Supporting Information for

Nitrogen-centred helical acridiniums with a 6-7-6-6 fused ring skeleton

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General

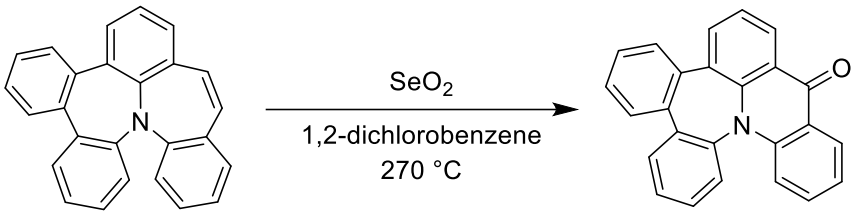
All reactions were carried out under an argon atmosphere. All commercially available compounds were used without further purification. Dry toluene, dry acetonitrile (for cyclic voltammetry measurement), and dry 1,2-dichlorobenzene were obtained by distillation from CaH_2 prior to use. Dry acetonitrile for cyclic voltammetry measurement was further purified by distillation from P_2O_5. Column chromatography was performed on aluminum oxide (Merck 90 active, neutral) of particle size 63-200 nm or on silica gel (Wakogel® 60N, neutral) of particle size 38-100 μm. ^1H and ^{13}C NMR spectra were recorded on a BRUKER Ascend™ 400 (^1H/400 MHz and ^{13}C/100MHz) spectrometer at 296 K unless otherwise indicated. IR spectra were measured on a Shimadzu IRAffinity-1S spectrophotometer using the attenuated total reflection (ATR) mode. Mass spectra were recorded on a Q Exactive spectrometer in FD mode or ESI positive mode by Dr. Eri Fukushi and Mr. Yusuke Takata (GS-MS & NMR Laboratory, Research Faculty of Agriculture, Hokkaido University). Melting points were measured on a Stanford Research Systems OptiMelt MPA100 and are uncorrected. UV-Vis spectra were recorded on a JASCO V-770 spectrophotometer. Redox potentials (E^{ox} and E^{red}) were measured on a BAS ALS-612EX by cyclic voltammetry in dry CH_2Cl_2 containing 0.1 M Bu_4NBF_4 as a supporting electrolyte. All of the values shown in the text are in E/V vs. Fc^+/Fc measured at the scan rate of 100 mVs^{-1}. Pt electrodes were used as the working (disk, ϕ = 1.6 mm) and counter electrodes. The working electrode was polished using a water suspension of aluminum oxide (0.05 μm) before use. CD spectra were measured on a JASCO J-820 spectropolarimeter.

A suitable crystal was selected and measured on a Rigaku XtaLAB Synergy (Cu-Kα radiation, λ = 1.54184 Å) with HyPix diffractometer. The crystal was kept at 150 K during data collection. Using Olex2,[1] the structure was solved with the SHELXT[2] structure solution program using Intrinsic Phasing and refined with the SHELXL[3] refinement package using Least Squares minimization.

DFT calculations were performed with the Gaussian 16W program package.[4] The geometries of the compounds were optimized by using the (U)CAM-B3LYP method[5] in combination with the 6-31+G(d,p) basis set[6-8] unless otherwise indicated.

Experimental Section

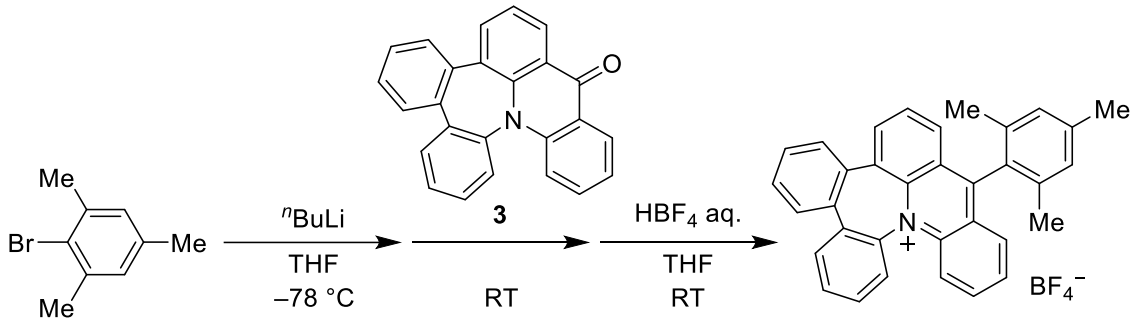
Synthetic procedures



2 **3**

dibenzo[4,5:6,7]cyclohept[1,2,3-*de*]acridone (3): A solution of **2**[9] (826 mg, 2.40 mmol) in dry *o*-dichlorobenzene (4 mL) was added SeO_2 (1.36 g, 12.3 mmol) at 24 °C. The mixture was heated at 270 °C for 5 min in a microwave reactor (74 W, Biotage® Initiator+). After cooling to 23 °C, the reaction mixture was purified by column chromatography on silica gel (hexane:EtOAc = 5:1) to give **3** (476 mg) as a yellow solid in 57% yield.

3; Mp: 245.3-245.8 °C; ^{1}H NMR ($CDCl_3$): δ/ppm 8.35 (1H, dd, *J* = 1.6, 7.6 Hz), 8.34 (1H, dd, *J* = 1.6, 7.6 Hz), 7.80 (1H, dd, *J* = 1.6, 7.6 Hz), 7.73 (1H, dd, *J* = 1.6, 7.6 Hz), 7.58-7.43 (5H, m), 7.34-7.27 (4H, m), 7.16 (1H, dt, *J* = 1.6, 7.6 Hz), 6.68 (1H, dd, *J* = 1.2, 8.4 Hz); ^{13}C NMR ($CDCl_3$): δ/ppm 179.85, 151.06, 149.78, 146.75, 139.24, 137.91, 136.03, 133.89, 133.04, 132.71, 131.21, 130.49, 128.76, 128.69, 128.39 (2C), 126.81 (2C), 126.73, 125.89, 125.84, 125.72, 124.87, 123.59, 122.86; IR (ATR): ν/cm^{-1} 3062, 3032, 3012, 2920, 2853, 1637, 1606, 1587, 1562, 1506, 1474, 1461, 1421, 1344, 1332, 1288, 1254, 1234, 1190, 1165, 1072, 1153, 1133, 1054, 1030, 1006, 976, 944, 924, 882, 866, 827, 773, 762, 754, 735, 698, 664, 650, 621, 597, 570, 535, 524; LR-MS (FD): m/z (%) 346.08 (27), 345.07 (M^+ , bp); HR-MS (FD) Calcd. for $C_{25}H_{15}NO$: 345.11402; Found: 345.11416.



1a^{+}BF_4^{-}

16-mesityldibenzo[4,5:6,7]cyclohept[1,2,3-*de*]acridinium tetrafluoroborate (1a^{+}BF_4^{-}): To a solution of 2-bromo-1,3,5-trimethylbenzene (641 mg, 3.22 mmol) in dry THF (30 mL) was added ^{n}BuLi (1.51 M in hexane, 2.17 mL, 3.22 mmol) dropwise over 5 min at –78 °C. After stirring at –78 °C for 1 h, acridone **3** (278 mg, 0.806 mmol) was added to the suspension and the mixture was warmed to 23 °C. The resulting solution was stirred at 24 °C for 4 h and then diluted with water. The mixture was extracted with EtOAc three times. The combined organic layers were washed with brine and dried over anhydrous Na_2SO_4. After filtration, the solvent was concentrated under reduced pressure. The crude solid was purified by column chromatography on aluminum oxide (hexane: EtOAc = 1:10) to give an intermediary alcohol as a white powder, which was used without further purification.

To a solution of the intermediary alcohol in THF (2 mL) was added 42% HBF_4 aq. (0.12 mL, 0.807 mmol) at 24 °C to give a deep red solution. After stirring at 23 °C for 5 min, the addition of dry Et_2O led to precipitation of the cation salt. The precipitates were collected, washed with dry CH_2Cl_2/dry Et_2O six times, and dried in vacuo to give **1a**$^{+}$$BF_4^{-}$ (213 mg) as deep red crystals in 49% yield over two steps.

1a^{+}BF_4^{-}; Mp: 176.4-180.2°C (decomp.); ^{1}H NMR ($CDCl_3$): δ/ppm 8.49 (1H, dd, *J* = 1.2, 7.6 Hz), 8.28-8.23 (1H, m), 8.14 (1H, d, *J* = 8.4 Hz), 8.00-7.96 (2H, m), 7.86-7.80 (4H, m), 7.72-7.67 (2H, m), 7.60 (1H, dt, *J* = 1.2, 7.6, Hz), 7.51 (1H, dt, *J* = 1.2, 7.6 Hz), 7.22 (1H, dd, *J* = 1.2, 7.6 Hz), 7.19 (2H, s), 6.67 (1H, d, *J* = 8.4 Hz), 2.49 (3H, s), 1.85 (3H, s), 1.82 (3H, s); ^{13}C NMR ($CDCl_3$): δ/ppm 166.34, 148.76, 145.05, 142.33, 140.95, 139.93, 138.63, 137.55, 135.76, 135.36, 135.22, 134.91, 133.47, 132.36, 132.06, 131.66, 130.52, 130.50, 130.38, 130.30, 129.96, 129.60, 129.48, 129.09, 129.08, 128.90, 128.63, 128.16, 127.34, 126.20, 122.29, 21.29, 20.15, 20.09; IR (ATR): ν/cm^{-1} 3068, 2916, 1610, 1595, 1584, 1569, 1538, 1520, 1506, 1460, 1444, 1432, 1413, 1390, 1366, 1269, 1203, 1163, 1048, 1033, 909, 853, 824, 768, 740, 688, 655, 613, 600, 570, 556, 520; LR-MS (FD): m/z (%) 450.18 (7), 449.17 (38), 448.17 (M^+ , bp); HR-MS (FD) Calcd. for $C_{34}H_{26}N$: 448.20652; Found: 448.20627.

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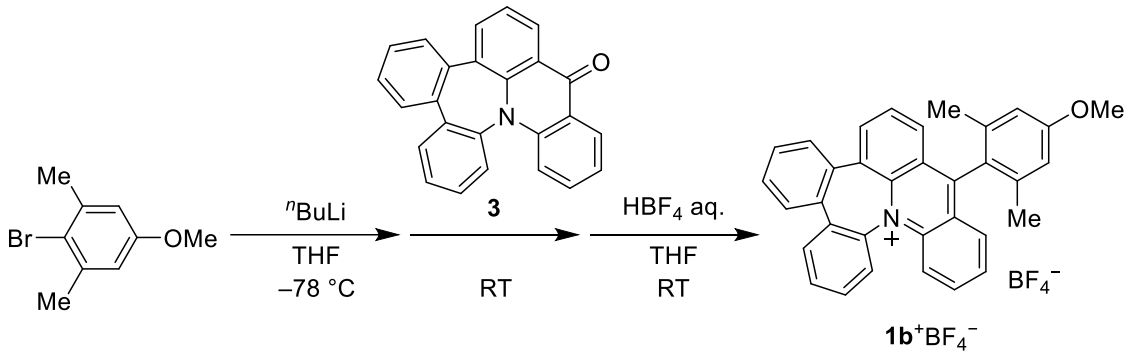

16-(2,6-dimethyl-4-methoxyphenyl)dibenzo[4,5:6,7]cyclohept[1,2,3-*de*]acridinium tetrafluoroborate ($\mathbf{1b}^{+}\mathbf{BF_4}^{-}$): To a solution of 2-bromo-5-methoxy-1,3-dimethylbenzene (615 mg, 3.29 mmol) in dry THF (30 mL) was added ^{n}BuLi (1.53 M in hexane, 2.14 mL, 3.27 mmol) dropwise over 5 min at –78 °C. After stirring at –78 °C for 1 h, acridone **3** (275 mg, 0.795 mmol) was added to the suspension and the mixture was warmed to 24 °C. The resulting solution was stirred at 24 °C for 4 h and then diluted with water. The mixture was extracted with EtOAc three times. The combined organic layers were washed with brine and dried over anhydrous Na_2SO_4. After filtration, the solvent was concentrated under reduced pressure. The crude solid was used without further purification.

To a solution of the crude solid in THF (2 mL) was added 42% HBF_4 aq. (0.12 mL, 0.807 mmol) at 24 °C to give a deep red solution. After stirring at 24 °C for 5 min, the addition of dry Et_2O led to precipitation of the cation salt. The precipitates were collected, washed with dry CH_2Cl_2/dry Et_2O three times, and dried in vacuo to give $\mathbf{1b}^{+}\mathbf{BF_4}^{-}$ (344 mg) as deep red crystals in 79% yield over two steps.

$\mathbf{1b}^{+}\mathbf{BF_4}^{-}$; Mp: 203.6-205.6 °C (decomp.); ^{1}H NMR (CD_3CN) δ/ppm 8.53 (1H, d, J = 7.1 Hz), 8.18-8.10 (2H, m), 8.07 (1H, dd, J = 1.3, 7.8 Hz), 7.98-7.92 (2H, m), 7.88-7.78 (3H, m), 7.78-7.71 (2H, m), 7.64 (1H, dt, J = 1.3, 7.8 Hz), 7.45 (1H, ddd, J = 1.5, 7.4, 8.3 Hz), 7.26 (1H, dd, J = 1.4, 7.6 Hz), 7.03 (1H, s), 7.02 (1H, s), 6.72 (1H, dd, J = 0.9, 8.3 Hz), 3.95 (3H, s), 1.87 (3H, s), 1.83 (3H, s); ^{13}C NMR (CD_3CN): δ/ppm; 166.35, 161.72, 150.14, 145.94, 143.22, 139.37, 139.15, 138.74, 138.45, 138.39, 135.96, 135.67, 134.01, 132.40, 131.82, 131.06, 130.68, 130.62, 130.42, 130.17, 129.61, 129.50, 129.34, 129.26, 128.20, 127.58, 125.06, 122.66, 114.26, 114.02, 55.76, 20.18, 19.94; IR (ATR): ν/cm^{-1} 3072, 2991, 2942, 2908, 2843, 1606, 1582, 1565, 1536, 1520, 1506, 1484, 1470, 1459, 1444, 1410, 1388, 1368, 1353, 1317, 1284, 1270, 1258, 1200, 1163, 1156, 1132, 1095, 1047, 1037, 995, 930, 907, 885, 867, 855, 825, 775, 764, 750, 740, 728, 709, 691, 654; LR-MS (ESI): m/z (%) 466.21 (7), 465.20 (37), 464.20 (M^+ , bp); HR-MS (ESI) Calcd. for $C_{34}H_{26}NO$: 464.20038; Found: 464.20199.

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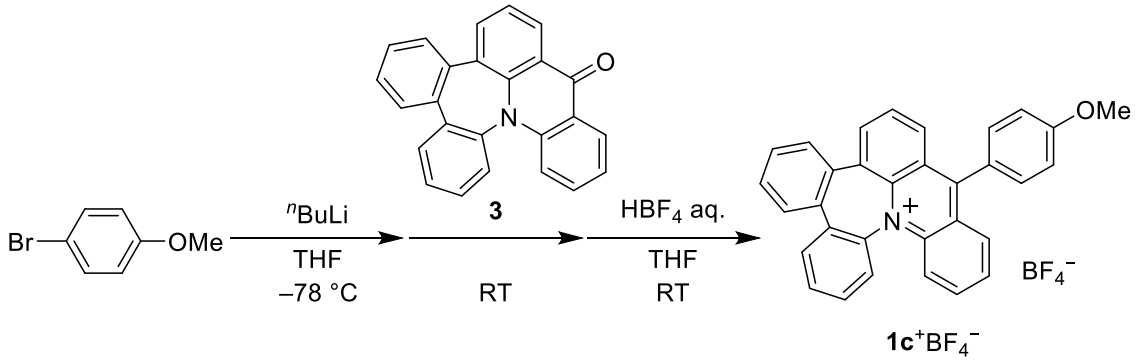
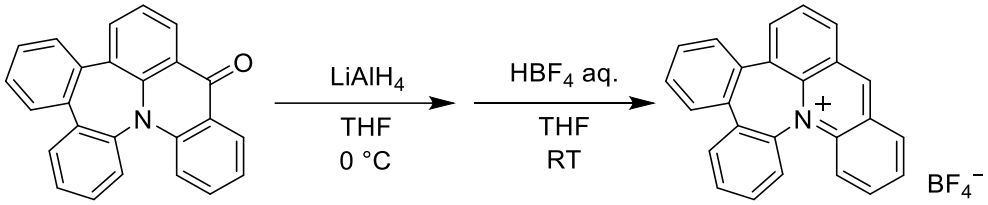


16-(4-methoxyphenyl)dibenzo[4,5:6,7]cyclohept[1,2,3-*de*]acridinium tetrafluoroborate ($\mathbf{1c}^{+}\mathbf{BF_4}^{-}$): To a solution of 1-bromo-4-methoxybenzene (603 mg, 3.22 mmol) in dry THF (30 mL) was added ^{n}BuLi (1.51 M in hexane, 2.17 mL, 3.22 mmol) dropwise over 5 min at –78 °C. After stirring at –78 °C for 1 h, acridone **3** (273 mg, 0.790 mmol) was added to the suspension and the mixture was warmed to 24 °C. The resulting solution was stirred at 24 °C for 4 h and then diluted with water. The mixture was extracted with EtOAc three times. The combined organic layers were washed with brine and dried over anhydrous Na_2SO_4. After filtration, the solvent was concentrated under reduced pressure. The crude solid was purified by column chromatography on aluminum oxide (hexane: EtOAc = 1:10) to give an intermediary alcohol as a white powder, which was used without further purification.

To a solution of the intermediary alcohol in THF (2 mL) was added 42% HBF_4 aq. (0.12 mL, 0.807 mmol) at 24 °C to give a deep red solution. After stirring at 24 °C for 5 min, the addition of dry Et_2O led to precipitation of the cation salt. The precipitates were collected, washed with dry CH_2Cl_2/dry Et_2O six times, and dried in vacuo to give $\mathbf{1c}^{+}BF_4^{-}$ (366 mg) as deep red crystals in 80% yield over two steps.

$\mathbf{1c}^{+}BF_4^{-}$; Mp: 168.3-172.3 °C (decomp.); ^{1}H NMR (CD_3CN) δ/ppm 8.48 (1H, dd, J = 1.2, 7.1 Hz), 8.19 (1H, dd, J = 1.1, 8.5 Hz), 8.12 (1H, ddd, J = 1.0, 6.7, 8.8 Hz), 8.08-8.03 (3H, m), 7.98-7.92 (2H, m), 7.80 (1H, ddd, J = 1.0, 6.7, 8.8 Hz), 7.77-7.70 (2H, m), 7.66-7.60 (3H, m), 7.46 (1H, ddd, J = 1.5, 7.3, 7.8 Hz), 7.37 (2H, d, J = 8.7 Hz), 7.23 (1H, dd, J = 0.8, 8.1 Hz), 6.82 (1H, dd, J = 0.8, 7.8 Hz), 4.02 (3H, s); ^{13}C NMR (CD_3CN): δ/ppm 165.33, 162.78, 150.03, 146.08, 143.13, 138.90, 138.76, 138.64, 135.99, 135.88, 133.83, 133.43, 132.28, 132.02, 131.71, 130.88, 130.74, 130.64, 130.59, 130.14, 129.57, 129.53, 129.29, 120.03, 128.68, 127.05, 125.66, 122.11, 115.14, 56.14; IR (ATR): ν/cm^{-1} 3070, 2940, 2844, 1598, 1580, 1567, 1540, 1515, 1506, 1477, 1459, 1441, 1423, 1410, 1391, 1363, 1313, 1297, 1287, 1256, 1178, 1115, 1047, 1036, 1018, 966, 842, 819, 804, 788, 779, 748, 741, 727, 682, 655, 640, 631, 618, 611, 598, 580, 551, 520; LR-MS (ESI): m/z (%) 438.18 (6), 467.17 (35), 436.17 (M^+ , bp); HR-MS (ESI) Calcd. for $C_{32}H_{22}NO$: 436.16922; Found: 436.16959.

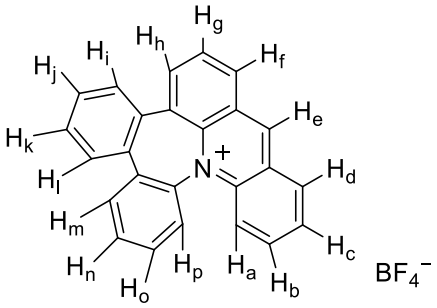


3 **1d**$^{+}$$BF_4^{-}$

dibenzo[4,5:6,7]cyclohept[1,2,3-*de*]acridinium tetrafluoroborate (1d^{+}BF_4^{-}): To a solution of acridone **3** (276 mg, 0.799 mmol) in dry THF (30 mL) was added $LiAlH_4$ (101 mg, 2.66 mmol) at 0 °C. The mixture was stirred at 0 °C for 4 h and then diluted with water. The solution was filtered through Celite® and dried over anhydrous Na_2SO_4. After drying, the solvent was concentrated under reduced pressure. The crude solid was purified by column chromatography on aluminum oxide (hexane: EtOAc = 10:1) to give an intermediary alcohol as a white powder, which was used without further purification.

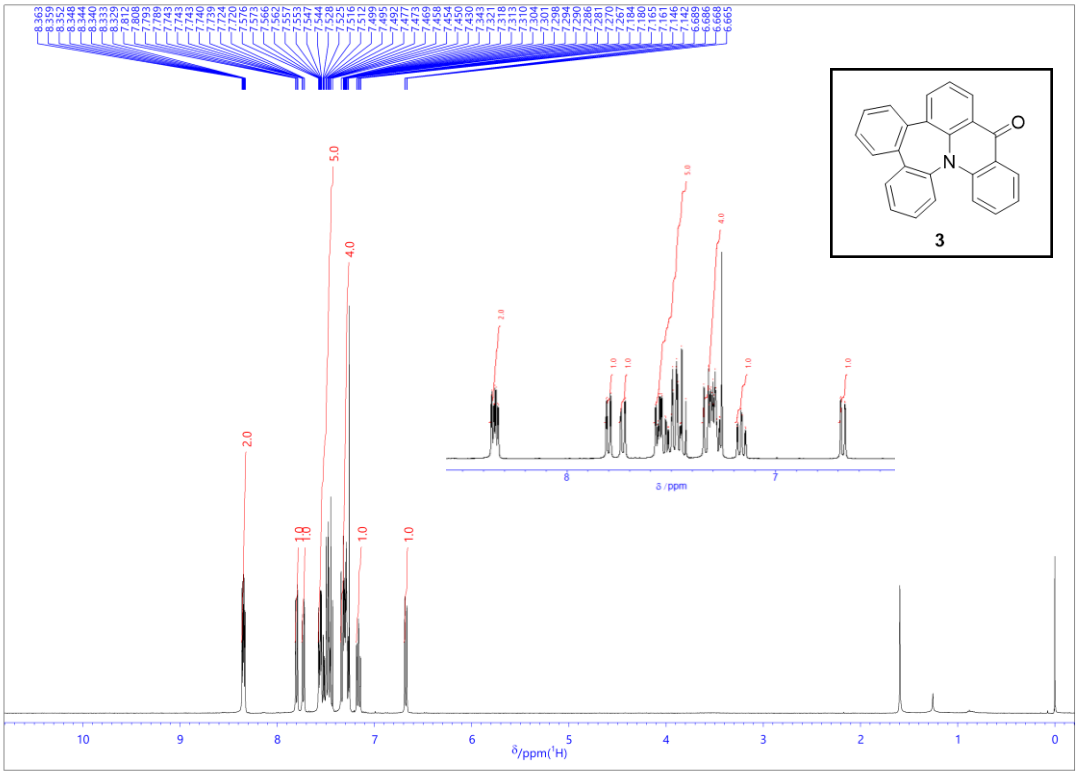
To a solution of the intermediary alcohol in THF (2 mL) was added 42% HBF_4 aq. (0.12 mL, 0.807 mmol) at 24 °C to give a deep red solution. After stirring at 24 °C for 5 min, the addition of dry Et_2O led to precipitation of the cation salt. The precipitates were collected, washed with dry CH_2Cl_2/dry Et_2O three times, and dried in vacuo to give **1d**$^{+}$$BF_4^{-}$ (71.8 mg) as red crystals in 25% yield over two steps.

1d^{+}BF_4^{-}; Mp: 193.3-194.5 °C; ^{1}H NMR (CD_3CN): δ/ppm 9.91 (H_e, 1H, s), 8.56 (H_h, 1H, dd, J = 0.9, 7.3 Hz), 8.53-8.48 (H_d, H_f, 2H, m), 8.18 (H_b, 1H, ddd, J = 1.6, 7.2, 8.5 Hz), 8.12-8.05 (H_a, H_g, 2H, m), 8.03 (H_l, 1H, dd, J = 1.2, 7.8 Hz), 7.97-7.89 (H_c, H_n, 2H, m), 7.76-7.67 (H_k, H_m, 2H, m), 7.61 (H_j, 1H, ddd, J = 1.2, 7.6, 7.9 Hz), 7.42 (H_o, 1H, ddd, J = 1.4, 7.5, 8.2 Hz), 7.21 (H_i, 1H, dd, J = 1.9, 7.9 Hz), 6.66 (H_p, 1H, d, J = 8.2 Hz); ^{13}C NMR (CD_3CN): δ/ppm 153.95, 149.93, 146.28, 142.83, 139.91, 139.41, 138.42, 136.00, 135.67, 133.98, 132.60, 132.14, 131.87, 131.79, 130.89, 130.67, 130.21, 130.17, 129.73, 129.34, 129.09, 127.52, 122.15; IR (ATR): ν/cm^{-1} 1622, 1602, 1584, 1570, 1536, 1508, 1485, 1460, 1445, 1434, 1423, 1399, 1376, 1360, 1331, 1286, 1265, 1256, 1185, 1172, 1157, 1147, 1135, 1093, 1034, 958, 947, 903, 888, 867, 843, 786, 760, 751, 740, 728, 667, 623, 614, 601, 581, 568, 560, 549, 517; LR-MS (FD): m/z (%) 331.13 (31), 330.12 (M^+, bp); HR-MS (FD) Calcd. for $C_{25}H_{16}N$: 330.12773; Found: 330.12688.



NMR Spectra of New Compounds (Figures S1-S9)

(a)



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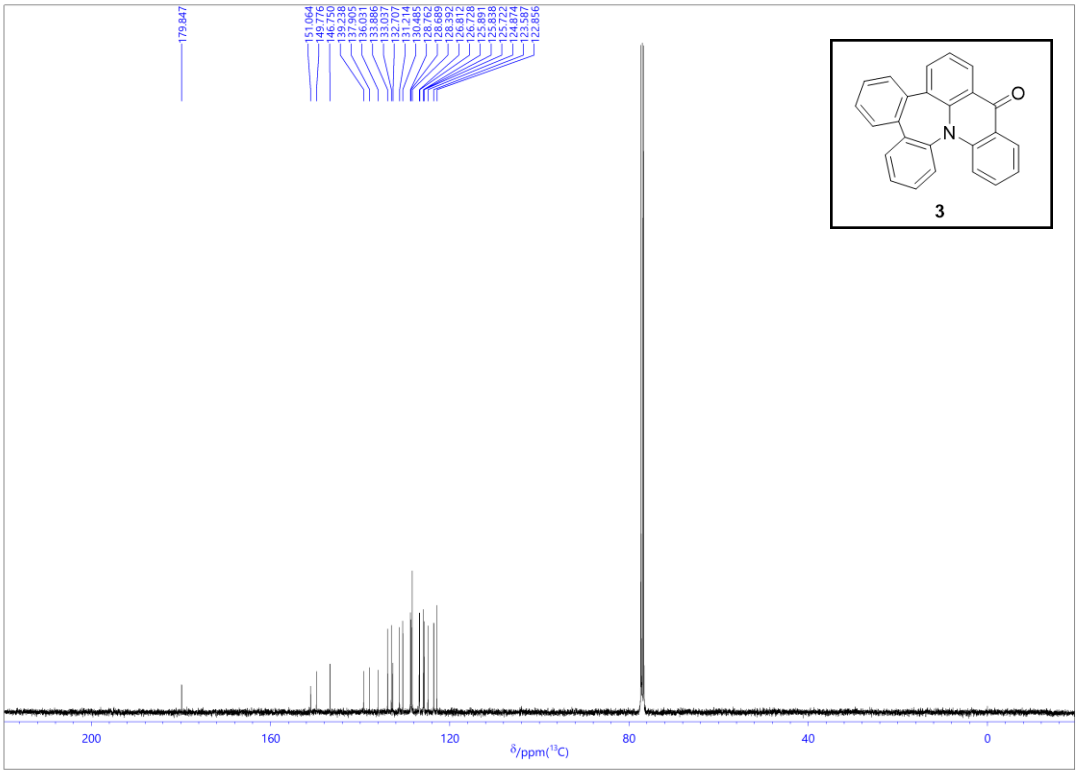
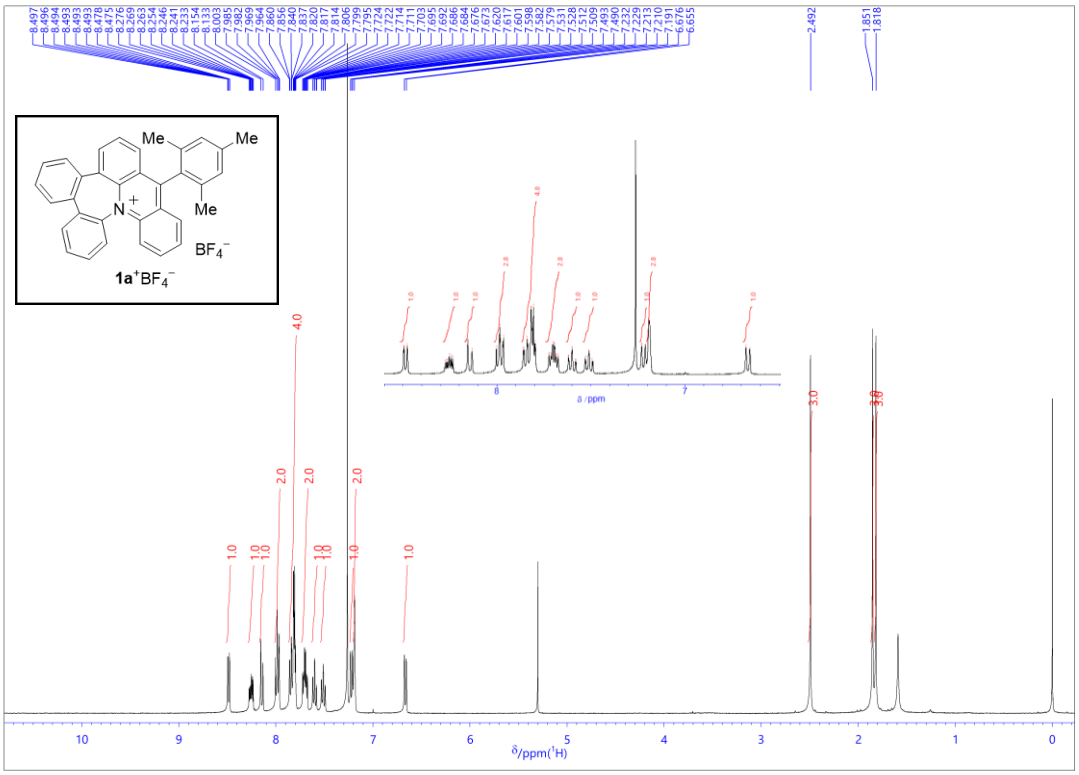


Figure S1. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of **3** in $CDCl_3$.

(a)



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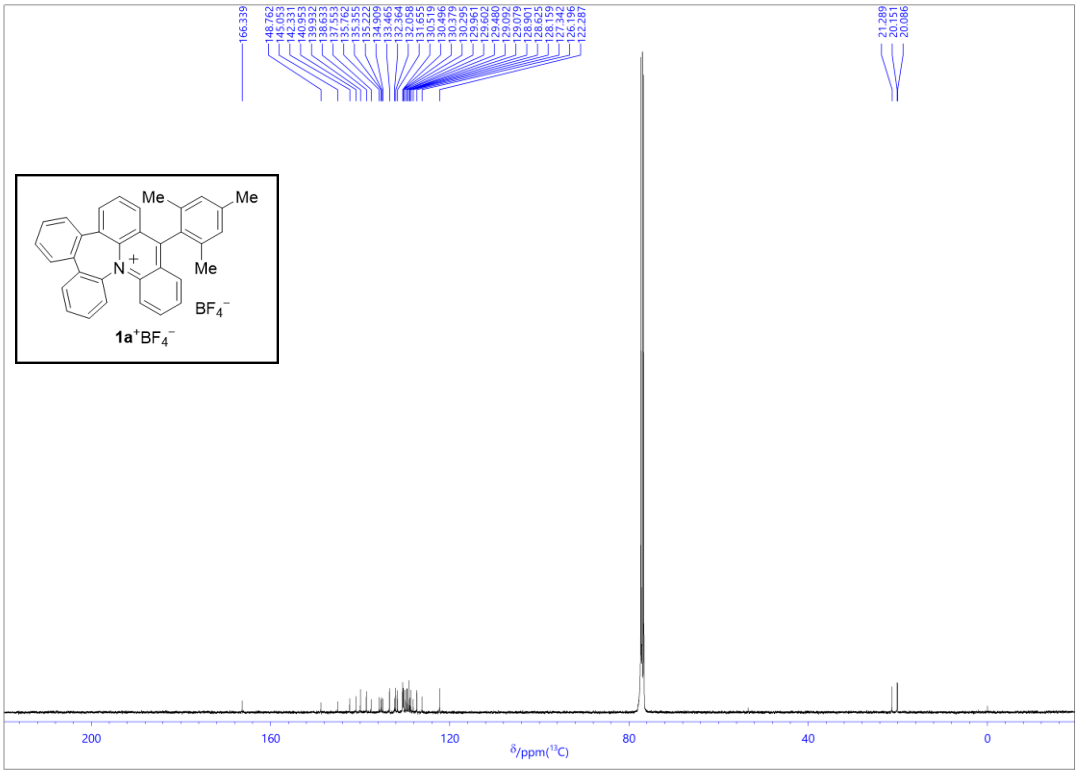
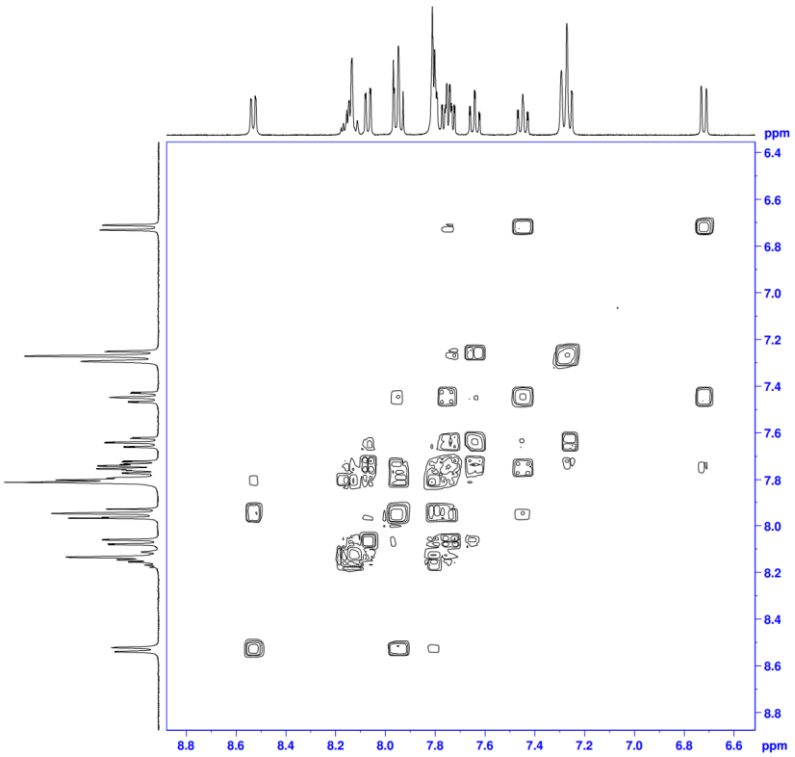


Figure S2. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of **1a**$^{+}$$BF_4^{-}$ in $CDCl_3$.

