

Electronic Supplementary Information

Modification at boron unit: tuning electronic and optical properties of π -conjugated acyclic anion receptors

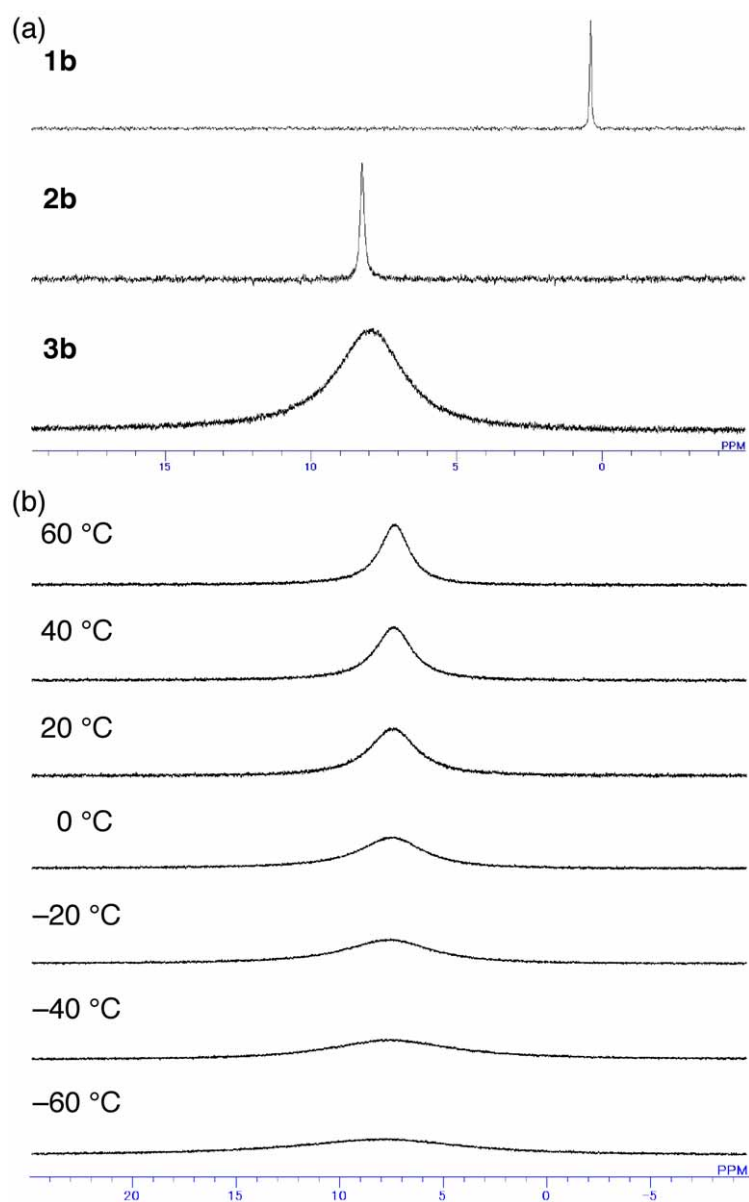
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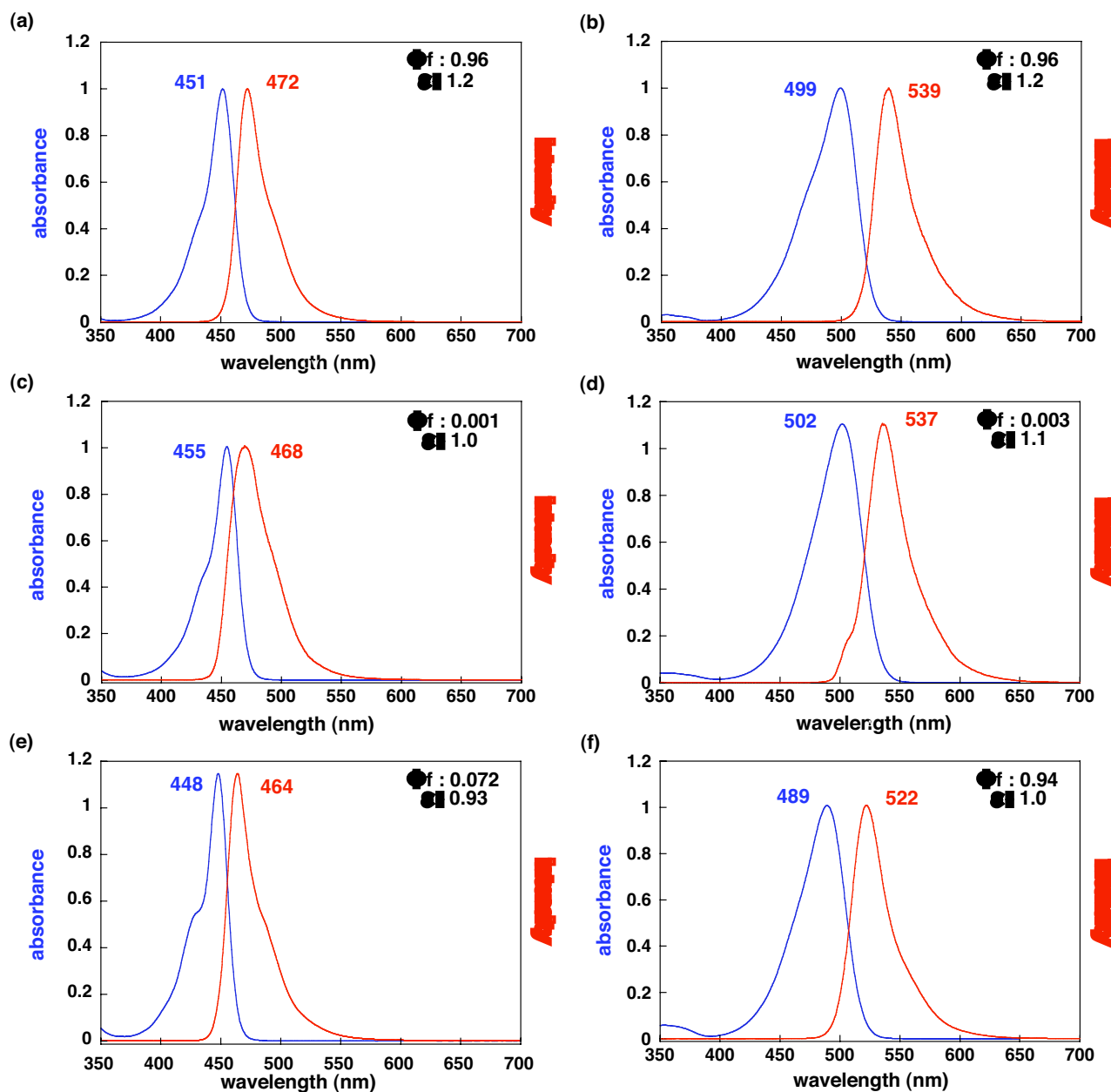
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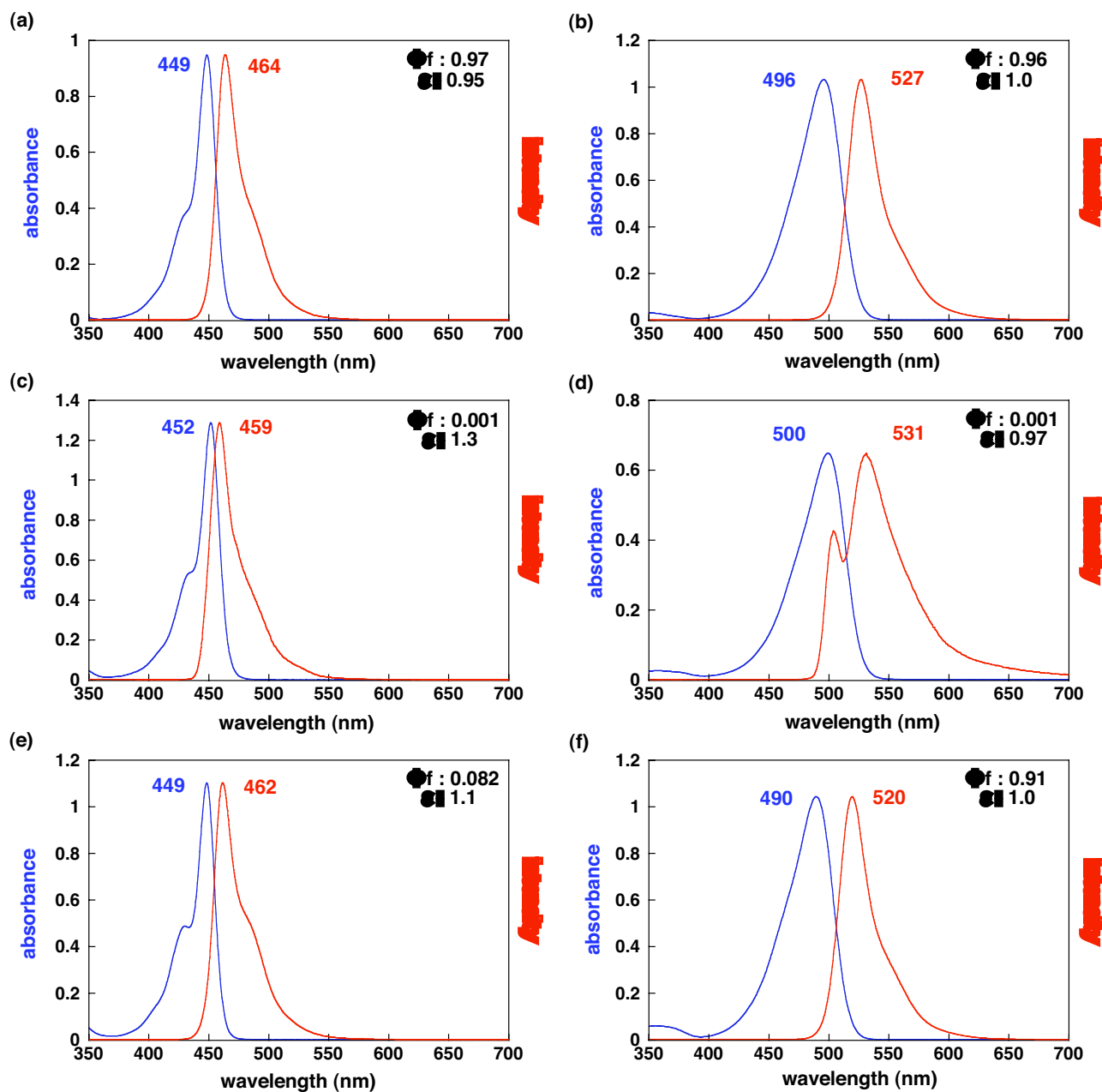
1. Spectroscopic data of acyclic anion receptors



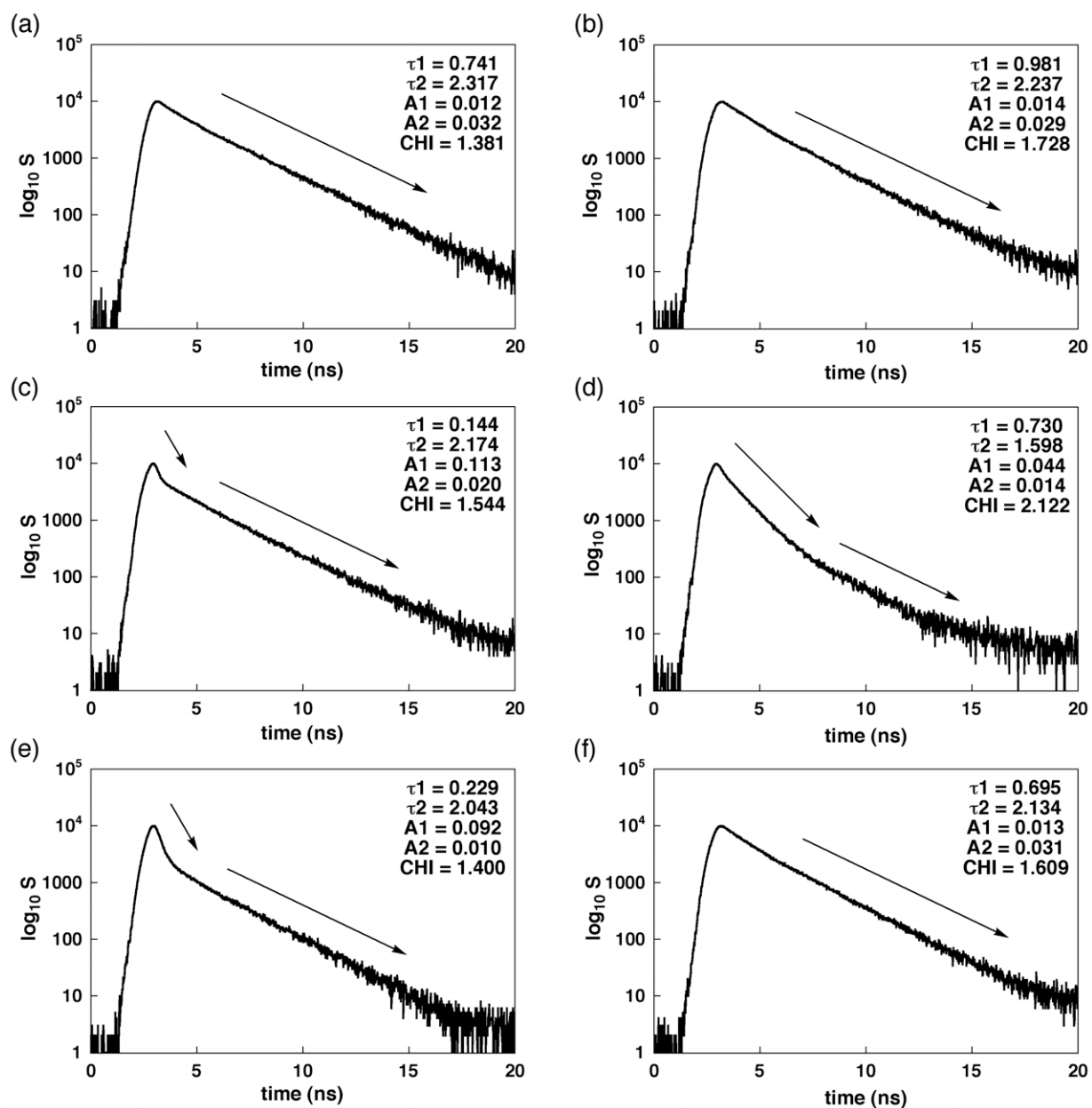
Supporting Figure 1 (a) ^{11}B NMR of **1b**,^[S1] **2b**,^[S2] and **3b** at 20 °C in CDCl_3 ; (b) VT ^{11}B NMR of **3b**.



Supporting Figure 2 UV/vis absorption (blue) and fluorescence emission (red) spectra of β -ethyl-substituted (a) **1b**, (b) **1d**, (c) **2b**, (d) **2d**, (e) **3b**, and (f) **3d** in CH_2Cl_2 ($1.0 \times 10^{-5} \text{ M}$). Absorption coefficients (ϵ , $10^5 \text{ M}^{-1} \text{ cm}^{-1}$) and fluorescence quantum yields (Φ_F) are 1.2 and 0.96 for **1b**, 1.2 and 0.96 for **1d**, 1.0 and 0.001 for **2b**, 1.1 and 0.003 for **2d**, 0.93 and 0.072 for **3b**, and 1.0 and 0.94 for **3d**. The Φ_F value of **2b** was reexamined.



Supporting Figure 3 UV/vis absorption (blue) and fluorescence emission (red) spectra of β -ethyl-substituted (a) **1b**, (b) **1d**, (c) **2b**, (d) **2d**, (e) **3b**, and (f) **3d** in toluene (1.0×10^{-5} M). Absorption coefficients (ϵ , $10^5 \text{ M}^{-1}\text{cm}^{-1}$) and fluorescence quantum yields (Φ_F) are 0.95 and 0.97 for **1b**, 1.0 and 0.96 for **1d**, 1.3 and 0.001 for **2b**, 0.97 and 0.001 for **2d**, 1.1 and 0.082 for **3b**, and 1.0 and 0.91 for **3d**.

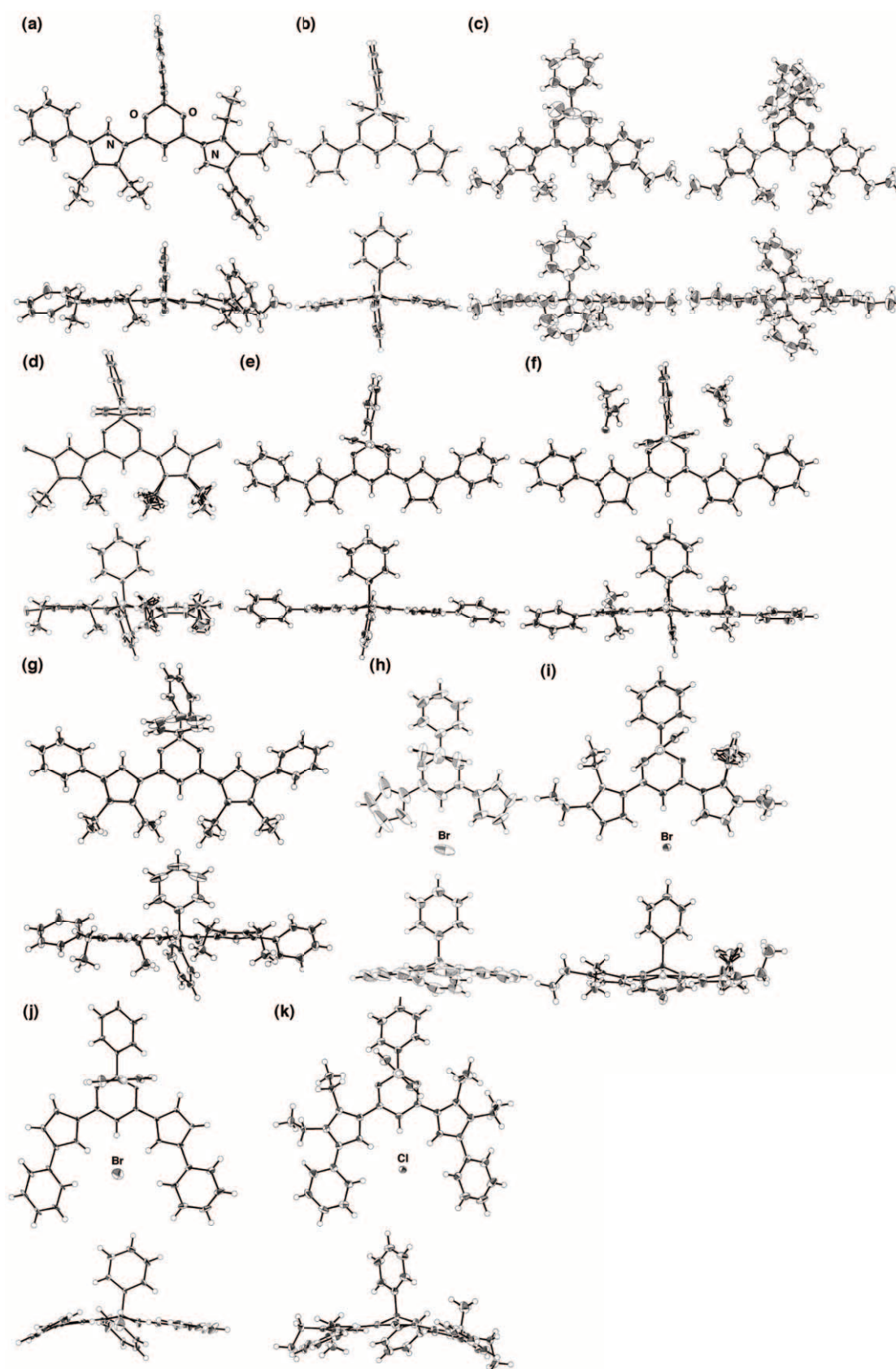


Supporting Figure 4 Fluorescence decay profiles at each λ_{em} for estimation of lifetime of β -ethyl-substituted derivatives (a) **1b**, (b) **1d**, (c) **2b**, (d) **2d**, (e) **3b**, and (f) **3d**, in CH_2Cl_2 (1.0×10^{-5} M). Excitation wavelength (λ_{ex}) is 399.5 nm.

