Supporting Information

Efficient 8-oxyquinolinato emitters based on 9,10-dihydro-9,10-diboraanthracene scaffold for applications in optoelectronic devices

Krzysztof Durka,[a] Ireneusz Głowacki,[b,*] Sergiusz Luliński,[a,*] Beata Łuszczyńska,[b] Jaromir Smętek,[a] Paweł Szczepanik,[a] Janusz Serwatowski,[a] Urszula E. Wawrzyniak,[c] Grzegorz Wesela-Bauman,[a,d,*] Ewelina Witkowska,[b] Gabriela Wiosna-Sałyga[b] and Krzysztof Woźniak[d]

[a]*Physical Chemistry Department, Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664 Warszawa, Poland*
[b]*Department of Molecular Physics, Faculty of Chemistry, Lodz University of Technology, Żeromskiego 116, 90-924 Łódź, Poland*
[c]*Department of Microbioanalytics, Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664 Warszawa, Poland*
[d]*Laboratory of Crystallochemistry, Department of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warszawa, Poland.*

Table of Contents

1. Synthesis and NMR spectra of new compounds

Synthesis and characterization of compounds 1-10. Solvents used for reactions were dried by heating to reflux with sodium/benzophenone and distilled under argon. *n*-BuLi (10 M in hexane), *t*-BuLi (1.7 M in pentane), trialkyl borates $B(OR)_3$, DMAE, Ph_2O, 1,2-dibromo-4,5-difluorobenzene, 8-hydroxyquinoline and its derivatives were used as received without further purification. Syntheses of **1-4** were reported recently.[1,2] Therefore only DSC, UV-Vis and fluorescence data are provided for these compounds. Complexes **5-10** were prepared on a 10 mmol scale in a simple manner by complexation of respective organoboron precursors with stoichiometric amounts of appropriate ligands in Et_2O. After precipitation from reaction mixtures as yellow microcrystalline solids, they were filtered, washed with Et_2O and dried *in vacuo*. All reaction yields are close to 95%. Compounds **5-7** are sparingly soluble in common solvents so we were unable to record reliable ^{13}C NMR spectra even after prolonged acquisition. In the ^{13}C NMR spectra the resonances of boron-bound carbon atoms were not observed in most cases as a result of broadening by a quadrupolar boron nucleus. ^{1}H and ^{13}C NMR chemical shifts are given relative to TMS using residual solvent resonances. ^{11}B and ^{19}F NMR chemical shifts are given relative to $BF_3{\cdot}Et_2O$ and $CFCl_3$, respectively. All complexes were characterized by elemental analyses and HRMS (ES).

Diisopropyl (2-bromo-4,5-difluorophenyl)boronate (**5a**): 2.5 M *n*-BuLi in hexane (42.0 mL, 0.105 mol *n*-BuLi) was added dropwise to the stirred solution of 1,2-dibromo-4,5-difluorobenzene (27.2 g, 0.1 mol) in PhMe/THF (4:1, 80 mL) at –70 °C. The resulting white slurry was stirred for 15 min followed by a slow addition of $B(O\textit{i}Pr)_3$ (18.8 g, 0.1 mol). The mixture was allowed to warm slowly to –30 °C. Then Me_3SiCl (14 mL, 0.11 mol) was added and the mixture was warmed to room temperature. The resultant suspension was filtered under argon and concentrated. The oily residue was distilled under reduced pressure (b.p. 64–68 °C /1 Tr) to give crude product in 53% (15.2 g) yield. ^{1}H NMR ($CDCl_3$, 400.0 MHz): δ = 7.30 (dd, J = 10.0, 7.0 Hz, 1H, Ph), 7.04 (t, J = 9.0, 1H, Ph), 4.35 (m, 2 H, O*i*Pr), 1.20 (d, J = 6.0 Hz, 12 H, O*i*Pr) ppm. $^{13}C\{^{1}H\}$NMR ($CDCl_3$, 100.6 MHz): δ = 151.1 (dd, $J_{C,F}$ = 52.0, 13.0 Hz, CF), 148.6 (dd, $J_{C,F}$ = 49.5, 13.5 Hz, CF), 121.0 (d, $J_{C,F}$ = 19.0 Hz), 120.5 (d, $J_{C,F}$ = 17.0 Hz), 118.6, 67.1, 24.2 ppm. ^{11}B NMR ($CDCl_3$, 64.2 MHz): δ = 27.0 ppm.

