

Supporting Information

BF₂ Complexes of β-Tetraethyl-Substituted Dipyrrolyldiketones as Anion Receptors: Potential Building Subunits for Oligomeric Systems

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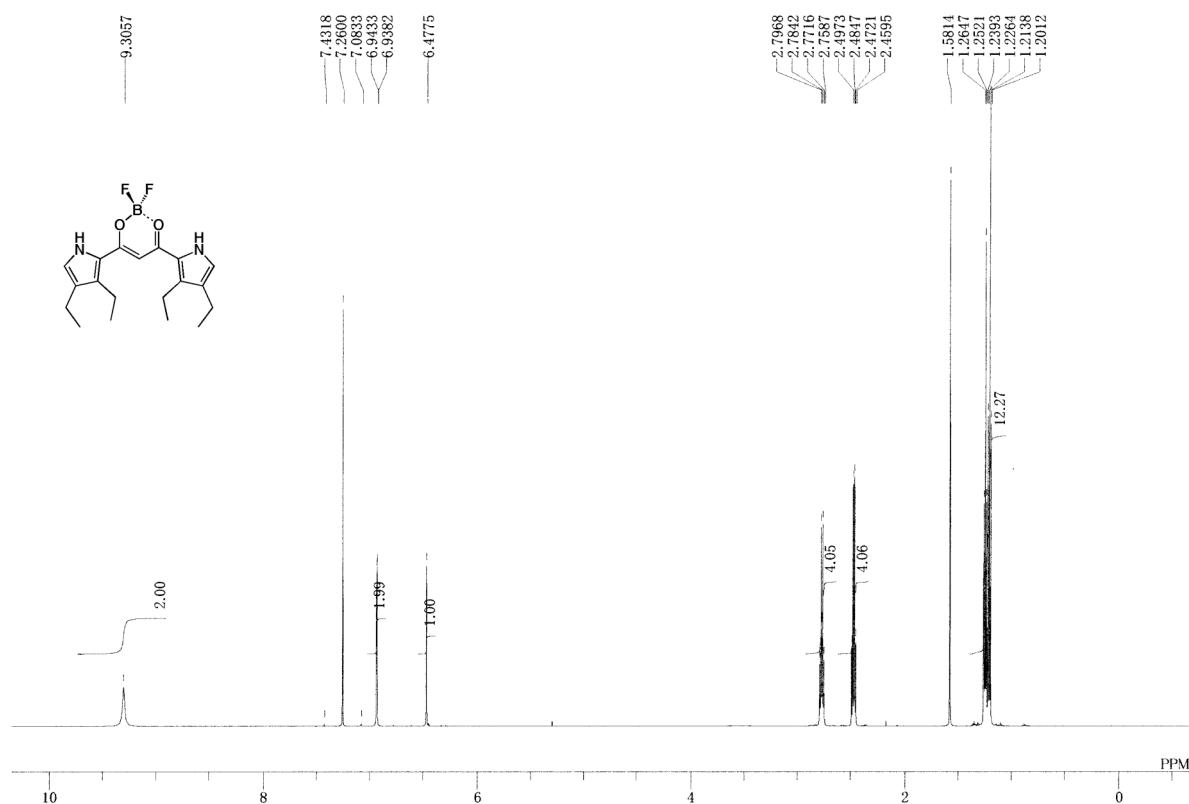
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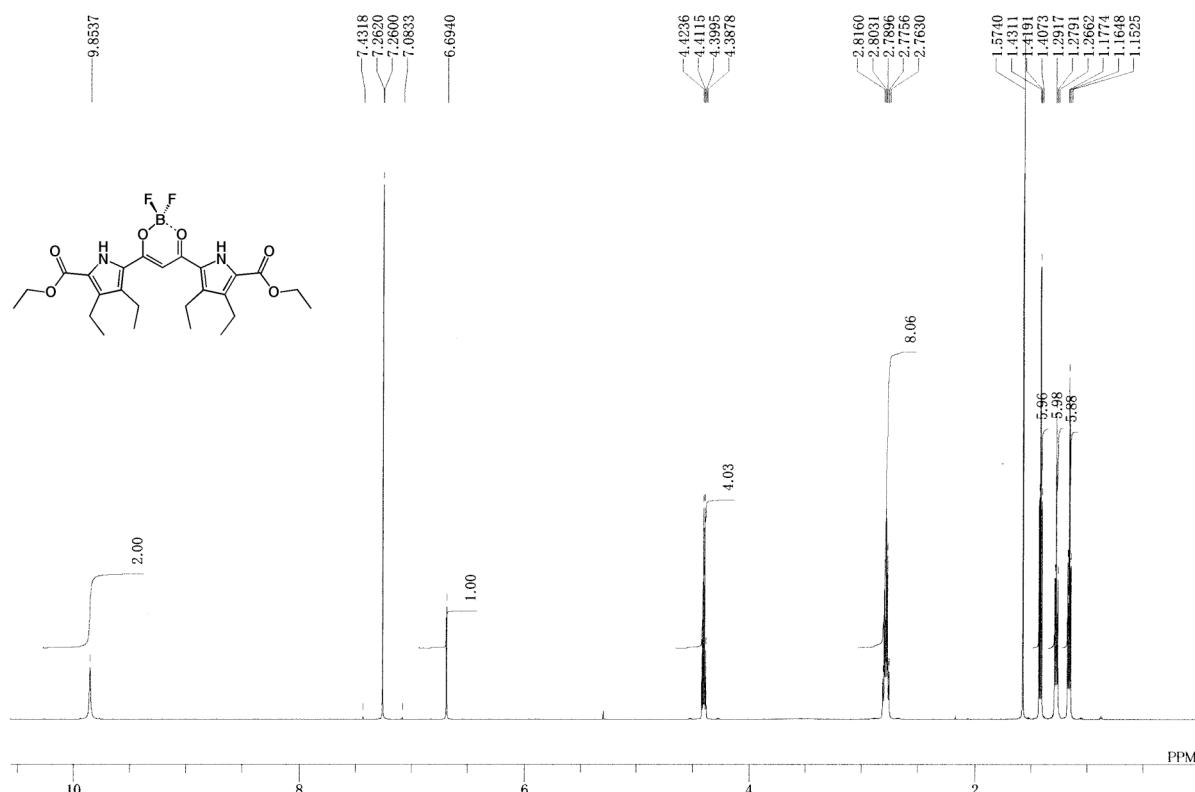
1. General procedures

Starting materials were purchased from Wako Chemical Co., Nacalai Chemical Co., and Aldrich Chemical Co. and used without further purification unless otherwise stated. UV-visible spectra were recorded on a Hitachi U-3500 spectrometer. NMR spectra used in the characterization of products were recorded on a JEOL ECA-600HR 600 MHz spectrometers. All NMR spectra were referenced to solvent. Fast atom bombardment mass spectrometric studies (FAB-MS) were made using a JEOL-HX110 instrument in the positive ion mode with a 3-nitrobenzylalcohol matrix. TLC analyses were carried out on aluminum sheets coated with silica gel 60 (Merck 5554). Column chromatography was performed on Sumitomo alumina KCG-1525, Wakogel C-200, C-300, and Merck silica gel 60 and 60H.

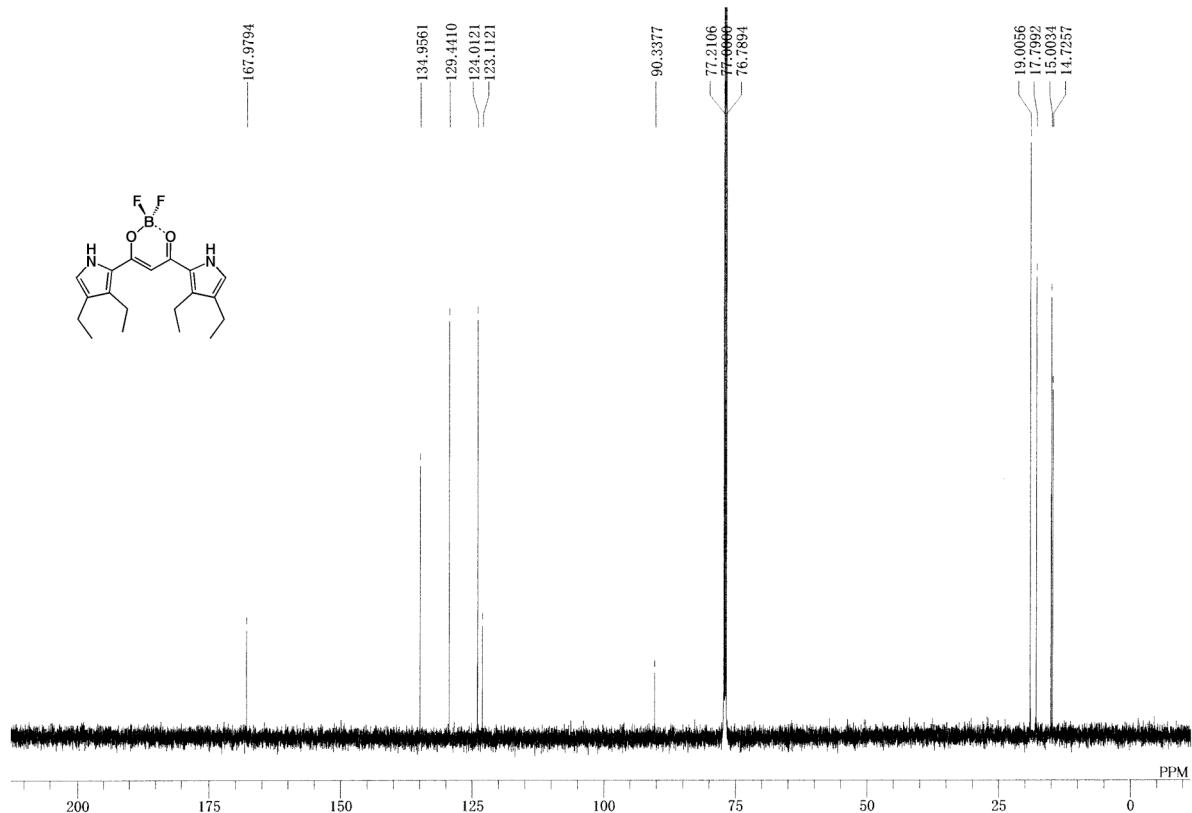
2. Spectroscopic data for 2 and 3



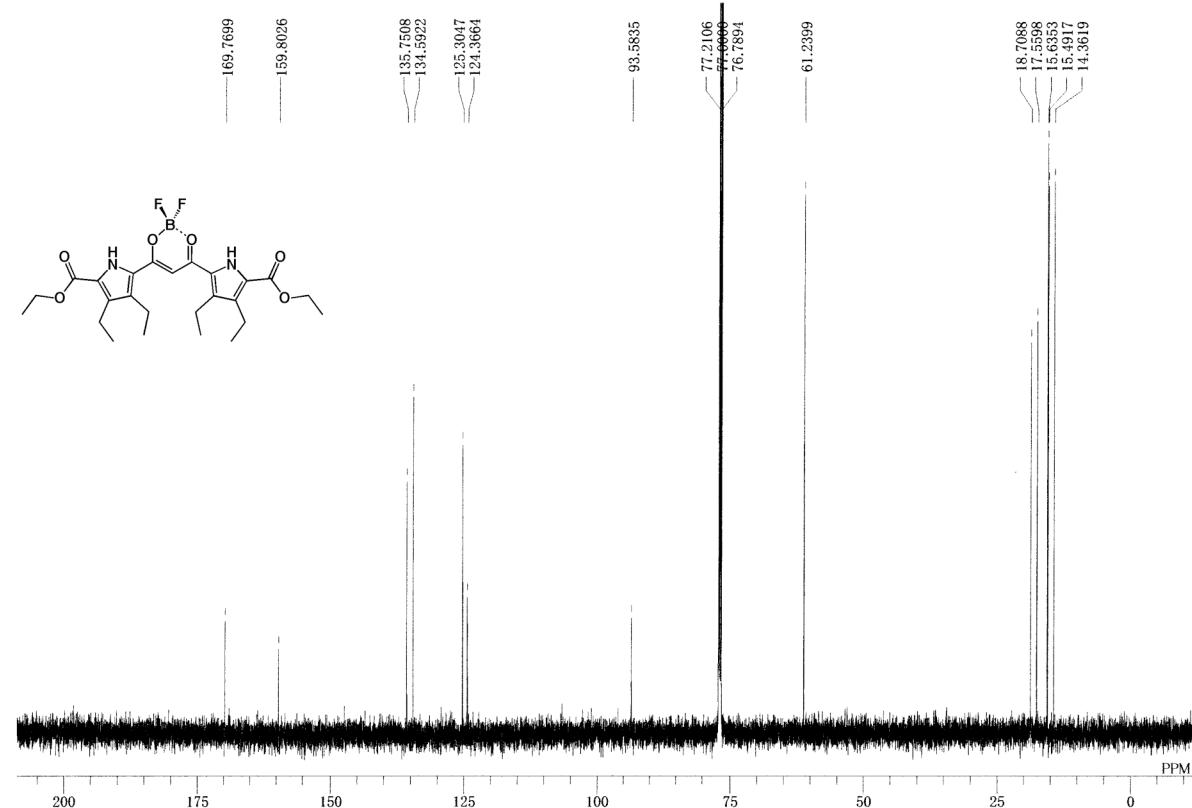
Supporting Figure 1 ^1H NMR spectrum of **2** in CDCl_3 .