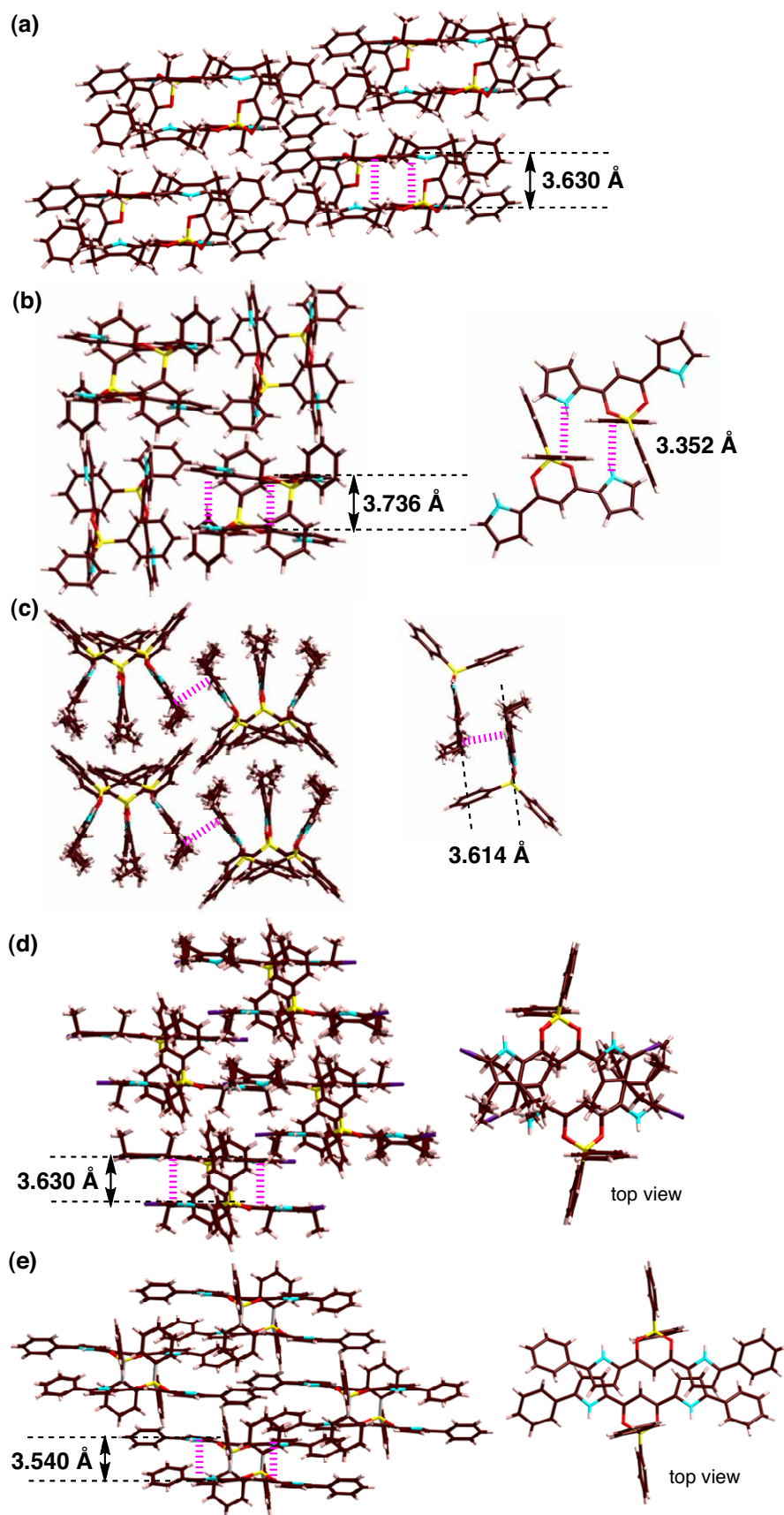
[S1] Maeda, H.; Kusunose, Y.; Mihashi, Y.; Mizoguchi, T. *J. Org. Chem.* **2007**, *72*, 2612–2616.

[S2] Maeda, H.; Fujii, Y.; Mihashi, Y. *Chem. Commun.* **2008**, 4285–4287.

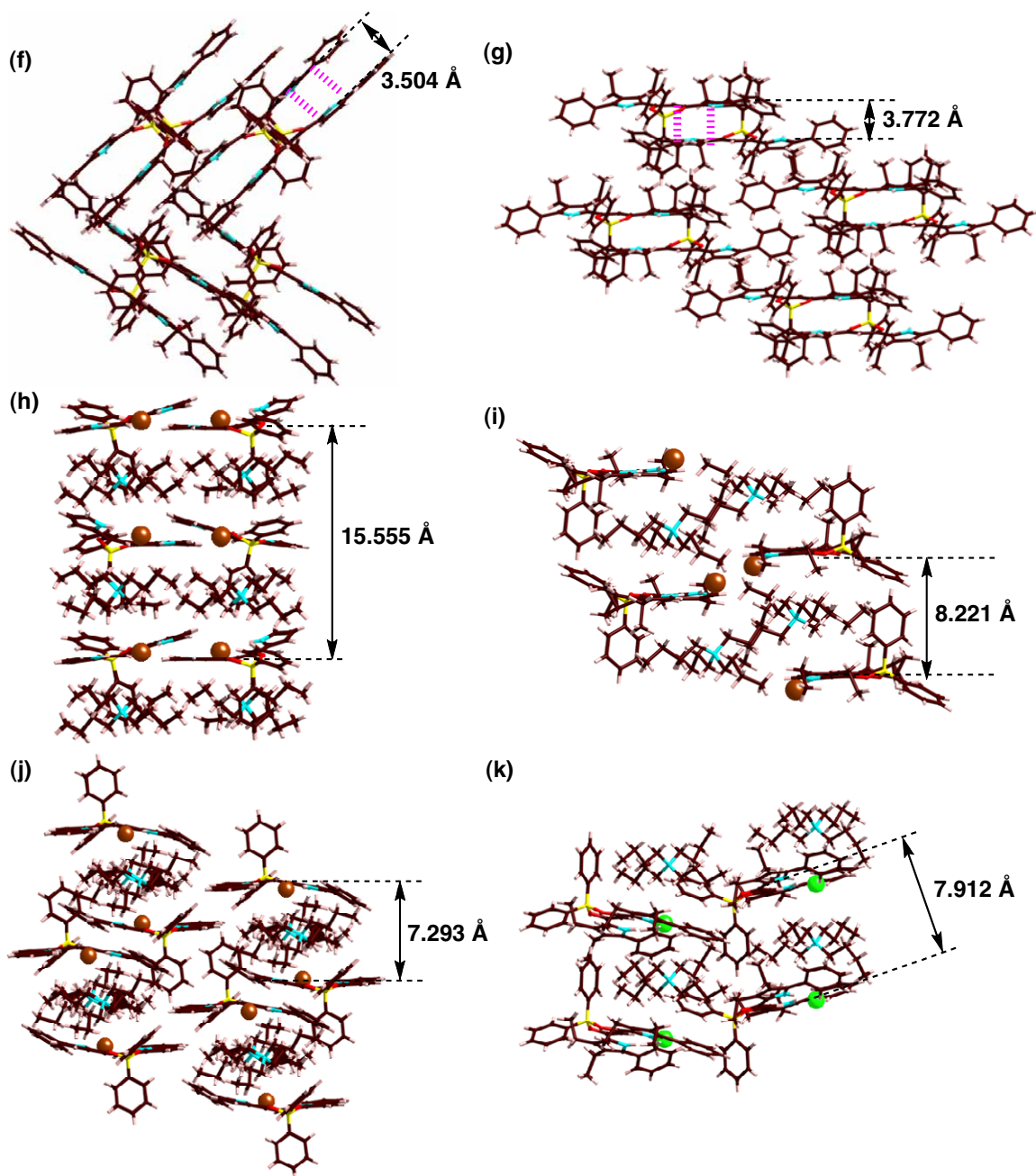
2. X-ray crystallographic data for acyclic anion receptors and their anion complexes



Supporting Figure 5 ORTEP drawings (top and side view) of single-crystal X-ray structures of (a) **2d**, (b) **3a**, (c) **3b** (two independent conformations), (d) **3b-I₂**, (e) **3c**, (f) **3c-acetone₂**, (g) **3d**, (h) **3a-TBABr**, (i) **3b-TBABr**, (j) **3c-TBABr**, and (k) **3d-TBACl**. TBA cations are omitted for clarity in (h)–(k). Thermal ellipsoids are scaled to the 50% probability level.

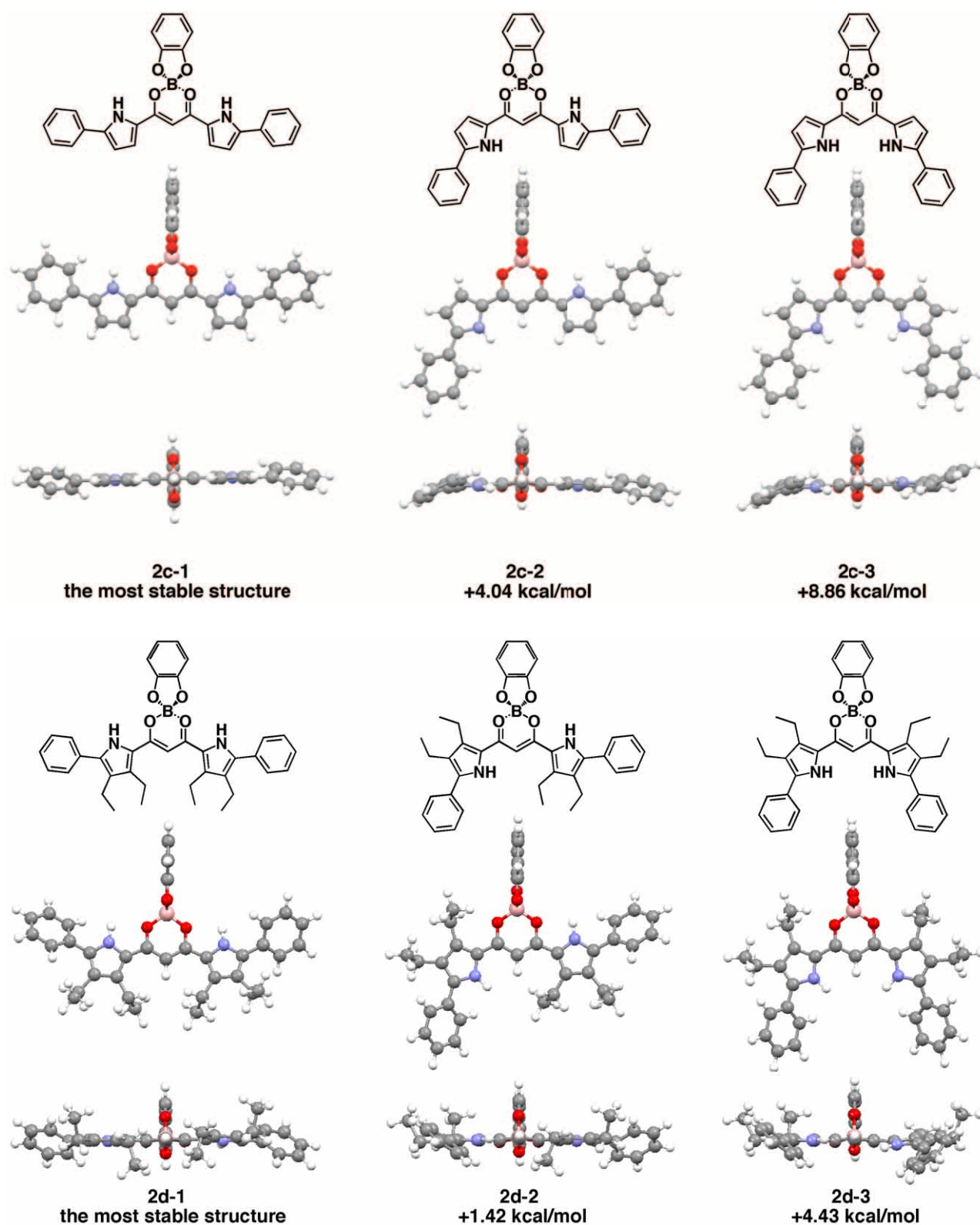


Supporting Figure 6 Assembled structures of (a) **2d**, (b) **3a**, (c) **3b**, (d) **3b-I₂**, (e) **3c**, (f) **3c**·acetone₂, (g) **3d**, (h) **3a**·TBABr, (i) **3b**·TBABr, (j) **3c**·TBABr, and (k) **3d**·TBACl. Atom color code: brown, pink, yellow, green, blue, and red represent carbon, hydrogen, boron, fluorine, nitrogen, and oxygen, respectively. The distances between π -planes of receptors and receptor-anion complexes are indicated.

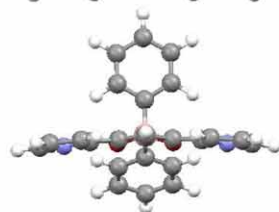
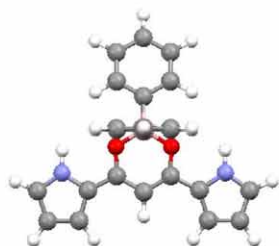
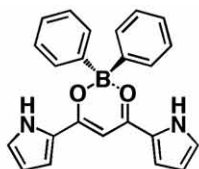


Supporting Figure 6 (continued).

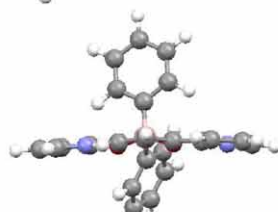
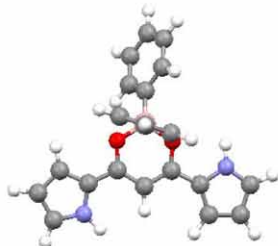
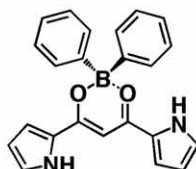
3. Optimization of acyclic anion receptors by DFT calculations^[S3]



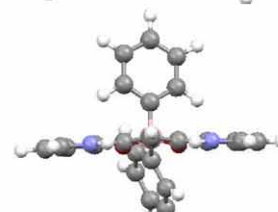
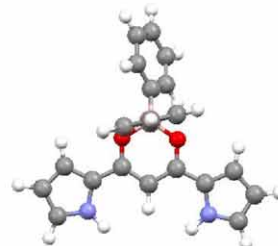
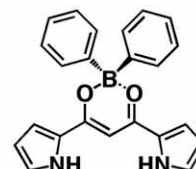
Supporting Figure 7 Optimized structures of newly synthesized **2c,d** and **3a-d** (three conformations in each compound) at B3LYP/6-31G(d,p) level.



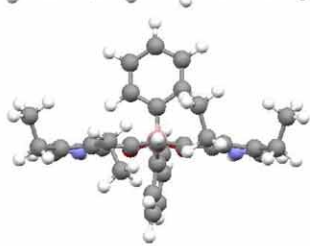
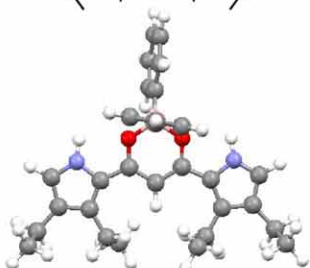
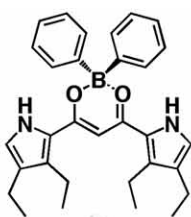
3a-1
the most stable structure



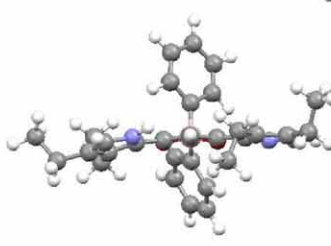
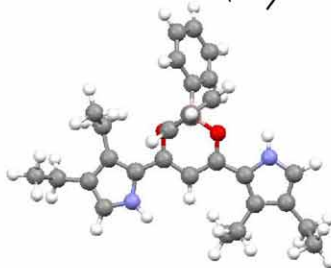
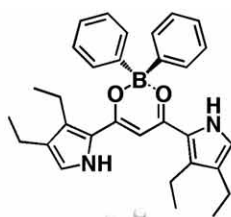
3a-2
+2.73 kcal/mol



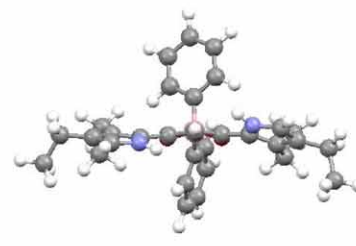
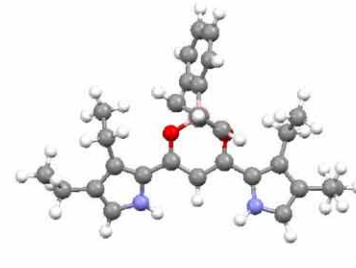
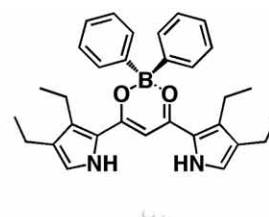
3a-3
+7.42 kcal/mol



