, *2*, 877-910. b) C. M. Cardona, W. Li, A. E. Kaifer, D. Stockdale, G. C. Bazan, *Adv. Mater.* **2011**, *23*, 2367-2371.

Computational Details. All calculations were performed using the computational chemistry software package Gaussian 16 ver. B.01[5] using (computational resource provided by Fujitsu PRIMERGY CX400) Super Computers at Information and Communications Headquarters in Nagoya University.

a) Ground State Details.

Ground state geometries of **4a,b** were computed at RB3LYP/6-31G(d,p) level of theory. At the optimized structures, no imaginary frequency was found through the frequency analysis. All coordinates are reported as XYZ Cartesian coordinates. And computed E (RB3LYP) and sum of zero-point and thermal correction energies of optimized structures are shown.

[5] Gaussian 16, Revision B.01, 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, Inc., Wallingford CT, 2016.

4a

E (RB3LYP) = -2604.434712 a.u.

Sum of electronic and thermal Energies = -2603.852902 a.u.

Imaginary Frequency = 0

Table S1. Cartesian coordinates of the optimized **4a**.

	Coordinates (Angstroms)		
Atom	X	Y	Z
C	-1.302587	0.296696	-0.178903
C	-1.135813	1.262569	-0.641161
C	-0.310731	-0.534105	0.184597
C	-0.611245	-1.509123	0.563213
C	-2.741576	-0.074322	-0.051169
N	-3.409253	0.81211	0.731417
C	-3.363575	-0.06148	-1.255068
H	-2.931427	-1.299724	0.485802
H	1.138025	-0.343567	0.097905
H	1.78638	0.920585	0.0353
C	1.938209	-1.50268	0.082948
H	3.185277	0.961545	-0.096029
C	3.319188	-1.451404	-0.049823
H	1.441513	-2.466475	0.159551
C	3.940482	-0.203284	-0.149681
H	3.676574	1.930065	-0.150192
C	3.903539	-2.365136	-0.072432
H	5.019541	-0.135223	-0.25276
C	1.067552	2.114207	0.078235
C	0.224126	2.083868	0.637484
C	1.631186	2.925078	0.29843
C	3.8614237	0.7802288	0.1389195
C	4.1411835	0.8452704	0.1495673
C	4.4209433	0.9103119	0.1602151
N	4.7007031	0.9753535	0.1708629
C	4.9804629	1.0403951	0.1815107
H	5.2602227	1.1054367	0.1921585
H	5.5399825	1.1704783	0.2028063
H	5.8197423	1.2355198	0.2134541
C	6.0995021	1.3005614	0.2241019
C	6.3792619	1.365603	0.2347498
C	6.6590217	1.4306446	0.2453976
H	6.9387815	1.4956861	0.2560454
H	7.2185413	1.5607277	0.2666932
C	7.4983011	1.6257693	0.277341
C	7.7780609	1.6908109	0.2879888
H	8.0578207	1.7558525	0.2986366
H	8.3375804	1.820894	0.3092844
C	8.6173402	1.8859356	0.3199323
H	8.8971	1.9509772	0.3305801
H	9.1768598	2.0160188	0.3412279
C	9.4566196	2.0810603	0.3518757
Cl	9.7363794	2.1461019	0.3625235
C	10.016139	2.2111435	0.3731713
C	10.295899	2.2761851	0.3838191
C	10.575659	2.3412267	0.3944669
H	10.855419	2.4062682	0.4051147
H	11.135178	2.4713098	0.4157626
H	11.414938	2.5363514	0.4264104
C	11.694698	2.601393	0.4370582
H	11.974458	2.6664345	0.447706
H	12.254218	2.7314761	0.4583538
H	12.533977	2.7965177	0.4690016
C	12.813737	2.8615593	0.4796494
H	13.093497	2.9266009	0.4902972
H	13.373257	2.9916424	0.500945
H	13.653017	3.056684	0.5115929
C	13.932776	3.1217256	0.5222407
H	14.212536	3.1867672	0.5328885
H	14.492296	3.2518087	0.5435363
H	14.772056	3.3168503	0.5541841

C	15.051816	3.3818919	0.5648319
C	15.331575	3.4469335	0.5754797
F	15.611335	3.5119751	0.5861275
F	15.891095	3.5770166	0.5967754
F	16.170855	3.6420582	0.6074232
F	16.450615	3.7070998	0.618071
F	16.730374	3.7721414	0.6287188
F	17.010134	3.8371829	0.6393666
F	17.289894	3.9022245	0.6500144
F	17.569654	3.9672661	0.6606622

4b

E (RB3LYP) = -1810.652960 a.u.