Supporting Figure 2 ^1H NMR spectrum of **3** in CDCl_3 .

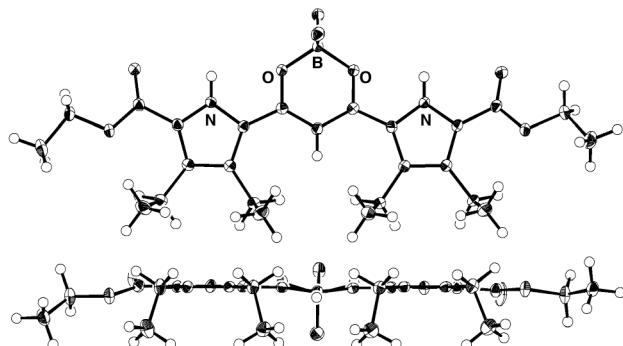


Supporting Figure 3 ^{13}C NMR spectrum of **2** in CDCl_3 .



Supporting Figure 4 ^{13}C NMR spectrum of **3** in CDCl_3 .

3. X-ray crystallographic data for 3

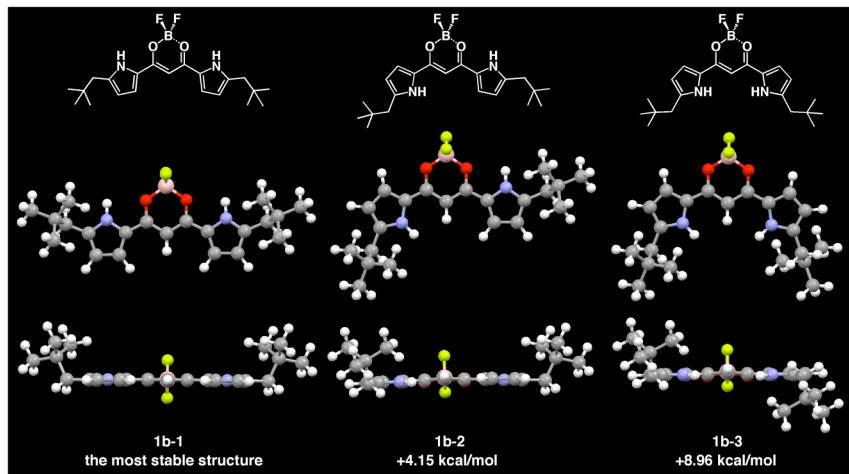


Supporting Figure 5 Ortep drawings (top and side view) of X-ray single crystal structure of **3**. Thermal ellipsoids are scaled to the 50% probability level.

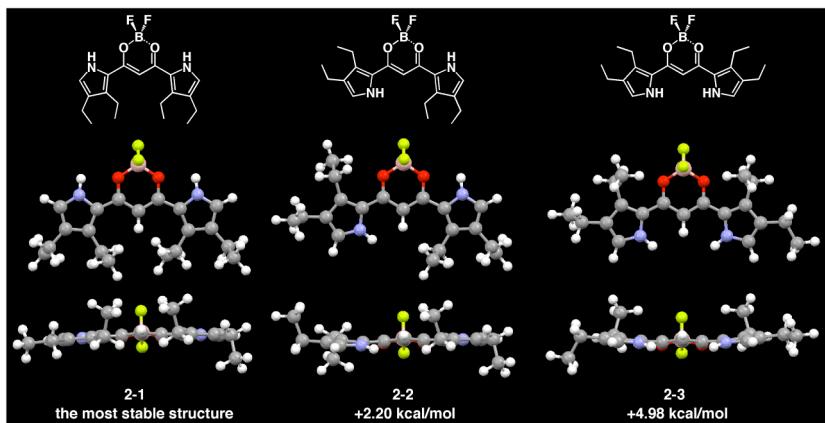
Supporting Table 1 Summary of crystallographic data for **3**

	3
formula	C ₂₅ H ₃₃ BF ₂ N ₂ O ₆
fw	506.35
crystal size (mm)	0.55 × 0.30 × 0.15
crystal system	monoclinic
space group	P2 ₁ /n (no. 14)
<i>a</i> (Å)	8.988(2)
<i>b</i> (Å)	19.159(6)
<i>c</i> (Å)	14.801(4)
α (deg)	90
β (deg)	103.31(1)
γ (deg)	90
<i>V</i> (Å ³)	2480(1)
<i>Z</i>	4
ρ _{calcd} (gcm ⁻³)	1.356
<i>T</i> (K)	123(2)
μ(Mo-Kα) (mm ⁻¹)	0.105
no. of reflns	24148
no. of unique reflns	5677
variables	326
λ _{Mo-Kα} (Å)	0.71075
<i>R</i> ₁ (<i>I</i> > 2σ(<i>I</i>))	0.0387
<i>wR</i> ₂ (<i>I</i> > 2σ(<i>I</i>))	0.1039
GOF	1.078

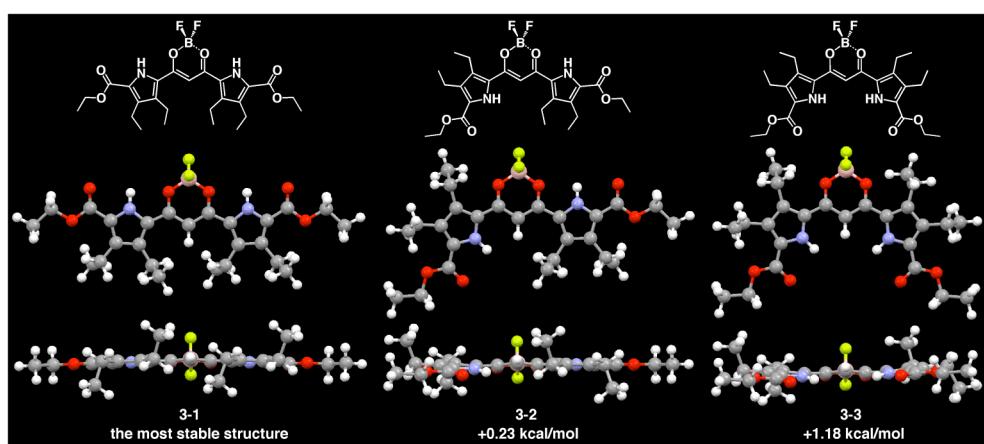
4. Optimization of 1b, 2, and 3 and anion complexes (F^- , Cl^-) by DFT calculations at the level of B3LYP/6-31G^[S1]**



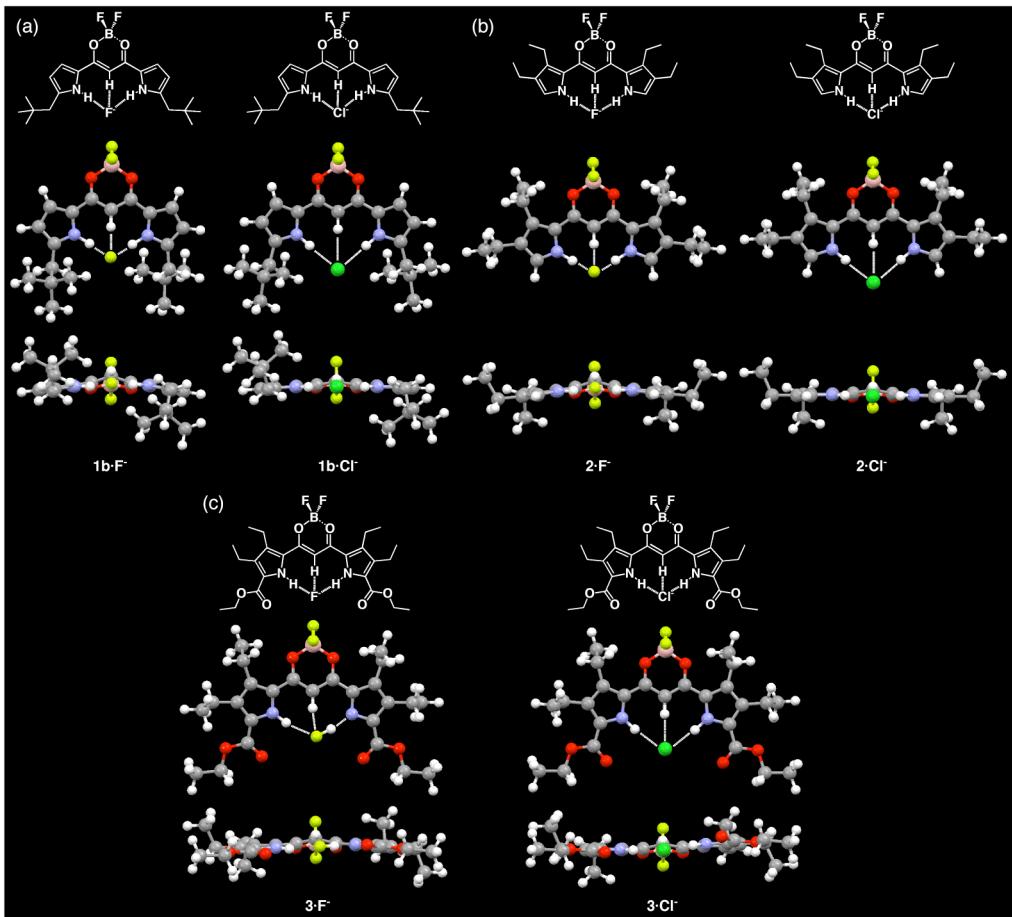
Supporting Figure 6 Optimized structures of **1b** (three conformations).



Supporting Figure 7 Optimized structures of **2** (three conformations).



Supporting Figure 8 Optimized structures of **3** (three conformations).



Supporting Figure 9 Optimized structures of anion (F^- , Cl^-) complexes of (a) **1b**, (b) **2**, and (c) **3**.

Cartesian Coordination of 1b-1.

-1302.4666461 hartree
 B,-0.0168026451,2.0196037928,-0.5445793126
 C,4.7696218226,-0.7486777222,-0.4753552829
 C,-4.7314189078,-0.8688851605,-0.6283332786
 C,4.3471043743,-2.080932818,-0.4717142619
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 C,2.940576898,-2.0934835308,-0.4825030598
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 C,2.5118808874,-0.7648903998,-0.4953553835
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 C,1.2124658221,-0.1489730315,-0.5178608383
 C,-1.1910471085,-0.1793795094,-0.5564990238
 C,0.0195488195,-0.8735143614,-0.5288502783
 C,6.1498482205,-0.1659590915,-0.4712724159
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 C,5.894578143,1.2708706652,1.6215092093
 C,-6.8864831883,-1.2187972531,1.5889507704
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 F,-0.0446683525,2.7617084965,0.6058422758
 F,-0.0079343482,2.7713695518,-1.6887146899
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 H,-5.8985043196,-1.6336115489,1.8103816832
 H,-7.4790798613,-2.002178294,1.1021646213
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Cartesian Coordination of 1b-2.

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Cartesian Coordination of 1b-3.

-1302.4523744 hartree
B,-0.0062617162,3.8653639778,0.6027738943
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Cartesian Coordination of 2-1.

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 H,-3.6547285389,1.9416603711,-0.6608331794

H,3.3095145048,2.4228305857,-0.8520880725
 H,-0.9396254771,-2.826934275,2.5990543281
 H,-2.3645754705,-1.8624479432,3.0208766945
 H,-0.9266786517,-1.0664922251,2.3802285979
 H,6.6528863698,-1.9958239375,2.4227582349
 H,4.9741642279,-1.5314752144,2.7472930585
 H,6.1894667268,-0.2848915306,2.4592721813

Cartesian Coordination of 2-2.