3b-1
the most stable structure

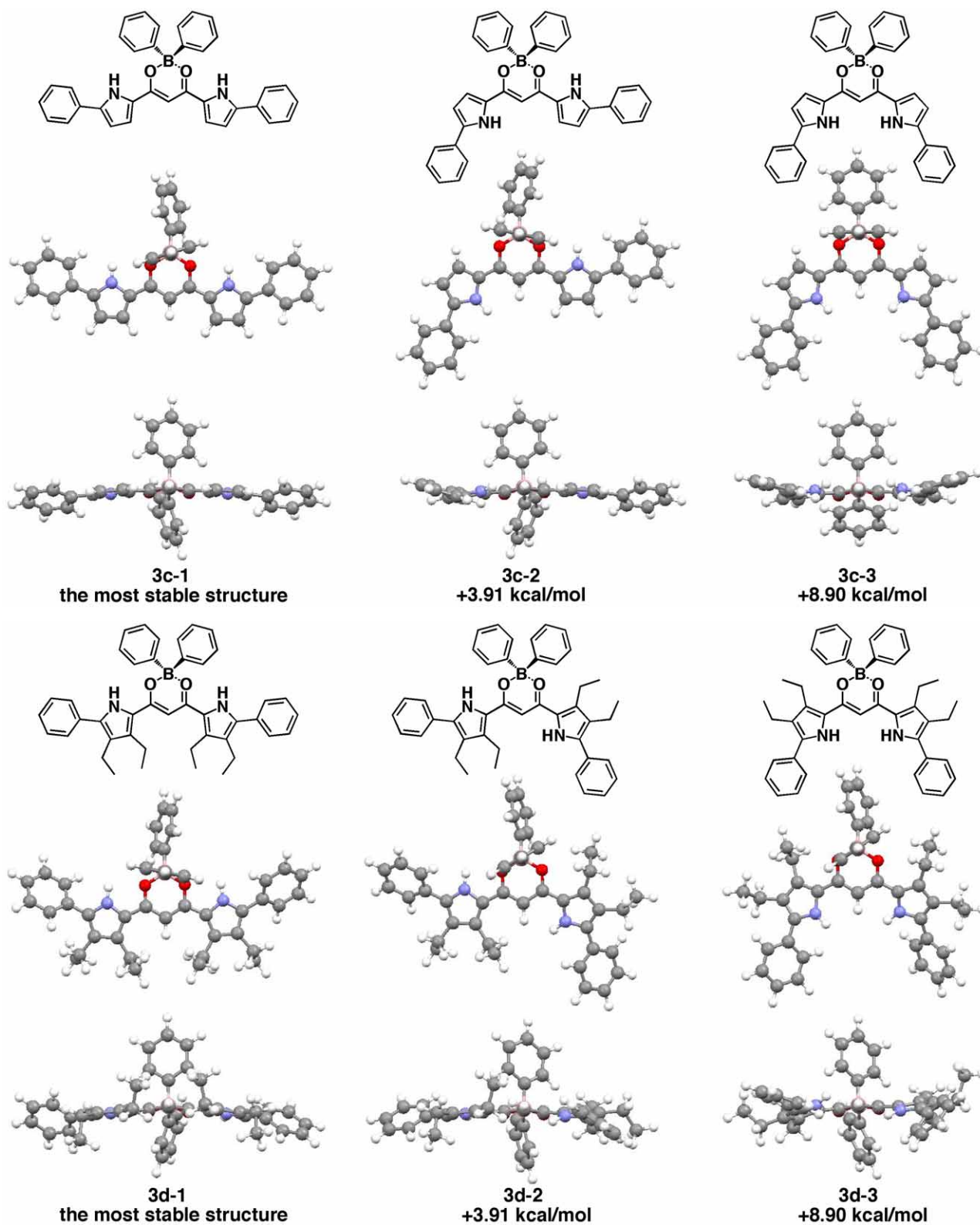


3b-2
+2.97 kcal/mol

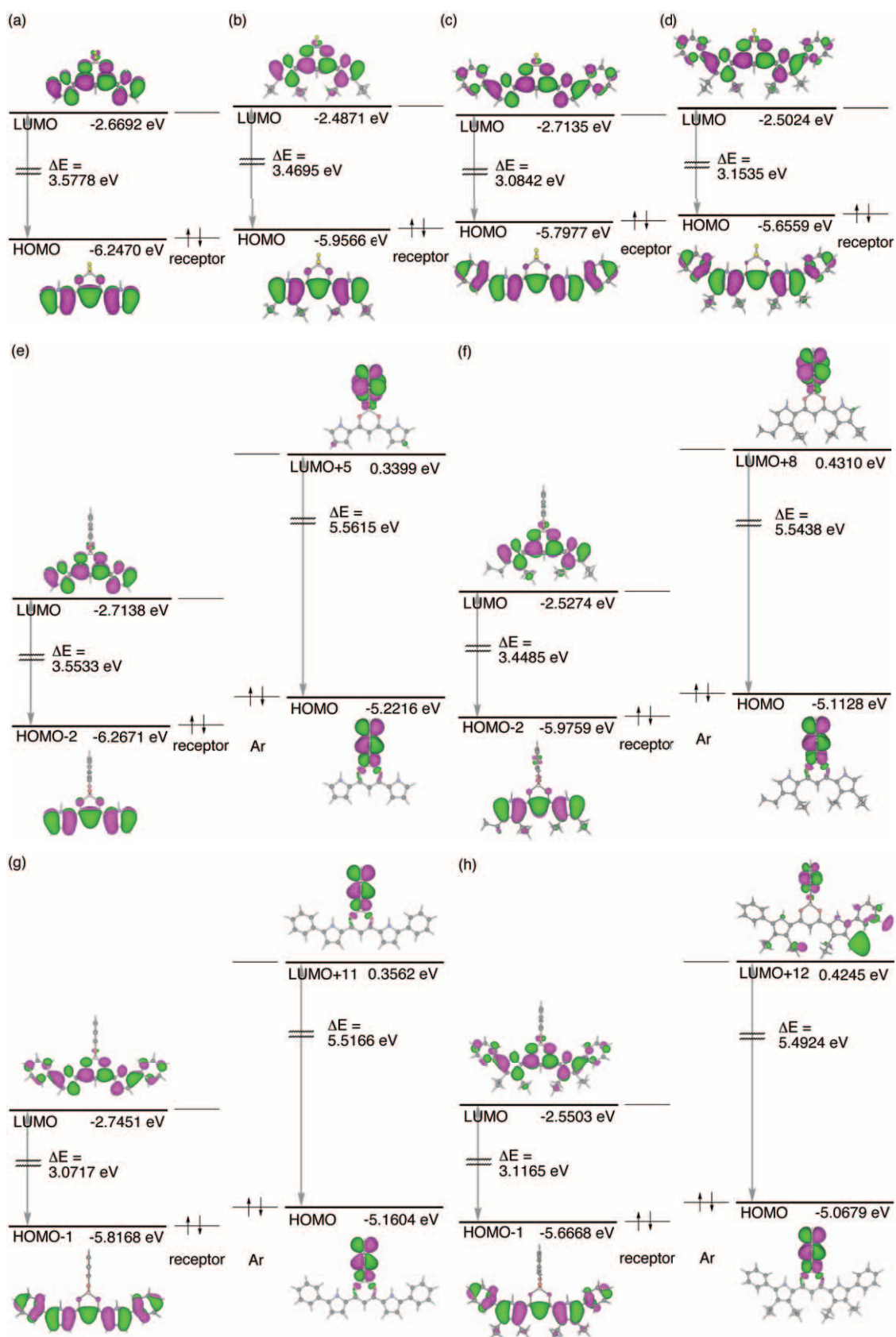


3b-3
+5.69 kcal/mol

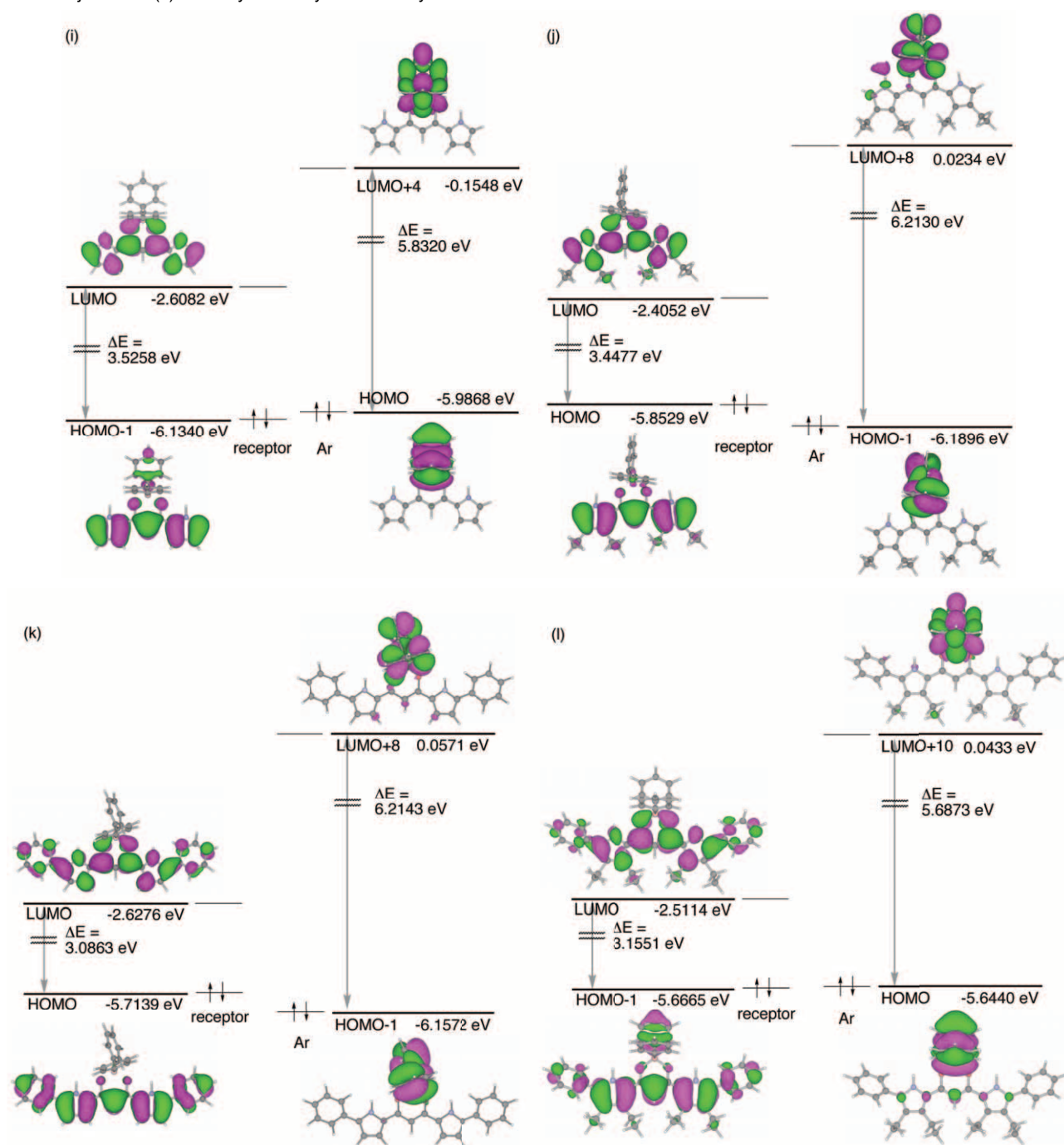
Supporting Figure 7 (continued).

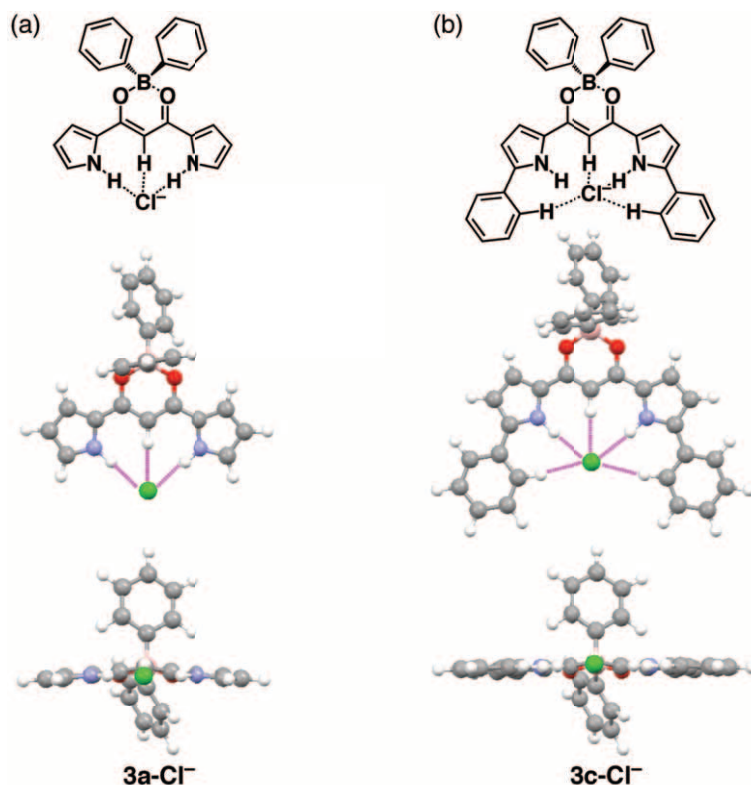


Supporting Figure 7 (continued).



Supporting Figure 8 Molecular orbitals (HOMO/LUMO) of (a) **1a**, (b) **1b**, (c) **1c**, (d) **1d**, (e) **2a**, (f) **2b**, (g) **2c**, (h) **2d**, (i) **3a**, (j) **3b**, (k) **3c**, and (l) **3d** at B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p) level. Fluorescence quantum yields (Φ_F) are controlled by the quenching process after excitation. One of the quenching processes is presumably intramolecular electron transfer between core π -units and aryl moieties around the boron, as suggested by the “overlap” of the steady state molecular orbital energy levels of the core π -units and the boron-aryl moieties as observed in less emissive **2a–d**. However, the energy levels of less emissive **3b** do not show such tendency whereas emissive **3d** exhibits the overlap. This suggests that the energy levels at the excited state are more essential to discuss the emission behavior.





Supporting Figure 9 Optimized structures of Cl^- complexes of (a) **3a** and (b) **3c** at B3LYP/6-31+G(d,p) level.

Cartesian Coordination of 2c-1.

-1553.2005937 hartree

C,-7.6604487295,0.6415510475,-0.4690939908
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 H,-9.7290862025,0.2712938862,0.0161881185
 H,-7.8424009529,1.6427426879,-0.8478263426
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Cartesian Coordination of 2c-2.

- 1553.1941489 hartree

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Cartesian Coordination of 2c-3.

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H,-2.1047179956,-1.8035478929,-0.265176869
H,-5.8089300857,0.1325265351,0.0781918937
H,-3.8608784237,2.0111276586,-0.1142980371
H,0.393132181,8.5276106601,-0.3687810801
H,0.4866349411,7.9822394401,2.0382577777
N,-2.7763310741,-1.076369043,-0.0779697062
N,2.650616115,-1.2948115764,-0.1122291551
O,0.1107837649,4.0242586358,-1.3165386542
O,0.2012380778,3.5058134856,0.9672243877
O,1.2685845239,2.0129803951,-0.6258957595
O,-1.1608754893,2.1307779396,-0.5012522598
B,0.1058140173,2.9382716815,-0.368786656
C,2.4807503537,0.0585674581,-0.3532162215
C,3.7470005285,0.5887420242,-0.6014815146
C,1.2116713645,0.7374689897,-0.3493739505
C,-0.0153452721,0.1077598232,-0.1023061431
C,-1.1943847425,0.8502328824,-0.2476664968
C,-2.5138750902,0.2816320693,-0.1589067187
C,4.6784641602,-0.4549994982,-0.4886131682
C,-4.1293399226,-1.293545695,-0.0137398467
C,-4.7468814051,-0.0396181949,-0.0185387115
C,-3.7429314738,0.9379913838,-0.1104680507
C,0.3552649946,7.489739968,-0.0507919139
C,0.4080692816,7.181921806,1.30817543
C,0.361532458,5.8478912748,1.7538542848
C,0.2615464905,4.8583954181,0.7917573692
C,0.2077289027,5.1688125328,-0.5773959255
C,0.2531672006,6.4774129875,-1.0232969568
C,-4.7035184517,-2.6369676033,0.0553997275
C,-3.9734398816,-3.7202993365,0.5772172402
C,-4.5305515128,-4.9960390252,0.6279132332
C,-5.8308459138,-5.2141647984,0.1697604199
C,-6.5696654407,-4.1444962889,-0.3412289863
C,-6.0123505403,-2.870566861,-0.403182003
C,4.4592027016,-2.9879329911,0.0522451648
C,5.767076705,-3.2084726237,0.5197012655
C,6.2348293942,-4.5013200709,0.7369515489
C,5.4060079344,-5.6007713004,0.5015367602
C,3.9797388984,-1.6244845244,-0.1735988615

Cartesian Coordination of 2d-1.

-1867.7373363 hartree
H,-1.4385557858,-3.5305619378,0.3273501212
H,-9.2433481791,-0.1403550553,1.0742042905

H,6.9466561873,-1.3811417409,-1.7119976467
H,9.0802251946,-0.1471420105,-1.851422792
H,9.394320067,1.9579606817,-0.5657904614
H,7.5547969054,2.8036008952,0.8793557804
H,5.4434606038,1.5369327809,1.0695071287
H,1.402723635,-3.3701519182,0.7711211948
H,2.9232198018,-4.2207415255,0.7356536404
H,6.3719509228,-3.0318750713,-0.3742561681
H,5.043394637,-4.1575297609,-0.249607045
H,4.889272744,-3.6748083844,2.2422318168
H,6.2402085939,-2.5484289644,2.0857510175
H,-5.3200898218,1.5854170338,-1.4157802184
H,-7.4281072995,2.8591698441,-1.4145594163
H,-9.4131844462,1.996710726,-0.1864669887
H,-7.1177210518,-1.3832450137,1.1320432059
H,0.032164613,6.7885637933,2.6264971819
H,0.0283231703,7.4238797286,0.2395733175
H,0.0124484373,5.6637006429,-1.5480080372
H,0.020357885,4.3728005736,3.3023587526
H,-1.3725771906,-4.7885845264,-1.8329067068
H,-1.2543112372,-3.0521749302,-2.1730228714
H,-2.7845550835,-3.8942114316,-2.4224864769
H,-6.4226125793,-4.7323043529,1.0842560752
H,-6.0790137073,-3.205042471,1.914556688
H,-4.7702088388,-4.3322995593,1.579238601
H,1.3980208361,-5.1202770403,-1.0200751762
H,2.8219968093,-4.3816912884,-1.772741945
H,1.283637155,-3.5189468167,-1.7731563183
H,6.4911835674,-4.2760290136,1.7793957972
N,3.5883955031,-0.0630140289,-0.2292199169
N,-3.6008668017,-0.0482402241,-0.1548683715
O,-1.2193205512,0.9755614996,-0.2041152488
O,1.2094109798,0.9704783252,-0.2139176096
O,0.0027581327,2.3498153328,1.3785718427
O,-0.001493472,2.9527273202,-0.8870494339
C,5.4450967421,-3.228602908,0.1711255669
H,-0.0094861919,-2.1270555039,-0.0845914612
H,3.467735923,0.9282388175,-0.380778155
H,-5.1118622234,-3.9969685044,-0.9006791213
H,-6.4169751466,-2.8787514996,-0.5846353585
H,-2.9565313943,-4.3365693156,0.0454795602
C,-1.9059148773,-3.8344786336,-1.7728126085
C,-5.6981216424,-3.9161913207,1.1745345806
C,1.9266354196,-4.1744306283,-1.1786523789
C,5.7861049401,-3.4469921221,1.6572061526
C,-6.0575121632,0.0022539423,-0.1404822784
C,6.0451601368,-0.0224270074,-0.2984202517
C,-6.1686699434,1.2149407263,-0.8479641777
C,-7.3646065924,1.9278383189,-0.8597689493
C,-8.4796356533,1.4424849822,-0.1738409101
C,-8.3848206282,0.2404882025,0.5288713172
C,-7.1867845058,-0.4709068734,0.5511470637
C,7.0891411182,-0.484354014,-1.1184596129
C,8.2866871971,0.222035587,-1.2084119194
C,8.4613561797,1.4074689977,-0.491702315
C,7.428031578,1.8832368119,0.3171701701
H,-3.4749143909,0.9501818488,-0.0703675073
C,6.2322453827,1.1748808645,0.416257886
C,0.0254520977,6.0150482389,1.8639930291
C,0.0231727015,6.3736666901,0.5166707529

C,0.0141468261,5.3961934979,-0.4963574318
C,0.0076658727,4.0699208994,-0.1025241026
C,0.0102198724,3.7081895412,1.255552469
C,0.0189752104,4.663498158,2.2568696025
C,1.1993243539,-0.3452817984,-0.1415453272
C,2.5168306351,-0.925663839,-0.1222346523
C,3.0486214973,-2.2246233122,0.0061802224
C,4.4607148308,-2.1076235948,-0.0510048045
C,4.7659501793,-0.7430340548,-0.2060851806
C,2.3022710869,-3.5219527805,0.1652547532
C,-5.461857112,-3.2394093517,-0.1889157358
C,-2.3211937926,-3.5249162705,-0.3219395681
C,-2.5315108509,-0.918777912,-0.1794868625
C,-1.21213117,-0.341321393,-0.1621406706
C,-0.0079640007,-1.0520210106,-0.1087619872
C,-3.0651863844,-2.223311088,-0.1889176528
C,-4.4769332803,-2.0990631563,-0.1518316384
C,-4.7818148023,-0.7241767036,-0.126858458
B,-0.0020927003,1.8228672203,0.0190345529

Cartesian Coordination of 2d-2.