2,3,7,8-Tetrafluoro-9,10-dihydroxy-9,10-dihydro-9,10-diboraanthracene (**5b**). A solution of *t*-BuLi (1.7 M, 14.0 mL, 0.024 mol) was slowly added to a stirred solution of **5a** (3.21 g, 10.0 mmol) in THF (40 mL) at –85 °C. The lithiate was stirred for 1 hr and then it was warmed to –30 °C, quenched with H_2SO_4 (1.5 M) to pH = 5 and stirred for *ca.* 10 min at room

temperature. The water phase was separated followed by the extraction with Et_2O (3 × 20 mL). The extracts were added to the organic phase, which was concentrated under reduced pressure. A solid residue was filtered and washed with hexane (10 mL). Drying *in vacuo* afforded a white powder of **5b**, m.p. > 350 °C (dec.), yield 0.63 g (41%).
^{1}H NMR (acetone-d_6, 400 MHz): δ = 9.49 (broad, 2H, OH), 7.93 (t, $J_{H,F}$ = 10.0 Hz, 4H, Ph) ppm. ^{19}F NMR (acetone-d_6, 367.5 MHz): δ = –135.5 (t, $J_{H,F}$ = 10.0 Hz) ppm. ^{13}C{^{1}H}NMR ($CDCl_3$, 100 MHz): δ = 154.2 (d, J = 248 Hz), 139.5 (d, J = 11 Hz) ppm. ^{11}B NMR (acetone-d_6, 64.2 MHz): δ = 40.5 ppm. Anal. calcd. for $C_{12}H_6B_2F_4O_2 \cdot 1.5H_2O$ (306.81): C, 46.98%; H, 2.96%. Found: C, 47.63%; H, 3.22%.

10-(*N,N*-Dimethylaminoethanolato)phenoxaborin (**9a**): A solution of diphenyl ether (34.0 g, 0.2 mol) in 50 ml THF was added dropwise to a stirred solution of *n*-BuLi (10 M in hexane, 41.0 ml, 0.41 mol) in 200 ml THF at −70 °C during 0.5 hr. The mixture was warmed slowly to 0 °C and stirred for 4 hrs. The mixture was cooled to −70 °C and $B(OMe)_3$ (22.4 mL, 0.21 mol) was added. The cooling bath was removed, the mixture was warmed to 0 °C and stirred for additional 1 hr. Then, the reaction was quenched with 1.5 M H_2SO_4 to pH = 5 and stirred at room temperature for 30 min. The aqueous phase was separated and extracted with Et_2O (2 × 50 mL). The extracts were added to the organic phase, dried over sodium sulfate and concentrated under reduced pressure. Et_2O (10 mL) and hexane (30 ml) were added to the remaining viscous residue followed by filtration of the resulting slurry. The obtained solid was washed with *n*-hexane (2 × 10 ml) and dried *in vacuo* to give crude 10-hydroxyphenoxaborin. It was dissolved in Et_2O (20 mL) and DMAE (5.2 g, 0.06 mol) was added. The mixture was stirred for 1 hr and then addition of hexane (100 mL) resulted in precipitation of a white solid. It was filtered, washed with hexane (2 × 20 mL) and dried *in vacuo* to give **9a**, m.p. = 105−108 °C, yield 29.4 g (56%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.64 (d, J = 7.0 Hz, 2H, Ph), 7.27 (t, J = 7.0 Hz, 2H, Ph), 7.13 (m, 4H, Ph), 4.47 (broad, 2H, $OCH_2CH_2N(CH_3)_2$), 3.11 (broad, 2H, $OCH_2CH_2N(CH_3)_2$), 2.14 (broad, 6H, $OCH_2CH_2N(CH_3)_2$) ppm. ^{13}C{^{1}H}NMR ($CDCl_3$, 100 MHz): δ = 158.7, 132.0, 128.1, 122.0, 115.8, 62.2, 58.1, 45.5 ppm. ^{11}B NMR ($CDCl_3$, 64.2 MHz): δ = 5.5 ppm. Anal. calcd for $C_{16}H_{18}BNO_2$ (267.13): C, 71.94%; H, 6.79%; N, 5.24%. Found: C, 71.85%; H, 6.97%; N, 4.87%.

10-Hydroxyphenoxaborin (**9b**): **9a** (4.0 g, 15.0 mmol) was dissolved in Et_2O (15 mL) and hydrolyzed by the addition of 1.5 M H_2SO_4 to pH = 5. The aqueous phase was separated and extracted with Et_2O (2 × 10 mL). Combined organic phases were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. To the remaining residue Et_2O (15 mL) and

hexane (40 mL) were added. The precipitated white solid was filtered and dried *in vacuo* to give **9b**, m.p. = 223−225 °C, yield 1.9 g (75%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.97 (d, J = 7.0 Hz, 2H), 7.65 (t, 2H), 7.45 (d, J = 8.5 Hz, 2H), 7.28 (t, 2H) ppm. $^{13}C\{^{1}H\}$NMR ($CDCl_3$, 100 MHz): δ = 162.1, 134.0, 132.3, 122.9, 118.0 ppm. ^{11}B NMR ($CDCl_3$, 64.2 MHz): δ = 36.5 ppm. Anal. calcd. for $C_{12}H_9BO_2$ (196.01): C, 73.53%; H, 4.63%. Found: C, 71.73%; H, 4.88%.