(a)



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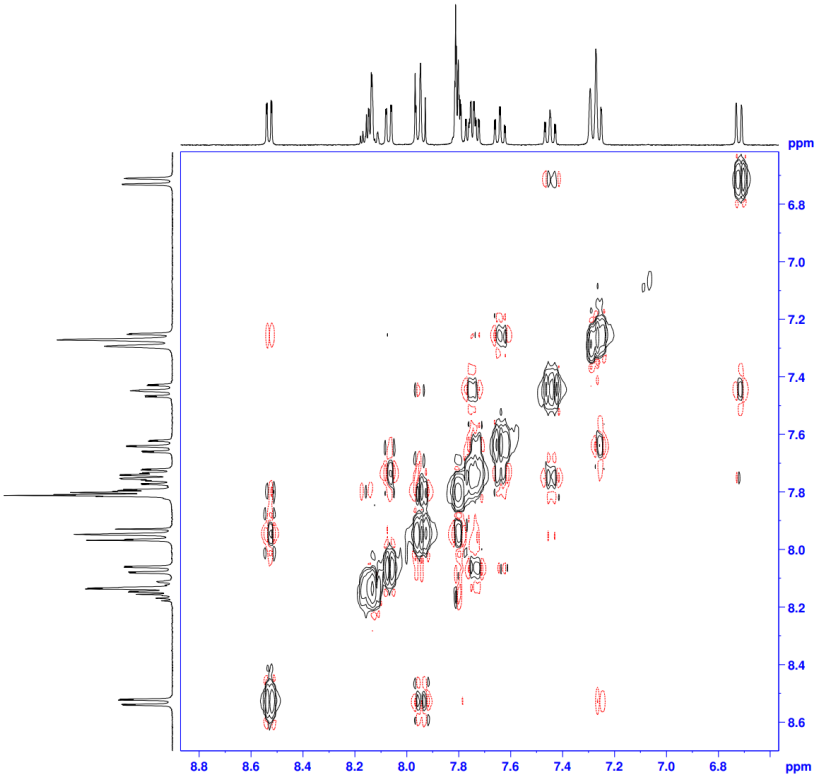
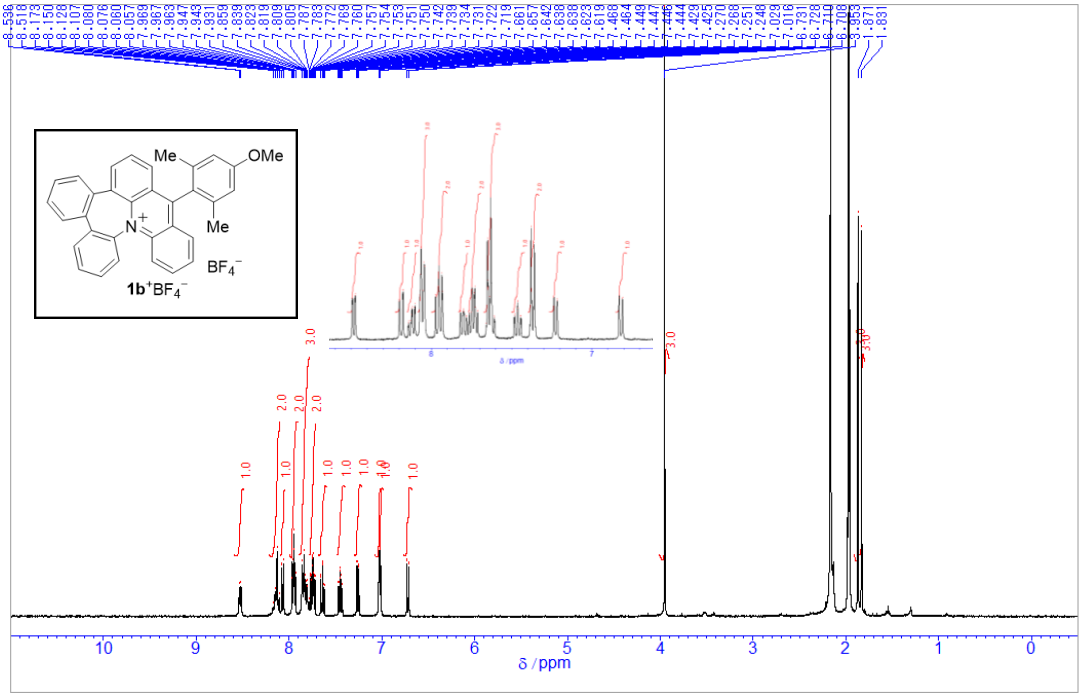


Figure S3. (a) ^{1}H-^{1}H COSY NMR and (b) ^{1}H-^{1}H NOESY spectra of **1a**$^{+}BF_4^{-}$ in CD_3CN.

(a)



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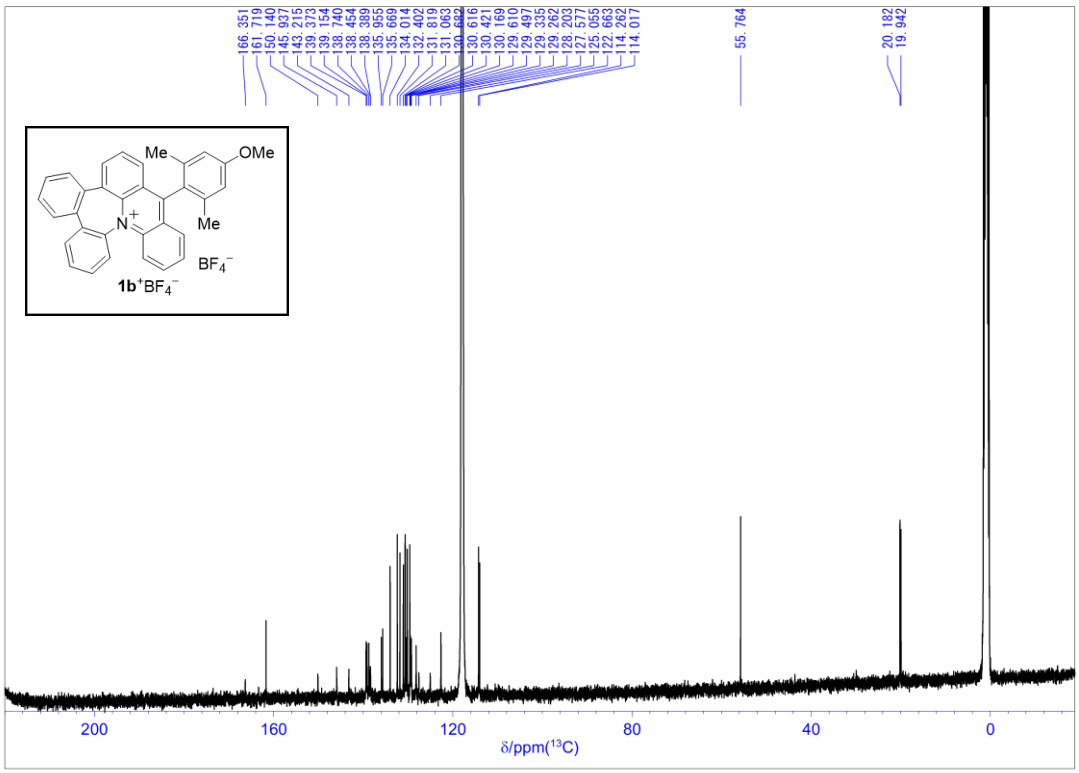
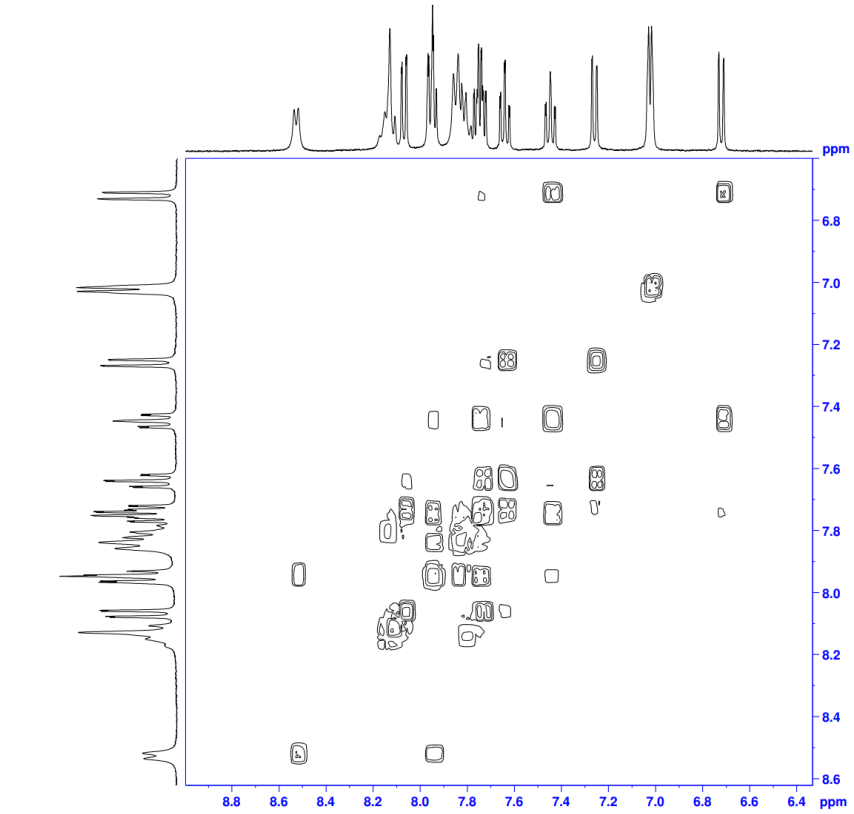


Figure S4. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of **1b**$^{+}$$BF_4^-$ in CD_3CN.

(a)



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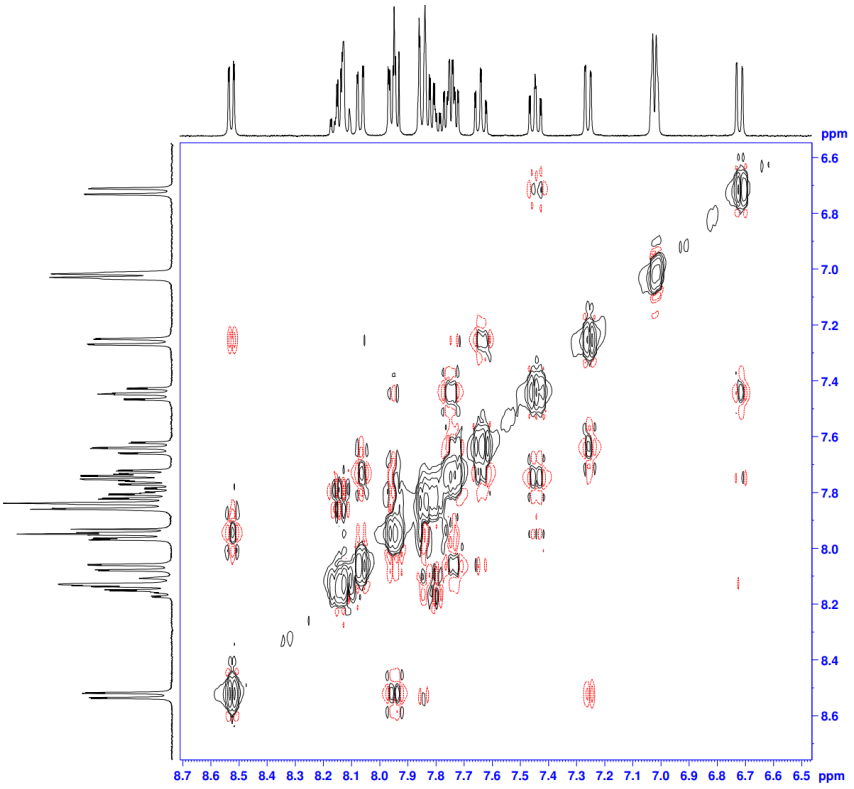
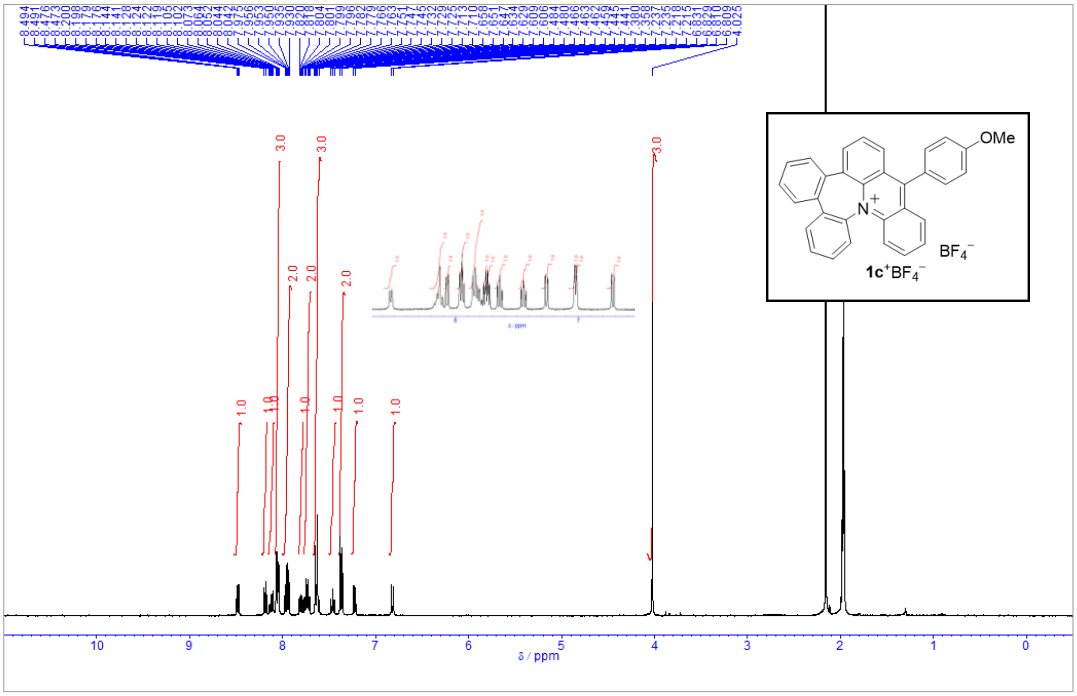


Figure S5. (a) ^{1}H-^{1}H COSY NMR and (b) ^{1}H-^{1}H NOESY spectra of **1b**$^{+}BF_4^{-}$ in CD_3CN.

(a)



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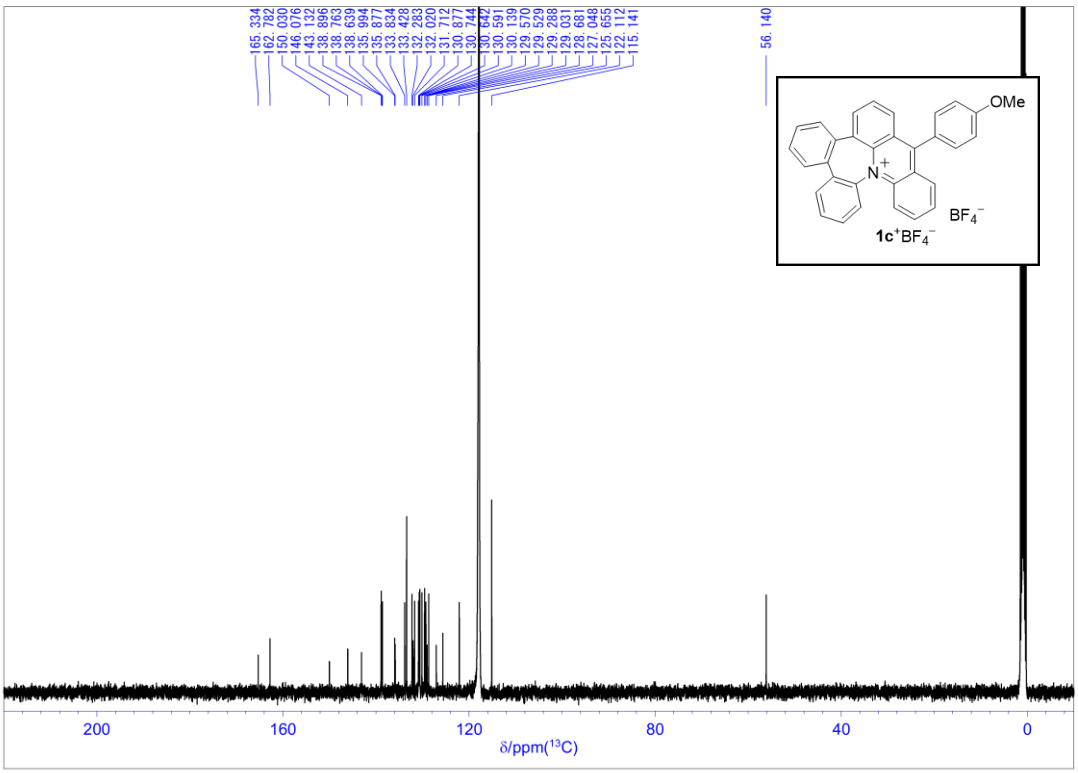
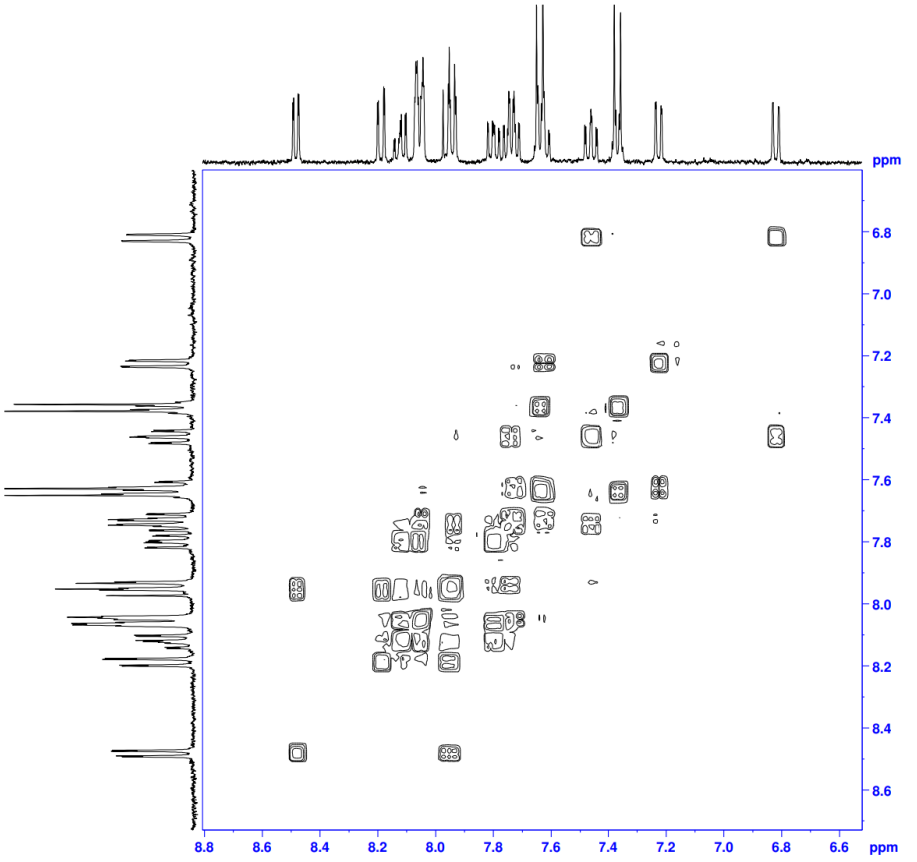


Figure S6. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of **1c**$^{+}$$BF_4^{-}$ in CD_3CN.

(a)



(b)

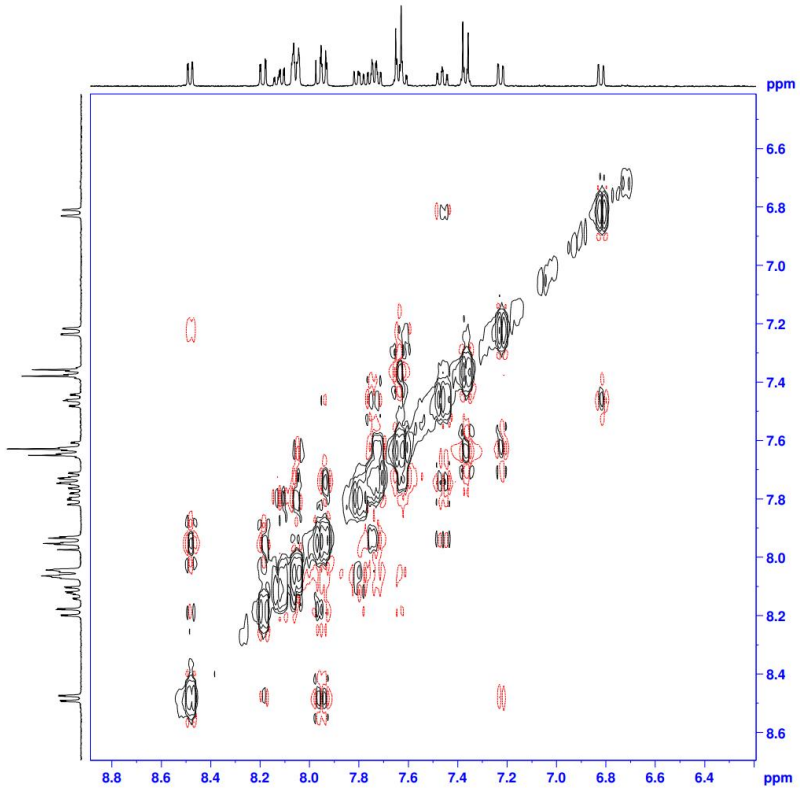
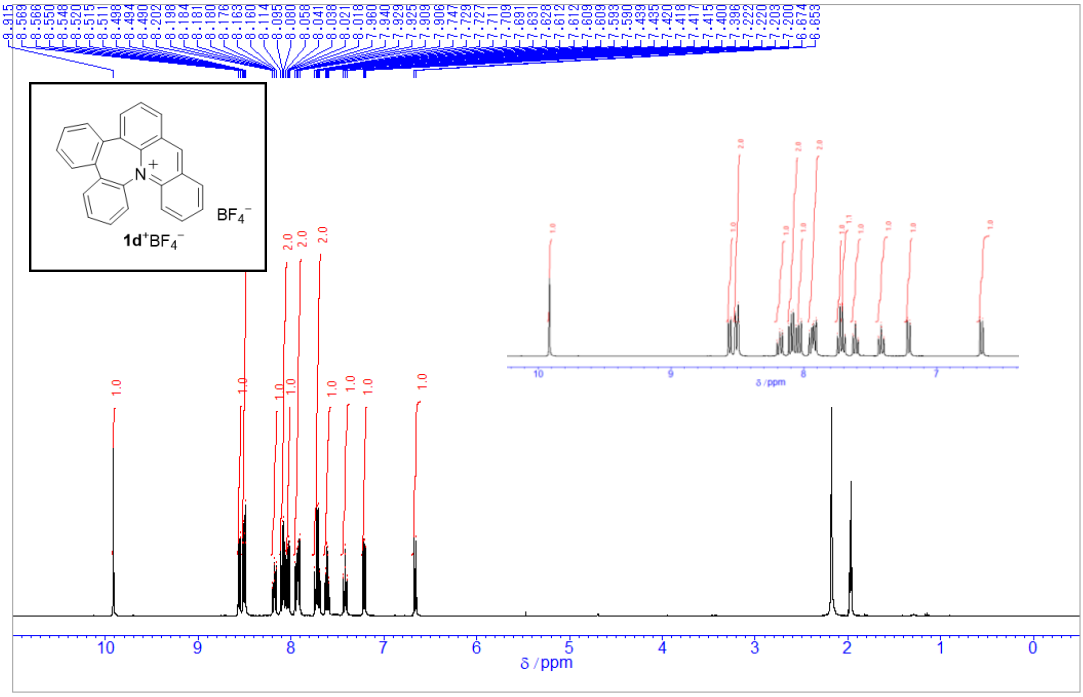


Figure S7. (a) ^{1}H-^{1}H COSY NMR and (b) ^{1}H-^{1}H NOESY spectra of **1c**$^{+}BF_4^{-}$ in CD_3CN.

(a)



(b)

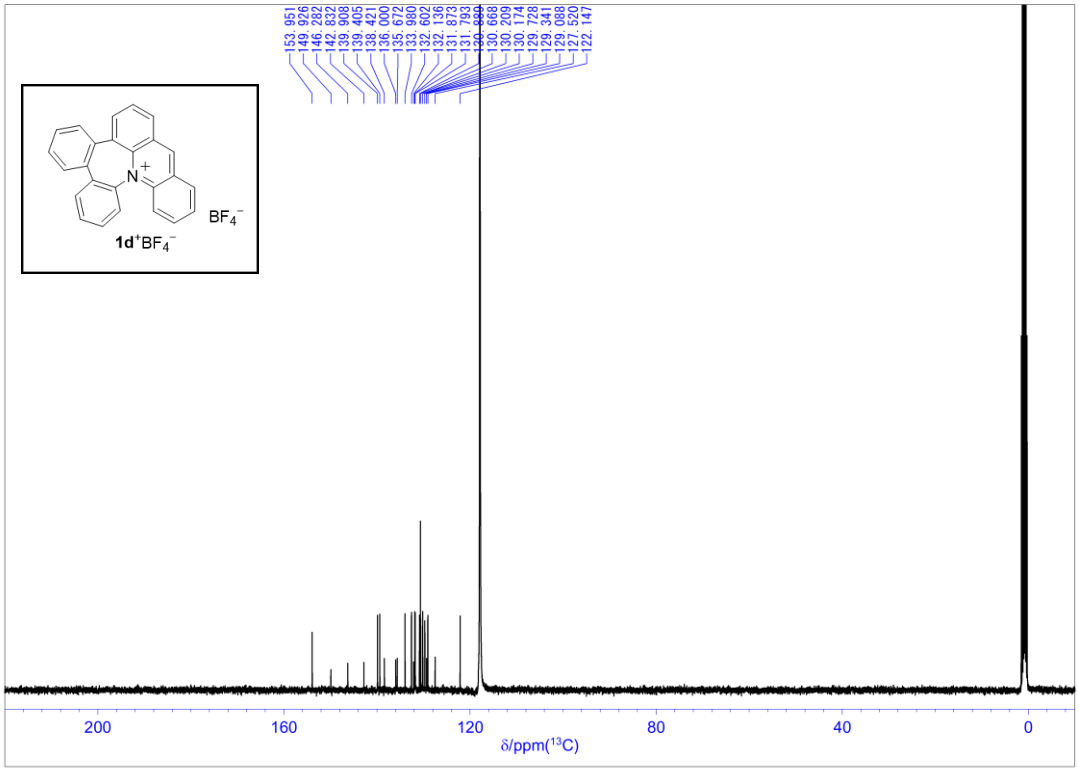
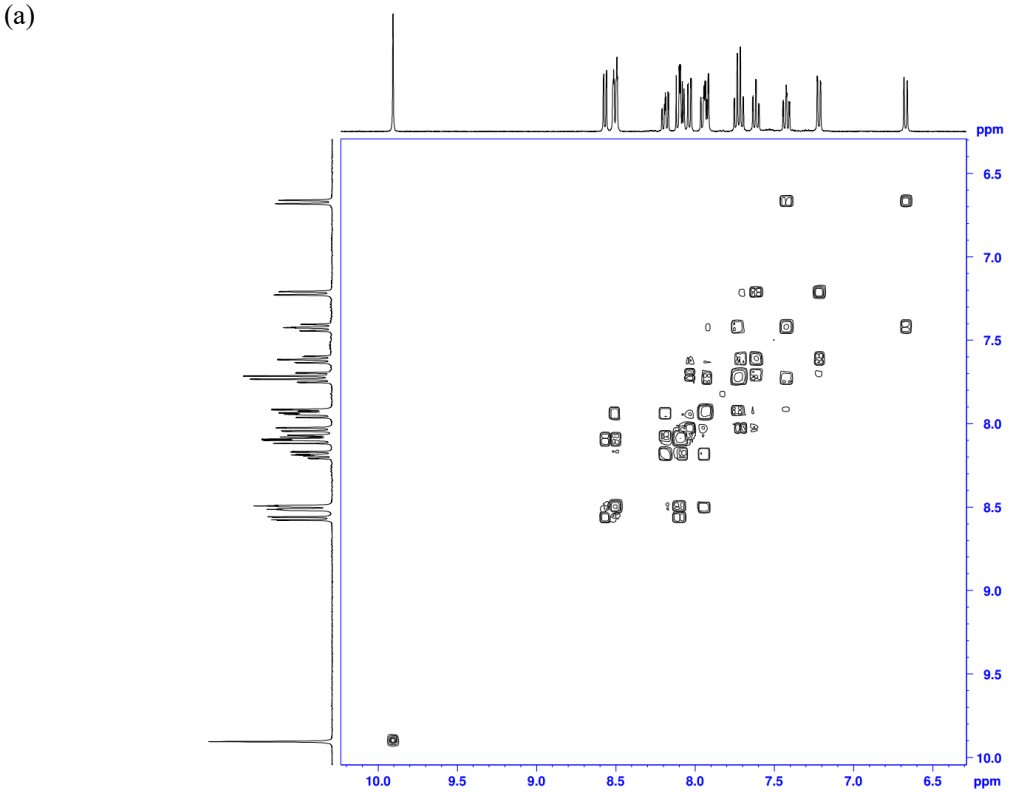


Figure S8. (a) ^{1}H NMR and (b) ^{13}C NMR spectra of **1d**$^{+}$$BF_4^-$ in CD_3CN.

(a)



(b)

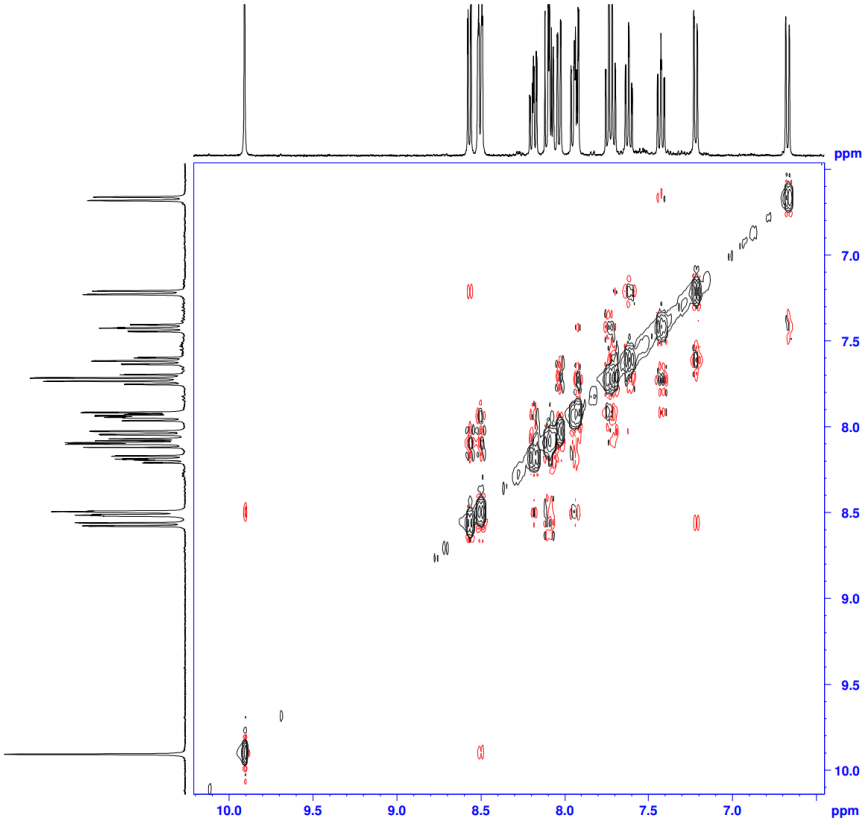


Figure S9. (a) ^{1}H-^{1}H COSY NMR and (b) ^{1}H-^{1}H NOESY spectra of **1d**$^{+}BF_4^{-}$ in CD_3CN.

Mass Spectra of New Compounds (Figures S10-S14 and Tables S1-S10)

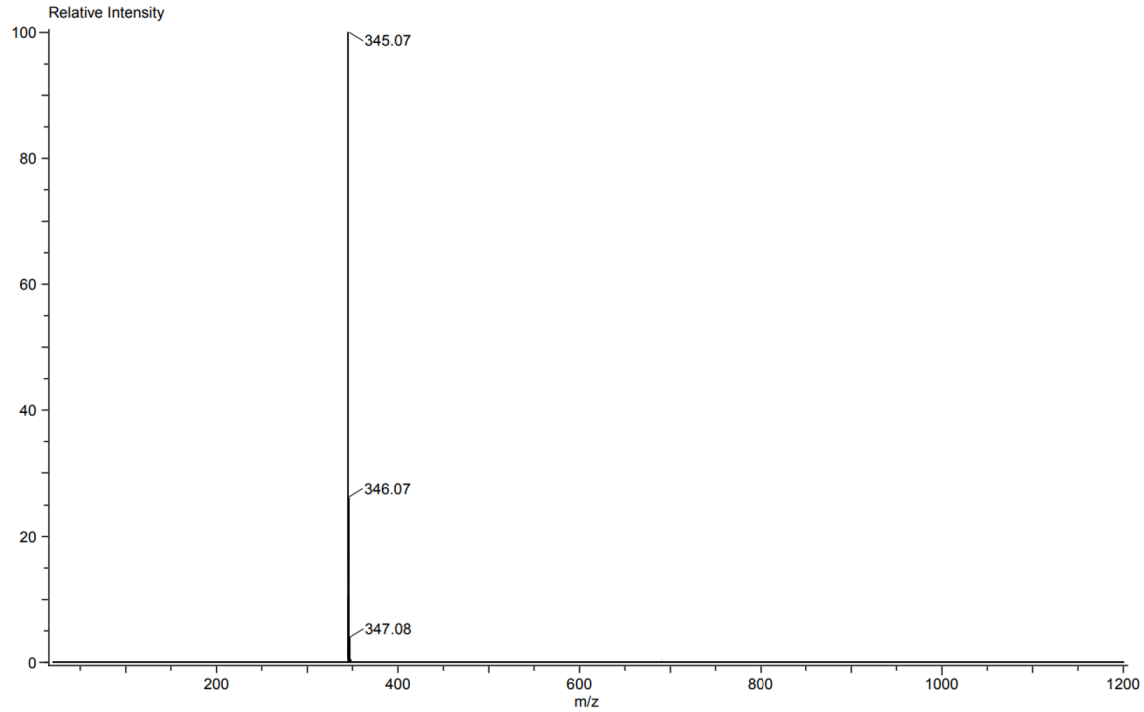


Figure S10. Low-resolution FD mass spectrum of **3**.

Table S1. Low-resolution FD mass data of **3**.

Peak Number	m/z	Relative Area
1	345.07	100.0000
2	346.08	26.9083
3	347.08	4.0360

Table S2. High-resolution FD mass data of **3**.

