Electronic Supplementary Information

Ion-pairing assemblies of anion-responsive helical Pt^{II} complexes

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1. Spectroscopic data

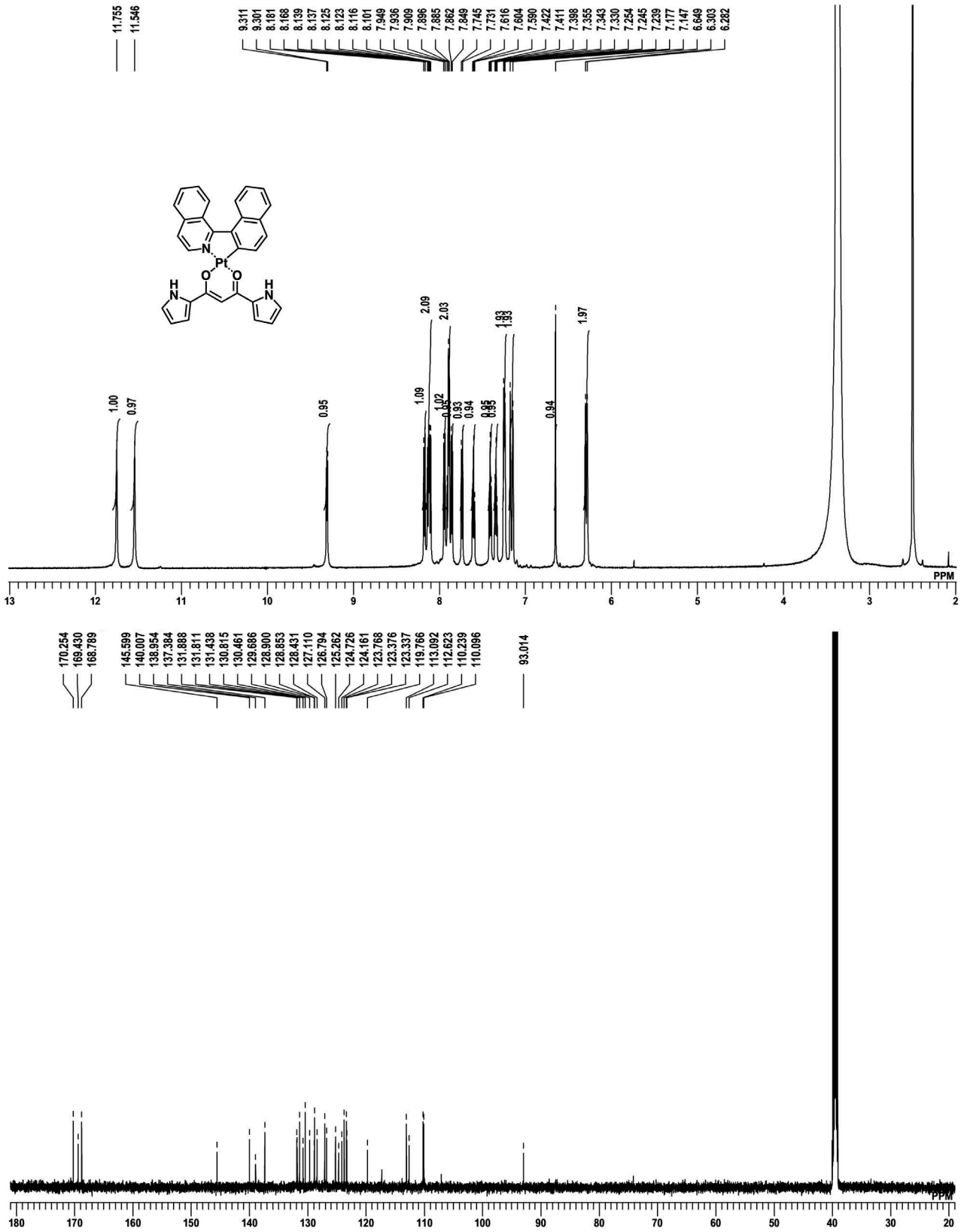

Fig. S1 ^{1}H NMR (top) and ^{13}C{^{1}H} NMR (bottom) spectra of **2a** in DMSO-d_6.

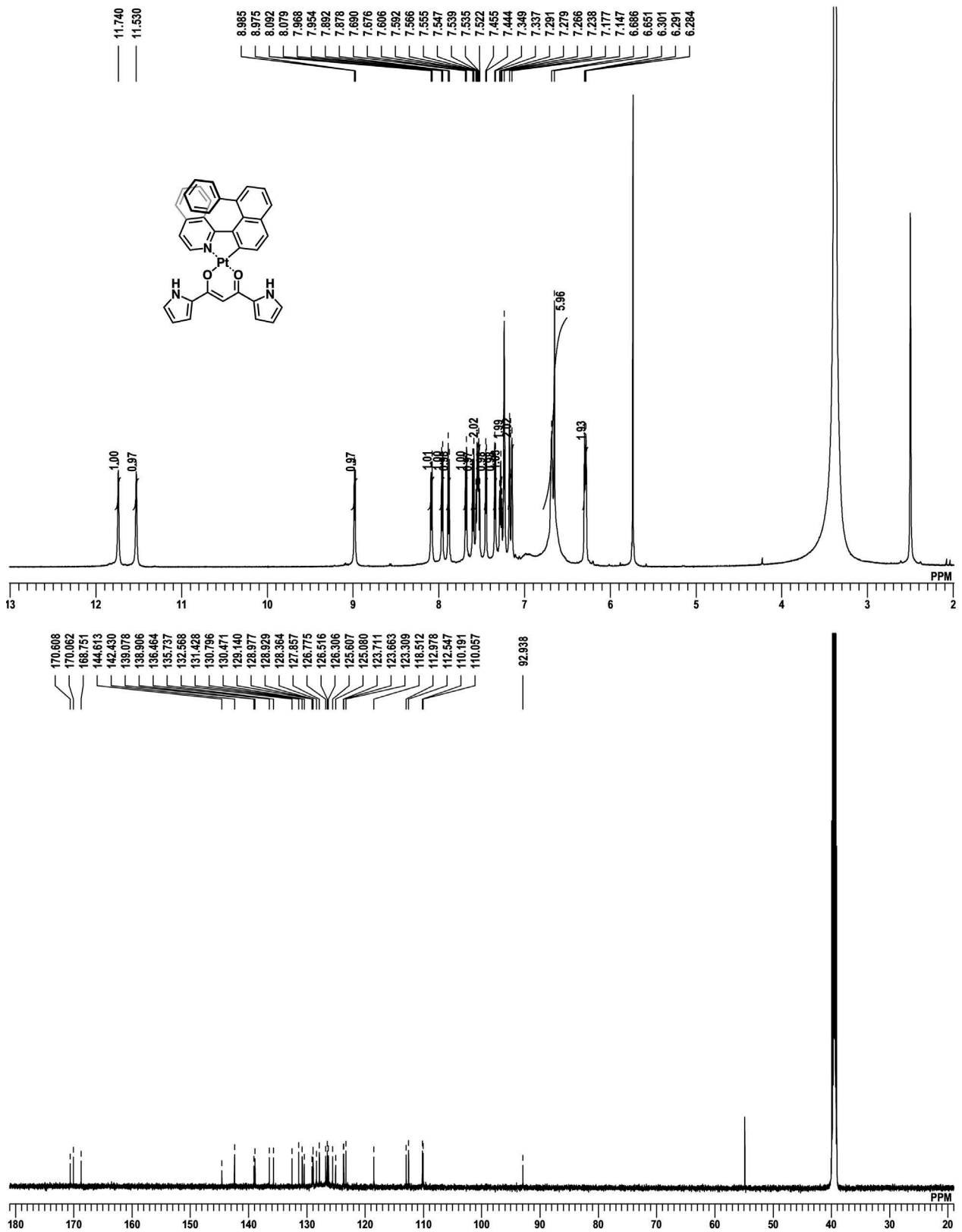

Fig. S2 ^{1}H NMR (top) and ^{13}C{^{1}H} NMR (bottom) spectra of **3a** in DMSO-d_6.

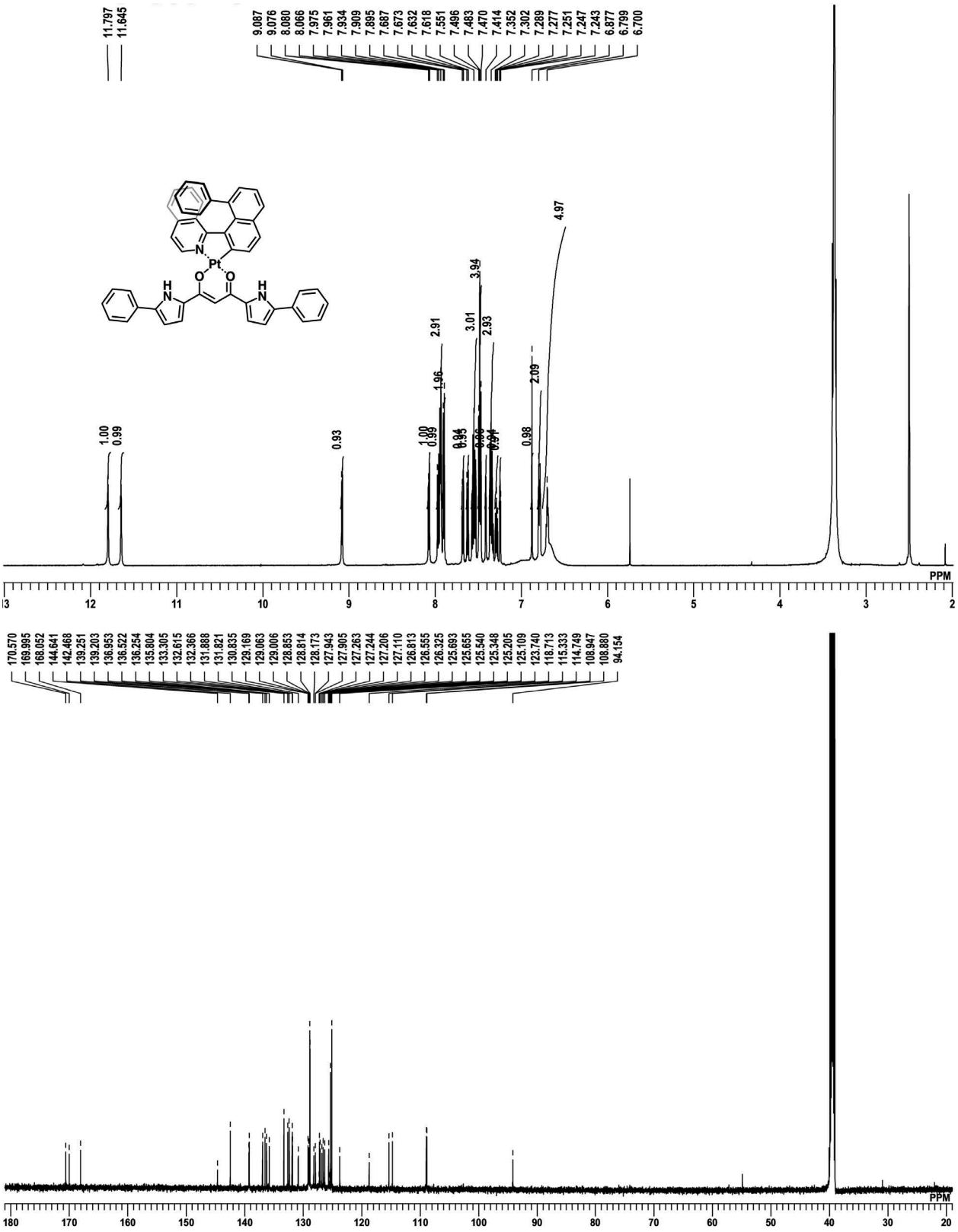

Fig. S3 ^{1}H NMR (top) and ^{13}C{^{1}H} NMR (bottom) spectra of **3b** in DMSO-d_6.

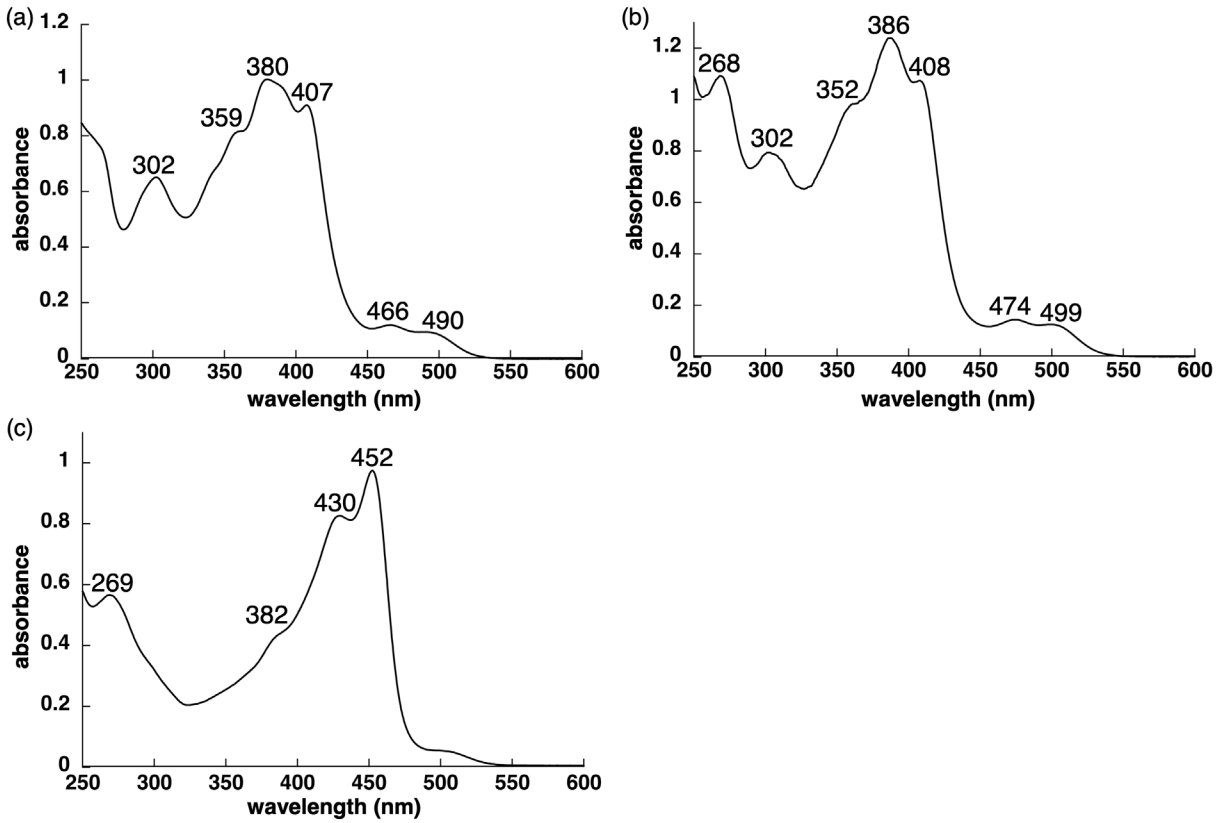

Fig. S4 UV/vis absorption spectra of (a) **2a** (0.03 mM), (b) **3a** (0.03 mM), and (c) **3b** (0.015 mM) in CH_2Cl_2.

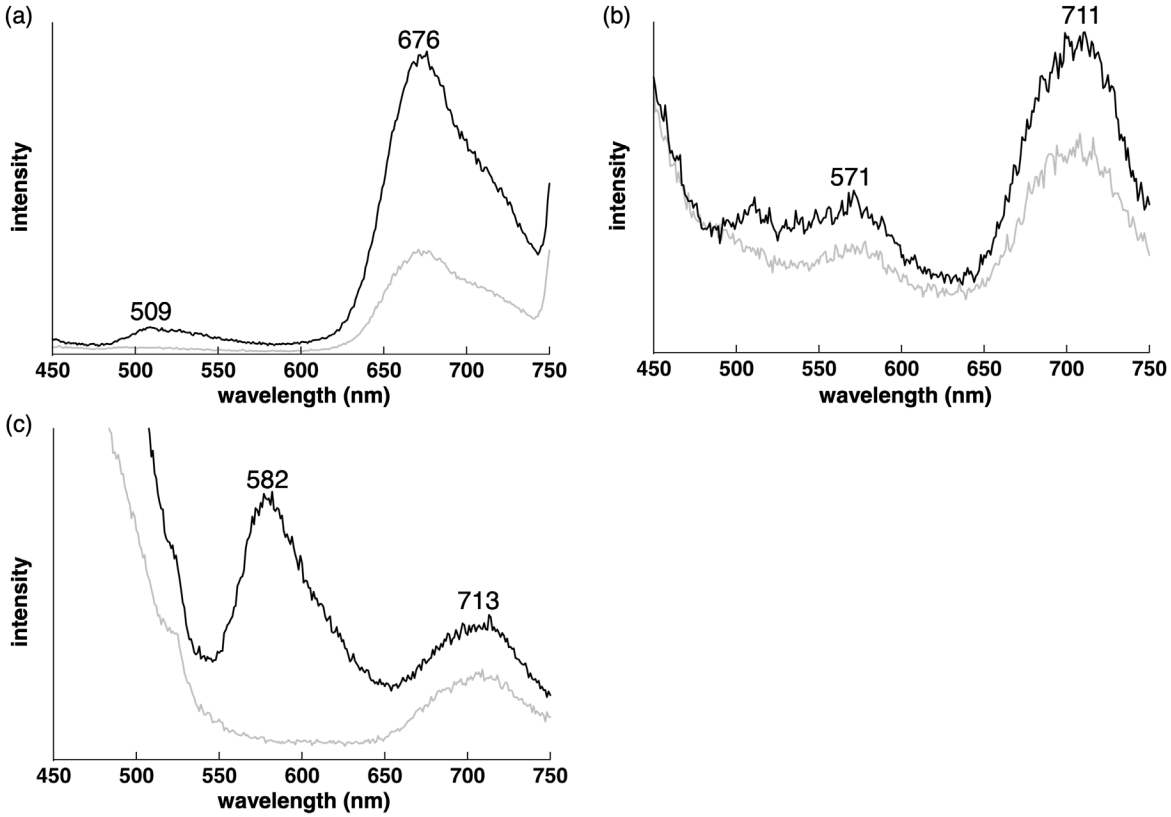

Fig. S5 Emission spectra of (a) **2a** (λ_{ex} = 380 nm), (b) **3a** (λ_{ex} = 387 nm), and (c) **3b** (λ_{ex} = 452 nm) in deoxygenated CH_2Cl_2 (black) and non-deoxygenated CH_2Cl_2 (gray) (0.03 mM) at r.t. Emission quantum yields (Φ_{em}) of **2a** and **3a** in deoxygenated CH_2Cl_2 at 20 °C were 1.1% and 0.5%, respectively, whereas Φ_{em} of **3b** was too low to determine.

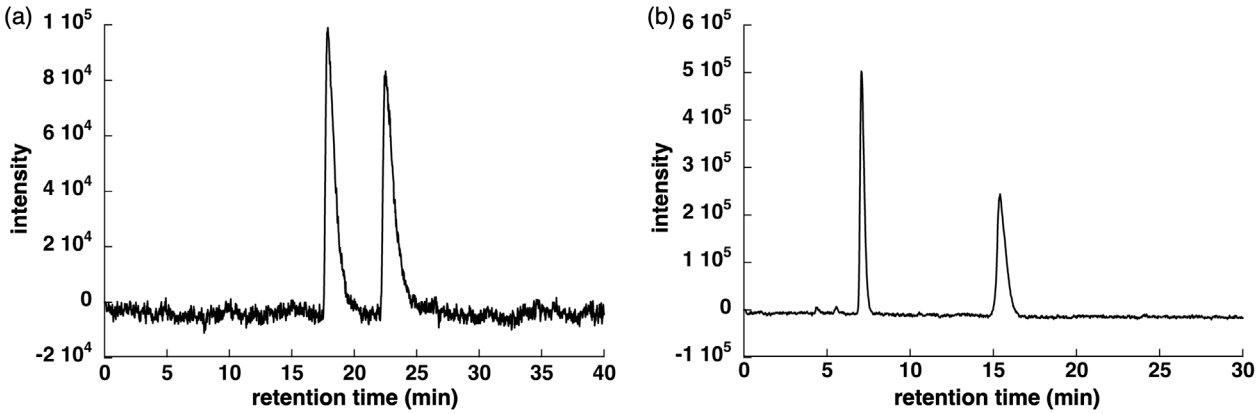

Fig. S6 Chiral HPLC profiles of dipyrrolyldiketone Pt^{II} complexes (Daicel CHIRALPAK IA, flow rate: 1.0 mL/min): (a) **3a** using CH_2Cl_2/*n*-hexane (1:1) as an eluent (monitored at 386 nm) and (b) **3b** using CH_2Cl_2/*n*-hexane (5:1) as an eluent (monitored at 452 nm).

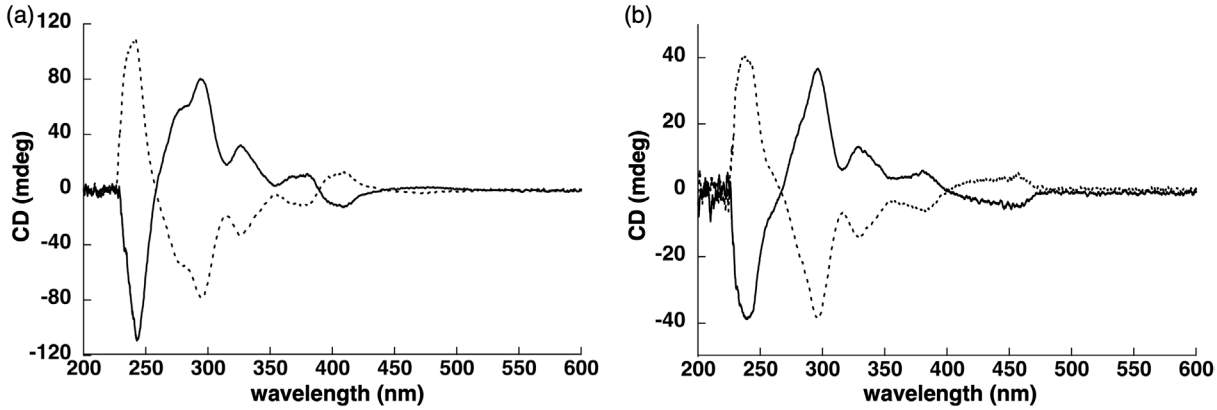

Fig. S7 CD spectra of (a) **3a** and (b) **3b** in CH_2Cl_2 (0.03 and 0.015 mM, respectively) after the separation of enantiomers. In (a), the solid and dotted lines correspond to the first and second fractions, respectively, whereas, in (b), dotted and solid lines correspond to the first and second fractions, respectively, in chiral HPLC separation (Fig. S6). Theoretical calculations for the CD spectra suggested that, in both Pt^{II} complexes, the solid and dotted lines are ascribable to *P*-type and *M*-type helices, respectively (Fig. S29).

2. X-ray crystallographic data

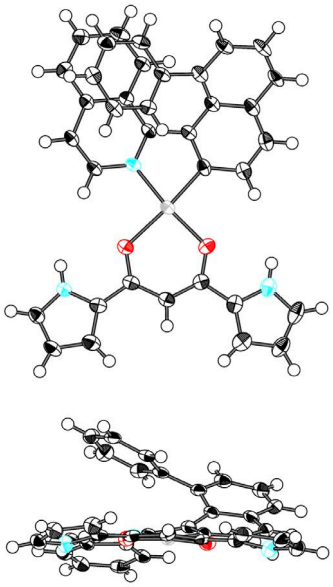

Fig. S8 Ortep drawings of single-crystal X-ray structure (top and side views) of **3a** in the form of the *P*-type helix as a representative. Thermal ellipsoids are scaled to the 50% probability level. Solvent molecules are omitted for clarity. Atom color code: black, white (sphere), blue, red, and gray refer to carbon, hydrogen, nitrogen, oxygen, and platinum, respectively.

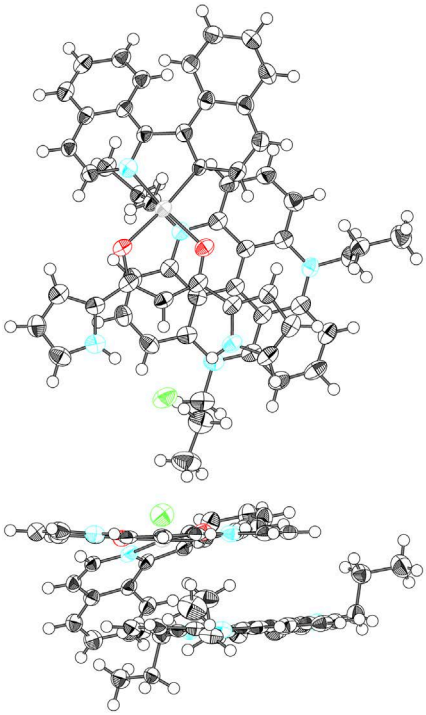

Fig. S9 Ortep drawings of single-crystal X-ray structure (top and side views) of **2a**·Cl^{-}-$TATA^{+}$ in the form of the *P*-type helix as a representative. Thermal ellipsoids are scaled to the 50% probability level. Atom color code: black, white (sphere), blue, red, yellow green, and gray refer to carbon, hydrogen, nitrogen, oxygen, chlorine, and platinum, respectively.

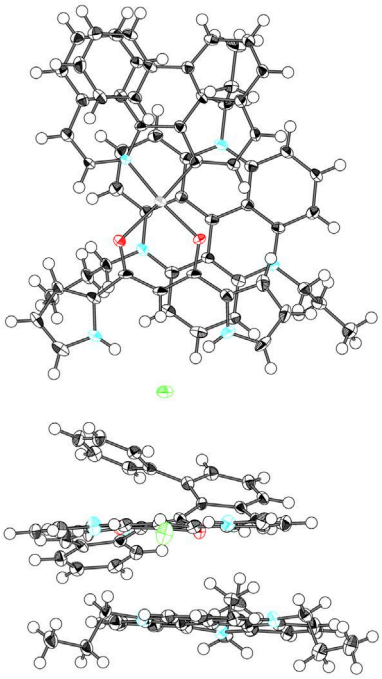

Fig. S10 Ortep drawings of single-crystal X-ray structure (top and side views) of **3a**·Cl^{-}-$TATA^{+}$ in the form of the *P*-type helix as a representative. Thermal ellipsoids are scaled to the 50% probability level. Solvent molecules are omitted for clarity. Atom color code: black, white (sphere), blue, red, yellow green, and gray refer to carbon, hydrogen, nitrogen, oxygen, chlorine, and platinum, respectively.

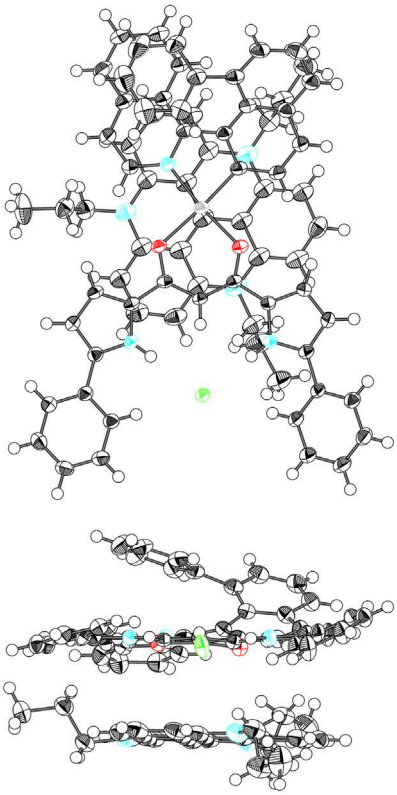

Fig. S11 Ortep drawings of single-crystal X-ray structure (top and side views) of **3b**·Cl^{-}-$TATA^{+}$ in the form of the *P*-type helix as a representative. Thermal ellipsoids are scaled to the 50% probability level. Solvent molecules are omitted for clarity. Atom color code: black, white (sphere), blue, red, yellow green, and gray refer to carbon, hydrogen, nitrogen, oxygen, chlorine, and platinum, respectively.

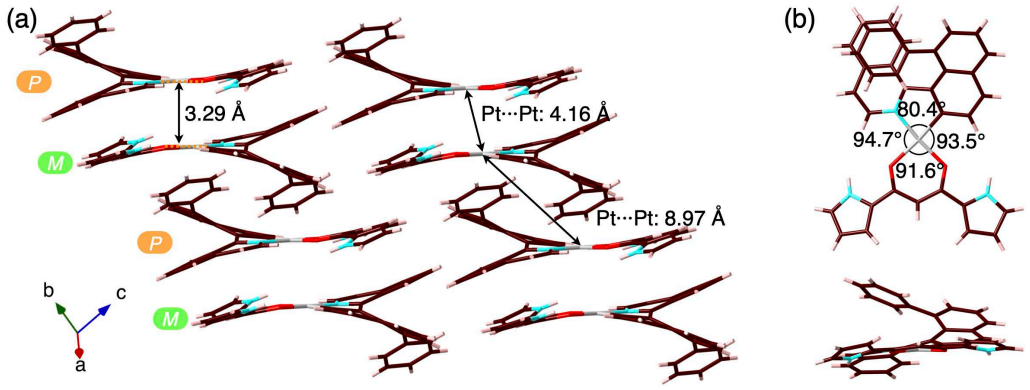

Fig. S12 Packing diagrams of **3a**: (a) side view of the packing structure and (b) enlarged top and side views of the constituting monomer. The distance between two **3a** mean planes (core five atoms of OOPtNC) is 3.29 Å with the Pt···Pt distances of 8.97 and 4.16 Å. The stacked dimer of **3a** is composed of the *P*- and *M*-type helices. The angles around Pt are 80.4°, 93.5°, 91.6°, and 94.7°. The τ_4 value,[S1] which serves as a geometry index for the four-coordinate Pt complex, is 0.09, suggesting an almost square planar structure. The colors orange and green in (a) represent *P*- and *M*-helical enantiomers, respectively. Atom color code: brown, pink, blue, red, and gray refer to carbon, hydrogen, nitrogen, oxygen, and platinum, respectively.