9,10-Bis(8-oxyquinolinato)-9,10-dihydro-9,10-diboraanthracene (**1**).

DSC (first heating cycle): T_m = 344.0 °C (dec.). UV-Vis (5×10^{-6} M in CH_2Cl_2): λ_{max} = 390 nm, ε = 4600 $cm^{-1}\,M^{-1}$. Fluorescence: λ_{exc} = 390 nm, λ_{em} = 494 nm, Φ = 48%.

1,6-Difluoro-9,10-bis(8-oxyquinolinato)-9,10-dihydro-9,10-diboraanthracene (**2**).

DSC (first heating cycle): **2a**, T_c = 274.0 °C, T_m = 368.9 °C; **2b**, T_c = 278.4 °C, T_m = 367.4 °C. UV-Vis (5×10^{-6}M in CH_2Cl_2): λ_{max} = 397 nm, ε = 8200 $cm^{-1}M^{-1}$. Fluorescence: λ_{exc} = 397 nm, λ_{em} = 503 nm, Φ = 52%.

1,6-Dichloro-9,10-bis(8-oxyquinolinato)-9,10-dihydro-9,10-diboraanthracene (**3**).

DSC (first heating cycle): T_m = 392.6 °C. UV-Vis (5×10^{-6} M in CH_2Cl_2): λ_{max} = 396 nm, ε = 7100 $cm^{-1}\,M^{-1}$. Fluorescence: λ_{exc} = 396 nm, λ_{em} = 502 nm, Φ = 53%.

1,6-Dibromo-9,10-bis(8-oxyquinolinato)-9,10-dihydro-9,10-diboraanthracene (**4**).

DSC (first heating cycle): T_m = 361.5 (dec.). UV-Vis (5×10^{-6} M in CH_2Cl_2): λ_{max} = 396 nm, ε = 3800 $cm^{-1}\,M^{-1}$. Fluorescence: λ_{exc} = 396 nm, λ_{em} = 502 nm, Φ = 41%.

2,3,7,8-Tetrafluoro-9,10-bis(8-oxyquinolinato)-9,10-dihydro-9,10-diboraanthracene (**5**).

M.p. = 283 °C (dec.). ^{1}H NMR ($CDCl_3$, 400.0 MHz): δ = 8.55 (dd, J = 5.0, 1.0 Hz, 2H, Q), 8.48 (dd, J = 8.5 Hz, 2H, Q), 7.77 (t, J = 8.0 Hz, 2H, Q), 7.65 (dd, 2H, Q), 7.38 (d, 2H, Q), 7.28 (d, 2H, Q), 6.65 (t, J = 10.0 Hz, 4H, Ph). ^{19}F NMR ($CDCl_3$, 367.5 MHz): δ = –142.1 (t, J = 9.5 Hz) ppm. ^{11}B NMR ($CDCl_3$, 64.2 MHz): δ = 11.3 ppm. Anal. calcd for $C_{30}H_{16}B_2F_4N_2O_2$ (534.08): C, 67.47%; H, 3.02%; N, 5.25%. Found: C, 67.28%; H, 3.35%; N, 5.22%. HRMS (ES): calcd. For $C_{30}H_{16}B_2F_4N_2O_2$ $[M+Na]^+$ 557.1232; found 557.1247. UV-Vis (5×10^{-6} M in CH_2Cl_2): λ_{max} = 396 nm, ε = 10000 $cm^{-1}\,M^{-1}$. Fluorescence: λ_{exc} = 396 nm, λ_{em} = 504 nm, Φ = 63%.