-1867.7350737 hartree
H,-1.535785035,-4.416968715,-0.558539827
H,6.4327422382,2.3365573627,-1.1436618929
H,3.9477316795,-3.3021843412,1.4383555497
H,5.1738919545,-5.4400019209,1.3575650662
H,7.3301059918,-5.600075954,0.1265829133
H,8.2220779021,-3.6012399588,-1.0530591317
H,6.9634776237,-1.4810618978,-1.0340253358
H,-2.0801062438,7.6323865114,0.1114259118
H,2.9998111392,2.9470431027,1.1965997324
H,3.4874007498,4.452525099,-0.7329207854
H,2.4667934097,3.0992227826,-1.2335859753
H,4.1943985247,3.1000436122,-1.6343889486
H,8.0378831141,1.7983621995,-0.6283454802
H,7.0171667671,0.7442399932,-1.6216530394
H,-1.8183581184,7.1144050712,-2.2894891072
H,-1.0850715861,4.8318942306,-3.028013406
H,-1.6168396237,5.8849008584,1.8504998507
H,0.2875457239,-4.5542212658,1.1339310315
H,-1.2512134706,-4.1794906032,1.925827158
H,-0.0628429045,-2.9009908719,1.6790287353
H,-4.7681983238,-5.6772265142,-1.6526474858
H,-3.3254783677,-4.7525532831,-2.0987090682
H,-4.9183218633,-4.0268926518,-2.2801245015
H,7.0400421229,0.0497159959,0.8305487879
H,6.4314326446,1.6289150705,1.2695499266
H,-5.4497871736,0.311319636,1.6585031022
H,-7.8355363175,0.8958400692,1.8392736156
H,-9.5340180585,-0.3433568742,0.5078077777
H,-8.803071384,-2.149623712,-1.0373749143
H,-6.4114137735,-2.6913957568,-1.2727757387
H,4.7247470912,3.0116984915,0.8545030934
N,3.2300817039,-1.0044192906,0.1921355046
N,-3.3858424697,-0.5582643269,0.1683909658
O,-0.7997014381,3.3195174984,1.1198827266
O,-0.5484736577,2.8273184451,-1.1596709899
O,-1.3906805445,1.1093943713,0.3437238067
O,0.9444229607,1.7814715324,0.440936545
C,-1.7623842399,6.6393601539,-0.1930374291

H,0.6273796571,-1.4855805666,-0.1423932385
H,2.6933497949,-1.8429614674,0.0424229606
H,-5.2328213908,-4.1209163033,0.2401064071
H,-3.6484754841,-4.8383412786,0.4066378644
H,-0.3581367688,-3.1679718865,-0.8478360114
C,-4.3165281905,-4.6797838781,-1.6397481295
C,-5.7479616043,-1.2358176509,0.1773721732
C,6.4036530199,0.8687783409,0.4793185387
C,-6.1772262889,-0.2144337975,1.0467733326
C,-7.5273611439,0.1063721084,1.160343847
C,-8.4808952787,-0.5911211385,0.4163893807
C,-8.0701237343,-1.6081626869,-0.4465255948
C,-6.7187917191,-1.9253787205,-0.5703321097
C,3.7621249134,2.6585748044,0.4686269124
C,3.460282538,3.3665461488,-0.8668855478
C,7.007581677,1.4708478704,-0.8022980448
C,4.8681052775,-3.3711798308,0.8649378939
C,5.5686667857,-4.5745346353,0.833554757
C,6.7812167399,-4.6635573788,0.1474014263
C,7.2836351387,-3.5393776434,-0.51002536
H,-3.5612070497,0.4351645939,0.2175406308
C,6.580435589,-2.3365363327,-0.4892749334
C,-1.6145936918,6.3470354273,-1.5483251204
C,-1.2040787807,5.0706539428,-1.9761806859
C,-0.9543409518,4.121129424,-1.0010080522
C,-1.1033202027,4.4158465452,0.364780105
C,-1.50625446,5.6681655368,0.7930281911
C,-0.4991603542,-3.7977943522,1.2289216979
C,1.3031984322,0.5376979358,0.238154325
C,2.7164115677,0.2796159117,0.260052653
C,5.3599583396,-2.2305881174,0.2013214017
C,4.5954306347,-0.9774377811,0.222579072
C,4.9907934564,0.3661737834,0.3314973298
C,3.8122199351,1.1580421919,0.3590994204
C,-4.2308780606,-4.1352991919,-0.2013458997
C,-1.1330317959,-3.4892561027,-0.1411438885
C,-2.1096912516,-1.0704195196,0.0791713197
C,-1.0145890718,-0.1374963401,0.1470069078
C,0.3389748853,-0.4639298117,0.0417613927
C,-2.2356951616,-2.4648776092,-0.0772723789
C,-3.6225375188,-2.7605144646,-0.0937150249
C,-4.3174034787,-1.5449535397,0.0601258173
B,-0.4501120194,2.2723308153,0.1864607197

Cartesian Coordination of 2d-3.

-1867.7302818 hartree
H,0.0236568899,6.4582287976,-2.2216892081
H,3.3336777532,2.5492588838,-1.9676309706
H,5.9062021737,-2.9485422165,1.4836690005
H,6.5869688132,-5.3155202868,1.3901255408
H,5.4396573151,-6.8910027999,-0.1544897828
H,3.621819217,-6.0551372669,-1.6335145823
H,2.9883035946,-3.6742389654,-1.5958507024
H,6.5518268295,0.4286118399,-0.3794984354
H,3.361938684,2.5709214274,0.5207489156
H,7.74426394,-0.0380193845,1.7549145946
H,6.3499654492,-0.9397211356,2.3731953538
H,6.219123618,0.7939520083,2.0960102307
H,4.5748218947,3.6590178614,-1.3692411924
H,5.0434909083,2.0732560217,-2.0081630621

H,6.6858223147,-1.2965068803,-0.1210994778
H,-6.591534583,-1.5439682835,-0.6259407062
H,-6.4607620371,0.0993578815,-1.2089633765
H,-5.1983005848,1.9322315776,-0.983917666
H,-3.5302405301,2.3241869031,-1.3825000244
H,-4.3925934895,3.7866816566,0.4449057739
H,-3.0278728819,2.8162916274,1.010396123
H,-4.6814032828,2.3702235292,1.4702146154
H,-8.0062409627,-0.0301421325,0.7435778058
H,-6.6091569227,0.980563029,1.1403284956
H,-6.7044723787,-0.664600355,1.7645590468
H,-2.712117439,-3.9383719578,-1.1523912255
H,-3.2859608064,-6.3198917516,-0.8625671102
H,-5.2676955336,-6.9729458681,0.4919237706
H,-6.6440788134,-5.2126920012,1.5827952951
H,-6.0311856644,-2.8346872972,1.3539153694
H,5.0697198525,2.1502525712,0.5353632695
N,-2.6246384048,-1.4401441811,-0.0915684077
N,2.6586672982,-1.3892998107,-0.1582026103
O,-0.0051349686,3.7973105248,-1.3842139949
O,-0.0989564882,3.3445421151,0.9157567689
O,1.2082272836,1.8887343062,-0.5305822692
O,-1.2221620924,1.8458551002,-0.6298448416
C,-0.1137350627,7.0348661116,1.1569386356
H,0.0182898971,-1.1210697156,0.2350946053
H,-1.872854522,-2.0801324613,0.1041196716
H,-0.0468166871,8.332631651,-0.5561672202
H,-0.1436578503,7.8572907157,1.8657614358
H,-0.1738808107,5.4913343428,2.6994858775
C,-4.1699601324,1.8948272384,-0.6076496509
C,-4.0609533853,2.7659138572,0.6594036697
C,-6.9215096673,-0.0379516038,0.8930118057
C,-3.5556221167,-4.2148419068,-0.5256627719
C,-3.8892493229,-5.5588308525,-0.3763926832
C,-5.0043305935,-5.9257226421,0.3791839915
C,-5.7793899301,-4.9364099456,0.9867024806
C,-5.4427169134,-3.5914010916,0.8476478688
C,4.1332787585,2.0118558187,-0.0151592588
C,6.65438059,-0.1294630006,1.702394791
C,4.2819151263,2.606024383,-1.4286543884
C,5.4197864327,-3.6179700755,0.7836925714
C,5.794180735,-4.9594981376,0.7388725102
C,5.1474402513,-5.8458185597,-0.123776682
C,4.1237277523,-5.3772923695,-0.9492666997
H,1.916623196,-2.0618659686,-0.2596291573
C,3.7538859923,-4.0349209823,-0.9141463831
C,-0.1310342396,5.7124597791,1.6379745259
C,-0.0911226436,4.6936088759,0.7025177492
C,-0.0357971767,4.9638296052,-0.6751331545
C,-0.0190115867,6.2610847211,-1.1555579055
C,6.196764102,-0.3915116508,0.2552667521
C,-6.2023226237,-0.5537899467,-0.3665939578
C,-1.2102412314,0.5721510405,-0.322585841
C,-2.4937513177,-0.0734189383,-0.2723156557
C,-0.059120524,7.3030930796,-0.210282195
C,-3.9437103488,-1.7962099562,-0.0601150105
C,-4.702134258,-0.6295437427,-0.2471930216
C,-3.7937417013,0.4541628801,-0.385231356
C,4.3929771446,-3.1304123139,-0.0441092305
C,-4.3248239192,-3.206439811,0.0863044894

C,3.7831149265,0.5475639184,-0.0207774963
C,1.2093064402,0.6079397744,-0.257648656
C,0.0045556802,-0.0884092591,-0.0852555695
C,2.5031191842,-0.0145612522,-0.1694139968
C,3.9761610945,-1.722821928,-0.0054426999
C,4.7044657968,-0.5266743463,0.0950942474
B,-0.031605313,2.7333070708,-0.4076460031

Cartesian Coordination of 3a-1.

-1172.7996873 hartree

C,1.2052399826,1.3037378236,2.1840368864
H,-2.1372945514,1.7883769843,4.0619791176
H,0.0140484024,2.0762663365,5.2789810759
H,2.1610716688,1.7585518295,4.061780144
H,2.1542180851,1.164564201,1.6711169616
H,5.7014850138,-1.726537994,-0.6746558828
H,4.8734954151,-4.2997288714,-0.3473770716
H,2.1832034399,-4.201101245,-0.1036000466
H,3.6152169203,-0.2832690958,-0.6204211312
H,-0.0197727979,-3.1100831958,0.0423098177
H,-2.2361329912,-4.1731649552,-0.1033050425
H,-4.9276177236,-4.2379323152,-0.3454229865
H,0.0335975365,5.2942417719,-3.3428255872
H,2.1760583362,4.2575414739,-2.6169453107
H,2.1604567781,2.2452512838,-1.1968730749
H,-2.1389164301,1.1944311104,1.6713000634
H,-5.723410427,-1.6544650672,-0.671581798
H,-3.6191922951,-0.2375180321,-0.6181701422
H,-2.1320841474,2.2688179538,-1.202325859
H,-2.1219817968,4.28125995,-2.622286823
N,-3.639707,-1.2406773625,-0.5116025268
N,3.6232482174,-1.2865661295,-0.5134657169
O,1.2354617497,-0.0600865121,-0.446111603
O,-1.2364592815,-0.0444201769,-0.4457053862
B,0.0049599458,0.802096596,-0.1153975921
C,2.8501593602,-3.3631278667,-0.2455709937
C,2.469793251,-2.0225730133,-0.3342653074
C,1.193756379,-1.3564687043,-0.2734378132
C,-0.0130150945,-2.0387148425,-0.0956259117
C,-1.2111101098,-1.3412325152,-0.2730082441
C,-2.4954877125,-1.9911602514,-0.333254868
C,-2.8926124803,-3.3268552089,-0.2446489733
C,4.7015926242,-2.1119559271,-0.5408398096
C,-4.7283542532,-2.0524490186,-0.5384984417
C,-4.2952101969,-3.3625162201,-0.3713605064
C,0.0130858447,2.0875405855,-1.0810575839
C,0.0073217881,1.1331942729,1.4692001135
C,-1.1794575151,2.6969136209,-1.5052771028
C,-1.1798729209,3.8371469808,-2.3102212131
C,0.0279136475,4.4067087031,-2.7158694512
C,1.2283367114,3.8238437076,-2.3072349888
C,1.2133433634,2.6837205104,-1.5022975342
C,-1.188045553,1.3203507989,2.1841456533
C,-1.1932814818,1.6548389052,3.539286716
C,0.0121913249,1.8158306163,4.2239832696
C,1.2152474448,1.6381296764,3.5391744544
C,4.2521228578,-3.4164404915,-0.373137491

Cartesian Coordination of 3a-2.

-1172.795341 hartree

C,-1.529808567,0.1256351111,2.2988307012
H,0.1331673163,-2.7371589081,1.5907109477
H,-1.4726971049,-1.4003992569,5.3429251304
H,-2.292911546,0.673346328,4.2408966599
H,-1.8936231425,1.0402421656,1.8367518681
H,-2.9062427127,5.1023964202,-0.9491957309
H,-0.5332373831,6.4061065449,-0.6609241478
H,1.3391071191,4.4920171112,-0.2904068668
H,-2.3946331696,2.6203393537,-0.7575037842
H,-3.6863656688,-3.7153222969,-3.45637671
H,-4.6485471032,-2.8103235606,-1.3479634871
H,-3.245219184,-1.4737019492,0.1809465119
H,-0.2534425236,-3.1032611736,3.9987197279
H,2.1537542125,2.1719344355,0.0202325659
H,4.2141382242,1.4486394042,-0.3213026461
H,6.3701489986,0.1864220724,-0.2956778113
H,5.7506511722,-2.463132336,-0.2506831506
H,3.0320104854,-2.5902746717,-0.2185685114
H,0.0830235131,-1.893135491,-2.495145595
H,-1.307764965,-3.252099947,-4.0178972548
N,4.2543283636,0.4440157604,-0.2661998623
N,-1.7116456508,3.3598099324,-0.6767924224
O,-0.8561798999,0.840337111,-0.4629045608
O,0.895810745,-0.8946231399,-0.3693540823
B,-0.588832542,-0.6325720954,-0.070633569
C,0.2797202658,4.3389454169,-0.4379647794
C,-0.3718516263,3.1048533771,-0.4678610069
C,0.0785113117,1.7416516868,-0.329964824
C,1.4162867791,1.3932610026,-0.1163640046
C,1.7861408715,0.0461486451,-0.2286474845
C,3.1572221847,-0.401958973,-0.2496561706
C,5.4016485102,-0.2912603279,-0.2754415724
C,-1.9193833224,4.697797206,-0.7800739588
C,5.0572803901,-1.6347996321,-0.2568514412
C,3.6498952502,-1.7054933367,-0.2428812937
C,-1.4722204088,-1.5612408333,-1.0419090819
C,-0.8435121768,-0.8155241127,1.5143497556
C,-0.9556228998,-2.0857964205,-2.238624994
C,-1.7384373882,-2.8551802165,-3.1017019232
C,-3.0732359952,-3.1161556202,-2.7881435984
C,-3.6119530437,-2.6066404832,-1.6052463899
C,-2.8164742911,-1.8459567964,-0.7466906035
C,-0.3969082466,-1.9808366215,2.1652489239
C,-0.614222698,-2.1929697432,3.526166626
C,-1.2987621403,-1.2381882989,4.2824704497
C,-1.7583906631,-0.0766907393,3.6628960982
C,-0.6947520254,5.3383554788,-0.6314985497

Cartesian Coordination of 3a-3.

-1172.7878571 hartree

C,-1.6499707306,1.0694240221,2.1913415637
H,-0.7026702816,-2.1553446621,1.7696083825
H,-1.9958533526,-0.1621908874,5.3467046834
H,-2.2788729365,1.9467873008,4.0563005848
H,-1.7836295982,1.9979146203,1.6406631552
H,2.1610960605,5.8303671595,-0.2038661146
H,4.5018729272,4.4446906647,-0.2731255775
H,3.9202187759,2.0160523926,-0.3301337144
H,0.1874502163,3.9553105729,-0.1909120784
H,-5.3084081221,-0.0271840369,-3.4326749923

H,-3.2523948282,1.2174376459,-4.0746935694
H,-1.2983997177,1.2435565616,-2.5656234624
H,-1.2074382453,-2.2146765465,4.1829226472
H,2.9980720557,0.03358754,0.0492898172
H,3.9708667771,-1.8850121743,-0.4619674246
H,4.6118908516,-4.2879495765,-0.6927724415
H,2.3059568214,-5.7234907779,-0.856964899
H,0.285530111,-3.9077183694,-0.6719372249
H,-3.4318946022,-1.1901934749,0.2519795476
H,-5.382904622,-1.2364399681,-1.2596038562
N,3.2900988452,-2.6246825499,-0.5113897319
N,3.2228820975,2.7384847661,-0.2597792925
O,-0.0701448785,1.2493168819,-0.3836487553
O,-0.0411028723,-1.2144216238,-0.4933387514
B,-0.9118988534,-0.0080037546,-0.0819653942
C,1.8526961729,2.532105711,-0.242776307
C,1.253708067,3.7896429663,-0.2192748481
C,1.2217432989,1.2334373036,-0.2351781018
C,1.9301724803,0.0280378629,-0.1256838497
C,1.2507317046,-1.1788211047,-0.3558663672
C,1.9152444484,-2.4528167637,-0.5018907531
C,3.587585598,-3.9471011111,-0.657945445
C,2.2791465158,4.7567841731,-0.2236007131
C,2.397184801,-4.6533445634,-0.741391142
C,1.3477931213,-3.7171820361,-0.6458751707
C,-2.2021765197,0.018028718,-1.0409052331
C,-1.1962636156,-0.07325224,1.5066123889
C,-3.3791586614,-0.6700568493,-0.7013151911
C,-4.4864973347,-0.6946573688,-1.5511689615
C,-4.4465242826,-0.016208058,-2.7704127004
C,-3.2920106603,0.6815822376,-3.1292812237
C,-2.1890078004,0.6923894572,-2.273762118
C,-1.0486502019,-1.2491636191,2.2606932534
C,-1.3325798452,-1.2875478244,3.6287000643
C,-1.7743912117,-0.1378613358,4.2829422649
C,-1.9325242102,1.045199946,3.5569096032
C,3.4867690968,4.0761700117,-0.2540848908

Cartesian Coordination of 3b-1.

-1487.3439558 hartree
H,1.9358434481,-4.6886087536,-0.7029419497
H,-0.9869892231,3.4716129338,4.217143885
H,1.1923953864,2.9106733935,5.2794259532
H,2.9987852785,1.8917938189,3.9052986441
H,2.6279956193,1.4382117394,1.5099356529
H,0.5776358249,-3.6003776466,-0.8184658606
H,-3.6116543264,-3.5356664626,0.6252174376
H,-1.9704531771,-2.9639640576,0.7473803163
H,-5.7838761599,-2.9786353053,-0.2571522295
H,-6.8288062352,-1.5811303955,-0.1484565949
H,0.6238224828,-4.713929653,1.4152507231
H,0.8921235252,-2.9746953265,1.6339081059
H,0.8002614633,6.2702274972,-3.5257461435
H,1.5570862542,6.4713887648,-1.1648261816
H,1.3474397717,4.5508496813,0.3728380264
H,-1.3496266307,3.0210123735,1.8207102443
H,2.2530252983,-4.0910787634,1.7222231793
H,5.7433017034,-5.5593879481,-0.0026186467
H,4.3702219694,-4.8516169984,0.8610811262
H,5.837987121,-3.9009623642,0.6168471762

H,-2.2173940603,-4.5230586433,-1.1927712031
H,-1.8284831956,-2.903091441,-1.8027894053
H,-3.4868881904,-3.498527315,-1.8836182703
H,-7.1172871896,-3.0485323968,1.8515048039
H,-6.4610674225,-1.4768264375,2.3441195214
H,-5.3992436827,-2.8829092952,2.2507044052
H,-0.3653930831,2.2045531285,-2.7864367204
H,-0.1636860978,4.1205542383,-4.3270071135
N,-3.5682533546,0.7395128226,-0.0922772407
N,3.4134686964,-0.626765227,-1.0777589134
O,1.3408546901,0.8752224788,-0.6246394336
O,-1.0460412477,1.3410902637,-0.3070810367
C,4.3781799946,-1.549008949,-1.299377018
H,5.4492705155,-3.9567099153,-1.8809874425
H,3.9813852431,-4.8751214351,-1.6375293533
C,1.8286305449,1.8880697073,2.0937541692
H,5.3714199351,-1.2624579668,-1.6150186303
H,3.4707248313,0.374280784,-1.1952472376
H,-0.3854526995,-1.9104497914,-0.0388442273
H,-5.6873559078,0.9074509609,-0.001230125
C,3.8506277792,-2.8152202652,-1.0618305178
C,2.4896745043,-2.6368721905,-0.6865153815
C,2.2366329475,-1.250775315,-0.7082760737
C,1.0921285878,-0.4045093497,-0.4678699405
C,-0.1953245034,-0.858853877,-0.1542957668
C,-1.2577566478,0.0545681207,-0.1584628781
C,-2.6542206387,-0.2968610183,-0.0582210231
C,-3.3875045836,-1.4918029545,0.0804677725
C,-4.7623765053,-1.1323825032,0.1228040671
C,-4.8268064271,0.2535462536,0.0106565755
C,0.4790972418,3.2205222232,-1.0805655684
H,-3.2793998997,1.7003812703,-0.2016240476
C,0.6090749971,2.1905906109,1.4652213621
C,4.6175444829,-4.1060370501,-1.1821456105
C,1.540238463,-3.7440868591,-0.3142022988
C,-2.8695313008,-2.9051121514,0.1245463666
C,-5.9447035844,-2.0486404303,0.3011506148
C,1.3116142177,-3.8885711802,1.2031170934
C,5.1744513192,-4.6362501332,0.1509593336
C,-2.5806985151,-3.4928842247,-1.2701242561
C,-6.2491441727,-2.3856952986,1.7723094421
C,0.0606031142,3.1368445609,-2.4214470884
C,0.1712026383,4.2170451113,-3.2969305755
C,0.7122299065,5.4245903853,-2.848498573
C,1.1362230705,5.5355674809,-1.5243067536
C,1.0174698752,4.4458417204,-0.6572096293
C,-0.3907535867,2.7688403437,2.2684623139
C,-0.1910703822,3.0262765585,3.6252044564
C,1.0312056376,2.7120203802,4.2231952202
C,2.0430702839,2.1414099855,3.4507758977
B,0.3594528056,1.9383988928,-0.1120670739

Cartesian Coordination of 3b-2.