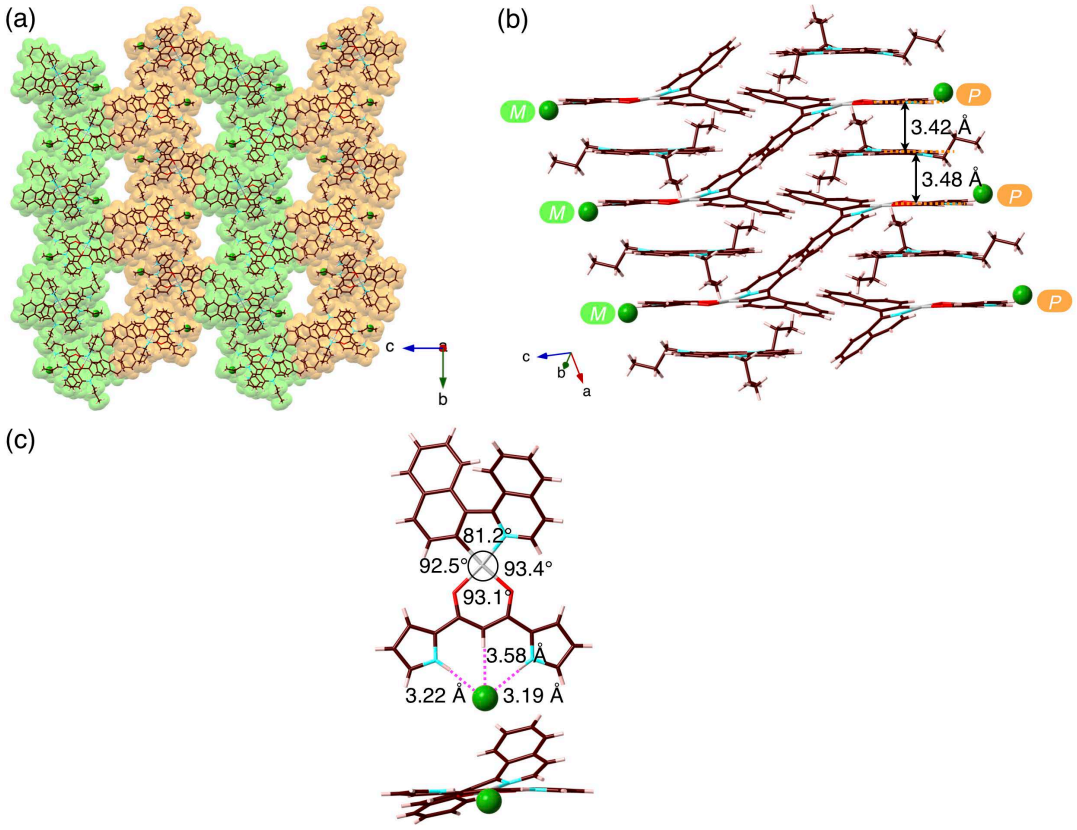

Fig. S13 Packing diagrams of **2a**·Cl^--$TATA^+$: (a) top view of the charge-by-charge assembly, (b) side view of the charge-by-charge columnar structure, and (c) top and side views of **2a**·Cl^-. The distances between the $TATA^+$ mean planes (core 22 atoms) and the dipyrrolyldiketone Pt^{II} complex units with Cl^- (17 atoms) are 3.42 and 3.48 Å. Each charge-by-charge column is composed of either of the enantiomers. The N(–H)···Cl^- and $C_{bridging}$(–H)···Cl^- hydrogen-bonding distances are 3.19/3.22 and 3.58 Å, respectively. The τ_4 value,[S1] which serves as geometry indices for the four-coordinate Pt complex, is 0.11, suggesting almost square planar structures. The colors orange and green in (a) represent *P*- and *M*-helical enantiomers, respectively. Atom color code: brown, pink, cyan, red, yellow green (spherical), and gray refer to carbon, hydrogen, nitrogen, oxygen, chlorine, and platinum, respectively.

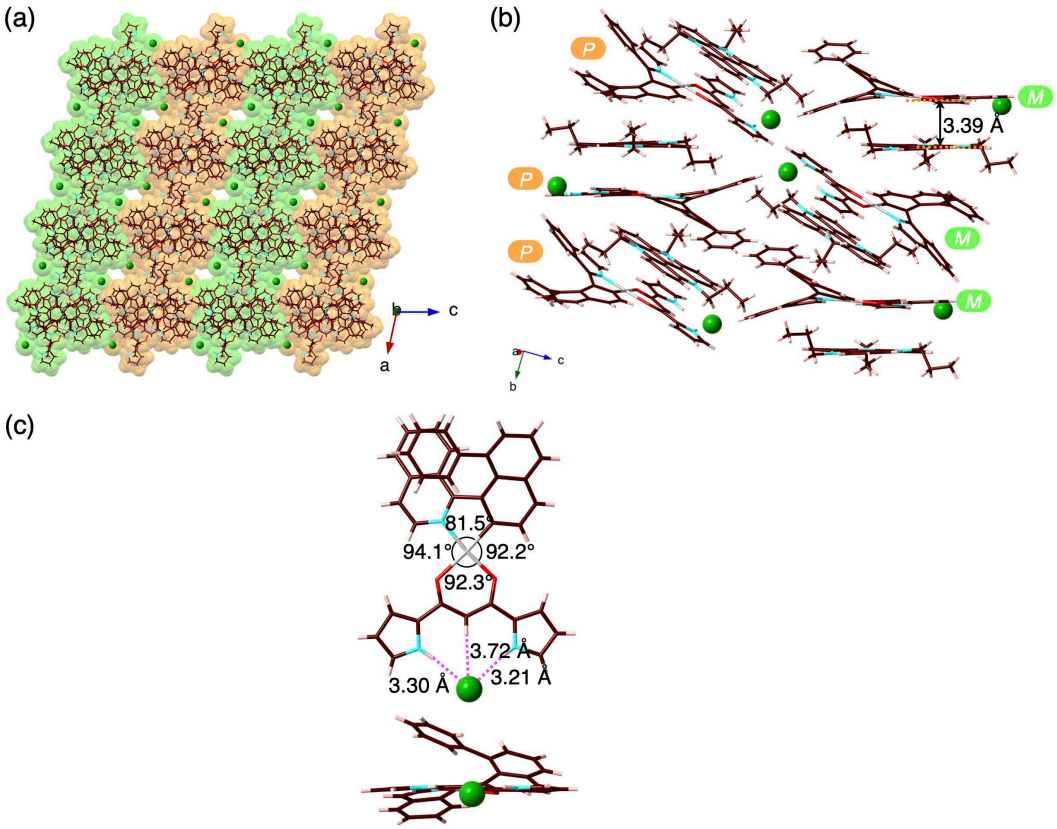

Fig. S14 Packing diagrams of **3a**·Cl^{-}-$TATA^{+}$: (a) top view of the charge-by-charge assembly, (b) side view of the charge-by-charge columnar structure, and (c) top and side views of **3a**·Cl^{-}. The distances between the $TATA^{+}$ mean planes (core 22 atoms) and the dipyrrolyldiketone Pt^{II} complex units with Cl^{-} (17 atoms) are 3.39 Å. Each charge-by-charge column is composed of either of the enantiomers. The N(–H)···Cl^{-} and $C_{bridging}$(–H)···Cl^{-} hydrogen-bonding distances are 3.30/3.21 and 3.72 Å, respectively. The τ_4 value,[S1] which serves as a geometry index for the four-coordinate Pt complex, is 0.09, suggesting an almost square planar structure. The colors orange and green in (a) represent *P*- and *M*-helical enantiomers, respectively. Atom color code: brown, pink, cyan, red, yellow green (spherical), and gray refer to carbon, hydrogen, nitrogen, oxygen, chlorine, and platinum, respectively.

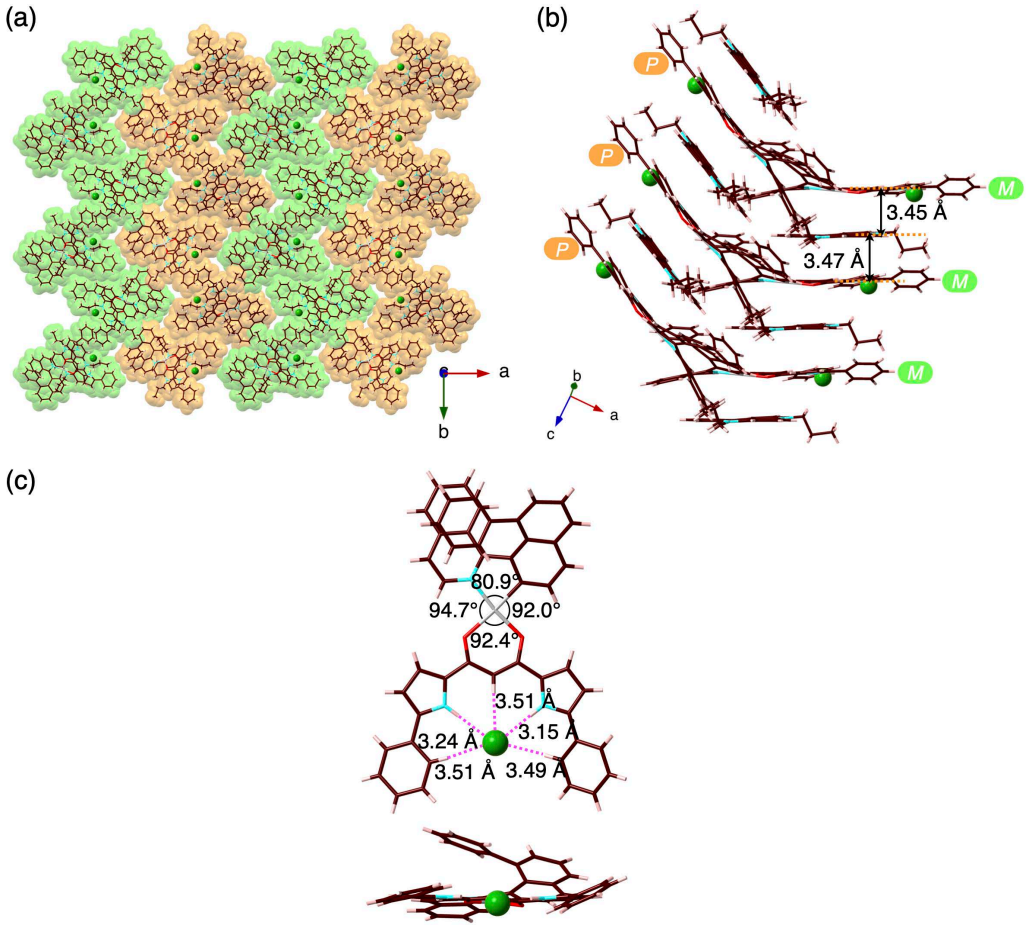

Fig. S15 Packing diagrams of **3b**·Cl^{-}-$TATA^{+}$: (a) top view of the charge-by-charge assembly, (b) side view of the charge-by-charge columnar structure, and (c) top and side views of **3b**·Cl^{-}-$TATA^{+}$. The distances between the $TATA^{+}$ mean planes (core 22 atoms) and the dipyrrolyldiketone Pt^{II} complex units with Cl^{-} (29 atoms) are 3.45 and 3.47 Å with the Pt···Pt distance of 8.48 Å. Each charge-by-charge column is composed of either of the enantiomer. The N(–H)···Cl^{-}, $C_{bridging}$(–H)···Cl^{-}, and *o*-C_{phenyl}(–H)···Cl^{-} hydrogen-bonding distances are 3.24/3.15, 3.51, and 3.51/3.49 Å, respectively. The τ_4 value,[S1] which serves as a geometry index for the four-coordinate Pt complex, is 0.09, suggesting an almost square planar structure. The colors orange and green in (a) represent *P*- and *M*-helical enantiomers, respectively. Atom color code: brown, pink, cyan, red, yellow green (spherical), and gray refer to carbon, hydrogen, nitrogen, oxygen, chlorine, and platinum, respectively.

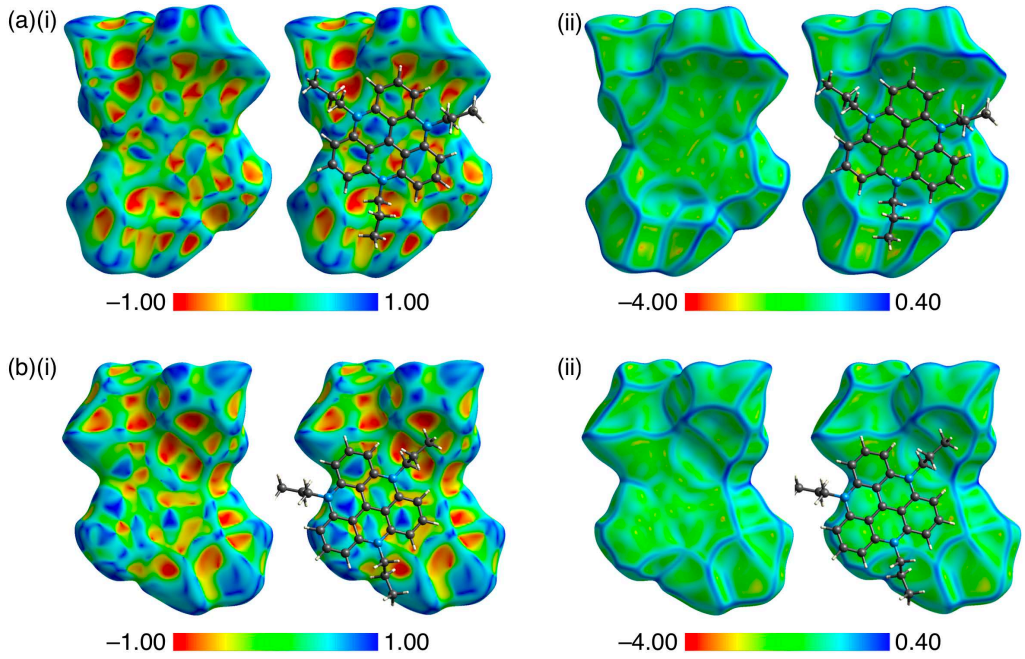

Fig. S16 Hirshfeld surfaces[S2] of **2a**·Cl^- (independent structures (a,b) and (c,d), wherein (b,d) show different sides of (a,c)) in the crystal structure of **2a**·Cl^--$TATA^+$ mapped over (i) shape-index and (ii) curvedness properties for only surface (left) and surface with a ball-and-stick model of the neighboring $TATA^+$ (right). Shape index is a qualitative measure of shape and is sensitive to subtle changes in surface shape, particularly in a flat region by differing by signs representing complementary bumps (blue) and hollows (red), whereas curvedness is a function of the root-mean-square curvature of the surface, and maps of curvedness typically show large regions of green (relatively flat) separated by dark blue edges (large positive curvature). The flat region on the curvedness surface suggested the characteristic mapping pattern for stacking between $TATA^+$ and **2a**·Cl^-.

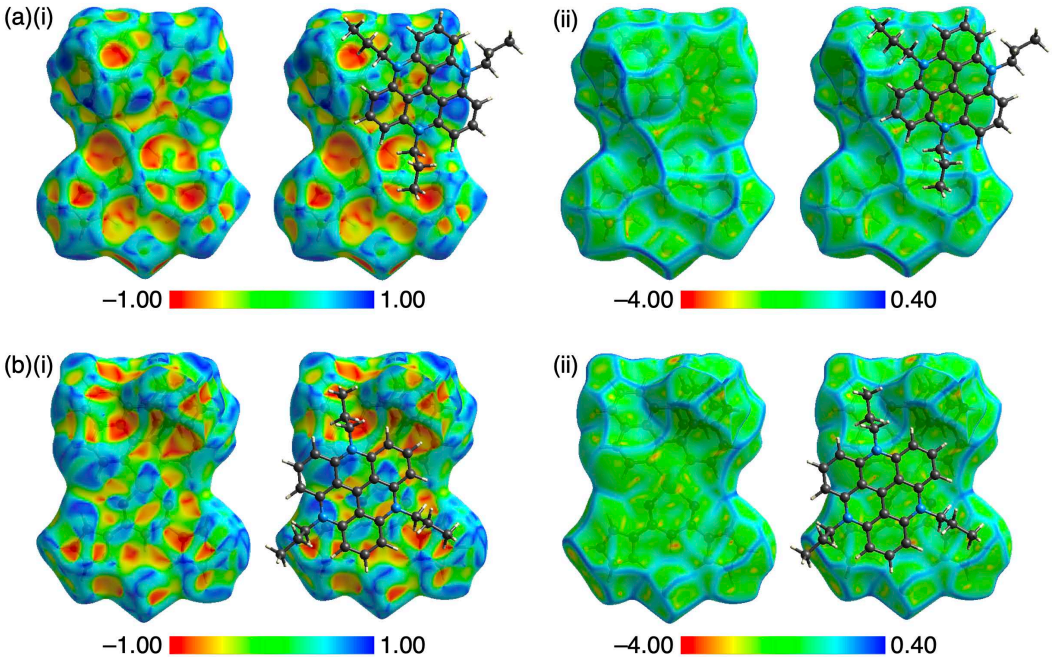

Fig. S17 Hirshfeld surfaces[S2] of **3a**·Cl^- ((a,b) for different sides) in the crystal structure of **3a**·Cl^--$TATA^+$ mapped over (i) shape-index and (ii) curvedness properties for only surface (left) and surface with a ball-and-stick model of the neighboring $TATA^+$ (right). Shape index is a qualitative measure of shape and is sensitive to subtle changes in surface shape, particularly in a flat region by differing by signs representing complementary bumps (blue) and hollows (red), whereas curvedness is a function of the root-mean-square curvature of the surface, and maps of curvedness typically show large regions of green (relatively flat) separated by dark blue edges (large positive curvature). The flat region on the curvedness surface suggested the characteristic mapping pattern for stacking between $TATA^+$ and **3a**·Cl^-.

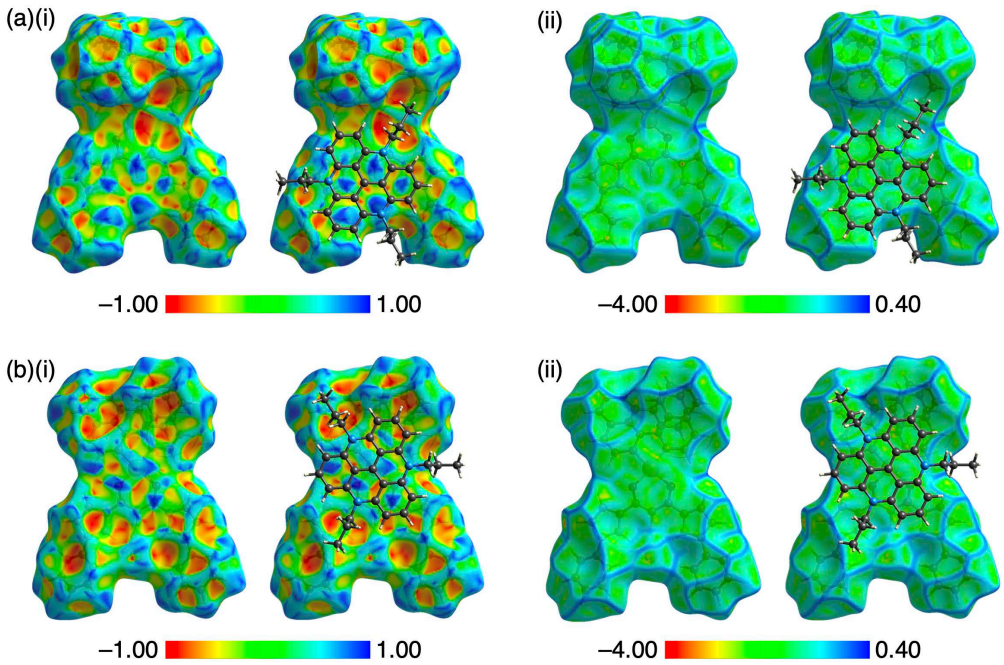

Fig. S18 Hirshfeld surfaces[S2] of **3b**·Cl^- ((a,b) for different sides) in the crystal structure of **3b**·Cl^--$TATA^+$ mapped over (i) shape-index and (ii) curvedness properties for only surface (left) and surface with a ball-and-stick model of the neighboring $TATA^+$ (right). Shape index is a qualitative measure of shape and is sensitive to subtle changes in surface shape, particularly in a flat region by differing by signs representing complementary bumps (blue) and hollows (red), whereas curvedness is a function of the root-mean-square curvature of the surface, and maps of curvedness typically show large regions of green (relatively flat) separated by dark blue edges (large positive curvature). The flat region on the curvedness surface suggested the characteristic mapping pattern for stacking between $TATA^+$ and **3b**·Cl^-.

[S1] L. Yang, D. R. Powell and R. P. Houser, *Dalton Trans.*, 2007, 955–964.
[S2] P. R. Spackman, M. J. Turner, J. J. McKinnon, S. K. Wolff, D. J. Grimwood, D. Jayatilaka and M. A. Spackman, *J. Appl. Cryst.*, 2021, **54**, 1006–1011.

3. Theoretical Studies

Computational Method. Calculations were performed using the *Gaussian 16* program.[S3] The ground states (S_0) and excited triplet states (T_1) were optimized at the B3LYP level by using 6-31G(d,p) basis set for C, H, N, O, and Cl and the LanL2DZ basis set and associated effective core potentials for Pt, whereas the excited singlet states (S_1) were optimized using the TD-DFT calculations at the same level to the ground states. For the discussion on the low phosphorescence intensities of the Pt^{II} complexes, T_1 were optimized at the TD-CAM-B3LYP level within the Tamm-Dancoff approximation by using 6-31+G(d,p) basis set for C, H, N, and O and the LanL2DZ basis set and associated effective core potentials for Pt. The solvent effect of CH_2Cl_2 was considered using a polarizable continuum model (PCM).

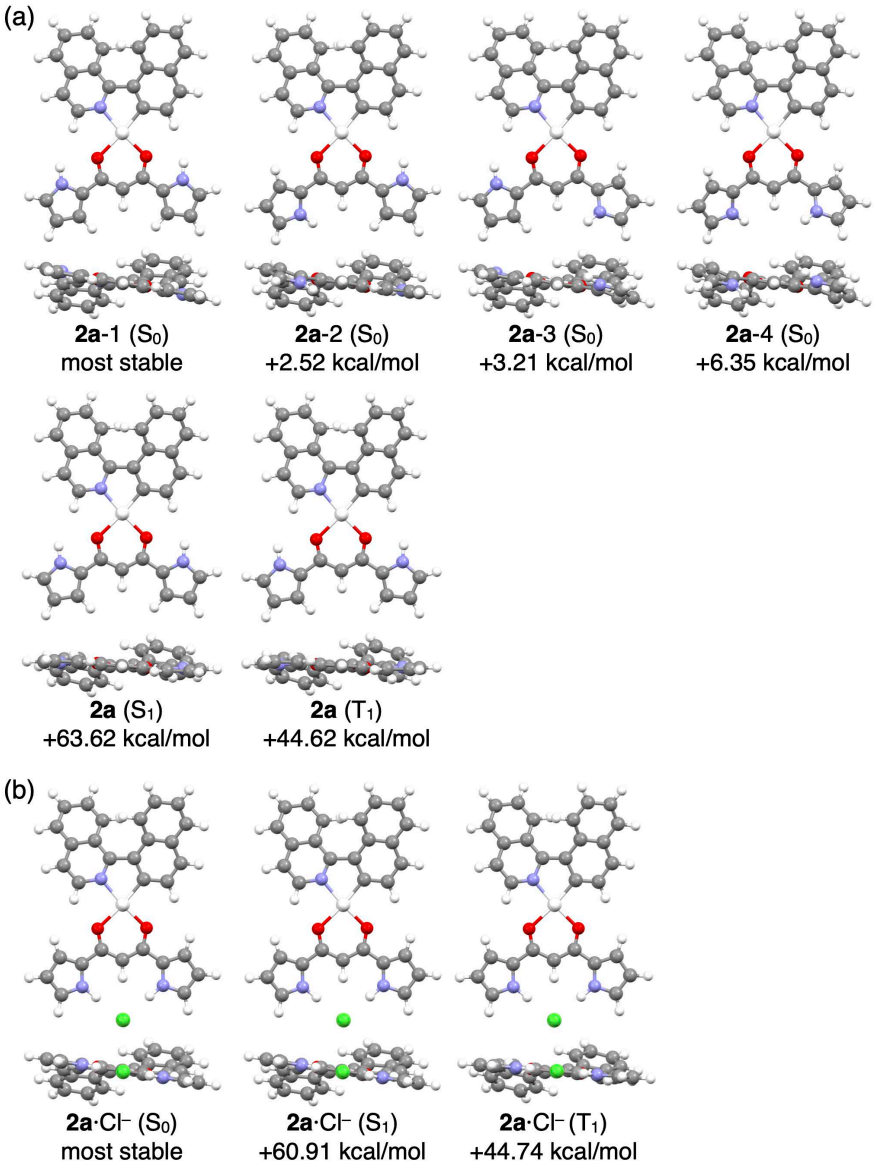

Fig. S19 Optimized structures and relative energies of (a) **2a** (four conformations for S_0) and (b) **2a**·Cl^-, calculated as *P*-tyle helices, in the ground (S_0) state and singlet (S_1) and triplet (T_1) excited states.

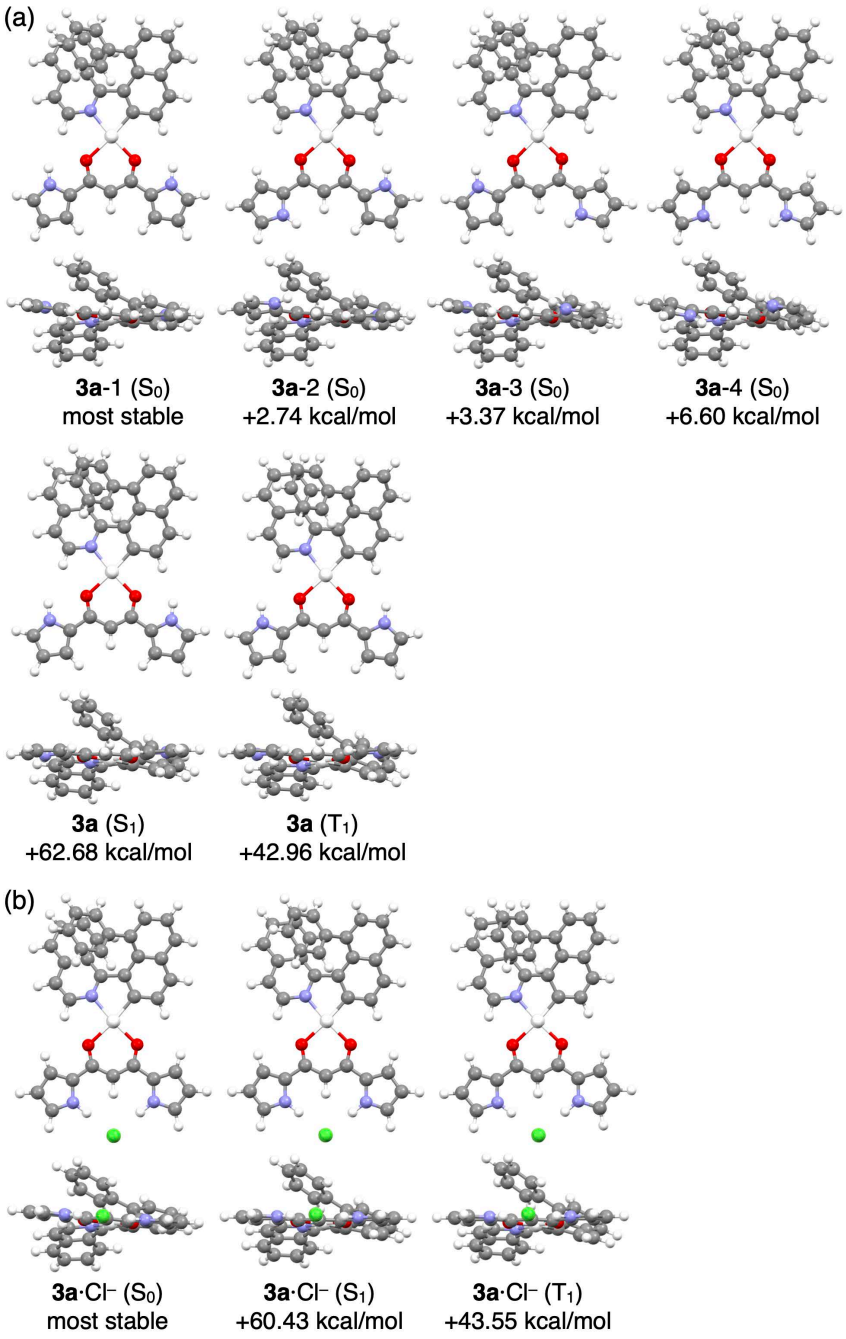

Fig. S20 Optimized structures and relative energies of (a) **3a** (four conformations for S_0) and (b) **3a**·Cl^-, calculated as *P*-tyle helices, in the ground (S_0) state and singlet (S_1) and triplet (T_1) excited states.