Mass	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
345.11416	345.11402	0.14	0.39	$^{12}C_{23}{}^{1}H_{13}{}^{14}N_4$	19.5
	345.11536	-1.21	-3.50	$^{12}C_{25}{}^{1}H_{15}{}^{14}N_1{}^{16}O_1$	19.0
	345.11268	1.47	4.27	$^{12}C_{22}{}^{1}H_{17}{}^{16}O_4$	14.5
	345.11134	2.82	8.16	$^{12}C_{20}{}^{1}H_{15}{}^{14}N_3{}^{16}O_3$	15.0
	345.10866	5.50	15.93	$^{12}C_{17}{}^{1}H_{17}{}^{14}N_2{}^{16}O_6$	10.5
	345.11989	-5.74	-16.62	$^{12}C_{16}{}^{1}H_{17}{}^{14}N_4{}^{16}O_5$	10.5
	345.12124	-7.08	-20.51	$^{12}C_{18}{}^{1}H_{19}{}^{14}N_1{}^{16}O_6$	10.0
	345.12392	-9.76	-28.28	$^{12}C_{21}{}^{1}H_{17}{}^{14}N_2{}^{16}O_3$	14.5

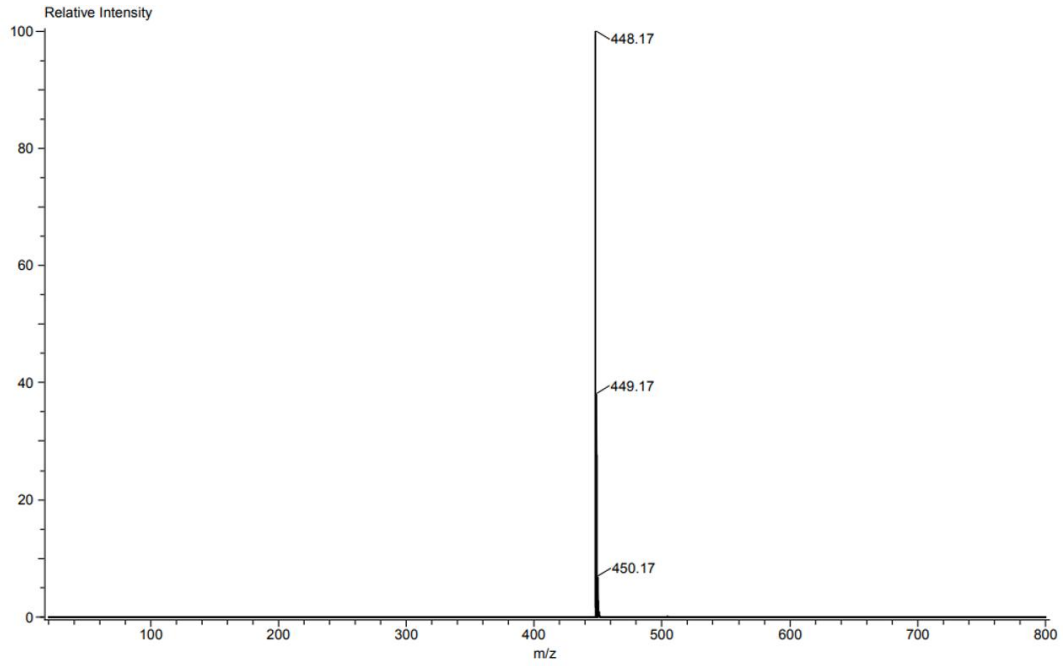


Figure S11. Low-resolution FD mass spectrum of **1a**$^{+}$ BF_4^{-}.

Table S3. Low-resolution FD mass data of **1a**$^{+}$ BF_4^{-}.

Peak Number	m/z	Relative Area
1	448.17	100.0000
2	449.17	37.5017
3	450.18	6.8388

Table S4. High-resolution FD mass data of **1a**$^{+}$ BF_4^{-}.

Mass	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
448.20627	448.20652	-0.25	-0.57	$^{12}C_{34}{}^{1}H_{26}{}^{14}N_1$	22.5
	448.20384	2.43	5.41	$^{12}C_{31}{}^{1}H_{28}{}^{16}O_3$	18.0
	448.20250	3.77	8.41	$^{12}C_{29}{}^{1}H_{26}{}^{14}N_3{}^{16}O_2$	18.5
	448.21105	-4.78	-10.67	$^{12}C_{25}{}^{1}H_{28}{}^{14}N_4{}^{16}O_4$	14.0
	448.21240	-6.13	-13.67	$^{12}C_{27}{}^{1}H_{30}{}^{14}N_1{}^{16}O_5$	13.5
	448.19982	6.45	14.39	$^{12}C_{26}{}^{1}H_{28}{}^{14}N_2{}^{16}O_5$	14.0
	448.21508	-8.81	-19.65	$^{12}C_{30}{}^{1}H_{28}{}^{14}N_2{}^{16}O_2$	18.0

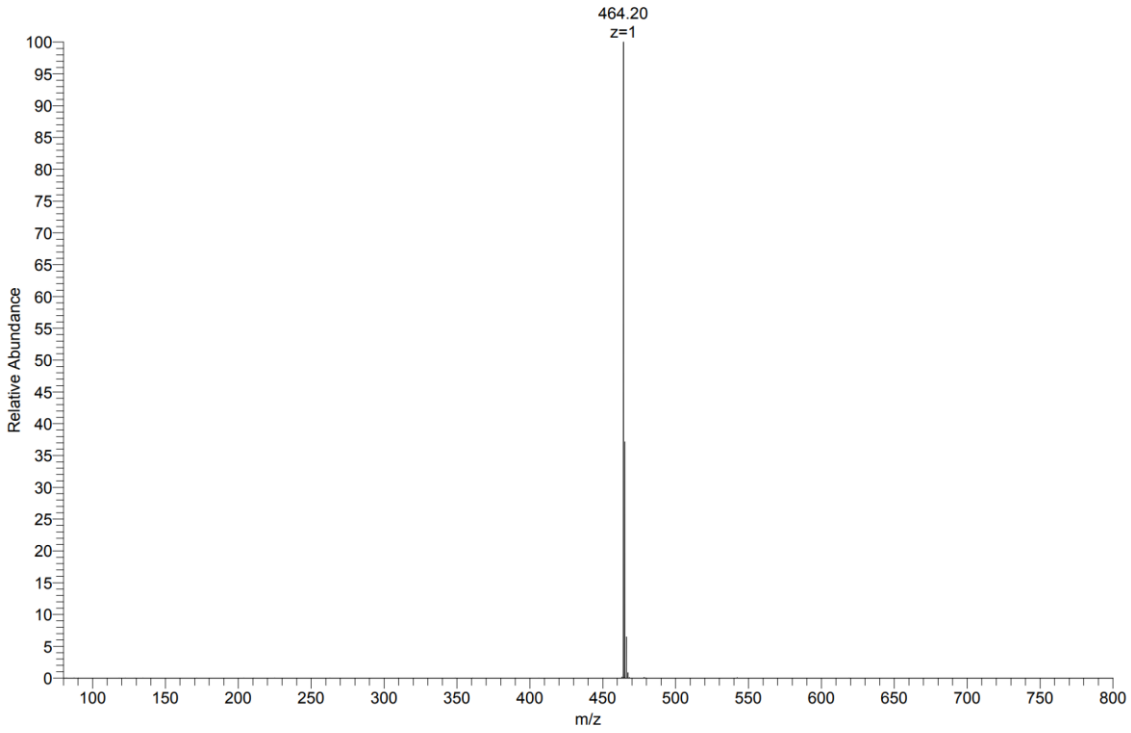


Figure S12. Low-resolution ESI mass spectrum of $\mathbf{1b}^{+}$ BF_4^{-}.

Table S5. Low-resolution ESI mass data of $\mathbf{1b}^{+}$ BF_4^{-}.

m/z= 80.00-800.00

m/z	Intensity	Relative	Charge
134.61	1398537.1	0.04	0.00
203.56	1445079.6	0.04	0.00
225.02	1403453.5	0.04	0.00
348.79	1537257.3	0.04	0.00
360.86	1489280.5	0.04	0.00
390.12	1450055.8	0.04	0.00
406.16	1450978.8	0.04	0.00
450.18	1472678.3	0.04	0.00
462.18	1566586.0	0.05	0.00
463.19	5775725.5	0.17	0.00
464.20	3472237312.0	100.00	1.00
464.53	3718599.8	0.11	0.00
465.20	1281229056.0	36.90	1.00
466.21	238021616.0	6.85	1.00
467.21	30139864.0	0.87	1.00
468.21	3063307.5	0.09	1.00
478.22	4210791.0	0.12	1.00
479.22	2533349.5	0.07	1.00
542.11	3580582.5	0.10	0.00
619.08	1552403.5	0.04	0.00

Table S6. High-resolution ESI mass data of **1b**$^{+}$ BF_4^{-}.

m/z= 459.20038-469.20038

m/z	Theo. Mass	Delta (mmu)	RDB equiv.	Composition
464.20038	464.20199	-1.61	22.5	$C_{34}H_{26}ON$
	464.19848	1.90	0.5	$C_{16}H_{34}O_{14}N$
	464.20786	-7.48	13.5	$C_{27}H_{30}O_6N$
	464.19260	7.78	9.5	$C_{23}H_{30}O_9N$
	464.21373	-13.35	4.5	$C_{20}H_{34}O_{11}N$
	464.18673	13.65	18.5	$C_{30}H_{26}O_4N$
	464.22312	-22.74	17.5	$C_{31}H_{30}O_3N$
	464.17735	23.03	5.5	$C_{19}H_{30}O_{12}N$
	464.22899	-28.61	8.5	$C_{24}H_{34}O_8N$
	464.17148	28.90	14.5	$C_{26}H_{26}O_7N$

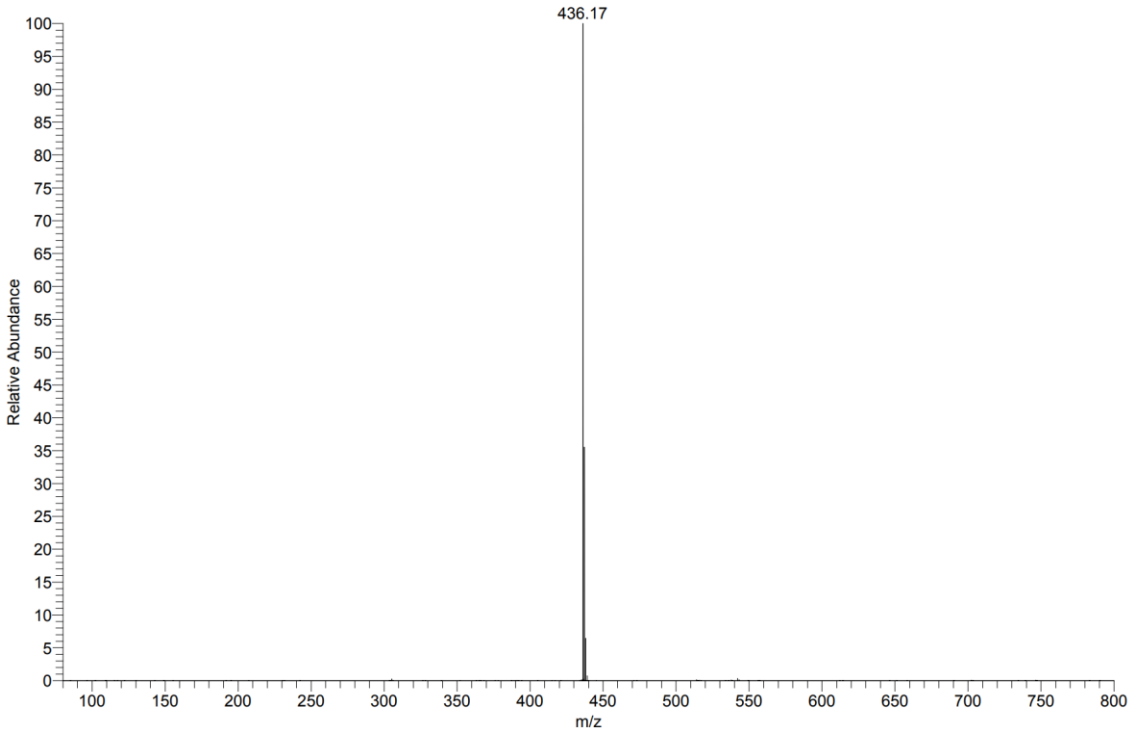


Figure S13. Low-resolution ESI mass spectrum of **1c**$^{+}$ BF_4^{-}.

Table S7. Low-resolution ESI mass data of **1c**$^{+}$ BF_4^{-}.

m/z	Intensity	Relative
436.17	358580320.0	100.00
437.17	124168576.0	34.63
438.18	22536806.0	6.29
439.18	2572685.5	0.72
542.21	1159974.0	0.32

Table S8. High-resolution ESI mass data of **1c**$^{+}$ BF_4^{-}.

m/z	Theo. Mass	Delta (mmu)	RDB equiv.	Composition
436.16922	436.16959	-0.37	22.5	$C_{32}H_{22}ON$
	436.16691	2.31	18.0	$C_{29}H_{24}O_4$
	436.17814	-8.92	18.0	$C_{28}H_{24}O_3N_2$
	436.15701	12.21	23.0	$C_{31}H_{20}ON_2$
	436.18217	-12.95	22.0	$C_{33}H_{24}O$
	436.15433	14.89	18.5	$C_{28}H_{22}O_4N$
	436.19072	-21.50	17.5	$C_{29}H_{26}O_3N$
	436.14578	23.44	23.0	$C_{32}H_{20}O_2$
	436.19340	-24.18	22.0	$C_{32}H_{24}N_2$
	436.14176	27.46	19.0	$C_{27}H_{20}O_4N_2$

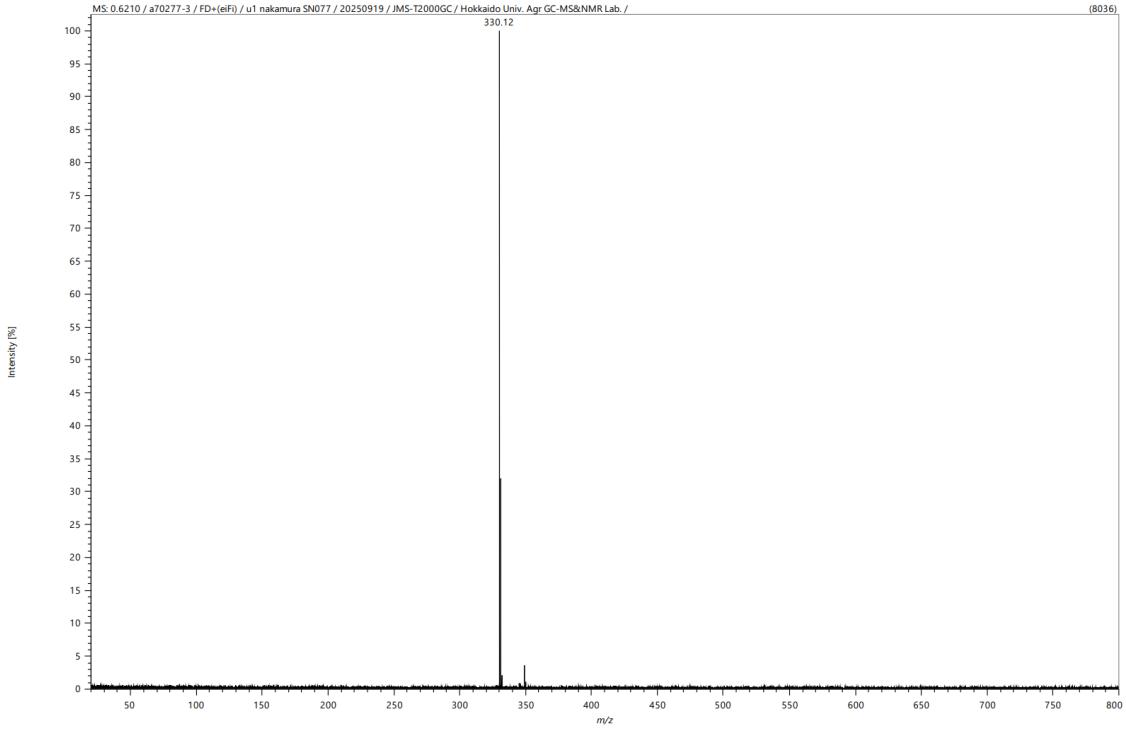


Figure S14. Low-resolution FD mass spectrum of **1d**$^{+}$ BF_4^{-}.

Table S9. Low-resolution FD mass data of **1d**$^{+}$ BF_4^{-}.

u1 nakamura SN077 / 20250919 / JMS-T2000GC / Hokkaido Univ. Agr GC-MS&NMR Lab.							
No.	m/z	Area	Area [%]	Height	Height [%]	Saturated	
1	330.12	57076.8	100.0	8035.9	100.0		
2	331.13	17577.7	30.8	2573.1	32.0		
3	349.12	1846.8	3.2	290.7	3.6		

Table S10. High-resolution FD mass data of **1d**$^{+}$ BF_4^{-}.

Results

Mass	Intensity	Formula	Charge	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
330.12688	5846.36	C25 H16 N	+1	330.12773	-0.84	-2.55	18.5
		C22 H18 O3	+1	330.12505	1.84	5.57	14.0

X-ray Analyses (Figures S15-S17 and Tables S11 and S12)

Compounds	*rac*-**3**	*P*-**1a**$^{+}BF_4^{-}$	*P*-**1b**$^{+}BF_4^{-}$
Solvent System	CH_2Cl_2/hexane	THF/hexane	MeCN/Et_2O
Empirical formula	$C_{25}H_{15}NO$	$C_{34}H_{26}BF_4N$	$C_{34}H_{26}BNOF_4$
Formula weight	345.38	535.37	551.37
Temperature/K	150	150	200
Flack parameter		$\chi = 0.02(5)$	$\chi = -0.03(4)$
Crystal system	monoclinic	orthorhombic	orthorhombic
Space group	$P2_1/n$	$P2_12_12_1$	$P2_12_12_1$
a/Å	8.95059(16)	11.24384(10)	11.5153(3)
b/Å	11.1282(2)	13.79725(13)	13.2614(3)
c/Å	17.1740(3)	17.01571(15)	17.5945(4)
α/°	90	90	90
β/°	101.9520(18)	90	90
γ/°	90	90	90
Volume/Å^3	1673.51(6)	2639.72(4)	2686.83(11)
Z	4	4	4
ρ_{calc} g/cm^3	1.371	1.347	1.363
μ/mm^{-1}	0.654	0.800	0.831
F(000)	720.0	1112.0	1144.0
Color and shape	yellow block	red plate	red block
Crystal size/mm^3	0.4 × 0.2 × 0.2	0.114 × 0.07 × 0.042	0.177 × 0.121 × 0.05
Reflections collected	13560	26421	26167
Independent reflections	3397 [R_{int} = 0.0225, R_{sigma} = 0.0175]	5436 [R_{int} = 0.0318, R_{sigma} = 0.0211]	5541 [R_{int} = 0.0257, R_{sigma} = 0.0168]
Data/restraints/parameters	3397/0/245	5436/21/391	5541/0/374
Goodness-of-fit on F_2	1.045	1.031	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0355, wR_2 = 0.0949	R_1 = 0.0340, wR_2 = 0.0877	R_1 = 0.0396, wR_2 = 0. 1102
Final R indexes [all data]	R_1 = 0.0369, wR_2 = 0.0959	R_1 = 0.0366, wR_2 = 0.0892	R_1 = 0.0413, wR_2 = 0.1117
Largest diff. peak/hole / e Å^{-3}	0.21/−0.17	0.22/−0.15	0.37/−0.33
CCDC No.	2496077	2496078	2496079

Table S11. Crystal data of *rac*-**3**, *P*-**1a**$^{+}BF_4^{-}$, and *P*-**1b**$^{+}BF_4^{-}$.

Table S12. Crystal data of *rac*-**1c**$^{+}BF_4^{-}$ and *rac*-**1d**$^{+}BF_4^{-}$.

Compounds	*rac*-**1c**$^{+}BF_4^{-}$	*rac*-**1d**$^{+}BF_4^{-}$
Solvent System	CH_2Cl_2/Et_2O	$MeCN/Et_2O$
Empirical formula	$C_{33}H_{24}BCl_2F_4NO$	$C_{25}H_{16}BNF_4$
Formula weight	608.24	417.20
Temperature/K	150	150
Flack parameter		
Crystal system	monoclinic	monoclinic
Space group	*I*2/*a*	$P2_1/n$
a/Å	24.5693(6)	9.75691(12)
b/Å	8.47276(18)	7.33195(9)
c/Å	26.6677(6)	26.2699(3)
α/°	90	90
β/°	93.9884(19)	96.4206(11)
γ/°	90	90
Volume/Å^3	5538.0(2)	1867.48(4)
Z	8	4
ρ_{calc} g/cm^3	1.459	1.484
μ/mm^{-1}	2.596	0.956
F(000)	2496.0	856.0
Color and shape	red needle	red plate
Crystal size/mm^3	0.265 × 0.039 × 0.034	0.3 × 0.03 × 0.02
Reflections collected	25961	17546
Independent reflections	5578 [R_{int} = 0.0574, R_{sigma} = 0.0446]	3780 [R_{int} = 0.0269, R_{sigma} = 0.0209]
Data/restraints/parameters	5578/2/399	3780/108/308
Goodness-of-fit on F_2	1.056	1.030
Final R indexes [I>=2σ (I)]	R_1 = 0.0588, wR_2 = 0.1320	R_1 = 0.0479, wR_2 = 0.1194
Final R indexes [all data]	R_1 = 0.0801, wR_2 = 0.1439	R_1 = 0.0546, wR_2 = 0.1240
Largest diff. peak/hole / e Å^{-3}	0.41/−0.51	0.49/−0.58
CCDC No.	2496080	2496081

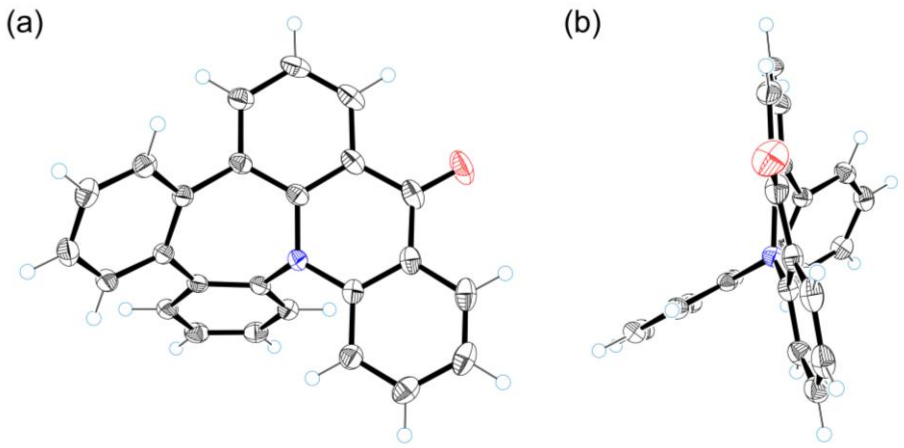


Figure S15. ORTEP drawings [(a) front view and (b) side view] of **3** determined at 150 K. Thermal ellipsoids are showed at 50% probability.

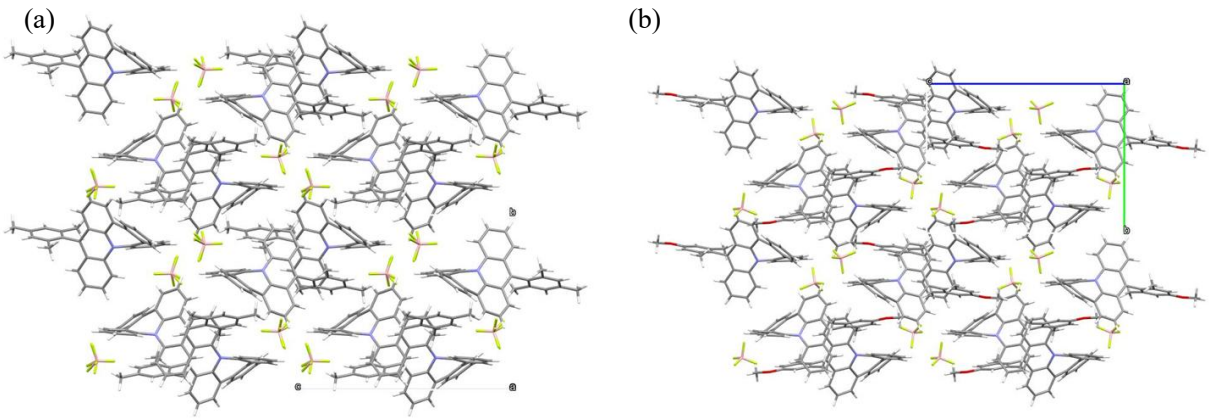
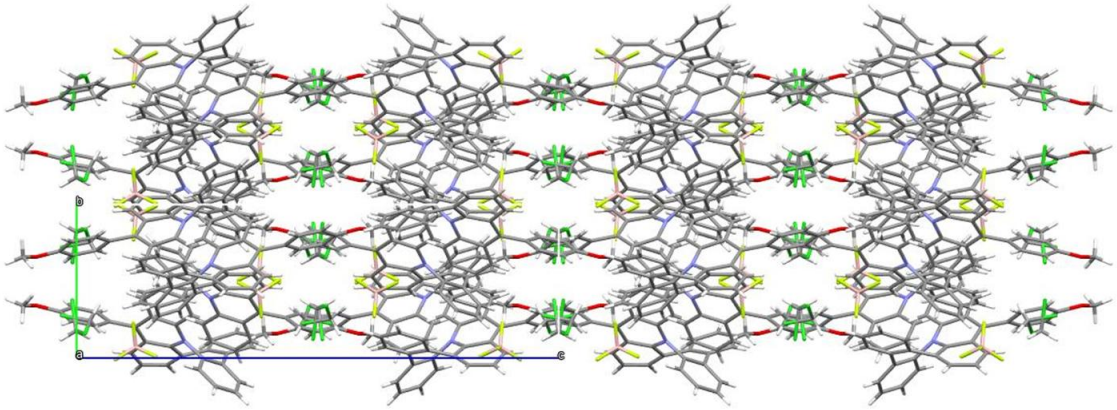


Figure S16. Crystal packing structures of (a) **1a**$^{+}BF_4^{-}$ and (b) **1b**$^{+}BF_4^{-}$ at 150 K.

(a)



(b)

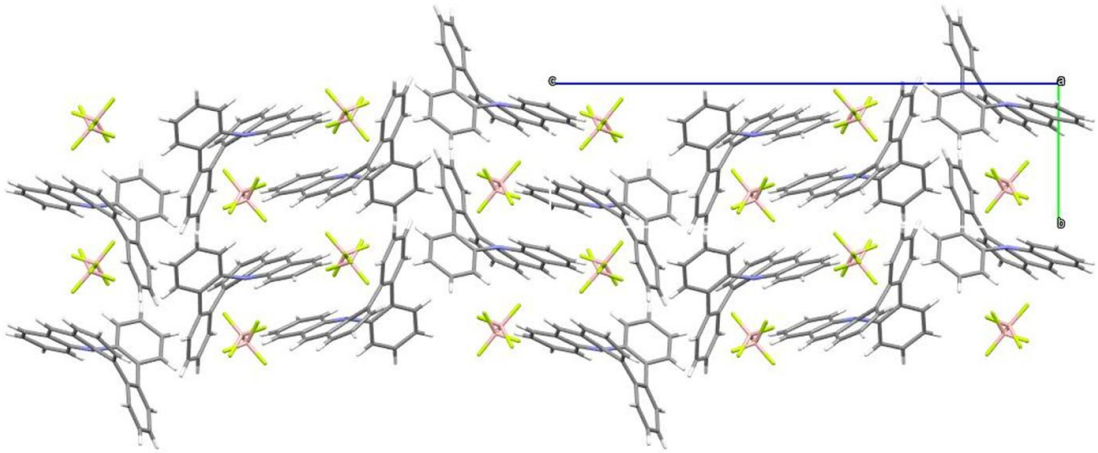


Figure S17. Crystal packing structures of (a) **1c**$^{+}BF_4^{-}$ and (b) **1d**$^{+}BF_4^{-}$ at 150 K.

UV-Vis Spectra (Figures S18)

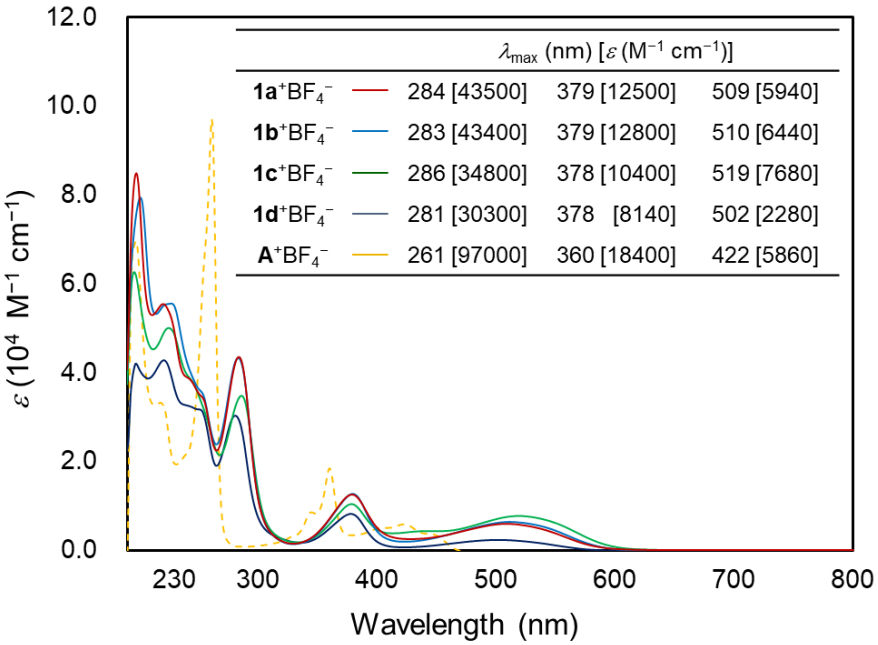


Figure S18. UV-Vis spectra of $\mathbf{A}^{+}BF_4^{-}$ (58.1 μM) , $\mathbf{1a}^{+}BF_4^{-}$ (20.9 μM), $\mathbf{1b}^{+}BF_4^{-}$ (21.2 μM), $\mathbf{1c}^{+}BF_4^{-}$ (23.3 μM), and $\mathbf{1d}^{+}BF_4^{-}$ (34.0 μM) in MeCN.

Cyclic Voltammetry (Figure S19)

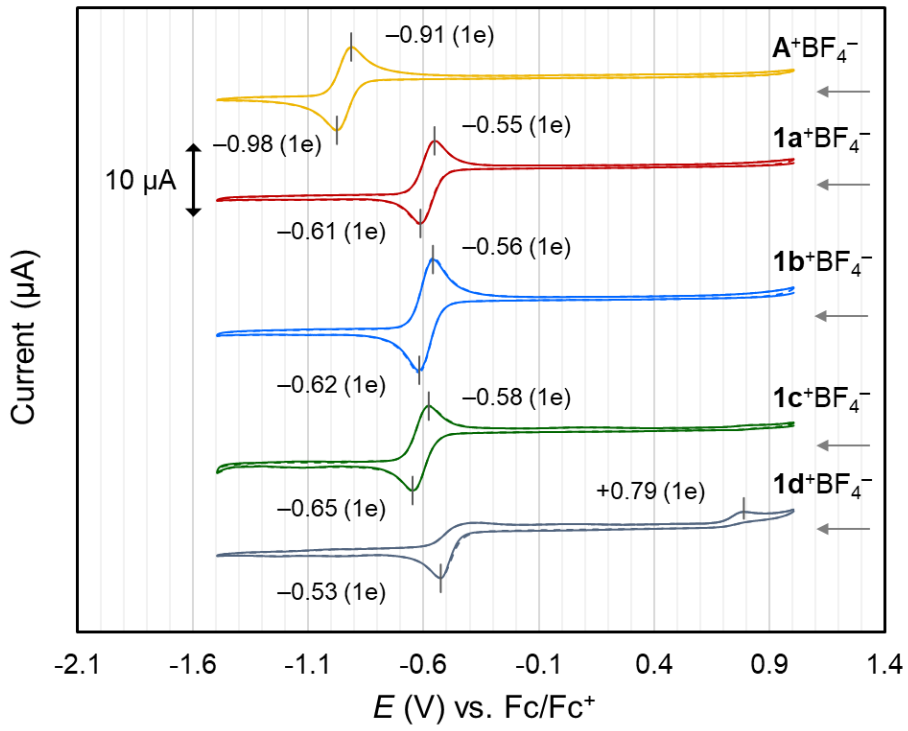


Figure S19. Cyclic voltammograms of 1.0 mM **1a**$^{+}BF_4^{-}$, **1b**$^{+}BF_4^{-}$, **1c**$^{+}BF_4^{-}$, and **1d**$^{+}BF_4^{-}$ in MeCN containing 0.1 M Et_4NClO_4 as the supporting electrolyte (Pt electrode, scan rate 100 mV s^{-1}, 1st cycle: solid line, 2nd cycle: dotted line).

Circular Dichroism (CD) Spectra (Figures S20 and S21)

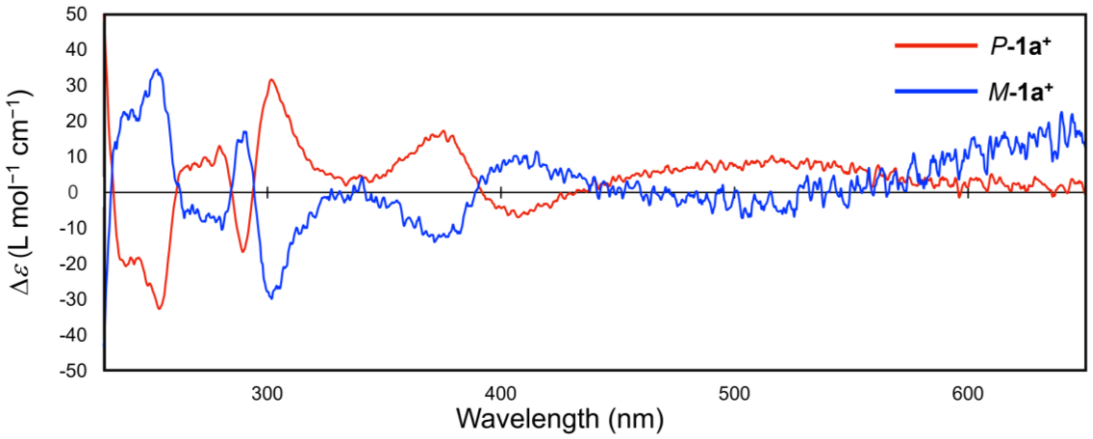


Figure S20. CD spectra for *P*/*M*-**1a**$^{+}BF_4^{-}$ in CH_2Cl_2 (*P* : $c = 4.57 \times 10^{-6}$ mol/L, *M* : $c = 1.82 \times 10^{-6}$ mol/L, 293 K).

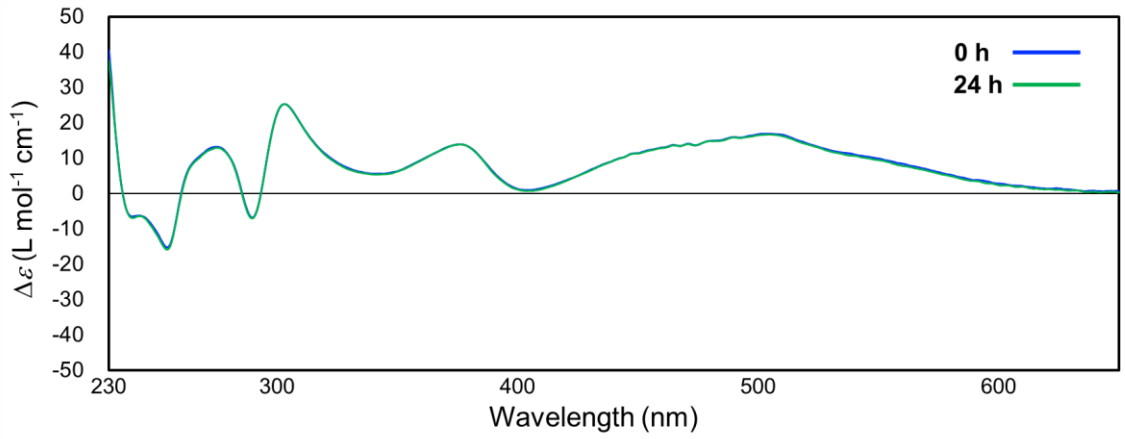


Figure S21. CD spectra for *P*-**1b**$^{+}BF_4^{-}$ and *P*-**1b**$^{+}BF_4^{-}$ after 24 h in CH_2Cl_2 ($c = 2.46 \times 10^{-5}$ M, 293 K).