Sum of electronic and thermal Energies = -1810.013174 a.u.

Imaginary Frequency = 0

Table S2. Cartesian coordinates of the optimized **4b**

	Coordinates (Angstroms)		
Atom	X	Y	Z
C	-1.302587	0.296696	-0.178903
C	-1.135813	1.262569	-0.641161
C	-0.310731	-0.534105	0.184597
C	-0.611245	-1.509123	0.563213
C	-2.741576	-0.074322	-0.051169
N	-3.409253	0.81211	0.731417
C	-3.363575	-0.06148	-1.255068
H	-2.931427	-1.299724	0.485802
H	1.138025	-0.343567	0.097905
H	1.78638	0.920585	0.0353
C	1.938209	-1.50268	0.082948
H	3.185277	0.961545	-0.096029
C	3.319188	-1.451404	-0.049823
H	1.441513	-2.466475	0.159551
C	3.940482	-0.203284	-0.149681
H	3.676574	1.930065	-0.150192
C	3.903539	-2.365136	-0.072432
H	5.019541	-0.135223	-0.25276
C	1.067552	2.114207	0.078235
C	0.224126	2.083868	0.637484
C	1.631186	2.925078	0.29843
C	3.8614237	0.7802288	0.1389195
C	4.1411835	0.8452704	0.1495673
C	4.4209433	0.9103119	0.1602151
N	4.7007031	0.9753535	0.1708629
C	4.9804629	1.0403951	0.1815107
H	5.2602227	1.1054367	0.1921585
H	5.5399825	1.1704783	0.2028063
H	5.8197423	1.2355198	0.2134541
C	6.0995021	1.3005614	0.2241019
C	6.3792619	1.365603	0.2347498
C	6.6590217	1.4306446	0.2453976
H	6.9387815	1.4956861	0.2560454
H	7.2185413	1.5607277	0.2666932
C	7.4983011	1.6257693	0.277341
C	7.7780609	1.6908109	0.2879888
H	8.0578207	1.7558525	0.2986366
H	8.3375804	1.820894	0.3092844
C	8.6173402	1.8859356	0.3199323
H	8.8971	1.9509772	0.3305801
H	9.1768598	2.0160188	0.3412279
C	9.4566196	2.0810603	0.3518757
Cl	9.7363794	2.1461019	0.3625235
C	10.016139	2.2111435	0.3731713
C	10.295899	2.2761851	0.3838191

C	10.575659	2.3412267	0.3944669
H	10.855419	2.4062682	0.4051147
H	11.135178	2.4713098	0.4157626
H	11.414938	2.5363514	0.4264104
C	11.694698	2.601393	0.4370582
H	11.974458	2.6664345	0.447706
H	12.254218	2.7314761	0.4583538
H	12.533977	2.7965177	0.4690016
C	12.813737	2.8615593	0.4796494
H	13.093497	2.9266009	0.4902972
H	13.373257	2.9916424	0.500945
H	13.653017	3.056684	0.5115929
C	13.932776	3.1217256	0.5222407
H	14.212536	3.1867672	0.5328885
H	14.492296	3.2518087	0.5435363
H	14.772056	3.3168503	0.5541841
C	15.051816	3.3818919	0.5648319
C	15.331575	3.4469335	0.5754797
H	15.611335	3.5119751	0.5861275
H	15.891095	3.5770166	0.5967754
H	16.170855	3.6420582	0.6074232
H	16.450615	3.7070998	0.618071
H	16.730374	3.7721414	0.6287188
H	17.010134	3.8371829	0.6393666
H	17.289894	3.9022245	0.6500144
H	17.569654	3.9672661	0.6606622