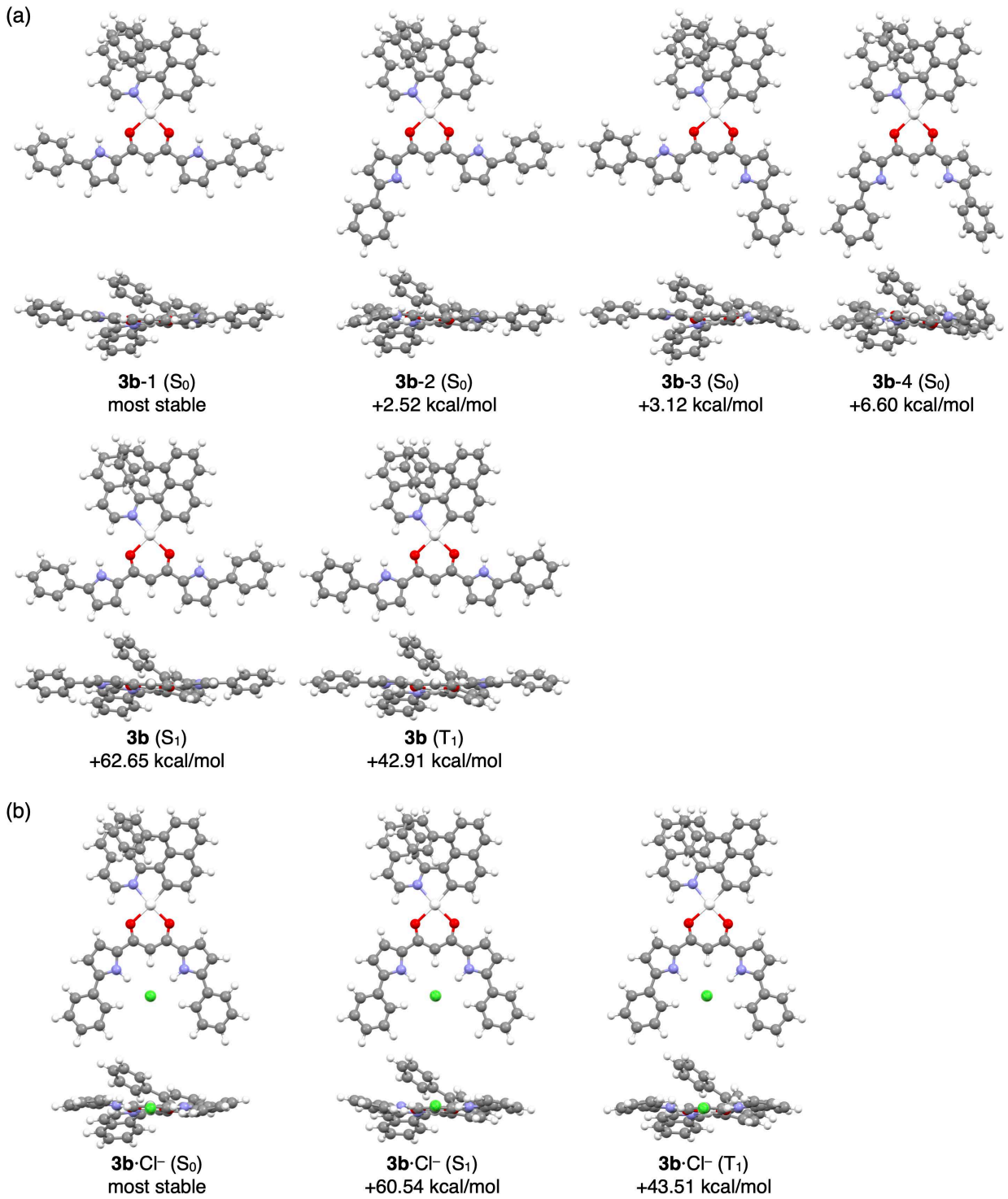

Fig. S21 Optimized structures and relative energies of (a) **3b** (four conformations for S_0) and (b) **3b**·Cl^-, calculated as *P*-tyle helices, in the ground (S_0) state and singlet (S_1) and triplet (T_1) excited states.

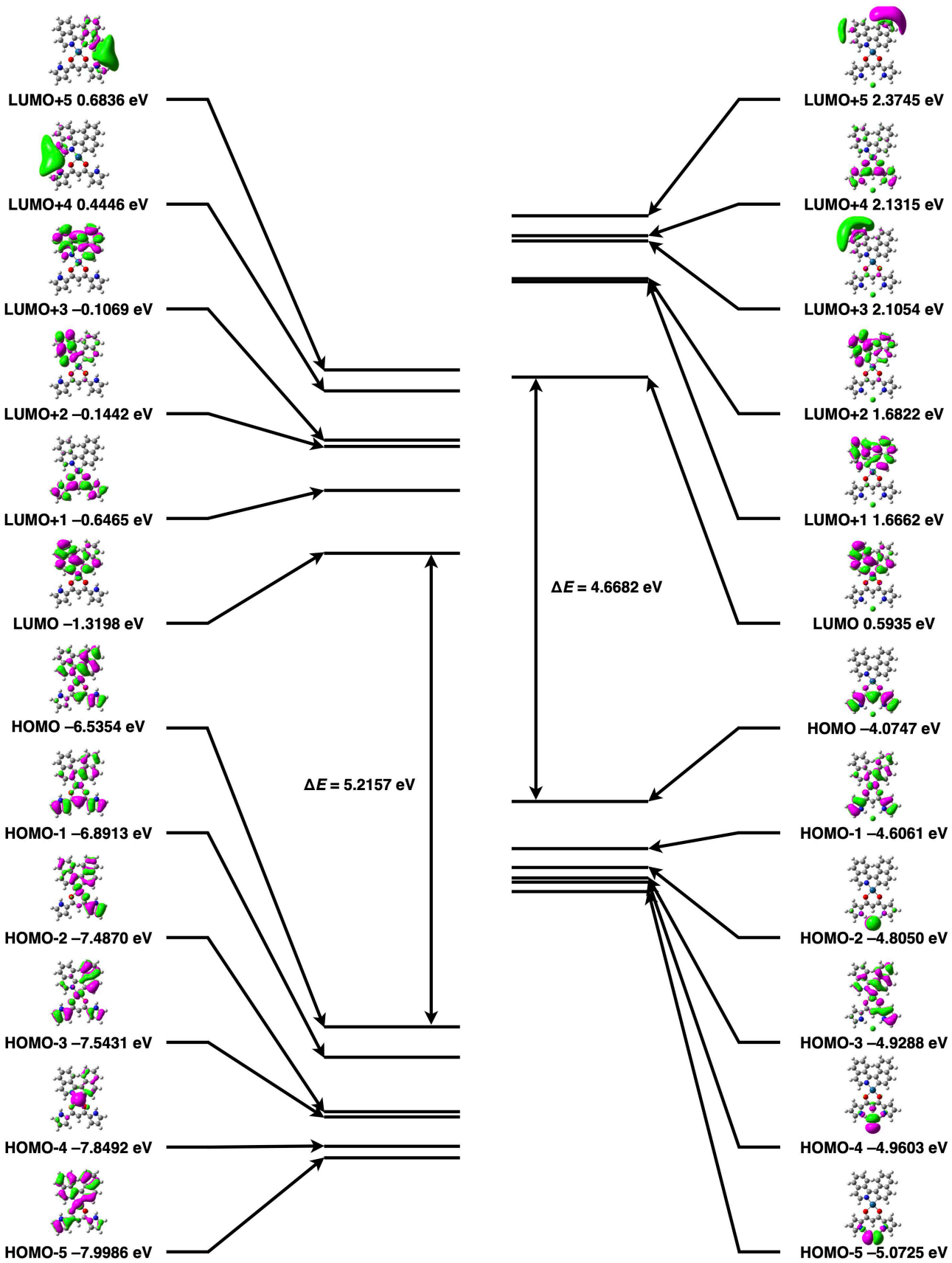

Fig. S22 Molecular orbitals (HOMO and LUMO) of **2a** (left) and **2a**·Cl^- (right) estimated at the CAM-B3LYP level by using 6-31+G(d,p) basis set for C, H, N, O, and Cl and the LanL2DZ basis set and associated effective core potentials for Pt.

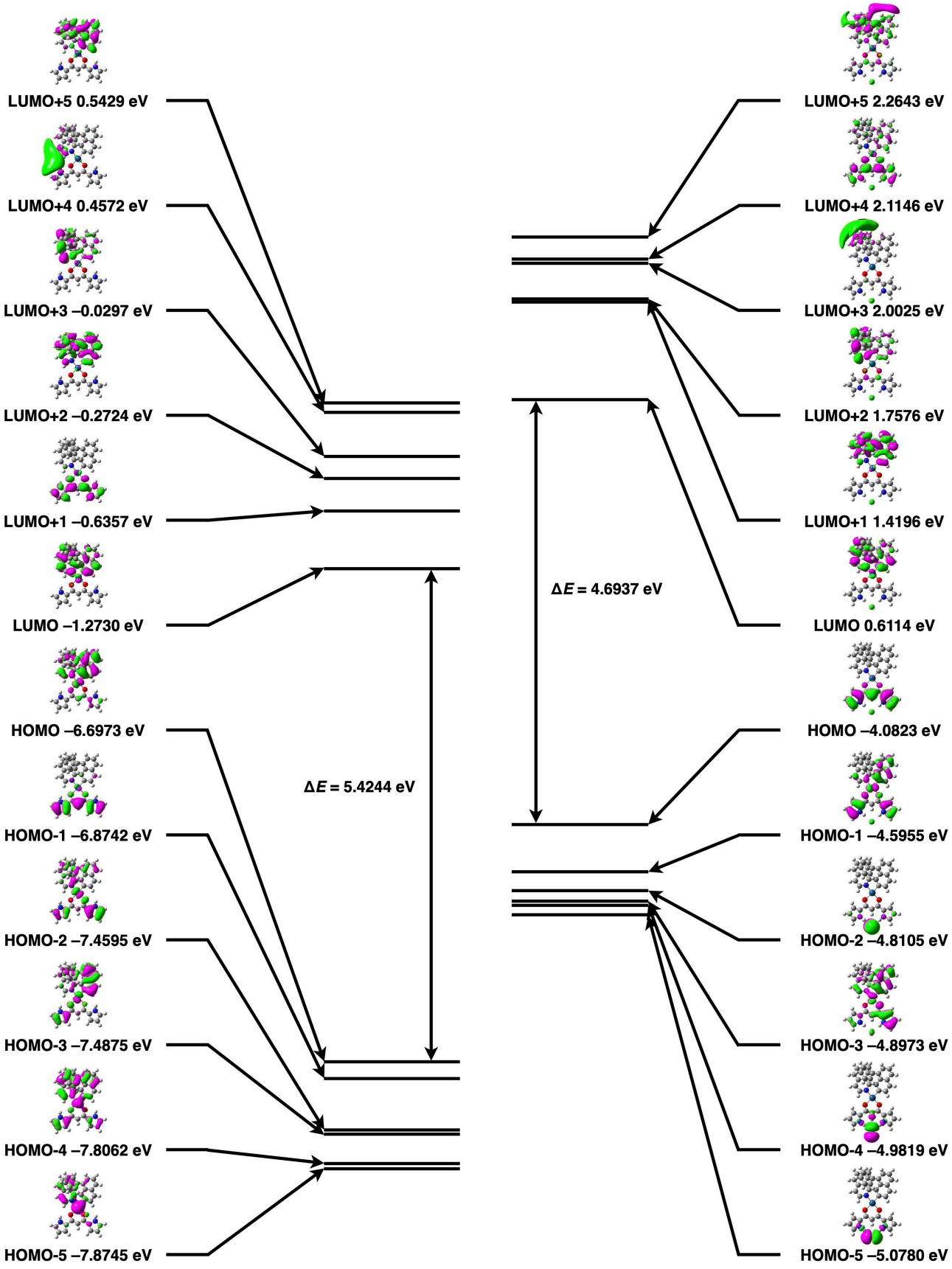

Fig. S23 Molecular orbitals (HOMO and LUMO) of **3a** (left) and **3a**·Cl^- (right) estimated at the CAM-B3LYP level by using 6-31+G(d,p) basis set for C, H, N, O, and Cl and the LanL2DZ basis set and associated effective core potentials for Pt.

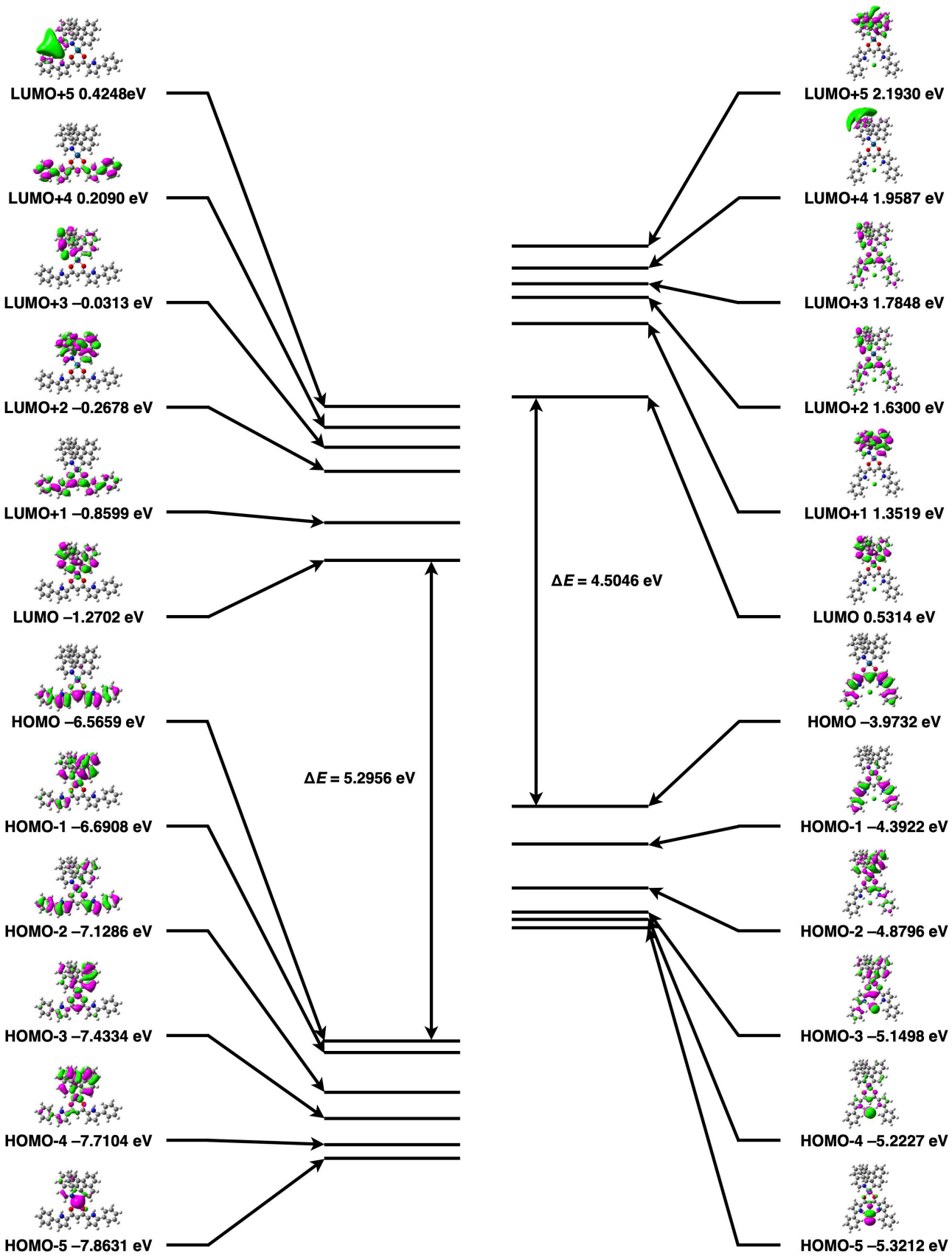

Fig. S24 Molecular orbitals (HOMO and LUMO) of **3b** (left) and **3b**·Cl^- (right) estimated at the CAM-B3LYP level by using 6-31+G(d,p) basis set for C, H, N, O, and Cl and the LanL2DZ basis set and associated effective core potentials for Pt.

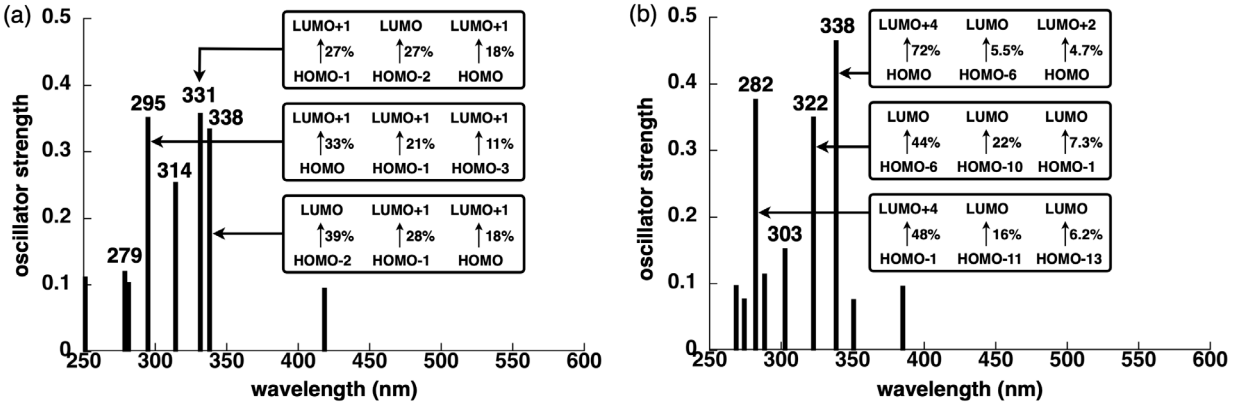

Fig. S25 TD-DFT-based UV/vis absorption stick spectra of (a) **2a** and (b) **2a**·Cl^- with the transitions correlated with molecular orbitals estimated at the CAM-B3LYP level by using 6-31+G(d,p) basis set for C, H, N, and O and the LanL2DZ basis set and associated effective core potentials for Pt.

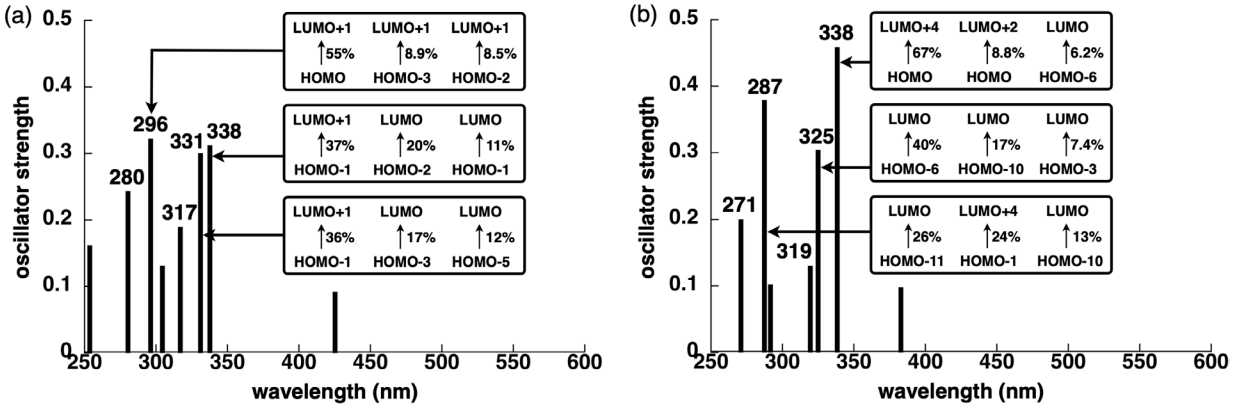

Fig. S26 TD-DFT-based UV/vis absorption stick spectra of (a) **3a** and (b) **3a**·Cl^- with the transitions correlated with molecular orbitals estimated at the CAM-B3LYP level by using 6-31+G(d,p) basis set for C, H, N, and O and the LanL2DZ basis set and associated effective core potentials for Pt.

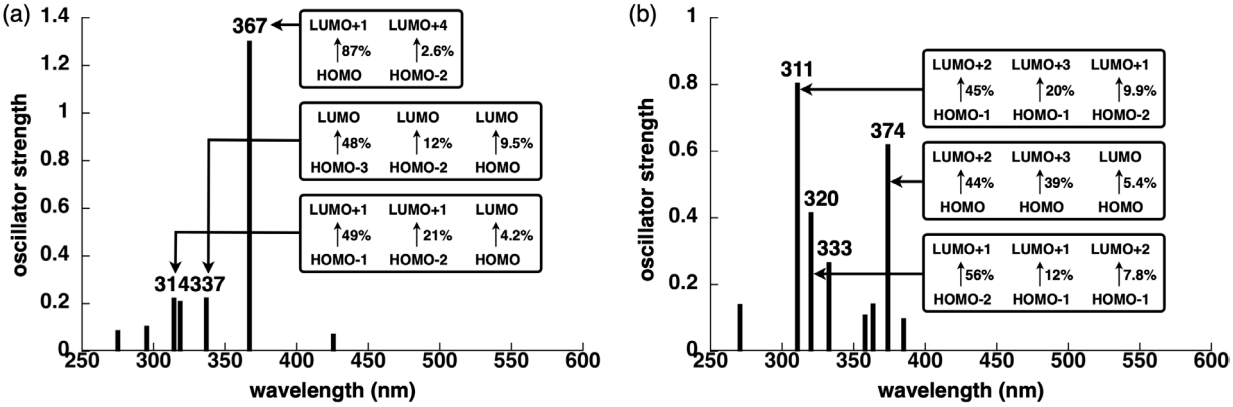

Fig. S27 TD-DFT-based UV/vis absorption stick spectra of (a) **3b** and (b) **3b**·Cl^- with the transitions correlated with molecular orbitals estimated at the CAM-B3LYP level by using 6-31+G(d,p) basis set for C, H, N, and O and the LanL2DZ basis set and associated effective core potentials for Pt.

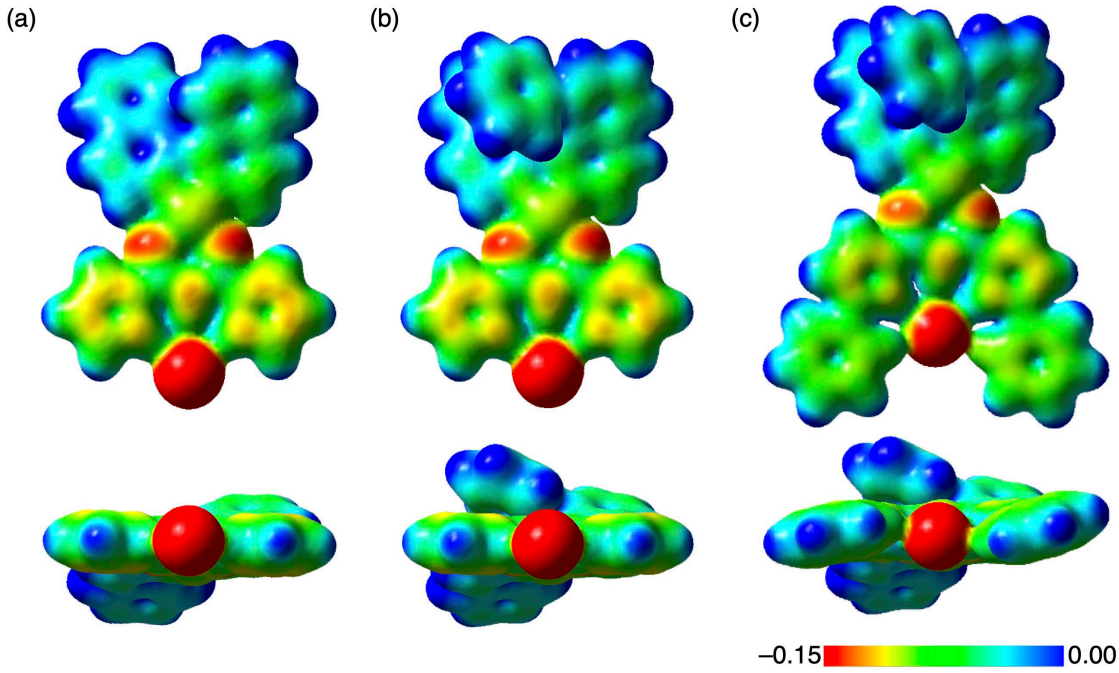

Fig. S28 Electrostatic potential (ESP) mapping (δ = 0.01) of (a) **2a**·Cl^-, (b) **3a**·Cl^-, and (c) **3b**·Cl^- calculated at the CAM-B3LYP level by using 6-31+G(d,p) basis set for C, H, N, O, and Cl and the LanL2DZ basis set and associated effective core potentials for Pt.

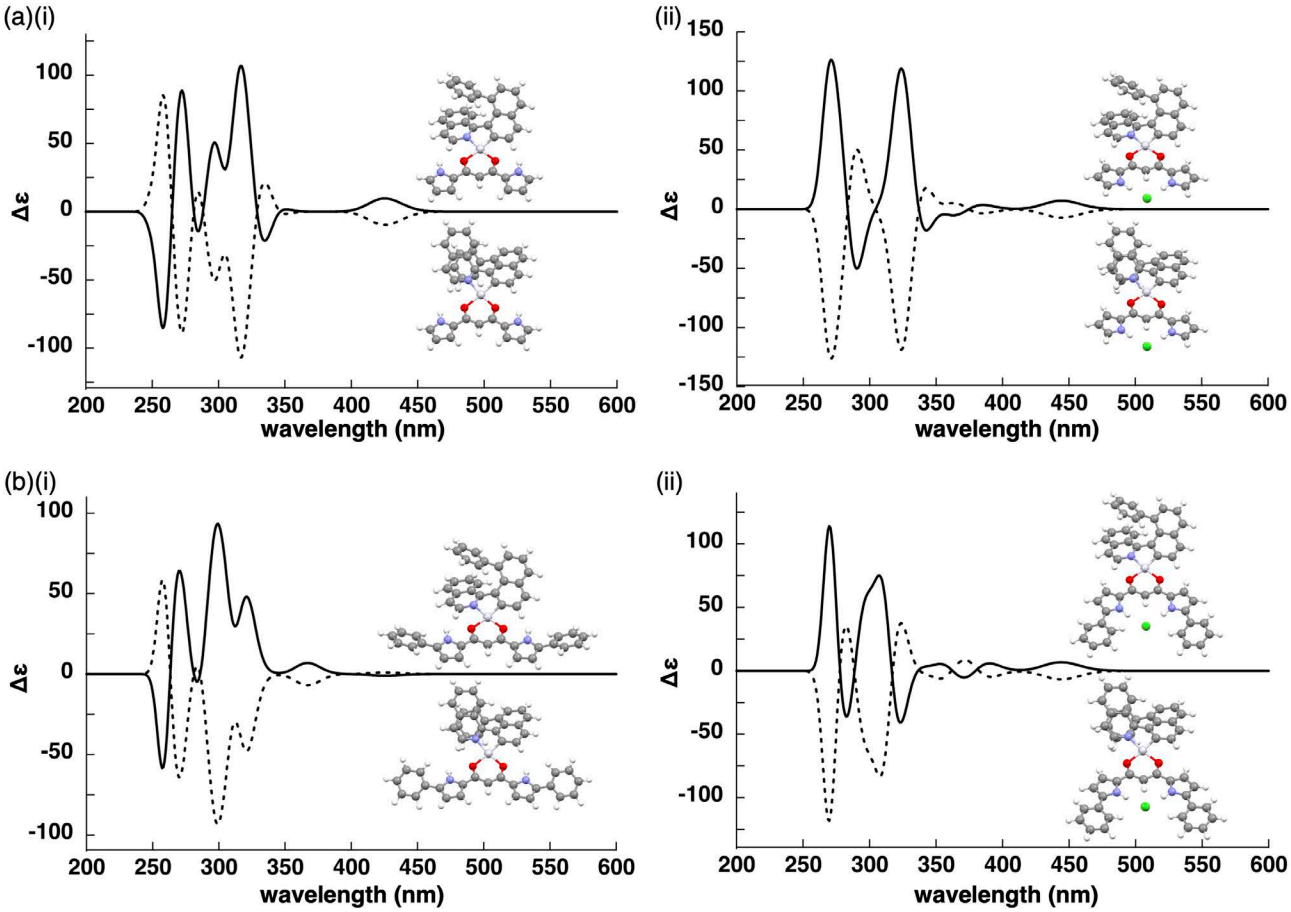

Fig. S29 Theoretical CD spectra of dipyrrolyldiketone Pt^{II} complexes estimated by using TD-DFT calculation at CAM-B3LYP/6-31+G(d,p) level: (a) **3a** and (b) **3b** for (i) Cl^--free states and (ii) Cl^- complexes (*P* helix: solid line; *M* helix: dotted line).