Theoretical Studies (Figures S22-S29 and Table S13)

DFT calculations

Computational details: The transition states for racemization were located using the TS optimization method [Opt=(TS, CalcFC, NoEigenTest, MaxStep=5)] from a reasonable transition-state guess. The obtained transition-state structures were confirmed by vibrational frequency analysis, exhibiting a single imaginary frequency corresponding to the helical inversion mode. Although the ground states are closed-shell, an unrestricted formalism was employed for the transition-state calculations to allow for possible electronic reorganization along the inversion pathway.

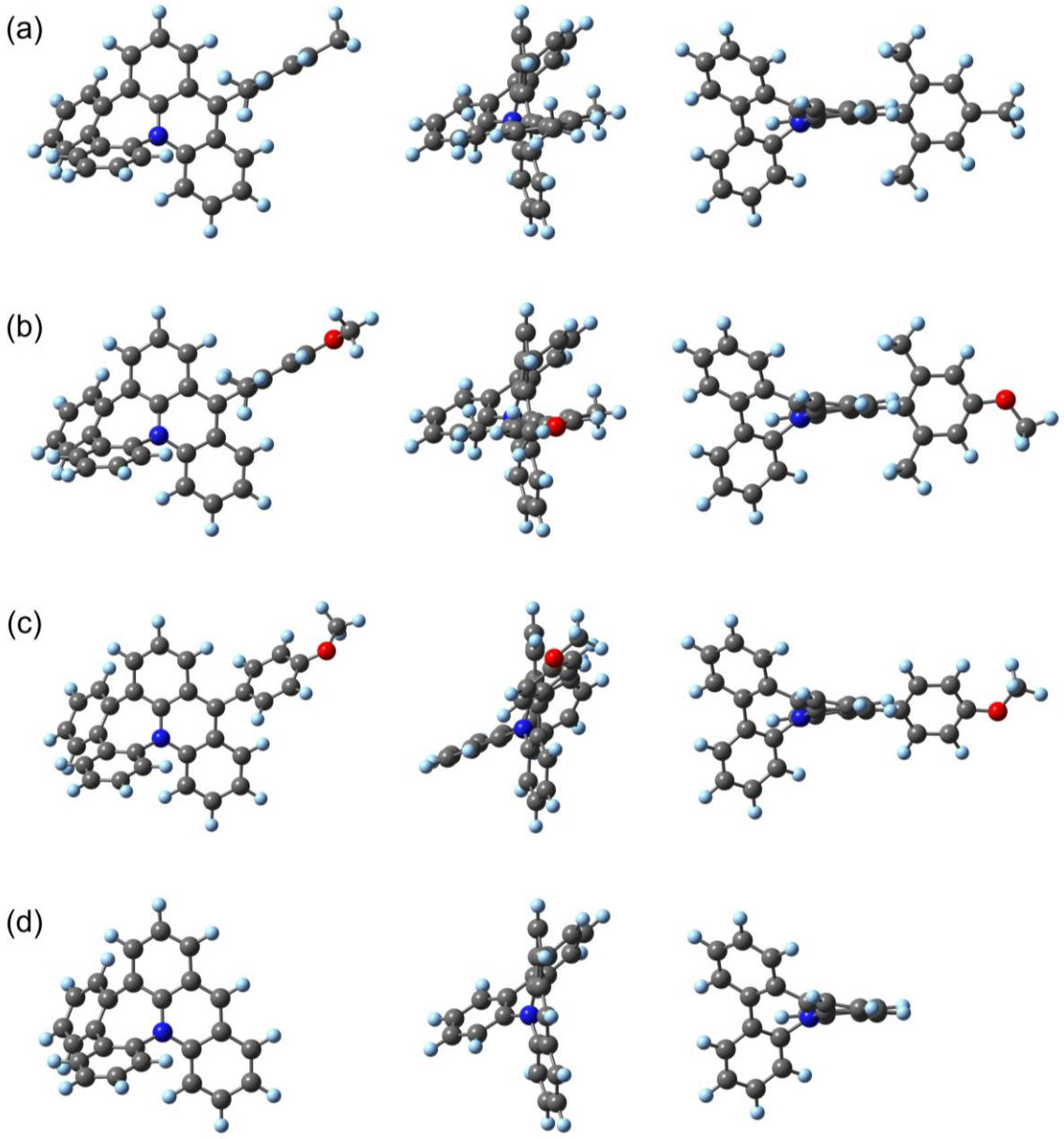


Figure S22. Optimized structures (front, side, and top views) of (a) *P*-**1a**$^+$, (b) *P*-**1b**$^+$, (c) *P*-**1c**$^+$, and (d) *P*-**1d**$^+$ obtained by DFT calculations at the CAM-B3LYP/6-31+G(d,p) level of theory. There were no imaginary frequencies in any of the optimized structures.

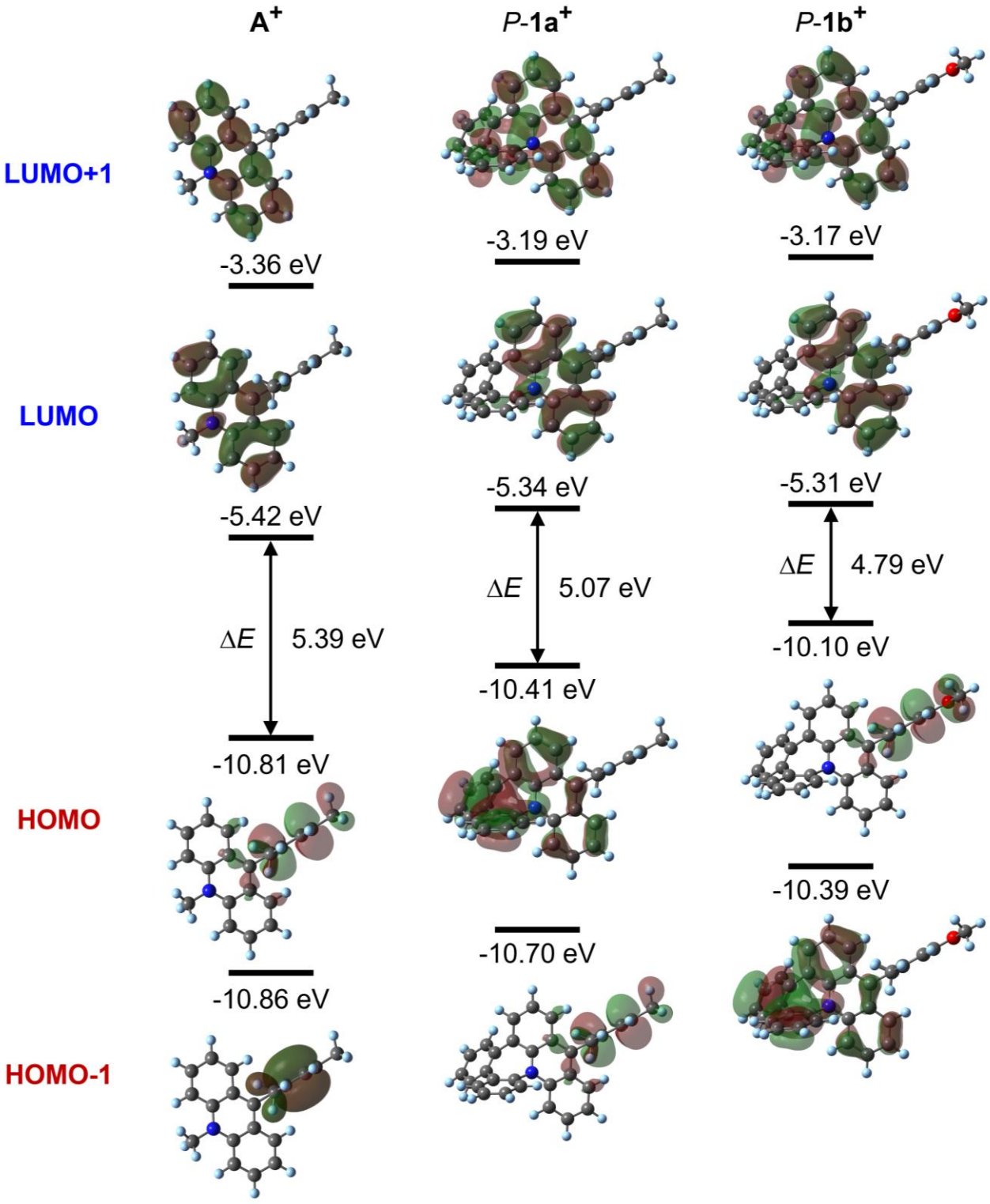


Figure S23. Kohn-Sham orbitals (isovalue = 0.02) calculated by DFT calculations at the CAM-B3LYP/6-31+G(d,p) level based on the optimized structures of $\mathbf{A}^+$, *P*-$\mathbf{1a}^+$, and *P*-$\mathbf{1b}^+$.

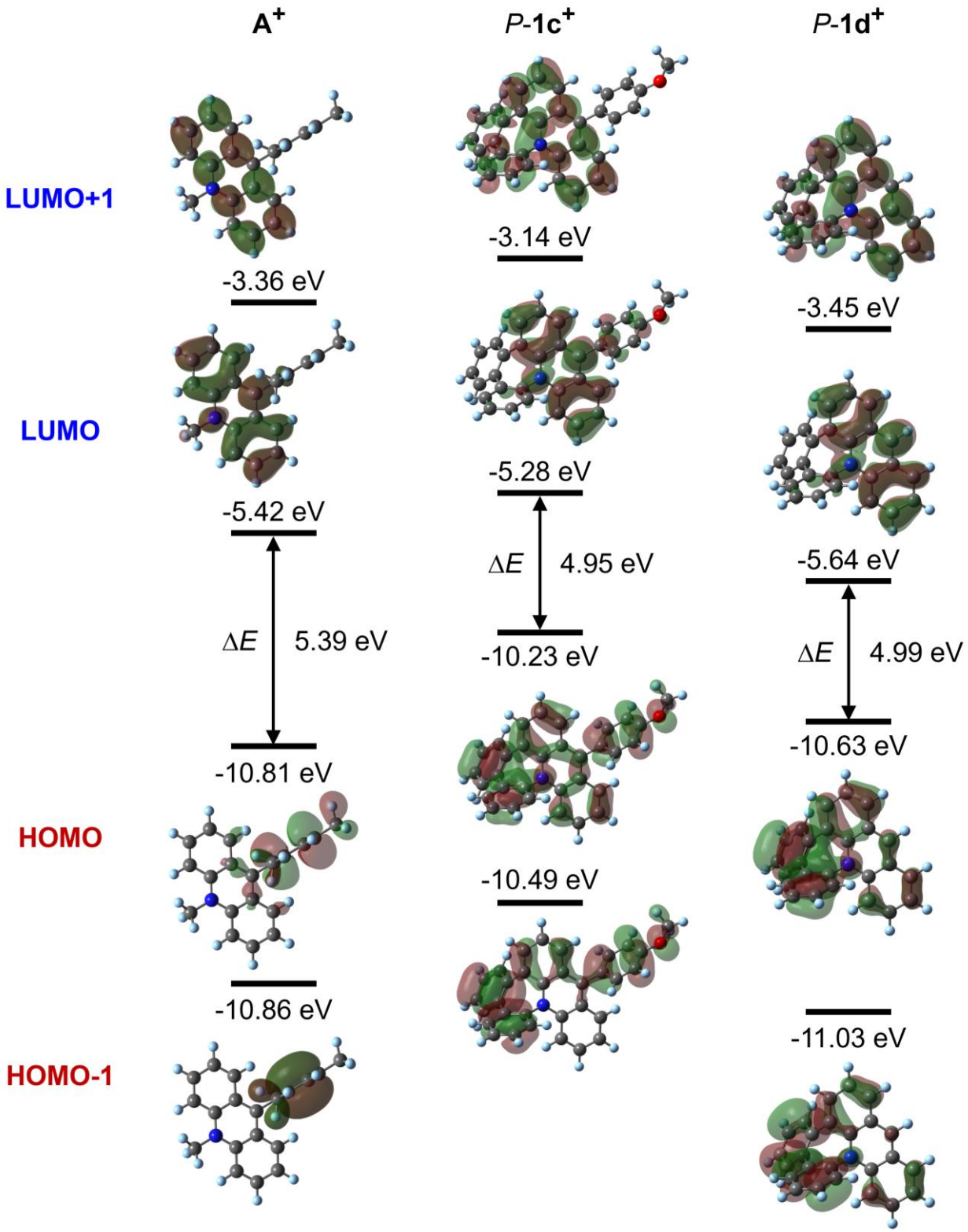


Figure S24. Kohn-Sham orbitals (isovalue = 0.02) calculated by DFT calculations at the CAM-B3LYP/6-31+G(d,p) level based on the optimized structures of $\mathbf{A}^+$, *P*-$\mathbf{1c}^+$, and *P*-$\mathbf{1d}^+$.

Racemization barrier

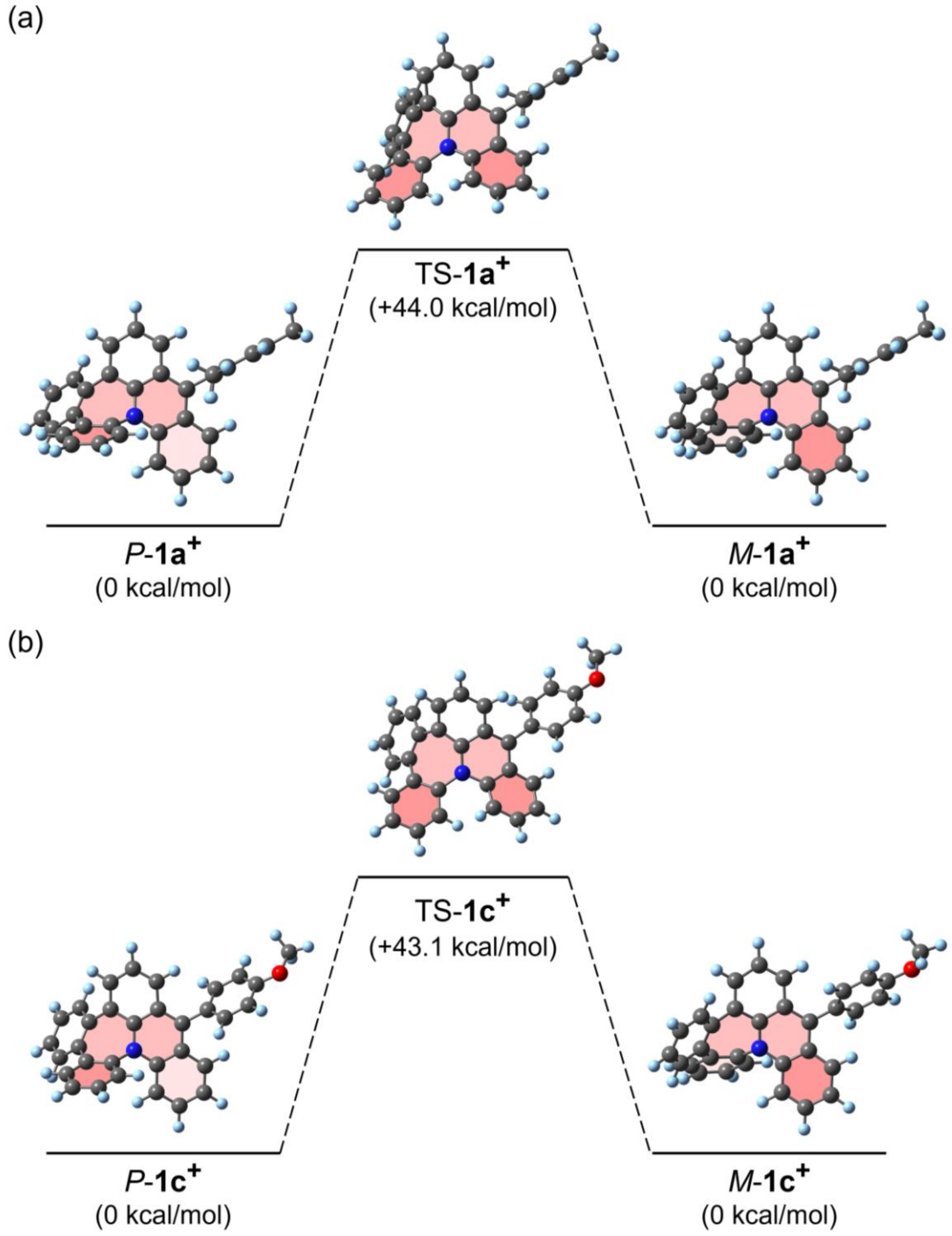


Figure S25. Computed racemization barrier of (a) **1a**$^+$ and (b) **1c**$^+$ obtained by DFT calculations at the (U)CAM-B3LYP/6-31+G(d,p) level.

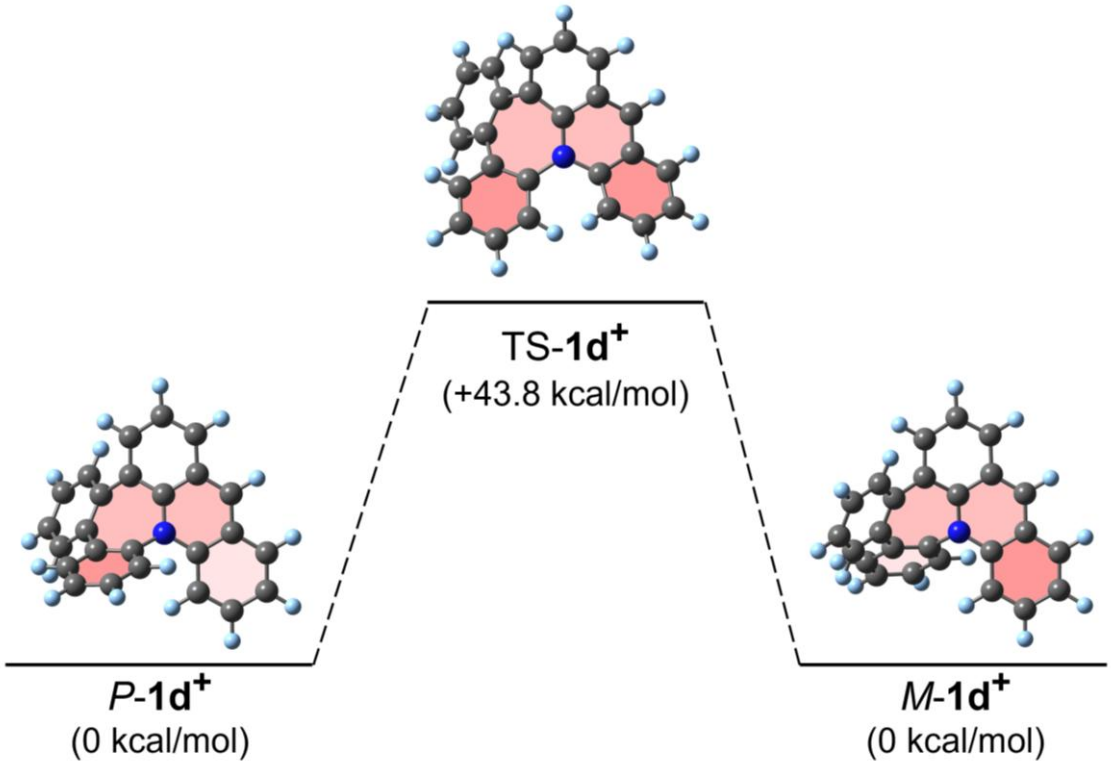


Figure S26. Computed racemization barrier of **1d**$^{+}$ obtained by DFT calculations at the (U)CAM-B3LYP/6-31+G(d,p) level.

Comparison of relative energy

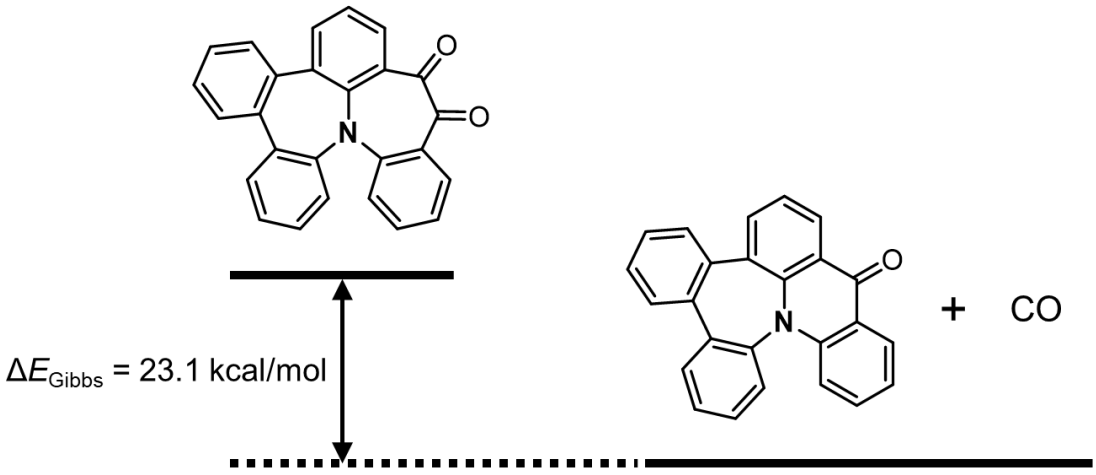


Figure S27. Comparison of relative energies between the assumed reaction intermediate and products (**3** and CO) at the CAM-B3LYP/6-31+G(d,p) level.

TD-DFT calculations

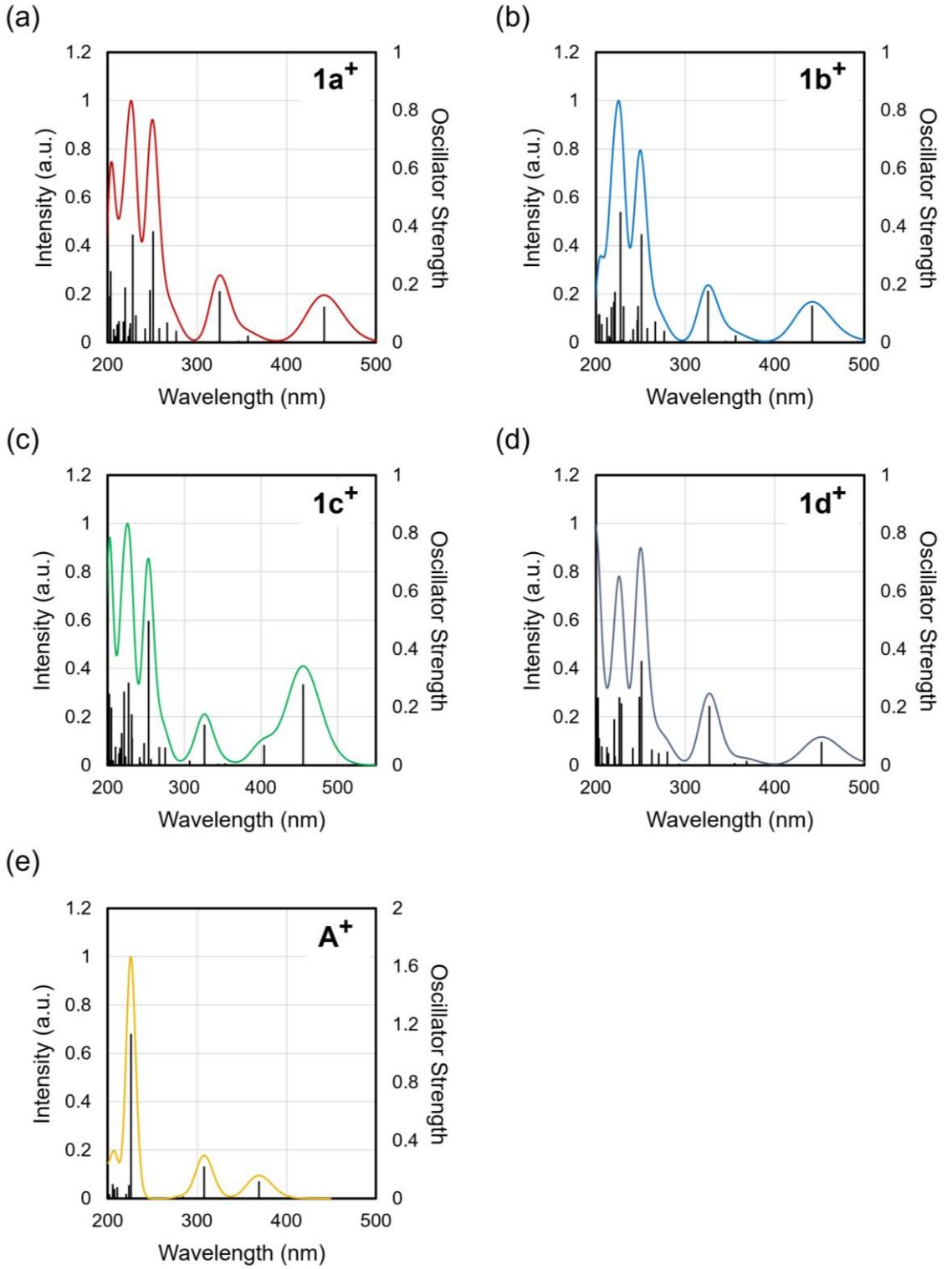


Figure S28. Simulated UV-Vis spectra by TD-DFT calculations at the CAM-B3LYP/6-31+G(d,p) level for (a) **1a**$^{+}$, (b) **1b**$^{+}$, (c) **1c**$^{+}$, (d) **1d**$^{+}$, and (e) **A**$^{+}$.

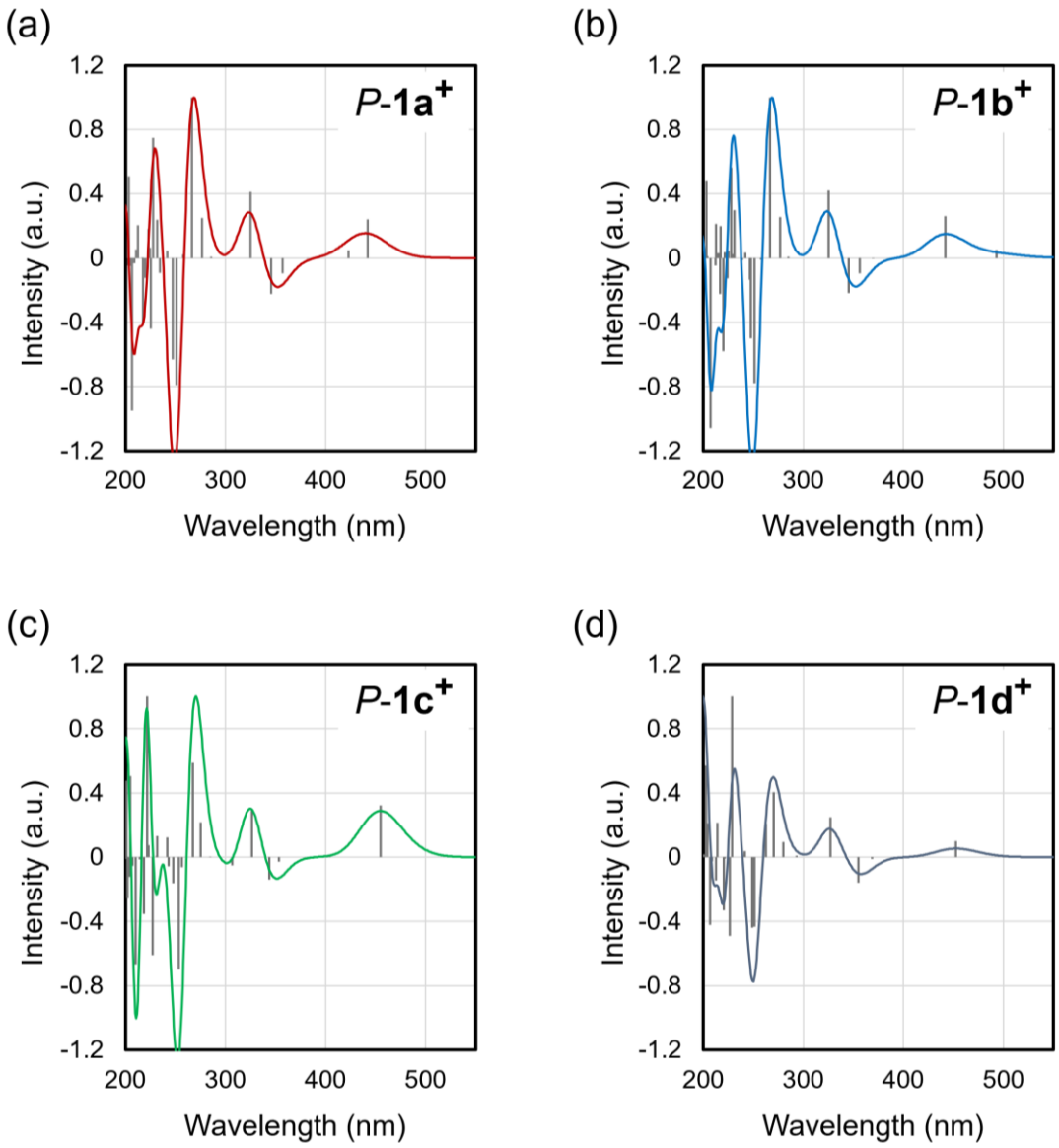


Figure S29. Simulated CD spectra by TD-DFT calculations at the CAM-B3LYP/6-31+G(d,p) level for (a) *P*-**1a**$^{+}$, (b) *P*-**1b**$^{+}$, (c) *P*-**1c**$^{+}$, and (d) *P*-**1d**$^{+}$.

P-**1a**$^+$; HOMO : 118, LUMO : 119

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.8041 eV
442.16 nm f=0.1238 <S**2>=0.000
115 -> 119 (LUMO) 0.17307
118 (HOMO) -> 119 0.66737
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1365.03781958
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.9304 eV
423.10 nm f=0.0037 <S**2>=0.000
107 ->119 -0.11149
117 ->119 0.69075

Excited State 3: Singlet-A 3.2452 eV
382.06 nm f=0.0002 <S**2>=0.000
116 ->119 0.70317

Excited State 4: Singlet-A 3.4740 eV
356.89 nm f=0.0236 <S**2>=0.000
110 ->119 -0.10937
114 ->119 0.38369
115 ->119 0.53595
118 ->119 -0.19518

Excited State 5: Singlet-A 3.5849 eV
345.85 nm f=0.0058 <S**2>=0.000
110 ->119 -0.15323
113 ->119 -0.22264
114 ->119 0.51567
115 ->119 -0.36961

Excited State 6: Singlet-A 3.8118 eV
325.26 nm f=0.1772 <S**2>=0.000
112 ->119 -0.23506
113 ->119 0.57481
114 ->119 0.17293
115 ->119 -0.13287
118 ->120 -0.17910

Excited State 7: Singlet-A 4.3421 eV
285.54 nm f=0.0021 <S**2>=0.000
110 ->119 -0.17335
112 ->119 0.58457
113 ->119 0.25442
115 ->119 -0.12631

Excited State 8: Singlet-A 4.4801 eV
276.74 nm f=0.0401 <S**2>=0.000
110 ->119 0.55163
111 ->119 0.16827
112 ->119 0.20867
114 ->119 0.16306
118 ->121 0.22212

Excited State 9: Singlet-A 4.6498 eV
266.64 nm f=0.0689 <S**2>=0.000
110 ->119 -0.13882
111 ->119 -0.28685
115 ->120 -0.14523
118 ->121 0.56783

Excited State 10: Singlet-A 4.8093 eV
257.80 nm f=0.0498 <S**2>=0.000
110 ->119 -0.24761
111 ->119 0.55891
115 ->121 0.14010
118 ->121 0.23328
118 ->123 -0.10271

Excited State 11: Singlet-A 4.9410 eV
250.93 nm f=0.3834 <S**2>=0.000
110 ->119 0.13889
112 ->119 -0.13932
113 ->119 0.13935
115 ->120 0.11377
115 ->121 0.12839
118 ->120 0.54736
118 ->123 -0.16490

Excited State 12: Singlet-A 5.0130 eV
247.32 nm f=0.1800 <S**2>=0.000
111 ->119 -0.21711
114 ->121 -0.10877
115 ->120 0.12877
115 ->121 0.38554
118 ->120 -0.24784
118 ->122 -0.20488
118 ->123 -0.23074
118 ->128 -0.10505

Excited State 13: Singlet-A 5.1265 eV
241.85 nm f=0.0482 <S**2>=0.000
111 ->122 -0.11385
114 ->120 -0.24472
114 ->121 -0.19811
114 ->122 0.12509
114 ->123 0.16943
115 ->120 -0.19418
115 ->122 -0.14887
115 ->124 -0.14692
118 ->122 0.28782
118 ->123 -0.11708
118 ->124 0.19948

Excited State 14: Singlet-A 5.2845 eV
234.62 nm f=0.0049 <S**2>=0.000
116 ->125 0.45185
116 ->126 -0.16611
117 ->120 -0.16741
117 ->121 0.13374
117 ->127 -0.41918

Excited State 15: Singlet-A 5.3543 eV
231.56 nm f=0.0930 <S**2>=0.000
106 ->119 0.10170
108 ->119 -0.24823
109 ->119 0.44641
114 ->120 -0.22790
115 ->120 -0.10067
118 ->122 -0.20615

Excited State 16: Singlet-A 5.4408 eV
227.88 nm f=0.3715 <S**2>=0.000
108 ->119 -0.17613
109 ->119 0.11559
115 ->120 0.33941
115 ->121 0.23055
115 ->123 -0.13560
118 ->122 0.35215
118 ->123 0.28951

Excited State 17: Singlet-A 5.5018 eV
225.35 nm f=0.0668 <S**2>=0.000
103 ->119 -0.13412
108 ->119 0.34295

114 ->120 -0.23746
114 ->122 -0.14402
115 ->122 -0.15940
117 ->120 0.25668
118 ->122 -0.11129
118 ->123 0.28639

Excited State 18: Singlet-A 5.5255 eV
224.39 nm f=0.0469 <S**2>=0.000
108 ->119 -0.18634
109 ->119 -0.17399
116 ->125 0.12713
117 ->120 0.53733
117 ->121 -0.18353
117 ->123 0.11804
118 ->123 -0.10348

Excited State 19: Singlet-A 5.5577 eV
223.08 nm f=0.0219 <S**2>=0.000
103 ->119 -0.17575
108 ->119 0.30714
109 ->119 0.38781
114 ->120 0.12534
114 ->122 0.14450
115 ->122 0.14930
117 ->120 0.11462
118 ->122 0.19894
118 ->123 -0.18770

Excited State 20: Singlet-A 5.6437 eV
219.68 nm f=0.1897 <S**2>=0.000
109 ->119 -0.19668
110 ->120 0.14418
113 ->121 0.13649
114 ->120 -0.26623
114 ->121 0.36032
114 ->122 0.10124
114 ->123 -0.10850
115 ->120 -0.10377
115 ->121 0.14307
115 ->122 0.10512
115 ->123 -0.11173
117 ->120 -0.12693
118 ->122 0.13876