1,6-Difluoro-9,10-bis(5-chloro-8-oxyquinolinato)-9,10-dihydro-9,10-diboraanthracene (**6**): M.p. = 400 °C (dec.). ^{1}H NMR ($CDCl_3$, 400.0 MHz): δ = 8.66 (d, J = 8.0, 2H, Q), 8.42 (d, J = 5.0 Hz, 2H, Q), 7.75 (d, J = 8.0 Hz, 2H, Q), 7.66 (dd, 2H, Q), 7.14 (d, 2H, Q), 7.00 (m, 2 H, Ph), 6.65 (d, J = 7.0 Hz, 2H, Ph), 6.52 (m, 2 H, Ph) ppm. ^{11}B NMR (DMSO-d_6, 64.2 MHz): δ = 9.7 ppm. Anal. calcd for $C_{30}H_{16}B_2Cl_2F_2N_2O_2$ (566.99): C, 63.55%; H, 2.84%; N, 4.94%. Found: C, 63.36%; H, 3.02%; N, 4.59%. HRMS (ES): calcd. for $C_{30}H_{16}B_2Cl_2F_4N_2O_2$

$[M+Na]^+$ 565.0894; found 565.0890. UV-Vis (5×10^{-6} M in CH_2Cl_2): λ_{max} = 414 nm, ε = 9400 cm^{-1} M^{-1}. Fluorescence: λ_{exc} = 414 nm, λ_{em} = 516 nm, Φ = 26%.

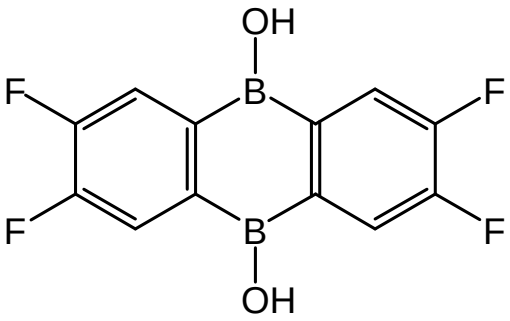
1,6-Difluoro-9,10-bis(5,7-dichloro-8-oxyquinolinato)-9,10-dihydro-9,10-diboraanthracene (**7**): M.p. = 440 °C (dec.). ^{1}H NMR (DMSO-d_6, 400.0 MHz): δ = 8.91 (d, J = 8.5, 2H, Q), 8.68 (d, J = 5.0 Hz, 2H, Q), 8.12 (s, 2H, Q), 8.04 (dd, 2H, Q), 7.05 (m, 2H, Q), 6.50 (d, J = 7.5 Hz, 2H, Ph), 6.49 (d, 2H, Ph) ppm. ^{11}B NMR (DMSO-d_6, 64.2 MHz): δ = 9.1 ppm. Anal. calcd. for $C_{30}H_{16}B_2Cl_4F_2N_2O_2$ (635.88): C, 56.67%; H, 2.22%; N, 4.39%. Found: C, 56.61%; H, 2.58%; N, 4.75%. HRMS (ES): calcd. for $C_{30}H_{16}B_2Cl_4F_2N_2O_2$ $[M+Na]^+$ 656.9880; found 656.9875. UV-Vis (5×10^{-6} M in CH_2Cl_2): λ_{max} = 390 nm, ε = 45800 $cm^{-1}M^{-1}$. Fluorescence: λ_{exc} = 390 nm, λ_{em} = 494 nm, Φ = 48%.

4,8-Bis(8-oxyquinolinato)-4,8-dihydro-p-diborino[2,3-b:5,6-b']dithiophene (**8**): ^{1}H NMR (DMSO-d_6, 400.0 MHz): δ = 8.59 (d, J = 4.0, 2H, Q), 8.15 (d, J = 7.5 Hz, 2H, Q), 7.78 (t, J = 8.0 Hz, 2H, Q), 7.38 (dd, 2H, Q), 7.25 (d, 2H, Q), 7.20 (d, 2H, Q), 6.90 (d, J = 7.5 Hz, 2H, Th), 6.71 (d, 2H, Th). ^{13}C NMR (DMSO-d_6, 100 MHz): δ = 158.1, 146.0, 141.7, 136.0, 132.1, 129.7, 129.3, 128.6, 121.0, 111.7, 108.6 ppm. ^{11}B NMR (DMSO-d_6, 64.2 MHz): δ = 7.9 ppm. Anal. calcd. for $C_{26}H_{16}B_2N_2O_2S_2$ (474.17): C, 65.86%; H, 3.40%; N, 5.91%. Found: C, 64.14%; H, 4.13%; N, 6.48%. HRMS (EI): calcd. for $C_{26}H_{16}B_2N_2O_2S_2$ $[M]^+$ 474.0839; found 474.0846. DSC (first heating cycle): T_m = 360.7 °C. UV-Vis (5×10^{-6} M in CH_2Cl_2): λ_{max} = 392 nm, ε = 4800 cm^{-1} M^{-1}. Fluorescence: λ_{exc} = 392 nm, λ_{em} = 506 nm, Φ = 22%.