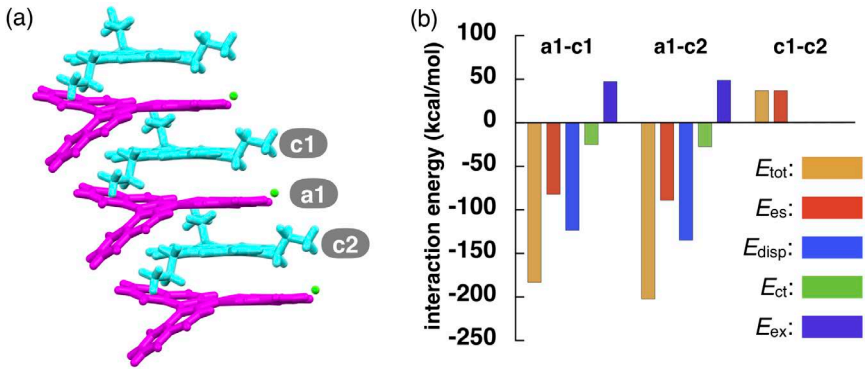

Fig. S30 Single-crystal X-ray structure of **2a**·Cl^{-}-$TATA^{+}$ for the EDA calculations (Table S1): (a) single-crystal X-ray structure and (b) intermolecular interaction energies (kcal/mol) between selected ions estimated at an FMO2-MP2 using mixed basis sets including NOSeC-V-TZP for Pt and NOSeC-V-DZP for the other atoms.[S4–6] The labels (c1–4 and a1,2) correspond to the fragments shown in Table S1.

Table S1 Energies between selected fragments in **2a**·Cl^{-}-$TATA^{+}$ (Fig. S30) estimated by EDA calculation based on an FMO2-MP2 using mixed basis sets including NOSeC-V-TZP for Pt and NOSeC-V-DZP for the other atoms.[S4–6]

fragments	total interaction energy (E_{tot}) (kcal/mol)	electrostatic interaction energy (E_{es}) (kcal/mol)	dispersion interaction energy (E_{disp}) (kcal/mol)	charge-transfer interaction energy (E_{ct+mix}) (kcal/mol)	exchange repulsion interaction energy (E_{ex}) (kcal/mol)
a1-c1	-183.318	-82.032	-123.371	-24.992	47.077
a1-c2	-202.377	-89.106	-134.735	-27.404	48.869
c1-c2	36.716	36.716	0.000	0.000	0.000

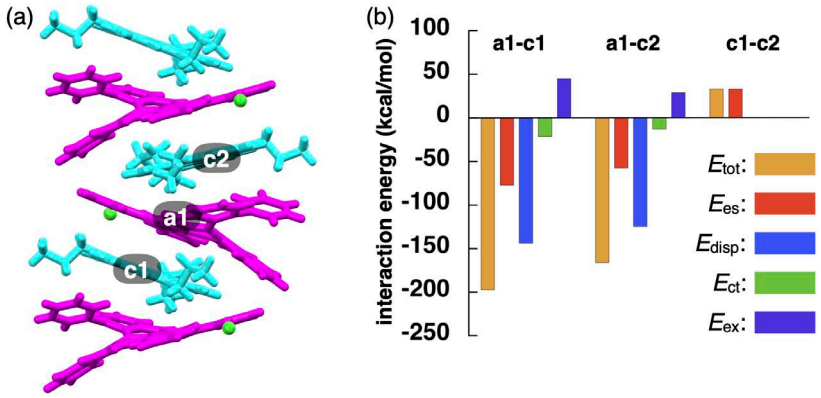

Fig. S31 Single-crystal X-ray structure of **3a**·Cl^{-}-$TATA^{+}$ for the EDA calculations (Table S2): (a) single-crystal X-ray structure and (b) intermolecular interaction energies (kcal/mol) between selected ions estimated at an FMO2-MP2 using mixed basis sets including NOSeC-V-TZP for Pt and NOSeC-V-DZP for the other atoms.[S4–6] The labels (c1,2 and a1) correspond to the fragments shown in Table S2.

Table S2 Energies between selected fragments in **3a**·Cl^{-}-$TATA^{+}$ (Fig. S31) estimated by EDA calculation based on an FMO2-MP2 using mixed basis sets including NOSeC-V-TZP for Pt and NOSeC-V-DZP for the other atoms.[S4–6]

fragments	total interaction energy (E_{tot}) (kcal/mol)	electrostatic interaction energy (E_{es}) (kcal/mol)	dispersion interaction energy (E_{disp}) (kcal/mol)	charge-transfer interaction energy (E_{ct+mix}) (kcal/mol)	exchange repulsion interaction energy (E_{ex}) (kcal/mol)
a1-c1	-197.553	-77.112	-143.814	-21.559	44.931
a1-c2	-166.012	-57.707	-124.570	-12.825	29.091
c1-c2	33.301	33.301	0.000	0.000	0.000

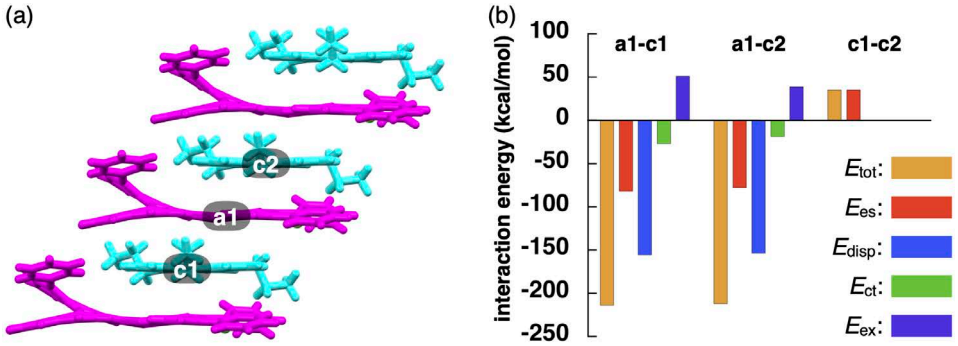

Fig. S32 Single-crystal X-ray structure of **3b**·Cl^--$TATA^+$ for the EDA calculations (Table S3): (a) single-crystal X-ray structure and (b) intermolecular interaction energies (kcal/mol) between selected ions estimated at an FMO2-MP2 using mixed basis sets including NOSeC-V-TZP for Pt and NOSeC-V-DZP for the other atoms.[S4–6] The labels (c1,2 and a1) correspond to the fragments shown in Table S3.

Table S3 Energies between selected fragments in **3b**·Cl^--$TATA^+$ (Fig. S32) estimated by EDA calculation based on an FMO2-MP2 using mixed basis sets including NOSeC-V-TZP for Pt and NOSeC-V-DZP for the other atoms.[S4–6]

fragments	total interaction energy (E_{tot}) (kcal/mol)	electrostatic interaction energy (E_{es}) (kcal/mol)	dispersion interaction energy (E_{disp}) (kcal/mol)	charge-transfer interaction energy (E_{ct+mix}) (kcal/mol)	exchange repulsion interaction energy (E_{ex}) (kcal/mol)
a1-c1	–213.982	–82.226	–155.735	-27.022	51.001
a1-c2	–211.938	–77.976	–153.770	-18.894	38.702
c1-c2	34.836	34.836	0.000	0.000	0.000

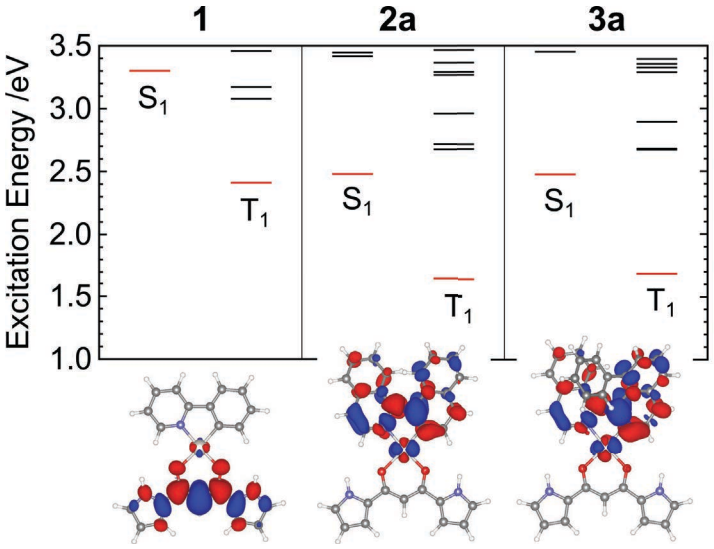

Fig. S33 Energy levels of excited singlet state S_1 and triplet state T_1 optimized structures for **1** (left), **2a** (center), and **3a** (right). Inset shows electron density differences between T_1 and S_0 at the T_1 optimized structures (isosurface value: 1×10^{-3} a.u.), in which red/blue regions are positive and negative, respectively. The T_1 excitation energies of **2a** and **3a** are lower than **1**, indicating the smaller T_1–S_0 energy gap. The smaller T_1–S_0 energy gap causes faster nonradiative decay, which results in the smaller luminescence intensities.

Cartesian Coordination

2a-1 (S_0)
(CAM-B3LYP/6-31G(d,p) for C, H, N, and O and CAM-B3LYP/LanL2DZ for Pt)
-1588.9231755 hartree
C,2.9763365376,-2.325826353,0.4449871257
C,4.3515675476,-2.4837047552,0.4261907334
C,4.689307956,-3.8365692082,0.7177126174
C,3.4187661082,-4.4699080291,0.9091929345
N,2.4343900038,-3.5502581838,0.7394384921
H,5.0766726781,-1.7108320227,0.2186646505
H,5.6027213696,-4.2995475032,0.7807908198
H,3.1940270106,-5.4975101911,1.1523322303
C,2.0873030946,-1.1852012624,0.2258420273
C,2.6530680338,0.0749716582,-0.0013849731
C,1.9678167456,1.2704649198,-0.2110006439
H,3.7322042966,0.1287850666,-0.0161163679
O,0.8371055268,-1.4574865484,0.2656605486
O,0.6913609754,1.448279682,-0.2240568997

C,2.72998369,2.4939969008,-0.4500945168
C,4.0828652737,2.7881719653,-0.4626701183
N,2.0609714715,3.6570507484,-0.731625267
C,4.216213259,4.1612411909,-0.7599614825
H,4.8861638984,2.0922013946,-0.2714346116
C,2.944234301,4.6696510971,-0.9231324047
H,5.1369662801,4.7194051096,-0.8449784102
H,2.6118695403,5.6691580147,-1.1598548564
Pt,-0.7024821634,-0.0066314254,0.0224990424
C,-2.1471576174,2.6336752018,-0.1249637185
C,-4.6424092802,1.432739461,0.4318809309
C,-3.2566743148,3.4166326858,0.0128934254
H,-1.1716510883,3.0801101623,-0.2775811355
H,-3.1832717635,4.498668852,-0.0606394518
C,-3.4987359595,0.6297701762,0.0843264505
C,-2.2402901337,1.223784789,-0.0564933627
C,-3.449780846,-0.8313996644,-0.0464529236
C,-1.9828918249,-2.6720766109,0.1662828469
C,-2.9784732396,-3.5822893265,0.002785724
H,-0.9479630932,-2.9410497972,0.3309478062
H,-2.7711653672,-4.6438770178,0.072809033
N,-2.2148673193,-1.3337445487,0.1267550567
H,1.0558868859,3.6939370289,-0.7908480163
H,1.4404378062,-3.6872670205,0.8234629625
C,-4.5152678593,2.8483408573,0.3421649101
C,-5.6186770669,3.678042421,0.6565138569
C,-6.7941452462,3.1495009696,1.1181287395
H,-7.6295173764,3.7949213232,1.3685394131
C,-6.8936848512,1.7567676678,1.3077255549
H,-7.7984058287,1.334732074,1.7341065565
C,-5.8524657618,0.9269181069,0.9771507397
H,-5.9482699624,-0.1337908207,1.1685300827
H,-5.5009777407,4.7528453822,0.5508246097
C,-4.268342458,-3.1270937088,-0.3633955397
C,-5.2989034721,-4.0284178231,-0.7247029432
C,-6.4826144538,-3.5646605058,-1.2309941723
H,-7.2622016109,-4.2616358751,-1.5210627813
H,-5.117029447,-5.0938507469,-0.6239530685
C,-6.6765862199,-2.1791291956,-1.4166613849
H,-7.591522738,-1.8205483215,-1.8759537588
C,-4.4991565762,-1.7272494716,-0.44662798
C,-5.7130053251,-1.2843056139,-1.0337382463
H,-5.8651674448,-0.2276966656,-1.2023978157

2a-2 (S_0)
(CAM-B3LYP/6-31G(d,p) for C, H, N, and O and CAM-B3LYP/LanL2DZ for Pt)
-1588.9191542 hartree
C,4.1793245492,2.2443120088,-0.419629976
C,4.6895953795,3.1170700832,0.5206220169
C,5.5375195579,4.0266423685,-0.1488811006
C,5.5323736213,3.6811562694,-1.4815731753
N,4.7012909069,2.6137416969,-1.6394673408
H,4.443954244,3.0993874128,1.5713956339
H,6.0890793263,4.8453160229,0.289422945
H,6.0575799234,4.1090117518,-2.3223126363
C,3.2426869247,1.1346973606,-0.229942057
C,2.5863592661,0.590814011,-1.3468866486
C,1.6926922494,-0.481309646,-1.3486577799
H,2.7386521542,1.0744136432,-2.3021687277
O,3.09298922,0.755293425,0.9762319137
O,1.3058241941,-1.1786177826,-0.3384292844
C,1.0926150643,-0.9044135262,-2.6133557251
C,1.2392789319,-0.4934331461,-3.9273971927
N,0.1738977057,-1.9213293762,-2.6091284896
C,0.3833560729,-1.2880723275,-4.7196214451
H,1.8930126114,0.2905258203,-4.2801119705
C,-0.2632840841,-2.1625404266,-3.8709878132
H,0.2521914643,-1.2309052028,-5.790170492
H,-0.9950628441,-2.9292095689,-4.0763396908
Pt,1.8679213444,-0.8600988385,1.5898739122
C,-0.1531059281,-3.1016939198,1.616462675
C,-0.296119524,-3.0848169606,4.436380465
C,-1.0351765422,-3.9278211029,2.2511983671
H,-0.1133545236,-3.0635629083,0.533876
H,-1.6972998586,-4.5747081246,1.6813088343
C,0.7556355148,-2.3833171718,3.74769415
C,0.7311701211,-2.2787474138,2.3529668129
C,1.8667671707,-1.6349875811,4.350950993
C,3.3400833329,0.1700192176,3.9336041937
C,3.8482080867,0.1414266491,5.1939199503
H,3.6560320359,0.8753973586,3.1750427735
H,4.5838601503,0.8738801893,5.5055312833
N,2.3855082222,-0.7088946634,3.5266066051
H,-0.1062638972,-2.3821629801,-1.7578431913
H,4.5765007405,2.0994253477,-2.4953400417
C,-1.1701125632,-3.9024502813,3.6641819996
C,-2.2085110448,-4.6240355579,4.3012649261
C,-2.4396657542,-4.4964053024,5.6445661706
H,-3.2465442328,-5.0435723616,6.120730177
C,-1.6439909303,-3.6102091253,6.3978690797
H,-1.8607829578,-3.4536736213,7.4499846731
C,-0.6080397876,-2.9270081247,5.8131364658
H,-0.038480952,-2.2276386715,6.4110792878
H,-2.8408350842,-5.2628010451,3.6910088489
C,3.481689862,-0.9182331622,6.0581329337
C,4.1118639662,-1.103694596,7.3129113813
C,3.8605040228,-2.2223627695,8.0595031687
H,4.3591945782,-2.3656223641,9.0126673127
H,4.8229634313,-0.357079724,7.6523825158
C,2.982908639,-3.214236139,7.571381323
H,2.8351078283,-4.127899763,8.1371444118
C,2.5151781329,-1.8605698661,5.6126100385
C,2.3268150287,-3.0383682984,6.3822319034
H,1.6760974925,-3.8164910556,6.0094918761

2a-3 (S_0)
(CAM-B3LYP/6-31G(d,p) for C, H, N, and O and CAM-B3LYP/LanL2DZ for Pt)
-1588.9180612 hartree
C,3.3426643519,-0.8602899826,-2.6453147301
C,2.7561800211,-1.0047749471,-3.8910117306
C,3.7528742717,-1.4589661106,-4.7814364403
C,4.9217880554,-1.5783753707,-4.0592479237
N,4.6592936001,-1.2171937791,-2.7771514792
H,1.721716682,-0.8115516149,-4.133706786
H,3.633092797,-1.6761972569,-5.832655024
H,5.9085874631,-1.8907981346,-4.3660767551
C,2.8496677936,-0.4328792324,-1.3346132224
C,1.5149071513,-0.0209852812,-1.2189500726

C,0.8752030458,0.4320638805,-0.0605392259
H,0.9164979529,-0.1006546766,-2.1161703553
O,3.7131407621,-0.4745871883,-0.3932275326
O,1.3799208402,0.5180582528,1.1145792138
C,-0.5224860094,0.8593558719,-0.1316452463
C,-1.4313096254,1.0254228434,0.8941521944
N,-1.1789872808,1.1506910903,-1.3068233235
C,-2.6582034153,1.4284498111,0.3220523989
H,-1.218851731,0.8452636524,1.936805671
C,-2.4658787005,1.508545024,-1.0386387596
H,-3.5814444228,1.6351676455,0.8430282836
H,-3.1415168386,1.796110991,-1.8301872829
Pt,3.2742279115,0.0275102271,1.6360335602
C,1.8657513688,1.1447657026,4.0431739463
C,4.2287744345,1.0889869525,5.6001336209
C,1.8496311188,1.6367887743,5.3162846201
H,0.98970492,1.2091593115,3.4079242351
H,0.9439428909,2.075872886,5.7268275516
C,4.1619967691,0.4009825292,4.3363574025
C,3.0374273955,0.5492969115,3.5186818645
C,5.2163887538,-0.3991192,3.7033068892
C,6.0218552452,-1.0811791405,1.588360204
C,7.144807377,-1.6406814432,2.1101224276
H,5.7989162884,-1.066563949,0.5296393522
H,7.8980735449,-2.0728063762,1.461512829
N,5.0779777334,-0.4927544368,2.368637638
H,-0.7383587188,1.2100516477,-2.2095234844
H,5.2989217623,-1.185719421,-1.9999144797
C,3.0304325,1.6696911837,6.1051928766
C,3.0429733151,2.3412211315,7.3514113886
C,4.2053800898,2.5094905687,8.055280509
H,4.2057260902,3.0370562181,9.0033781276
C,5.4128610874,2.0275706971,7.5126361157
H,6.3483823821,2.2125370098,8.0313983236
C,5.4239266813,1.3418690364,6.3241542961
H,6.3724623304,1.0167255328,5.9172036944
H,2.1079408703,2.7488874118,7.7252069282
C,7.2666645281,-1.7430933385,3.5173805163
C,8.3184633582,-2.4745192982,4.120255218
C,8.3259558354,-2.6975341154,5.4704799489
H,9.12672768,-3.2728189644,5.9238425441
H,9.0985283745,-2.8829297129,3.4853510532
C,7.2690333037,-2.2152531049,6.2715278806
H,7.2470921068,-2.4475639416,7.3308666088
C,6.2580173844,-1.1628901617,4.3332594633
C,6.2633806804,-1.4669493829,5.7193682779
H,5.4482876323,-1.1227370629,6.3399607704

2a-4 (S_0)
(CAM-B3LYP/6-31G(d,p) for C, H, N, and O and CAM-B3LYP/LanL2DZ for Pt)
-1588.9130576 hartree
C,1.8439441189,1.297348597,2.6147723324
C,0.6776192018,1.4169580126,3.3422178397
C,0.9860610274,2.0905764837,4.545622679
C,2.3364054972,2.3548611454,4.5291081373
N,2.8451943645,1.8892248272,3.3531187083
H,-0.290196892,1.0732850587,3.0102726593
H,0.299871595,2.3565649587,5.3361820651
H,2.9705551847,2.8300750126,5.2624593397
C,2.0450561266,0.6956964934,1.2930885011
C,3.1923827233,1.0358173832,0.5533564234
C,3.5651281374,0.5254476052,-0.6968366226
H,3.8592486369,1.765346676,0.9942892276
O,1.126329062,-0.0977924598,0.9156835703
O,2.9621382818,-0.3804416303,-1.3707619665
C,4.776824958,1.0331484455,-1.3442193706
C,5.5395230547,0.4501046886,-2.3350331198
N,5.3810620755,2.2264300337,-1.0138800943
C,6.6226432317,1.3153071126,-2.6102714502
H,5.3347773313,-0.5113662878,-2.7806594542
C,6.4874775847,2.41113786,-1.7893440859
H,7.4153999928,1.1560779568,-3.3263200675
H,7.0864794998,3.305258481,-1.7027137448
Pt,1.2025388025,-1.2550264839,-0.8649874996
C,1.9986383532,-2.269520405,-3.581722154
C,-0.4494290972,-3.6506119373,-3.9085200583
C,1.7398079611,-2.9195104777,-4.7539228925
H,2.9029437537,-1.6846515056,-3.4555958004
H,2.4537554836,-2.8868826461,-5.5729972484
C,-0.0635258162,-3.1297711726,-2.6225897307
C,1.0810696263,-2.3347805048,-2.5064475062
C,-0.8061595354,-3.237731086,-1.3598584265
C,-1.1482846765,-2.1240422535,0.7010804367
C,-2.1552417909,-2.9595382685,1.0692227521
H,-0.8019773576,-1.2982853487,1.3103956372
H,-2.6908587581,-2.798180932,1.9975850084
N,-0.4863323292,-2.2753492613,-0.4769664386
H,4.9731717686,2.9253160973,-0.4153793663
H,3.8247884498,1.8427009627,3.1267185331
C,0.500008907,-3.5785376229,-4.9679940096
C,0.171817083,-4.0941513412,-6.2450936011
C,-1.0732725994,-4.5993882757,-6.5081017727
H,-1.3180416429,-4.9801041194,-7.4942130729
C,-2.051208256,-4.5790673008,-5.4940120453
H,-3.0597171591,-4.9170987155,-5.7112556794
C,-1.7494380996,-4.1186295395,-4.2372782303
H,-2.5327436945,-4.0827018228,-3.4915308176
H,0.9261760335,-4.0522655682,-7.0257760246
C,-2.4233632847,-4.1015372593,0.2763479457
C,-3.3310127475,-5.1027161528,0.7002493761
C,-3.4529429957,-6.2728138215,0.0014805285
H,-4.138687713,-7.0422463321,0.341367413
H,-3.9010935597,-4.9360597073,1.608890313
C,-2.6553471309,-6.499547468,-1.1406810392
H,-2.7099878384,-7.4531517067,-1.6548567249
C,-1.6984738036,-4.2794596279,-0.9333646321
C,-1.8028701796,-5.5297093716,-1.597127296
H,-1.1810741807,-5.7248457273,-2.4592842929

2a (S_1)
(CAM-B3LYP/6-31G(d,p) for C, H, N, and O and CAM-B3LYP/LanL2DZ for Pt)
-1588.82178332 hartree
C,4.0551225089,2.3779585265,-0.1477386572
C,5.4262832566,2.5650162207,-0.2114735906
C,5.6644208936,3.9546258879,-0.2446571232
C,4.4355657924,4.5813935872,-0.1974913982
N,3.477889204,3.6221614424,-0.1436919096
H,6.1726686618,1.7850790516,-0.2411814904

H,6.6242391921,4.446895188,-0.2983407379
H,4.1822510144,5.630880717,-0.1973951019
C,3.1996117976,1.1971020773,-0.0893014075
C,3.7926385435,-0.0658464966,0.014645865
C,3.1341855987,-1.2935866664,0.0901409015
H,4.8727502916,-0.0960989027,0.0291435536
O,1.9412887493,1.4454393048,-0.1401941188
O,1.8622268253,-1.4974960651,0.1046745617
C,3.9205886014,-2.5209350752,0.155005775
C,5.2765279633,-2.7831546221,0.2600384111
N,3.2767368891,-3.7311194326,0.1087950044
C,5.4376321591,-4.1843275864,0.2753622472
H,6.0624039327,-2.0457138637,0.3296523589
C,4.1791505282,-4.7419764991,0.1758186008
H,6.3670714919,-4.7290246727,0.352111404
H,3.8695191514,-5.7758406443,0.1475100289
Pt,0.4307708594,-0.0372361862,-0.0148761497
C,-0.9432693565,-2.652974705,0.4477015519
C,-3.4535148731,-1.5504411885,-0.3060043551
C,-2.0499487931,-3.4559967189,0.4145968472
H,0.0327597731,-3.0588487279,0.6874277172
H,-1.97618833,-4.5152744007,0.6428291707
C,-2.3457904089,-0.6758205828,-0.0184957682
C,-1.0414091115,-1.2742781467,0.1703858332
C,-2.3408894643,0.7535259777,0.0287923611
C,-0.874216522,2.5842059483,-0.383328363
C,-1.9012479441,3.4779839379,-0.3523770215
H,0.1470575499,2.8731032074,-0.5979612192
H,-1.7145871759,4.5234463148,-0.5698595326
N,-1.0518447074,1.2665124184,-0.1411448124
H,2.2763542067,-3.8001162587,0.0079959954
H,2.4802424205,3.7477267417,-0.0812323888
C,-3.3095780436,-2.9422606038,-0.023764868
C,-4.3989386592,-3.8011084572,-0.2457613783
C,-5.5743336156,-3.3358018025,-0.8018719762
H,-6.3992813213,-4.0185297123,-0.9779406824
C,-5.6866810671,-1.9891635762,-1.1702387672
H,-6.5884488102,-1.6307322613,-1.6550604261
C,-4.6453482798,-1.1172786272,-0.9269633956
H,-4.7344912642,-0.0827536169,-1.2317888171
H,-4.2924942212,-4.8527867174,0.0036190621
C,-3.1991119595,3.0604628444,0.0784244165
C,-4.2329373654,3.9789261886,0.3149248398
C,-5.4432515642,3.5673562838,0.8411353837
H,-6.2335502624,4.2879654553,1.0234089897
H,-4.0566535853,5.0278837926,0.0959877115
C,-5.6289693464,2.2212387922,1.1667754545
H,-6.5585291773,1.8968873621,1.6234515872
C,-3.4120774252,1.6725059502,0.3288383029
C,-4.6322494058,1.2931858654,0.9234170334
H,-4.7889517956,0.260968733,1.2069144865

2a (T_1)
(CAM-B3LYP/6-31G(d,p) for C, H, N, and O and CAM-B3LYP/LanL2DZ for Pt)
-1588.8520616 hartree
C,4.0962892947,2.3912789216,-0.1015013296
C,5.4657127224,2.5705686581,-0.1967510419
C,5.7140530277,3.959944434,-0.1926371299
C,4.4928039263,4.5934041116,-0.0919488857
N,3.5293119686,3.6382505814,-0.0423863696
H,6.2048644853,1.7867947361,-0.2715865646
H,6.6761135896,4.4466399506,-0.2572463843
H,4.2474717492,5.6440135727,-0.0515111663
C,3.2300188692,1.2140309284,-0.0568395612
C,3.8194589797,-0.0550598797,-0.003073516
C,3.1572567697,-1.2803414947,0.064825265
H,4.8995375047,-0.090858433,-0.0156323339
O,1.9753929819,1.4695472904,-0.068320519
O,1.8856276459,-1.48053907,0.1053742576
C,3.9381228728,-2.5146321062,0.090714004
C,5.2933050672,-2.7895967462,0.1575142668
N,3.2824275547,-3.7177824451,0.041071405
C,5.4421583564,-4.1929602627,0.1461026801
H,6.0871741871,-2.0599386131,0.21848173
C,4.1769416165,-4.7380123855,0.0697295155
H,6.3684312034,-4.7467352378,0.1902072689
H,3.8569903589,-5.7684694305,0.0332021953
Pt,0.461463183,-0.0285515664,0.0322588297
C,-0.9596356359,-2.629008229,0.5182213049
C,-3.4753425237,-1.5539772056,-0.2828400944
C,-2.0917157133,-3.4241955892,0.552965743
H,0.0079177355,-3.0491114059,0.7715231029
H,-2.0290681137,-4.4682325029,0.8436780622
C,-2.3429941828,-0.6651969572,-0.0160047888
C,-1.0220396282,-1.2837232413,0.1708519512
C,-2.3448411551,0.7245194973,0.0677474752
C,-0.8755916598,2.5618995587,-0.3321571883
C,-1.9249557121,3.4528082317,-0.3781454303
H,0.1506251974,2.862979808,-0.5052592733
H,-1.7383974452,4.4926928539,-0.6200656267
N,-1.0447737921,1.2659109512,-0.0620400667
H,2.2786047507,-3.7737649411,-0.0318799594
H,2.5348667868,3.7664341729,0.0526229119
C,-3.3499862392,-2.9226980488,0.0758098484
C,-4.4391566448,-3.7827930532,-0.1289191801
C,-5.5963357319,-3.3367336311,-0.743022718
H,-6.4232696941,-4.0210369151,-0.9039832483
C,-5.6829877676,-2.0166374574,-1.1853134413
H,-6.5672649876,-1.6718780813,-1.7105972394
C,-4.6317146295,-1.1423255188,-0.9569816931
H,-4.7031555851,-0.1221918993,-1.3135004825
H,-4.3489273833,-4.8212777385,0.1757983998
C,-3.2327685551,3.0330754728,0.018899908
C,-4.2739679246,3.9569463605,0.2069953497
C,-5.4896122528,3.5549330335,0.7233200487
H,-6.2871622871,4.2755668844,0.8700073017
H,-4.0973515614,4.9997179913,-0.0392239887
C,-5.6724226557,2.2183211915,1.0853995098
H,-6.6085108064,1.9006874661,1.5329378296
C,-3.4425157965,1.6590403308,0.3068867606
C,-4.6642321216,1.2895523365,0.887078281
H,-4.8230701992,0.2626157608,1.188534015