Excited State 21: Singlet-A 5.7015 eV
217.46 nm f=0.0720 <S**2>=0.000
113 ->120 0.11173
114 ->120 -0.13761
114 ->121 0.11028
115 ->120 0.39621
115 ->121 -0.36331
115 ->122 -0.10181
116 ->120 -0.16834
118 ->121 0.13270
118 ->123 -0.18906

Excited State 22: Singlet-A 5.7103 eV
217.12 nm f=0.0067 <S**2>=0.000
115 ->120 0.10201
115 ->121 -0.10026
116 ->120 0.60169
116 ->121 -0.25419
117 ->125 0.12005

Excited State 23: Singlet-A 5.8281 eV
212.73 nm f=0.0735 <S**2>=0.000
114 ->120 0.19837
114 ->121 0.32961
114 ->123 0.20661
115 ->120 -0.11983
115 ->121 0.12059
115 ->122 -0.30906
115 ->123 -0.19517
117 ->121 -0.12118
118 ->124 0.17323

Excited State 24: Singlet-A 5.8851 eV
210.67 nm f=0.0627 <S**2>=0.000
116 ->120 -0.17454
116 ->127 0.30528
117 ->121 0.26804
117 ->125 0.43578
117 ->126 -0.17134

Excited State 25: Singlet-A 5.9389 eV
208.77 nm f=0.0222 <S**2>=0.000
107 ->119 -0.16202
115 ->123 -0.13905
116 ->127 -0.16399
117 ->120 0.15355
117 ->121 0.47081
117 ->122 0.11049
117 ->123 0.11384
117 ->125 -0.20972
117 ->128 -0.11366

Excited State 26: Singlet-A 5.9956 eV
206.79 nm f=0.0462 <S**2>=0.000
107 ->119 -0.11884
111 ->121 -0.10397
112 ->122 -0.14592
113 ->120 0.12511
114 ->121 0.22749
114 ->122 0.19204
114 ->124 0.11930
115 ->121 0.10914
115 ->122 0.22732
115 ->123 0.32550
117 ->121 0.12545
118 ->120 -0.11991
118 ->123 0.14651
118 ->124 0.14213

Excited State 27: Singlet-A 6.0485 eV
204.98 nm f=0.0035 <S**2>=0.000
98 ->119 -0.19730
99 ->119 -0.12667
107 ->119 0.54197
116 ->121 0.12051
117 ->121 0.21729

Excited State 28: Singlet-A 6.0952 eV
203.41 nm f=0.2456 <S**2>=0.000
112 ->120 -0.13567
113 ->120 0.40727
113 ->121 -0.36881
114 ->120 -0.15947
115 ->122 0.10964
118 ->122 0.13380

Excited State 29: Singlet-A 6.1047 eV
203.10 nm f=0.0048 <S**2>=0.000
106 ->119 -0.14375
107 ->119 -0.11098
116 ->120 0.18901
116 ->121 0.57243
116 ->122 0.10057
116 ->123 0.13414
117 ->125 0.10231

Excited State 30: Singlet-A 6.1233 eV
202.48 nm f=0.1584 <S**2>=0.000
103 ->119 -0.15271
106 ->119 -0.24529
110 ->120 -0.10060

114 ->120	-0.20067	116 ->121	-0.15476
114 ->122	0.24669	118 ->122	-0.13850
114 ->123	0.15071	118 ->123	0.10565
115 ->123	-0.17690	118 ->124	-0.23837

Ground to excited state transition electric dipole moments (Au):

state	X	Y	Z	Dip. S.	Osc.
1	1.3043	-0.3063	-0.0793	1.8014	0.1238
2	-0.2220	-0.0305	-0.0374	0.0516	0.0037
3	-0.0040	-0.0317	-0.0336	0.0021	0.0002
4	0.4796	-0.0199	0.2176	0.2777	0.0236
5	0.0425	-0.2420	0.0759	0.0661	0.0058
6	0.4637	1.0749	0.7261	1.8977	0.1772
7	-0.0443	0.0178	-0.1308	0.0194	0.0021
8	-0.3159	-0.4560	-0.2409	0.3658	0.0401
9	-0.7216	0.1829	-0.2256	0.6050	0.0689
10	-0.6305	0.1593	0.0113	0.4230	0.0498
11	0.6507	1.4694	0.7645	3.1671	0.3834
12	-0.5639	-1.0231	-0.3181	1.4660	0.1800
13	-0.1946	-0.4961	-0.3160	0.3839	0.0482
14	0.0851	-0.0185	0.1739	0.0378	0.0049
15	-0.7683	0.0918	-0.3324	0.7092	0.0930
16	-0.8392	-0.9309	1.1028	2.7870	0.3715
17	-0.5507	-0.4310	0.0801	0.4954	0.0668
18	0.5463	-0.1932	-0.1030	0.3464	0.0469
19	-0.3932	-0.0537	0.0549	0.1605	0.0219
20	0.6509	-0.8132	-0.5357	1.3720	0.1897
21	0.2966	0.6486	-0.0821	0.5155	0.0720
22	0.1453	0.1527	-0.0591	0.0479	0.0067
23	0.7078	-0.1089	-0.0433	0.5148	0.0735
24	0.6575	0.0096	-0.0490	0.4348	0.0627
25	-0.1391	0.3445	0.1216	0.1528	0.0222
26	-0.0176	-0.4806	-0.2886	0.3145	0.0462
27	-0.0619	-0.0294	-0.1366	0.0234	0.0035
28	-1.2009	0.3472	0.2868	1.6449	0.2456
29	0.1426	0.0893	0.0605	0.0320	0.0048
30	-0.9698	0.3312	-0.0763	1.0560	0.1584

Ground to excited state transition velocity dipole moments (Au):

state	X	Y	Z	Dip. S.	Osc.
1	-0.1403	0.0312	0.0091	0.0207	0.1341
2	0.0237	0.0031	0.0038	0.0006	0.0036
3	-0.0001	0.0013	0.0029	0.0000	0.0001
4	-0.0632	0.0046	-0.0268	0.0047	0.0248
5	-0.0054	0.0309	-0.0107	0.0011	0.0056
6	-0.0643	-0.1425	-0.0972	0.0339	0.1612
7	0.0016	-0.0043	0.0177	0.0003	0.0014
8	0.0512	0.0756	0.0399	0.0099	0.0402
9	0.1205	-0.0336	0.0371	0.0170	0.0664
10	0.1102	-0.0277	-0.0020	0.0129	0.0487
11	-0.1155	-0.2584	-0.1340	0.0981	0.3601
12	0.1025	0.1846	0.0598	0.0482	0.1743
13	0.0360	0.0899	0.0553	0.0124	0.0440
14	-0.0159	0.0049	-0.0349	0.0015	0.0051
15	0.1447	-0.0180	0.0660	0.0256	0.0868
16	0.1634	0.1824	-0.2176	0.1073	0.3578
17	0.1072	0.0848	-0.0140	0.0189	0.0623
18	-0.1083	0.0334	0.0255	0.0135	0.0443
19	0.0768	0.0108	-0.0120	0.0062	0.0201
20	-0.1358	0.1651	0.1051	0.0568	0.1824
21	-0.0595	-0.1337	0.0169	0.0217	0.0690
22	-0.0327	-0.0307	0.0124	0.0022	0.0069
23	-0.1444	0.0215	0.0104	0.0214	0.0667
24	-0.1396	-0.0018	0.0109	0.0196	0.0605
25	0.0302	-0.0747	-0.0268	0.0072	0.0220
26	0.0039	0.1071	0.0634	0.0155	0.0469
27	0.0134	0.0051	0.0285	0.0010	0.0031
28	0.2641	-0.0768	-0.0629	0.0796	0.2369
29	-0.0306	-0.0209	-0.0138	0.0016	0.0046
30	0.2154	-0.0748	0.0163	0.0523	0.1549

Ground to excited state transition magnetic dipole moments (Au):

state	X	Y	Z
1	-0.1252	-0.0564	0.2157

2	0.1578	0.0113	-0.0430
3	0.0051	-0.1361	0.0709
4	-0.0391	-0.2953	0.3667
5	0.0163	-0.3681	0.8684
6	-0.0408	0.1994	-0.6868
7	-0.0175	-0.0487	0.0415
8	0.0893	0.0749	0.4790
9	0.2060	-0.1141	2.5041
10	0.0051	-0.1464	0.9858
11	0.0144	0.2116	0.3413
12	0.0423	-0.4284	-0.1306
13	-0.0155	0.1496	-0.1266
14	0.1181	0.5904	0.3969
15	-0.0690	0.3476	0.7527
16	0.2526	-1.0532	-1.1827
17	-0.0769	-0.5706	0.4595
18	0.0307	0.4087	-0.0449
19	0.1833	0.2603	-0.7781
20	0.0192	0.1669	-0.4117
21	0.1569	0.4784	0.6912
22	-0.0147	0.0985	0.2388
23	-0.0756	0.1414	1.6494
24	-0.0342	-0.1621	0.2860
25	0.1446	0.0076	0.3228
26	-0.0643	-0.5113	-1.4767
27	-0.1011	-0.0627	-0.2220
28	0.1845	0.0127	-0.5299
29	0.0348	0.3489	-0.0562
30	0.2971	0.2728	-0.0674

Ground to excited state transition velocity quadrupole moments (Au):

state	XX	YY	ZZ	XY	XZ	YZ
1	0.1507	0.0133	-0.0527	0.0092	0.0267	-0.1951
2	0.1270	-0.0081	-0.0191	-0.0032	-0.0174	-0.0113
3	-0.0034	0.0064	-0.0011	-0.0171	0.0252	0.0020
4	-0.2723	0.1280	0.0006	-0.1817	0.0688	-0.0373
5	-0.1588	0.0665	0.0432	-0.2787	0.0708	0.0815
6	0.0717	-0.1457	-0.1425	0.0159	-0.0182	-0.1938
7	-0.4834	0.0865	0.0316	0.0565	-0.1131	0.2493
8	-0.5425	0.1338	0.0864	0.0465	0.2745	0.2676
9	-0.4872	0.0795	-0.0108	0.1458	-0.0862	0.3279
10	-0.0148	-0.1879	-0.0393	-0.0517	-0.1307	0.0233
11	0.3168	-0.0898	-0.1758	0.2816	-0.1857	-0.3072
12	-0.6809	0.0681	0.1420	-0.3584	0.3007	0.3384
13	0.0802	0.0183	0.1134	0.0096	0.1100	0.0442
14	0.0102	-0.0004	-0.0074	0.0936	-0.1146	-0.0237
15	0.6552	-0.3063	-0.0963	0.4741	-0.5079	0.0526
16	-0.9084	-0.2527	0.0280	-2.3534	1.2831	-0.2076
17	-1.2090	0.1899	0.1226	-0.6342	0.3359	0.6142
18	-0.1469	0.2506	0.0882	0.5295	-0.1892	0.0663
19	1.8853	-0.6476	-0.1514	-0.2517	-0.0079	-0.9318
20	-0.6251	0.5272	0.2609	0.2645	0.3596	0.2625
21	-0.1305	0.4143	0.0046	0.8357	-0.3118	-0.1240
22	-0.0573	0.1528	-0.0226	0.2809	-0.0747	0.0726
23	1.2833	0.1596	0.0778	-0.0400	0.0979	-0.5146
24	-1.2663	0.2730	0.0064	0.2150	0.2663	0.1194
25	0.3646	0.0820	-0.0008	-0.1843	0.2620	-0.0903
26	0.3064	-0.1799	0.1467	-0.1790	-0.3614	-0.0876
27	-0.4079	0.1004	0.0847	0.0363	0.0256	0.1456
28	0.1407	-0.2415	0.0629	-0.1073	-0.0157	0.3912
29	-1.1189	0.2362	0.0722	0.4229	-0.1866	0.2574
30	-1.2950	0.4325	-0.0315	0.6812	-0.2063	0.4238

<0|del|b> * <b|rxdel|0> + <0|del|b> * <b|delr+rdel|0>

Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)

state	XX	YY	ZZ	R(velocity)	E-M Angle
1	-1.8690	160.5891	-36.8449	40.6251	61.16
2	-0.2840	10.9198	13.1170	7.9176	24.49
3	-0.1489	0.7647	-0.4267	0.0630	90.00
4	-18.3976	-27.3768	-2.5815	-16.1186	105.57
5	-53.4341	-34.4475	-23.7455	-37.2091	131.62
6	86.2561	210.3804	-89.9592	68.8924	71.91
7	3.2355	0.2307	0.6065	1.3576	40.88
8	12.6725	76.3337	37.0950	42.0337	53.29
9	205.1538	314.0033	-16.4870	167.5567	68.28

10	-2.8031	2.1701	11.3343	3.5671	88.65
11	-362.4313	50.2801	-85.3553	-132.5022	144.21
12	-314.4496	101.0676	-103.5041	-105.6287	146.74
13	-5.4702	-12.2023	39.7740	7.3672	74.42
14	-24.9547	-22.0292	0.0979	-15.6287	117.48
15	117.8489	28.7834	-26.4649	40.0558	75.46
16	607.1898	-437.4954	207.0900	125.5948	78.30
17	-130.2275	73.9515	-164.3558	-73.5439	128.55
18	56.3210	-43.8149	19.4931	10.6664	78.94
19	26.4449	-88.5752	152.9933	30.2877	66.56
20	-80.6155	-186.3947	204.5719	-20.8128	99.95
21	-134.6506	-7.4273	-65.8199	-69.2993	119.28
22	1.9016	-4.0744	3.5773	0.4682	88.02
23	29.2554	169.7894	-96.1597	34.2950	82.62
24	10.1427	-18.1982	34.7480	8.8975	79.84
25	24.7550	-19.3947	-21.1102	-5.2500	99.31
26	-194.2077	-132.9851	-149.8028	-158.9985	139.75
27	-9.1339	-10.7577	-5.5636	-8.4851	174.75
28	59.8090	281.9889	-85.7924	85.3352	59.20
29	-25.6406	-3.6694	5.3675	-7.9809	122.77
30	-40.6117	224.8557	-50.6937	44.5168	62.97

1/2[<0|r|b>*<b|rxdel|0> + (<0|rxdel|b>*<b|r|0>)*]

Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)

state	XX	YY	ZZ	R(length)
1	115.4521	-12.2099	12.1000	38.4474
2	24.7702	0.2441	-1.1370	7.9591
3	0.0144	-3.0488	1.6854	-0.4497
4	13.2618	-4.1458	-56.4389	-15.7743
5	-0.4883	-62.9852	-46.5987	-36.6907
6	13.3876	-151.5447	352.6175	71.4868
7	-0.5481	0.6117	3.8416	1.3017
8	19.9506	24.1387	81.6038	41.8977
9	105.1028	14.7499	399.4170	173.0899
10	2.2592	16.5011	-7.8447	3.6385
11	-6.6349	-219.8441	-184.5155	-136.9982
12	16.8854	-309.9677	-29.3691	-107.4838
13	-2.1311	52.4821	-28.2840	7.3557
14	-7.1030	7.7062	-48.8234	-16.0734
15	-37.4961	-22.5761	176.9574	38.9617
16	149.8974	-693.3373	922.3022	126.2874
17	-29.9412	-173.8971	-26.0433	-76.6272
18	-11.8544	55.8405	-3.2662	13.5733
19	50.9628	9.8802	30.2310	30.3580
20	-8.8262	96.0061	-155.9689	-22.9297
21	-32.9150	-219.4407	40.1366	-70.7397
22	1.5061	-10.6383	9.9780	0.2819
23	37.8292	10.8894	50.5004	33.0730
24	15.8795	1.0992	9.9080	8.9622
25	14.2203	-1.8589	-27.7561	-5.1316
26	-0.8027	-173.7501	-301.3821	-158.6450
27	-4.4237	-1.3050	-21.4561	-9.0616
28	156.7177	-3.1256	107.4440	87.0120
29	-3.5044	-22.0261	2.4039	-7.7089
30	203.7563	-63.8996	-3.6363	45.4068

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)

state	X	Y	Z	Dip. S.	Osc.(frdel)
1	-0.1829	-0.0096	-0.0007	0.1932	0.1288
2	-0.0053	-0.0001	-0.0001	0.0055	0.0037
3	0.0000	-0.0000	-0.0001	0.0001	0.0001
4	-0.0303	-0.0001	-0.0058	0.0363	0.0242
5	-0.0002	-0.0075	-0.0008	0.0085	0.0057
6	-0.0298	-0.1532	-0.0705	0.2535	0.1690
7	-0.0001	-0.0001	-0.0023	0.0025	0.0016
8	-0.0162	-0.0345	-0.0096	0.0603	0.0402
9	-0.0870	-0.0061	-0.0084	0.1015	0.0676
10	-0.0695	-0.0044	-0.0000	0.0739	0.0493
11	-0.0752	-0.3797	-0.1024	0.5573	0.3715
12	-0.0578	-0.1889	-0.0190	0.2657	0.1771
13	-0.0070	-0.0446	-0.0175	0.0691	0.0461
14	-0.0014	-0.0001	-0.0061	0.0075	0.0050
15	-0.1112	-0.0017	-0.0219	0.1348	0.0899
16	-0.1371	-0.1698	-0.2399	0.5468	0.3646
17	-0.0590	-0.0366	-0.0011	0.0967	0.0645

18	-0.0592	-0.0065	-0.0026	0.0683	0.0455
19	-0.0302	-0.0006	-0.0007	0.0314	0.0210
20	-0.0884	-0.1343	-0.0563	0.2790	0.1860
21	-0.0177	-0.0867	-0.0014	0.1058	0.0705
22	-0.0048	-0.0047	-0.0007	0.0102	0.0068
23	-0.1022	-0.0023	-0.0005	0.1050	0.0700
24	-0.0918	-0.0000	-0.0005	0.0923	0.0616
25	-0.0042	-0.0257	-0.0033	0.0332	0.0221
26	-0.0001	-0.0515	-0.0183	0.0698	0.0465
27	-0.0008	-0.0002	-0.0039	0.0049	0.0032
28	-0.3172	-0.0267	-0.0180	0.3619	0.2413
29	-0.0044	-0.0019	-0.0008	0.0071	0.0047
30	-0.2089	-0.0248	-0.0012	0.2349	0.1566

P-**1b**$^{+}$; HOMO : 122, LUMO : 123

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.5147 eV
493.04 nm f=0.0040 <S**2>=0.000
113 ->123 (LUMO) -0.13406
122 (HOMO) ->123 0.68723
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1440.23736390
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.8056 eV
441.92 nm f=0.1268 <S**2>=0.000
120 ->123 -0.17155
121 ->123 0.66780

Excited State 3: Singlet-A 3.3571 eV
369.32 nm f=0.0006 <S**2>=0.000
119 ->123 0.70253

Excited State 4: Singlet-A 3.4801 eV
356.27 nm f=0.0243 <S**2>=0.000
114 ->123 -0.11266
118 ->123 0.39145
120 ->123 0.53067
121 ->123 0.19311

Excited State 5: Singlet-A 3.5898 eV
345.38 nm f=0.0058 <S**2>=0.000
114 ->123 -0.15194
117 ->123 -0.22622
118 ->123 0.50889
120 ->123 -0.37665

Excited State 6: Singlet-A 3.8106 eV
325.37 nm f=0.1774 <S**2>=0.000
116 ->123 -0.22820
117 ->123 0.57646
118 ->123 0.17448
120 ->123 -0.13643
121 ->124 0.17867

Excited State 7: Singlet-A 4.3493 eV
285.07 nm f=0.0020 <S**2>=0.000
114 ->123 -0.17453
116 ->123 0.58748
117 ->123 0.24680
120 ->123 -0.12614

Excited State 8: Singlet-A 4.4822 eV
276.61 nm f=0.0399 <S**2>=0.000
114 ->123 0.54967
115 ->123 0.16767
116 ->123 0.21024
118 ->123 0.16392
121 ->125 -0.22487

Excited State 9: Singlet-A 4.6518 eV
266.53 nm f=0.0719 <S**2>=0.000
114 ->123 0.14529
115 ->123 0.27699
120 ->124 0.14477
121 ->125 0.56911

Excited State 10: Singlet-A 4.8149 eV
257.50 nm f=0.0502 <S**2>=0.000
114 ->123 -0.24321
115 ->123 0.55980
120 ->125 0.14470
121 ->125 -0.22208
121 ->127 0.10608

Excited State 11: Singlet-A 4.9397 eV
251.00 nm f=0.3724 <S**2>=0.000
114 ->123 -0.14195
116 ->123 0.13388
117 ->123 -0.13902
120 ->124 -0.11093
120 ->125 -0.11949
121 ->124 0.54090
121 ->127 -0.15785

Excited State 12: Singlet-A 5.0128 eV
247.33 nm f=0.1256 <S**2>=0.000
115 ->123 -0.21820
118 ->125 -0.10795
120 ->124 0.13520
120 ->125 0.37087
121 ->124 0.20718
121 ->126 -0.20013
121 ->127 0.22842
122 ->124 -0.15584

Excited State 13: Singlet-A 5.0312 eV
246.43 nm f=0.0770 <S**2>=0.000
121 ->124 0.15168
122 ->124 0.52917
122 ->125 -0.25317
122 ->130 0.16769
122 ->131 -0.15851

Excited State 14: Singlet-A 5.1259 eV
241.88 nm f=0.0456 <S**2>=0.000
115 ->126 0.11373

118 ->124	-0.24554	
118 ->125	-0.19679	
118 ->126	-0.12726	
118 ->127	0.16690	
120 ->124	-0.19097	
120 ->126	0.14895	
120 ->128	-0.14726	
121 ->126	0.28896	
121 ->127	0.11940	
121 ->128	-0.19793	

Excited State 15:	Singlet-A	5.1901 eV
238.88 nm f=0.0094	<S**2>=0.000	
119 ->130	0.20114	
119 ->131	0.16921	
119 ->133	0.10201	
122 ->124	-0.32051	
122 ->127	-0.13088	
122 ->128	-0.11413	
122 ->130	0.37184	
122 ->131	-0.31259	

Excited State 16:	Singlet-A	5.3693 eV
230.92 nm f=0.1241	<S**2>=0.000	
110 ->123	0.15700	
111 ->123	0.36711	
112 ->123	-0.29788	
118 ->124	0.24596	
120 ->124	0.13306	
121 ->126	0.24477	

Excited State 17:	Singlet-A	5.4066 eV
229.32 nm f=0.0085	<S**2>=0.000	
105 ->123	0.14510	
113 ->123	0.55973	
122 ->123	0.13740	
122 ->124	-0.10337	
122 ->125	-0.28401	
122 ->126	0.11773	

Excited State 18:	Singlet-A	5.4453 eV
227.69 nm f=0.4496	<S**2>=0.000	
111 ->123	-0.13583	
112 ->123	0.13277	
120 ->124	0.33374	
120 ->125	0.23760	
120 ->127	-0.13221	
121 ->126	0.32097	
121 ->127	-0.32059	

Excited State 19:	Singlet-A	5.5076 eV
225.12 nm f=0.0062	<S**2>=0.000	
113 ->123	0.32504	
122 ->124	0.16611	
122 ->125	0.52722	
122 ->127	0.12584	
122 ->131	-0.13407	

Excited State 20:	Singlet-A	5.5284 eV
224.27 nm f=0.0048	<S**2>=0.000	
110 ->123	-0.13850	
111 ->123	-0.16817	
112 ->123	0.18186	
118 ->124	0.25366	
118 ->126	-0.20777	
120 ->126	-0.21864	
121 ->126	0.23408	
121 ->127	0.33066	

Excited State 21:	Singlet-A	5.5978 eV
221.49 nm f=0.1748	<S**2>=0.000	
107 ->123	0.14024	
109 ->123	-0.27830	
110 ->123	0.37512	
111 ->123	-0.16859	
112 ->123	0.23242	
118 ->124	0.12549	
118 ->125	-0.15254	
122 ->130	0.12482	
122 ->131	0.14164	

Excited State 22:	Singlet-A	5.6336 eV
220.08 nm f=0.1403	<S**2>=0.000	
107 ->123	0.11329	
109 ->123	-0.14392	
110 ->123	0.28623	
114 ->124	0.11015	
118 ->124	-0.18846	
118 ->125	0.28643	
119 ->130	0.11102	
120 ->125	0.12314	
121 ->126	0.13029	
122 ->130	-0.15045	
122 ->131	-0.16698	

Excited State 23:	Singlet-A	5.7020 eV
217.44 nm f=0.1220	<S**2>=0.000	
112 ->123	0.12759	
118 ->127	0.10496	
119 ->124	0.10806	
119 ->130	0.13115	
119 ->131	-0.10626	
120 ->124	0.30620	
120 ->125	-0.29921	
120 ->126	0.12293	
121 ->125	-0.11284	
122 ->130	-0.23852	
122 ->131	-0.20689	
122 ->133	-0.12725	

Excited State 24:	Singlet-A	5.7161 eV
216.90 nm f=0.0160	<S**2>=0.000	
112 ->123	-0.15421	
118 ->124	-0.20306	
118 ->125	0.19262	
119 ->124	-0.12554	
119 ->130	-0.11032	
119 ->131	0.10297	
120 ->124	0.27109	
120 ->125	-0.24519	
121 ->127	0.16861	
122 ->130	0.19668	
122 ->131	0.16302	
122 ->133	0.10849	

Excited State 25:	Singlet-A	5.7687 eV
214.93 nm f=0.0227	<S**2>=0.000	
122 ->126	0.56198	
122 ->127	0.24954	
122 ->128	0.22235	
122 ->130	0.12408	

Excited State 26:	Singlet-A	5.8321 eV
212.59 nm f=0.0860	<S**2>=0.000	
118 ->124	0.18658	
118 ->125	0.30980	
118 ->127	0.19297	
119 ->124	-0.20403	
120 ->124	-0.11499	
120 ->125	0.12060	
120 ->126	0.29481	
120 ->127	-0.18551	
121 ->128	-0.16159	

Excited State 27:	Singlet-A	5.8466 eV
212.06 nm f=0.0030	<S**2>=0.000	

118 ->125	0.12111		
119 ->124	0.58665		
119 ->125	-0.21801		
119 ->127	0.10252		
120 ->126	0.10528		
122 ->130	0.10686		
122 ->131	0.10591		

Excited State 28: Singlet-A 5.9914 eV
206.94 nm f=0.0639 <S**2>=0.000

115 ->125	-0.10700
116 ->126	0.15495
117 ->124	0.11865
117 ->125	0.10273
118 ->125	0.21926
118 ->126	-0.20367
118 ->128	0.12113
120 ->125	0.11090
120 ->126	-0.24137
120 ->127	0.34241
121 ->124	0.13592
121 ->127	-0.15406
121 ->128	-0.14507

Excited State 29: Singlet-A 6.0812 eV
203.88 nm f=0.0976 <S**2>=0.000

107 ->123	-0.23186
111 ->123	0.33854
112 ->123	0.31704
117 ->124	0.23343
117 ->125	-0.17643
118 ->124	-0.21219
121 ->128	0.14308

Excited State 30: Singlet-A 6.1003 eV
203.24 nm f=0.0977 <S**2>=0.000

109 ->123	0.10840
111 ->123	-0.20222
112 ->123	-0.14606
114 ->125	-0.10821
116 ->124	-0.13973
117 ->124	0.34122
117 ->125	-0.32094
118 ->126	0.14507
120 ->127	0.10786
121 ->126	0.15640

Ground to excited state transition electric dipole moments (Au):

state	X	Y	Z	Dip. S.	Osc.
1	-0.2536	-0.0167	-0.0143	0.0648	0.0040
2	-1.3245	0.2972	0.0457	1.8448	0.1268
3	-0.0396	-0.0490	-0.0538	0.0069	0.0006
4	0.4794	-0.0114	0.2351	0.2853	0.0243
5	0.0374	-0.2440	0.0700	0.0658	0.0058
6	0.4384	1.0773	0.7397	1.8999	0.1774
7	-0.0391	0.0221	-0.1306	0.0191	0.0020
8	-0.3077	-0.4526	-0.2524	0.3632	0.0399
9	0.7342	-0.1880	0.2386	0.6313	0.0719
10	-0.6321	0.1606	0.0155	0.4256	0.0502
11	-0.6349	-1.4350	-0.7839	3.0768	0.3724
12	-0.4694	-0.8424	-0.3046	1.0228	0.1256
13	-0.3227	-0.7101	-0.1295	0.6251	0.0770
14	-0.1781	-0.4774	-0.3219	0.3632	0.0456
15	-0.0949	-0.1057	0.2321	0.0741	0.0094
16	0.8354	-0.2222	0.4426	0.9432	0.1241
17	-0.1731	-0.0922	-0.1604	0.0642	0.0085
18	-1.1555	-0.9653	1.0504	3.3703	0.4496
19	-0.0960	0.1461	0.1247	0.0461	0.0062
20	0.0766	0.1655	0.0432	0.0351	0.0048
21	-1.0281	0.3307	0.3290	1.2745	0.1748
22	0.5833	-0.6541	-0.4987	1.0167	0.1403
23	0.6146	0.7022	-0.0471	0.8731	0.1220
24	-0.1571	0.2946	-0.0554	0.1145	0.0160
25	-0.3759	0.1346	0.0307	0.1603	0.0227
26	0.7717	-0.0683	-0.0434	0.6021	0.0860
27	-0.1348	-0.0140	0.0509	0.0210	0.0030
28	0.0014	-0.5751	-0.3229	0.4350	0.0639
29	-0.7572	0.2850	-0.0145	0.6548	0.0976
30	-0.7244	0.1765	0.3127	0.6537	0.0977

Ground to excited state transition velocity dipole moments (Au):

state	X	Y	Z	Dip. S.	Osc.
1	0.0228	0.0020	0.0015	0.0005	0.0038
2	0.1423	-0.0303	-0.0055	0.0212	0.1370
3	0.0043	0.0035	0.0056	0.0001	0.0003
4	-0.0633	0.0035	-0.0292	0.0049	0.0254
5	-0.0047	0.0312	-0.0101	0.0011	0.0055
6	-0.0608	-0.1429	-0.0990	0.0339	0.1615
7	0.0009	-0.0050	0.0176	0.0003	0.0014
8	0.0498	0.0751	0.0418	0.0099	0.0399
9	-0.1227	0.0344	-0.0392	0.0178	0.0693
10	0.1106	-0.0278	-0.0026	0.0130	0.0490
11	0.1126	0.2528	0.1368	0.0953	0.3499
12	0.0851	0.1532	0.0562	0.0339	0.1226
13	0.0593	0.1243	0.0283	0.0198	0.0713
14	0.0329	0.0865	0.0564	0.0117	0.0416

15	0.0197	0.0226	-0.0477	0.0032	0.0111
16	-0.1577	0.0422	-0.0867	0.0342	0.1155
17	0.0330	0.0171	0.0313	0.0024	0.0079
18	0.2246	0.1899	-0.2078	0.1297	0.4320
19	0.0190	-0.0284	-0.0255	0.0018	0.0060
20	-0.0154	-0.0334	-0.0095	0.0014	0.0047
21	0.2075	-0.0646	-0.0666	0.0517	0.1675
22	-0.1222	0.1326	0.0984	0.0422	0.1359
23	-0.1250	-0.1446	0.0118	0.0367	0.1167
24	0.0322	-0.0606	0.0096	0.0048	0.0152
25	0.0771	-0.0260	-0.0075	0.0067	0.0210
26	-0.1576	0.0133	0.0098	0.0251	0.0781
27	0.0273	0.0028	-0.0102	0.0009	0.0026
28	-0.0005	0.1275	0.0707	0.0213	0.0644
29	0.1675	-0.0633	0.0032	0.0321	0.0957
30	0.1585	-0.0385	-0.0688	0.0313	0.0932

Ground to excited state transition magnetic dipole moments (Au):

state	X	Y	Z
1	0.1397	0.0270	-0.0223
2	0.1395	0.0714	-0.1916
3	0.0155	-0.1536	0.0446
4	-0.0538	-0.3242	0.3710
5	-0.0117	-0.3716	0.8541
6	-0.0156	0.1459	-0.6166
7	-0.0188	-0.0399	0.0334
8	0.0697	0.0933	0.4525
9	-0.1371	0.0804	-2.5470
10	-0.0184	-0.1234	0.9630
11	-0.0157	-0.1438	-0.4445
12	0.0430	-0.3708	-0.1956
13	-0.0226	-0.1029	-0.1123
14	-0.0112	0.1723	-0.1795
15	-0.0349	0.0410	0.0398
16	0.0994	-0.4332	-0.8657
17	-0.1328	0.1225	0.1836
18	0.2682	-1.1582	-1.1474
19	-0.0188	-0.1243	-0.1168
20	0.2434	0.6692	-0.8431
21	0.0701	-0.0018	0.1414
22	-0.0043	-0.1466	-0.6612
23	0.0011	-0.1585	0.5191
24	0.1952	0.7390	0.6076
25	0.0349	0.0369	-0.3575
26	-0.1080	0.0387	1.4470
27	-0.0264	0.2619	0.6832
28	-0.0767	-0.4272	-1.5319
29	0.1479	0.3598	-0.1394
30	0.1129	-0.3847	-0.6095

Ground to excited state transition velocity quadrupole moments (Au):

state	XX	YY	ZZ	XY	XZ	YZ
1	0.1746	-0.0231	-0.0222	-0.0078	-0.0213	-0.0267
2	-0.2579	-0.0163	0.0495	0.0068	-0.0315	0.1918
3	0.0117	0.0048	0.0014	-0.0173	0.0206	0.0029
4	-0.2331	0.1282	0.0005	-0.1910	0.0783	-0.0409
5	-0.1577	0.0633	0.0465	-0.2952	0.0700	0.0773
6	0.1323	-0.1493	-0.1575	0.0910	0.0339	-0.2045
7	-0.4794	0.0859	0.0263	0.0493	-0.1351	0.2498
8	-0.6162	0.1353	0.1093	-0.0032	0.2427	0.2774
9	0.5655	-0.0706	0.0118	-0.1569	0.1271	-0.3273
10	-0.0527	-0.1962	-0.0498	-0.0283	-0.1402	0.0104
11	-0.4200	0.0868	0.1985	-0.4405	0.1343	0.3116
12	-0.7383	0.0676	0.1385	-0.4784	0.3152	0.2930
13	-0.2484	0.0174	0.1219	0.0470	-0.2067	0.2115
14	0.0378	0.0234	0.1252	-0.0618	0.1143	0.0441
15	0.2529	-0.1197	0.0072	0.3097	-0.4398	-0.0352
16	-0.9011	0.3373	0.1462	-0.6150	0.6212	-0.0549
17	0.2964	-0.0536	0.0145	0.0551	-0.0807	0.0326
18	-0.9145	-0.3488	0.0568	-2.5151	1.3337	-0.2456
19	-0.0340	-0.1257	-0.0178	-0.0416	0.0159	-0.0583
20	2.2919	-0.5395	-0.1927	0.3199	-0.1972	-1.0398
21	1.7586	-0.6825	-0.2182	-0.3453	-0.2478	-0.4801
22	-0.9173	0.2810	0.2115	-0.0795	0.4755	0.0378
23	-1.4002	0.2857	-0.0844	0.4759	0.0936	-0.1333

24	1.1416	0.3003	0.0434	0.7798	-0.4831	-0.0444
25	-0.0624	-0.0589	-0.0795	0.0116	-0.0927	0.0870
26	0.8920	0.2117	0.0948	-0.0514	0.2265	-0.4672
27	1.6411	-0.0423	-0.0159	0.0180	-0.1575	-0.1642
28	0.3703	-0.1984	0.1375	-0.1688	-0.4851	-0.0613
29	-0.7076	0.2478	0.1105	0.6154	-0.2447	0.6005
30	0.3447	-0.4523	0.0313	-0.7103	0.3485	-0.0068