10-(8-Oxyquinolinato)phenoxaborin (**9**): M.p. = 365 °C (dec.). ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.40 (d, J = 8.5 Hz, 1H), 8.03 (d, J= 5.0 Hz, 1H), 7.74 (t, J= 8.0 Hz, 1H), 7.49 (dd, 1H), 7.30 (m, 6H), 7.09 (dd, J = 7.0, 1.0 Hz, 2H), 6.96 (td, J= 1.5 Hz, 2H) ppm. ^{13}C{^{1}H}NMR (acetone-d_6, 100 MHz): δ = 159.7, 157.7, 141.6, 140.3, 133.5, 133.4, 129.6, 129.0, 124.9, 122.8, 118.0, 116.7, 113.6, 109.1 ppm. ^{11}B NMR ($CDCl_3$, 64.2 MHz): δ = 8.8 ppm. Anal. calcd. for $C_{21}H_{14}BNO_2$ (323.15): C, 78.05%; H, 4.37%; N, 4.33%. Found: C, 76.00%; H, 4.37%; N, 4.64%. HRMS (ES): calcd. for $C_{21}H_{14}BNO_2$ $[M+Na]^+$ 346.1015; found 346.1015. UV-Vis (5×10^{-6} M in CH_2Cl_2): λ_{max} = 390 nm, ε = 4200 cm^{-1} M^{-1}. Fluorescence: λ_{exc} = 390 nm, λ_{em} = 510 nm, Φ = 19%.

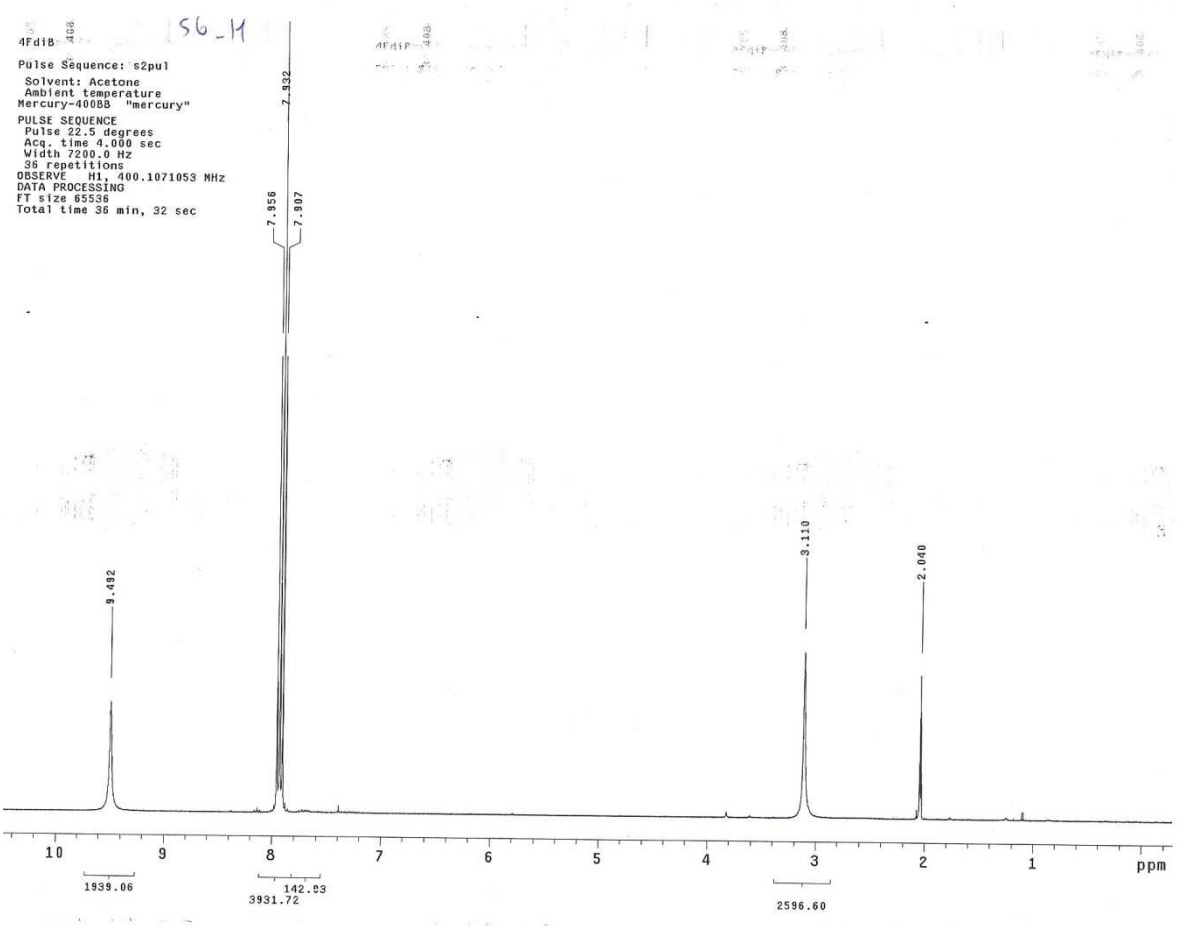
1,6-Difluoro-9,10-bis(benzo[h]-10-oxyquinolinato)-9,10-dihydro-9,10-diboraanthracene (**10**): M.p. = 460 °C (dec.). ^{1}H NMR (DMSO-d_6, 400 MHz): δ = 8.86 (d, J = 8.0 Hz, 2H, BQ – benzo[h]-10-oxyquinolinato ligand), 8.55 (d, J = 6.0 Hz, 2H, BQ), 8.15 (d, J = 9.0 Hz, 2H, BQ), 8.05 (d, 2H, BQ), 7.82 (dd, 2H, BQ), 7.72 (t, J = 8.0 Hz, 2H, BQ), 7.50 (d, 2H, BQ), 6.99 (d, 2H, BQ), 6.86 (m, 2H, Ph), 6.64 (d, J = 8.0 Hz, 2H), 6.54 (m, 2H, Ph) ppm. ^{19}F NMR