2a·Cl^- (S_0)
(CAM-B3LYP/6-31G(d,p) for C, H, N, O, and Cl and CAM-B3LYP/LanL2DZ for Pt)
-2049.2355085 hartree
C,1.5453760783,1.0299567796,2.4160603382
C,0.4733107854,0.8581004511,3.2799487314

C,0.6729711708,1.7126469028,4.3808875061
C,1.8635778549,2.3806466232,4.153851808
N,2.3807246868,1.9676445542,2.9756781429
H,-0.3525547859,0.1836643463,3.1097022763
H,0.029435438,1.8330014625,5.2411327406
H,2.3810878143,3.1209281648,4.7461702119
C,1.7894055876,0.3656914966,1.1379679324
C,2.9366878733,0.694660756,0.4066887396
C,3.3378626855,0.1741775835,-0.8230576392
H,3.587929737,1.4365809402,0.84452506
O,0.8987543575,-0.4916219968,0.7869080248
O,2.7175389592,-0.7133761191,-1.532400758
C,4.5827048658,0.6446126839,-1.4237933014
C,5.153008677,0.2608956661,-2.6288537341
N,5.4113998768,1.5819422375,-0.8531221514
C,6.3501459775,0.9860361772,-2.7817921004
H,4.7296637778,-0.466089268,-3.3053831731
C,6.4731979427,1.7908764024,-1.6629762753
H,7.0457257686,0.9329146024,-3.6075712714
H,7.2402524239,2.498067224,-1.3833891179
Pt,0.9855072364,-1.5891905684,-0.9970932772
C,1.7406733624,-2.5846595413,-3.7386717794
C,-0.7074076125,-3.9715971079,-4.0359546889
C,1.4687392579,-3.2287618027,-4.9089695641
H,2.6461127409,-2.0006269107,-3.6138310358
H,2.1715319809,-3.191879671,-5.7379942398
C,-0.3043435741,-3.457465381,-2.7516820944
C,0.8386444399,-2.6530659372,-2.6458136922
C,-1.0279824103,-3.577722569,-1.4802154378
C,-1.3383214162,-2.4841332104,0.5968471422
C,-2.3428738895,-3.3205838931,0.9718995793
H,-0.976074705,-1.6617475709,1.2033799998
H,-2.8649700688,-3.1662798061,1.909306231
N,-0.6927379074,-2.6270047886,-0.5903189436
H,5.2836063319,2.0727830711,0.049311887
H,3.2733202476,2.3281443965,2.5924635659
C,0.225177715,-3.889696831,-5.1101128511
C,-0.1216046499,-4.3968270197,-6.3842963935
C,-1.3694992128,-4.9052632531,-6.6343916339
H,-1.6268128094,-5.2795604217,-7.620246193
C,-2.3313944702,-4.8947411502,-5.606064226
H,-3.3427789838,-5.2344332885,-5.8089569006
C,-2.010524867,-4.440270407,-4.3509172217
H,-2.7824721783,-4.4104874063,-3.5928960897
H,0.621504981,-4.3461724989,-7.1757171434
C,-2.6227094211,-4.4558967454,0.1734124368
C,-3.5239599042,-5.4619035996,0.6013349733
C,-3.65751938,-6.6267638667,-0.1043201194
H,-4.3384271895,-7.3989059633,0.2403325092
H,-4.0796391986,-5.302164623,1.5204586425
C,-2.8769350066,-6.8437156623,-1.2597295942
H,-2.9381902186,-7.7928877865,-1.7819377912
C,-1.9163461944,-4.6235036597,-1.0485054135
C,-2.0306112931,-5.8689596557,-1.7187622684
H,-1.4200615487,-6.0560264261,-2.5908728945
Cl,5.1217900433,3.1486353749,1.9001200503

2a·Cl⁻ (S_1)
(CAM-B3LYP/6-31G(d,p) for C, H, N, O, and Cl and CAM-B3LYP/LanL2DZ for Pt)

-2049.13844331 hartree
C,3.5657211393,2.4149198474,-0.240901042
C,3.1650797509,3.7400960635,-0.3588810441
C,4.3261959487,4.5289163891,-0.4334224904
C,5.4027823212,3.6599525469,-0.3593888127
N,4.9411642648,2.3965938044,-0.2439830747
H,2.1381264638,4.0724230236,-0.3806832564
H,4.3817688393,5.6040532557,-0.5289905726
H,6.465508006,3.8519786881,-0.3807451784
C,2.7281563344,1.2297278222,-0.1293870179
C,3.3286860795,-0.0225028688,0.0209779538
C,2.6975131274,-1.2643406607,0.1192439388
H,4.4081279567,-0.034311079,0.053141625
O,1.4570553037,1.4546052258,-0.1859130164
O,1.4227757438,-1.4897687534,0.1199210967
C,3.5097384158,-2.466305202,0.2321203201
C,3.0819021682,-3.7833763481,0.3509064803
N,4.8855407193,-2.4760687689,0.2343742446
C,4.2263105056,-4.5951272013,0.4266803411
H,2.0481270982,-4.0932902744,0.3745225532
C,5.3207481163,-3.7481699846,0.3506401554
H,4.2600383949,-5.6709207066,0.5248036345
H,6.3793493626,-3.9618967962,0.3705410967
Pt,0.0127283769,-0.036422516,-0.0336669151
C,-1.3404145524,-2.6774939103,0.3559096442
C,-3.8617813898,-1.5661081005,-0.3370570128
C,-2.4397931822,-3.4888463696,0.2995006261
H,-0.3521322635,-3.0788955482,0.5509791381
H,-2.3543574292,-4.5570414731,0.4778191149
C,-2.7571157653,-0.6917800196,-0.0323916524
C,-1.4568090281,-1.2875538639,0.1414906751
C,-2.7592836143,0.742046707,0.0334382198
C,-1.2961799808,2.5954779418,-0.3111323677
C,-2.3252529689,3.4845848836,-0.244784977
H,-0.2696356227,2.8918241568,-0.4927467471
H,-2.1385784997,4.5399582879,-0.4078693673
N,-1.4770599756,1.2678906963,-0.1333017657
H,5.5249372285,-1.66388608,0.1533603495
H,5.5623927631,1.5698793755,-0.1733371556
C,-3.7056262185,-2.9668197377,-0.1046611657
C,-4.7951569976,-3.8255935137,-0.3488516858
C,-5.9751932245,-3.3527637937,-0.8792105097
H,-6.797355547,-4.0350972834,-1.0727633461
C,-6.0983439116,-1.9926633014,-1.2037438418
H,-7.0052831938,-1.6244011159,-1.6724337321
C,-5.0623591661,-1.1245980795,-0.9392338707
H,-5.1592639175,-0.0813653226,-1.2103289254
H,-4.6760052562,-4.884673844,-0.1376002575
C,-3.6233661479,3.0449099246,0.1659275982
C,-4.6620878048,3.9489212929,0.4345197828
C,-5.873067678,3.5167175822,0.9461627148
H,-6.6657804519,4.2291941558,1.1518079158
H,-4.4877919921,5.0057569821,0.2530734877
C,-6.053024778,2.1605539233,1.2264668917
H,-6.9810522776,1.8154936642,1.6721373582
C,-3.831720358,1.6471694127,0.3662416214
C,-5.0508844202,1.2462814669,0.9520651538
H,-5.2020468646,0.2047446084,1.2022654783
Cl,6.9224240493,-0.0651202118,-0.0065574096

2a·Cl⁻ (T_1)
(CAM-B3LYP/6-31G(d,p) for C, H, N, O, and Cl and CAM-B3LYP/LanL2DZ for Pt)
-2049.164205 hartree
C,3.601306956,2.4382122669,-0.1941465102
C,3.2040845993,3.7645439848,-0.2917490473
C,4.3678142911,4.5527513788,-0.3622628007
C,5.4417062108,3.6809024981,-0.3056456811
N,4.9762036136,2.4167609089,-0.2047843741
H,2.1777825969,4.0997760527,-0.3037746544
H,4.4253815896,5.6291077564,-0.4440741771
H,6.5049928431,3.8694521807,-0.3296257404
C,2.7577177116,1.2511517836,-0.0938468668
C,3.3624077495,-0.0066433648,0.0172936111
C,2.7348246266,-1.2479727203,0.1167695642
H,4.4422350924,-0.0191044461,0.0225142884
O,1.492025736,1.4769704471,-0.1187188464
O,1.4607213938,-1.477442504,0.1388579751
C,3.5513361753,-2.4536044986,0.2085466293
C,3.1264706641,-3.7709390091,0.308906814
N,4.9265389852,-2.4607082165,0.2064400551
C,4.2742266505,-4.5833705739,0.3685267949
H,2.0931607426,-4.0827656163,0.3302972744
C,5.3658596283,-3.7349761449,0.3021598242
H,4.3093232438,-5.6607271826,0.4496643808
H,6.425080827,-3.9460598944,0.3155486991
Pt,0.0460900982,-0.0401942437,0.0171558825
C,-1.3394527303,-2.6803982127,0.3763914228
C,-3.8799708422,-1.5859417844,-0.3044286071
C,-2.4547918747,-3.4869171332,0.3794582426
H,-0.3547577637,-3.0928964593,0.5692698661
H,-2.3736922952,-4.5483312775,0.595107345
C,-2.7486065113,-0.6986367548,-0.0349494013
C,-1.4295195824,-1.3075495121,0.1209541746
C,-2.7600115507,0.6943065283,0.0686787801
C,-1.2925691875,2.5499373146,-0.3085079741
C,-2.3498520006,3.4345769966,-0.319513414
H,-0.2649870847,2.8582008482,-0.4699534404
H,-2.1707766351,4.482309494,-0.5320220914
N,-1.4563446938,1.2485171869,-0.0685476421
H,5.5630078505,-1.6467728235,0.1380677041
H,5.5963888819,1.5887410681,-0.1452313131
C,-3.7297523918,-2.9715602504,-0.0262318483
C,-4.820379422,-3.8330605181,-0.2419111802
C,-6.0000736927,-3.3712645239,-0.7895756452
H,-6.8254904188,-4.0558370653,-0.9603599125
C,-6.1142089044,-2.0271301592,-1.1582661739
H,-7.0184875363,-1.6656613119,-1.6372022429
C,-5.0664961672,-1.156498275,-0.9199802394
H,-5.1585016455,-0.1211429488,-1.2232241234
H,-4.7055227035,-4.8855506915,0.0016548486
C,-3.6516666449,3.0014641635,0.0980234988
C,-4.6879847616,3.9156322545,0.3319015825
C,-5.8956673694,3.5010739881,0.8675032829
H,-6.6901264275,4.2185138836,1.0464068796
H,-4.5174620556,4.9643741623,0.1059466114
C,-6.0670912368,2.1597784802,1.2035974916
H,-6.9923566398,1.8274529322,1.663900503
C,-3.8520755898,1.6193160246,0.3597886278
C,-5.0577472054,1.2377333263,0.9629152789
H,-5.2062754651,0.2040101757,1.2466464422
Cl,6.9725192722,-0.0389849686,-0.0091734279

3a-1 (S_0)
(CAM-B3LYP/6-31G(d,p) for C, H, N, and O and CAM-B3LYP/LanL2DZ for Pt)
-1819.8359884 hartree
C,-3.0849687355,-1.9226102768,-2.9551934013
C,-3.2380902139,-2.6651989149,-4.1133066779
C,-4.6228158528,-2.8165747614,-4.3416640776
C,-5.2795895188,-2.1664540462,-3.3177651855
N,-4.3426381595,-1.6303293881,-2.4941330081
H,-2.4400154888,-3.0472110885,-4.7324943953
H,-5.0909833043,-3.3401522152,-5.1622128834
H,-6.3349035178,-2.0511896763,-3.1212356688
C,-1.9229996849,-1.4394615111,-2.2098612798
C,-0.64545085,-1.8436438991,-2.6161358655
C,0.5645833685,-1.515362103,-2.0066662885
H,-0.5927020752,-2.5105402758,-3.4648687578
O,-2.1974655815,-0.6811127951,-1.2157001636
C,1.8064074862,-2.066665108,-2.5440142684
C,2.1105008861,-2.8239217662,-3.662256335
N,2.9816640329,-1.8439522897,-1.8740381884
C,3.5026844377,-3.0557156865,-3.651930932
H,1.4085197927,-3.1631550929,-4.4095522476
C,4.0118852164,-2.4378709773,-2.528523906
H,4.0727119025,-3.6101851996,-4.3828299536
H,5.0232283437,-2.3816282383,-2.1549670459
Pt,-0.7270822182,0.1944237754,0.0453385413
H,3.0127724326,-1.3263593226,-1.0099336728
H,-4.4909640604,-1.1101142514,-1.6446590706
C,-3.332859924,1.4304818199,0.7353675106
C,-1.5050732704,2.0261825213,2.1054897561
C,-4.1485736318,2.3640629065,1.29086375
H,-3.6441691584,0.7565392705,-0.0519472247
C,-2.2395457985,3.1625817607,2.5835017454
C,-3.6000305789,3.3004067501,2.2018829195
H,-5.1845703498,2.4429990691,0.9819104699
C,-1.6402388095,4.2107470688,3.3261606832
C,-4.3476823805,4.4072704797,2.6703110681
C,-2.3737348207,5.2970690974,3.7235639807
C,-3.7485005888,5.3838830756,3.4190332341
H,-4.3225169628,6.2406008457,3.7572705793
C,0.5062866478,1.0118391786,1.3489177967
C,1.9188591981,0.9343346852,1.3236588073
C,-0.1156502227,1.6689152985,2.4150533598
C,2.6578365457,1.4605101282,2.3440875952
H,2.4001261112,0.4926324825,0.4584801222
C,0.6140625173,1.9346129303,3.6277332694
C,2.0365658535,1.9273510965,3.5344466389
H,3.7435734124,1.4706081484,2.2950019973
C,0.0359600804,2.090747317,4.9329525348
C,2.82303219,2.3193829725,4.6427778537
C,0.8484822582,2.4574735501,5.9876691107
C,2.2370051258,2.6253522852,5.8406825135
H,2.8387667512,2.920084882,6.693930408
N,-2.0376649011,1.2832600009,1.1226761631
O,0.7414700579,-0.7668004933,-0.9727690274
H,-1.8932426581,6.0986405392,4.2746050553
H,0.4067739192,2.5493171322,6.9747406246

H,-5.3945664439,4.4831252458,2.3933552994
C,-1.3712114942,1.7127277914,5.2452526561
C,-2.1699727141,2.5126099879,6.0664096813
C,-1.8925931482,0.4937919697,4.7978736352
C,-3.4558535776,2.1187820657,6.4155644568
H,-1.7850288248,3.4653537528,6.4151941731
C,-3.1777764047,0.0986965525,5.1468557001
H,-1.2798464378,-0.153779596,4.1796894832
C,-3.9666411698,0.9110128785,5.9544509547
H,-4.0619267109,2.7613788663,7.0465827348
H,-3.5597382025,-0.8536056347,4.7925488506
H,-4.9713700827,0.6027610083,6.2255607256
H,-0.5862578863,4.1598301679,3.5605958323
H,3.9028649176,2.3456806732,4.5291813425

3a-2 (S_0)
(CAM-B3LYP/6-31G(d,p) for C, H, N, and O and CAM-B3LYP/LanL2DZ for Pt)
-1819.8316172 hartree
C,4.3353093692,-2.6402484186,0.3369200263
C,4.9750258691,-3.391866337,-0.6285792175
C,5.5579711004,-4.5092330258,0.008461729
N,4.5250845848,-3.2829351509,1.5403842439
H,5.0235974009,-3.1332540885,-1.6751628945
H,6.1386479079,-5.2930157694,-0.4552636144
C,3.5993779621,-1.3834387314,0.1826640663
C,3.2957745937,-0.6200162894,1.3231060878
C,2.5656006108,0.5684721222,1.3615965509
H,3.6804982664,-0.9625174211,2.2740265585
O,3.2929853431,-1.0821106236,-1.0158754804
C,2.32820098,1.2185795815,2.6499921194
C,2.7547529867,0.9686566205,3.9430868379
N,1.5213316457,2.3254140545,2.6976836897
C,2.1839211726,1.9543088632,4.7767747201
H,3.414810858,0.1718972681,4.2529595076
C,1.4225033583,2.777648461,3.9735402805
H,2.314297714,2.0552548202,5.8441958789
H,0.8249957569,3.6424446656,4.219632726
Pt,2.1984711637,0.6397496803,-1.5800623955
H,1.0764466218,2.6950657913,1.8722406931
H,4.0949132116,-3.013099942,2.4090715457
C,3.1097111914,-0.7342215821,-4.0404579435
C,1.7372212781,1.1634258094,-4.3549253322
C,3.4064595964,-0.8252130505,-5.3636179795
H,3.4797962364,-1.424117385,-3.2922069841
C,2.1776096946,1.253325572,-5.7167930818
C,2.9915580087,0.2118230841,-6.2351552932
H,4.018818508,-1.6395902818,-5.7333537652
C,1.931497476,2.3859830579,-6.5330038954
C,3.4303920024,0.2744428594,-7.5797397082
C,2.4125643707,2.4445297552,-7.8139120461
C,3.1445498526,1.3659934323,-8.3542977134
H,3.5025943372,1.4167831881,-9.3776078163
C,1.1417391698,2.1538817261,-2.2760043113
C,0.6370233011,3.2383100722,-1.5202981835
C,0.8446670332,2.0852729938,-3.6406602323
C,-0.1533153298,4.1833159876,-2.1092196293
H,0.9285601126,3.3284924636,-0.4798716541
C,-0.2278086465,2.8737938997,-4.1898057918
C,-0.6422024967,4.0083773124,-3.432284851
H,-0.4810558784,5.0579263344,-1.5533128048
C,-1.5848101564,4.9158454853,-3.9698675291
C,-1.9069295798,3.4621409825,-5.8430516253
C,-2.175738489,4.6727828153,-5.1795851477
H,-2.9035486016,5.3642261628,-5.5910006543
N,2.3158664973,0.2571357785,-3.5523604077
O,2.0366623616,1.1934068235,0.3686888153
H,2.231688265,3.3278420645,-8.4173739267
H,-2.4912543978,3.1987457904,-6.7188743025
H,4.0275477756,-0.5434257939,-7.9707873367
H,1.3769616234,3.2211193954,-6.1282808324
H,-1.8484898722,5.7946760349,-3.3886387653
C,-0.9515117923,1.2057949149,-6.0073346695
C,-0.9273365404,1.0665340355,-7.3973355668
C,-1.0404653898,0.0479579252,-5.2268114366
C,-0.9706857892,-0.1890127264,-7.9907524225
H,-0.8488902287,1.9532512852,-8.0179086909
C,-1.084171136,-1.2078416387,-5.8189311865
H,-1.0851178521,0.1350252287,-4.1463733905
C,-1.0459773795,-1.3322609199,-7.2036120154
H,-0.9398556757,-0.2733438274,-9.0726025448
H,-1.1565848812,-2.0922168003,-5.1937402674
H,-1.0777683812,-2.3137332058,-7.6658695844
C,-0.9850953178,2.5509157227,-5.3668916331
C,5.2517906533,-4.4184954479,1.3476648626
H,5.4910568987,-5.0746096446,2.1710933257

3a-3 (S_0)
(CAM-B3LYP/6-31G(d,p) for C, H, N, and O and CAM-B3LYP/LanL2DZ for Pt)
-1819.8306187 hartree
C,3.8253801464,-1.0598177117,-2.6998175464
C,3.2429945515,-1.7728825253,-3.7335053838
C,4.2175475661,-1.9334893386,-4.7422059569
N,5.1179093888,-0.7955409133,-3.0712244434
H,2.2306952882,-2.1486491804,-3.7560332692
H,4.0963924649,-2.4462802243,-5.6850669307
C,3.3495825117,-0.5822582651,-1.4001726643
C,1.9989168023,-0.7568941208,-1.0697496427
C,1.3625236169,-0.3421622598,0.1053095489
H,1.4012151603,-1.2916160174,-1.7952116347
O,4.2409574313,-0.025019611,-0.6731741689
C,-0.0749883508,-0.5673606418,0.2613941306
C,-0.8371640528,-0.5378088135,1.4120761674
N,-0.9216916967,-0.8837903876,-0.7778952738
C,-2.169800078,-0.8397555367,1.0547238842
H,-0.4495491389,-0.3400862477,2.3996054378
C,-2.1910637746,-1.0364718617,-0.3075289863
H,-3.0204950589,-0.9087969573,1.7165920746
H,-3.0088914278,-1.267131045,-0.9736305841
Pt,3.8669176212,0.7083226565,1.292698756
H,-0.6620690595,-0.8800473969,-1.7500379849
H,5.7423467573,-0.2679619147,-2.4826630639
C,6.8114311844,0.727258962,0.9179438195
C,6.0106687665,1.6692543551,2.9284380812
C,8.1052506553,0.7596573884,1.3312180279
H,6.5031211501,0.3536310715,-0.0497768015
C,7.3174287599,1.5355816207,3.5057606847
C,8.3881549015,1.1173288211,2.6729345607
H,8.9022615945,0.4390797249,0.6701645138

C,7.5649302637,1.6930327596,4.8924604737
C,9.6874382301,0.9885411911,3.2194459188
C,8.8220340051,1.5114073943,5.4051234705
C,9.9011983662,1.1848666998,4.5571594213
H,10.8961412623,1.0635981368,4.9734566479
C,3.6433059817,1.5253842914,3.0717068344
C,2.4307025554,1.5977400981,3.797104328
C,4.7879617474,2.1380712827,3.5897661842
C,2.3827848258,2.2711411343,4.9838245321
H,1.5582095405,1.0873793982,3.4054253095
C,4.6755639541,3.1015166034,4.6544922984
C,3.4760689642,3.066949671,5.4239509369
H,1.4764847367,2.2709174277,5.5838060429
C,3.3488694896,3.8765392996,6.5767257334
C,5.4329255709,4.932226629,6.0596124664
C,4.3328326588,4.763644593,6.9191124633
H,4.2343864456,5.3894611113,7.7998774554
N,5.7904622843,1.1526766755,1.7089620852
O,1.9053631619,0.2345231422,1.1131035613
H,8.9890478753,1.6171570945,6.4718919796
H,6.1301999559,5.7427159537,6.2463436801
H,10.5016702016,0.6959940789,2.563763632
H,6.7448543501,1.9378863489,5.5529398495
H,2.4411255304,3.7975087978,7.1678196028
C,6.6653704144,4.5761611875,3.9658205284
C,7.9550506322,4.8955623808,4.3980522541
C,6.3579209031,4.7519181239,2.6121300126
C,8.914506042,5.3573699834,3.5054483548
H,8.2135319112,4.7570973283,5.4428291228
C,7.3160960267,5.2141137895,1.7189080421
H,5.3550259356,4.5336418674,2.2606547237
C,8.5999490291,5.5156466322,2.1607384978
H,9.9130674644,5.5895264827,3.862483031
H,7.0536336363,5.3477533889,0.6740963911
H,9.3488681965,5.8752488145,1.4622689761
C,5.6088309197,4.1576524391,4.9297762379
C,5.3675707972,-1.3126936053,-4.3015140445
H,6.3326025226,-1.2043716753,-4.7732189573

3a-4 (S_0)
(CAM-B3LYP/6-31G(d,p) for C, H, N, and O and CAM-B3LYP/LanL2DZ for Pt)
-1819.82547 hartree
C,3.8706014355,-1.0489654247,-2.6543787851
C,3.7628879221,-0.4433314002,-3.8894165578
C,4.4565344654,-1.2437327559,-4.8250213981
N,4.6092327976,-2.1987631602,-2.829010433
H,3.213296367,0.4657730468,-4.0804689861
H,4.5598915819,-1.0632556424,-5.8849065109
C,3.3076762596,-0.621865123,-1.3699069389
C,3.1734229174,-1.5641784899,-0.3338130976
C,2.704616124,-1.3230347149,0.9642748389
H,3.463744535,-2.5819580364,-0.5600263885
O,2.9681538603,0.6017373504,-1.3103626773
C,2.5849375288,-2.4431766968,1.9004307842
C,2.5234318392,-2.4189639177,3.2784939858
N,2.5422033525,-3.7650296346,1.5141465646
C,2.4364800667,-3.7553944311,3.7296783693
H,2.5641853708,-1.522847957,3.8785779879
C,2.4341399319,-4.5621996723,2.6151576503
H,2.3834485841,-4.0929455048,4.7542785231
H,2.3574942708,-5.6351182151,2.5217898514
Pt,2.2934888394,1.5649705131,0.4558725289
H,2.4396511512,-4.0779204647,0.5630854634
H,4.9520812762,-2.775757685,-2.0789761267
C,2.7906157347,3.6527517666,-1.5860245077
C,1.882174469,4.3947117823,0.4658480361
C,3.0308519213,4.9188394796,-2.0178979969
H,3.0188181971,2.7674298304,-2.1667514449
C,2.302143286,5.7323900822,0.1643162827
C,2.8437655738,5.9992837744,-1.120622379
H,3.4367573884,5.0926348532,-3.0078271006
C,2.3055147257,6.7730436406,1.1268866844
C,3.2563075893,7.3147358927,-1.4428277669
C,2.7595053442,8.0242827152,0.804504701
C,3.2123414601,8.3073907466,-0.5015641272
H,3.5503935106,9.3085313268,-0.7494289189
C,1.5831335391,2.5882561057,1.9834565864
C,1.3364099775,2.073610953,3.2780546163
C,1.2442202674,3.9141364216,1.6980415975
C,0.7622924211,2.8650067637,4.2312041297
H,1.6374802698,1.0560636959,3.5007311287
C,0.3634138618,4.6411935309,2.5752870791
C,0.2284218626,4.1415164184,3.9037993604
H,0.6361227449,2.5036253474,5.2485063756
C,-0.4963132008,4.8788994081,4.8691497363
C,-1.1726843786,6.4253633409,3.173360725
C,-1.1489921923,6.0304947903,4.5228779188
H,-1.7100017356,6.5943048002,5.2607950307
N,2.2508661908,3.4045997935,-0.3618820191
O,2.3648298823,-0.1948298349,1.4642342944
H,2.7732001348,8.8034953028,1.5593402127
H,-1.8185349826,7.2445439354,2.873736446
H,3.6412098965,7.5101206129,-2.43889438
H,1.9655962083,6.5662434056,2.1321473502
H,-0.545399082,4.4955670084,5.884209564
C,-0.7574662517,6.0956566835,0.7759449324
C,-0.7947716739,7.4257429752,0.3498105013
C,-1.0918859791,5.0957878063,-0.1439693028
C,-1.1356114596,7.7482634405,-0.9579693824
H,-0.529413323,8.2135534102,1.047291747
C,-1.433140511,5.4169587296,-1.4516090495
H,-1.0930644516,4.0583361415,0.1732772238
C,-1.4531826717,6.7445406329,-1.8656849459
H,-1.1474327529,8.7881972046,-1.2692810096
H,-1.6926109088,4.6249010482,-2.1470413807
H,-1.7176638955,6.9950198437,-2.8881081
C,-0.471067282,5.7471069229,2.1961978509
C,4.9816823585,-2.3125656689,-4.1355921897
H,5.5927370397,-3.1366681739,-4.4721178974

3a (S_1)
(CAM-B3LYP/6-31G(d,p) for C, H, N, and O and CAM-B3LYP/LanL2DZ for Pt)
-1819.73609357 hartree
C,4.3684156258,-2.6659039625,0.0923253608
C,5.7080632246,-2.9756884923,0.2609006552
C,5.8309682995,-4.3793141469,0.1985177417
N,3.6975708729,-3.8513384474,-0.0670809477
H,6.5086148924,-2.2680768123,0.4178098106