-1223.825164 hartree
 B,-1.116177404,-2.3632399572,-0.2019918621
 C,-1.1342520684,0.0683273045,0.1209712378
 C,4.6874415245,-1.013985637,-0.3096301676
 C,7.1847893535,-1.5348639712,-0.4566576781
 C,6.0888622858,-0.4654404922,-0.4048808787
 C,4.958882216,3.4721837702,0.328960867
 C,-4.3729480147,0.3259407793,-0.0354755609
 C,-3.3444149422,1.4035356395,0.1892764706
 C,3.4859308196,-0.2545313469,-0.2560878044
 C,0.2539204181,0.1147087033,-0.0883459882
 C,4.3236179862,-2.3567729678,-0.2660738399
 C,0.9845615318,-1.0763216356,-0.0951716195
 C,-2.389406165,3.4378199697,0.4526921804
 C,2.4219564408,-1.1720614044,-0.1777382883
 C,-1.9485392963,1.2475176199,0.2452182236
 C,-3.6130361572,2.7959972862,0.3134649617
 C,3.4256274385,1.2496951985,-0.2587219236
 C,-5.6462506926,3.4460593609,1.7059018827
 C,3.2553935746,1.863540852,1.1441426517
 C,-4.4023461111,-0.2141477613,-1.4787423736
 F,-1.5702962057,-3.3708839431,0.5950268224
 F,-1.3730733596,-2.5408980652,-1.5428854172
 N,1.3958630881,2.5118454829,0.3945462848
 N,2.9739391905,-2.4376465724,-0.1886234766
 O,-1.7612407609,-1.0716211586,0.2309852181
 O,0.3779695778,-2.2375753784,-0.0040917247
 H,8.1733389915,-1.0725625212,-0.5286437692
 H,7.0599996448,-2.1910118294,-1.3244986639
 H,7.1742205061,-2.1599391444,0.4424896481
 H,6.2809292894,0.2007262886,0.4472904254
 H,6.170800093,0.1714645456,-1.2966185503
 H,-4.839066676,4.5135500229,0.006986974
 H,-5.6161715549,3.0031784393,-0.4124660218
 H,-4.1868111235,-0.506296492,0.6484201162
 H,-5.3588137135,0.7313552316,0.2162334695
 H,0.7597275924,1.0571342495,-0.2216215686
 H,4.9365127114,-3.245199314,-0.288745877
 H,-2.1690586974,4.4873191574,0.5890242006
 H,4.3502652328,1.634989789,-0.7016799153
 H,2.6220143768,1.5978342191,-0.9181473703
 H,-5.8084784201,2.4195081136,2.0488616834
 H,-5.0322628812,3.9512262775,2.4583813815
 H,-6.6189150451,3.9476507089,1.6674257848
 H,3.2365920267,2.957727319,1.093781053
 H,4.0815946618,1.5708779903,1.7988802497
 H,2.3293020094,1.5229075102,1.6180905622
 H,-5.224129021,-0.9279773186,-1.5965084284
 H,-3.4736938557,-0.7347903705,-1.7234429787

H,-4.5508677531,0.5951934391,-2.2014224337
H,-0.4221786954,2.6979213754,0.5708969674
H,2.4037659805,-3.269577509,-0.147501996

Cartesian Coordination of 2-3.

-1223.8207372 hartree
B,0.0196348481,2.0408754591,0.685083097
C,1.2400041774,0.0122415799,0.0612051249
C,-4.616577608,-1.3563406365,0.5291265372
C,-6.8228975993,-2.6464206641,0.500921499
C,-6.1193677316,-1.2914296062,0.6276385736
C,6.085853746,-0.7501249148,-1.4216275984
C,4.0505588663,1.5600657662,-0.4743524309
C,3.737527057,0.0912520906,-0.5944673714
C,-3.7141182537,-0.2620561852,0.6639830359
C,0.0246497797,-0.6822295259,-0.0442791246
C,-3.8522689177,-2.4893699464,0.2876705009
C,-1.1454315424,-0.1012069006,0.4683838805
C,3.9353551294,-2.1143493335,-1.0610567786
C,-2.4187314799,-0.7718502474,0.4849179476
C,2.5031081209,-0.5363971393,-0.3560420715
C,4.6359534149,-0.9159289012,-1.0488389924
C,-4.1075383668,1.1738621995,0.8906869747
C,7.0391049562,-0.7671553521,-0.2132593897
C,-3.9733670053,2.0605493706,-0.3631286528
C,3.4223981229,2.4228105762,-1.5865003804
F,0.1580260984,2.895408615,1.7349401301
F,-0.2154116933,2.6588527738,-0.527446433
N,2.6558146616,-1.8811379681,-0.6633323109
N,-2.5390223865,-2.1324094082,0.2397309199
O,1.2791853562,1.2192807096,0.5589034245
O,-1.1300511927,1.1055819162,0.9680012819
H,-7.9065919677,-2.529056637,0.5898510462
H,-6.4976342425,-3.3390933532,1.2845903591
H,-6.618701217,-3.1142411147,-0.4683172688
H,-6.5063338179,-0.6125441141,-0.1440269407
H,-6.398012232,-0.8316886547,1.5851407963
H,6.3701832758,-1.5510933038,-2.1144644195
H,6.2199685228,0.1864362682,-1.9752014216
H,3.7064838608,1.9296244231,0.4951850993
H,5.1386070321,1.6847218952,-0.4949401203
H,-0.0207061456,-1.629064812,-0.5651784166
H,-4.1531474518,-3.5176823069,0.1532288989
H,4.2670385469,-3.1085431482,-1.3258715
H,-5.1463844785,1.1961009964,1.2378413771
H,-3.4945976474,1.5995699774,1.6892703479
H,6.8041763308,0.0388430445,0.4888299218
H,6.9602928914,-1.7127371697,0.3327152171
H,8.07904818,-0.644478829,-0.5334809755
H,-4.3555738539,3.0653407334,-0.1560936246
H,-4.5418776184,1.6487881331,-1.20373955
H,-2.9277267493,2.1588034052,-0.664083182
H,3.7553414038,3.4612721948,-1.4897200357
H,2.3319990683,2.4167942272,-1.5214783865
H,3.7156629955,2.0644637592,-2.5789127473
H,1.9691235051,-2.5937821353,-0.480065314
H,-1.7682505073,-2.7790860245,0.2101464644

Cartesian Coordination of 3-1.

-1758.2415695 hartree
B,-0.2400338239,2.8885846371,-0.0073403557
C,-4.7512739,-0.1493503016,-0.3045399019
C,4.3050293863,-1.4767476603,-0.4207475757
C,-2.8891466656,-1.4388348619,-0.3731862077
C,-2.5143259951,-0.084263476,-0.2182030293
C,-1.2580559254,0.6296117386,-0.1019123099
C,0.0086272173,0.0356331998,-0.1419931462
C,1.1372691493,0.8298845134,0.0911405338
C,2.4960215634,0.3340134555,0.1830671453
C,3.1025370771,-0.9423232319,0.1392001629
C,4.4974414918,-0.7466227433,0.2943859067
C,4.7000659603,0.636314023,0.4394117115
C,-6.066855388,0.5038198367,-0.2847616968
C,-8.4136828625,0.2385248632,-0.428958473
C,-9.4225868799,-0.8758202431,-0.6217187259
C,-5.1614939058,-2.7030381725,-0.5972137201
C,-5.5401211287,-2.9734841511,-2.0645905107
C,-1.995291647,-2.6493320491,-0.4353692469
C,2.4380411437,-2.2779137936,-0.0664576247
C,2.1884327911,-2.6185665219,-1.5483001887
C,5.5514667606,-1.8215768901,0.334202522
C,5.8751748927,1.4966904023,0.6303588561
C,8.2234173115,1.6131443014,0.8975962275
C,9.407698294,0.6703210993,0.9711031225
F,-0.3982538138,3.8250926803,0.9672997669
F,-0.1775623646,3.3899988151,-1.279936396
N,-3.6640067789,0.6565147046,-0.1827679578
N,3.4917518065,1.2540251437,0.3672218353
O,-1.4000678492,1.9172169871,0.069935429
O,1.0358318976,2.1204699467,0.269763224
O,-6.203133074,1.7065881455,-0.1415722862
O,-7.0924648905,-0.358312421,-0.4445814358
O,5.7979776761,2.7109102029,0.7040570626
O,7.0317805874,0.8071825473,0.717670358
C,-1.5504275853,-3.1548967983,0.9501916549
C,5.9053347551,-2.2712664578,1.7632992145
H,0.1100270086,-1.0226013906,-0.2963731531
H,-8.4677442982,0.9872045705,-1.2249173361
H,-8.5505049069,0.7599855074,0.5231126936
H,-10.4346846589,-0.4598550609,-0.6169559277
H,-9.352136562,-1.6141171662,0.1821642739
H,-9.2665952858,-1.3868262238,-1.5759518859
H,-6.0761353744,-2.589967087,-0.0096921977
H,-4.6340979238,-3.5733139473,-0.1916193045
H,-6.152247399,-3.8776485818,-2.1466018743
H,-4.6502688141,-3.1083156679,-2.6880496505
H,-6.1131976654,-2.13646062,-2.4727400157
H,-1.1182379488,-2.4428991598,-1.0578203992
H,-2.5297463939,-3.4531627132,-0.9513692221
H,1.4960692675,-2.319684714,0.4904893952
H,3.0688477845,-3.0566143808,0.3741601649
H,1.7110120395,-3.5988447517,-1.6487517478
H,3.1302738589,-2.6423167975,-2.1048138833
H,1.5459001542,-1.8735924234,-2.0279518376
H,5.2075653448,-2.6856288453,-0.2445499683
H,6.4567059933,-1.4562846794,-0.15742852

H,8.1095398432,2.2059147133,1.8100849722
 H,8.3026671928,2.3116095264,0.0591636211
 H,10.328138655,1.2463709052,1.1065324395
 H,9.5021345362,0.0850693195,0.051967562
 H,9.308882288,-0.0206318941,1.8130429788
 H,-3.7015970121,1.6624483555,-0.0809144342
 H,3.3510699683,2.2534549726,0.4379175273
 H,-0.9108641118,-4.0387140028,0.8569263278
 H,-2.4172220901,-3.4270128953,1.5600342526
 H,-0.995321045,-2.3860133516,1.4964126112
 H,6.6618687793,-3.0626169262,1.7449704639
 H,5.0253199573,-2.6547207993,2.2897819445
 H,6.3040607414,-1.4327031263,2.3407874119

Cartesian Coordination of 3-2.

-1758.2411703 hartree
 B,0.0317139319,3.1696115757,0.636706941
 C,4.1053837366,-1.1374928084,-0.267905116
 C,4.8377873916,0.0562768499,-0.1907623507
 C,3.8992833534,1.1007364555,0.0142822898
 C,2.6202477759,0.5082609741,0.0575962632
 C,1.313566716,1.1080377705,0.2112071368
 C,0.1275842075,0.4140380577,-0.0731706288
 C,-1.0975389357,1.0068576015,0.2451349272
 C,-2.3871715465,0.3587646389,0.1285390493
 C,-2.8195885477,-0.9519834108,-0.174922325
 C,-4.2354866616,-0.947704771,-0.1166084295
 C,-4.6236441153,0.3574019457,0.2311101972
 C,4.4376724882,-2.556937824,-0.4279281847
 C,6.137050913,-4.1753606835,-0.7443123562
 C,7.6437547849,-4.2187185774,-0.9020261666
 C,6.3276877968,0.2139096698,-0.337013578
 C,6.7886078614,0.2893898841,-1.8039449442
 C,4.2248724323,2.5642027649,0.1516676052
 C,-1.974580832,-2.1507243127,-0.5165066215
 C,-5.1414121282,-2.1284308561,-0.3476003254
 C,-5.5464208697,-2.8484471092,0.9514865345
 C,-5.9100434215,1.0318214206,0.4504129299
 C,-8.267892383,0.8274787187,0.5119997627
 C,-9.320163287,-0.2410599649,0.29181179
 F,-0.0156719738,3.8542122289,-0.5493565356
 F,0.0231922499,3.9520797364,1.7494586538
 N,2.780891434,-0.8418708219,-0.1275509056
 N,-3.5022932769,1.113133822,0.3709835066
 O,1.2960832107,2.3316609106,0.6541898869
 O,-1.1557227869,2.2309751047,0.7028222575
 O,3.5875407248,-3.4344775668,-0.414556339
 O,5.7547344991,-2.7852679804,-0.5905315695
 O,-5.9949024604,2.2148528751,0.7316223057
 O,-6.9714457098,0.2104757164,0.3123024508
 C,4.3978417422,3.0163204276,1.6135611716
 C,-1.6047208153,-2.2433101456,-2.0094383702
 H,0.1592188725,-0.5688877463,-0.5130793835
 H,5.6181209044,-4.5857238692,-1.6157684061
 H,5.7967749625,-4.7308638235,0.1346958619
 H,7.9715333272,-5.2555164311,-1.0242255722
 H,8.1425666001,-3.8026491395,-0.0222432385
 H,7.9626090519,-3.6518096372,-1.781079731