<0|del|b> * <b|rxdel|0> + <0|del|b> * <b|delr+rdel|0>

Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)

state	XX	YY	ZZ	R(velocity)	E-M Angle
1	0.2033	9.7568	14.5391	8.1664	13.94
2	-7.2045	165.3866	-29.6775	42.8349	58.66
3	-1.3159	1.2233	-1.1827	-0.4251	100.08
4	-18.4374	-28.8075	-0.1226	-15.7892	104.34
5	-51.9298	-31.8005	-24.0610	-35.9304	130.75
6	91.0156	210.7185	-93.9238	69.2701	69.36
7	2.1568	-0.1381	1.3942	1.1377	40.46
8	16.2304	78.0417	31.9210	42.0644	50.71
9	215.8913	311.6317	-33.4957	164.6758	69.45
10	-5.8209	-6.9415	8.2868	-1.4919	90.58
11	-372.7215	63.8064	-76.4186	-128.4445	133.28
12	-274.3722	85.4015	-57.2176	-82.0628	145.78
13	21.1516	12.8174	-100.1966	-22.0759	143.07
14	-16.1207	-10.4196	43.1129	5.5242	80.59
15	-10.7355	21.2946	-16.7079	-2.0496	116.07
16	150.4493	26.3966	-29.3903	49.1519	76.78
17	19.5086	1.2917	-8.4249	4.1251	73.88
18	508.7539	-493.1485	262.8372	92.8142	82.39
19	14.0187	0.7877	6.6941	7.1668	32.80
20	-41.7131	40.6371	-61.9140	-20.9967	115.56
21	-3.9838	-201.9621	223.9725	6.0089	81.59
22	-265.4000	-104.7443	83.3141	-95.6100	127.13
23	81.4109	28.7529	-12.5048	32.5530	73.84
24	-102.3002	5.3825	-13.1351	-36.6843	118.90
25	-1.2789	20.3138	-4.2779	4.9190	81.38
26	18.5196	173.8511	-87.5746	34.9320	82.06
27	-9.7958	-19.6699	6.6598	-7.6020	108.90
28	-181.3373	-154.7468	-186.7724	-174.2855	134.53
29	-58.1596	194.4110	-131.4527	1.5996	88.83
30	187.6473	15.5850	32.1245	78.4523	54.70

1/2[<0|r|b>*<b|rxdel|0> + (<0|rxdel|b>*<b|r|0>)*]

Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)

state	XX	YY	ZZ	R(length)
1	25.0429	0.3182	-0.2248	8.3788
2	130.6379	-15.0081	6.1961	40.6086
3	0.4343	-5.3162	1.6972	-1.0616
4	18.2474	-2.6063	-61.6937	-15.3509
5	0.3088	-64.1095	-42.2540	-35.3515
6	4.8243	-111.1740	322.5122	72.0542
7	-0.5189	0.6227	3.0835	1.0625
8	15.1647	29.8501	80.7768	41.9305
9	71.1773	10.6942	429.7927	170.5548
10	-8.2119	14.0137	-10.5575	-1.5852
11	-7.0340	-145.8754	-246.4467	-133.1187
12	14.2686	-220.8909	-42.1391	-82.9205
13	-5.1604	-51.6696	-10.2859	-22.3720
14	-1.4111	58.1865	-40.8625	5.3043
15	-2.3443	3.0668	-6.5387	-1.9387
16	-58.7292	-68.0650	270.9561	48.0540
17	-16.2478	7.9859	20.8217	4.1866
18	219.1846	-790.5839	852.3223	93.6410
19	-1.2785	12.8432	10.3002	7.2883
20	-13.1944	-78.3447	25.7661	-21.9243
21	50.9430	0.4285	-32.8983	6.1577
22	1.7910	-67.7884	-233.1642	-99.7205
23	-0.4630	78.7015	17.3047	31.8478
24	21.6918	-153.9436	23.8110	-36.1469
25	9.2645	-3.5122	7.7544	4.5022
26	58.9182	1.8680	44.4176	35.0679
27	-2.5195	2.6009	-24.5941	-8.1709
28	0.0755	-173.7230	-349.8360	-174.4945
29	79.1785	-72.5137	-1.4298	1.7450
30	57.8386	48.0298	134.7780	80.2155

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)

state	X	Y	Z	Dip. S.	Osc.(frdel)
1	-0.0058	-0.0000	-0.0000	0.0058	0.0039
2	-0.1885	-0.0090	-0.0003	0.1977	0.1318
3	-0.0002	-0.0002	-0.0003	0.0006	0.0004
4	-0.0303	-0.0000	-0.0069	0.0372	0.0248
5	-0.0002	-0.0076	-0.0007	0.0085	0.0057
6	-0.0267	-0.1539	-0.0733	0.2539	0.1692
7	-0.0000	-0.0001	-0.0023	0.0024	0.0016
8	-0.0153	-0.0340	-0.0106	0.0599	0.0399
9	-0.0901	-0.0065	-0.0094	0.1059	0.0706
10	-0.0699	-0.0045	-0.0000	0.0744	0.0496
11	-0.0715	-0.3627	-0.1072	0.5414	0.3610
12	-0.0400	-0.1291	-0.0171	0.1861	0.1241
13	-0.0191	-0.0883	-0.0037	0.1111	0.0741
14	-0.0059	-0.0413	-0.0181	0.0653	0.0435
15	-0.0019	-0.0024	-0.0111	0.0153	0.0102
16	-0.1318	-0.0094	-0.0384	0.1795	0.1197
17	-0.0057	-0.0016	-0.0050	0.0123	0.0082
18	-0.2596	-0.1833	-0.2183	0.6611	0.4407
19	-0.0018	-0.0042	-0.0032	0.0092	0.0061
20	-0.0012	-0.0055	-0.0004	0.0071	0.0047
21	-0.2133	-0.0214	-0.0219	0.2566	0.1711
22	-0.0712	-0.0868	-0.0491	0.2071	0.1381
23	-0.0768	-0.1016	-0.0006	0.1790	0.1193
24	-0.0051	-0.0179	-0.0005	0.0234	0.0156
25	-0.0290	-0.0035	-0.0002	0.0327	0.0218
26	-0.1216	-0.0009	-0.0004	0.1229	0.0820
27	-0.0037	-0.0000	-0.0005	0.0042	0.0028
28	-0.0000	-0.0733	-0.0228	0.0962	0.0641
29	-0.1268	-0.0181	-0.0000	0.1449	0.0966
30	-0.1148	-0.0068	-0.0215	0.1431	0.0954

P-**1c**$^{+}$; HOMO : 114, LUMO : 115

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.7245 eV
455.07 nm f=0.2793 <S**2>=0.000
112 ->115 (LUMO) -0.11905
114 (HOMO) ->115 0.67974
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1361.64054855
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.0671 eV
404.23 nm f=0.0694 <S**2>=0.000
112 ->115 0.16730
113 ->115 0.66270

Excited State 3: Singlet-A 3.5084 eV
353.40 nm f=0.0063 <S**2>=0.000
111 ->115 -0.37398
112 ->115 0.53236
113 ->115 -0.18183
114 ->115 0.12063

Excited State 4: Singlet-A 3.6047 eV
343.96 nm f=0.0057 <S**2>=0.000
106 ->115 -0.15504
109 ->115 0.22303
111 ->115 0.51971
112 ->115 0.34952

Excited State 5: Singlet-A 3.7998 eV
326.29 nm f=0.1403 <S**2>=0.000
108 ->115 -0.23596
109 ->115 0.37504
110 ->115 0.43802
111 ->115 -0.16580
112 ->115 -0.13437
114 ->116 0.18495

Excited State 6: Singlet-A 4.0413 eV
306.79 nm f=0.0159 <S**2>=0.000
108 ->115 0.15803
109 ->115 -0.39592
110 ->115 0.52915

Excited State 7: Singlet-A 4.3551 eV
284.69 nm f=0.0014 <S**2>=0.000
106 ->115 0.16211
108 ->115 0.55132
109 ->115 0.31541
112 ->115 -0.12928
114 ->116 -0.11038

Excited State 8: Singlet-A 4.5052 eV
275.20 nm f=0.0617 <S**2>=0.000
106 ->115 0.53922
107 ->115 -0.16402
108 ->115 -0.20704
111 ->115 0.14651
113 ->117 -0.15812
114 ->117 0.19455

Excited State 9: Singlet-A 4.6398 eV
267.22 nm f=0.0630 <S**2>=0.000
106 ->115 -0.19574
107 ->115 0.25064

111 ->115 -0.10637
112 ->116 0.11457
113 ->117 -0.31825
114 ->117 0.47962

Excited State 10: Singlet-A 4.8305 eV
256.67 nm f=0.0211 <S**2>=0.000
106 ->115 0.22956
107 ->115 0.56386
112 ->117 0.16827
114 ->117 -0.18432

Excited State 11: Singlet-A 4.8911 eV
253.49 nm f=0.4975 <S**2>=0.000
106 ->115 0.15978
108 ->115 0.18198
109 ->115 -0.14847
113 ->116 -0.21999
114 ->116 0.53992

Excited State 12: Singlet-A 5.0065 eV
247.65 nm f=0.0765 <S**2>=0.000
107 ->115 -0.24909
111 ->117 0.11014
112 ->116 0.10839
112 ->117 0.39492
113 ->118 0.10537
113 ->119 -0.17256
114 ->116 0.12657
114 ->118 -0.16390
114 ->119 0.20943

Excited State 13: Singlet-A 5.0982 eV
243.19 nm f=0.0107 <S**2>=0.000
111 ->116 0.19009
111 ->117 0.19553
111 ->118 0.11859
111 ->119 -0.16146
112 ->116 -0.15281
113 ->118 -0.10023
113 ->120 0.22804
114 ->117 0.15969
114 ->118 0.28852
114 ->119 0.11891
114 ->121 0.12089

Excited State 14: Singlet-A 5.1265 eV
241.85 nm f=0.0282 <S**2>=0.000
110 ->121 -0.14405
112 ->120 0.10570
113 ->116 -0.26244
113 ->117 0.19994
113 ->118 0.13172
113 ->120 0.20373
113 ->121 0.13655
113 ->123 -0.14157
114 ->116 -0.13293
114 ->119 0.14896
114 ->120 0.30054

Excited State 15: Singlet-A 5.3535 eV
231.60 nm f=0.0943 <S**2>=0.000
103 ->115 -0.10227
105 ->115 0.13941
111 ->116 0.19979
111 ->118 -0.10499
112 ->117 -0.11117
113 ->116 0.39640
113 ->118 0.17216
113 ->121 0.11216
114 ->116 0.11556
114 ->118 -0.19719
114 ->120 0.16825

Excited State 16: Singlet-A 5.3605 eV
231.29 nm f=0.1750 <S**2>=0.000
111 ->117 -0.14468
112 ->116 0.19944
112 ->117 0.12654
113 ->117 -0.25532
113 ->119 0.15170
114 ->117 -0.18288
114 ->118 0.40515

Excited State 17: Singlet-A 5.4523 eV
227.40 nm f=0.2843 <S**2>=0.000
111 ->116 -0.15931
111 ->118 0.14867
112 ->116 -0.17572
112 ->117 -0.19071
112 ->118 -0.19804
113 ->116 0.10733
113 ->118 0.14183
113 ->119 -0.20992
114 ->118 0.13831
114 ->119 0.35513
114 ->121 -0.11984

Excited State 18: Singlet-A 5.5535 eV
223.25 nm f=0.0300 <S**2>=0.000
100 ->115 0.10161
102 ->115 -0.11947
103 ->115 -0.20370
105 ->115 0.36481
106 ->116 -0.12120
111 ->116 0.24007
111 ->117 -0.14034
113 ->116 -0.28128
114 ->116 -0.12644

Excited State 19: Singlet-A 5.5972 eV
221.51 nm f=0.2538 <S**2>=0.000
103 ->115 -0.10329
105 ->115 0.25028
111 ->116 -0.19465
112 ->116 0.18728
112 ->118 -0.12627
113 ->116 0.20137
113 ->117 0.14797
113 ->118 -0.18764
113 ->119 0.12676
113 ->121 0.16137
114 ->116 0.10404
114 ->117 0.12284
114 ->118 0.10889
114 ->121 0.18528
114 ->122 -0.11395
114 ->123 0.12718

Excited State 20: Singlet-A 5.6796 eV
218.30 nm f=0.1107 <S**2>=0.000
109 ->116 0.11996
111 ->119 -0.12126
112 ->116 0.42815
112 ->117 -0.34646
112 ->118 0.11597
113 ->119 -0.13452
114 ->116 0.10208
114 ->117 -0.11064
114 ->119 0.16808

Excited State 21: Singlet-A 5.7344 eV
216.21 nm f=0.0598 <S**2>=0.000
100 ->115 0.13130
111 ->116 0.11737
111 ->117 0.30110

111 ->119	0.10757	
112 ->116	0.21376	
112 ->119	0.12923	
113 ->117	0.25324	
113 ->118	0.12623	
113 ->120	-0.10863	
114 ->117	0.15614	
114 ->121	-0.25752	
Excited State 22:	Singlet-A	5.7719 eV
214.80 nm f=0.0408	<S**2>=0.000	
96 ->115	0.16050	
99 ->115	0.11985	
100 ->115	-0.29971	
102 ->115	0.25189	
105 ->115	-0.13692	
111 ->116	0.30970	
113 ->117	0.10003	
113 ->121	0.11313	
Excited State 23:	Singlet-A	5.7831 eV
214.39 nm f=0.0028	<S**2>=0.000	
100 ->115	0.36770	
102 ->115	-0.16662	
105 ->115	-0.36447	
110 ->120	0.10950	
111 ->116	0.11122	
111 ->117	-0.11265	
113 ->121	0.12446	
114 ->121	0.14078	
Excited State 24:	Singlet-A	5.9025 eV
210.05 nm f=0.0641	<S**2>=0.000	
111 ->118	0.15306	
112 ->118	-0.28197	
112 ->119	0.35664	
113 ->116	-0.15319	
113 ->117	-0.16975	
113 ->118	0.10064	
113 ->121	0.15854	
114 ->119	-0.17857	
114 ->121	0.13598	
Excited State 25:	Singlet-A	5.9898 eV
206.99 nm f=0.0172	<S**2>=0.000	
95 ->115	-0.26208	
99 ->115	0.16280	
103 ->115	0.37819	
104 ->115	0.34729	
105 ->115	0.17411	
Excited State 26:	Singlet-A	6.0567 eV
204.70 nm f=0.1987	<S**2>=0.000	
108 ->116	-0.17112	
109 ->116	0.31484	
109 ->117	-0.26040	
110 ->116	0.24208	
110 ->117	-0.15797	
111 ->116	0.12540	
111 ->117	-0.18057	
112 ->117	0.12744	
112 ->118	-0.11697	
Excited State 27:	Singlet-A	6.0871 eV
203.68 nm f=0.0184	<S**2>=0.000	
107 ->116	-0.11137	
107 ->117	-0.12649	
109 ->116	-0.21672	
110 ->116	-0.10974	
111 ->117	-0.17064	
111 ->118	0.25108	
111 ->119	-0.17411	
113 ->117	0.19932	
113 ->118	0.19822	
114 ->118	-0.11901	
114 ->119	-0.16228	
114 ->120	-0.11071	
114 ->123	-0.10189	
Excited State 28:	Singlet-A	6.1380 eV
202.00 nm f=0.2464	<S**2>=0.000	
102 ->115	-0.11999	
106 ->116	0.12327	
109 ->117	-0.13005	
111 ->116	0.13616	
111 ->118	0.17057	
111 ->119	-0.13196	
111 ->120	0.10116	
112 ->117	-0.10950	
112 ->119	-0.13466	
113 ->121	0.15375	
114 ->120	0.27187	
114 ->121	-0.11693	
114 ->123	0.23683	
114 ->125	0.12323	
Excited State 29:	Singlet-A	6.1880 eV
200.36 nm f=0.2069	<S**2>=0.000	
108 ->116	-0.11700	
109 ->116	0.10541	
111 ->117	0.32713	
112 ->119	-0.22021	
113 ->117	-0.10457	
113 ->118	0.20373	
113 ->119	0.14210	
114 ->117	-0.10123	
114 ->122	-0.26322	
Excited State 30:	Singlet-A	6.1930 eV
200.20 nm f=0.0020	<S**2>=0.000	
108 ->116	-0.14549	
108 ->117	-0.11879	
112 ->119	-0.14269	
112 ->122	-0.10288	
113 ->118	0.11541	
114 ->121	0.20388	
114 ->122	0.38792	
114 ->123	0.13644	
114 ->125	0.10105	

Ground to excited state transition electric dipole moments (Au):

state	X	Y	Z	Dip. S.	Osc.
1	2.0227	0.3020	-0.0467	4.1845	0.2793
2	0.9593	-0.0007	0.0519	0.9230	0.0694
3	-0.1482	0.0753	-0.2137	0.0733	0.0063
4	-0.0518	0.2200	0.1138	0.0640	0.0057
5	-0.2970	1.0637	-0.5357	1.5067	0.1403
6	-0.0851	-0.2488	0.3024	0.1606	0.0159
7	0.0619	0.0663	0.0709	0.0133	0.0014
8	-0.4487	0.5270	-0.2831	0.5592	0.0617
9	-0.7036	-0.0197	-0.2432	0.5546	0.0630

10	0.3627	0.1951	-0.0912	0.1779	0.0211
11	0.7403	-1.7589	0.7143	4.1520	0.4975
12	0.3685	-0.6921	0.0949	0.6239	0.0765
13	0.0623	-0.0957	0.2700	0.0859	0.0107
14	0.0571	0.4657	0.0636	0.2242	0.0282
15	-0.0000	0.3905	0.7527	0.7191	0.0943
16	-0.5049	-0.9595	-0.3965	1.3327	0.1750
17	-1.1425	0.5133	0.7482	2.1285	0.2843
18	0.3538	-0.2567	0.1720	0.2207	0.0300
19	1.1596	0.2216	-0.6761	1.8509	0.2538
20	-0.3946	0.7880	0.1380	0.7957	0.1107
21	0.3839	0.4594	-0.2588	0.4253	0.0598
22	0.4939	-0.0035	0.2115	0.2887	0.0408
23	-0.0553	0.0113	0.1289	0.0198	0.0028
24	0.4714	-0.3362	0.3288	0.4433	0.0641
25	-0.3128	-0.1291	0.0508	0.1171	0.0172
26	1.1007	0.0505	-0.3538	1.3392	0.1987
27	-0.0970	-0.3373	-0.0189	0.1235	0.0184
28	1.0306	0.7497	0.1183	1.6383	0.2464
29	1.0540	-0.1169	-0.4901	1.3648	0.2069
30	0.0553	0.0782	-0.0616	0.0130	0.0020

Ground to excited state transition velocity dipole moments (Au):

state	X	Y	Z	Dip. S.	Osc.
1	-0.2050	-0.0302	0.0056	0.0430	0.2861
2	-0.0995	0.0001	-0.0065	0.0100	0.0589
3	0.0237	-0.0082	0.0271	0.0014	0.0071
4	0.0058	-0.0276	-0.0163	0.0011	0.0053
5	0.0420	-0.1428	0.0721	0.0273	0.1306
6	0.0125	0.0303	-0.0424	0.0029	0.0129
7	-0.0043	-0.0121	-0.0086	0.0002	0.0010
8	0.0728	-0.0870	0.0470	0.0151	0.0607
9	0.1173	0.0060	0.0401	0.0154	0.0602
10	-0.0645	-0.0332	0.0156	0.0055	0.0207
11	-0.1304	0.3060	-0.1253	0.1263	0.4686
12	-0.0668	0.1260	-0.0202	0.0207	0.0752
13	-0.0120	0.0136	-0.0475	0.0026	0.0092
14	-0.0125	-0.0902	-0.0135	0.0085	0.0300
15	0.0021	-0.0781	-0.1492	0.0284	0.0961
16	0.0999	0.1836	0.0776	0.0497	0.1682
17	0.2244	-0.1012	-0.1464	0.0820	0.2729
18	-0.0676	0.0531	-0.0317	0.0084	0.0274
19	-0.2334	-0.0461	0.1361	0.0751	0.2435
20	0.0785	-0.1619	-0.0299	0.0333	0.1063
21	-0.0761	-0.0947	0.0535	0.0176	0.0557
22	-0.1005	0.0000	-0.0406	0.0118	0.0369
23	0.0100	-0.0041	-0.0277	0.0009	0.0028
24	-0.0989	0.0744	-0.0703	0.0202	0.0622
25	0.0667	0.0300	-0.0116	0.0055	0.0166
26	-0.2403	-0.0112	0.0779	0.0639	0.1915
27	0.0205	0.0726	0.0046	0.0057	0.0170
28	-0.2287	-0.1671	-0.0259	0.0809	0.2392
29	-0.2369	0.0257	0.1085	0.0686	0.2010
30	-0.0106	-0.0195	0.0150	0.0007	0.0021

Ground to excited state transition magnetic dipole moments (Au):

state	X	Y	Z
1	-0.1864	0.0234	0.2875
2	-0.0110	0.0321	0.1257
3	0.0413	-0.2278	-0.2754
4	0.0415	0.2994	0.8822
5	0.0720	0.0747	0.7887
6	0.0182	-0.2690	0.0294
7	0.0345	-0.0306	-0.0232
8	0.1065	-0.0653	0.6390
9	0.2047	-0.1766	2.4672
10	0.0175	-0.0180	-0.8124
11	-0.0150	-0.3004	0.4972
12	-0.0474	-0.2971	0.0979
13	-0.0102	0.1113	0.3044
14	-0.0741	-0.3230	0.1382
15	0.1818	0.5285	-0.4840
16	-0.0890	-0.5005	1.3290
17	0.0709	1.1498	0.3298
18	-0.0785	0.1674	-0.1429

19	-0.2632	-0.3262	1.2758
20	-0.1014	0.6094	-0.5747
21	-0.0609	-0.0739	0.2908
22	-0.0922	0.0782	0.2899
23	-0.0439	0.0290	0.1140
24	0.1139	-0.4425	1.8695
25	-0.0956	-0.1438	0.3384
26	-0.2919	-0.4968	0.7858
27	-0.1877	-0.4007	-0.0147
28	-0.1465	0.5964	0.1693
29	-0.4597	-0.3946	0.3062
30	-0.1490	-0.0568	-0.3890

Ground to excited state transition velocity quadrupole moments (Au):

state	XX	YY	ZZ	XY	XZ	YZ
1	0.6483	-0.1361	-0.0795	0.0969	-0.0679	-0.1087
2	1.5562	-0.3354	-0.1060	0.1583	-0.0662	0.2496
3	0.1666	0.0030	-0.0025	0.2130	0.0556	0.1143
4	-0.0106	-0.0340	-0.0249	-0.3048	-0.0840	0.0553
5	0.1567	-0.2093	-0.0906	-0.0312	-0.0137	0.1836
6	-0.2453	0.1090	0.0358	-0.0002	0.0079	-0.0810
7	-0.3688	0.1048	-0.0273	-0.0033	-0.1309	-0.1882
8	0.4703	-0.1794	-0.0289	0.0062	-0.2714	0.2787
9	0.5395	-0.1410	0.0872	0.1473	0.1519	0.3099
10	-0.1295	-0.1527	-0.0661	-0.0224	-0.1445	-0.0184
11	-0.3578	0.2193	0.0943	0.3140	0.2399	-0.4195
12	-0.4042	0.0878	0.0411	0.1742	0.1952	-0.2529
13	0.0546	0.0444	0.0655	0.1524	0.2202	-0.0034
14	-0.0074	-0.0064	-0.0629	0.7424	0.4141	0.0340
15	0.1568	0.2559	-0.0868	-0.7883	-0.5879	-0.2734
16	-1.5639	0.0653	0.2308	0.9350	1.0722	0.0978
17	0.9466	0.0507	0.0845	-1.8081	-1.0260	0.4977
18	0.2392	-0.2941	-0.0559	-0.1096	-0.0942	0.2402
19	2.4228	-0.9007	-0.1876	1.1690	0.5920	0.5588
20	0.4517	0.2044	0.0337	-0.7904	-0.4708	0.4213
21	-2.4811	0.3017	-0.1645	-0.3213	-0.1610	-0.6179
22	0.4007	0.4110	0.0490	-0.0486	0.0100	-0.3754
23	0.9356	0.4852	0.1552	0.1985	0.1543	-0.3034
24	0.8795	-0.4474	-0.0467	0.1307	-0.5665	-0.0263
25	-0.9797	0.2125	0.1179	-0.2304	-0.0474	-0.0929
26	-0.6070	-0.0217	0.0750	0.4043	0.1647	-0.3746
27	-1.2812	0.5652	0.1743	0.1958	0.1661	0.0391
28	-0.4949	0.0367	-0.3247	-0.7135	-0.4557	-0.1511
29	-1.1058	-0.2011	-0.0965	0.7919	0.8133	-0.0049
30	-0.7638	0.3877	0.0086	0.2354	0.0814	0.0651

<0|del|b> * <b|rxdel|0> + <0|del|b> * <b|delr+rdel|0>

Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)

state	XX	YY	ZZ	R(velocity)	E-M Angle
1	-2.1266	217.4170	61.0397	92.1100	56.67
2	-5.7995	-73.8488	81.3522	0.5680	88.80
3	1.7597	-26.2181	-0.8488	-8.4357	110.32
4	-53.3391	-50.0531	-16.0907	-39.8276	137.45
5	106.3580	176.8813	-33.9191	83.1067	68.02
6	-22.9025	-4.8459	-15.8656	-14.5380	129.10
7	-2.1686	1.8279	2.1958	0.6183	58.11
8	26.5119	123.4447	35.7849	61.9138	57.05
9	213.0607	317.8714	-25.8999	168.3440	66.72
10	-34.3538	-24.4686	6.1438	-17.5595	102.66
11	-525.1170	66.3016	-140.1875	-199.6677	137.49
12	-129.7474	41.5350	-51.0729	-46.4284	142.67
13	-43.7470	-13.3243	8.6527	-16.1395	141.06
14	102.5445	16.2055	-12.8925	35.2858	31.44
15	184.3992	-81.9212	10.0207	37.4996	75.44
16	-202.8054	56.4576	154.8750	2.8424	89.57
17	-6.4910	-327.2456	-191.0853	-174.9406	115.68
18	37.9280	-17.1155	44.0605	21.6243	29.02
19	644.4907	-93.6227	308.7740	286.5474	47.21
20	-227.1168	31.6095	-107.5216	-101.0097	125.53
21	-16.5664	141.6545	-33.8153	30.4243	47.98
22	-16.3315	55.4397	-47.4388	-2.7769	94.21
23	-13.5348	-1.8943	3.0763	-4.1176	174.45
24	-214.0921	-213.2904	-144.8951	-190.7592	129.87
25	-6.6545	-30.8154	-9.4953	-15.6551	121.31
26	159.0726	301.6589	-25.6266	145.0350	56.24

27	-63.6969	-6.3464	-34.2507	-34.7647	170.54
28	-253.5158	70.8763	-38.5331	-73.7242	112.91
29	136.9843	89.2128	184.2649	136.8206	42.05
30	0.6034	-13.1737	2.7969	-3.2578	106.21

1/2[<0|r|b>*<b|rxdel|0> + (<0|rxdel|b>*<b|r|0>)*]

Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)

state	XX	YY	ZZ	R(length)
1	266.6563	-4.9945	9.4875	90.3831
2	7.4327	0.0169	-4.6178	0.9439
3	4.3304	12.1218	-41.6197	-8.3892
4	1.5182	-46.5766	-70.9727	-38.6770
5	15.1131	-56.2105	298.8197	85.9075
6	1.0977	-47.3332	-6.2781	-17.5045
7	-1.5117	1.4331	1.1651	0.3622
8	33.8027	24.3233	127.9301	62.0187
9	101.8548	-2.4651	424.2889	174.5595
10	-4.4897	2.4772	-52.4048	-18.1391
11	7.8555	-373.6617	-251.1285	-205.6449
12	12.3478	-145.4314	-6.5716	-46.5517
13	0.4477	7.5353	-58.1237	-16.7136
14	2.9908	106.3634	-6.2148	34.3798
15	0.0013	-145.9467	257.6423	37.2323
16	-31.7956	-339.5733	372.6213	0.4175
17	57.3011	-417.3870	-174.4923	-178.1927
18	19.6343	30.3935	17.3833	22.4704
19	215.8602	51.1051	609.9505	292.3053
20	-28.2954	-339.6109	56.0654	-103.9470
21	16.5280	24.0089	53.2166	31.2512
22	32.2172	0.1950	-43.3723	-3.6534
23	-1.7156	-0.2310	-10.3937	-4.1134
24	-37.9668	-105.1978	-434.6793	-192.6146
25	-21.1467	-13.1302	-12.1685	-15.4818
26	227.2378	17.7361	196.5793	147.1844
27	-12.8803	-95.5785	-0.1960	-36.2183
28	106.7585	-316.2234	-14.1571	-74.5407
29	342.6626	-32.6345	106.1197	138.7160
30	5.8243	3.1428	-16.9596	-2.6642

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)

state	X	Y	Z	Dip. S.	Osc.(frdel)
1	-0.4147	-0.0091	-0.0003	0.4241	0.2827
2	-0.0955	-0.0000	-0.0003	0.0958	0.0639
3	-0.0035	-0.0006	-0.0058	0.0099	0.0066
4	-0.0003	-0.0061	-0.0019	0.0082	0.0055
5	-0.0125	-0.1519	-0.0386	0.2030	0.1353
6	-0.0011	-0.0075	-0.0128	0.0214	0.0143
7	-0.0003	-0.0008	-0.0006	0.0017	0.0011
8	-0.0327	-0.0458	-0.0133	0.0918	0.0612
9	-0.0825	-0.0001	-0.0097	0.0924	0.0616
10	-0.0234	-0.0065	-0.0014	0.0313	0.0209
11	-0.0965	-0.5382	-0.0895	0.7242	0.4828
12	-0.0246	-0.0872	-0.0019	0.1137	0.0758
13	-0.0008	-0.0013	-0.0128	0.0149	0.0099
14	-0.0007	-0.0420	-0.0009	0.0436	0.0291
15	-0.0000	-0.0305	-0.1123	0.1428	0.0952
16	-0.0504	-0.1761	-0.0308	0.2573	0.1715
17	-0.2564	-0.0519	-0.1096	0.4178	0.2786
18	-0.0239	-0.0136	-0.0054	0.0430	0.0287
19	-0.2707	-0.0102	-0.0920	0.3729	0.2486
20	-0.0310	-0.1276	-0.0041	0.1627	0.1085
21	-0.0292	-0.0435	-0.0139	0.0866	0.0577
22	-0.0496	-0.0000	-0.0086	0.0582	0.0388
23	-0.0006	-0.0000	-0.0036	0.0042	0.0028
24	-0.0466	-0.0250	-0.0231	0.0947	0.0631
25	-0.0209	-0.0039	-0.0006	0.0253	0.0169
26	-0.2645	-0.0006	-0.0276	0.2926	0.1951
27	-0.0020	-0.0245	-0.0001	0.0265	0.0177
28	-0.2358	-0.1253	-0.0031	0.3641	0.2427
29	-0.2497	-0.0030	-0.0532	0.3059	0.2039
30	-0.0006	-0.0015	-0.0009	0.0030	0.0020

P-**1d**$^{+}$; HOMO : 86, LUMO : 87

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.7403 eV
452.45 nm f=0.0803 <S**2>=0.000
85 -> 87 (LUMO) -0.17841
86 (HOMO) -> 87 0.66476
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1016.21623777
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.3635 eV
368.61 nm f=0.0147 <S**2>=0.000
84 -> 87 -0.27699
85 -> 87 0.59511
86 -> 87 0.21208

Excited State 3: Singlet-A 3.4912 eV
355.13 nm f=0.0076 <S**2>=0.000
80 -> 87 0.16491
83 -> 87 0.17459
84 -> 87 0.59275
85 -> 87 0.27140

Excited State 4: Singlet-A 3.7924 eV
326.93 nm f=0.2034 <S**2>=0.000
82 -> 87 -0.25402
83 -> 87 0.57661
84 -> 87 -0.14788
85 -> 87 -0.10854
86 -> 88 0.18292

Excited State 5: Singlet-A 4.2296 eV
293.14 nm f=0.0054 <S**2>=0.000
80 -> 87 -0.13736
82 -> 87 0.58059
83 -> 87 0.28343
85 -> 87 -0.12817

Excited State 6: Singlet-A 4.4280 eV
280.00 nm f=0.0467 <S**2>=0.000
80 -> 87 0.57209
81 -> 87 -0.21678
82 -> 87 0.18143
84 -> 87 -0.14192
86 -> 89 0.17664

Excited State 7: Singlet-A 4.5882 eV
270.23 nm f=0.0426 <S**2>=0.000
81 -> 87 0.44750
85 -> 88 -0.13882
86 -> 89 0.49232

Excited State 8: Singlet-A 4.7195 eV
262.71 nm f=0.0547 <S**2>=0.000
80 -> 87 0.30246
81 -> 87 0.45628
86 -> 89 -0.39844

Excited State 9: Singlet-A 4.9342 eV
251.28 nm f=0.3596 <S**2>=0.000
82 -> 87 0.14452
83 -> 87 -0.12332
85 -> 88 -0.11148
85 -> 89 0.19957
86 -> 88 0.53321
86 -> 91 -0.19799

Excited State 10: Singlet-A 4.9848 eV
248.73 nm f=0.2361 <S**2>=0.000
81 -> 87 -0.14729
84 -> 89 0.10077
85 -> 89 0.42913
86 -> 88 -0.29066
86 -> 90 0.14262
86 -> 91 -0.23859
86 -> 94 0.11756

Excited State 11: Singlet-A 5.1379 eV
241.31 nm f=0.0602 <S**2>=0.000
81 -> 90 -0.10961
84 -> 88 0.21787
84 -> 89 -0.21681
84 -> 91 -0.20028
85 -> 88 -0.20363
85 -> 90 0.14182
85 -> 92 -0.14860
86 -> 89 -0.11094
86 -> 90 0.30223
86 -> 92 -0.22839

Excited State 12: Singlet-A 5.4196 eV
228.77 nm f=0.2130 <S**2>=0.000
79 -> 87 -0.17231
84 -> 88 -0.26603
84 -> 90 0.10621
85 -> 88 0.28036
85 -> 89 -0.18775
85 -> 91 -0.10011
86 -> 90 0.37375
86 -> 91 -0.24050

Excited State 13: Singlet-A 5.4724 eV
226.56 nm f=0.2352 <S**2>=0.000
79 -> 87 -0.17575
80 -> 88 -0.13276
83 -> 89 0.13927
84 -> 88 -0.35002
84 -> 90 0.13770
85 -> 88 -0.18099
85 -> 89 0.17044
85 -> 90 -0.15633
86 -> 91 0.37100

Excited State 14: Singlet-A 5.5981 eV
221.47 nm f=0.0301 <S**2>=0.000
79 -> 87 0.22076
83 -> 88 -0.12524
84 -> 88 0.10523
84 -> 89 0.28835
84 -> 90 0.23395
85 -> 88 0.10520
85 -> 90 -0.18402
85 -> 91 -0.11115
86 -> 90 0.29055
86 -> 91 0.21579

Excited State 15: Singlet-A 5.6213 eV
220.56 nm f=0.1591 <S**2>=0.000
83 -> 88 0.12816
84 -> 91 -0.11513
85 -> 88 0.45529
85 -> 89 0.34492
85 -> 90 0.11172
86 -> 88 0.15311
86 -> 89 0.12459
86 -> 91 0.16845

Excited State 16:	Singlet-A	5.7903 eV
214.12 nm f=0.0419	<S**2>=0.000	
70 -> 87	-0.11627	
72 -> 87	0.14121	
73 -> 87	0.15547	
76 -> 87	0.27075	
78 -> 87	-0.25846	
79 -> 87	0.31364	
84 -> 88	-0.25552	
84 -> 89	-0.25872	
85 -> 91	0.10589	