($CDCl_3$, 367.5 MHz): δ = –103.1 (m) ppm. ^{11}B NMR ($CDCl_3$, 64.2 MHz): δ = 8.3 ppm. Anal. calcd. for $C_{38}H_{22}B_2F_2N_2O_2$ (598.21): C, 76.30%; H, 3.71%; N, 4.68%. Found: C, 76.24%; H, 3.73%; N, 4.37%. HRMS (ES): calcd. for $C_{38}H_{22}B_2F_2N_2O_2$ $[M+Na]^+$ 597.1986; found 597.1974. UV-Vis (5×10^{-6} M in CH_2Cl_2): λ_{max} = 427 nm, ε = 12000 $cm^{-1}\,M^{-1}$. Fluorescence: λ_{exc} = 427 nm, λ_{em} = 550 nm, Φ = 19%.

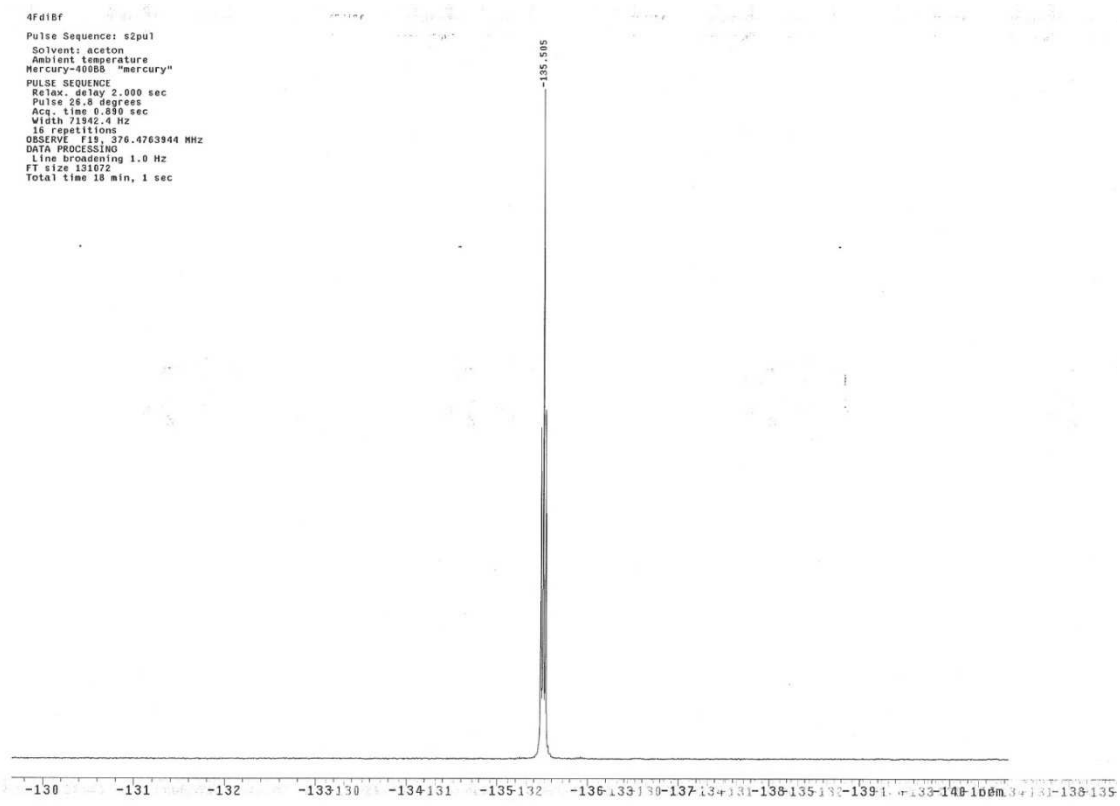


5b

^{1}H NMR ($CDCl_3$ solution)