-1487.3392249 hartree
H,-2.8533492542,2.8336820444,0.743255482
H,3.7196152361,-0.3075360021,0.8182206107
H,6.7660934102,4.3937034411,-0.0512828757
H,5.9928255768,2.9346240153,0.5865146918
H,5.428370275,4.5260273801,1.10415065
H,-4.5481100014,3.1168080826,0.4539660728

H,-3.1785776349,4.4342510669,-1.1580178212
H,-4.1521636418,3.2360062394,-2.0252438652
H,-2.4310172229,2.9481326734,-1.7759171992
H,4.6835222831,5.0234217789,-1.2584977103
H,5.227060404,3.4408903712,-1.7698635878
H,5.1378369078,-0.6889537264,-0.1673247984
H,5.116064956,0.7836497081,0.8173566947
H,-8.0250921361,1.9328713133,1.2695021922
H,-6.3599242756,2.0483741129,1.8633458913
H,-7.1516553843,0.4743090214,1.772783155
H,2.527940116,-3.3655004489,0.1314620203
H,3.3313880238,-4.9859266496,-1.5478794864
H,2.1467207778,-5.2218143048,-3.7231663507
H,0.1595854151,-3.803024152,-4.198078944
H,-0.6232022572,-2.1665554588,-2.5229781757
H,1.6485799369,-0.2490120904,2.2652433251
H,1.706385944,-0.9471042176,4.6256010269
H,0.6204147988,-3.0709943331,5.3306381008
H,-0.5156624638,-4.4900954035,3.6305475705
H,-0.5557172889,-3.7960648423,1.2646816206
H,4.6936986045,1.2467812393,-1.6482881548
H,3.2911519648,0.1852713718,-1.5849272151
N,1.2918861677,3.3490107337,0.0082257049
N,-3.6493811144,-1.0422813006,-0.364388836
O,-1.0470620201,-1.1662888826,-0.2812916128
O,1.2501327082,-0.2523972954,-0.2250120279
C,-4.9804463246,-0.7970368843,-0.3849065394
H,-7.2554109194,0.6626440816,-0.7388666359
H,-6.4787954325,2.2272652631,-0.6672207978
C,5.8070815053,3.9580783832,0.2483074743
H,-5.699884487,-1.5954376298,-0.4993771698
H,-3.1797317413,-1.9328309156,-0.4354707228
H,-1.0543328738,2.1431590416,-0.0238360923
H,0.4015625673,3.629797407,0.3847725353
C,-5.1839131847,0.5721232708,-0.2406982126
C,-3.9009876515,1.1752492505,-0.126989556
C,-2.950988462,0.1394421256,-0.2112438789
C,-1.5097002974,0.0536723774,-0.1588489294
C,-0.6463768434,1.1461058837,-0.0380261105
C,0.7413573916,0.9438952348,-0.1464885019
C,1.680000029,2.0369170255,-0.2229766233
C,0.8930727502,-2.6265903917,-1.0628480294
C,2.3500101804,4.1790817821,-0.1878131314
C,3.4481027311,3.4261543841,-0.580770287
C,3.0348153103,2.0621428808,-0.5997951606
H,2.2590300805,5.2460114534,-0.0396412981
C,0.5286134555,-1.9560960032,1.568085322
C,-6.526684711,1.2514853167,-0.1691808223
C,-3.6562325243,2.6539869674,0.0187764004
C,-3.3321303437,3.3605916806,-1.3116841853
C,-7.047373931,1.4394980591,1.2674061168
C,2.0098289121,-3.4457366504,-0.821038841
C,2.464234263,-4.3673739453,-1.7658306517
C,1.8004142235,-4.5013260741,-2.9867092687
C,0.6855166894,-3.7046239205,-3.2513719612
C,0.2459979961,-2.781044069,-2.3006160205
C,1.1645302869,-1.1793929909,2.5506986837
C,1.2014921179,-1.5710483181,3.8920445761
C,0.5937055746,-2.7615398388,4.2891470121
C,-0.0445221664,-3.5562689563,3.3335660407

C,-0.0695071031,-3.1560802207,1.9980297311
C,3.8882286551,0.8873621996,-0.9973318141
C,4.8041694584,3.9877396119,-0.9186335835
C,4.5024701359,0.1265642677,0.1926305273
B,0.4228020238,-1.5240084338,0.0136139303

Cartesian Coordination of 3b-3.

-1487.3348816 hartree
H,0.2031673542,4.7916823406,-4.2098993705
H,3.3148778564,0.41828529,-1.4978277128
H,4.8047183064,2.1597011049,-0.5066947769
H,5.3492059492,1.0143680833,0.732105846
H,3.6590027209,1.5487060268,0.6944792494
H,0.8780776026,5.5146607594,-1.9273835002
H,0.7527644865,3.9319814826,-0.0374453936
H,-1.9652772425,2.8275010003,1.1150448974
H,-2.2140524718,3.7498257625,3.3880444466
H,7.5798599059,-2.8506202997,-1.685313716
H,6.0293058122,-2.2433180421,-2.2887527478
H,6.1250838604,-3.8583952888,-1.5821991149
H,5.0007914027,-0.0857098032,-1.5355590622
H,-0.473885071,3.3106993623,5.1131120825
H,1.5111446991,1.931243446,4.5264554013
H,1.7465605224,0.9969325577,2.2597902096
H,-3.5220329741,0.7296636465,0.851927433
H,-5.1888996056,0.1911936481,0.695767117
H,-6.4570099099,-1.6844566845,0.81751278
H,-6.3978190776,-3.4119422744,0.5447429266
H,-4.7012181193,1.9400565907,-0.9850692297
H,-4.9860485328,0.4140229437,-1.8366459168
H,-3.3314402306,1.0109578536,-1.6111415791
H,-7.8782107488,-2.3237067471,-1.1326366888
H,-6.4732984564,-3.0281772531,-1.9524516288
H,-6.5517750046,-1.2854851914,-1.676697733
H,6.7019998496,-2.853501506,0.6553151666
H,6.626092378,-1.2456315257,-0.0319547386
N,-2.4641130315,-3.0876935667,-0.0403865945
N,2.6869822157,-2.8084285382,0.9032905322
O,1.2554050297,0.3395591682,-0.122455201
O,-1.2178159697,0.2841173993,-0.2115100274
C,4.7229560868,-2.1907828351,0.2120553517
H,-0.6945012801,0.8796873303,-2.6855004409
H,-0.5859643799,2.4604370632,-4.575429433
C,4.5152315818,1.2771427532,0.0725330905
H,4.333669854,-4.0976070927,1.3202439664
H,1.9842389638,-3.2562712933,1.4692020771
H,0.0553260078,-2.6728910055,0.6268584794
H,-1.6692349899,-3.6739450046,-0.2364326132
C,3.9990101313,-3.1738169032,0.8694271902
C,2.5407309399,-1.557467731,0.3180730098
C,3.8058100132,-1.156670272,-0.1372404763
C,1.2486184451,-0.9237613646,0.1996747137
C,0.0443331778,-1.6216915855,0.3746946859
C,-1.1710529458,-0.9856050809,0.0720785147
C,-2.4232532597,-1.7013274243,0.0126104562
C,0.0238950652,2.2758262084,-1.205812887
C,-3.7589796263,-3.5053894543,-0.0386221833
C,-4.5897467683,-2.3979080475,0.0533979349
C,-3.7497881379,-1.2451654587,0.0769808851
H,-4.0085328648,-4.5554294637,-0.0994611938

C,-0.096694984,1.8201088836,1.5011339362
C,-0.3464953415,1.8949869541,-2.5083705025
C,-0.2869029913,2.7849941719,-3.5816412828
C,0.1557412928,4.0936397676,-3.3780730307
C,0.5336524798,4.4974997548,-2.0971718337
C,0.464421526,3.5979562587,-1.0306532966
C,-1.2038062154,2.6126184864,1.8617192857
C,-1.3460865392,3.1421618224,3.1441489677
C,-0.3698343975,2.8977080784,4.1132377229
C,0.7418714292,2.1238424092,3.7824640994
C,0.8700961644,1.5954725528,2.4945127
C,-4.2101585691,0.1822432206,0.2017258226
C,-6.0937756124,-2.4480573154,0.1192081189
C,-4.3138800959,0.9280044245,-1.1419647997
C,-6.7902909693,-2.2595479056,-1.2402701107
C,6.1937154573,-2.2499644741,-0.1063953047
C,6.5012266609,-2.8337721106,-1.4972338308
C,4.1540113427,0.1128000541,-0.8684991956
B,-0.0009870767,1.2144914699,0.0057844532

Cartesian Coordination of 3c-1.

-1634.9387117 hartree

H,0.2031673542,4.7916823406,-4.2098993705
H,3.3148778564,0.41828529,-1.4978277128
H,4.8047183064,2.1597011049,-0.5066947769
H,5.3492059492,1.0143680833,0.732105846
H,3.6590027209,1.5487060268,0.6944792494
H,0.8780776026,5.5146607594,-1.9273835002
H,0.7527644865,3.9319814826,-0.0374453936
H,-1.9652772425,2.8275010003,1.1150448974
H,-2.2140524718,3.7498257625,3.3880444466
H,7.5798599059,-2.8506202997,-1.685313716
H,6.0293058122,-2.2433180421,-2.2887527478
H,6.1250838604,-3.8583952888,-1.5821991149
H,5.0007914027,-0.0857098032,-1.5355590622
H,-0.473885071,3.3106993623,5.1131120825
H,1.5111446991,1.931243446,4.5264554013
H,1.7465605224,0.9969325577,2.2597902096
H,-3.5220329741,0.7296636465,0.851927433
H,-5.1888996056,0.1911936481,0.695767117
H,-6.4570099099,-1.6844566845,0.81751278
H,-6.3978190776,-3.4119422744,0.5447429266
H,-4.7012181193,1.9400565907,-0.9850692297
H,-4.9860485328,0.4140229437,-1.8366459168
H,-3.3314402306,1.0109578536,-1.6111415791
H,-7.8782107488,-2.3237067471,-1.1326366888
H,-6.4732984564,-3.0281772531,-1.9524516288
H,-6.5517750046,-1.2854851914,-1.676697733
H,6.7019998496,-2.853501506,0.6553151666
H,6.626092378,-1.2456315257,-0.0319547386
N,-2.4641130315,-3.0876935667,-0.0403865945
N,2.6869822157,-2.8084285382,0.9032905322
O,1.2554050297,0.3395591682,-0.122455201
O,-1.2178159697,0.2841173993,-0.2115100274
C,4.7229560868,-2.1907828351,0.2120553517
H,-0.6945012801,0.8796873303,-2.6855004409
H,-0.5859643799,2.4604370632,-4.575429433
C,4.5152315818,1.2771427532,0.0725330905
H,4.333669854,-4.0976070927,1.3202439664
H,1.9842389638,-3.2562712933,1.4692020771

H,0.0553260078,-2.6728910055,0.6268584794
H,-1.6692349899,-3.6739450046,-0.2364326132
C,3.9990101313,-3.1738169032,0.8694271902
C,2.5407309399,-1.557467731,0.3180730098
C,3.8058100132,-1.156670272,-0.1372404763
C,1.2486184451,-0.9237613646,0.1996747137
C,0.0443331778,-1.6216915855,0.3746946859
C,-1.1710529458,-0.9856050809,0.0720785147
C,-2.4232532597,-1.7013274243,0.0126104562
C,0.0238950652,2.2758262084,-1.205812887
C,-3.7589796263,-3.5053894543,-0.0386221833
C,-4.5897467683,-2.3979080475,0.0533979349
C,-3.7497881379,-1.2451654587,0.0769808851
H,-4.0085328648,-4.5554294637,-0.0994611938
C,-0.096694984,1.8201088836,1.5011339362
C,-0.3464953415,1.8949869541,-2.5083705025
C,-0.2869029913,2.7849941719,-3.5816412828
C,0.1557412928,4.0936397676,-3.3780730307
C,0.5336524798,4.4974997548,-2.0971718337
C,0.464421526,3.5979562587,-1.0306532966
C,-1.2038062154,2.6126184864,1.8617192857
C,-1.3460865392,3.1421618224,3.1441489677
C,-0.3698343975,2.8977080784,4.1132377229
C,0.7418714292,2.1238424092,3.7824640994
C,0.8700961644,1.5954725528,2.4945127
C,-4.2101585691,0.1822432206,0.2017258226
C,-6.0937756124,-2.4480573154,0.1192081189
C,-4.3138800959,0.9280044245,-1.1419647997
C,-6.7902909693,-2.2595479056,-1.2402701107
C,6.1937154573,-2.2499644741,-0.1063953047
C,6.5012266609,-2.8337721106,-1.4972338308
C,4.1540113427,0.1128000541,-0.8684991956
B,-0.0009870767,1.2144914699,0.0057844532

Cartesian Coordination of 3c-2.

-1634.9324768 hartree

C,-8.0460252606,-3.5479295008,0.0866190988
C,-8.351363605,-2.2045878007,0.317684044
C,-7.3676371097,-1.2279405512,0.1921550978
H,-4.769233432,-3.2193685029,-0.747176739
H,-8.8137424133,-4.3086315723,0.1893113272
H,-9.3578366674,-1.9175893228,0.6073004664
H,-7.6051799428,-0.1896890073,0.4008946727
H,0.5690811783,3.4382065168,5.2889794163
H,2.2819706415,1.8641266585,4.4069581589
H,2.2224132496,1.1646437517,2.0441816535
H,-6.5030104953,-4.9454715335,-0.4744388742
H,2.9005067038,-4.6883633516,0.1531983387
H,0.4653478445,-3.5463797594,0.254874196
H,3.3238133546,-0.5123968531,-0.263744452
H,-1.1325231605,-1.6597502694,0.2328192372
H,-3.3321270993,-1.679581568,0.1803041008
H,-6.0739990149,1.3353280936,-0.8258199144
H,-3.5784810889,2.398507604,-0.8210063319
H,5.2969192662,-0.8499408232,-1.3518283529
H,7.7443842957,-0.9919831495,-1.5271566964
H,8.9626802765,-2.9377043158,-0.5688633623
H,7.6915648918,-4.7301767523,0.5975389209
H,5.2402105192,-4.5638756241,0.8305317851
H,-0.3245719211,2.5063807464,-2.677385755

H,0.6250411914,4.1115053481,-4.2954507503
H,2.5347974614,5.5641752844,-3.6382181304
H,3.4709960051,5.3949321967,-1.3393692485
H,2.5022239852,3.8028798335,0.2794390109
H,-1.2464672817,3.6106272665,1.4002184797
H,-1.1981509055,4.3053642413,3.7662940984
N,-3.6952612497,-0.8017969388,-0.1547177379
N,2.9390264211,-1.4414036499,-0.1714529202
O,1.2442310251,0.6186851939,-0.2460754787
O,-1.0078700418,1.6088980278,-0.4325366916
B,0.4409368549,1.926375318,-0.0385373509
C,1.410636404,-3.0378597659,0.1308466089
C,1.5862241187,-1.6604076015,-0.0272056698
C,0.6787846997,-0.5427332241,-0.0519565647
C,-0.7088594672,-0.6782686026,0.0708636609
C,-1.5199925643,0.4298528314,-0.2062404455
C,-2.9546322912,0.3560601792,-0.3201481006
C,1.0212401043,3.0138325543,-1.0728720212
C,-5.0313904369,-0.5380321209,-0.3076682295
C,-5.1488586223,0.8234247648,-0.6044011939
C,-3.8589255227,1.3769598412,-0.6135768832
C,3.6287820129,-2.6176446834,-0.1034032874
C,0.4830724437,2.3289240467,1.5257126282
C,5.0837878664,-2.694350324,-0.2363668144
C,5.8140520516,-1.6900022083,-0.8969715493
C,7.1994991838,-1.7765235531,-1.0107808526
C,7.8830065798,-2.8703107919,-0.4770486727
C,7.1681854523,-3.8777511041,0.1747236004
C,5.7846139884,-3.790280076,0.2982966057
C,0.5120133055,3.1326791097,-2.3774374673
C,1.0450451,4.0396908933,-3.2949962048
C,2.1165574466,4.8557522618,-2.9277600254
C,2.6413466196,4.7587141308,-1.6379857159
C,2.0940162394,3.8529283847,-0.7271860666
C,-0.4686427159,3.2211862969,2.05306293
C,-0.4452383346,3.6169159067,3.3903021889
C,0.5458723476,3.1312312237,4.2466871143
C,1.5056611407,2.249541757,3.7503327462
C,1.4682302941,1.8578666343,2.4093239732
C,-6.0555302622,-1.5744329144,-0.1771704959
C,-5.7630776683,-2.9294100133,-0.4167802086
C,-6.7476689199,-3.9053625604,-0.2804443697
C,2.6807894179,-3.6327189832,0.0888561195

Cartesian Coordination of 3c-3.

-1634.9245216 hartree

C,-5.5365652517,5.6710038099,0.23611747
C,-4.2076667294,5.4783325841,-0.14483335303
C,-3.7105259081,4.1902670958,-0.3295876074
H,-6.5090873618,2.4179482201,0.4417153916
H,-5.9247108312,6.6751546027,0.3760818375
H,-3.5596026209,6.3334648358,-0.3125589434
H,-2.6874331799,4.05846719,-0.6715089376
H,5.9300297008,6.6699256727,0.3794499207
H,7.4021233203,4.6967634412,0.7353435179
H,6.5108591897,2.412207252,0.4433394093
H,-7.3985253736,4.7033717174,0.7324963373
H,-5.7432304526,0.4409282529,-0.8528464567
H,-2.0087041664,2.0299453371,0.2035562185
H,-3.9034441505,-1.5480726036,-0.9256308777

H,0.0004789613,1.1577359825,-0.0739105628
H,2.0102872,2.0280424787,0.2042647001
H,5.743602751,0.4363632821,-0.852351492
H,3.9022106285,-1.5510892893,-0.9260676995
H,2.1440170114,-4.2025973003,-1.2371293667
H,2.1454150853,-6.2213098066,-2.6528331562
H,-0.0047853022,-7.2507687826,-3.3661250337
H,-2.1532520878,-6.2269409919,-2.6395839251
H,-2.1484426367,-4.2083746135,-1.2237497198
H,2.1460841048,-3.1224617852,1.6353503478
H,2.149533024,-3.6864779105,4.0355439639
H,0.000393896,-3.9682098289,5.2581496185
H,-2.1494597095,-3.6770651374,4.0390229248
H,-2.1474119039,-3.1128961052,1.6388518458
H,2.6908348149,4.056382091,-0.6700753796
H,3.5648051804,6.3305027883,-0.3099121885
N,2.6925697031,1.3962046286,-0.1828416573
N,-2.6914955112,1.3984868864,-0.1832693305
O,-1.237612489,-1.9028707794,-0.4795794808
O,1.2359028372,-1.9038491043,-0.4802177938
B,-0.0010966326,-2.7558729831,-0.1493826027
C,-2.4924946129,0.0427437965,-0.3855199718
C,-3.7380798171,-0.5098150319,-0.6809796632
C,-1.2093470892,-0.6125998688,-0.3156564029
C,0.0000223395,0.0779165177,-0.1415235977
C,1.2087764444,-0.613589412,-0.3159285356
C,2.492470229,0.0406983294,-0.3856163479
C,-0.0020385137,-4.0419769462,-1.1111534887
C,4.0233478617,1.70389281,-0.3075777983
C,4.6888672486,0.5192794294,-0.6342158699
C,3.7376360076,-0.5127773221,-0.6811208121
C,-4.6884589952,0.5230471874,-0.6345840777
C,-0.0007312764,-3.0734486543,1.4379815644
C,1.1953683714,-4.6415826432,-1.5358860344
C,1.200938011,-5.7833445247,-2.3388776487
C,-0.0040201658,-6.3619102109,-2.7406908752
C,-1.208012485,-5.7864867297,-2.3314641669
C,-1.2004775379,-4.6447490559,-1.5284999854
C,1.1973609037,-3.2455789635,2.1525778965
C,1.2044393308,-3.5627441654,3.51209643
C,0.0000785892,-3.7204112651,4.1999193946
C,-1.2046770829,-3.5574807483,3.5140497844
C,-1.1984046023,-3.2403064742,2.1545114569
C,4.53360102,3.0623053196,-0.1237583548
C,3.7139567417,4.1871883201,-0.3278602904
C,4.2121208916,5.4747590345,-0.1424155909
C,5.5410872274,5.6661594657,0.2389400476
C,6.3678916059,4.5575236768,0.435092024
C,5.8704123847,3.2692910614,0.2612183161
C,-4.53115053,3.0661540383,-0.1251825802
C,-5.8678820819,3.2744196697,0.2593819549
C,-6.3643351921,4.5631408847,0.4325633448
C,-4.0219980126,1.7072363835,-0.3083188156

Cartesian Coordination of 3d-1.