H,6.7394903924,-4.955496639,0.2938915482
C,3.6191836379,-1.4131827022,0.0579436001
C,4.3183932455,-0.2047247016,0.1555153011
C,3.7725522498,1.0789931037,0.1415974335
H,5.3911519398,-0.2712108648,0.2676659837
O,2.3488025903,-1.5518574544,-0.059260156
C,4.6527091649,2.2327733091,0.2974024844
C,6.0266273797,2.3856815277,0.3785431738
N,4.0991534209,3.4837394991,0.3958866724
C,6.2915375961,3.763082557,0.5298189621
H,6.7581999363,1.593112172,0.3241632178
C,5.0752292944,4.4150084443,0.5407353073
H,7.2610529103,4.2305043144,0.6195872934
H,4.8418517902,5.464274544,0.6413891915
Pt,0.9884842132,0.070591145,-0.1970343537
H,3.1013557517,3.6268604212,0.384662324
H,2.7024547032,-3.8852708263,-0.2196394515
C,-0.5690461404,-2.4405973348,-0.4085056206
C,-1.8176576639,-0.4283612791,-0.6133546321
C,-1.656413966,-3.2061428644,-0.7003179351
H,0.3968478279,-2.8635259937,-0.1626721801
C,-2.9347058897,-1.1650550422,-1.1473082027
C,-2.8649799971,-2.5874955863,-1.1476110876
H,-1.5814717334,-4.2871233905,-0.6693424862
C,-4.0630846142,-0.5575469646,-1.72994095
C,-3.9480562391,-3.3369441419,-1.6332564297
C,-5.106348794,-1.317943567,-2.2252377331
C,-5.063141061,-2.7137502692,-2.1593774445
H,-5.890718022,-3.3041729802,-2.5387586233
C,-0.336024417,1.4582764131,-0.4346744163
C,-0.1045254364,2.8200518473,-0.6956851405
C,-1.6996081286,0.9741098373,-0.3697561617
C,-1.1580050612,3.6923359146,-0.7979594754
H,0.9159577619,3.1546878827,-0.8442296369
C,-2.7393885866,1.9279320174,-0.0721669581
C,-2.4805131149,3.2876169841,-0.4426694661
H,-0.9952766663,4.7325479559,-1.064470417
C,-3.5241397398,4.2235965768,-0.3958180798
C,-4.9691716434,2.5939915744,0.6204809229
C,-4.7661924688,3.870951179,0.09647479
H,-5.5647113646,4.6045559387,0.138085364
N,-0.6099795792,-1.0891081245,-0.4136411991
O,2.53160076,1.3970386321,0.0112710986
H,-5.9624071542,-0.8227330654,-2.6726118501
H,-5.8989968443,2.3654061556,1.1295437507
H,-3.8845008694,-4.4207676174,-1.6070915958
H,-4.1101832171,0.5210156883,-1.8031554649
H,-3.3338557653,5.2389530304,-0.7304211081
C,-4.1863425083,0.3751395094,1.3507316222
C,-5.4126211362,-0.2948364924,1.3037557618
C,-3.1906789123,-0.1125752292,2.2049979551
C,-5.6321101267,-1.430386226,2.0715512089
H,-6.1881817305,0.060388406,0.6334481222
C,-3.4124932811,-1.2449927614,2.9770393673
H,-2.2436492284,0.4115334882,2.275777291
C,-4.631852203,-1.9104213814,2.9100374167
H,-6.5853297411,-1.9454799331,2.0095023354
H,-2.6303429325,-1.6045451498,3.6378812313
H,-4.803175466,-2.7975429563,3.5113615287
C,-3.9693807437,1.6249506271,0.5821300963
C,4.5662181828,-4.8917071259,-0.0079838261
H,4.230999123,-5.9122534198,-0.1161830452

3a (T_1)
(CAM-B3LYP/6-31G(d,p) for C, H, N, and O and CAM-B3LYP/LanL2DZ for Pt)
-1819.7675347 hartree
C,4.3602082358,-2.6907401035,0.1335099562
C,5.7010802181,-2.9949435707,0.2962494923
C,5.8240343813,-4.4007964139,0.2779754387
N,3.6885075339,-3.8803798331,0.0194347919
H,6.5042447409,-2.2826364822,0.4132649243
H,6.734390044,-4.9732162168,0.3789963925
C,3.6083098046,-1.4376663703,0.0672268349
C,4.3037353676,-0.2299650134,0.2077986109
C,3.7598754395,1.0536050302,0.1843431273
H,5.3697239474,-0.2983784647,0.3719737765
O,2.3475391306,-1.5741138985,-0.1106266302
C,4.6324373809,2.2083838566,0.3818492244
C,5.9996515819,2.3645683628,0.5321206689
N,4.0713589258,3.4576285478,0.4478313473
C,6.2531011561,3.7437933398,0.6919956136
H,6.7346585137,1.5733517954,0.5199089994
C,5.0364467654,4.3925466516,0.6377263654
H,7.2155982742,4.213978393,0.8304244237
H,4.795533266,5.4416254269,0.721116634
Pt,0.9983277597,0.070676315,-0.2836953629
H,3.0748205824,3.5952771403,0.3781514539
H,2.6901296119,-3.9181974091,-0.1058828847
C,-0.5679666616,-2.405458756,-0.6660617566
C,-1.8292156015,-0.3914816351,-0.7501998102
C,-1.6707884404,-3.1752534325,-0.9287328069
H,0.4133898173,-2.8280141102,-0.4910829639
C,-2.9847765708,-1.1347831244,-1.2239774072
C,-2.90561743,-2.5499865171,-1.2701089749
H,-1.5851946456,-4.2555681275,-0.9469952961
C,-4.1466364958,-0.5183080553,-1.7199764357
C,-4.0125234563,-3.2988782409,-1.7143749544
C,-5.2098922861,-1.2701560659,-2.1768819045
C,-5.1545809203,-2.6701668178,-2.1554324578
H,-5.9996240141,-3.2539848236,-2.5053100856
C,-0.3291636667,1.4789248898,-0.5108871905
C,-0.1558404287,2.7962151251,-0.8852517738
C,-1.7151193949,0.9683046493,-0.442194526
C,-1.2509335954,3.6478326791,-1.0453224176
H,0.8484866098,3.1633348984,-1.0708870636
C,-2.7733261337,1.9296500348,-0.1191830052
C,-2.5575309577,3.2595698272,-0.5857649201
H,-1.112664441,4.6682611972,-1.3883623745
C,-3.5968487274,4.1910685499,-0.4942991087
C,-4.9347533982,2.6121243048,0.7281528645
C,-4.7880107457,3.8575277926,0.1340561798
H,-5.585533374,4.589871282,0.2098578018
N,-0.6190096569,-1.0649079339,-0.6130250875
O,2.5252886919,1.3755594141,0.0124487491
H,-6.0932189672,-0.7696249439,-2.5600193707
H,-5.8217785218,2.3901718785,1.3112137008
H,-3.9389016522,-4.3821493348,-1.7246267927
H,-4.2049167094,0.5613602616,-1.7546762888
H,-3.4473552995,5.1898243922,-0.8930514841

C,-4.088305478,0.3912685283,1.4214186489
C,-5.3000245302,-0.304753997,1.4229507696
C,-3.0502543133,-0.0728145927,2.236447824
C,-5.4647787406,-1.4443131552,2.2002382024
H,-6.1114397039,0.0372253802,0.7888313481
C,-3.2155828525,-1.210129711,3.0156312523
H,-2.1126369496,0.4722486772,2.2696961707
C,-4.4222842004,-1.9020574912,2.9977028155
H,-6.4098430139,-1.9776746193,2.1792252306
H,-2.4004636296,-1.5509082524,3.64599343
H,-4.5507859233,-2.790996972,3.6070178784
C,-3.9269456939,1.6421309202,0.6357823484
C,4.557707645,-4.9196884996,0.10522258
H,4.2207077963,-5.9431935562,0.0383162644

3a·Cl⁻ (S_0)
(CAM-B3LYP/6-31G(d,p) for C, H, N, O, and Cl and CAM-B3LYP/LanL2DZ for Pt)
-2280.148028 hartree
C,3.5928003288,2.4559748169,-0.3095660585
C,3.2104502429,3.7736708552,-0.5160634343
C,4.3829818671,4.5487220557,-0.5977653736
C,5.4464504424,3.6777280769,-0.4371544893
N,4.96660998,2.4260774032,-0.2660181764
H,2.1884906874,4.1116446648,-0.6015256697
H,4.4523908334,5.6159153512,-0.7556559911
H,6.5113686648,3.8582607064,-0.4314102256
C,2.7370088372,1.2812573182,-0.1626588625
C,3.3284109354,0.0210518958,-0.0149804753
C,2.6854480221,-1.2049278566,0.1517205556
H,4.4079420774,-0.0062363982,-0.0291150652
O,1.4739907183,1.517867836,-0.184104007
O,1.4087658377,-1.4165749254,0.1832625426
C,3.4876093008,-2.4145119065,0.3103056366
C,3.0489498182,-3.7242923175,0.4393748057
N,4.8618654462,-2.4314732421,0.3535140489
C,4.1878590231,-4.5429875688,0.5621344631
H,2.0131253321,-4.0284816271,0.4359987642
C,5.2877403475,-3.7052898779,0.5053064833
H,4.2112300345,-5.6174898574,0.6782138045
H,6.3441475124,-3.9229070024,0.5627801406
Pt,0.0167525417,0.0278414463,0.0139475812
C,-1.4067944941,-2.6288667583,0.3023852235
C,-3.8851661984,-1.4803538359,-0.4514546287
C,-2.5288004565,-3.403471334,0.2736033452
H,-0.4302819507,-3.0536806409,0.5084849366
H,-2.4760704163,-4.4660739482,0.4980474234
C,-2.7603625553,-0.6524333568,-0.0984610647
C,-1.4988807194,-1.2271175198,0.1064375443
C,-2.7408523635,0.8034126213,0.0860593349
C,-1.3056083856,2.6804918089,0.0243909447
C,-2.3194225482,3.5533759225,0.2677874345
H,-0.272617324,2.9756987586,-0.1207289362
H,-2.1310695867,4.6207848013,0.2884271804
N,-1.5164542705,1.338678939,-0.0385442516
H,5.5060452236,-1.6234357421,0.2910007899
H,5.5765475075,1.6012627426,-0.1203483564
C,-3.7811397939,-2.8691575168,-0.1432673203
C,-4.8950702362,-3.7203807111,-0.3212262586
C,-6.0566784856,-3.2504719875,-0.8738280871
H,-6.9097047312,-3.9061898367,-1.0164345652
C,-6.0991377509,-1.9298460906,-1.352655412
H,-6.9568145798,-1.6040755597,-1.9329447339
C,-5.0413486827,-1.0554081081,-1.1904031113
H,-4.798515919,-4.7639812174,-0.0347339749
C,-3.5996986031,3.0449662945,0.5993195637
C,-4.6439246354,3.8895061748,1.0490068836
C,-5.8182584429,3.3610259009,1.512896201
H,-6.6052857908,4.0154105864,1.8750694985
H,-4.4784148054,4.9626951388,1.0510574418
C,-5.9948836404,1.9619388153,1.5539080747
H,-6.9075636943,1.5456826238,1.9680917496
C,-3.8090900485,1.6415646997,0.5536414711
C,-5.0201408123,1.1249534776,1.0781415764
H,-5.1626240311,0.0539666506,1.1207948492
Cl,6.9345837479,-0.028722188,0.1412038146
C,-5.0917215464,0.2272348202,-1.9477050872
C,-4.0142311309,0.6185630059,-2.750335545
C,-6.242499782,1.0198221119,-1.9553028695
C,-4.0817556865,1.7727903539,-3.5199374689
H,-3.1172647838,0.0090120194,-2.772273522
C,-6.3116732828,2.174469501,-2.7251564229
H,-7.0822944585,0.7391188076,-1.3279190379
C,-5.2299402214,2.5578199988,-3.5093003812
H,-3.2323469276,2.0559536385,-4.1336303092
H,-7.2121953244,2.7809647522,-2.7044450791
H,-5.2800308134,3.4623852491,-4.1074491254

3a·Cl⁻ (S_1)
(CAM-B3LYP/6-31G(d,p) for C, H, N, O, and Cl and CAM-B3LYP/LanL2DZ for Pt)
-2280.05172171 hartree
C,3.5663366607,2.4704058592,-0.1308820262
C,3.1748358518,3.8020697802,-0.1874850191
C,4.3415013528,4.5855384514,-0.2305026413
C,5.4119471447,3.7068079777,-0.1996657276
N,4.9415643002,2.4426435821,-0.1401564147
H,2.1502663483,4.1423477196,-0.1929705687
H,4.4042914099,5.6635026104,-0.277793609
H,6.4759681235,3.8920667333,-0.2154944501
C,2.7207305714,1.2865727629,-0.071651612
C,3.3135282999,0.0242962487,0.0068940704
C,2.6742599402,-1.2170680925,0.0472948784
H,4.393208759,0.0031656435,0.0238709109
O,1.4508249756,1.5235417895,-0.1050487864
O,1.3987152504,-1.4331176045,0.0515053434
C,3.4782611202,-2.4296540474,0.0847476705
C,3.0394244484,-3.7474963386,0.1233503386
N,4.8538082204,-2.4505456472,0.0813749681
C,4.1774833291,-4.5719809644,0.1447392729
H,2.0026556787,-4.0484537546,0.128327908
C,5.2786829243,-3.7312023519,0.1175452558
H,4.2024237404,-5.6520719815,0.1755299937
H,6.33549913,-3.9544638979,0.120999696
Pt,0.0002157456,0.0371793558,0.0013215992
C,-1.3879129045,-2.5776482361,0.5183431773
C,-3.8651825481,-1.4672969613,-0.3464533926
C,-2.5239017103,-3.3430827689,0.5635741712
H,-0.4119147034,-2.9961500243,0.7379026635
H,-2.4830366173,-4.3846680998,0.8692777059

C,-2.7633562709,-0.60079445,-0.0027711048
C,-1.4706392536,-1.2084789936,0.2021176298
C,-2.7628833982,0.8229933961,0.1500291858
C,-1.3035219547,2.697717625,-0.0186808302
C,-2.3285497165,3.5762417073,0.1574555568
H,-0.2779627187,3.0084340577,-0.1809717822
H,-2.140761256,4.6428122827,0.1081874736
N,-1.4875279312,1.3583010878,0.0183319949
H,5.4992339018,-1.6399663679,0.0488643936
H,5.5571725363,1.6094341118,-0.1084350965
C,-3.7689540692,-2.8286306053,0.0914705867
C,-4.895253825,-3.664753581,-0.0109251925
C,-6.0494214981,-3.2224535496,-0.6192842672
H,-6.9100642791,-3.8790303656,-0.7029271013
C,-6.0822258942,-1.9549660497,-1.2105296209
H,-6.9373989656,-1.6664039791,-1.81228099
C,-5.0033228405,-1.0847355076,-1.118822472
H,-4.8284149907,-4.6784553085,0.3735890619
C,-3.6266234855,3.0960476334,0.5184948552
C,-4.6653976541,3.96583459,0.8863329802
C,-5.8778239441,3.4788559743,1.3383335924
H,-6.6691010876,4.1642874208,1.6258438749
H,-4.4894286895,5.0363345273,0.8291364443
C,-6.0668898711,2.098633949,1.4476955183
H,-7.002103656,1.7072811094,1.8368354798
C,-3.8397851809,1.6877845175,0.5596747221
C,-5.068178714,1.220554498,1.0676921663
H,-5.229047126,0.1556325248,1.1724077554
Cl,6.9071324687,-0.0414555723,-0.0280454938
C,-5.0346503589,0.1421844354,-1.9567287532
C,-3.9337545987,0.487210857,-2.7483508742
C,-6.1874850177,0.9272649029,-2.0428376049
C,-3.9832577835,1.5901694486,-3.5904162135
H,-3.036788236,-0.121251062,-2.7089802915
C,-6.2367509245,2.0322472291,-2.8828749854
H,-7.0413862648,0.6857808569,-1.4186490512
C,-5.1336885492,2.3687649169,-3.659135712
H,-3.1176156553,1.840036262,-4.1955772452
H,-7.1369523194,2.6378854817,-2.9222743626
H,-5.1688927697,3.2345765754,-4.3131403031

3a·Cl⁻ (T_1)
(CAM-B3LYP/6-31G(d,p) for C, H, N, O, and Cl and CAM-B3LYP/LanL2DZ for Pt)
-2280.0786299 hartree
C,3.566428345,2.4849692274,-0.1324502662
C,3.1771934721,3.8166152558,-0.1668102297
C,4.3453458927,4.5997108772,-0.2260885753
C,5.4136016826,3.7194995182,-0.2255504868
N,4.9405862024,2.4551230473,-0.1698826049
H,2.1533413297,4.1591274931,-0.1510581643
H,4.4090624331,5.6781587995,-0.264682936
H,6.4776788772,3.9018222302,-0.2600848849
C,2.7167428788,1.2989802689,-0.0693348367
C,3.3138170562,0.0335217298,-0.0610600051
C,2.67947715,-1.2079735447,-0.002988351
H,4.3924963589,0.0129995306,-0.1089827456
O,1.4526334627,1.5345576427,-0.0291981319
O,1.4068066267,-1.4306824018,0.0565872672
C,3.4881494593,-2.4225229191,-0.0095206087
C,3.0518339176,-3.7395414422,0.0096812263
N,4.8627853873,-2.4406775035,-0.041178325
C,4.1926550924,-4.5639449683,-0.0106105877
H,2.0151684076,-4.040536817,0.0288346284
C,5.2911952676,-3.7224561788,-0.0414264845
H,4.2187928211,-5.6446227942,-0.0047220617
H,6.3483237863,-3.9431577975,-0.0634376504
Pt,0.0052055907,0.0205731237,0.0900396487
C,-1.4587328568,-2.5609483194,0.6689174377
C,-3.9161638441,-1.4599498121,-0.2941601496
C,-2.636661836,-3.2888264682,0.7780139861
H,-0.5039944753,-3.0144844627,0.9145045234
H,-2.6261235908,-4.309114469,1.1494907369
C,-2.7865344616,-0.5946633119,0.0589411518
C,-1.4724831318,-1.2366413338,0.2545435325
C,-2.7849262262,0.7866010929,0.2743125403
C,-1.3147614306,2.6591739782,0.1511869736
C,-2.3535684685,3.5479780568,0.2741520318
H,-0.2819378986,2.9663216675,0.0272635558
H,-2.1604230631,4.6134382686,0.2245867076
N,-1.5016393128,1.3318392075,0.1904186643
H,5.5050603271,-1.6289374293,-0.0623983572
H,5.5557250532,1.6213676444,-0.1547902869
C,-3.8667268533,-2.7849499656,0.2311388355
C,-4.9948514293,-3.6077825878,0.109320931
C,-6.1030486659,-3.1839899995,-0.6038679288
H,-6.9674417052,-3.8338360558,-0.7027430631
C,-6.0813146653,-1.9574089792,-1.258413195
H,-6.8998998265,-1.6763102909,-1.9121714002
C,-4.9862815675,-1.0949367464,-1.1382563386
H,-4.9718981202,-4.5990528802,0.5524848936
C,-3.6667295249,3.0722169979,0.5708816792
C,-4.7171658476,3.9541711717,0.8854177098
C,-5.9454823582,3.4756731996,1.2880406041
H,-6.7461790909,4.1651940284,1.5365817283
H,-4.5332068073,5.0230368754,0.8268685196
C,-6.1446048498,2.0951341649,1.4006380823
H,-7.096992317,1.7110336675,1.752619503
C,-3.8876936935,1.6714347273,0.6155180375
C,-5.1342096976,1.2116389238,1.0715529665
H,-5.3033630682,0.1477685285,1.1742698402
Cl,6.9233182489,-0.0200766897,-0.1357872287
C,-4.9635546403,0.1200907289,-1.9954490753
C,-3.8313761969,0.4291845717,-2.7569649523
C,-6.0929482794,0.9327553391,-2.1219996228
C,-3.8259252552,1.527819432,-3.6058540027
H,-2.9522454364,-0.2026806862,-2.6874523502
C,-6.0879181479,2.0330407494,-2.9705816261
H,-6.973632988,0.7141837898,-1.5269471196
C,-4.9534386362,2.3356734864,-3.7141734905
H,-2.9368039868,1.749660913,-4.1873777247
H,-6.971634458,2.6594953651,-3.044144313
H,-4.9467434174,3.1962858638,-4.3758584811

3b-1 (S_0)
(CAM-B3LYP/6-31G(d,p) for C, H, N, and O and CAM-B3LYP/LanL2DZ for Pt)
-2281.6901114 hartree
C,-1.54823435,-4.1824711013,-0.4539721044
C,-1.4930501685,-5.5664892494,-0.4443072753

C,-2.8166712389,-6.0422943499,-0.3967441613
N,-2.872257278,-3.8324006107,-0.4245539996
H,-0.5966494643,-6.1673058581,-0.4854573829
H,-3.1319943943,-7.075357856,-0.4115818116
C,-0.533762407,-3.1305687407,-0.4768276467
C,0.8162840972,-3.493923426,-0.3989424103
C,1.9103023453,-2.6298837061,-0.3714001328
H,1.0328510095,-4.5495976237,-0.3174279214
O,-0.995139473,-1.9388234585,-0.5538650159
C,3.2546341683,-3.186447239,-0.2514612505
C,3.7560792101,-4.4774905745,-0.2233937388
N,4.3214476177,-2.3363875503,-0.1258913092
C,5.1513890757,-4.3848961309,-0.0671433993
H,3.1804214695,-5.3857758154,-0.3228490638
C,5.4832479878,-3.0385184794,-0.0029288843
H,5.8534410254,-5.2054061584,-0.0409647241
Pt,0.225880272,-0.1997144023,-0.6188079487
H,4.1997103386,-1.3393112413,-0.0401441004
H,-3.166659883,-2.8724907534,-0.3404541585
C,-2.5555456085,0.6503643162,-1.1973990366
C,-0.9650911906,2.3805704517,-0.9740430528
C,-3.5208815117,1.4953599258,-1.6442085282
H,-2.7049579197,-0.4135639084,-1.0677561444
C,-1.8624219492,3.2847898874,-1.634568519
C,-3.1782808234,2.8404556614,-1.9287222281
H,-4.518453814,1.1279678355,-1.85595149
C,-1.4621894096,4.5601629862,-2.1062972578
C,-4.0844579606,3.7186606324,-2.5699015093
C,-2.344232658,5.370721354,-2.770372847
C,-3.6775683712,4.9597549092,-2.9791907871
H,-4.371604977,5.6201522093,-3.4891385362
C,1.2130962501,1.5072790937,-0.5999632208
C,2.6197290703,1.6575338273,-0.5788651383
C,0.4099670314,2.6501268354,-0.5374455016
C,3.1802495096,2.8970914808,-0.4624756374
H,3.2387849615,0.776069732,-0.7019777628
C,0.9658908299,3.9037778101,-0.0982547411
C,2.3830508626,4.0382880139,-0.1746031946
H,4.2579343617,3.0262329936,-0.5191344396
C,2.9941023584,5.2839599817,0.1002949319
C,0.8754603631,6.167259291,0.7768906673
C,2.2472881833,6.348477046,0.5257419289
H,2.7147672115,7.3029984383,0.7433657608
N,-1.3037470494,1.0844695419,-0.8910533354
O,1.8917563202,-1.3424442478,-0.42597372
H,-2.014463132,6.3355283655,-3.1411217633
H,0.3171776498,6.9627822104,1.259947767
H,-5.0958255421,3.3741404632,-2.7618937751
H,-0.4417589785,4.884550439,-1.9581849343
H,4.0715467117,5.3682237614,-0.0075489264
C,-1.1574000166,4.8121452907,1.0301698097
C,-2.1221540626,5.8048057481,0.8405180457
C,-1.4969502429,3.6971839352,1.8043621093
C,-3.3925366626,5.6811169912,1.3894545666
H,-1.8788278394,6.6721743055,0.2355076997
C,-2.7665261636,3.5727346595,2.3541863342
H,-0.7546849778,2.9267970914,1.9847284051
H,-4.1291753331,6.4603567485,1.2203668649
H,-3.0063360162,2.7015226541,2.9556518541
C,0.2300153552,4.9755877987,0.5116367762
C,-3.6628376705,-4.9424123703,-0.3787916083
C,-3.7212983118,4.5624709746,2.1462818056
H,-4.7136850601,4.4640337963,2.5746068215
C,-5.1241638395,-4.8667775711,-0.3382643092
C,-5.8098027253,-3.7658694745,-0.8632381366
C,-5.8682213693,-5.9072850172,0.2287797858
C,-7.1961280027,-3.7034464861,-0.8143125737
H,-5.2557302791,-2.9634923803,-1.34135346
C,-7.2538458008,-5.8485442717,0.2663975988
H,-5.3492015209,-6.7577080673,0.6582500657
C,-7.924786508,-4.7447764928,-0.2509016358
H,-7.7099552519,-2.842179576,-1.2295129562
H,-7.813390428,-6.6648365014,0.7121044646
H,-9.008256323,-4.6976818269,-0.216154718
C,6.7853733684,-2.386116585,0.1451507327
C,7.0098979398,-1.0934650876,-0.3410132733
C,7.8397883624,-3.0536414708,0.7778880768
C,8.2485711319,-0.4841611971,-0.190840074
H,6.2176988713,-0.5690578701,-0.8670611813
C,9.0800086077,-2.4475357617,0.916869342
H,7.6740676616,-4.0483621179,1.1780988765
C,9.2897062235,-1.1584445111,0.4370109938
H,8.4038192055,0.5182360457,-0.5771092895
H,9.885144154,-2.9807205958,1.4124504756
H,10.2586030647,-0.6834145995,0.5508998421

3b-2 (S_0)
(CAM-B3LYP/6-31G(d,p) for C, H, N, and O and CAM-B3LYP/LanL2DZ for Pt)
-2281.6860958 hartree
C,-3.8796159607,3.2007437365,0.1494823162
C,-4.0314250478,4.0863477699,-0.8992425355
C,-4.5303156683,5.2941774748,-0.3730668757
N,-4.2644113073,3.8604733658,1.2950813429
H,-3.771120366,3.8739571736,-1.9249036005
H,-4.7234037015,6.2072157164,-0.917130982
C,-3.390666477,1.8218336172,0.1227671705
C,-2.9992723097,1.2108683758,1.3264813474
C,-2.5397388044,-0.0975199348,1.4858037978
H,-2.9925251988,1.8229580085,2.2182037928
O,-3.3497387758,1.2862911381,-1.0321174793
C,-2.1489220015,-0.5592323936,2.8156865921
C,-2.1848163839,0.010514804,4.0778079397
N,-1.61007474,-1.8106476028,2.9539607019
C,-1.6442104503,-0.9250520747,4.979321149
H,-2.5733908943,0.9873477172,4.3251198778
C,-1.2870620342,-2.0543116158,4.2553848195
H,-1.5545685041,-0.8125097846,6.0498691279
Pt,-2.7719448099,-0.7155017526,-1.4056620041
H,-1.4120389831,-2.3943576368,2.1559536832
H,-4.41927024,3.4127482081,2.183731835
C,-3.8053000726,0.4408138579,-3.9269639981
C,-2.9242964587,-1.7477724214,-4.0699010488
C,-4.3036197406,0.3977898399,-5.190587439
H,-3.8988659714,1.2990712963,-3.2730892218
C,-3.6023693688,-1.9361892096,-5.3195976652
C,-4.263403128,-0.8245580825,-5.905584322
H,-4.7963519465,1.2648869321,-5.6151610829
C,-3.7379513942,-3.2037958013,-5.9397872689
C,-4.9309401229,-0.984119185,-7.1438985235

C,-4.4338252481,-3.3401577512,-7.111417219
C,-5.0118136989,-2.2149971754,-7.7366785154
H,-5.5433712063,-2.333897693,-8.6754234142
C,-2.2084898919,-2.5288935093,-1.9405753287
C,-1.8274561433,-3.5770288148,-1.0700273042
C,-2.1380496073,-2.7373430433,-3.3214901579
C,-1.366170836,-4.7598582802,-1.5727281576
H,-1.952614719,-3.4381662328,-0.001815121
C,-1.36607943,-3.831542272,-3.8505545789
C,-1.0804619068,-4.9056153713,-2.9573730656
H,-1.1423149405,-5.5940366369,-0.9128880775
C,-0.4557365925,-6.0808718422,-3.43644869
C,-0.1532285933,-5.0428154007,-5.5711589736
C,-0.0389360758,-6.1690591768,-4.7365055466
H,0.4461618047,-7.0670489694,-5.1044020941
N,-3.1532260588,-0.6204240898,-3.3791607775
O,-2.4005506091,-0.9939857764,0.572754387
H,-4.5438951372,-4.3212612974,-7.5613542791
H,0.3172693931,-5.0601045714,-6.5490178107
H,-5.4068082209,-0.1183005278,-7.5937067819
H,-3.3050270265,-4.0745974632,-5.4676269973
H,-0.2901086088,-6.8998758667,-2.7425610221
C,-0.6239558176,-2.6752939614,-6.0233916229
C,-0.8534938194,-2.7448387319,-7.3998306544
C,-0.1607908552,-1.4680142985,-5.4889294886
C,-0.6463623361,-1.6394988736,-8.2157611835
H,-1.2218675195,-3.6704835798,-7.8299941625
C,0.0470944859,-0.3623785259,-6.3037399594
H,0.0471914802,-1.3998406634,-4.4263767579
H,-0.8415240159,-1.7138738854,-9.2810501657
H,0.4105668335,0.562929983,-5.8679339121
C,-0.7674308494,-3.8780454879,-5.15540623
C,-4.6830228688,5.127848934,0.9931907644
C,-0.1980614405,-0.4420428192,-7.6704293391
H,-0.0376352134,0.4226915459,-8.3064197478
C,-5.1725673995,6.0505134058,2.0189585899
C,-4.7507834734,5.9472807407,3.3491243709
C,-6.0774307209,7.0631329983,1.6819585894
C,-5.2277929076,6.8236865859,4.3149744173
H,-4.018865359,5.1942225889,3.6260227896
C,-6.5429860318,7.9457544873,2.6458197547
H,-6.4283409708,7.1414350469,0.6583304858
C,-6.1244774745,7.8276555549,3.9676500045
H,-4.8869975181,6.729064875,5.3411014961
H,-7.2458899445,8.7239798469,2.3659005745
H,-6.4939695329,8.5150196579,4.7215203462
C,-0.6942596089,-3.3183618742,4.6961840711
C,-0.897909381,-4.5041203069,3.9819996091
C,0.0900700177,-3.3625884478,5.8539464842
C,-0.3270197579,-5.6959164269,4.4083824537
H,-1.5314519727,-4.5017351819,3.1000162414
C,0.650241536,-4.5565677157,6.2846468278
H,0.273708195,-2.4468336419,6.4060304321
C,0.4479869929,-5.7283118079,5.5621202414
H,-0.4985457018,-6.6058028743,3.8420508332
H,1.2575283841,-4.5705926205,7.1841532025
H,0.8909697315,-6.6605182708,5.8969670936