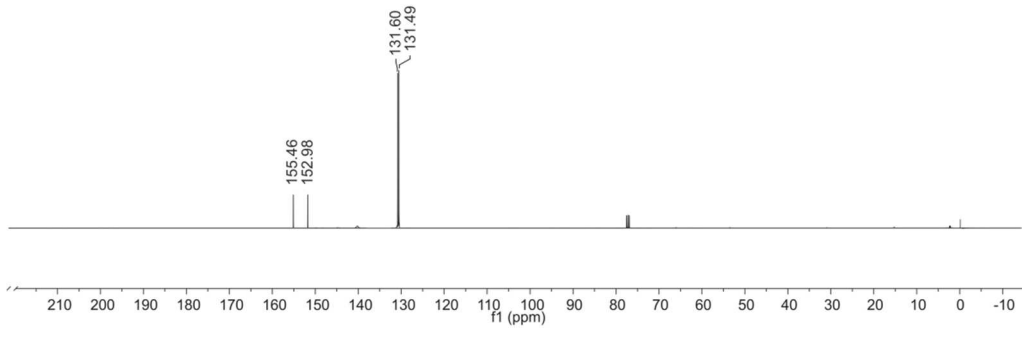


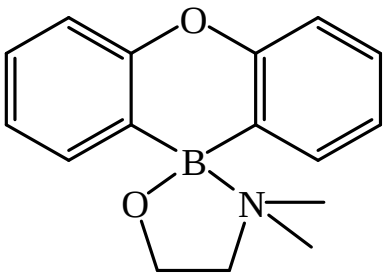
^{19}F NMR ($CDCl_3$ solution)



^{13}C NMR ($CDCl_3$ solution)

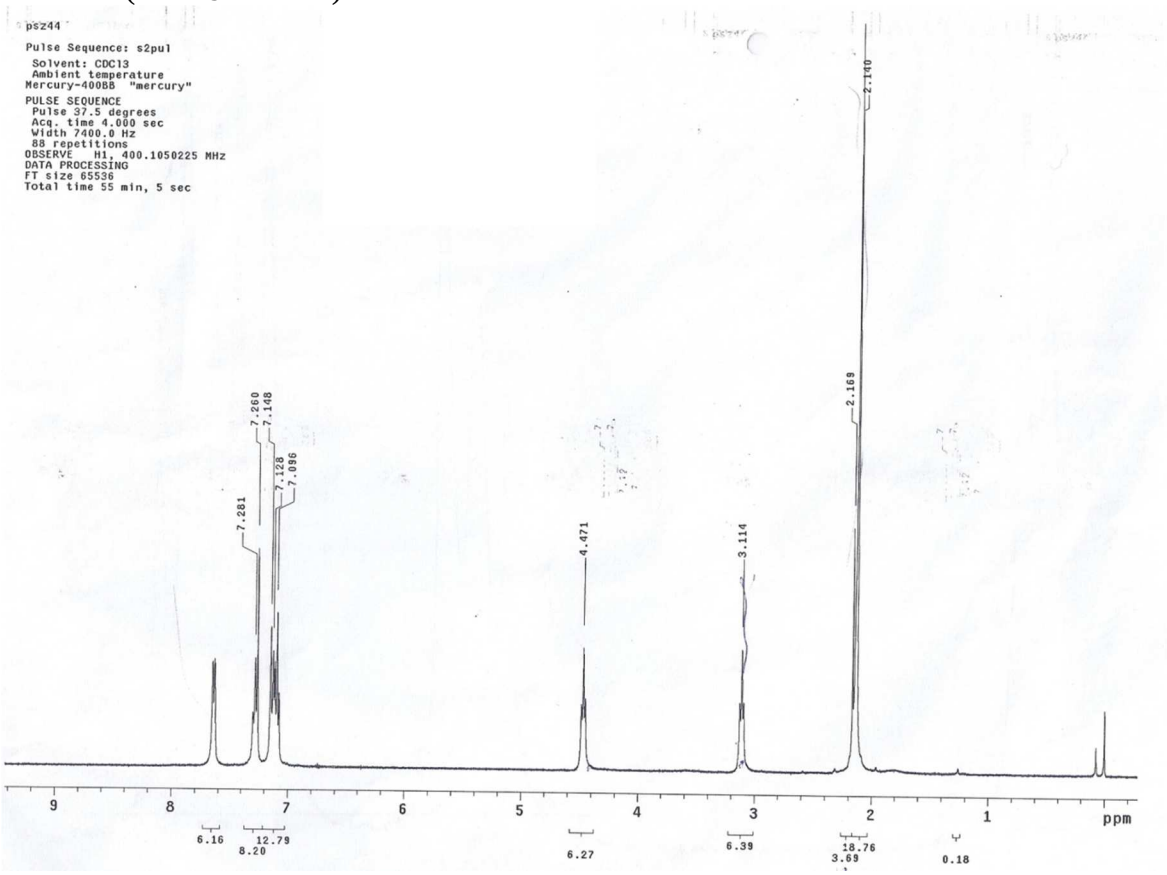
Parameter	Value
1 Origin	Varian
2 Solvent	cdcl3
3 Temperature	25.0
4 Number of Scans	2000
5 Spectrometer Freq.	100.57
6 Nucleus	13C