-1949.4757104 hartree

H,-2.8088290766,-4.3670081892,-0.3435306222
H,-2.0739875437,2.6494529653,1.8313778887
H,-0.0251456584,2.9811949577,5.5897028877
H,2.0787528401,2.2265076323,4.4970716605

H,2.0997598353,1.6803157395,2.0924237189
H,-6.3616280737,-3.0843856307,0.1354736274
H,-5.0231993877,-4.179487483,0.3773483617
H,0.1031375389,6.1397460177,-3.2590583152
H,0.9221541408,6.381852584,-0.9227511812
H,0.8493037697,4.4574910709,0.6224962003
H,-2.1032940641,3.1867821712,4.2358968327
H,1.4066518191,-2.8510478558,2.2959641717
H,2.9373441303,-3.7107670791,2.4674008142
H,1.4521648295,-4.6154175818,2.1259705939
H,6.1412271411,-5.0417540064,-1.3014761166
H,5.7363747101,-3.6087242912,-2.2617787643
H,4.4512323818,-4.6422427303,-1.6472242109
H,-1.4210620702,-4.8902159311,1.6612776931
H,-2.91493184,-4.0728164456,2.1508267426
H,-1.3961440323,-3.1771454914,2.1195644439
H,-6.2112944065,-4.7017107499,-1.7534906902
H,-4.5688006405,-4.1488337707,-2.1249760627
H,-5.9355833044,-3.0511952889,-2.337668561
H,5.4772633708,1.5528660266,0.559338718
H,7.5947474122,2.7475932712,0.1622967189
H,9.3973842348,1.6884862287,-1.187261309
H,9.0320460288,-0.5680833579,-2.1671260067
H,6.8902536577,-1.737259893,-1.8297829188
H,-7.0807796317,-1.2484190875,1.1349552948
H,-9.2275376685,-0.0657534311,0.8372083764
H,-9.4212092759,1.7776701943,-0.82036936
H,-7.4456894894,2.4105988087,-2.1929850316
H,-5.315581129,1.1859368909,-1.9411993775
H,-0.8351681394,2.0212940688,-2.4819900238
H,-0.7790768467,3.9444127474,-4.0290553934
N,-3.5948909088,-0.1184252259,-0.1888632122
N,3.5842396718,-0.1502511172,-0.2917847499
O,1.2278491644,0.9373572997,-0.1837249089
O,-1.2205124277,0.9486193708,-0.1686647458
C,0.0151471951,2.1147073525,1.7610453767
C,-1.1789423066,2.8565910109,3.7681699909
C,-0.0135869013,2.7420358239,4.5296221359
C,1.165009508,2.3194642971,3.9149822582
C,1.1718236278,2.0124942866,2.5517598844
H,2.8284749663,-4.4107312617,0.0550591494
H,1.3088492714,-3.5811136702,-0.1471357017
H,-1.3003289013,-3.4938728017,-0.4117015513
C,8.4583831382,1.1679288228,-1.0254598329
C,8.2543356808,-0.1006027652,-1.5703191687
C,7.0485526241,-0.769402307,-1.3684473681
C,-7.1671057616,-0.4708846897,0.3833638268
C,-8.3733658157,0.2083168756,0.225008118
C,-8.4810908312,1.2476590927,-0.701045974
C,-7.3716295126,1.6043076301,-1.4692865576
C,-6.1663660999,0.9211583857,-1.3198181637
C,-0.4450996139,2.9744594455,-2.1322017588
C,-0.4163974543,4.0586763437,-3.0102156601
C,0.0788299469,5.2915199744,-2.5797411394
C,0.5385258298,5.4252822231,-1.2691873046
C,0.4989868249,4.3331477613,-0.3989986563
H,3.4639595124,0.8323957859,-0.4919421267
H,-0.0072015512,-2.0951371675,0.4292893488
H -3.4976546425,0.8865469193,-0.191992234
H,5.0945685009,-4.0371702793,0.7204816263

H,6.3743270061,-3.0080358141,0.1239323742
C,1.9950625752,-3.6891600609,1.9113093882
C,-1.1564970059,2.549421814,2.4076207266
C,5.3714547535,-3.3789970088,-0.1119955236
C,2.2576906968,-3.5430763072,0.4000353071
C,-2.2463563635,-3.5594166233,0.1367590889
C,-5.3745384881,-3.3525459871,-0.2505234215
C,5.4294929114,-4.215858641,-1.4039521987
C,-1.9758034209,-3.9478216453,1.6029715052
C,-5.5314184773,-3.8446409559,-1.7016169054
C,6.0217414429,-0.1853095941,-0.6055261129
C,-6.0457454143,-0.1299686763,-0.3926062749
C,6.2429962916,1.0938717673,-0.0592448586
C,7.445253896,1.7633118488,-0.2714708122
C,4.4123987742,-2.2174303039,-0.1676362594
C,-3.0168627755,-2.2744904867,-0.0070723436
C,-4.4284540384,-2.1854018434,-0.120313496
C,-4.7585567842,-0.8229201001,-0.2273043951
C,-1.2070236584,-0.3502489905,0.0304143623
C,-2.5120005006,-0.9595632281,-0.0374871971
C,0.010423523,3.0808312438,-0.8059186688
C,3.011915932,-2.2893057328,0.0472892162
C,2.508224579,-0.9771569971,-0.0451687015
C,1.2064147432,-0.3599452338,0.024530621
C,-0.0026317707,-1.0382717012,0.2319410371
C,4.7396982037,-0.8656206034,-0.3850741029
B,0.0105353643,1.8014466287,0.173530273

Cartesian Coordination of 3d-2.

-1949.473257 hartree
H,-0.4100811544,1.807926788,2.9969405304
H,-3.6285447693,-3.4066406869,-1.7529914841
H,-6.8702927079,-6.0972831031,-0.9148582056
H,-7.9679734024,-4.3356039682,0.4548148242
H,-6.8822588811,-2.1434354302,0.7630438833
H,-8.2181050589,1.0571452813,0.6952380987
H,-6.6998715313,1.6547606804,1.37890301
H,-7.1648222273,-0.028151598,1.6186107585
H,-4.6834193661,-5.6232337798,-2.0022858588
H,-4.8808070407,2.7137389933,-0.4743032456
H,-3.1271612298,2.7962842128,-0.5736356681
H,-6.9941273463,-0.3960485521,-0.9004435558
H,-6.4924781922,1.2679249436,-1.0926586957
H,-3.9915549518,4.0228268476,1.4254092224
H,-2.9288982316,2.6895885389,1.8990057022
H,-4.6865755087,2.5248472656,2.0658110634
N,-3.1466607189,-1.2389643223,-0.2263969793
N,3.3676746031,-0.5749904316,0.1866892132
O,1.3230991164,1.0213225264,0.4365678886
O,-1.0683198807,1.6219688588,0.4590369822
C,-3.8966926842,0.8723600532,-0.070940679
C,8.4308166345,-0.5790148487,0.8203117325
C,7.9384656462,-1.8387780363,1.1640616198
C,6.6031354339,-2.1621400538,0.9309457221
C,-0.3684022552,3.9824462641,-1.4454827652
C,-0.2943042296,4.6229998458,-2.6822948794
C,0.6622744076,4.2244978992,-3.6191883666
C,1.5388191699,3.1876026051,-3.3012135824
C,1.4516375401,2.5528321818,-2.0589348671
C,1.334662397,4.3367971068,1.5730957971

C,1.5920311098,5.1019792552,2.7135602987
C,1.1226487703,4.6816043281,3.9581689427
C,0.3990994732,3.4906323705,4.0515538848
C,0.1534267957,2.7338936443,2.9053983728
C,-3.9546586653,2.3742346633,0.0036364148
C,-6.4478661638,0.4136862095,-0.4056220614
C,-3.8880824333,2.932852831,1.4378297691
C,-7.1740851031,0.7954911805,0.8969314158
C,-5.1741567607,-2.6085293892,-0.4716891007
C,-4.5651621331,-3.6164940089,-1.2441466055
C,-5.1681287197,-4.8624896535,-1.3973649041
C,-6.3977161646,-5.12760012,-0.7915091276
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Cartesian Coordination of 3d-3.

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C,-0.0116641978,0.2047650354,0.0309892643
C,1.1969446755,-0.4865828124,-0.1465412839
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Cartesian Coordination of 3a•Cl⁻

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C,2.2733257723,1.3016258652,3.4626380143
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C,-2.0827743748,-4.6585768226,-0.1247363973
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Cartesian Coordination of 3c•Cl⁻

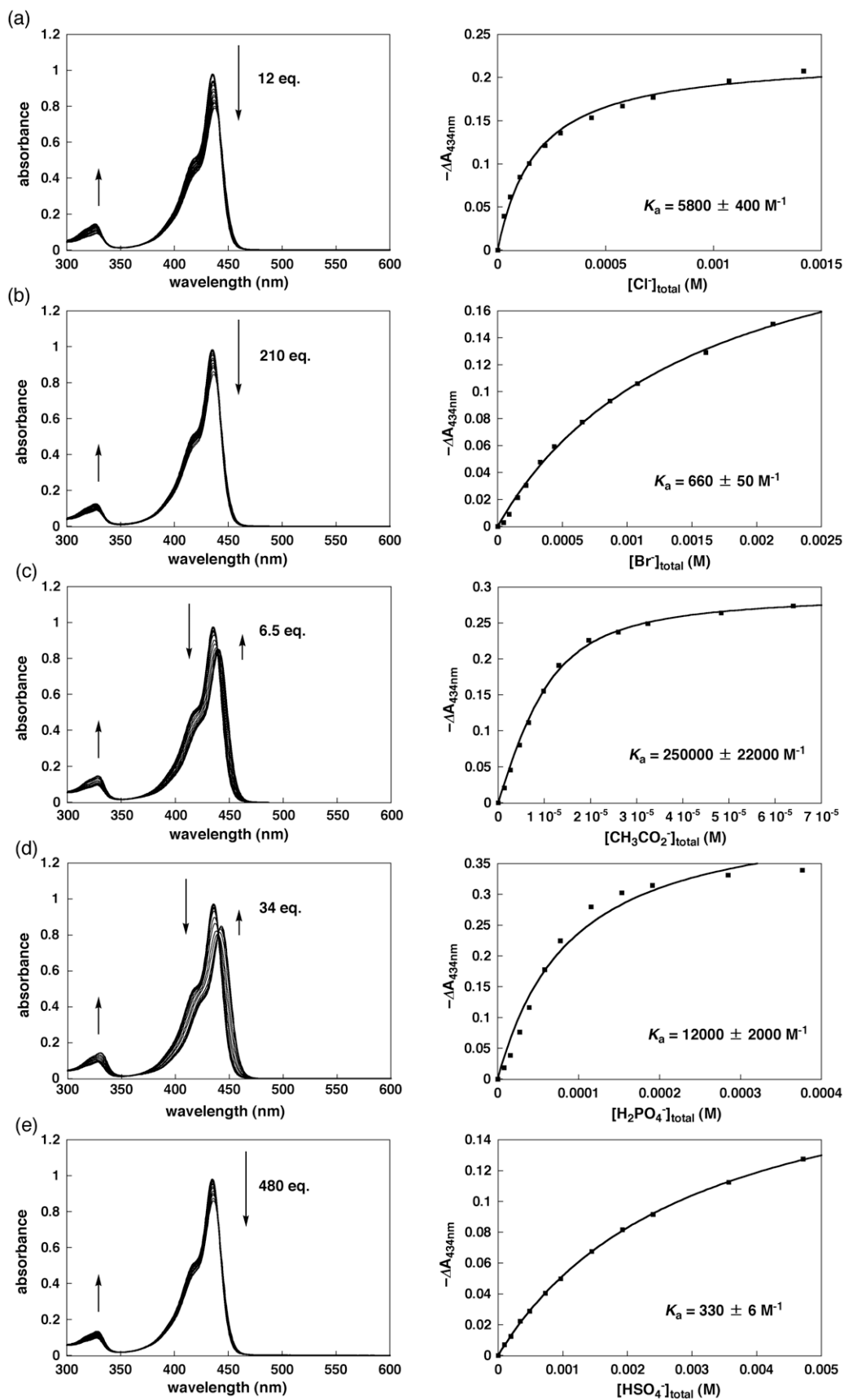
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H,-1.913452121,-1.7955322299,-0.0531008917
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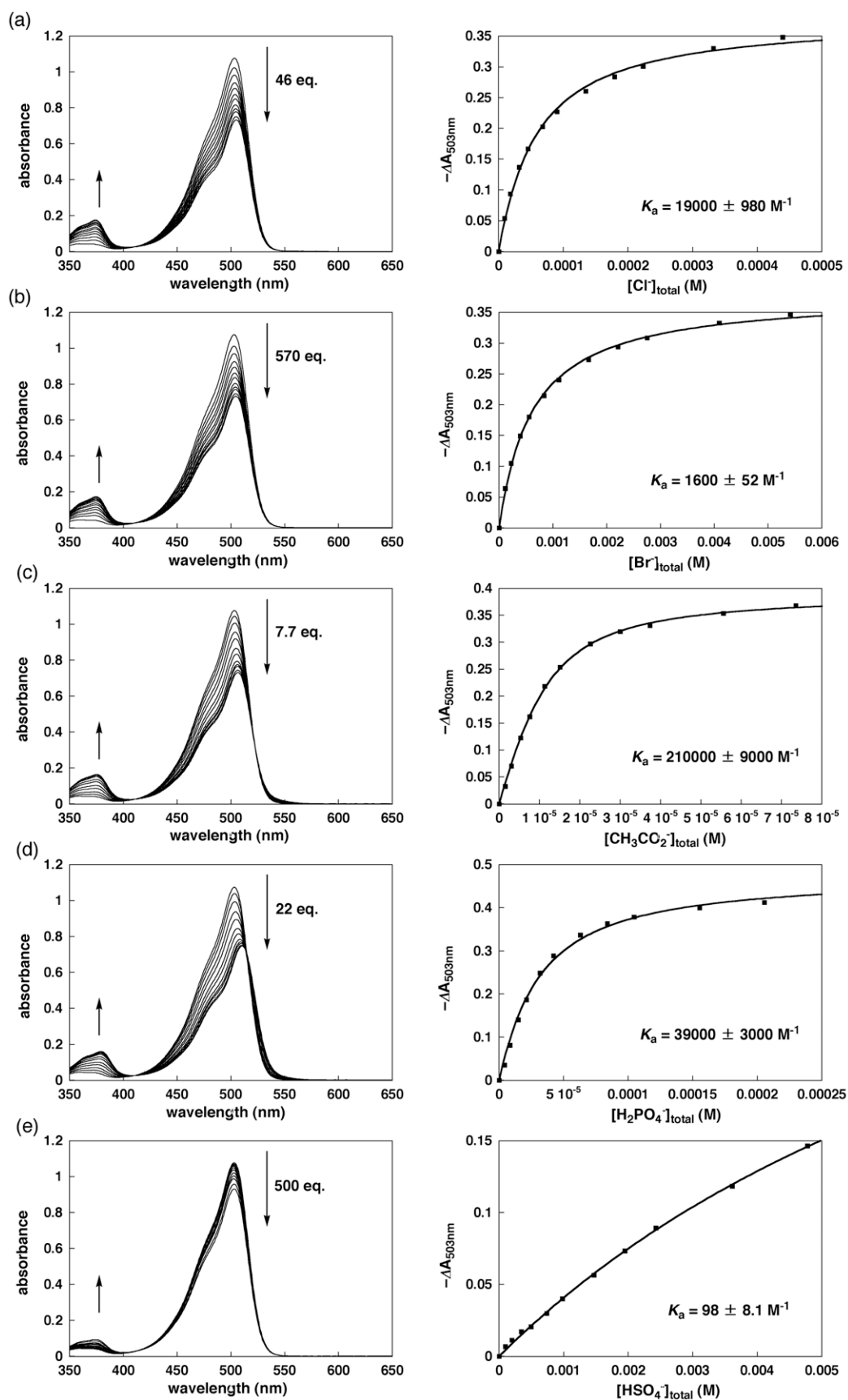
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[S3] *Gaussian 03*, (Revision C.01), Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, 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.