3b-3 (S_0)
(CAM-B3LYP/6-31G(d,p) for C, H, N, and O and CAM-B3LYP/LanL2DZ for Pt)
-2281.6851463 hartree
C,-1.7025423697,1.325718955,2.5849143844
C,-1.9469329009,1.1385374185,3.9355118807
C,-1.0259638689,1.9307180118,4.6462815889
N,-0.655110278,2.2015307846,2.4844745229
H,-2.706283658,0.5006164596,4.3629593159
H,-0.9240481859,1.9964487136,5.7196551499
C,-2.3178642068,0.8127909491,1.3608918991
C,-3.3146631298,-0.1670509316,1.4662021689
C,-3.9903189052,-0.7908994636,0.4116330024
H,-3.5317213687,-0.5160499711,2.4666227926
O,-1.8647870451,1.3200450046,0.2784190805
C,-5.0231735683,-1.7818179377,0.709768511
C,-5.5882546058,-2.7240907866,-0.1267474563
N,-5.6013042132,-1.9402544373,1.9492501322
C,-6.5338134186,-3.4509107216,0.6231935407
H,-5.3085161459,-2.8756349537,-1.1580358964
C,-6.5382604744,-2.9372468426,1.9090224669
H,-7.125495383,-4.2878488146,0.2821000557
Pt,-2.503549853,0.7156311376,-1.6634480798
H,-5.5113246836,-1.2824042251,2.706328292
H,-0.3236045524,2.532610627,1.5924416778
C,-0.7244432139,3.06071118,-2.0411320182
C,-1.4670301251,1.9890370889,-4.0090868367
C,-0.195075198,4.1097991926,-2.7228530951
H,-0.6891465315,2.9710328638,-0.9632773628
C,-1.1216255695,3.1565472495,-4.7687802563
C,-0.431566394,4.2117368221,-4.1163008131
H,0.3307017046,4.8984807101,-2.1970102975
C,-1.5365238183,3.3522243813,-6.1099213056
C,-0.0724060553,5.3684463863,-4.8487211574
C,-1.2204580912,4.5038318587,-6.780777182
C,-0.4554878132,5.5105662706,-6.1551147823
H,-0.1949999033,6.4095007118,-6.7046377386
C,-2.9263865453,0.1815891248,-3.5116441536
C,-3.8999236342,-0.7728129402,-3.8906966155
C,-2.128545669,0.7729866316,-4.4952515189
C,-4.036594803,-1.1257871568,-5.2025152717
H,-4.5507984903,-1.1836582827,-3.1271348509
C,-2.0440076817,0.1856206737,-5.8076629966
C,-3.0981107939,-0.6982103272,-6.1817948383
H,-4.8288597521,-1.8015186071,-5.5140630042
C,-3.1672106111,-1.2012438365,-7.501837393
C,-1.0492334918,-0.2002122133,-7.98950252
C,-2.182247955,-0.9195772251,-8.4090311965
H,-2.2306754503,-1.3096796975,-9.4202458622
N,-1.3623206555,2.0385092997,-2.6713894352
O,-3.7997124466,-0.6074924726,-0.8428275593
H,-1.5631248194,4.6441857585,-7.8005593937
H,-0.200825998,-0.111887576,-8.660577426
H,0.4802512883,6.1541683003,-4.3430872135
H,-2.1282164299,2.5907988408,-6.5984821389
H,-4.0050915511,-1.8379362373,-7.7705663712
C,0.3883278742,0.8545601605,-6.3007408449
C,1.1079833273,1.7267881403,-7.1214068328
C,0.9888038904,0.4117617786,-5.1170104224
C,2.3791407571,2.159423219,-6.7643117659
H,0.6541780652,2.0872784133,-8.0388322742
C,2.2598643071,0.8430446261,-4.7592757664

H,0.4571632839,-0.2852839614,-4.4779142076
H,2.9153137252,2.8451844846,-7.4129557475
H,2.7082379387,0.4820630692,-3.8389357541
C,-0.9405207836,0.3232316724,-6.7160283447
C,-0.2273998045,2.5869062612,3.7199203424
C,2.9595980153,1.7216417672,-5.5795561127
H,3.9521249549,2.0596245421,-5.2990026954
C,0.8906949469,3.5123478851,3.9127153424
C,1.9045096711,3.6362139779,2.9563521171
C,0.9668115288,4.293517194,5.0709851996
C,2.95725479,4.5211357202,3.1487809292
H,1.8875916424,3.0132431556,2.0669317146
C,2.025284082,5.1689225186,5.2665901063
H,0.1772142357,4.2226457933,5.8116812432
C,3.023506897,5.2903969684,4.3049166144
H,3.7360608654,4.6002284532,2.3968890651
H,2.0659402704,5.7679156253,6.170823055
H,3.8483192516,5.9788255188,4.4568948168
C,-7.3304192892,-3.307370884,3.0830066629
C,-6.8463879562,-3.1018710613,4.3797356202
C,-8.5968353952,-3.8813792054,2.9262284746
C,-7.6101513326,-3.4501746546,5.4860150527
H,-5.8501964461,-2.6945138705,4.5251975177
C,-9.353001701,-4.2404746773,4.0325797136
H,-8.9926485738,-4.0272178719,1.9266723158
C,-8.8658685229,-4.0224259944,5.3177027103
H,-7.2162607597,-3.2852200016,6.4838741231
H,-10.3339039013,-4.6830818178,3.8911410987
H,-9.4608878208,-4.2984644635,6.1820469174

3b-4 (S_0)
(CAM-B3LYP/6-31G(d,p) for C, H, N, and O and CAM-B3LYP/LanL2DZ for Pt)
-2281.6795984 hartree
C,-1.7484372691,1.5330700842,2.4377483949
C,-1.7374997431,2.8386396198,2.8847508175
C,-1.0379817023,2.8680458662,4.1082840536
N,-1.0554526577,0.7816488301,3.3612310285
H,-2.1637525361,3.6741559276,2.3506450414
H,-0.8108732845,3.7407303137,4.7030909936
C,-2.3393184637,0.9870368056,1.2134860714
C,-1.9007271883,-0.2640792438,0.7432651819
C,-2.3832423568,-0.9560701151,-0.3754106878
H,-1.1065841807,-0.7396702286,1.3039912402
O,-3.2157814582,1.7249839723,0.6617153794
C,-1.7737605462,-2.2340770197,-0.7467020802
C,-2.2850325901,-3.2357324501,-1.5489921481
N,-0.5441202396,-2.6611395546,-0.3020337035
C,-1.3461667018,-4.284865291,-1.5759667101
H,-3.2441839075,-3.1973678065,-2.0420089527
C,-0.2627258032,-3.9027634238,-0.8021368175
H,-1.4256053777,-5.2110179514,-2.1261406864
Pt,-4.3718668545,1.1430963213,-1.0197189304
H,0.0814126049,-2.1227880698,0.2736162095
H,-1.0732839589,-0.2248468635,3.3982847131
C,-5.5240770923,3.6522025249,0.0530778546
C,-6.5028394039,2.8187196553,-1.9301485224
C,-6.4988716954,4.5833027732,0.2261020606
H,-4.6837624655,3.5313939162,0.7256300514
C,-7.6641030806,3.6260079678,-1.6924459415
C,-7.6354032507,4.5552842651,-0.6194638633
H,-6.4459271757,5.2859153444,1.0497906649
C,-8.8766277048,3.4592339143,-2.4076253379
C,-8.7673233958,5.3689957968,-0.3725070409
C,-9.9743581322,4.2235811554,-2.1136836768
C,-9.9117904772,5.2092554226,-1.1059596558
H,-10.782839586,5.8220718645,-0.8968674247
C,-5.4713138145,0.7889309045,-2.617065148
C,-5.43293985,-0.3878871498,-3.4013948748
C,-6.2953006192,1.8471963335,-3.0114068186
C,-6.1855303682,-0.4786438134,-4.5371017268
H,-4.820707135,-1.2177693415,-3.0666872206
C,-6.8316460992,1.888192181,-4.3472686965
C,-6.867006324,0.6541634501,-5.0605013045
H,-6.2200565505,-1.4041413424,-5.1060190882
C,-7.5135975033,0.578564058,-6.3163205241
C,-7.835296375,2.9493483647,-6.2881222383
C,-8.0338152389,1.7000480626,-6.902581203
H,-8.5250263977,1.6448691546,-7.8683940566
N,-5.5459010321,2.7786499749,-0.9899400497
O,-3.3457331789,-0.6037098228,-1.1427883909
H,-10.8999914294,4.0688780172,-2.6581099871
H,-8.1053153281,3.8520411795,-6.8268072751
H,-8.7202762061,6.0954641466,0.4327876155
H,-8.9377491311,2.7035469862,-3.1783848056
H,-7.5631310037,-0.3843096317,-6.8164333488
C,-6.8436287539,4.44528486,-4.6124686731
C,-7.7495530326,5.5064905985,-4.6851348969
C,-5.534437694,4.7189928192,-4.2014369131
C,-7.3680281168,6.7971936683,-4.3401345711
H,-8.7715838488,5.3110049147,-4.9930155669
C,-5.1516974162,6.0090113874,-3.856597286
H,-4.8087444164,3.9135396335,-4.161618711
H,-8.0922230882,7.6041186643,-4.3942654628
H,-4.1295503272,6.1985811353,-3.5442131373
C,-7.2223341688,3.074282208,-5.0569356647
C,-0.638385274,1.5748988094,4.3973791147
C,-6.0676983278,7.0535711661,-3.9210288792
H,-5.7689041369,8.0610492951,-3.6494125573
C,0.0958827263,1.0349301335,5.5428459331
C,0.8664589566,-0.127466312,5.4292773368
C,0.0404360298,1.6799914727,6.7833475119
C,1.552324063,-0.6350638736,6.5249149257
H,0.9547185323,-0.6242238425,4.4675594056
C,0.7368888677,1.1789079968,7.8735146783
H,-0.5702052721,2.5702010925,6.8913221469
C,1.4923357939,0.0166605818,7.7513412998
H,2.1457576098,-1.5372895505,6.4160616991
H,0.6804696782,1.6923902357,8.8280703798
H,2.0313879023,-0.3774756114,8.6065248885
C,0.998338694,-4.591777058,-0.5198778204
C,2.1726606677,-3.8820271266,-0.2455273954
C,1.0502370855,-5.9901357983,-0.5238732531
C,3.359306165,-4.5501447734,0.0273212099
H,2.1709132734,-2.7962233673,-0.2784688729
C,2.2391943274,-6.6557591574,-0.2629292443
H,0.1431911096,-6.5534405944,-0.7162098384
C,3.3985284686,-5.9396463906,0.018800071
H,4.2601798993,-3.9811334476,0.2340283577
H,2.2587790639,-7.7409492879,-0.2691711492

H,4.3266002898,-6.4615219462,0.2276503297

3b (S_1)
(CAM-B3LYP/6-31G(d,p) for C, H, N, and O and CAM-B3LYP/LanL2DZ for Pt)
-2281.59027104 hartree
C,-4.1890937572,3.1657958458,0.0564730092
C,-5.4414296545,3.7149699344,0.2849422757
C,-5.3243402597,5.1087230307,0.1414414519
N,-3.3412262082,4.2039052273,-0.226825673
H,-6.3414705547,3.1684929414,0.524685591
H,-6.1192741961,5.8352927282,0.2245606221
C,-3.666087508,1.804080914,0.0746524467
C,-4.5495310635,0.7440451077,0.3096118776
C,-4.2291478519,-0.612771597,0.3628986924
H,-5.5847639913,1.0024210239,0.4813927768
O,-2.4022297066,1.7130236428,-0.1300815358
C,-5.2760554517,-1.5835136973,0.659652901
C,-6.6450856709,-1.4884456207,0.8519727283
N,-4.937327057,-2.902572224,0.8120964474
C,-7.1218106514,-2.7812183684,1.133721361
H,-7.2366960217,-0.5879401361,0.7786550996
C,-6.0376407264,-3.6489581115,1.1101210098
H,-8.1498627087,-3.0670455078,1.3013603351
Pt,-1.3484668745,-0.1261991377,-0.2279479178
H,-3.9767059965,-3.2091120231,0.7966746762
H,-2.3549630252,4.0611449977,-0.3757389298
C,0.5879877884,2.055321793,-0.7452850276
C,1.4610013365,-0.1524415026,-0.8626230978
C,1.7632872446,2.5984186301,-1.1664313151
H,-0.2715985424,2.6559087078,-0.4760387285
C,2.6420255493,0.3403171989,-1.5246788969
C,2.8130416684,1.7497143078,-1.6365219144
H,1.8736876014,3.6755263698,-1.218781745
C,3.6041890284,-0.4929033966,-2.1260320138
C,3.9668550969,2.2640228588,-2.2487720895
C,4.7199448216,0.0383595304,-2.7463478317
C,4.9177342511,1.4215733301,-2.7915956809
H,5.8017595946,1.8314222103,-3.2690308352
C,-0.2986975757,-1.7357234445,-0.4360452032
C,-0.775722937,-3.0513704069,-0.5682721404
C,1.1278564073,-1.4925600168,-0.4982028875
C,0.1046773815,-4.0985191923,-0.665629215
H,-1.8466065052,-3.2125613333,-0.6219011085
C,2.0119321133,-2.5895389797,-0.1903734812
C,1.4999176408,-3.9060231532,-0.4303634006
H,-0.2508613107,-5.1108467355,-0.833966679
C,2.3712657786,-5.0036767726,-0.3730681807
C,4.1439801803,-3.5831682084,0.4117161251
C,3.6890935587,-4.838869958,0.0084962092
H,4.3532942555,-5.6954717051,0.0595633026
N,0.4005183361,0.7203667529,-0.6414823498
O,-3.0715538181,-1.1484017263,0.1844391173
H,5.4437769882,-0.6279190215,-3.2049877574
H,5.1352682009,-3.484660377,0.840215404
H,4.0890487467,3.3415659001,-2.306790255
H,3.4632360056,-1.5656718551,-2.1139501669
H,1.9873587955,-5.991422148,-0.6098923734
C,3.8046026145,-1.2164610448,1.0056744149
C,5.1188578586,-0.7746270872,0.8258707745
C,2.9738765678,-0.5048148308,1.8788599361
C,5.5846231851,0.3563944573,1.482401202
H,5.7697826423,-1.3051355306,0.1389494279
C,3.4416736621,0.6230845177,2.5396182317
H,1.9605149581,-0.8503647548,2.0527435039
H,6.6033170269,0.6924872626,1.3177509478
H,2.7842968871,1.1583406821,3.2171791735
C,3.32184351,-2.460094718,0.3574816464
C,-4.0028235144,5.3934036183,-0.178032373
C,4.7468045448,1.0603169644,2.3406340431
H,5.1105947052,1.9440994961,2.8549312433
C,-3.3443576217,6.6724195,-0.4497096056
C,-2.2107733965,6.7468094552,-1.2665594021
C,-3.8461849414,7.8543963622,0.1058848119
C,-1.5927068658,7.9656904086,-1.5125174315
H,-1.8249149335,5.8485377061,-1.7394574375
C,-3.2335386375,9.0726364839,-0.1498409848
H,-4.7125791845,7.8088506229,0.7573297933
C,-2.1016370003,9.1340006189,-0.9567155453
H,-0.716298264,8.0035950615,-2.1516605458
H,-3.6360505518,9.9787293948,0.2917708064
H,-1.6206268454,10.086762468,-1.1521906557
C,-5.973349046,-5.0949685065,1.3289507054
C,-4.9521152342,-5.8703305734,0.7690502845
C,-6.9454607228,-5.7329936181,2.1072319567
C,-4.9002717346,-7.2404692433,0.9880616741
H,-4.2055182537,-5.4035793361,0.1334714643
C,-6.8982836512,-7.1037536458,2.3157068084
H,-7.7314928657,-5.1416704981,2.5649620949
C,-5.8735677223,-7.8638770247,1.7606050463
H,-4.1013130506,-7.8251679661,0.5432858015
H,-7.6603624607,-7.5803736303,2.9240819173
H,-5.8347816796,-8.9351453891,1.928577992

3b (T_1)
(CAM-B3LYP/6-31G(d,p) for C, H, N, and O and CAM-B3LYP/LanL2DZ for Pt)
-2281.6217224 hartree
C,-4.1698398062,3.1994727832,0.1374732825
C,-5.4222937521,3.7471443039,0.3635222033
C,-5.3049142255,5.1426998386,0.2268922282
N,-3.3171184958,4.2400152914,-0.1186283179
H,-6.32125006,3.2003008214,0.6063238495
H,-6.0879899546,5.873288728,0.3679932293
C,-3.6534578867,1.832048755,0.113350138
C,-4.5288785131,0.7792595878,0.4090994035
C,-4.2154155089,-0.5788510339,0.4508000813
H,-5.5471739545,1.0465191521,0.6536884348
O,-2.4103950559,1.7306787305,-0.1772452811
C,-5.2477094147,-1.5435528154,0.8173834135
C,-6.6048096047,-1.4477141092,1.0786112681
N,-4.9030575388,-2.8626075053,0.9463432913
C,-7.0715579324,-2.7448418718,1.3600758526
H,-7.1926774234,-0.5418276331,1.06742626
C,-5.9918197434,-3.6139027497,1.2725505574
H,-8.0792878547,-3.022554663,1.6323976624
Pt,-1.3847287486,-0.135821197,-0.3273575795
H,-3.9657133317,-3.1846273961,0.758813152
H,-2.3555970781,4.0884166155,-0.3778131083
C,0.5348706579,1.9911636762,-1.0489693389

C,1.4207596805,-0.215458682,-1.0681330732
C,1.7212172343,2.5334826915,-1.4686314953
H,-0.3380882512,2.5922276069,-0.8280601348
C,2.6343457179,0.2771556405,-1.6980759271
C,2.7925609967,1.677394002,-1.8578413239
H,1.8183794004,3.6079352921,-1.5726942832
C,3.6210066055,-0.5679659975,-2.2350652849
C,3.9619527697,2.1861149122,-2.4555401973
C,4.7469180743,-0.0494976711,-2.8416691175
C,4.9323365105,1.3363120896,-2.9353129749
H,5.8260662283,1.7357560278,-3.4033316083
C,-0.3458643203,-1.7694668918,-0.5492702761
C,-0.7768425354,-3.0565550318,-0.7998224338
C,1.1069540883,-1.5095189992,-0.6393955648
C,0.1362096466,-4.0978194512,-0.9806739058
H,-1.8419882741,-3.2517540526,-0.8720461044
C,2.0116641839,-2.6199260569,-0.3280233429
C,1.5279005528,-3.9183091899,-0.6644040349
H,-0.2071227345,-5.0974889625,-1.227231169
C,2.3965886909,-5.0115027513,-0.5834853825
C,4.0960794951,-3.6177983988,0.3895391854
C,3.6820827736,-4.8539790827,-0.0857673872
H,4.3462328892,-5.7096906008,-0.0166485844
N,0.3622014498,0.6696209473,-0.8865870741
O,-3.0757194716,-1.1257612606,0.2061424762
H,5.4909788778,-0.7236952561,-3.2532759523
H,5.060032282,-3.5186642578,0.8763623701
H,4.0724293439,3.2619548125,-2.552192066
H,3.4915546519,-1.6406972082,-2.1824374354
H,2.0409234612,-5.9919313254,-0.8853411625
C,3.7130098487,-1.2405111445,0.9649649685
C,5.0202601553,-0.7725440405,0.8074013809
C,2.8536131118,-0.5458894504,1.8229381033
C,5.4520440774,0.3688118047,1.4713210805
H,5.6959063867,-1.2949426391,0.1380330303
C,3.2857548496,0.5933021086,2.4888751675
H,1.8443135547,-0.9120860989,1.9795809204
H,6.4678589368,0.7229661895,1.3272529927
H,2.6059859316,1.1148368852,3.1550763813
C,3.2648018627,-2.4924017063,0.3017614832
C,-3.9811901351,5.4296391018,-0.0764961032
C,4.5855035338,1.056809131,2.3127745248
H,4.9226492034,1.9473058209,2.8336800802
C,-3.313574535,6.7121114165,-0.3059517952
C,-1.9482769826,6.8770364661,-0.047751906
C,-4.0383325957,7.8074326119,-0.7883997694
C,-1.3253999216,8.0973479838,-0.274010392
H,-1.3732609002,6.0524371362,0.3631834558
C,-3.4166422126,9.0290186739,-1.0031957045
H,-5.0932360891,7.6883692884,-1.0121805781
C,-2.056478798,9.179248359,-0.751312357
H,-0.2660440822,8.2064957331,-0.0640898464
H,-3.9953441402,9.866534027,-1.3797104166
H,-1.5704552687,10.1338149676,-0.9243445035
C,-5.9160461776,-5.0603525009,1.4858623732
C,-4.7218020701,-5.676432237,1.8759437392
C,-7.050629026,-5.8590324034,1.3047808101
C,-4.6629121168,-7.0500739608,2.0706763989
H,-3.8359811679,-5.0748171903,2.056398923
C,-6.9923967008,-7.2298142687,1.5105322399
H,-7.9783511689,-5.3980876133,0.9823605924
C,-5.7975670325,-7.8330159113,1.8907227156
H,-3.7276003172,-7.5085503747,2.375793891
H,-7.8829182166,-7.832655127,1.3631206526
H,-5.7519278596,-8.9058769315,2.0466567997

3b·Cl⁻ (S_0)
(CAM-B3LYP/6-31G(d,p) for C, H, N, O, and Cl and CAM-B3LYP/LanL2DZ for Pt)
-2742.0064252 hartree
C,3.6515183165,2.464927214,-0.4275785421
C,3.196326373,3.7348142344,-0.7489074817
C,4.3148558629,4.5715586717,-0.8505380361
C,5.4425986756,3.8001769006,-0.5852241253
N,5.0219039384,2.5257749924,-0.3375723085
H,2.16089179,3.9942585307,-0.9073143508
H,4.3156354289,5.6189277698,-1.1153996036
C,2.8288925318,1.2710708096,-0.2318686994
C,3.4295586295,0.0177334068,-0.0549198831
C,2.7771358882,-1.2003452181,0.1423271708
H,4.5100495476,-0.0103264853,-0.0766837906
O,1.5645322383,1.4988800518,-0.2536117926
O,1.4990991453,-1.3996592735,0.1883121602
C,3.5448549074,-2.4326498666,0.314872391
C,3.0310789336,-3.7150176995,0.4361872639
N,4.9151898134,-2.5263532127,0.3763265693
C,4.1141127917,-4.5923924961,0.5701341141
H,1.9802169917,-3.9586888847,0.4220059822
C,5.279630762,-3.8326027896,0.5307148584
H,4.0631062692,-5.6629473175,0.7053800326
Pt,0.0990657164,0.0312912255,0.0010045898
C,-1.327446042,-2.6127579319,0.3821942539
C,-3.8092193403,-1.4824910718,-0.3863854064
C,-2.4507534981,-3.3862395473,0.3834438084
H,-0.3512722617,-3.0339891689,0.5963733992
H,-2.3978704238,-4.441788187,0.6387388645
C,-2.6804983565,-0.6470061757,-0.065512754
C,-1.4183682135,-1.2175437817,0.1453608797
C,-2.657328566,0.8129535622,0.0814543214
C,-1.2184526999,2.6844744876,-0.0347494042
C,-2.227949668,3.5653671243,0.1965386864
H,-0.1861801191,2.9746493209,-0.1930084912
H,-2.0365639476,4.6323993472,0.1921926827
N,-1.432875256,1.3420737494,-0.0663404424
H,5.5704478448,-1.7336018155,0.3181900484
H,5.6375923702,1.7399681919,-0.0806453262
C,-3.704913176,-2.8621928352,-0.0401932159
C,-4.821287205,-3.7164307832,-0.186358844
C,-5.9860426168,-3.2599985514,-0.7433296777
H,-6.8410094009,-3.9179738882,-0.8615785526
C,-6.0303940302,-1.9528513773,-1.2578789258
H,-6.8921502539,-1.6418086247,-1.8401609448
C,-4.9704693821,-1.0757969442,-1.1275931922
H,-4.7242048761,-4.7518042103,0.1282800044
C,-3.5070952344,3.0679954445,0.5485762949
C,-4.5457124396,3.9256766777,0.98601605
C,-5.7177690184,3.411191335,1.4708599393
H,-6.5004702682,4.0758456538,1.823470389
H,-4.377557756,4.9981492483,0.9617572581
C,-5.8973597855,2.0139216949,1.5460509742

H,-6.8078384434,1.6099030547,1.9767955992
C,-3.7200447518,1.6644404419,0.537294752
C,-4.9283582798,1.1633825362,1.0828464784
H,-5.0733511889,0.0941472113,1.1519838087
Cl,6.9456289922,0.0010189054,0.2912392269
C,-5.0252715072,0.1864837632,-1.9180453206
C,-3.9542428809,0.5543765148,-2.7401415893
C,-6.1747361843,0.9807670251,-1.9363392984
C,-4.0266159029,1.6880380848,-3.5393181978
H,-3.0587843202,-0.0576249787,-2.7543569041
C,-6.2487062208,2.1148962319,-2.7356815532
H,-7.0095697257,0.7181609456,-1.2946664715
C,-5.1733006795,2.4753239752,-3.5391590633
H,-3.182451298,1.9530988398,-4.1681397629
H,-7.1480110734,2.7233716715,-2.7231902989
H,-5.2272324052,3.3637791611,-4.1606292913
C,6.6697683775,-4.2887999035,0.6428866835
C,7.7298072107,-3.4050082184,0.8798092036
C,6.9597643137,-5.6550000894,0.5211189028
C,9.0301909584,-3.8813759936,0.9927167165
H,7.5502800866,-2.337214314,0.9645706143
C,8.2588010366,-6.1253896536,0.6430261987
H,6.1566251506,-6.354356848,0.3142773609
C,9.3050508247,-5.2394159802,0.8808936038
H,9.8344061231,-3.1739444033,1.1708057173
H,8.4555360123,-7.1892284744,0.5435386305
H,10.3238055686,-5.6045765917,0.9720107472
C,6.8495753066,4.2165644051,-0.5705773827
C,7.901258968,3.2925284258,-0.5971605733
C,7.1655591082,5.5819348146,-0.5412153361
C,9.2202452103,3.7293708221,-0.5970957705
H,7.6979646905,2.2256124038,-0.6031874098
C,8.4841730492,6.0120824363,-0.5506083666
H,6.365627702,6.3134553318,-0.4957098199
C,9.5224391754,5.0861566942,-0.5792146391
H,10.0172252764,2.9921549481,-0.6114297534
H,8.701591903,7.0762715475,-0.5266294473
H,10.5558432367,5.4201732101,-0.5812348001

3b·Cl⁻ (S_1)
(CAM-B3LYP/6-31G(d,p) for C, H, N, O, and Cl and CAM-B3LYP/LanL2DZ for Pt)
-2741.90994228 hartree
C,3.6355352006,2.4933421573,-0.1723509279
C,3.1713591587,3.8000917667,-0.2482812281
C,4.2864240274,4.6403994432,-0.3230941829
C,5.4235838886,3.8352980403,-0.2933028906
N,5.010059468,2.5397102767,-0.1985793953
H,2.130444165,4.0835907455,-0.2371914463
H,4.2791799353,5.7196064347,-0.3672601681
C,2.8195180775,1.2887444473,-0.079958237
C,3.4179882439,0.030003325,0.0345527411
C,2.7660245853,-1.2034410125,0.122134424
H,4.498809034,0.0056373028,0.0458783623
O,1.5489610841,1.5191199254,-0.1204700375
O,1.4881956232,-1.4056180649,0.1384083307
C,3.5319033666,-2.4410400082,0.2003820929
C,3.013270985,-3.7290534378,0.2385332801
N,4.9031089572,-2.5438605501,0.238969237
C,4.0922271774,-4.6155119415,0.304760777
H,1.9612433602,-3.9659651523,0.2032254722
C,5.261855501,-3.857168168,0.307326088
H,4.040721961,-5.6942787215,0.3223454679
Pt,0.0858321867,0.0529426306,0.0353079277
C,-1.307054982,-2.5372944999,0.6501768374
C,-3.7821156615,-1.4624231503,-0.2634872484
C,-2.4435511571,-3.2998052228,0.7248089537
H,-0.3327394402,-2.9472239176,0.8921472243
H,-2.403795154,-4.3275992272,1.0741223305
C,-2.6800457959,-0.5832938767,0.0462752943
C,-1.387711189,-1.1823818313,0.2773840669
C,-2.6785253056,0.8447523074,0.1431982442
C,-1.2168681035,2.7094771078,-0.0972252435
C,-2.2412202344,3.5957763373,0.0386011311
H,-0.1911245428,3.0128725769,-0.270718011
H,-2.0522495875,4.6591211353,-0.0551922226
N,-1.4016330145,1.3729373304,-0.0044616969
H,5.5623371631,-1.7513386043,0.2355232209
H,5.6358150406,1.7210005563,-0.168754934
C,-3.6874231455,-2.8048126451,0.2292987659
C,-4.8135716768,-3.6441970807,0.1584621014
C,-5.9665020504,-3.2264822148,-0.4696052771
H,-6.8271736286,-3.8856609342,-0.5284088841
C,-5.9976547006,-1.983942879,-1.1113715793
H,-6.8516070419,-1.7194759143,-1.7257805832
C,-4.9184992787,-1.1109468772,-1.0527946202
H,-4.747876756,-4.6415158893,0.5838006812
C,-3.5407717629,3.1320992081,0.4158527594
C,-4.5793715064,4.0173465399,0.7450408507
C,-5.7933425987,3.5504440457,1.21369169
H,-6.5845473138,4.2478230495,1.4709575952
H,-4.4021946004,5.0844183688,0.6444156404
C,-5.9841276347,2.1760675355,1.3791657767
H,-6.9206441504,1.8019821824,1.781843135
C,-3.7555195372,1.7270140506,0.5142524626
C,-4.9854849997,1.2821471575,1.0378864423
H,-5.1477264389,0.2225680541,1.1857580798
Cl,6.941847004,-0.0406270015,0.0585306233
C,-4.9477746625,0.0811685776,-1.9395138109
C,-3.8454864308,0.3931929803,-2.742847541
C,-6.09995053,0.8628660773,-2.0589257178
C,-3.8929644682,1.4613273274,-3.6287521073
H,-2.9491810026,-0.214051541,-2.6778855598
C,-6.1471296674,1.9331764638,-2.9428155102
H,-6.955067885,0.6471919425,-1.4269960481
C,-5.0426918336,2.2373781483,-3.7303810159
H,-3.026473908,1.685808956,-4.2425861522
H,-7.0468450582,2.5372738473,-3.0080188271
H,-5.0763887568,3.0760119749,-4.4189384292
C,6.6507970765,-4.3262305328,0.3597115043
C,7.7317288372,-3.4934447465,0.0455314147
C,6.9171230025,-5.6535081128,0.7235917301
C,9.0314029514,-3.9821169006,0.0939349626
H,7.5677826259,-2.4548279851,-0.226387299
C,8.2161742872,-6.1376650779,0.7619896838
H,6.0952531331,-6.3081275814,0.9935260288
C,9.2837670475,-5.303005445,0.4460361853
H,9.8526711723,-3.3147468984,-0.1486568771
H,8.3958098036,-7.1700730274,1.0482065347
H,10.3022196051,-5.6784489523,0.4799957779

C,6.8313137711,4.2457377203,-0.3380607736
C,7.8729692704,3.3765956173,0.0085068192
C,7.1567477868,5.5522264287,-0.7280997473
C,9.1922905496,3.8100776098,-0.0341540415
H,7.6629003043,2.3520742008,0.3012997679
C,8.4751263985,5.9814620656,-0.7607314733
H,6.3660119614,6.2338402425,-1.0230925761
C,9.5033812876,5.1110198999,-0.4124990253
H,9.9822266326,3.1151586626,0.2338063079
H,8.7007919388,6.9987726147,-1.0676786486
H,10.5368545053,5.4433303072,-0.44181387

3b·Cl⁻ (T_1)
(CAM-B3LYP/6-31G(d,p) for C, H, N, O, and Cl and CAM-B3LYP/LanL2DZ for Pt)
-2741.9370853 hartree
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C,-2.984914044,4.6867127466,-0.0265701985
C,-4.1673960596,3.9521198411,-0.027599505
N,-3.8319526723,2.6302248293,-0.072718281
H,-0.8652995236,3.9964561442,-0.0831189546
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C,-1.7196100139,1.2425609767,-0.1609294234
C,-2.3928326213,0.0182962431,-0.0607711923
C,-1.8221271705,-1.2559649203,-0.09536375
H,-3.4653704693,0.0623376523,0.0684865961
O,-0.4486137259,1.3935289029,-0.286950717
O,-0.5675944104,-1.5442669175,-0.2184290616
C,-2.6598958813,-2.4469516748,0.0261971837
C,-2.2155816086,-3.7563593621,0.1342247681
N,-4.0338832855,-2.4678051616,0.0671420374
C,-3.3455484637,-4.5765452759,0.2394051786
H,-1.177175604,-4.0494254266,0.1505450959
C,-4.4688454174,-3.7555728398,0.1902946854
H,-3.3538876365,-5.6494921274,0.3650579228
Pt,0.914708914,-0.1926820431,-0.4026214789
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C,4.7604721212,-1.8811669913,-0.1267440969
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H,1.2111372285,-3.2893419941,-1.0984998374
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C,2.30907878,-1.5415716269,-0.5738258888
C,3.7313794394,0.3959926701,-0.7673772713
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[S6] Report for pair interaction energy decomposition analysis (PIEDA): D. G. Fedorov and K. Kitaura, *J. Comput. Chem.*, 2007, **28**, 222–237.