H,6.8297257368,-0.6255666819,0.1515545219
 H,6.6425435281,1.1204390618,0.1899271452
 H,7.8738972182,0.4216965974,-1.8622204393
 H,6.316200748,1.1274187138,-2.3261926833
 H,6.5288758571,-0.6299009715,-2.3363886224
 H,5.1446960689,2.7734309919,-0.4056432781
 H,3.4319591286,3.1586324121,-0.3090616865
 H,-2.5182395931,-3.0569436203,-0.2308241594
 H,-1.0658374347,-2.153970915,0.0955395465
 H,-4.6431403528,-2.8385549387,-1.0163834503
 H,-6.0444748366,-1.793528034,-0.8643036199
 H,-6.1913693183,-3.7061711139,0.7341419011
 H,-6.0937586291,-2.1697279896,1.6112446952
 H,-4.6692670418,-3.2131414916,1.4958137906
 H,-8.3711624363,1.6604599144,-0.189672542
 H,-8.3053514057,1.2421612154,1.5237979729
 H,-10.3163604447,0.1875440397,0.4374987591
 H,-9.1949790313,-1.0667112386,0.9979155472
 H,-9.2648229871,-0.6427237138,-0.7239318018
 H,2.0807359031,-1.5670932335,-0.0712488087
 H,-3.496931889,2.0939099671,0.6191886133
 H,4.6693695971,4.0758354223,1.6545819493
 H,5.1833043331,2.4439716843,2.1184660527
 H,3.4651906358,2.885247809,2.1671984343
 H,-0.990516358,-3.1282561215,-2.2046914405
 H,-1.0491466385,-1.3608868205,-2.3419763477
 H,-2.5047690769,-2.3113596344,-2.627925058

Cartesian Coordination of 3-3.

-1758.2396836 hartree
 B,-0.0720580795,3.4814590281,0.2752452131
 C,-3.9365047946,-1.0693013775,-0.0168681635
 C,-4.7131910496,0.0987121067,-0.0423256122
 C,-3.8148763931,1.1920354223,0.0666624929
 C,-2.5122736716,0.6532154248,0.1352943035
 C,-1.2313402776,1.3181891997,0.208084465
 C,-0.0133692475,0.6616111719,-0.0160910073
 C,1.1843262855,1.3675119381,0.166359838
 C,2.4841051512,0.7387721814,0.0966396433
 C,3.7687041383,1.3078891804,-0.0262924864
 C,4.6975063279,0.2368376704,-0.0865137357
 C,3.9544685541,-0.9494249275,-0.0006656064
 C,-4.2126754388,-2.5094856087,-0.0525265782
 C,-5.8474561815,-4.2181372384,-0.1651824932
 C,-7.3552579132,-4.3384038951,-0.2599028874
 C,-6.2136705797,0.1786793208,-0.1382861756
 C,-6.9137658941,0.0973999124,1.2300915483
 C,-4.1941056145,2.6501202038,0.053659666
 C,4.1095998771,2.7732436393,-0.0841822979
 C,4.2722857054,3.41533669,1.3061139431
 C,6.1886513959,0.360031946,-0.2526188218
 C,4.2728185591,-2.3809617553,0.031592181
 C,5.9524892845,-4.0458292525,-0.0768376087
 C,7.4565513073,-4.1283153248,-0.2436880348
 F,-0.0591695227,4.4488025761,1.230867178
 F,-0.1360826856,3.9476405902,-1.0163136609
 N,-2.6232717695,-0.7130691901,0.0759429286
 N,2.6327658877,-0.6256754138,0.0984806222

O,-1.2669222506,2.5856062075,0.5080233538
O,1.1824715865,2.6445412585,0.4259562083
O,-3.3236436514,-3.3465624001,-0.0134826931
O,-5.5243369302,-2.8051825985,-0.1249113881
O,3.4144064401,-3.2389101596,0.170682349
O,5.586075262,-2.6432286019,-0.1093724114
C,-3.8857222312,3.3628508704,-1.2775725017
C,6.6453673913,0.2527817264,-1.7188226094
H,0.0037801585,-0.3697558957,-0.3387876498
H,-5.4506644491,-4.6926733849,0.737315056
H,-5.3415669782,-4.6681933715,-1.0245491452
H,-7.6390044687,-5.3948327158,-0.2873963749
H,-7.7311149285,-3.8584135069,-1.1678259809
H,-7.8407249311,-3.8745632443,0.6032324459
H,-6.5774634515,-0.6324526829,-0.7740502363
H,-6.4907972237,1.1152664376,-0.6334099561
H,-7.9998215393,0.173939956,1.114205536
H,-6.5857913694,0.9039876775,1.8934190217
H,-6.6905131247,-0.8542944749,1.720939176
H,-3.6721816643,3.168974471,0.8615986143
H,-5.2651042742,2.7303542443,0.2659694252
H,3.3288672518,3.3086172255,-0.6301499632
H,5.0378249668,2.8962811682,-0.6528270105
H,4.5520968177,4.4690136071,1.2087312543
H,5.0480498473,2.9097976202,1.8908794827
H,3.3330484962,3.3650011991,1.8616291148
H,6.5145606805,1.3200943633,0.1608717605
H,6.6833329491,-0.4197093336,0.3326081601
H,5.4183057126,-4.5645481745,-0.8784735978
H,5.6176682591,-4.4727052369,0.8733027331
H,7.7717102135,-5.1759968,-0.2248214146
H,7.9706115624,-3.6007513442,0.5646547714
H,7.7704153867,-3.6923527888,-1.1961959579
H,-1.8948075943,-1.4064382382,0.1650159463
H,1.92747598,-1.3315808738,0.2525632134
H,-4.2602501884,4.3910466117,-1.2485120358
H,-4.363170113,2.8521173062,-2.1204146572
H,-2.8096178142,3.4080052136,-1.4608888166
H,7.7318250436,0.3646777178,-1.795195448
H,6.1802373531,1.0267636605,-2.3375086783
H,6.3734930825,-0.7210128189,-2.1359934781

Cartesian Coordination of 1b·F⁻.

-1402.4002395 hartree

N,-2.1073801475,0.1413699234,0.4867682174
N,2.271086012,-0.1247424488,-0.2986014954
O,1.4335077833,3.3873092697,-0.4346341039
O,-0.9845066811,3.5398320377,0.0390913892
C,0.267353329,1.6242572538,0.6052259712
C,-2.074804799,-2.2589151403,2.5784522383
C,2.8264606452,-4.480792267,-1.7613347889
C,-3.4683814116,-4.1164649165,1.6090531209
C,3.8358324643,-2.7008525087,-3.2189895572
C,-4.5825735711,-2.2352389447,2.8474120285
C,3.4182819362,-2.2703340439,-0.7488684223
F,0.5956717664,4.796137791,1.2678785919
F,0.1958621924,5.304425161,-0.9369691585
C,-3.5718554761,-1.8525714782,0.5485699059

C,2.882077572,-2.9667076647,-2.0408268192
C,-3.4206495233,-2.6061250423,1.9089824936
C,1.4679021896,-2.4583730315,-2.3871581048
C,4.3336061988,0.1935698408,-1.0929868482
C,1.392992736,2.1387557219,-0.0338448823
C,-0.9443458014,2.2845892669,0.4174476118
C,-3.5096823996,1.8937367278,0.6066435783
C,2.4640516513,1.2431762186,-0.3903186891
C,-2.166093467,1.5244177716,0.5079175612
C,-4.2616487552,0.703404009,0.6599723989
C,3.7505492503,1.4597756768,-0.8903584779
C,-3.3606207238,-0.3674099961,0.5757154407
C,3.3833488051,-0.7702292025,-0.7263646651
B,0.317473122,4.3129343551,0.0037115953
H,-1.229003285,-0.4517251,0.3369770378
H,0.2648801671,0.6037827665,0.9522453208
H,-2.1013470273,-1.24989835,3.0019830067
H,-1.2405579634,-2.2797662109,1.8680338868
H,-1.8694880072,-2.9572276768,3.399718333
H,2.50771338,-5.0317070291,-2.6542102775
H,2.1157979014,-4.7057438973,-0.9581968474
H,3.8080907875,-4.8693040459,-1.461865622
H,-3.4275362483,-4.7012780886,2.5357531182
H,-2.6200609169,-4.419336236,0.9851597987
H,-4.3904010635,-4.3912160151,1.0810856461
H,4.8333251108,-3.117339487,-3.0278068411
H,3.4545318262,-3.1572028536,-4.140430263
H,3.9473848692,-1.6263057538,-3.3948378443
H,-5.5493696605,-2.5414095466,2.4272630088
H,-4.6162119315,-1.1541009927,3.0158211918
H,-4.4707579235,-2.7269661133,3.8213151688
H,4.4480731077,-2.609476776,-0.5757099091
H,2.8153658343,-2.6296340465,0.0940916128
H,-2.8419045893,-2.2826751066,-0.1482514614
H,-4.5687072064,-2.0669249469,0.142180919
H,1.5069285512,-1.4379263161,-2.7814377178
H,0.8107170272,-2.4330523112,-1.5106100465
H,1.0165591233,-3.0940843427,-3.159332979
H,5.3328399246,-0.014205869,-1.4531292744
H,-3.8731474282,2.9107804446,0.6491067032
H,-5.337506103,0.6146921073,0.7383780835
H,4.195529384,2.4301296449,-1.059499233
H,1.3551326227,-0.6158196281,-0.0498920611
F,0.0336892813,-1.320925428,0.3033869736

Cartesian Coordination of 1b·Cl⁻.

-1762.7909501 hartree

N,-2.4714657793,-0.0162365197,0.3876344012
N,2.5181893639,0.0023666668,-0.33981337
O,1.2097132223,3.3858364141,-0.3202282367
O,-1.2374930046,3.3763757861,0.0272403124
C,0.0530213708,1.4145214771,0.2711623438
C,-2.9558853826,-2.3030279673,2.774016727
C,4.4371182922,-4.0127435219,-1.8702482078
C,-4.469181555,-4.0361499529,1.7632421382
C,5.3141416056,-1.9014747601,-2.9110048074
C,-5.4450667677,-1.9224552617,2.7084257955
C,4.1532857734,-1.8504139,-0.6448786595

F,0.1965096625,4.6698807618,1.369953348
 F,-0.1183002229,5.2358622506,-0.8334984792
 C,-4.1122939021,-1.8827512356,0.5407410237
 C,4.1806708586,-2.5059493883,-2.0630371627
 C,-4.2431798822,-2.524933448,1.9592027565
 C,2.8309673137,-2.3060049279,-2.7764504012
 C,4.5748823931,0.7569574027,-0.7420515221
 C,1.2098213585,2.0911060098,-0.1102109574
 C,-1.1692615426,2.0823225072,0.2295384058
 C,-3.7225978328,1.8408181602,0.437399237
 C,2.4424430788,1.3848422326,-0.3450411705
 C,-2.4126887931,1.3666049343,0.3505373949
 C,-4.5689766938,0.7202215436,0.5285874141
 C,3.7260141208,1.8702804541,-0.5999965137
 C,-3.7640985509,-0.4246715464,0.4928449084
 C,3.7953825715,-0.3951368531,-0.583194498
 B,0.0148046262,4.2175629441,0.0777381297
 H,-1.6742064326,-0.6648375422,0.2816267977
 H,1.7296444854,-0.6523214537,-0.2115215531
 H,0.0849855925,0.3524778107,0.4666275806
 H,-2.8058277966,-1.2416602215,2.9937939976
 H,-2.070707762,-2.6534543229,2.2325754334
 H,-3.0127258439,-2.8378448566,3.7300417941
 H,4.4997710305,-4.5251218467,-2.8375682309
 H,3.6284246396,-4.4779299845,-1.2964062729
 H,5.3782051969,-4.192723016,-1.3356787676
 H,-4.6012049202,-4.540115326,2.7279762855
 H,-3.6142432315,-4.4981559017,1.2579228863
 H,-5.364822214,-4.2305726169,1.1600611974
 H,6.2929656612,-2.0633142574,-2.4417134726
 H,5.3415976952,-2.361592319,-3.9059709157
 H,5.1772715919,-0.8236312699,-3.0417994186
 H,-6.3832047795,-2.1040196444,2.168556089
 H,-5.3305212143,-0.8409624475,2.8306383272
 H,-5.5435557945,-2.366556344,3.7062202816
 H,5.1411152169,-1.9902199973,-0.1864079814
 H,3.4341871862,-2.4052938435,-0.0311549348
 H,-3.3428894087,-2.4361391266,-0.0105720104
 H,-5.0601297277,-2.0357731159,0.0084312899
 H,2.6524158288,-1.2487102286,-2.9949254555
 H,1.9949148935,-2.6594761324,-2.1635192485
 H,2.8187316957,-2.850318462,-3.7287692537
 H,5.640476529,0.7691207895,-0.9271699564
 H,-3.9976626398,2.8854704347,0.4357479875
 H,-5.6481556289,0.7227336229,0.6027473365
 H,3.9857789144,2.9175343035,-0.6524365137
 Cl,0.0376193712,-2.1152044058,0.0880889967

Cartesian Coordination of 2·F⁻.