Excited State 17:	Singlet-A	5.8318 eV
212.60 nm f=0.0630	<S**2>=0.000	
84 -> 88	-0.17083	
84 -> 89	0.32950	
84 -> 90	-0.11317	
84 -> 91	-0.17143	
85 -> 90	0.29295	
85 -> 91	-0.27917	
86 -> 92	-0.17579	

Excited State 18:	Singlet-A	5.9428 eV
208.63 nm f=0.0063	<S**2>=0.000	
72 -> 87	-0.16482	
74 -> 87	-0.10351	
76 -> 87	-0.41213	
78 -> 87	0.13764	
79 -> 87	0.43041	
83 -> 88	-0.10849	
84 -> 88	-0.14423	

Excited State 19:	Singlet-A	5.9999 eV
206.64 nm f=0.0652	<S**2>=0.000	
81 -> 89	-0.10960	
82 -> 90	0.14457	
83 -> 89	-0.10948	
84 -> 89	0.26318	
84 -> 90	0.16037	
84 -> 91	-0.13425	
84 -> 92	-0.14110	
85 -> 89	-0.14956	
85 -> 90	-0.12399	
85 -> 91	0.37723	
86 -> 88	0.13492	
86 -> 90	-0.14352	
86 -> 91	-0.10846	
86 -> 92	-0.14236	

Excited State 20:	Singlet-A	6.0835 eV
203.81 nm f=0.0930	<S**2>=0.000	
79 -> 87	0.10909	
82 -> 88	-0.15634	
83 -> 88	0.40538	
83 -> 89	0.33110	
84 -> 88	0.10903	
84 -> 90	-0.12147	
85 -> 91	0.14265	
86 -> 90	0.18079	

Excited State 21:	Singlet-A	6.1245 eV
202.44 nm f=0.2332	<S**2>=0.000	
77 -> 87	0.10524	
78 -> 87	-0.12277	
81 -> 89	-0.12439	
82 -> 88	-0.10770	
83 -> 89	0.27669	
84 -> 88	0.16795	
84 -> 90	0.26360	
84 -> 91	-0.17939	
85 -> 90	-0.15513	
85 -> 91	-0.18172	
86 -> 90	-0.16492	
86 -> 91	-0.18976	
86 -> 92	0.13918	

Excited State 22:	Singlet-A	6.1786 eV
200.67 nm f=0.0815	<S**2>=0.000	
70 -> 87	-0.11795	
72 -> 87	-0.18686	
73 -> 87	0.18743	
76 -> 87	-0.10677	
77 -> 87	0.27272	
78 -> 87	-0.16036	
80 -> 88	-0.14536	
82 -> 88	0.17435	
83 -> 90	-0.14344	
84 -> 89	0.14675	
84 -> 92	0.13063	
85 -> 90	0.10294	
85 -> 91	0.15479	
85 -> 92	-0.14029	
86 -> 91	0.10541	
86 -> 92	0.17015	

Excited State 23:	Singlet-A	6.1982 eV
200.03 nm f=0.0175	<S**2>=0.000	
69 -> 87	0.10849	
71 -> 87	-0.11105	
72 -> 87	-0.31547	
73 -> 87	0.36448	
74 -> 87	0.19235	
76 -> 87	0.16276	
78 -> 87	0.31721	
84 -> 90	0.10034	

Excited State 24:	Singlet-A	6.2735 eV
197.63 nm f=0.0714	<S**2>=0.000	
71 -> 87	0.10742	
72 -> 87	-0.14666	
77 -> 87	0.23842	
78 -> 87	-0.14728	
82 -> 89	0.12880	
83 -> 88	0.20377	
83 -> 89	-0.21343	
84 -> 89	-0.10742	
84 -> 90	-0.13228	
85 -> 90	-0.22171	
85 -> 91	-0.13202	
85 -> 92	0.20338	
86 -> 92	-0.18797	

Excited State 25:	Singlet-A	6.2887 eV
197.15 nm f=0.0519	<S**2>=0.000	
82 -> 89	-0.29418	
84 -> 92	-0.10646	
85 -> 88	0.16063	
85 -> 89	-0.10909	
86 -> 91	0.11175	
86 -> 93	-0.21863	
86 -> 94	0.34458	
86 -> 95	0.11588	

Excited State 26:	Singlet-A	6.2986 eV
196.84 nm f=0.1532	<S**2>=0.000	
73 -> 87	-0.11578	
83 -> 88	0.32870	
83 -> 89	-0.17715	
84 -> 90	0.23030	
85 -> 90	0.12780	
85 -> 91	-0.13142	
85 -> 92	-0.11614	
86 -> 92	0.32624	
86 -> 93	-0.11042	
86 -> 94	0.11099	

Excited State 27:	Singlet-A	6.3486 eV
195.29 nm f=0.1390	<S**2>=0.000	
71 -> 87	0.14008	
72 -> 87	-0.11959	
77 -> 87	0.19617	
78 -> 87	-0.12274	
79 -> 87	-0.15800	
80 -> 88	0.10603	
82 -> 88	-0.22140	
82 -> 89	0.16180	
83 -> 88	-0.10917	
83 -> 90	0.22080	
84 -> 90	0.12052	
84 -> 91	0.14679	
84 -> 92	-0.12856	
85 -> 90	0.28097	

Excited State 28:	Singlet-A	6.4359 eV
192.64 nm f=0.0332	<S**2>=0.000	
71 -> 87	-0.16537	
73 -> 87	0.12313	
76 -> 87	-0.10481	
77 -> 87	-0.11315	
78 -> 87	-0.11465	
81 -> 89	-0.13381	
82 -> 88	-0.27198	
83 -> 89	-0.11136	
84 -> 90	-0.15817	
84 -> 91	-0.12590	
85 -> 91	0.13749	
85 -> 92	0.14056	
86 -> 90	0.16161	
86 -> 92	0.30407	

Excited State 29:	Singlet-A	6.4612 eV
191.89 nm f=0.0926	<S**2>=0.000	
78 -> 87	-0.10586	
80 -> 88	0.11535	
82 -> 89	-0.22316	
82 -> 90	-0.10446	
85 -> 93	-0.11365	
86 -> 93	0.41733	
86 -> 95	0.14809	
86 -> 96	0.21838	

Excited State 30:	Singlet-A	6.4860 eV
191.16 nm f=0.0242	<S**2>=0.000	
71 -> 87	0.17033	
73 -> 87	-0.11565	
75 -> 87	-0.14064	
76 -> 87	0.20607	
77 -> 87	0.16384	
78 -> 87	0.25962	
79 -> 87	0.10629	
80 -> 88	-0.10327	
82 -> 88	-0.21520	
82 -> 90	0.12482	
83 -> 90	-0.11474	
86 -> 92	0.13849	
86 -> 93	0.22163	

Ground to excited state transition electric dipole moments (Au):

state	X	Y	Z	Dip. S.	Osc.
1	0.6848	-0.8412	0.1378	1.1956	0.0803
2	-0.3190	0.2396	0.1407	0.1789	0.0147
3	0.0258	-0.2268	-0.1919	0.0889	0.0076
4	-1.1447	-0.7206	0.5998	2.1892	0.2034
5	0.1584	-0.0139	-0.1641	0.0522	0.0054
6	0.6062	0.2024	-0.1485	0.4306	0.0467
7	0.4561	-0.3754	-0.1732	0.3790	0.0426
8	-0.4938	0.4702	0.0884	0.4727	0.0547
9	1.2711	1.0223	-0.5605	2.9750	0.3596
10	-1.2370	-0.6224	0.1247	1.9332	0.2361
11	0.4502	0.4237	-0.3105	0.4785	0.0602
12	0.2590	0.2644	1.2113	1.6042	0.2130
13	-1.1861	-0.0968	-0.5812	1.7542	0.2352
14	0.0910	0.4106	-0.2058	0.2192	0.0301
15	-0.7438	-0.7736	-0.0613	1.1555	0.1591
16	-0.0042	-0.3119	0.4450	0.2953	0.0419
17	-0.5946	0.2901	0.0576	0.4410	0.0630
18	0.0165	0.0198	0.2063	0.0432	0.0063
19	0.3416	0.5486	-0.1613	0.4436	0.0652
20	0.2959	-0.6297	0.3737	0.6238	0.0930
21	0.8496	-0.8531	0.3232	1.5541	0.2332
22	-0.4784	-0.0737	-0.5517	0.5386	0.0815
23	0.3001	0.1377	0.0767	0.1149	0.0175
24	0.5652	-0.2133	-0.3153	0.4644	0.0714
25	0.5031	0.1695	0.2345	0.3368	0.0519
26	0.5659	-0.7172	0.3975	0.9927	0.1532
27	-0.2100	0.8230	0.4149	0.8935	0.1390
28	0.3305	-0.2155	-0.2339	0.2104	0.0332
29	0.4189	-0.6273	0.1265	0.5850	0.0926
30	0.3243	0.1563	-0.1504	0.1522	0.0242

Ground to excited state transition velocity dipole moments (Au):

state	X	Y	Z	Dip. S.	Osc.
1	-0.0745	0.0878	-0.0152	0.0135	0.0893
2	0.0404	-0.0329	-0.0163	0.0030	0.0161
3	-0.0035	0.0300	0.0248	0.0015	0.0080
4	0.1531	0.0928	-0.0797	0.0384	0.1837
5	-0.0183	0.0008	0.0228	0.0009	0.0037
6	-0.0985	-0.0332	0.0242	0.0114	0.0467
7	-0.0738	0.0640	0.0283	0.0104	0.0409

8	0.0839	-0.0823	-0.0142	0.0140	0.0539
9	-0.2234	-0.1792	0.0982	0.0917	0.3370
10	0.2230	0.1112	-0.0246	0.0627	0.2281
11	-0.0819	-0.0772	0.0548	0.0157	0.0553
12	-0.0532	-0.0496	-0.2388	0.0623	0.2086
13	0.2301	0.0219	0.1151	0.0667	0.2210
14	-0.0154	-0.0835	0.0389	0.0087	0.0283
15	0.1492	0.1565	0.0133	0.0469	0.1514
16	0.0005	0.0626	-0.0924	0.0124	0.0390
17	0.1223	-0.0574	-0.0116	0.0184	0.0572
18	-0.0014	-0.0066	-0.0439	0.0020	0.0060
19	-0.0760	-0.1216	0.0352	0.0218	0.0659
20	-0.0648	0.1372	-0.0822	0.0298	0.0889
21	-0.1865	0.1911	-0.0722	0.0765	0.2265
22	0.1061	0.0171	0.1217	0.0264	0.0774
23	-0.0655	-0.0293	-0.0175	0.0055	0.0160
24	-0.1258	0.0502	0.0718	0.0235	0.0680
25	-0.1163	-0.0387	-0.0544	0.0180	0.0519
26	-0.1308	0.1623	-0.0893	0.0514	0.1482
27	0.0491	-0.1864	-0.0970	0.0466	0.1331
28	-0.0800	0.0512	0.0537	0.0119	0.0335
29	-0.0988	0.1456	-0.0286	0.0318	0.0892
30	-0.0746	-0.0362	0.0330	0.0080	0.0223

Ground to excited state transition magnetic dipole moments (Au):

state	X	Y	Z
1	-0.0843	0.0296	-0.3381
2	0.0714	0.0651	0.1654
3	-0.0192	-0.2072	-0.8990
4	-0.1256	-0.4824	-1.4066
5	0.0761	0.0898	0.1374
6	-0.0810	0.1103	0.6911
7	-0.3114	0.2332	2.0129
8	0.1297	-0.1982	-1.6278
9	0.3223	0.5088	0.5443
10	-0.2762	-0.6056	-0.7022
11	0.0453	0.0232	0.2757
12	-0.0923	0.2409	-1.1911
13	-0.2180	-0.5324	-0.6519
14	-0.2873	-0.1305	-0.4503
15	-0.2875	-0.3271	-0.0799
16	0.0332	-0.0392	-0.7135
17	-0.2802	-0.1540	1.5520
18	-0.0149	0.0093	0.1761
19	0.5989	0.4876	-0.7031
20	-0.0476	-0.0462	-0.8366
21	-0.2327	0.3615	-0.9132
22	0.2645	-0.4316	-0.1274
23	-0.0614	-0.0395	0.0773
24	-0.0039	0.3350	0.5635
25	0.1101	0.4556	0.5541
26	-0.4842	-0.0435	-0.5175
27	0.1419	0.1339	-0.3611
28	0.2151	0.0488	0.8421
29	-0.0288	0.3572	-0.0106
30	0.1030	0.2351	0.6523

Ground to excited state transition velocity quadrupole moments (Au):

state	XX	YY	ZZ	XY	XZ	YZ
1	0.1448	0.2355	-0.0139	-0.1335	-0.0919	-0.2414
2	-0.3434	0.0470	0.0315	0.1633	0.0257	0.0882
3	0.3321	-0.2308	-0.0350	-0.0256	0.0645	0.0081
4	-0.8035	0.3583	-0.0108	-0.0785	0.3116	-0.0809
5	-0.1297	-0.1224	-0.0103	0.2752	-0.1354	-0.1828
6	0.4159	-0.2613	-0.0371	0.1184	-0.3743	0.0931
7	0.1734	0.0798	-0.0938	0.1101	-0.2618	-0.1861
8	-0.0245	-0.0933	0.0773	0.0549	0.0799	0.2430
9	0.9080	-0.6206	-0.0189	0.1533	-0.5205	0.2183
10	-0.3083	0.3038	0.0402	-0.0771	0.5897	-0.0665
11	0.6110	-0.3439	0.0380	0.0139	-0.2276	0.1728
12	-1.8406	1.2946	0.0487	-0.5263	-0.4059	0.4245
13	1.0802	-0.7214	0.1321	0.0510	0.8795	0.1692
14	0.9042	-0.3823	0.0794	-0.3440	0.2377	0.6271
15	-0.0639	0.0179	0.0187	0.2984	0.5410	-0.2040
16	-0.9191	0.3077	-0.1681	-0.6610	0.3006	-0.0064

17	-0.0823	0.4059	0.1063	-0.2110	0.1662	0.5124
18	-0.5350	0.0824	-0.1323	-0.7346	0.3210	0.3613
19	0.1693	-0.2553	0.1936	-0.3056	0.2672	-0.0602
20	-0.1179	0.6007	0.0039	-0.7054	-0.0564	-0.3623
21	-0.4848	0.2404	-0.0880	0.5572	-0.3488	-0.3034
22	0.8810	-0.5991	-0.0329	0.0769	0.3575	-0.3649
23	-0.0281	0.0905	-0.0182	0.0579	-0.1258	0.1927
24	0.6858	-0.4550	-0.0555	0.1857	-0.1384	-0.0997
25	-0.5740	0.2012	-0.0323	0.1766	-0.5403	0.0092
26	-0.4489	0.0889	-0.1813	-0.3957	-0.0678	0.0406
27	-0.7727	0.8784	0.2525	-0.0673	-0.5895	0.2692
28	0.2603	-0.3880	-0.1687	-0.2232	0.0279	-0.2888
29	-0.1306	0.2851	-0.2500	0.0947	-0.0850	-0.1190
30	0.4218	-0.3283	-0.1061	-0.2307	-0.0931	0.3254

<0|del|b> * <b|rxdel|0> + <0|del|b> * <b|delr+rdel|0>

Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)

state	XX	YY	ZZ	R(velocity)	E-M Angle
1	62.6958	96.1214	-60.2999	32.8391	69.80
2	-19.0151	18.3269	-10.5001	-3.7295	100.78
3	-85.7740	-59.6816	-11.5480	-52.3346	142.09
4	113.2535	188.2363	-57.5375	81.3174	80.54
5	21.7677	-2.6948	-10.8658	2.7357	70.06
6	7.6905	27.5827	56.2915	30.5215	73.73
7	192.5693	189.9953	15.5543	132.7063	62.93
8	92.1376	112.4139	0.4541	68.3352	75.04
9	-225.9533	-160.6514	-41.1890	-142.5979	116.51
10	-219.6265	-117.7514	-93.6354	-143.6711	117.44
11	-6.5430	-6.6187	49.1000	11.9794	74.13
12	671.1655	250.5153	63.2996	328.3268	24.24
13	-175.9582	-162.0151	-143.2338	-160.4024	127.56
14	-0.2927	-16.1123	8.8376	-2.5224	92.46
15	-227.5794	-134.0975	35.9847	-108.5641	172.74
16	175.6357	8.0796	27.2052	70.3068	37.33
17	4.5697	13.0036	-161.0633	-47.8300	101.68
18	42.9962	-65.4949	-2.6483	-8.3823	171.34
19	-99.9006	-88.0971	-227.4804	-138.4927	147.16
20	202.7225	59.0966	-54.5453	69.0913	63.11
21	253.5913	323.7746	-16.8955	186.8235	50.28
22	-30.6245	-55.3104	102.0338	5.3663	86.50
23	-7.6033	-13.8771	33.3716	3.9637	60.84
24	118.8829	61.5769	-3.3648	59.0317	54.94
25	-119.6743	-52.6514	-12.9506	-61.7588	128.47
26	130.6091	105.2820	77.3068	104.3993	50.47
27	-141.3608	73.7845	119.2296	17.2177	78.91
28	51.2365	94.2527	-54.3628	30.3755	71.27
29	92.2684	26.2064	45.7478	54.7409	30.34
30	2.9973	-4.2357	16.9889	5.2502	85.13

1/2[<0|r|b>*<b|rxdel|0> + (<0|rxdel|b>*<b|r|0>)*]

Rotatory Strengths (R) in cgs (10**-40 erg-esu-cm/Gauss)

state	XX	YY	ZZ	R(length)
1	40.8200	17.5853	32.9538	30.4531
2	16.1016	-11.0291	-16.4530	-3.7935
3	0.3500	-33.2251	-121.9989	-51.6247
4	-101.6289	-245.8223	596.5795	83.0427
5	-8.5244	0.8821	15.9428	2.7669
6	34.7132	-15.7840	72.5974	30.5089
7	100.4307	61.9274	246.5425	136.3002
8	45.2720	65.9067	101.7075	70.9621
9	-289.6782	-367.7834	215.7296	-147.2440
10	-241.5940	-266.5240	61.9134	-148.7349
11	-14.4261	-6.9553	60.5405	13.0530
12	16.9078	-45.0289	1020.2678	330.7156
13	-182.8412	-36.4624	-267.9661	-162.4232
14	18.4887	37.8885	-65.5215	-3.0481
15	-151.2249	-178.9405	-3.4648	-111.2101
16	0.0998	-8.6517	224.5239	71.9907
17	-117.8247	31.6051	-63.2426	-49.8208
18	0.1738	-0.1308	-25.6906	-8.5492
19	-144.6865	-189.1426	-80.1695	-137.9996
20	9.9614	-20.5609	221.1119	70.1708
21	139.7795	218.1012	208.7424	188.8744
22	89.4830	-22.4976	-49.6837	5.7672
23	13.0421	3.8513	-4.1956	4.2326

24	1.5539	50.5256	125.6629	59.2475
25	-39.1756	-54.6145	-91.9118	-61.9006
26	193.8013	-22.0638	145.4849	105.7408
27	21.0760	-77.9159	105.9534	16.3712
28	-50.2779	7.4319	139.2771	32.1437
29	8.5251	158.4553	0.9446	55.9750
30	-23.6321	-25.9873	69.3949	6.5918

1/2[<0|del|b>*<b|r|0> + (<0|r|b>*<b|del|0>)*] (Au)

state	X	Y	Z	Dip. S.	Osc.(frdel)
1	-0.0510	-0.0739	-0.0021	0.1270	0.0847
2	-0.0129	-0.0079	-0.0023	0.0231	0.0154
3	-0.0001	-0.0068	-0.0048	0.0117	0.0078
4	-0.1753	-0.0669	-0.0478	0.2899	0.1933
5	-0.0029	-0.0000	-0.0037	0.0066	0.0044
6	-0.0597	-0.0067	-0.0036	0.0700	0.0467
7	-0.0337	-0.0240	-0.0049	0.0626	0.0417
8	-0.0415	-0.0387	-0.0013	0.0814	0.0543
9	-0.2840	-0.1831	-0.0551	0.5222	0.3481
10	-0.2758	-0.0692	-0.0031	0.3481	0.2321
11	-0.0369	-0.0327	-0.0170	0.0866	0.0577
12	-0.0138	-0.0131	-0.2893	0.3161	0.2108
13	-0.2729	-0.0021	-0.0669	0.3419	0.2279
14	-0.0014	-0.0343	-0.0080	0.0437	0.0291
15	-0.1110	-0.1211	-0.0008	0.2328	0.1552
16	-0.0000	-0.0195	-0.0411	0.0606	0.0404
17	-0.0727	-0.0166	-0.0007	0.0900	0.0600
18	-0.0000	-0.0001	-0.0091	0.0092	0.0061
19	-0.0260	-0.0667	-0.0057	0.0983	0.0656
20	-0.0192	-0.0864	-0.0307	0.1363	0.0909
21	-0.1584	-0.1630	-0.0233	0.3447	0.2298
22	-0.0508	-0.0013	-0.0671	0.1192	0.0794
23	-0.0197	-0.0040	-0.0013	0.0250	0.0167
24	-0.0711	-0.0107	-0.0226	0.1045	0.0696
25	-0.0585	-0.0066	-0.0128	0.0778	0.0519
26	-0.0741	-0.1164	-0.0355	0.2260	0.1506
27	-0.0103	-0.1534	-0.0402	0.2040	0.1360
28	-0.0264	-0.0110	-0.0125	0.0500	0.0333
29	-0.0414	-0.0913	-0.0036	0.1363	0.0909
30	-0.0242	-0.0057	-0.0050	0.0348	0.0232

$\mathbf{A}^{+}$; HOMO : 83, LUMO : 84

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.9712 eV
417.29 nm f=0.0000 <S**2>=0.000
76 -> 84 (LUMO) 0.11188
83 (HOMO) -> 84 0.69074
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -943.665444064
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.2751 eV
378.57 nm f=0.0002 <S**2>=0.000
82 -> 84 0.70323

Excited State 3: Singlet-A 3.3580 eV
369.22 nm f=0.1178 <S**2>=0.000
81 -> 84 0.69809

Excited State 4: Singlet-A 4.0265 eV
307.92 nm f=0.2202 <S**2>=0.000
80 -> 84 0.64569
81 -> 85 0.26564

Excited State 5: Singlet-A 4.3620 eV
284.24 nm f=0.0139 <S**2>=0.000
79 -> 84 0.68312
81 -> 85 -0.11457

Excited State 6: Singlet-A 5.2768 eV
234.96 nm f=0.0028 <S**2>=0.000
82 -> 89 0.46543
83 -> 85 -0.29946
83 -> 90 0.40976

Excited State 7: Singlet-A 5.4219 eV
228.67 nm f=0.0034 <S**2>=0.000
82 -> 89 0.21713
83 -> 85 0.62740
83 -> 86 -0.10734
83 -> 90 0.18332

Excited State 8: Singlet-A 5.4869 eV
225.96 nm f=1.1342 <S**2>=0.000
79 -> 84 0.14771
80 -> 84 -0.25598
81 -> 85 0.62373

Excited State 9: Singlet-A 5.5411 eV
223.75 nm f=0.0914 <S**2>=0.000
72 -> 84 -0.16737
75 -> 84 -0.18315

77 -> 84 0.24625
78 -> 84 0.57117
79 -> 85 -0.10697

Excited State 10: Singlet-A 5.6009 eV
221.37 nm f=0.0000 <S**2>=0.000
82 -> 85 0.69892

Excited State 11: Singlet-A 5.6172 eV
220.72 nm f=0.0323 <S**2>=0.000
72 -> 84 -0.28190
73 -> 84 0.11537
77 -> 84 0.53536
78 -> 84 -0.27105

Excited State 12: Singlet-A 5.8870 eV
210.61 nm f=0.0787 <S**2>=0.000
79 -> 85 -0.10837
80 -> 85 -0.13829
82 -> 86 0.14923
82 -> 90 -0.34979
83 -> 89 0.53467

Excited State 13: Singlet-A 5.9682 eV
207.74 nm f=0.0671 <S**2>=0.000
73 -> 84 -0.13859
74 -> 84 0.13094
75 -> 84 0.20819
78 -> 84 0.20279
79 -> 85 0.36058
79 -> 86 -0.12078
80 -> 85 0.28692
80 -> 86 0.26918
81 -> 97 0.12851
82 -> 90 -0.12732

Excited State 14: Singlet-A 6.0319 eV
205.55 nm f=0.0998 <S**2>=0.000
79 -> 87 -0.13317
81 -> 86 0.66220

Excited State 15: Singlet-A 6.0853 eV
203.74 nm f=0.0012 <S**2>=0.000
69 -> 84 0.12527
71 -> 84 -0.13250
76 -> 84 0.64229
83 -> 84 -0.12355
83 -> 87 0.12989

Excited State 16: Singlet-A 6.1312 eV
202.22 nm f=0.0127 <S**2>=0.000
82 -> 89 0.12486
83 -> 86 0.67150

Excited State 17: Singlet-A 6.1486 eV
201.65 nm f=0.0303 <S**2>=0.000
73 -> 84 0.17415
75 -> 84 -0.14018
79 -> 85 -0.18536
79 -> 86 -0.14238
80 -> 85 0.44950
80 -> 86 -0.13806
81 -> 87 0.36739

Excited State 18: Singlet-A 6.2994 eV
196.82 nm f=0.0869 <S**2>=0.000
75 -> 84 -0.15883
82 -> 86 0.64800
83 -> 89 -0.14775

Excited State 19: Singlet-A 6.3595 eV
194.96 nm f=0.0113 <S**2>=0.000
73 -> 84 0.20870
74 -> 84 0.16583
75 -> 84 0.51441
78 -> 84 0.12298
79 -> 85 -0.14679
80 -> 86 -0.16374
82 -> 86 0.20241
82 -> 90 0.15781

Excited State 20: Singlet-A 6.4057 eV
193.55 nm f=0.0010 <S**2>=0.000
71 -> 84 0.54608
76 -> 84 0.20474
83 -> 87 -0.34920

Excited State 21: Singlet-A 6.4538 eV
192.11 nm f=0.0001 <S**2>=0.000
69 -> 84 -0.21883
71 -> 84 0.34157
83 -> 87 0.54326
83 -> 88 0.11651

Excited State 22: Singlet-A 6.5309 eV
189.84 nm f=0.1016 <S**2>=0.000
64 -> 84 0.11154
72 -> 84 0.46998
73 -> 84 -0.20347
77 -> 84 0.24635
80 -> 85 0.10053
81 -> 87 -0.10294
82 -> 89 0.18697
83 -> 90 -0.23551

Excited State 23: Singlet-A 6.5606 eV
188.98 nm f=0.5282 <S**2>=0.000
72 -> 84 0.12877
79 -> 85 0.11610
80 -> 85 -0.33382
81 -> 87 0.50971
82 -> 90 0.19732

Excited State 24: Singlet-A 6.6284 eV
187.05 nm f=0.0028 <S**2>=0.000
82 -> 87 0.67988
82 -> 88 0.14266

Excited State 25: Singlet-A 6.6427 eV
186.65 nm f=0.0148 <S**2>=0.000
81 -> 88 0.63058
81 -> 91 -0.20227
81 -> 93 0.10188

Excited State 26: Singlet-A 6.6554 eV
186.29 nm f=0.0019 <S**2>=0.000
69 -> 84 0.61831
71 -> 84 0.17831
72 -> 86 0.12323
76 -> 84 -0.12052
83 -> 87 0.14089

Excited State 27: Singlet-A 6.6610 eV
186.13 nm f=0.3311 <S**2>=0.000
72 -> 84 0.19912
73 -> 84 -0.15071
77 -> 84 0.21493
82 -> 89 -0.38386
83 -> 90 0.44785

Excited State 28: Singlet-A 6.7246 eV
184.38 nm f=0.0479 <S**2>=0.000
72 -> 84 0.25121
73 -> 84 0.52388
75 -> 84 -0.10628
79 -> 85 0.10884

80 -> 86 0.23830
82 -> 90 -0.12122

Excited State 29: Singlet-A 6.7428 eV
183.88 nm f=0.0088 <S**2>=0.000
82 -> 88 0.10438
83 -> 88 -0.34990
83 -> 91 0.31113
83 -> 93 0.36148
83 -> 96 -0.19255
83 -> 97 -0.11015
83 ->105 0.11973

Excited State 30: Singlet-A 6.7513 eV
183.65 nm f=0.0021 <S**2>=0.000
82 -> 88 -0.34117
82 -> 91 0.32989
82 -> 93 0.37154
82 -> 96 -0.20294
82 -> 97 -0.11601
82 ->105 0.12206

Low-lying triplet states

The TD-DFT calculations described in the preceding subsections include multiple singlet excited states to comprehensively describe the absorption and CD spectra. In this subsection, low-lying triplet excited states of the helical acridiniums (**1a**$^+$, **1b**$^+$, **1c**$^+$, and **1d**$^+$) as well as the non-helical analogue (**A**$^+$) were also calculated by TD-DFT.[10] The structure optimization was performed at ωB97XD[11]/6-31G(d,p)[6, 7] level of theory with solvent effect by Solvation Model based on solute electron Density (SMD) model[12] with the parameter set for CH_2Cl_2 solvent. Excited states were calculated by TD-DFT at CAM-B3LYP[5]/6-311+G(2d,p)[13, 8] level with the solvent effect in the same way as for the structure optimization. For geometry optimization, GRRM23 program[14, 15] was used, and necessary entities (energy, its first and second derivatives) were computed by using Gaussian 16 suit of program.[4] For excited state, Gaussian 16 was used.

In Table S13, the TD-DFT results were compared with the experimental absorption energy. Calculated vertical excitation energies were compared with the absorption maxima. The experimental absorption shows spectral broadening, and comparison between theory and experiment is not straight-forward and out of our focus in the present study. Although the calculated vertical excitation energies overestimated the absorption peak position by about 0.4 eV, this is a systematic deviation. In Table S13, we also show the peak position shifted by −0.4 eV. Then the deviation is at most -11 nm. With this result, we are confident to assign the experimentally observed peaks around 513 nm – 530 nm to the lowest singlet excited state. The first singlet excited state is characterized as one-electron excitation from HOMO to LUMO. An exemption is **1b**$^+$ in which next-HOMO to LUMO excited configuration and HOMO-LUMO configuration are strongly coupled.

Table S13. Low-lying excited states of helical and non-helical acridiniums ($\mathbf{1}^+$ and $\mathbf{A}^+$).[a]

state	CAM-B3LYP/6-311+G(2d,p)				CAM-B3LYP/6-311+G(2d,p) (shifted)[c]		exptl.		
	E_{abs} / eV	λ_{abs} / nm	wave function[b] (|c|>0.30)	f	λ_{abs} / nm	error / nm	E_{abs} / eV	λ_{abs} / nm	ε / $M^{-1}cm^{-1}$
$1a^+$									
T_1	1.71	723	0.62 (118→119)	—	943				
T_2	2.58	480	0.52 (113→119)	—	567				
S_1	2.82	439	0.68 (118→119)	0.18	512	−6	2.39	518	5760
T_3	2.88	430	0.40 (113→119) +0.38 (114→119)	—	499				
$1b^+$									
T_1	1.72	721	0.62 (121→123)	—	939				
T_2	2.58	481	0.50 (117→123)	—	569				
T_3	2.81	441	0.64 (122→123)	—	514				
S_1	2.82	439	0.53 (121-123) -0.42 (122-123)	0.15	512	–11	2.37	523	5600
$1c^+$									
T_1	1.74	713	0.63 (114→115)	—	925				
T_2	2.60	477	0.39 (113→115) -0.34 (110→115)	—	564				
S_1	2.74	452	0.69 (114→115)	0.33	528	−2	2.34	530	9250
T_3	2.82	440	0.42 (113→115) +0.32 (110→115)	—	512				
$1d^+$									
T_1	1.72	720	0.61 (86→87)	—	937				
T_2	2.58	481	0.54 (83→87)	—	569				
S_1	2.83	438	0.68 (86→87)	0.13	509	–5	2.42	513	3000
T_3	2.89	429	0.39 (83→87) –0.38 (84→87)	—	497				
A^+									
T_1	1.94	640	0.65 (83→84)	—	806				
T_2	2.87	432	0.63 (80→84)	—	502				
S_1	3.29	377	0.68 (83→84)	0.16	429	0	2.89	429	6000
T_3	3.30	376	0.56 (79→84)	—	427				

[a] E_{abs}, λ_{abs}, f, and ε denote absorption energy, absorption wavelength, oscillator strength, and extinction coefficient, respectively. The CAM-B3LYP/6-311+G(2d,p)//wB97XD/6-31G(d,p) level of calculations were performed with the Gaussian16 suit of program.[4] For the structural optimization, the GRRM23 program[14, 15] was used. Solvation effect was taken into account by the SMD model[12] with the parameter set for CH_2Cl_2 solvent.

[b] "c" is the coefficient for the excited-state configuration.

[c] A systematic error was observed in the CAM-B3LYP excitation energy. Therefore, the calculated excitation energies were shifted by –0.4 eV. The energy shift was determined as the excitation energy to the S1 state of compound $\mathbf{A}^+$ exactly agrees with the experimentally observed value. Then, the shifted λ_{abs} was calculated from the shifted E_{abs}.