4.Anion-binding behaviors

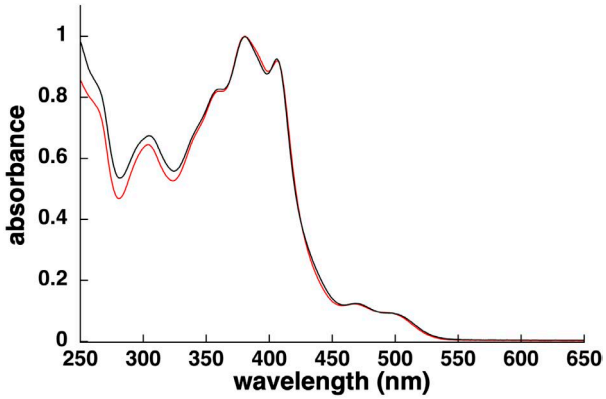

Fig. S34 UV/vis absorption spectra of **2a** in CH_2Cl_2 (0.03 mM) in the absence (black) and presence (red) of 3000 equiv of Cl^- as a tetrabutylammonium (TBA) salt. Anion-free and anion-binding forms show the similar UV/vis absorption spectra, as conformation changes in the anion-free and anion-binding forms result in the very small change in the directions of their transition dipole moments. Such UV/vis absorption spectral changes were also supported by TD-DFT calculations (Fig. S25).

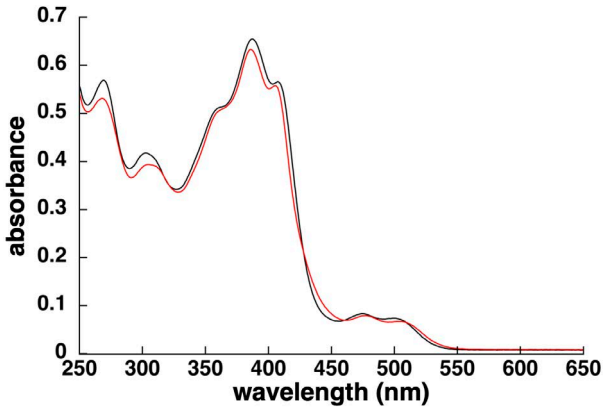

Fig. S35 UV/vis absorption spectra of **3a** in CH_2Cl_2 (0.015 mM) in the absence (black) and presence (red) of 2000 equiv of Cl^- as a TBA salt. Anion-free and anion-binding forms show the similar UV/vis absorption spectra, as conformation changes in the anion-free and anion-binding forms result in the very small change in the directions of their transition dipole moments. Such UV/vis absorption spectra were also supported by TD-DFT calculations (Fig. S26).

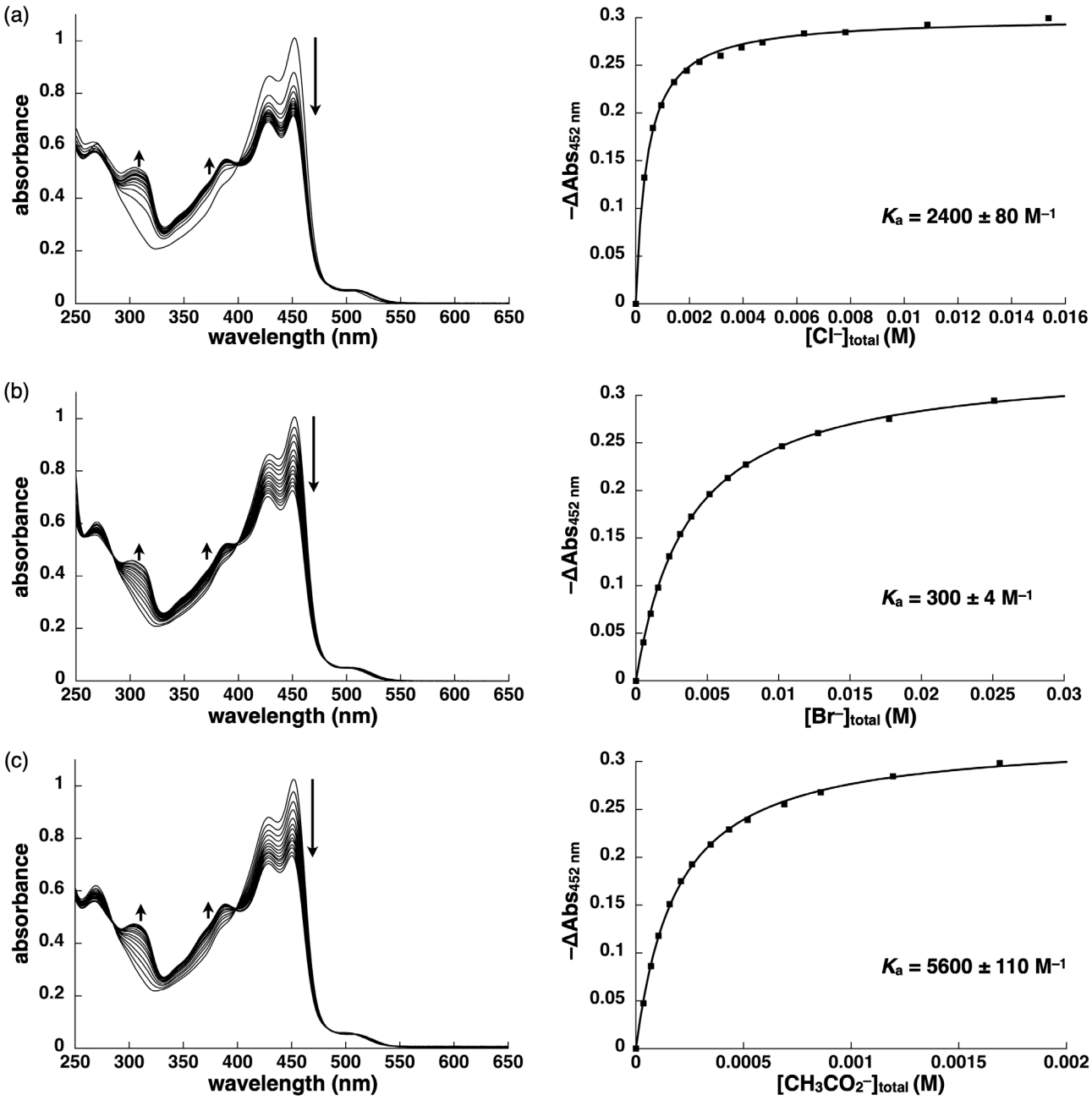

Fig. S36 UV/vis absorption spectral changes (left) and titration plots and 1:1 fitting curves (left) of **3b** (0.015 mM) upon the addition of (a) Cl^-, (b) Br^-, and (c) $CH_3CO_2^-$ as TBA salts in CH_2Cl_2.

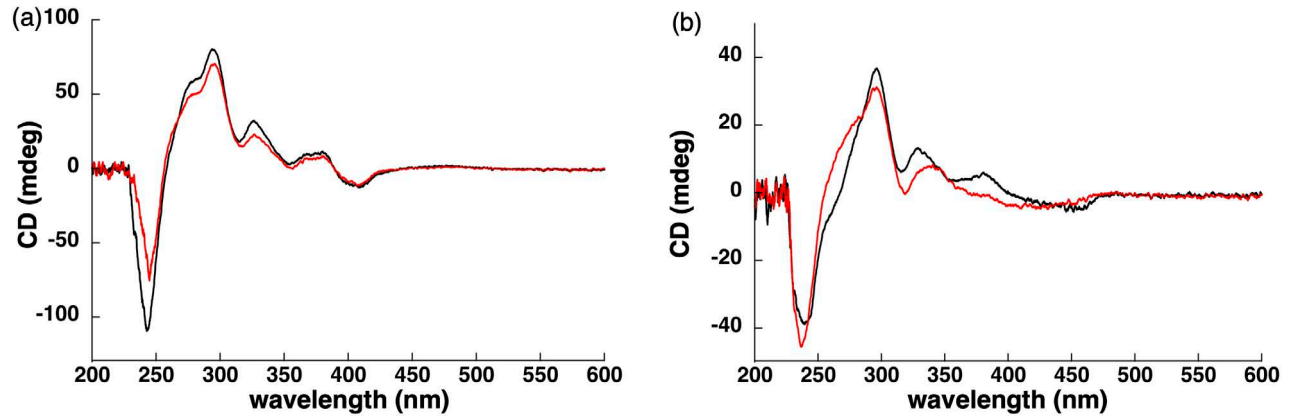

Fig. S37 CD spectral changes of (a) **3a** (0.03 mM) and (b) **3b** (0.015 mM) in the absence (black) and presence (red) of Cl^- as a TBA salt (2000 and 1000 equiv for **3a** and **3b**, respectively) in CH_2Cl_2.

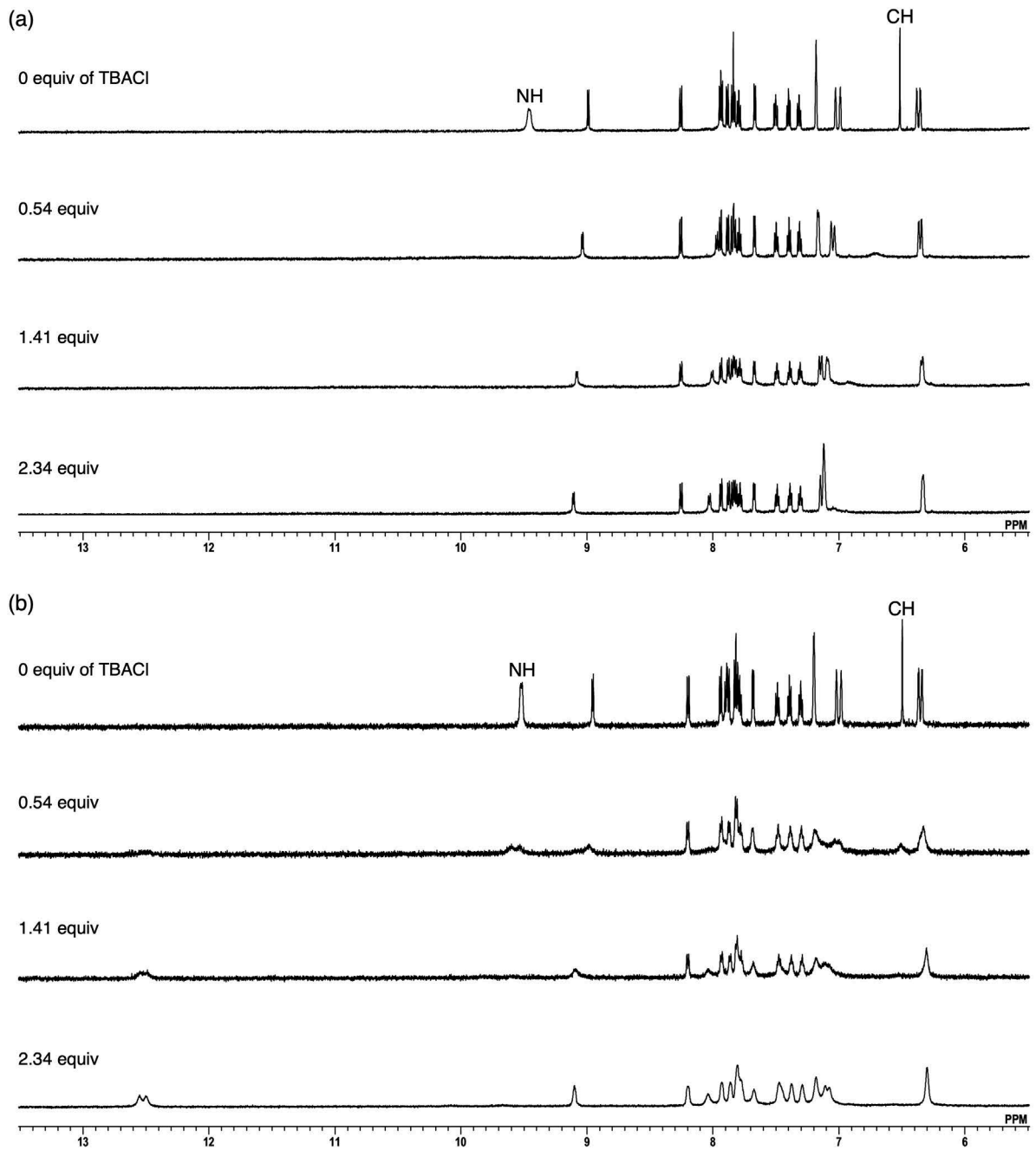

Fig. S38 ^{1}H NMR spectral changes of **2a** (1.0×10^{-3} M) upon the addition of Cl^- (0–2.34 equiv) added as a TBA salt in CD_2Cl_2 at (a) 20 °C and (b) –50 °C. Upon the addition of 2.34 equiv of TBACl at –50 °C, the signals of pyrrole NH (9.53 and 9.51 ppm) and bridging CH (6.50 ppm) were decreased and new signals were emerged in the downfield region, whose signals were identified as anion-binding pyrrole NH (12.55 and 12.50 ppm) and bridging CH (8.04 ppm). The equilibrium constant (K_a) was estimated to be 1×10^3 M^{-1} by the integrals of NH signals in the ^{1}H NMR spectrum at –50 °C upon the addition of 0.54 equiv of TBACl.

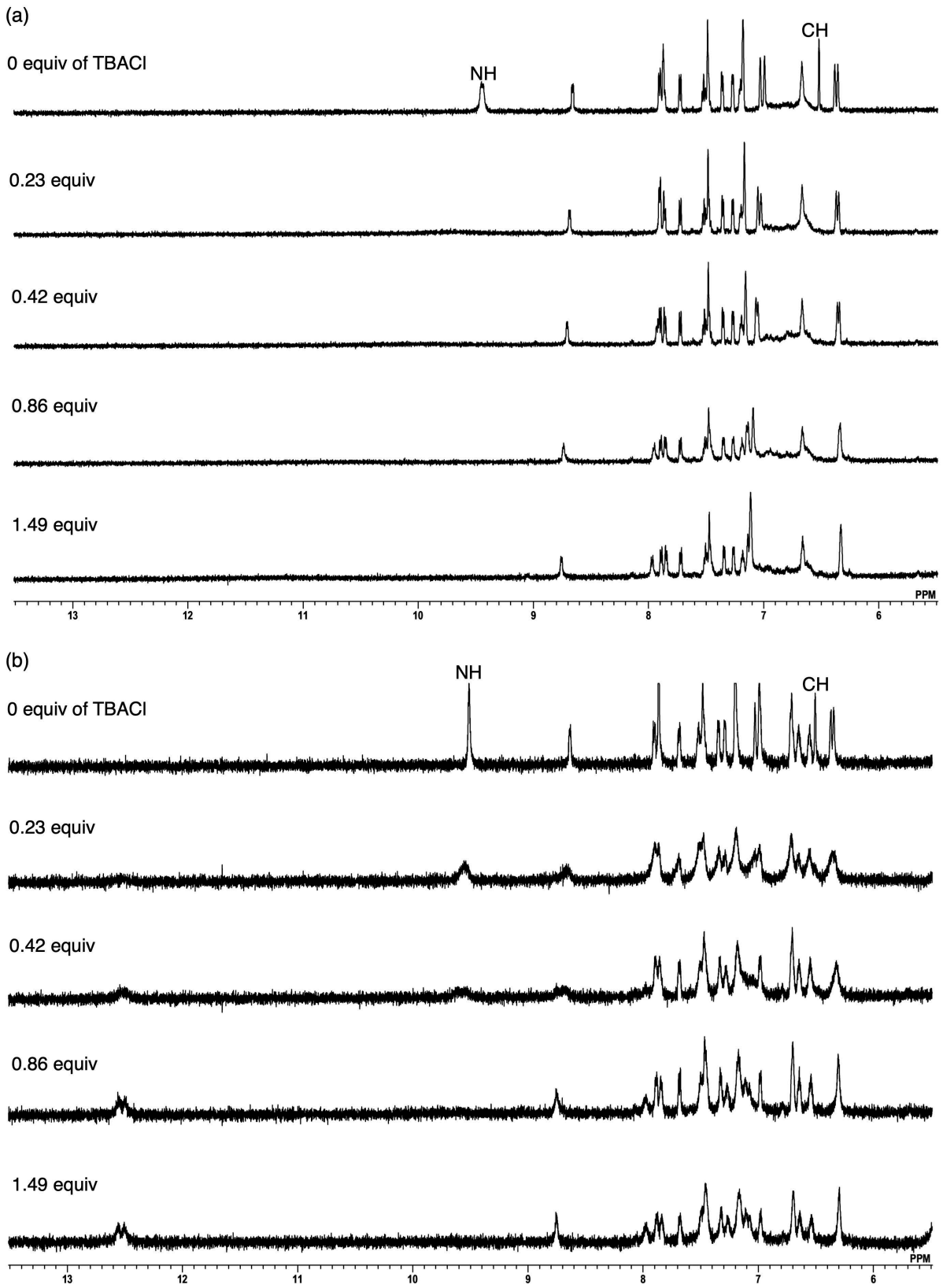

Fig. S39 ^{1}H NMR spectral changes of **3a** (1.0×10^{-3} M) upon the addition of Cl^- (0–1.49 equiv) added as a TBA salt in CD_2Cl_2 at (a) 20 °C and (b) –50 °C. Upon the addition of 1.49 equiv of TBACl at –50 °C, the signals of pyrrole NH (9.51 ppm) and bridging CH (6.51 ppm) were decreased and new signals were emerged in the downfield region, whose signals were identified as anion-binding pyrrole NH (12.56 and 12.51 ppm) and bridging CH (7.98 ppm). The equilibrium constant (K_a) was estimated to be 2×10^3 M^{-1} by the integrals of NH signals in the ^{1}H NMR spectrum at –50 °C upon the addition of 0.42 equiv of TBACl.

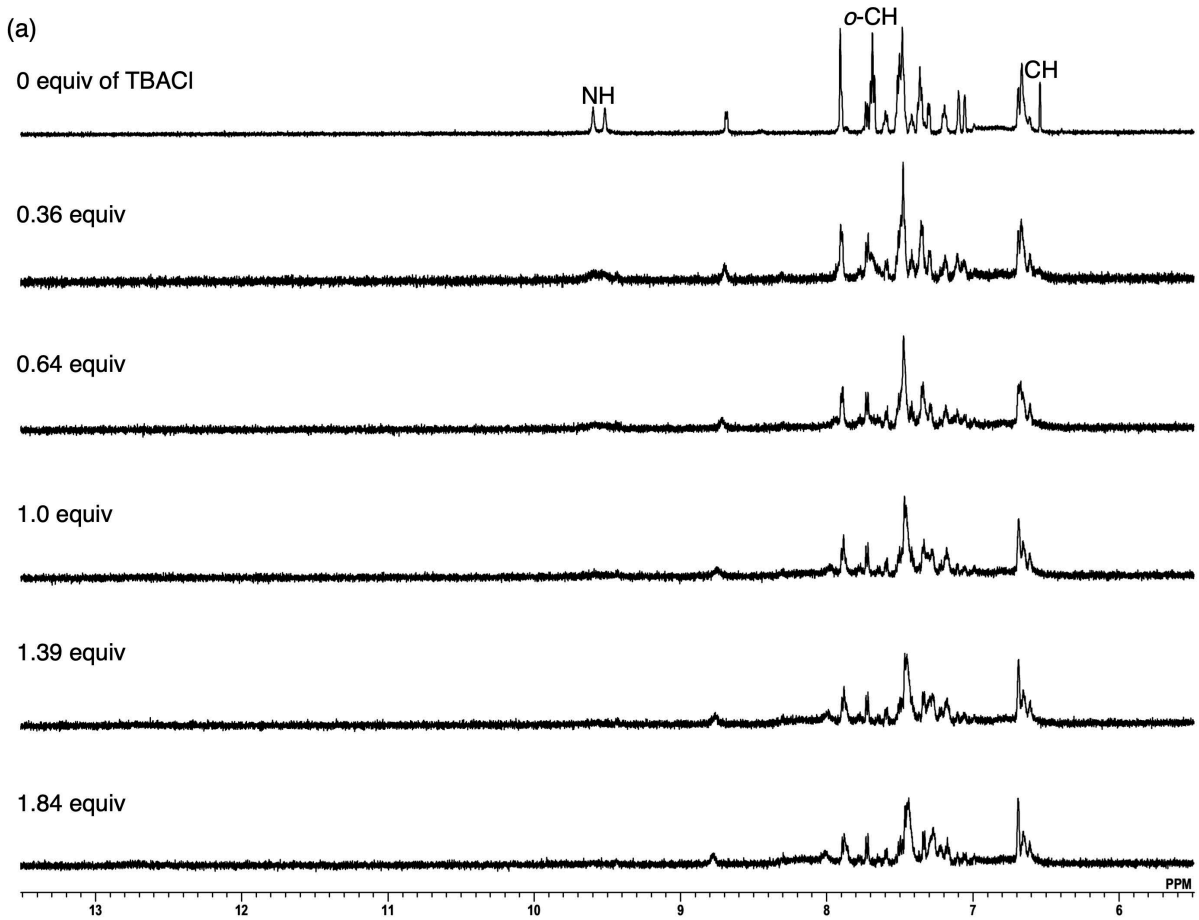

Fig. S40 ^{1}H NMR spectral changes of **3b** (1.0×10^{-3} M) upon the addition of Cl^- (0–1.84 equiv) added as a TBA salt in CD_2Cl_2 at (a) 20 °C and (b) –50 °C. Upon the addition of 1.84 equiv of TBACl at –50 °C, the signals of pyrrole NH (9.63 and 9.56 ppm), bridging CH (6.51 ppm), and phenyl *o*-CH (7.66 ppm) were decreased and new signals were emerged in the downfield region, whose signals were identified as anion-binding pyrrole NH (12.65 and 12.60 ppm), bridging CH (8.00 ppm), and phenyl *o*-CH (8.22 ppm).

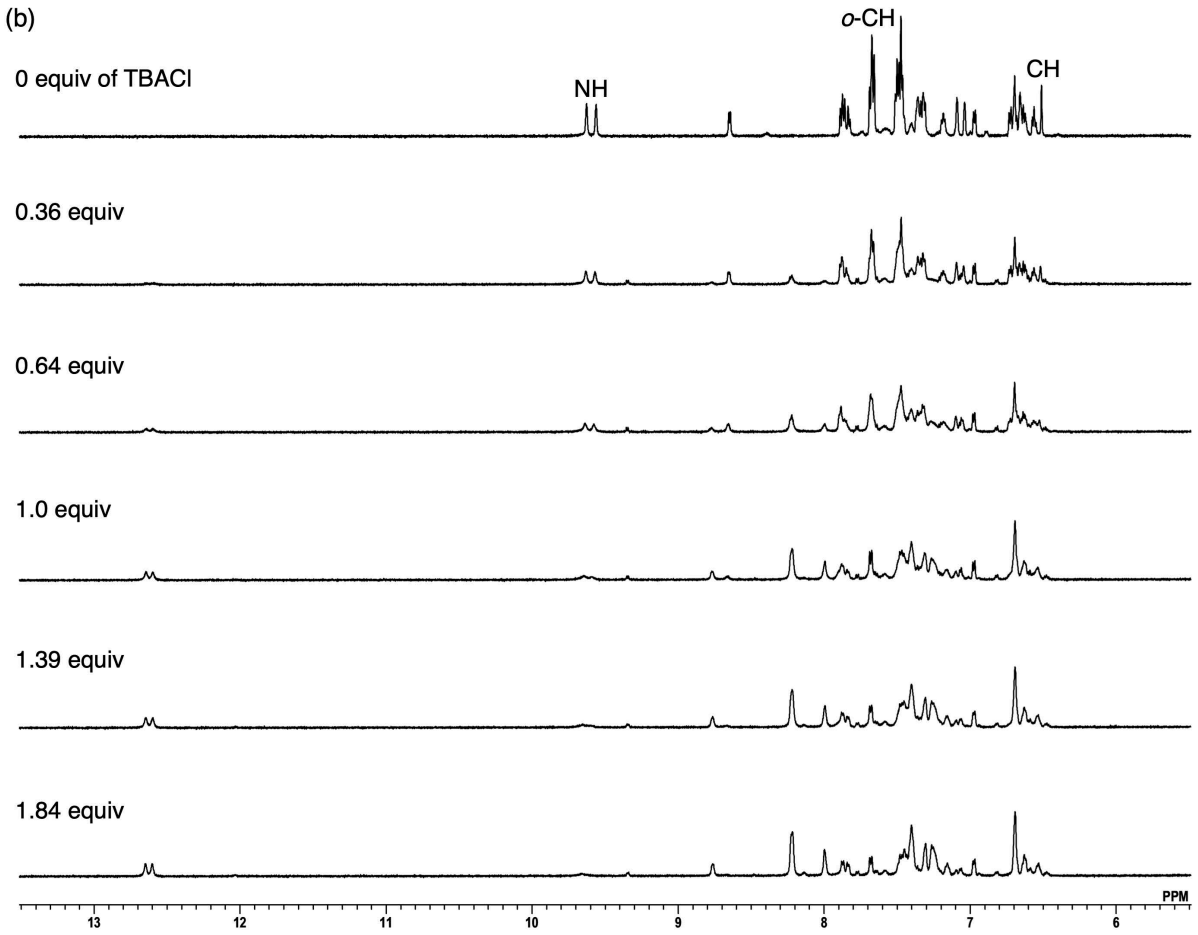

Fig. S40 (Continued)