-1323.758287 hartree
 H,3.6789234148,-3.2798756133,-0.298017574
 H,0.0162857076,-1.0707851956,-1.1154000631
 H,-3.5504272749,-3.4209898622,-0.2679217256
 H,6.1592627927,-2.3733634738,0.5150711138
 H,6.3559996607,-0.6618726412,0.831356725
 H,7.7762789228,-1.3578435701,-1.1038113519
 H,6.5287481626,-0.2228074991,-1.6549556791
 H,6.3384330162,-1.949298705,-1.9619063207

H,5.323521206,1.4386854216,-0.0748735421
 H,3.7231857438,2.130079936,-0.3221404063
 H,-5.3760602823,1.2298072121,-0.0306967894
 H,-3.8060230214,1.9830797881,-0.2910970184
 H,-6.3182408923,-0.9092744618,0.883807372
 H,-6.0574604075,-2.6118474547,0.5657231771
 H,-7.7262163957,-1.6605773644,-1.0396214592
 H,-6.2735207971,-2.1956334675,-1.909643518
 H,-6.5285473984,-0.4778222458,-1.6009418844
 H,1.3550122107,-2.2511939114,-0.4292210658
 H,-1.2696309361,-2.3024272066,-0.4183393617
 H,4.6698186157,2.824382156,1.8859030491
 H,4.7610028971,1.1245210478,2.3904019614
 H,3.1835389276,1.8776306189,2.0807987865
 H,-4.7607529751,2.6403583107,1.9247764896
 H,-3.2370959287,1.7523735328,2.1072660137
 H,-4.7813529218,0.9383363282,2.4298095242
 F,0.0540801093,-2.9117242388,-0.6713309559

Cartesian Coordination of 2·C⁺.

-1684.1549762 hartree
 B,0.026867962,2.5350906631,0.2040816668
 C,3.7639703851,-2.1185946192,-0.1919961794
 C,4.6131021347,-1.0200816794,-0.0578159367
 C,3.7845673602,0.1287847347,0.0345905787
 C,2.4534255397,-0.3216848721,-0.0514235632
 C,1.2078618292,0.4011292401,-0.0271738359
 C,-0.0031135396,-0.2241292462,-0.3225582454
 C,-1.199374237,0.4261759477,-0.0214381288
 C,-2.4598149328,-0.2705599827,-0.0397316216
 C,-3.7808530316,0.2075895071,0.0525170481
 C,-4.6336106677,-0.9237309297,-0.0356678624
 C,-3.8082483551,-2.0397372236,-0.173719087
 C,6.1180979311,-1.0690116364,-0.0618425258
 C,6.7423267416,-0.8604521284,-1.4541450002
 C,4.251569795,1.5494254099,0.2119651063
 C,-4.2172244264,1.6377182788,0.2316970691
 C,-6.1393041821,-0.941290126,-0.0323942223
 C,-6.7658161012,-0.7201438536,-1.4217292411
 F,0.0301167288,3.1328201544,-1.0416840439
 F,0.0387617646,3.4440612762,1.2344341019
 N,2.4804303756,-1.6993442518,-0.1939418507
 N,-2.5162632606,-1.6473878333,-0.1819591096
 O,1.2499301384,1.6654113635,0.3343551256
 O,-1.2134189205,1.6910398407,0.3402145808
 C,4.2446224472,2.0155477623,1.6794675967
 C,-4.1934482997,2.1039997172,1.698966536
 H,3.9987994668,-3.1708973327,-0.2749951738
 H,-0.0146562384,-1.2540350269,-0.6490477599
 H,-4.0653916624,-3.0868979503,-0.2553842565
 H,6.4487800293,-2.0384896679,0.3326132008
 H,6.5188683677,-0.3134529323,0.6255245583
 H,7.83733157,-0.9086268344,-1.4123675164
 H,6.4612984586,0.11288687,-1.8692708692
 H,6.393110353,-1.6270229488,-2.1535390381
 H,5.2672172856,1.6447391901,-0.1921763059
 H,3.6120043911,2.221174355,-0.3674168242
 H,-5.23260952,1.7541031173,-0.1675615807

H,-3.5665910366,2.295819296,-0.3510208407
 H,-6.5209078183,-0.1773772515,0.6566474583
 H,-6.4881794583,-1.9035749364,0.3640139102
 H,-7.8613681138,-0.7454898041,-1.3746075089
 H,-6.4360464672,-1.4940134628,-2.1225198478
 H,-6.4665899955,0.2470160927,-1.8385696049
 H,1.6626187187,-2.3367769952,-0.2305068523
 H,-1.7121941909,-2.3018432243,-0.2226114629
 H,4.6318158092,3.0376653916,1.7651980569
 H,4.8627150601,1.3628186286,2.3062963943
 H,3.2246038159,2.0056737447,2.0703116901
 H,-4.5587946173,3.1340073118,1.7861488273
 H,-3.1719827254,2.0729429873,2.0848839674
 H,-4.8220196098,1.4645106738,2.3290107236
 Cl,-0.0393974126,-3.7089680189,-0.3802867083

Cartesian Coordination of 3-F⁻.

-1858.1701396 hartree
 B,-0.1689160652,3.6920300545,-0.4428177784
 C,3.7222188682,-0.7361917924,0.2199183363
 C,4.5725975457,0.3925149589,-0.0261609057
 C,3.7156738598,1.4839536528,-0.182685395
 C,2.3931894588,0.9697874926,-0.0041374696
 C,1.1412932966,1.6595271154,-0.0557211
 C,-0.0548576792,1.0140522535,0.3184270878
 C,-1.2581923325,1.5500060051,-0.0791206011
 C,-2.4717783734,0.7449100028,-0.0514443956
 C,-3.8249546119,1.1189024433,-0.1203923396
 C,-4.5888035464,-0.0718713655,-0.0504157315
 C,-3.6762921094,-1.1362408176,0.0589106232
 C,4.0506400772,-2.1471696553,0.4471791557
 C,5.7731402416,-3.767004453,0.5795574374
 C,7.2843713975,-3.8593208651,0.4602231101
 C,6.076136124,0.4226829374,-0.1233154088
 C,6.6108162637,0.0357777062,-1.514215161
 C,4.1047390958,2.9178301573,-0.4350053579
 C,-4.3606444535,2.5211680895,-0.2502949861
 C,-4.4726088564,3.0003922499,-1.7087736789
 C,-6.0925726079,-0.153565473,-0.0582133627
 C,-3.8321675241,-2.5845425798,0.1353446212
 C,-5.346907166,-4.3980772003,0.2361766215
 C,-6.8441775441,-4.6461734193,0.248074707
 F,-0.1955514919,4.5641982714,-1.5020361427
 F,-0.2114542305,4.3282055367,0.7846662837
 N,2.4207420349,-0.3806758181,0.2368555606
 N,-2.4069875937,-0.619033802,0.0566192118
 O,1.1005538886,2.8847242889,-0.5261045425
 O,-1.3582772365,2.7713297341,-0.5658068952
 O,3.2575906356,-3.0379453615,0.6917078995
 O,5.4011055192,-2.4004075058,0.356581524
 O,-2.9117836577,-3.3819191373,0.1649037585
 O,-5.1423972813,-2.9753053136,0.173020838
 C,3.9534958528,3.8293959633,0.7973411028
 C,-6.7062453579,-0.2450840574,1.3505737209
 H,-0.0076978012,0.0326501842,0.7541836946
 H,5.2691865174,-4.4067421263,-0.1534924907
 H,5.4250284231,-4.0839434138,1.5689863778
 H,7.6125083749,-4.8914344585,0.624708182

H,7.774487373,-3.2201710465,1.2010053053
 H,7.6183791223,-3.5459300765,-0.5334463977
 H,6.5092621385,-0.2534917217,0.6191502718
 H,6.4312445479,1.4302284697,0.1249750319
 H,7.7068395172,0.0818308484,-1.5456786119
 H,6.2201625464,0.7085781324,-2.2851465945
 H,6.3052196484,-0.9825782492,-1.7698187071
 H,3.4912596203,3.3267429029,-1.243687994
 H,5.1452453653,2.9514453311,-0.7801143245
 H,-3.7056175483,3.209510373,0.2902967381
 H,-5.3460645558,2.575337783,0.2289084866
 H,-4.8962665272,4.0102442962,-1.7544973048
 H,-5.1124738386,2.3355294584,-2.3000626914
 H,-3.4820158996,3.0266680114,-2.1685304325
 H,-6.4930294089,0.7298803079,-0.5679987332
 H,-6.4098608714,-1.0246572612,-0.6380225952
 H,-4.861260167,-4.7922858455,1.135079459
 H,-4.8620512665,-4.8709464587,-0.6242885493
 H,-7.0443124939,-5.7217077625,0.2953272424
 H,-7.3136987434,-4.2483639091,-0.6565791778
 H,-7.3133233091,-4.1705421656,1.1144289019
 H,1.1930474787,-1.3800614131,0.3039162099
 H,-1.5504975635,-1.1811119557,0.084405127
 H,4.2926328215,4.847718354,0.5718958995
 H,4.5436512154,3.4525979482,1.6402676518
 H,2.9073777178,3.8883045296,1.1080639041
 H,-7.8009340389,-0.2830022786,1.3007367309
 H,-6.4237205798,0.6186381546,1.9613946604
 H,-6.3563051418,-1.1472172431,1.8597141945
 F,0.3291059565,-1.8770338488,0.371623368

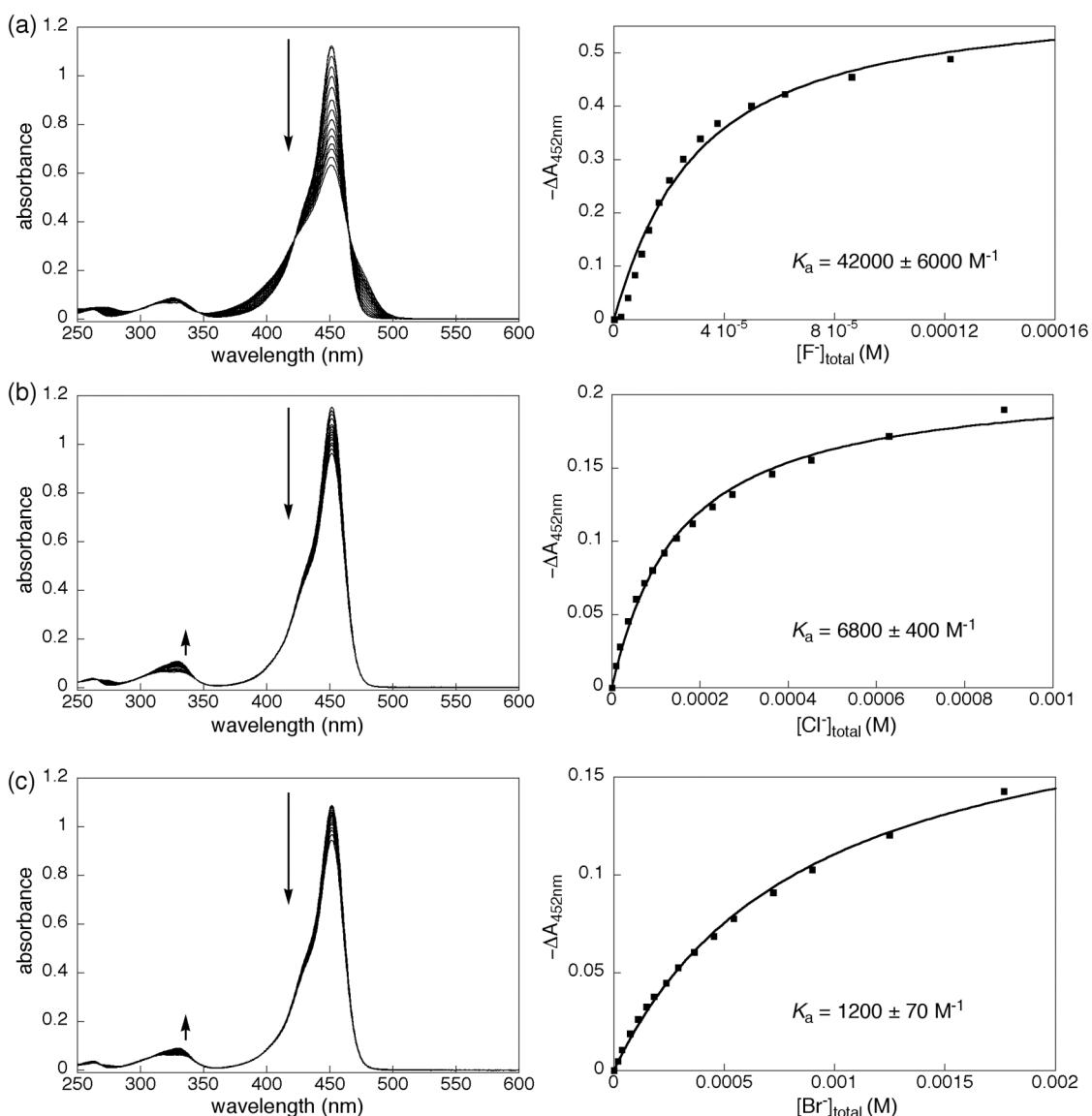
Cartesian Coordination of 3-Cl⁻.