Optimized Coordinates [at the (U)CAM-B3LYP/6-31+G(d,p) level]

P-**1a**$^{+}$ (with no imaginary frequency)										
SCF Done: E(RCAM-B3LYP) = -1365.14086737 A.U. after 12 cycles										
Center Number	Atom	X	Y	Z		Center Number	Atom	X	Y	Z
1	N	-1.162484	0.612572	0.127195		31	H	-6.297271	-2.118231	2.061627
2	C	1.084765	1.134086	0.863794		32	C	-4.518543	-3.099741	1.345687
3	C	-3.860484	-0.633664	0.200712		33	H	-4.759212	-4.058235	1.792511
4	C	-2.321069	1.222997	-0.518772		34	C	0.059761	3.334688	2.255012
5	C	-3.589876	0.649577	-0.476233		35	H	-0.334532	4.174176	2.817951
6	C	-1.663162	-1.648516	-0.627716		36	C	1.947508	1.991333	1.609807
7	C	1.579598	0.054124	0.107468		37	H	3.006778	1.763810	1.625995
8	C	-2.079552	2.388542	-1.248924		38	C	0.174012	-2.885413	-1.677717
9	H	-1.076271	2.796595	-1.296499		39	H	0.490693	-3.751382	-2.247681
10	C	0.663291	-0.840976	-0.485628		40	C	1.449103	3.062461	2.292151
11	C	-5.045099	-0.796616	0.925530		41	H	2.108154	3.702383	2.867513
12	H	-5.709450	0.052071	1.049112		42	C	3.047044	-0.165036	-0.030571
13	C	-0.732972	-0.614107	-0.335559		43	C	3.743819	0.471599	-1.070633
14	C	-0.309166	1.425353	0.836470		44	C	3.713903	-0.998195	0.883112
15	C	-2.986401	-1.721356	0.053176		45	C	5.115341	0.254920	-1.180413
16	C	-0.802294	2.551623	1.532520		46	C	5.087251	-1.179603	0.733368
17	H	-1.862912	2.766654	1.519291		47	C	5.806514	-0.567415	-0.291823
18	C	1.092641	-1.993804	-1.201736		48	H	5.659032	0.745612	-1.982963
19	H	2.155110	-2.147606	-1.347052		49	H	5.609364	-1.817617	1.440996
20	C	-4.623150	1.313303	-1.153184		50	C	3.038257	1.372687	-2.053317
21	H	-5.612881	0.870736	-1.149642		51	H	2.233387	0.849126	-2.579302
22	C	-1.187516	-2.734153	-1.339887		52	H	2.595175	2.242446	-1.557238
23	H	-1.882142	-3.524570	-1.603592		53	H	3.735478	1.744151	-2.805749
24	C	-3.334332	-2.945882	0.639435		54	C	2.979422	-1.681267	2.010140
25	H	-2.651367	-3.785064	0.564759		55	H	2.473059	-0.962216	2.662005
26	C	-3.117812	3.028599	-1.905859		56	H	2.218475	-2.374531	1.637723
27	H	-2.922365	3.934598	-2.468571		57	H	3.671303	-2.254880	2.628556
28	C	-4.400844	2.490887	-1.848540		58	C	7.284204	-0.806181	-0.449546
29	H	-5.221537	2.976693	-2.364838		59	H	7.758341	-1.020636	0.510773
30	C	-5.377336	-2.016280	1.496302		60	H	7.469013	-1.662813	-1.106288
						61	H	7.783016	0.059277	-0.891518

Transition State (TS) of **1a**$^+$ (with only one imaginary frequency)										
SCF Done: E(UCAM-B3LYP) = -1365.07137556 A.U. after 9 cycles										
Center Number	Atom	X	Y	Z		Center Number	Atom	X	Y	Z
1	N	1.224894	0.936026	0.177714		31	H	5.232748	-3.334499	-2.305429
2	C	-1.054306	1.433821	-0.545022		32	C	3.540897	-3.799634	-1.056214
3	C	3.599602	-1.103960	-0.318205		33	H	3.507074	-4.846442	-1.337914
4	C	2.675591	1.270588	0.120942		34	C	-0.582135	4.136973	-0.613422
5	C	3.711126	0.306045	0.104128		35	H	-0.465379	5.207792	-0.482788
6	C	1.533772	-1.425618	1.048783		36	C	-1.943287	2.300652	-1.239472
7	C	-1.541403	0.262091	0.057970		37	H	-2.873791	1.882464	-1.605290
8	C	3.097133	2.605819	0.034858		38	C	-0.296882	-2.215527	2.486282
9	H	2.421486	3.392003	-0.214672		39	H	-0.636924	-2.891317	3.262009
10	C	-0.660732	-0.455338	0.875265		40	C	-1.677688	3.637091	-1.340798
11	C	4.530031	-1.616435	-1.230386		41	H	-2.353713	4.307346	-1.858474
12	H	5.271785	-0.955511	-1.664412		42	C	-2.967589	-0.145502	-0.077539
13	C	0.750264	-0.273341	0.690317		43	C	-3.951999	0.451724	0.728929
14	C	0.238464	1.892683	-0.155501		44	C	-3.304467	-1.133680	-1.017828
15	C	2.624341	-1.939562	0.199289		45	C	-5.274107	0.041926	0.571761
16	C	0.337810	3.299018	-0.021359		46	C	-4.642419	-1.499537	-1.144907
17	H	1.072196	3.746281	0.622517		47	C	-5.642117	-0.928860	-0.358812
18	C	-1.159733	-1.413879	1.806704		48	H	-6.039014	0.496895	1.194908
19	H	-2.230106	-1.459122	1.965207		49	H	-4.910018	-2.253196	-1.880236
20	C	5.030406	0.726757	0.338424		50	C	-3.605569	1.498089	1.759414
21	H	5.788476	-0.043696	0.413985		51	H	-2.851021	1.139737	2.466973
22	C	1.034216	-2.267021	2.022618		52	H	-3.212448	2.409778	1.298874
23	H	1.678348	-3.070389	2.364395		53	H	-4.489252	1.776642	2.335387
24	C	2.595912	-3.288525	-0.178541		54	C	-2.257093	-1.782734	-1.888257
25	H	1.810524	-3.935020	0.197047		55	H	-1.700839	-1.045977	-2.476654
26	C	4.418149	2.999147	0.189551		56	H	-1.528697	-2.342354	-1.292908
27	H	4.657856	4.054607	0.124032		57	H	-2.717190	-2.482332	-2.587626
28	C	5.398774	2.054160	0.430957		58	C	-7.075454	-1.368142	-0.491574
29	H	6.428500	2.335301	0.619847		59	H	-7.297943	-1.701282	-1.507721
30	C	4.506335	-2.955021	-1.595025		60	H	-7.286473	-2.205066	0.182478
						61	H	-7.765505	-0.560446	-0.237506

M-**1a**$^+$ (with no imaginary frequency)										
SCF Done: E(RCAM-B3LYP) = -1365.14086735 A.U. after 11 cycles										
Center Number	Atom	X	Y	Z		Center Number	Atom	X	Y	Z
1	N	1.162491	0.612544	0.127402		31	H	6.297834	-2.117747	2.060960
2	C	-1.084793	1.133935	0.864004		32	C	4.518994	-3.099420	1.345508
3	C	3.860559	-0.633466	0.200471		33	H	4.759809	-4.057876	1.792335
4	C	2.320901	1.223098	-0.518768		34	C	-0.059827	3.334401	2.255472
5	C	3.589749	0.649715	-0.476510		35	H	0.334439	4.173847	2.818494
6	C	1.663195	-1.648551	-0.627488		36	C	-1.947548	1.991050	1.610158
7	C	-1.579591	0.054094	0.107507		37	H	-3.006817	1.763514	1.626308
8	C	2.079204	2.388659	-1.248809		38	C	-0.173971	-2.885717	-1.677177
9	H	1.075918	2.796726	-1.296145		39	H	-0.490666	-3.751838	-2.246903
10	C	-0.663255	-0.841025	-0.485543		40	C	-1.449164	3.062106	2.292624
11	C	5.045341	-0.796295	0.925030		41	H	-2.108218	3.701923	2.868099
12	H	5.709700	0.052423	1.048362		42	C	-3.047014	-0.165104	-0.030541
13	C	0.732995	-0.614170	-0.335426		43	C	-3.713846	-0.998345	0.882926
14	C	0.309137	1.425225	0.836721		44	C	-3.743791	0.471688	-1.070619
15	C	2.986509	-1.721228	0.053231		45	C	-5.087266	-1.179786	0.733113
16	C	0.802236	2.551449	1.532872		46	C	-5.115226	0.255009	-1.180461
17	H	1.862849	2.766514	1.519612		47	C	-5.806472	-0.567495	-0.291946
18	C	-1.092606	-1.993966	-1.201439		48	H	-5.609342	-1.817937	1.440624
19	H	-2.155074	-2.147795	-1.346748		49	H	-5.658919	0.745798	-1.982966
20	C	4.622846	1.313443	-1.153698		50	C	-2.979407	-1.681627	2.009857
21	H	5.612590	0.870902	-1.150377		51	H	-2.218496	-2.374877	1.637335
22	C	1.187544	-2.734374	-1.339404		52	H	-2.473006	-0.962707	2.661838
23	H	1.882177	-3.524851	-1.602916		53	H	-3.671318	-2.255299	2.628183
24	C	3.334627	-2.945686	0.639480		54	C	-3.038171	1.372865	-2.053186
25	H	2.651717	-3.784932	0.564946		55	H	-2.594757	2.242372	-1.556967
26	C	3.117314	3.028749	-1.905967		56	H	-2.233551	0.849232	-2.579483
27	H	2.921720	3.934776	-2.468584		57	H	-3.735452	1.744710	-2.805373
28	C	4.400357	2.491045	-1.848986		58	C	-7.284178	-0.805893	-0.450080
29	H	5.220920	2.976865	-2.365478		59	H	-7.785135	0.065811	-0.877203
30	C	5.377758	-2.015898	1.495846		60	H	-7.469295	-1.652103	-1.120104
						61	H	-7.755888	-1.036158	0.507726

P-**1b**$^{+}$ (with no imaginary frequency)										
SCF Done: E(RCAM-B3LYP) = -1440.32977761 A.U. after 11 cycles										
Center Number	Atom	X	Y	Z		Center Number	Atom	X	Y	Z
1	N	-1.422296	0.614577	0.128433		31	H	-6.601482	-2.131951	1.916011
2	C	0.800868	1.142394	0.930272		32	C	-4.799840	-3.108005	1.251745
3	C	-4.117231	-0.640330	0.124802		33	H	-5.050068	-4.067082	1.692025
4	C	-2.563651	1.220990	-0.550775		34	C	-0.271038	3.338428	2.293379
5	C	-3.831354	0.643546	-0.544610		35	H	-0.684239	4.176165	2.845276
6	C	-1.893765	-1.648295	-0.639727		36	C	1.638163	1.999549	1.704648
7	C	1.322393	0.063928	0.188973		37	H	2.696496	1.772425	1.753772
8	C	-2.305180	2.387334	-1.273788		38	C	-0.023499	-2.879105	-1.636875
9	H	-1.302301	2.798713	-1.292233		39	H	0.312222	-3.743764	-2.197870
10	C	0.425153	-0.833479	-0.430417		40	C	1.116900	3.068560	2.373270
11	C	-5.321609	-0.806790	0.815457		41	H	1.756409	3.707954	2.970858
12	H	-5.991981	0.039786	0.919519		42	C	2.793063	-0.152636	0.097306
13	C	-0.975617	-0.610958	-0.321062		43	C	3.528487	0.500221	-0.900262
14	C	-0.592358	1.430044	0.862105		44	C	3.430889	-1.011192	1.017366
15	C	-3.235754	-1.725213	0.002960		45	C	4.906191	0.289613	-0.982073
16	C	-1.109002	2.554401	1.543958		46	C	4.800017	-1.197663	0.917452
17	H	-2.169258	2.766954	1.499058		47	C	5.544301	-0.555904	-0.076576
18	C	0.878158	-1.984314	-1.135003		48	H	5.465176	0.794394	-1.759735
19	H	1.944909	-2.133648	-1.250433		49	H	5.322493	-1.847250	1.611201
20	C	-4.846882	1.303776	-1.251186		50	C	2.859710	1.422464	-1.889885
21	H	-5.834854	0.857965	-1.275969		51	H	2.061030	0.915133	-2.440262
22	C	-1.394505	-2.732614	-1.337620		52	H	2.416075	2.291083	-1.392577
23	H	-2.078789	-3.525372	-1.620665		53	H	3.578195	1.794899	-2.621471
24	C	-3.596385	-2.950603	0.579615		54	C	2.655375	-1.715537	2.102825
25	H	-2.908812	-3.787565	0.524939		55	H	2.118527	-1.007598	2.742195
26	C	-3.326175	3.023973	-1.960433		56	H	1.914452	-2.406140	1.687856
27	H	-3.117653	3.930694	-2.517268		57	H	3.324458	-2.294592	2.740561
28	C	-4.608553	2.482043	-1.940042		58	O	6.867609	-0.817233	-0.077245
29	H	-5.415651	2.965120	-2.479806		59	C	7.694122	-0.201916	-1.054788
30	C	-5.666092	-2.027270	1.377161		60	H	7.668795	0.888919	-0.962738
						61	H	8.703249	-0.558537	-0.856235
						62	H	7.396013	-0.497515	-2.066123

Transition State (TS) of **1b**$^{+}$ (with only one imaginary frequency)										
SCF Done: E(UCAM-B3LYP) = -1440.26040441 A.U. after 10 cycles										
Center Number	Atom	X	Y	Z		Center Number	Atom	X	Y	Z
1	N	1.496689	0.932087	0.178620		31	H	5.445317	-3.404461	-2.286502
2	C	-0.768757	1.475949	-0.554752		32	C	3.733440	-3.842062	-1.054747
3	C	3.837149	-1.151071	-0.304677		33	H	3.682003	-4.886827	-1.341327
4	C	2.953684	1.239113	0.132968		34	C	-0.240411	4.168464	-0.623057
5	C	3.971132	0.255298	0.123405		35	H	-0.102858	5.236835	-0.492525
6	C	1.754250	-1.438500	1.043382		36	C	-1.632534	2.359341	-1.259938
7	C	-1.283606	0.312738	0.042157		37	H	-2.566389	1.957953	-1.635840
8	C	3.401187	2.566141	0.050846		38	C	-0.099245	-2.196022	2.468869
9	H	2.742568	3.364739	-0.204858		39	H	-0.456747	-2.866434	3.241409
10	C	-0.419353	-0.424428	0.860784		40	C	-1.338666	3.689920	-1.360824
11	C	4.765915	-1.677607	-1.210560		41	H	-1.994574	4.372862	-1.887743
12	H	5.524058	-1.029285	-1.635171		42	C	-2.714369	-0.069411	-0.102317
13	C	0.995720	-0.270107	0.684105		43	C	-3.700429	0.566449	0.666033
14	C	0.530965	1.908292	-0.157580		44	C	-3.059038	-1.091086	-1.013308
15	C	2.841405	-1.969903	0.200332		45	C	-5.034294	0.182525	0.515954
16	C	0.657367	3.312577	-0.022700		46	C	-4.391486	-1.440879	-1.152698
17	H	1.395641	3.745138	0.626807		47	C	-5.384089	-0.813115	-0.394537
18	C	-0.941907	-1.373559	1.788493		48	H	-5.787645	0.669868	1.121700
19	H	-2.013686	-1.394994	1.942459		49	H	-4.691686	-2.212259	-1.853402
20	C	5.295896	0.650872	0.370173		50	C	-3.352121	1.634842	1.674043
21	H	6.038663	-0.133808	0.451238		51	H	-2.579890	1.298134	2.372620
22	C	1.232331	-2.273768	2.011016		52	H	-2.980371	2.543505	1.190804
23	H	1.858561	-3.090928	2.353365		53	H	-4.228598	1.911611	2.261709
24	C	2.790548	-3.316506	-0.183374		54	C	-2.010531	-1.790478	-1.842156
25	H	1.989556	-3.949296	0.182487		55	H	-1.420912	-1.082882	-2.433566
26	C	4.727965	2.934432	0.217481		56	H	-1.312701	-2.353536	-1.214568
27	H	4.988175	3.985174	0.154315		57	H	-2.473551	-2.494612	-2.534650
28	C	5.688326	1.971040	0.467508		58	O	-6.644057	-1.241004	-0.611228
29	H	6.721388	2.232621	0.666039		59	C	-7.711082	-0.653015	0.119289
30	C	4.719886	-3.014000	-1.581064		60	H	-7.785168	0.419990	-0.085884
						61	H	-8.615498	-1.150951	-0.225640
						62	H	-7.591498	-0.819602	1.194879

M-**1b**$^+$ (with no imaginary frequency)										
SCF Done: E(RCAM-B3LYP) = -1440.32972985 A.U. after 8 cycles										
Center Number	Atom	X	Y	Z		Center Number	Atom	X	Y	Z
1	N	1.438693	0.606217	0.134522		31	H	6.442151	-2.347745	2.085170
2	C	-0.793841	1.206845	0.855021		32	C	4.633764	-3.249863	1.339580
3	C	4.084648	-0.746142	0.219148		33	H	4.832145	-4.222479	1.776571
4	C	2.626755	1.177941	-0.492980		34	C	0.302107	3.349938	2.281989
5	C	3.871636	0.554653	-0.444764		35	H	0.723146	4.167125	2.858229
6	C	1.857929	-1.663529	-0.643487		36	C	-1.629593	2.087875	1.603872
7	C	-1.324463	0.155379	0.082086		37	H	-2.696786	1.900459	1.607190
8	C	2.438662	2.360236	-1.211783		38	C	-0.014599	-2.812609	-1.729802
9	H	1.452717	2.807981	-1.264556		39	H	-0.358665	-3.656647	-2.316553
10	C	-0.436543	-0.767119	-0.513448		40	C	-1.096937	3.131172	2.303350
11	C	5.254412	-0.964281	0.953513		41	H	-1.736297	3.789445	2.880236
12	H	5.950236	-0.143920	1.094063		42	C	-2.797205	-0.003456	-0.072608
13	C	0.965957	-0.597091	-0.347204		43	C	-3.505089	-0.839601	0.801051
14	C	0.610496	1.443939	0.844589		44	C	-3.464724	0.695757	-1.099505
15	C	3.170130	-1.796732	0.049519		45	C	-4.886291	-0.975231	0.645808
16	C	1.140178	2.542076	1.558506		46	C	-4.834120	0.538574	-1.234943
17	H	2.208422	2.715837	1.557711		47	C	-5.552412	-0.291373	-0.369351
18	C	-0.902510	-1.891578	-1.251387		48	H	-5.425945	-1.619356	1.328365
19	H	-1.968432	-1.999064	-1.412137		49	H	-5.377101	1.057958	-2.017020
20	C	4.937051	1.184813	-1.103670		50	C	-2.808249	-1.589605	1.910028
21	H	5.908569	0.703620	-1.095656		51	H	-2.085781	-2.312275	1.517747
22	C	1.347811	-2.720467	-1.374715		52	H	-2.263545	-0.914082	2.577052
23	H	2.013727	-3.534170	-1.641678		53	H	-3.527691	-2.141289	2.516750
24	C	3.463816	-3.040997	0.623727		54	C	-2.714959	1.599310	-2.046284
25	H	2.749369	-3.851766	0.531593		55	H	-2.249922	2.437764	-1.517717
26	C	3.507945	2.966359	-1.850966		56	H	-1.920637	1.062095	-2.574398
27	H	3.353890	3.885611	-2.404974		57	H	-3.387679	2.015830	-2.797104
28	C	4.768263	2.378076	-1.787291		58	O	-6.880147	-0.363991	-0.595802
29	H	5.612633	2.837012	-2.289813		59	C	-7.680882	-1.186783	0.240372
30	C	5.532744	-2.202884	1.512221		60	H	-7.638585	-0.850662	1.281655
						61	H	-8.698843	-1.085211	-0.131624
						62	H	-7.372080	-2.235277	0.174513

P-**1c**$^{+}$ (with no imaginary frequency)										
SCF Done: E(RCAM-B3LYP) = -1361.74067345 A.U. after 11 cycles										
Center Number	Atom	X	Y	Z		Center Number	Atom	X	Y	Z
1	N	1.251880	0.616764	-0.047913		31	H	6.250344	-2.069759	-2.345529
2	C	-0.970017	1.304440	-0.721478		32	C	4.437186	-3.054300	-1.726933
3	C	3.893519	-0.714378	-0.293441		33	H	4.634160	-3.963049	-2.285232
4	C	2.433736	1.099010	0.659284		34	C	0.159772	3.588833	-1.890062
5	C	3.679711	0.488586	0.534450		35	H	0.594297	4.464906	-2.359847
6	C	1.664513	-1.728340	0.442433		36	C	-1.778436	2.241814	-1.430785
7	C	-1.516629	0.168801	-0.076412		37	H	-2.837262	2.041091	-1.530037
8	C	2.241425	2.176757	1.525671		38	C	-0.188919	-2.977156	1.433805
9	H	1.254776	2.613782	1.630840		39	H	-0.526291	-3.864902	1.956320
10	C	-0.631838	-0.823468	0.417935		40	C	-1.230393	3.355487	-1.999988
11	C	5.064581	-0.839672	-1.046928		41	H	-1.852758	4.051535	-2.550439
12	H	5.763928	-0.010842	-1.078023		42	C	-2.977498	0.013724	0.042753
13	C	0.770993	-0.635900	0.272845		43	C	-3.747800	0.996194	0.690561
14	C	0.432428	1.539599	-0.656352		44	C	-3.635613	-1.096469	-0.494519
15	C	2.975437	-1.774822	-0.263951		45	C	-5.114355	0.857105	0.814990
16	C	0.977348	2.710105	-1.227560		46	H	-3.261465	1.864424	1.123670
17	H	2.044117	2.884152	-1.173502		47	C	-5.015677	-1.231846	-0.404398
18	C	-1.081087	-2.008252	1.069410		48	H	-3.069699	-1.855658	-1.024921
19	H	-2.135603	-2.124822	1.278543		49	C	-5.763556	-0.256520	0.262319
20	C	4.741981	1.026809	1.274618		50	H	-5.710856	1.599061	1.333387
21	H	5.714189	0.551617	1.207044		51	H	-5.493897	-2.091743	-0.854950
22	C	1.164136	-2.860657	1.057001		52	O	-7.096874	-0.294174	0.421253
23	H	1.832325	-3.698458	1.225757		53	C	-7.831848	-1.391296	-0.108464
24	C	3.266077	-2.936004	-0.992205		54	H	-7.511674	-2.333843	0.346697
25	H	2.548894	-3.749668	-1.004629		55	H	-8.872214	-1.199607	0.146855
26	C	3.307565	2.693951	2.243682		56	H	-7.726822	-1.444813	-1.196678
27	H	3.150551	3.532560	2.912852						
28	C	4.568800	2.119743	2.108603						
29	H	5.410557	2.509357	2.670539						
30	C	5.339832	-1.996758	-1.760774						

Transition State (TS) of **1c**$^{+}$ (with only one imaginary frequency)										
SCF Done: E(UCAM-B3LYP) = -1361.67262006 A.U. after 9 cycles										
Center Number	Atom	X	Y	Z		Center Number	Atom	X	Y	Z
1	N	1.368716	0.907520	0.240099		31	H	4.789596	-3.624736	-2.633000
2	C	-0.865194	1.680916	-0.380393		32	C	3.125909	-3.980177	-1.311934
3	C	3.486990	-1.337608	-0.472784		33	H	2.975926	-5.005829	-1.631161
4	C	2.840587	1.094283	0.133255		34	C	-0.102517	4.321095	-0.300641
5	C	3.766045	0.031183	0.006165		35	H	0.128003	5.363843	-0.109128
6	C	1.462144	-1.515602	0.979969		36	C	-1.640663	2.673813	-1.040292
7	C	-1.457056	0.516692	0.153966		37	H	-2.589245	2.380445	-1.471198
8	C	3.395057	2.382663	0.108612		38	C	-0.376250	-2.152467	2.476634
9	H	2.792463	3.248606	-0.047499		39	H	-0.748724	-2.797306	3.263623
10	C	-0.626375	-0.324954	0.914873		40	C	-1.233815	3.979856	-1.061304
11	C	4.314580	-1.896700	-1.454077		41	H	-1.822339	4.742533	-1.557521
12	H	5.095691	-1.292077	-1.900993		42	C	-2.892526	0.223995	0.026044
13	C	0.788529	-0.276054	0.696178		43	C	-3.882309	1.162286	0.374542
14	C	0.474046	1.978974	0.008333		44	C	-3.305438	-1.032293	-0.433608
15	C	2.459417	-2.097176	0.061857		45	C	-5.221359	0.853326	0.262707
16	C	0.725024	3.353752	0.228825		46	H	-3.595754	2.128148	0.776287
17	H	1.512755	3.674362	0.886128		47	C	-4.650122	-1.343168	-0.582596
18	C	-1.177693	-1.241942	1.859564		48	H	-2.562103	-1.772983	-0.709897
19	H	-2.230535	-1.158350	2.096301		49	C	-5.619538	-0.398490	-0.230131
20	C	5.132507	0.300277	0.188516		50	H	-5.988482	1.561995	0.553138
21	H	5.808363	-0.546478	0.179249		51	H	-4.930474	-2.314692	-0.968005
22	C	0.915119	-2.339077	1.943339		52	O	-6.943986	-0.595784	-0.320428
23	H	1.483321	-3.217883	2.229764		53	C	-7.433765	-1.842114	-0.802648
24	C	2.280180	-3.419082	-0.366058		54	H	-7.118154	-2.664528	-0.153111
25	H	1.454184	-4.002317	0.025680		55	H	-8.518640	-1.759244	-0.783088
26	C	4.756075	2.628542	0.211163		56	H	-7.099484	-2.023588	-1.828892
27	H	5.101722	3.656238	0.198958						
28	C	5.642920	1.574612	0.335911						
29	H	6.704939	1.736302	0.480968						
30	C	4.140800	-3.209166	-1.869631						

M-**1c**$^{+}$ (with no imaginary frequency)										
SCF Done: E(RCAM-B3LYP) = -1361.74067345 A.U. after 11 cycles										
Center Number	Atom	X	Y	Z		Center Number	Atom	X	Y	Z
1	N	-1.251902	0.616823	-0.047825		31	H	-6.250179	-2.069403	-2.345882
2	C	0.969969	1.304335	-0.721634		32	C	-4.437070	-3.054011	-1.727309
3	C	-3.893493	-0.714292	-0.293451		33	H	-4.634020	-3.962662	-2.285778
4	C	-2.433726	1.099019	0.659430		34	C	-0.159802	3.588616	-1.890426
5	C	-3.679698	0.488590	0.534582		35	H	-0.594317	4.464674	-2.360252
6	C	-1.664525	-1.728320	0.442381		36	C	1.778336	2.241492	-1.431268
7	C	1.516626	0.168827	-0.076317		37	H	2.837130	2.040709	-1.530629
8	C	-2.241417	2.176636	1.525990		38	C	0.188799	-2.977149	1.433869
9	H	-1.254770	2.613654	1.631182		39	H	0.526152	-3.864899	1.956392
10	C	0.631809	-0.823404	0.418132		40	C	1.230300	3.355110	-2.000583
11	C	-5.064516	-0.839484	-1.047022		41	H	1.852615	4.050990	-2.551307
12	H	-5.763858	-0.010655	-1.078050		42	C	2.977490	0.013770	0.042780
13	C	-0.771017	-0.635861	0.272941		43	C	3.747808	0.996220	0.690673
14	C	-0.432453	1.539584	-0.656370		44	C	3.635667	-1.096369	-0.494530
15	C	-2.975418	-1.774740	-0.264083		45	C	5.114334	0.857143	0.815113
16	C	-0.977353	2.710068	-1.227652		46	H	3.261452	1.864423	1.123797
17	H	-2.044087	2.884237	-1.173502		47	C	5.015716	-1.231790	-0.404297
18	C	1.080977	-2.008190	1.069641		48	H	3.069799	-1.855513	-1.025037
19	H	2.135458	-2.124770	1.278894		49	C	5.763554	-0.256485	0.262455
20	C	-4.741938	1.026646	1.274911		50	H	5.710855	1.599087	1.333509
21	H	-5.714117	0.551404	1.207353		51	H	5.493951	-2.091704	-0.854794
22	C	-1.164196	-2.860678	1.056910		52	O	7.096836	-0.294207	0.421549
23	H	-1.832400	-3.698491	1.225526		53	C	7.831871	-1.391062	-0.108605
24	C	-3.266007	-2.935822	-0.992504		54	H	7.726579	-1.444346	-1.196802
25	H	-2.548818	-3.749475	-1.004994		55	H	8.872258	-1.199206	0.146498
26	C	-3.307526	2.693692	2.244126		56	H	7.512018	-2.333781	0.346422
27	H	-3.150505	3.532201	2.913421						
28	C	-4.568743	2.119458	2.109045						
29	H	-5.410465	2.508944	2.671124						
30	C	-5.339711	-1.996469	-1.761046						

P-**1d**$^+$ (with no imaginary frequency)										
SCF Done: E(RCAM-B3LYP) = -1016.31694107 A.U. after 11 cycles										
Center Number	Atom	X	Y	Z		Center Number	Atom	X	Y	Z
1	N	-1.166674	0.622469	0.040329		21	H	-5.755463	0.826414	-0.610965
2	C	1.156010	1.170130	0.441099		22	C	-1.364564	-2.783255	-1.281661
3	C	-3.826792	-0.631051	0.528669		23	H	-2.081016	-3.585070	-1.424708
4	C	-2.411633	1.207828	-0.454234		24	C	-3.241594	-2.931720	0.956960
5	C	-3.657612	0.631493	-0.217200		25	H	-2.573142	-3.773969	0.815646
6	C	-1.758247	-1.672311	-0.556660		26	C	-3.404408	2.963052	-1.777211
7	C	1.514602	0.058077	-0.316572		27	H	-3.294906	3.848860	-2.392778
8	C	-2.280734	2.348210	-1.249624		28	C	-4.663193	2.425071	-1.523371
9	H	-1.296699	2.755207	-1.453038		29	H	-5.551010	2.891077	-1.936512
10	C	0.559984	-0.863290	-0.749854		30	C	-5.149190	-1.973292	2.058724
11	C	-4.900263	-0.770881	1.413614		31	H	-5.982619	-2.056884	2.747655
12	H	-5.543013	0.082225	1.603109		32	C	-4.317762	-3.062757	1.822596
13	C	-0.806578	-0.625444	-0.427647		33	H	-4.493092	-4.007507	2.325473
14	C	-0.230701	1.465475	0.594281		34	C	0.346471	3.431765	1.853090
15	C	-2.979739	-1.725057	0.293947		35	H	0.039911	4.299306	2.427920
16	C	-0.616010	2.626245	1.301076		36	C	2.124198	2.050740	1.007538
17	H	-1.666081	2.853188	1.431821		37	H	3.175508	1.813794	0.881521
18	C	0.912735	-2.043966	-1.460839		38	C	-0.053665	-2.953253	-1.780681
19	H	1.952051	-2.204448	-1.727038		39	H	0.190552	-3.845055	-2.346252
20	C	-4.778795	1.270831	-0.765662		40	C	1.729515	3.155405	1.702038
						41	H	2.462004	3.820287	2.144784
						42	H	2.562447	-0.116044	-0.546633

Transition State (TS) of **1d**$^{+}$ (with only one imaginary frequency)										
SCF Done: E(UCAM-B3LYP) = -1016.24742288 A.U. after 11 cycles										
Center Number	Atom	X	Y	Z		Center Number	Atom	X	Y	Z
1	N	-1.153839	0.784595	-0.070489		21	H	-5.751905	0.447269	-0.849281
2	C	1.078394	1.057946	0.885903		22	C	-1.270542	-2.681449	-1.379906
3	C	-3.883300	-0.780198	0.349756		23	H	-1.990586	-3.428261	-1.697377
4	C	-2.526812	1.330292	-0.283406		24	C	-3.256279	-3.083473	0.671371
5	C	-3.701702	0.541015	-0.282747		25	H	-2.550966	-3.892055	0.514974
6	C	-1.748638	-1.623331	-0.631798		26	C	-3.933805	3.254449	-0.871928
7	C	1.394653	-0.248885	0.532485		27	H	-4.000577	4.328954	-1.000808
8	C	-2.727367	2.707049	-0.461801		28	C	-5.019446	2.433297	-1.116388
9	H	-1.969696	3.419773	-0.230933		29	H	-5.955721	2.823466	-1.498717
10	C	0.534465	-0.974127	-0.271330		30	C	-5.241569	-2.240661	1.727638
11	C	-4.992511	-0.991426	1.177312		31	H	-6.103292	-2.385926	2.369988
12	H	-5.658785	-0.165341	1.398731		32	C	-4.375109	-3.296628	1.463224
13	C	-0.836926	-0.551586	-0.330607		33	H	-4.554103	-4.275760	1.893839
14	C	-0.071079	1.634790	0.267369		34	C	1.082711	3.765923	0.504833
15	C	-3.009026	-1.825732	0.105608		35	H	1.160552	4.808147	0.213315
16	C	0.086685	3.002218	-0.065851		36	C	2.057562	1.866341	1.526599
17	H	-0.490085	3.460527	-0.846442		37	H	2.870565	1.366699	2.043470
18	C	0.989631	-2.147158	-0.943695		38	C	0.100854	-2.917550	-1.623401
19	H	2.050134	-2.373128	-0.917913		39	H	0.415499	-3.766782	-2.218140
20	C	-4.891941	1.101952	-0.773883		40	C	2.022477	3.225263	1.402222
						41	H	2.765939	3.855905	1.875022
						42	H	2.364902	-0.660015	0.796882

M-**1d**$^{+}$ (with no imaginary frequency)										
SCF Done: E(RCAM-B3LYP) = -1016.31694107 A.U. after 10 cycles										
Center Number	Atom	X	Y	Z		Center Number	Atom	X	Y	Z
1	N	-1.166335	0.622101	0.078296		21	H	-5.694104	0.752234	1.080846
2	C	1.120700	1.210650	-0.449437		22	C	-1.268315	-2.876482	1.143804
3	C	-3.856243	-0.603199	-0.307624		23	H	-1.972805	-3.690512	1.276928
4	C	-2.370789	1.161306	0.707348		24	C	-3.306084	-2.860960	-0.954779
5	C	-3.631338	0.598789	0.519180		25	H	-2.629631	-3.708261	-0.928861
6	C	-1.713776	-1.714846	0.538019		26	C	-3.261514	2.804126	2.231954
7	C	1.533592	0.045229	0.191363		27	H	-3.106053	3.640284	2.904442
8	C	-2.180472	2.237490	1.576748		28	C	-4.536045	2.281078	2.030994
9	H	-1.183770	2.632472	1.737748		29	H	-5.390461	2.709345	2.543464
10	C	0.612999	-0.911598	0.621409		30	C	-5.289326	-1.829823	-1.835062
11	C	-4.992413	-0.679609	-1.118979		31	H	-6.171552	-1.864112	-2.464919
12	H	-5.646798	0.182364	-1.193851		32	C	-4.443505	-2.930106	-1.746062
13	C	-0.773493	-0.656412	0.420428		33	H	-4.656305	-3.834047	-2.306227
14	C	-0.273328	1.510018	-0.476419		34	C	0.210491	3.570480	-1.618540
15	C	-2.994949	-1.707824	-0.221526		35	H	-0.137150	4.478271	-2.100305
16	C	-0.709062	2.719954	-1.060888		36	C	2.044931	2.137185	-1.016045
17	H	-1.765765	2.951061	-1.095728		37	H	3.102512	1.896469	-0.986778
18	C	1.016550	-2.141875	1.210891		38	C	0.075811	-3.077958	1.529941
19	H	2.072603	-2.317254	1.386355		39	H	0.360583	-4.009540	2.005212
20	C	-4.708329	1.188245	1.196852		40	C	1.600717	3.290186	-1.591933
						41	H	2.298898	3.990911	-2.034830
						42	H	2.595466	-0.140897	0.329214

$\mathbf{A}^+$ (with no imaginary frequency)										
SCF Done: E(RCAM-B3LYP) = -943.774633585 A.U. after 11 cycles										
Center Number	Atom	X	Y	Z		Center Number	Atom	X	Y	Z
1	N	-2.905243	0.017922	0.084254		21	C	2.096390	-0.302659	-1.165168
2	C	-0.132208	2.373327	-0.646439		22	C	1.328504	0.599534	2.482432
3	C	-0.810732	1.166853	-0.303776		23	C	5.698529	0.014262	0.050465
4	C	-0.823538	3.502385	-0.974826		24	C	1.377188	-0.620640	-2.452573
5	C	-2.236220	3.471181	-0.985792		25	H	0.951081	2.364864	-0.645941
6	C	-2.932059	2.338208	-0.648239		26	H	-0.299481	4.413773	-1.238089
7	C	-2.237101	1.160232	-0.281624		27	H	-2.788331	4.359181	-1.275115
8	C	-2.939609	-2.375670	0.520888		28	H	-4.010614	2.356896	-0.700738
9	C	-2.240844	-1.165006	0.295052		29	H	-4.018256	-2.413478	0.482442
10	C	-2.247410	-3.537157	0.752390		30	H	-2.802395	-4.455774	0.911169
11	C	-0.834817	-3.563885	0.777715		31	H	-0.313682	-4.494226	0.971252
12	C	-0.139828	-2.414336	0.540934		32	H	0.943508	-2.409989	0.538265
13	C	-0.814537	-1.185543	0.279594		33	H	-4.655847	-0.642843	1.035243
14	C	-0.097611	-0.006647	0.003519		34	H	-4.883573	-0.165381	-0.667853
15	C	-4.364574	0.065232	0.265575		35	H	-4.653128	1.051733	0.615078
16	C	1.393310	-0.006534	0.014997		36	H	3.997066	0.495525	2.119482
17	C	2.072947	0.284468	1.208725		37	H	4.037939	-0.531482	-2.032726
18	C	3.466399	0.274638	1.197554		38	H	2.025654	0.797509	3.297819
19	C	4.193704	-0.011114	0.043575		39	H	0.685514	-0.230253	2.793395
20	C	3.488548	-0.299661	-1.124540		40	H	0.691231	1.483006	2.372584
						41	H	6.068728	1.006347	-0.228746
						42	H	6.097015	-0.217885	1.040573
						43	H	6.112838	-0.702627	-0.661902
						44	H	0.735434	-1.502053	-2.353450
						45	H	2.090609	-0.822851	-3.252715
						46	H	0.742563	0.209336	-2.779685

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