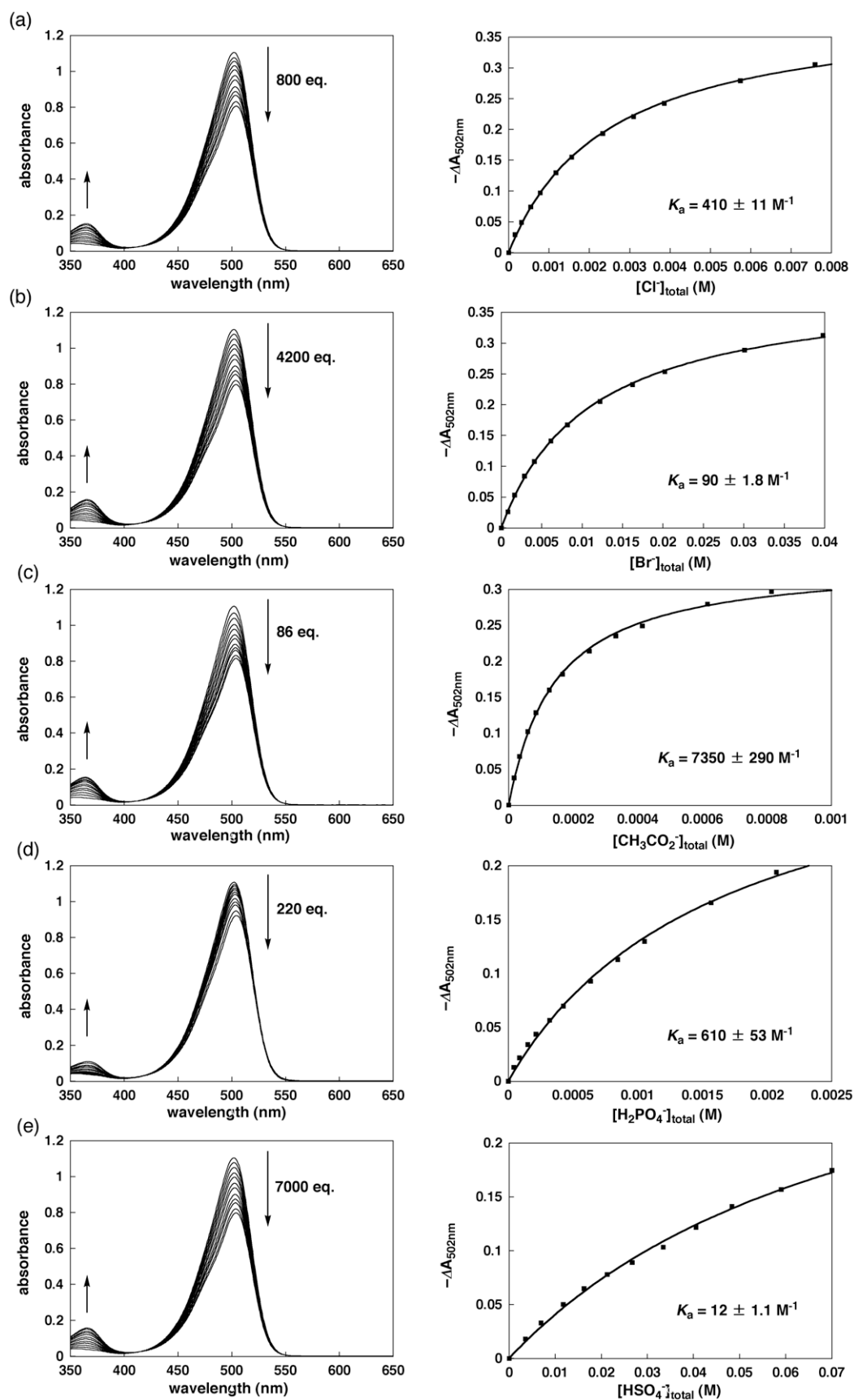
4. Anion-binding behavior



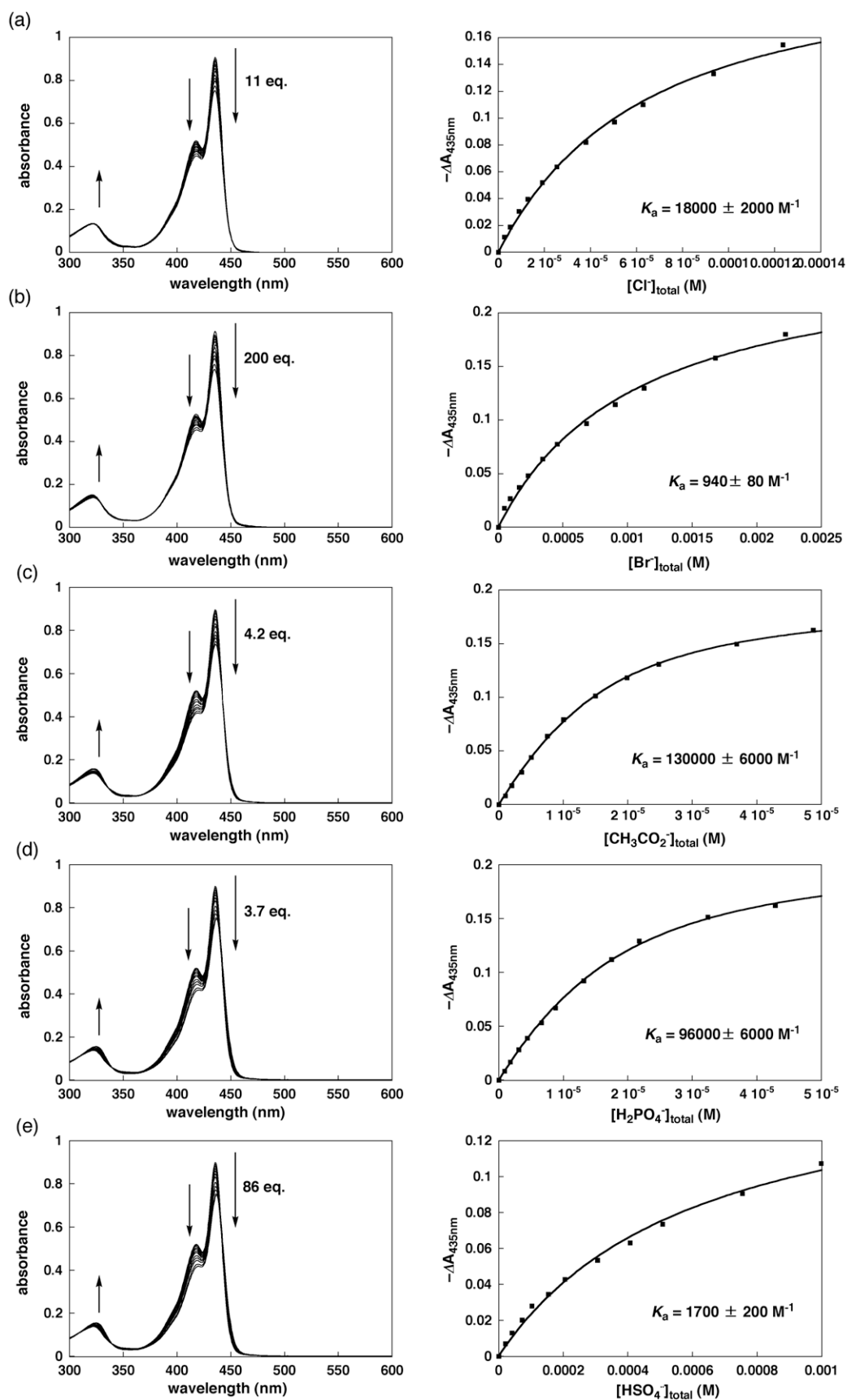
Supporting Figure 10 UV-vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **2a** (1.0×10^{-5} M) upon the addition of (a) Cl^- , (b) Br^- , (c) CH_3CO_2^- , (d) H_2PO_4^- , and (e) HSO_4^- as tetrabutylammonium (TBA) salts in CH_2Cl_2 . Complexation with H_2PO_4^- may include other binding modes.



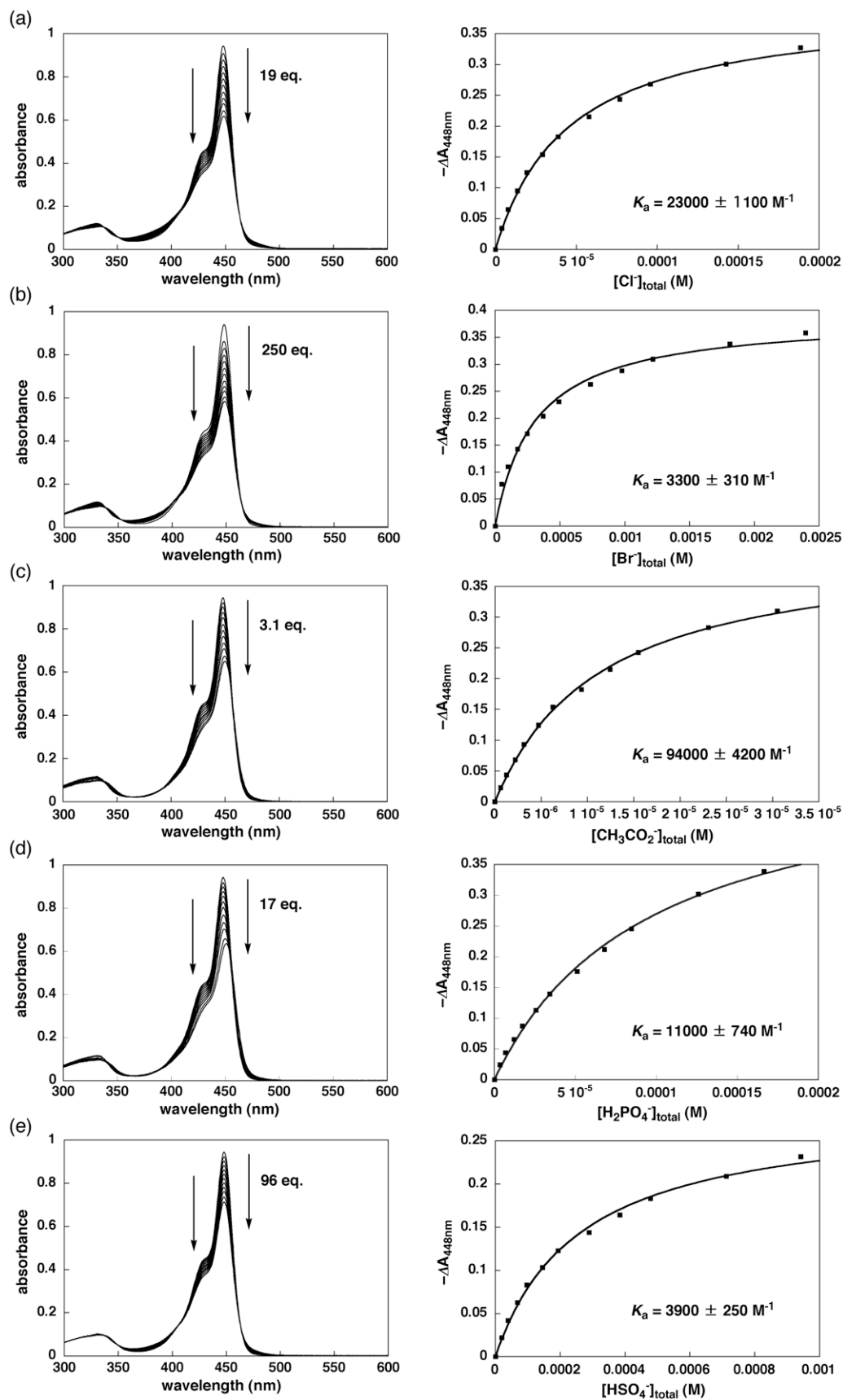
Supporting Figure 11 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **2c** ($1.0 \times 10^{-5} \text{ M}$) upon the addition of (a) Cl^- , (b) Br^- , (c) CH_3CO_2^- , (d) H_2PO_4^- , and (e) HSO_4^- as TBA salts in CH_2Cl_2 .



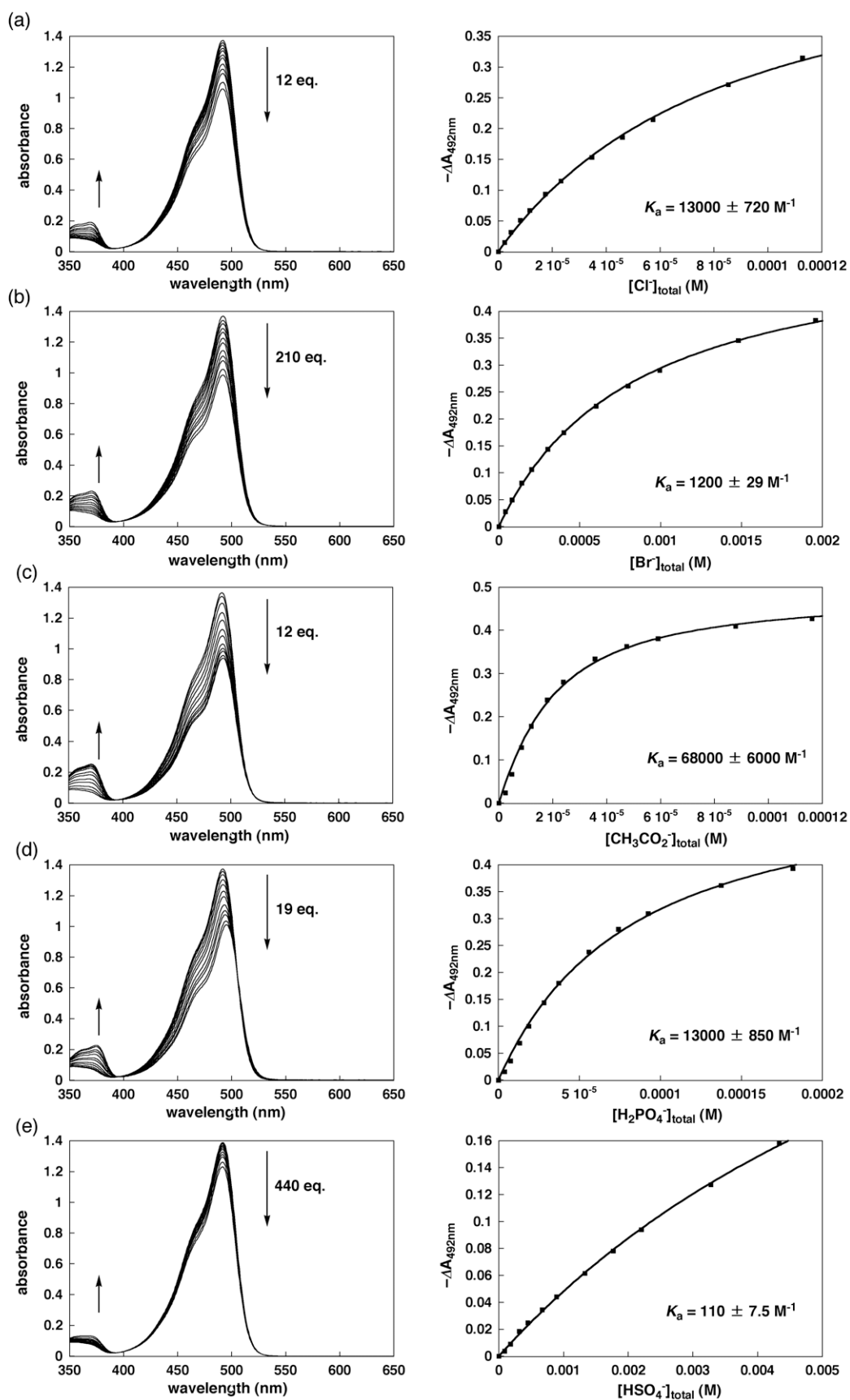
Supporting Figure 12 UV-vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **2d** (1.0×10^{-5} M) upon the addition of (a) Cl^- , (b) Br^- , (c) CH_3CO_2^- , (d) H_2PO_4^- , and (e) HSO_4^- as TBA salts in CH_2Cl_2 .



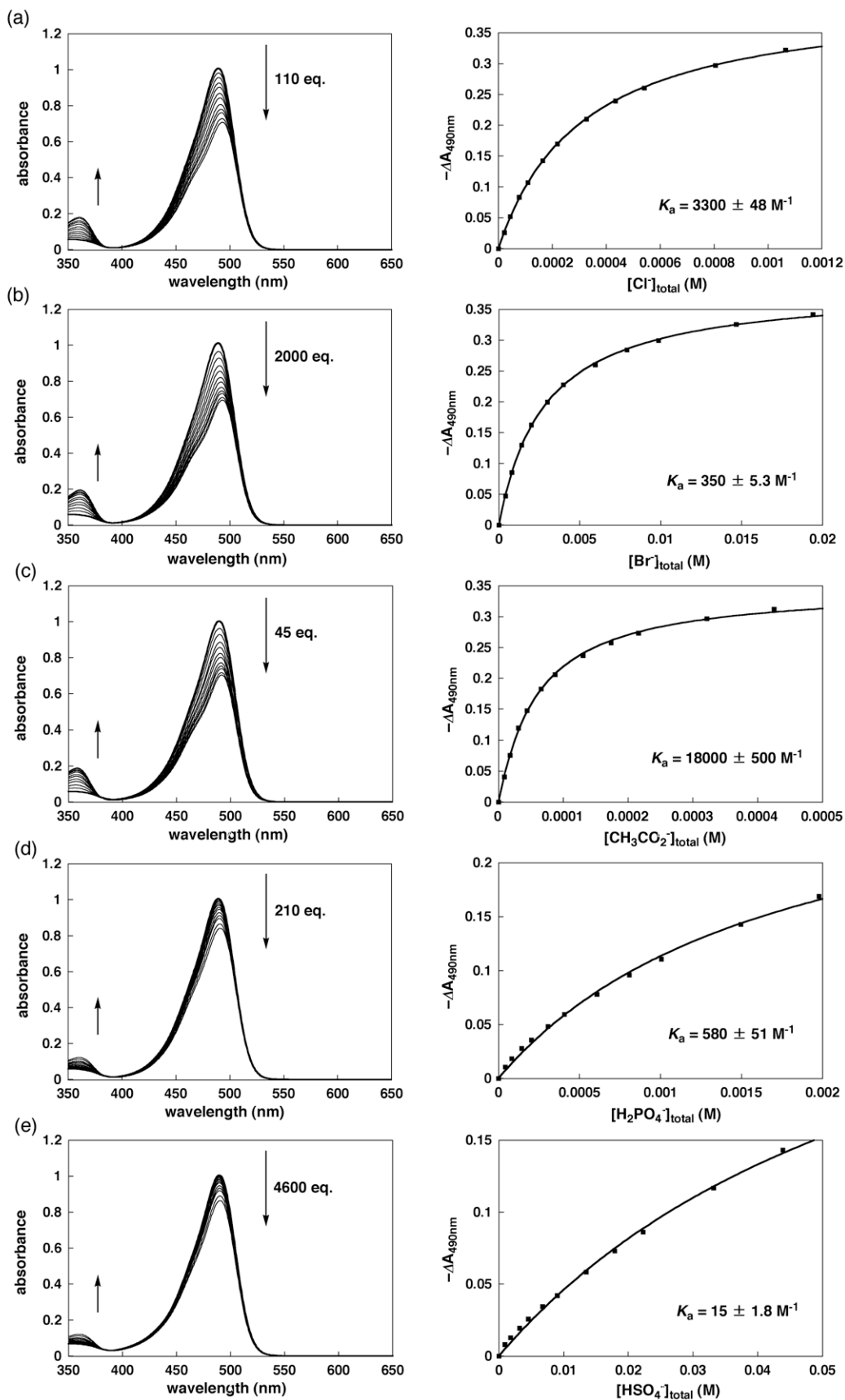
Supporting Figure 13 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **3a** (1.2×10^{-5} M) upon the addition of (a) Cl^- , (b) Br^- , (c) CH_3CO_2^- , (d) H_2PO_4^- , and (e) HSO_4^- as TBA salts in CH_2Cl_2 .



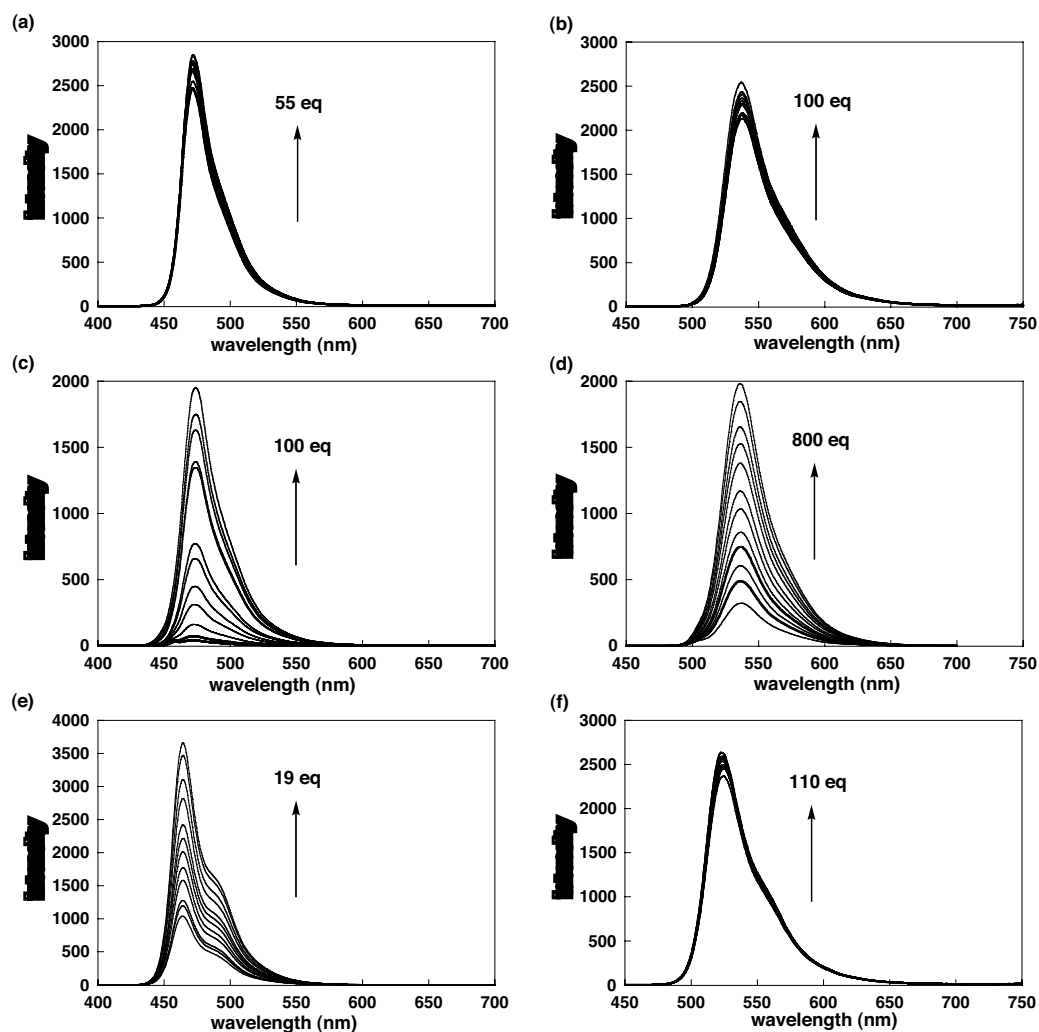
Supporting Figure 14 UV-vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **3b** (1.0×10^{-5} M) upon the addition of (a) Cl^- , (b) Br^- , (c) CH_3CO_2^- , (d) H_2PO_4^- , and (e) HSO_4^- as TBA salts in CH_2Cl_2 .