-2218.553051 hartree
 B,-0.1560840668,3.5659047679,-0.4602023642
 C,3.9796214118,-0.6804354699,0.2162404272
 C,4.681049798,0.5294310336,0.0365565764
 C,3.7115028377,1.5374625296,-0.1547045958
 C,2.4474587193,0.9100262975,-0.0757857997
 C,1.1319999236,1.5050753555,-0.1802234598
 C,-0.0378229266,0.8059517708,0.112056577
 C,-1.2653733171,1.3970978409,-0.1788188106
 C,-2.515427782,0.6663990332,-0.124320749
 C,-3.8353048383,1.1690644675,-0.1367427461
 C,-4.699460663,0.057427864,-0.0407574699
 C,-3.8812591004,-1.0883790951,0.0266114638
 C,4.4374236719,-2.0495486803,0.4775960943
 C,6.3004580087,-3.5019507622,0.5814790345
 C,7.8035465014,-3.4637398384,0.3739652243
 C,6.1740894809,0.7323318519,0.0361900305
 C,6.8163446152,0.5233052497,-1.3468588057
 C,3.9923326061,3.0060418771,-0.3495924142
 C,-4.2633804672,2.6109786659,-0.2295049067
 C,-4.3619502099,3.1304732704,-1.6752487967
 C,-6.2039551743,0.12191052,0.0087865472
 C,-4.2007568571,-2.5177214764,0.103500158
 C,-5.9204870085,-4.1283865535,0.3035238117
 C,-7.4317615299,-4.1899624413,0.4306179116
 F,-0.215426975,4.4524467836,-1.504890328

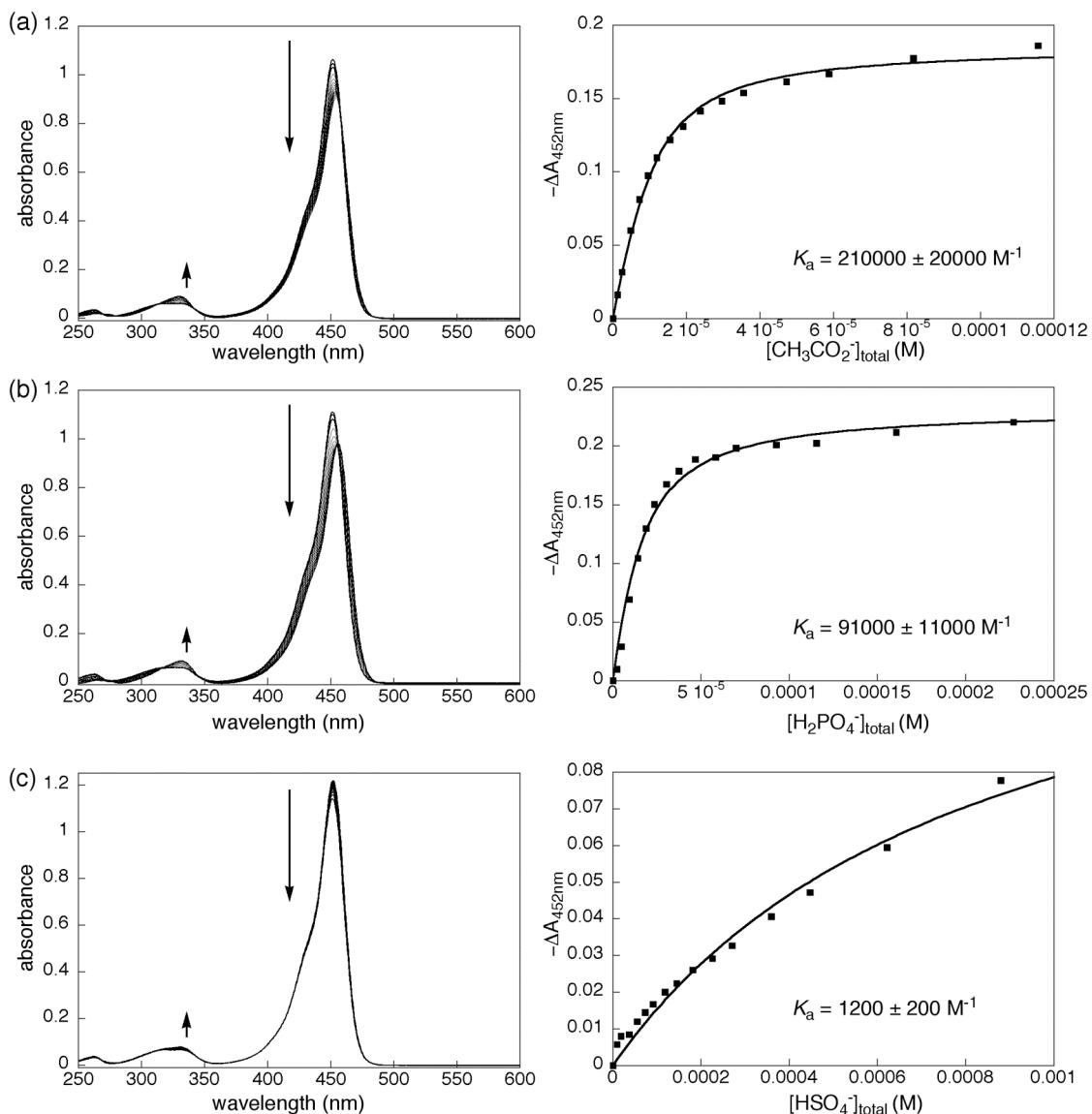
F,-0.1460899834,4.1848527205,0.7772064459
 N,2.6399734328,-0.4294541546,0.156055614
 N,-2.5726458708,-0.7016081676,-0.0224842939
 O,1.0974653821,2.7513704756,-0.5926873234
 O,-1.3511571353,2.6554226029,-0.5460919459
 O,3.7266335354,-2.9796326631,0.7971404666
 O,5.7923327182,-2.1811012204,0.3227522408
 O,-3.393652051,-3.4226647543,0.0613424565
 O,-5.5465949809,-2.7410501393,0.2338653014
 C,3.7194728045,3.8642917972,0.9003133712
 C,-6.7683628744,0.1091832859,1.440916582
 H,0.0078133584,-0.2299730196,0.4271350466
 H,5.8131358063,-4.2128441656,-0.0937912252
 H,6.0365313766,-3.7972765642,1.6024965351
 H,8.2314946467,-4.4550141437,0.5565074814
 H,8.2759112531,-2.753430956,1.0592617646
 H,8.0491884977,-3.1657049402,-0.6495830936
 H,6.6375078616,0.0453233866,0.7484019703
 H,6.3968940199,1.7469234661,0.3856939616
 H,7.8987691943,0.6945452303,-1.307855942
 H,6.3904944192,1.2085663726,-2.0872701895
 H,6.6439503868,-0.4986697862,-1.6950030335
 H,3.3863078937,3.3888269955,-1.1743583657
 H,5.0413208959,3.1250583531,-0.644262898
 H,-3.5561370024,3.2387605587,0.3179531687
 H,-5.237019237,2.7232657373,0.2626866908
 H,-4.7124486594,4.1688469997,-1.6906982146
 H,-5.05815526,2.527062281,-2.2685317697
 H,-3.3808741502,3.0973436321,-2.1541993169
 H,-6.5363225346,1.0341897072,-0.4991627353
 H,-6.6268118937,-0.7198958586,-0.5451278681
 H,-5.4196917683,-4.5936897082,1.1589831665
 H,-5.5649636061,-4.6437891634,-0.5948708304
 H,-7.7599195245,-5.2329939013,0.4895394607
 H,-7.9163887131,-3.7250616952,-0.4332419449
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 H,-6.4855344597,-0.8144567784,1.9528734714
 Cl,0.1452379462,-2.4697949687,0.039280122

[S1] *Gaussian 03*, (Revision C.01), Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian, Inc., Wallingford CT, 2004.

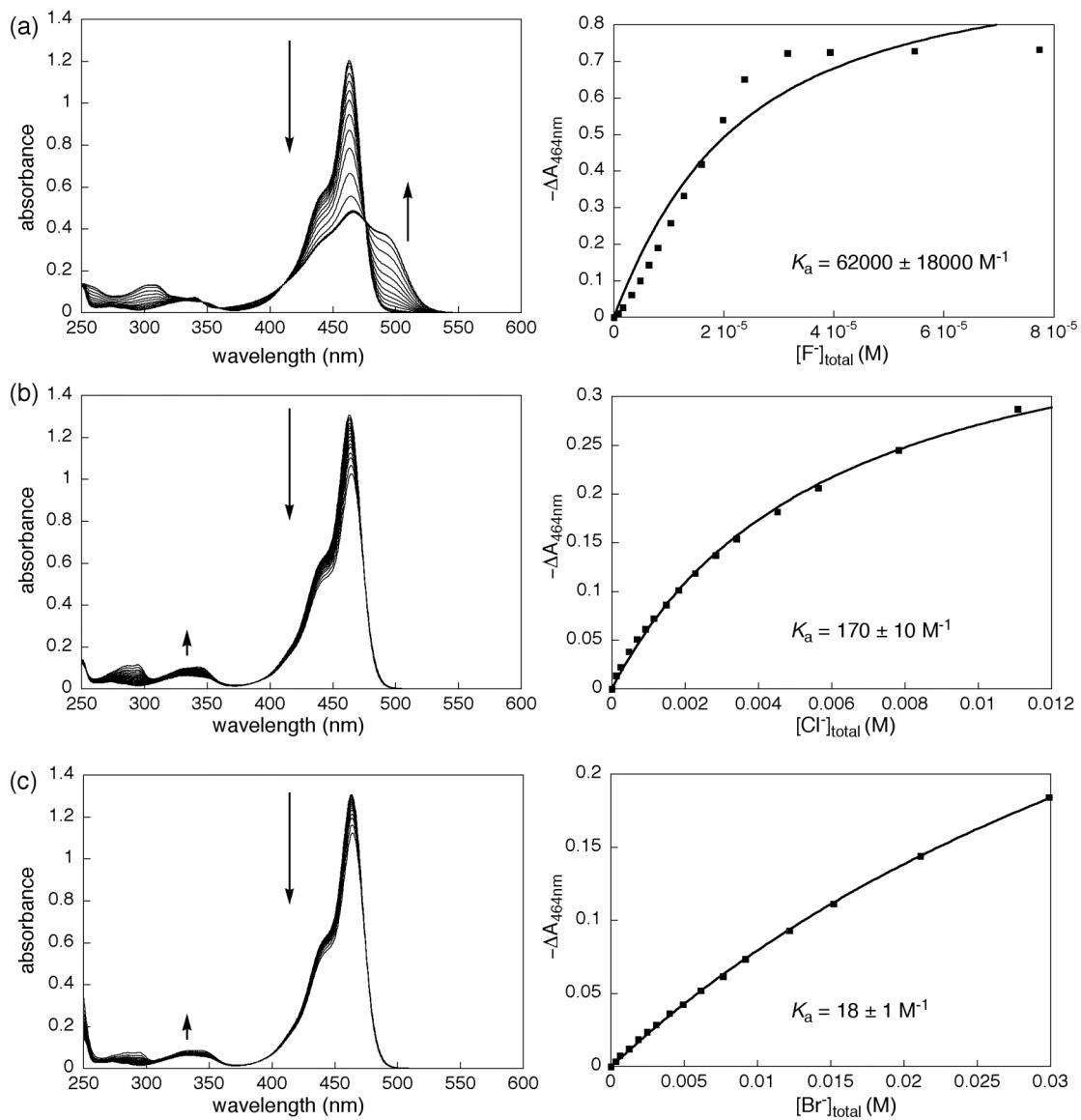
5. Anion binding behavior



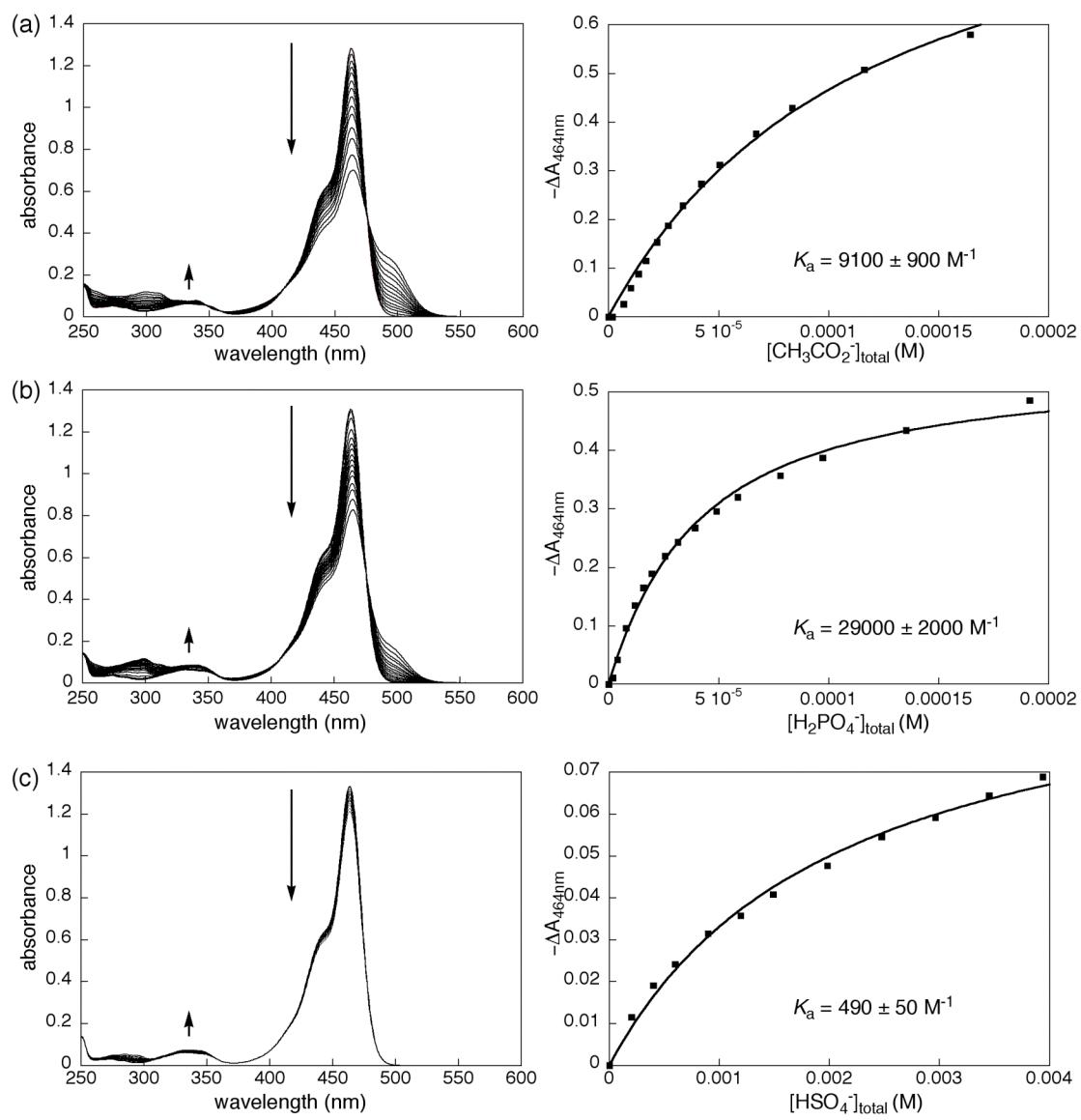
Supporting Figure 10 UV-vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **2** (9.2 × 10⁻⁶ M) upon the addition of (a) F⁻, (b) Cl⁻, and (c) Br⁻ as tetrabutylammonium salts in CH₂Cl₂.



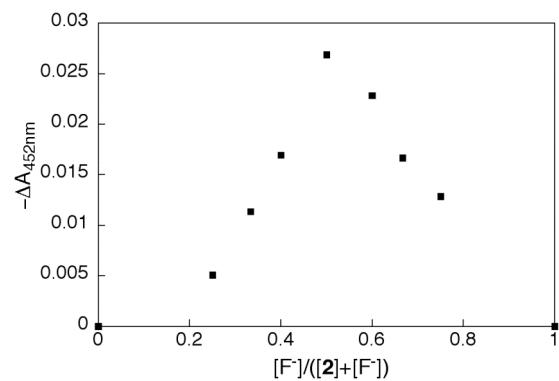
Supporting Figure 11 UV-vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **2** (9.2×10^{-6} M) upon the addition of (a) CH_3CO_2^- , (b) H_2PO_4^- , and (c) HSO_4^- as tetrabutylammonium salts in CH_2Cl_2 .



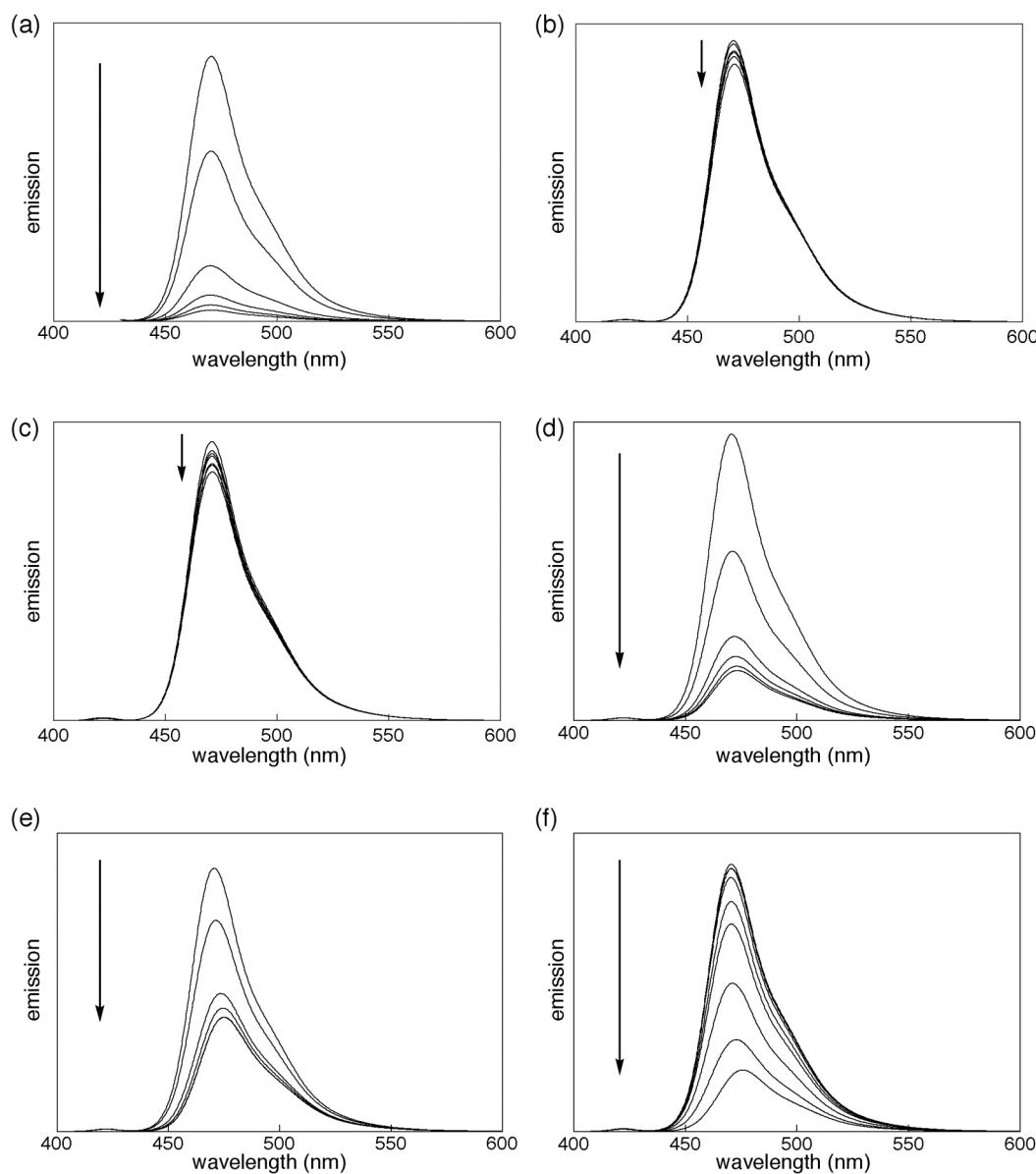
Supporting Figure 12 UV-vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **3** ($1.0 \times 10^{-5} \text{ M}$) upon the addition of (a) F^- , (b) Cl^- , and (c) Br^- as tetrabutylammonium salts in CH_2Cl_2 . Sigmoidal curve of F^- binding would be derived from the effect of water even using dried solvent.^[S2] TBAF is not a salt that can be obtained completely pure, anhydrous form and it often contain impurities such as $[\text{F}-\text{H}-\text{F}]^-$.^[S3]



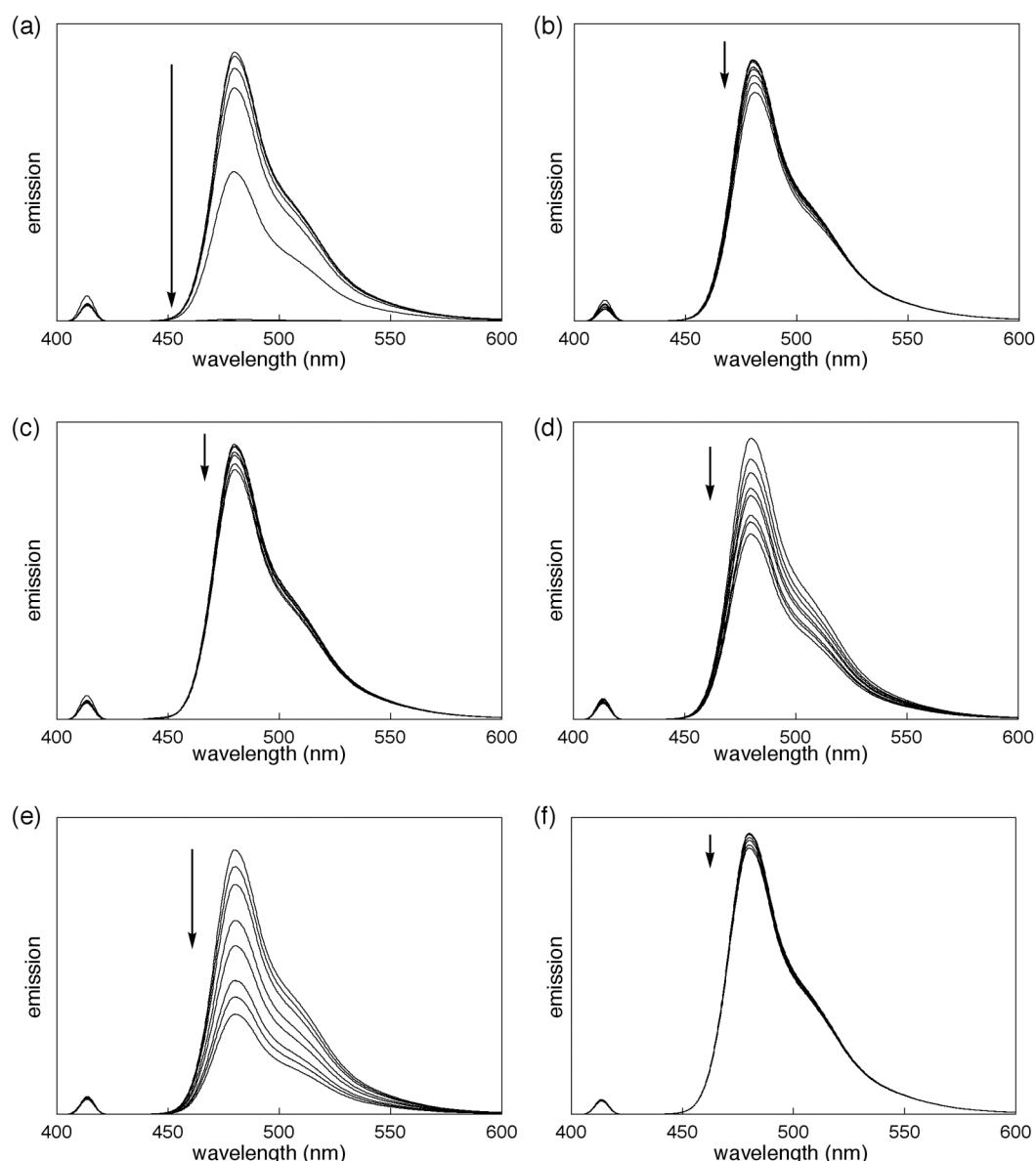
Supporting Figure 13 UV-vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **3** ($1.0 \times 10^{-5} \text{ M}$) upon the addition of (a) CH_3CO_2^- , (b) H_2PO_4^- , and (c) HSO_4^- as tetrabutylammonium salts in CH_2Cl_2 .