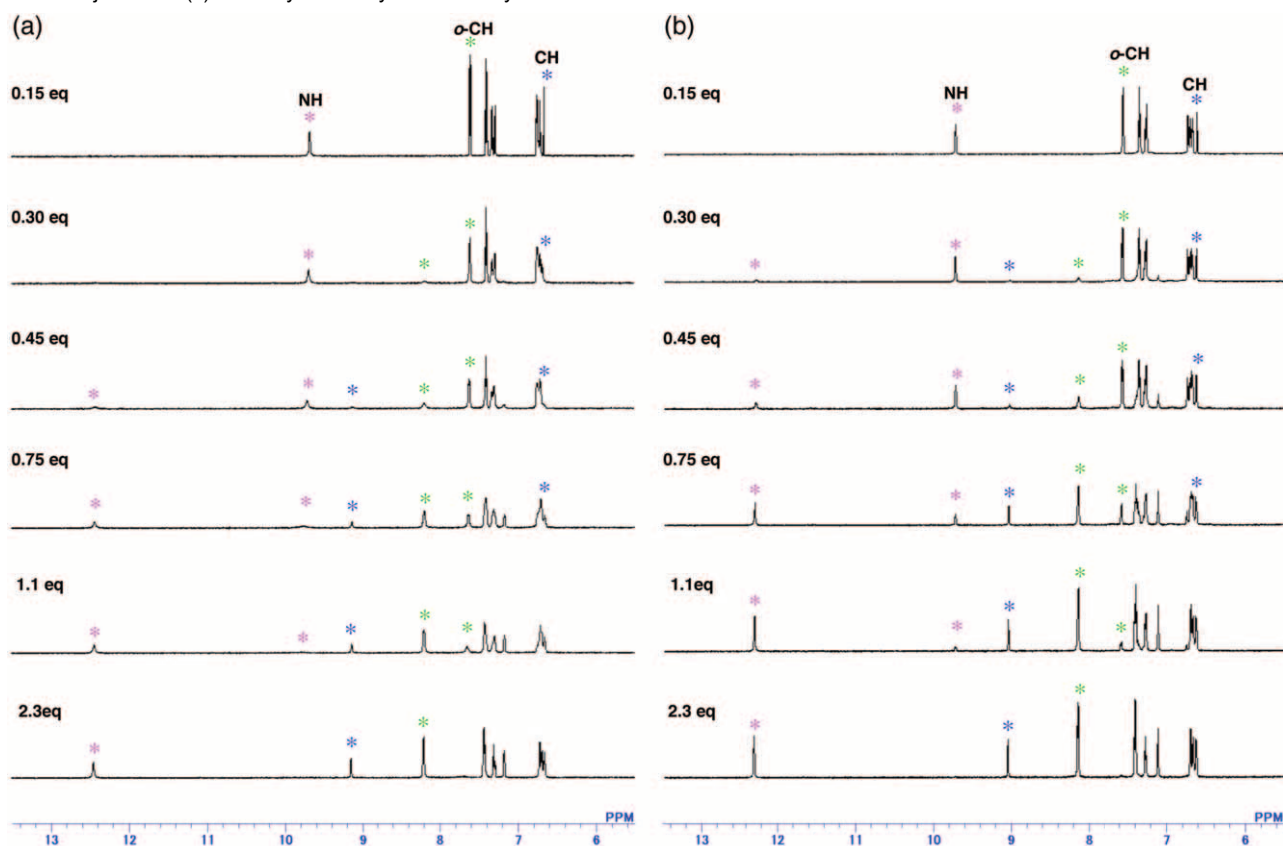
Supporting Figure 15 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **3c** (1.0×10^{-5} M) upon the addition of (a) Cl^- , (b) Br^- , (c) CH_3CO_2^- , (d) H_2PO_4^- , and (e) HSO_4^- as TBA salts in CH_2Cl_2 .



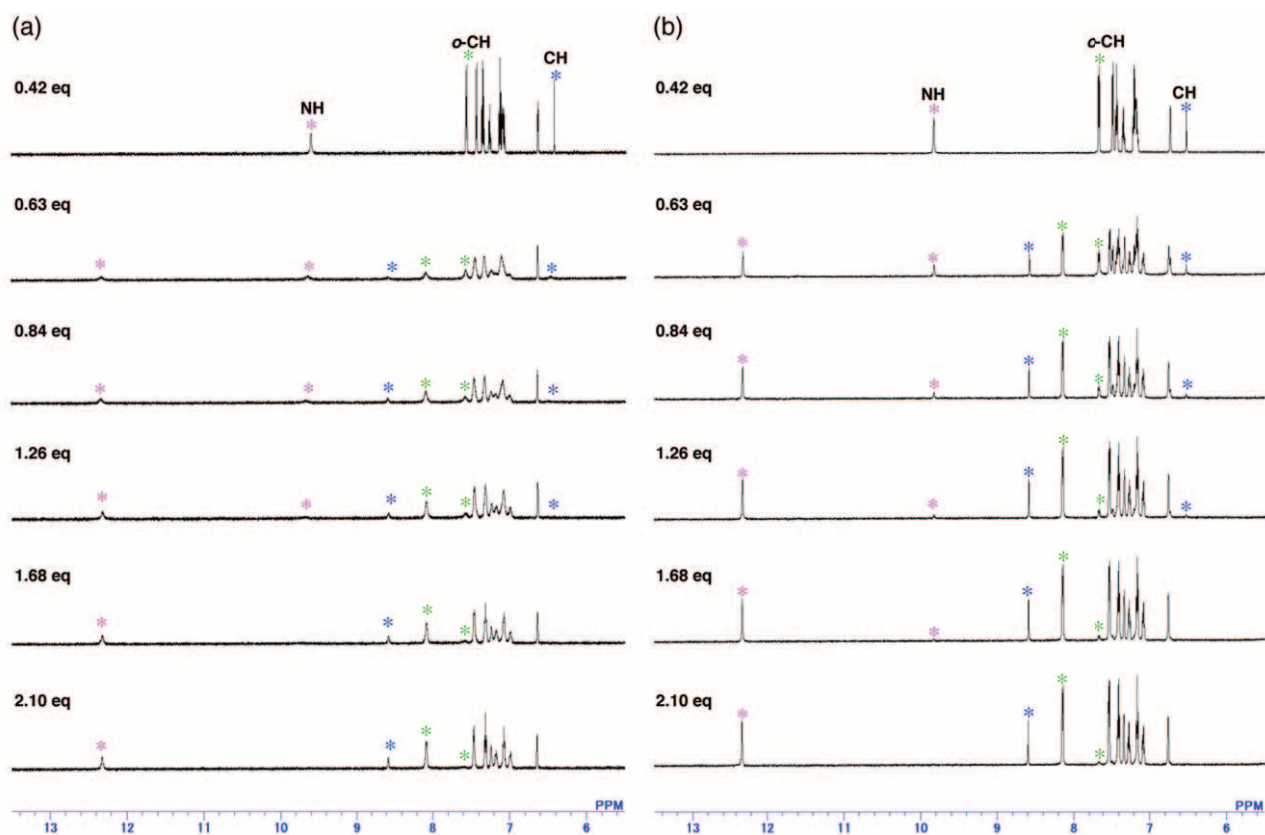
Supporting Figure 16 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) of **3d** (1.0×10^{-5} M) upon the addition of (a) Cl^- , (b) Br^- , (c) CH_3CO_2^- , (d) H_2PO_4^- , and (e) HSO_4^- as TBA salts in CH_2Cl_2 .



Supporting Figure 17 Fluorescence spectral changes of (a) **1b** ($\Phi_F = 0.84$), (b) **1d** (0.90), (c) **2b** (0.029), (d) **2d** (0.017), (e) **3b** (0.40), and (f) **3d** (0.83) (1.0×10^{-5} M, $\lambda_{\text{ex}} = \lambda_{\text{max}}$) upon the addition of Cl^- as a TBA salt in CH_2Cl_2 . Slightly decreased Φ_F values of **1b**, **1d**, and **3d**, whose emissions are inconsiderably increased by anion binding, may be within the error.



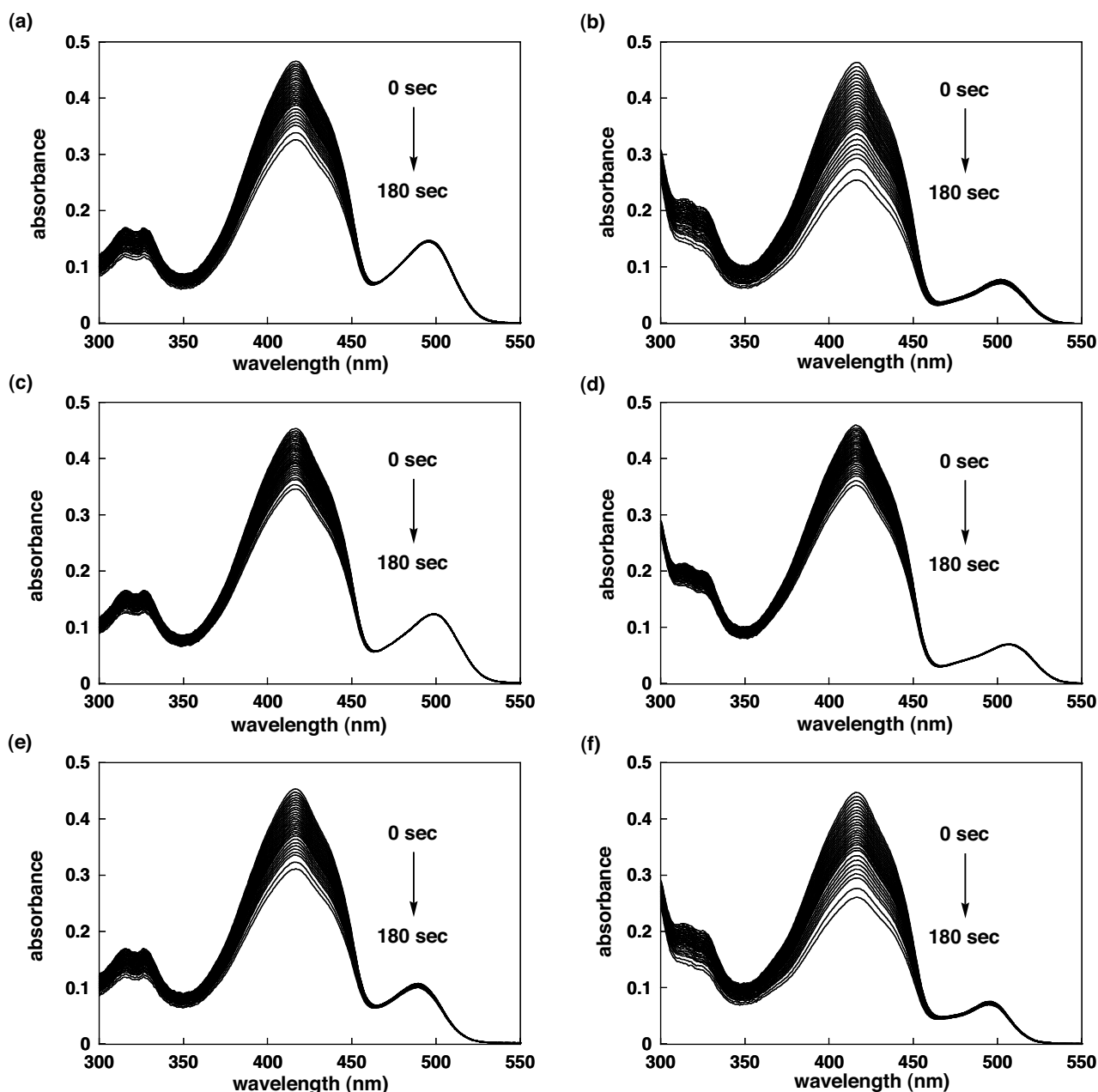
Supporting Figure 18 ^1H NMR spectral changes of **2c** (1.0×10^{-3} M) upon the addition of Cl^- as a TBA salt in CH_2Cl_2 at (a) 20°C and (b) -50°C .



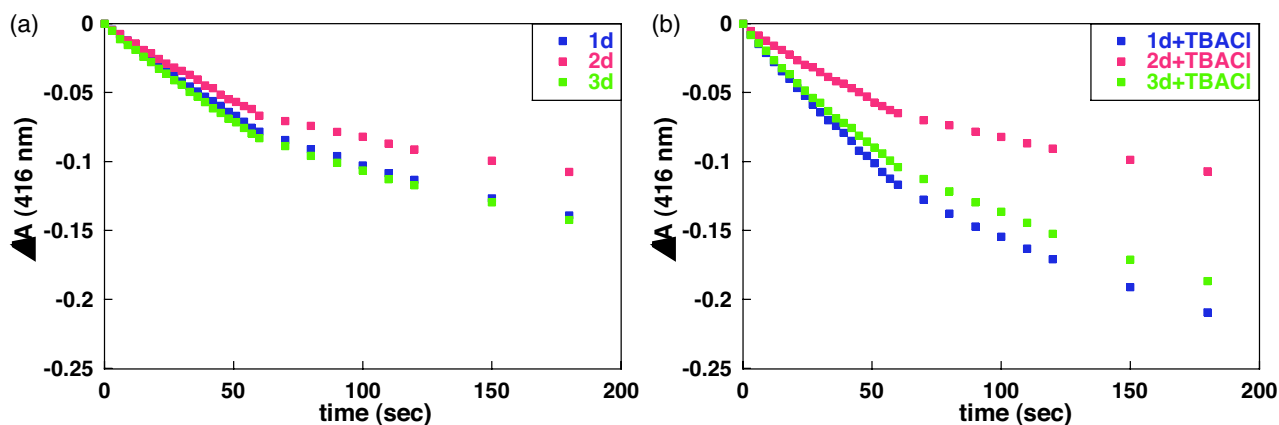
Supporting Figure 19 ^1H NMR spectral changes of **3c** (1.0×10^{-3} M) upon the addition of Cl^- as a TBA salt in CH_2Cl_2 at (a) 20°C and (b) -50°C .

5. Singlet oxygen generation properties

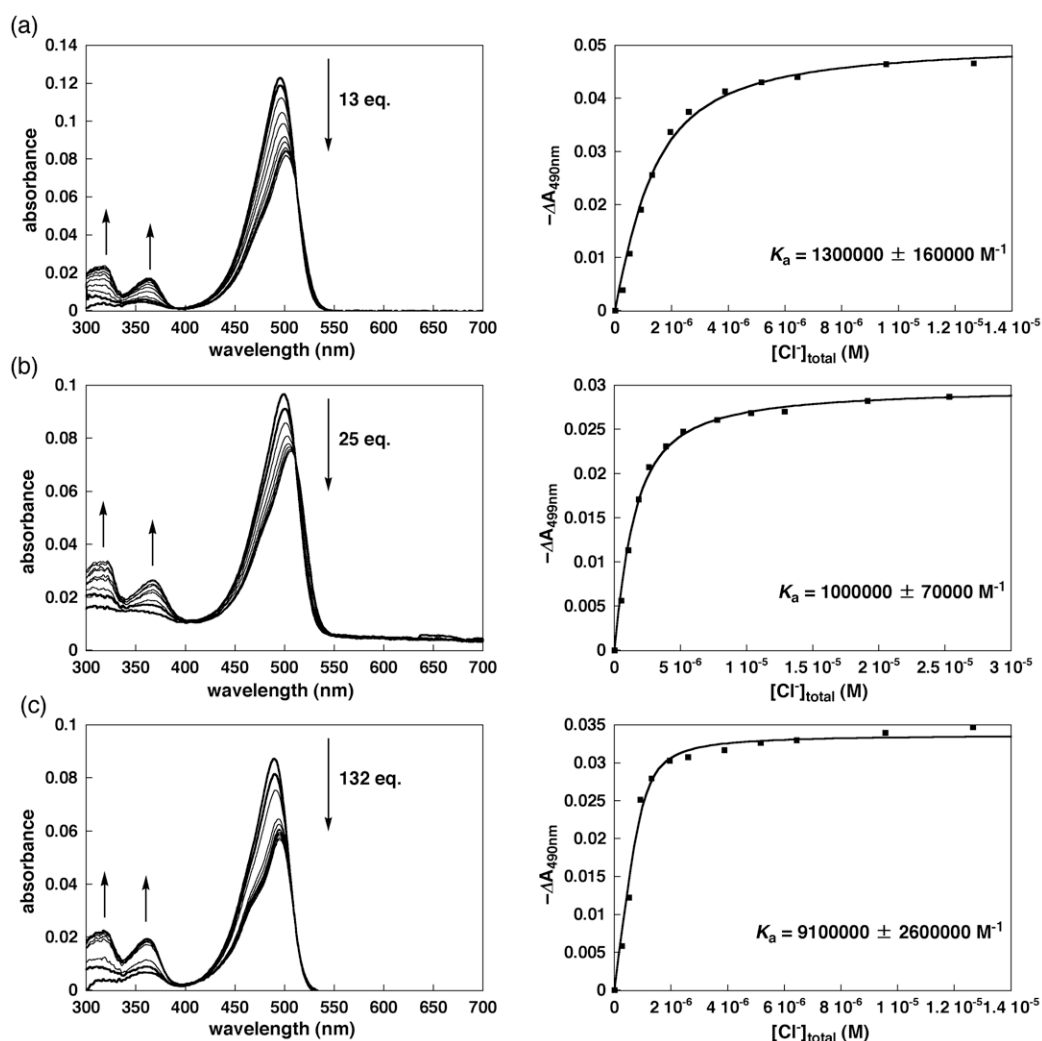
Method: The photosensitizing ability yielding singlet oxygen was evaluated by photo-degradation of 1,3-diphenylisobenzofuran (DPBF)^[S4,5] in toluene using a xenon lamp equipped with a light filter (>490 nm; ATG Y-50). Measurements were carried out in a quartz cell (1 cm × 1 cm) at room temperature. A toluene solutions (3.0 ml) containing 1×10^{-6} M sensitizers (**1d**, **2d**, and **3d**), tetrabutylammonium (TBA) chloride (0 or 3.5×10^{-5} M) and 2.0×10^{-5} M DPBF as chemical quencher for singlet oxygen were freshly prepared in the dark, and then photoirradiated. A decrease of DPBF concentration was followed by an absorbance at 416 nm. Quantum yields (ϕ_{Δ}) of singlet oxygen photogeneration were calculated from the kinetic profiles analyzed by the initial rate of DPBF degradation using the relative method with *meso*-tetraphenylporphyrin ($\phi_{\Delta s} = 0.73$) as a standard compound.



Supporting Figure 20 UV/vis absorption spectral changes of DPBF (2×10^{-5} M) with the existence of (a) **1d**, (b) **1d** along with 35 equiv of TBACl, (c) **2d**, (d) **2d** along with 35 equiv of TBACl, (e) **3d**, and (f) **3d** along with 35 equiv of TBACl in toluene (1×10^{-6} M) at r.t. At this concentration, based on the examination of anion binding in toluene, 35 equiv of TBACl is enough to form >95% receptor-anion complexes in this solvent.



Supporting Figure 21 Time-dependent decomposition profiles of DPBF by photoirradiation of (a) **1d**, **2d**, and **3d**, and (b) Cl^- complexes (>95%) of **1d**, **2d**, and **3d** as TBA salts.



Supporting Figure 22 UV/vis absorption spectral changes (left) and corresponding titration plots and 1:1 fitting curves (right) for (a) **1d**, (b) **2d**, and (c) **3d** upon the addition of Cl^- as a tetrabutylammonium (TBA) salt in 1% CH_2Cl_2 /toluene (1×10^{-6} M). This result suggests that 35 equiv of Cl^- affords >95% complexes in this concentration.

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[S5] Spiller, W.; Kliesch, H.; Wöhrle, D.; Hackbarth, S.; Röder, B.; Schnurpfeil, G. *J. Porphyrins Phthalocyanines* **1998**, *2*, 145–158.