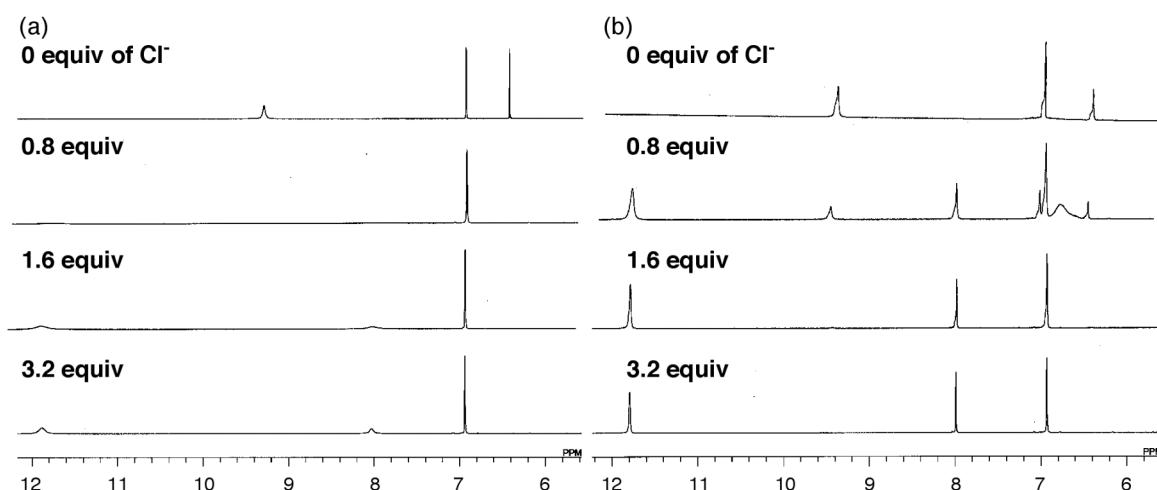
Supporting Figure 14 Job plots of **2** for F^- binding (total concentration: $9.5 \times 10^{-6} \text{ M}$) in CH_2Cl_2 .



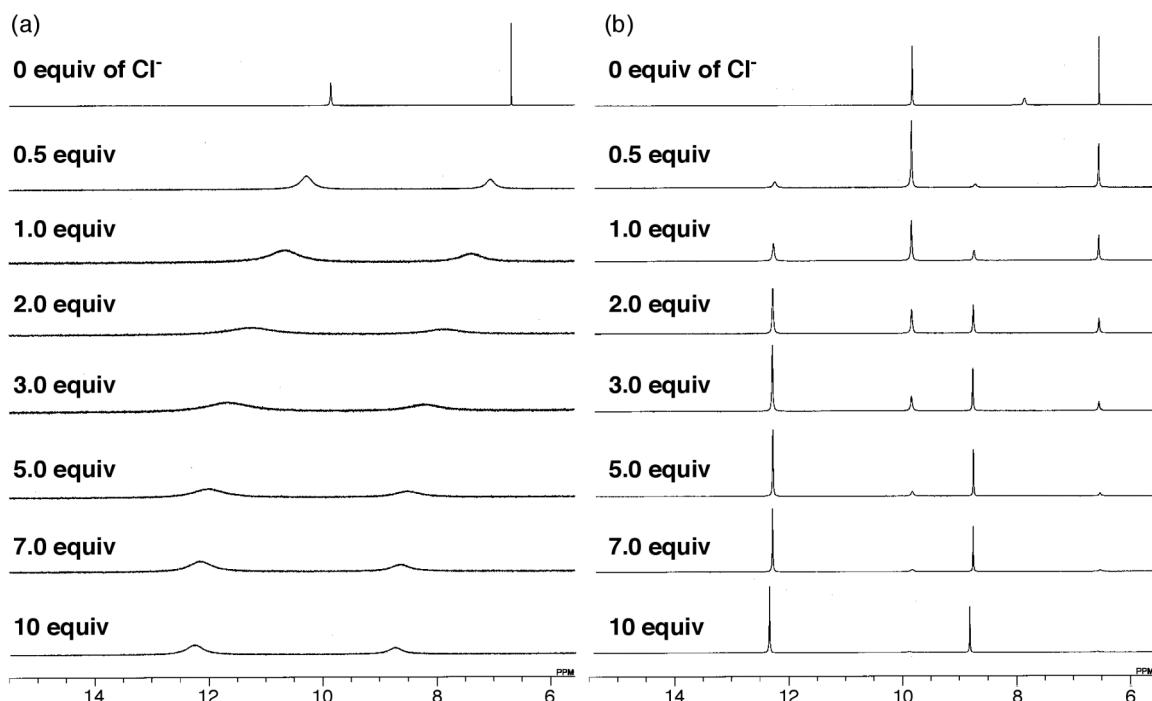
Supporting Figure 15 Fluorescence emission spectral changes of **2** ($2.4\text{--}2.9 \times 10^{-6}$ M) excited at 423 nm for F^- or 420 nm for the other anions as isosbestic points upon the addition of (a) F^- (0–20 equiv), (b) Cl^- (0–160 equiv), (c) Br^- (0–470 equiv), (d) CH_3CO_2^- (0–26 equiv), (e) H_2PO_4^- (0–32 equiv), and (f) HSO_4^- (0–1000 equiv).



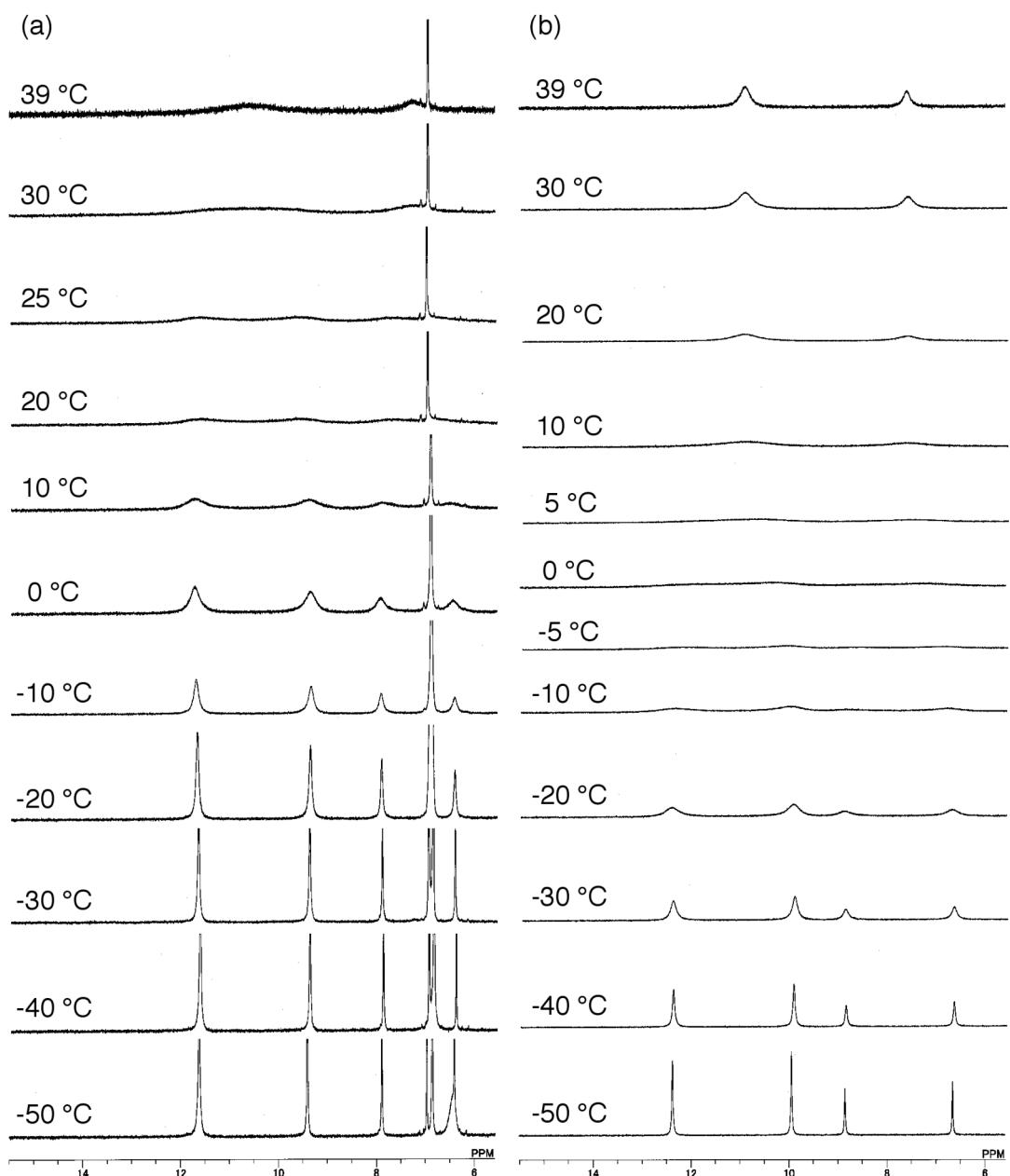
Supporting Figure 16 Fluorescence emission spectral changes of **3** ($1.2\text{--}1.4 \times 10^{-6}$ M) excited at 411 nm as an isosbestic point upon the addition of (a) F^- (0–13 equiv), (b) Cl^- (0–2300 equiv), (c) Br^- (0–2500 equiv), (d) CH_3CO_2^- (0–20 equiv), (e) H_2PO_4^- (0–30 equiv), and (f) HSO_4^- (0–1300 equiv).



Supporting Figure 17 ^1H NMR spectral changes of **2** (5.4×10^{-3} M) in CD_2Cl_2 at (a) r.t. and (b) -50 °C upon the addition of Cl^- (0–3.2 equiv) added as a tetrabutylammonium salt.



Supporting Figure 18 ^1H NMR spectral changes of **3** (5.3×10^{-3} M) in CD_2Cl_2 at (a) r.t. and (b) -50 °C upon the addition of Cl^- (0–10 equiv) added as a tetrabutylammonium salt.



Supporting Figure 19 Various-temperature ^1H NMR spectral changes from 40 to $-50\text{ }^\circ\text{C}$ in CD_2Cl_2 : (a) **2** ($5.8 \times 10^{-3}\text{ M}$) and with 0.55 equiv. of Cl^- and (b) **3** ($5.6 \times 10^{-3}\text{ M}$) with 1.40 equiv. of Cl^- . Cl^- was added as a tetrabutylammonium salt.

[S3] Footnote 18 in Takeuchi, M.; Shioya, T.; Swager, T. M. *Angew. Chem., Int. Ed.* **2001**, *40*, 3372.

[S2] Sharma, R. K.; Fry, J. L. *J. Org. Chem.* **1983**, *48*, 2112.