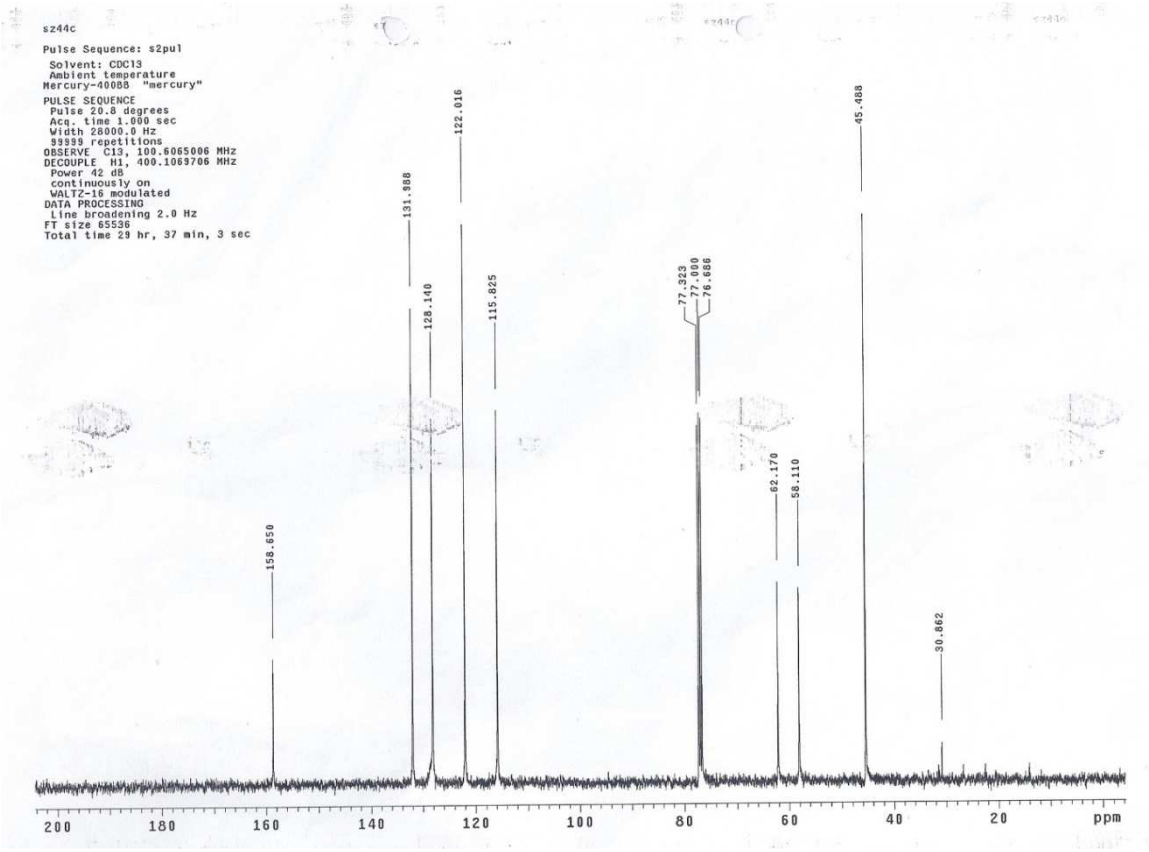


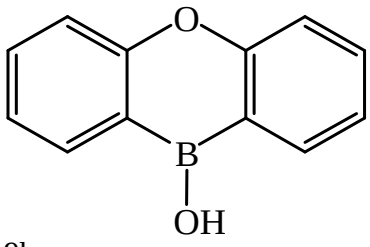
9a

^{1}H NMR ($CDCl_3$ solution)



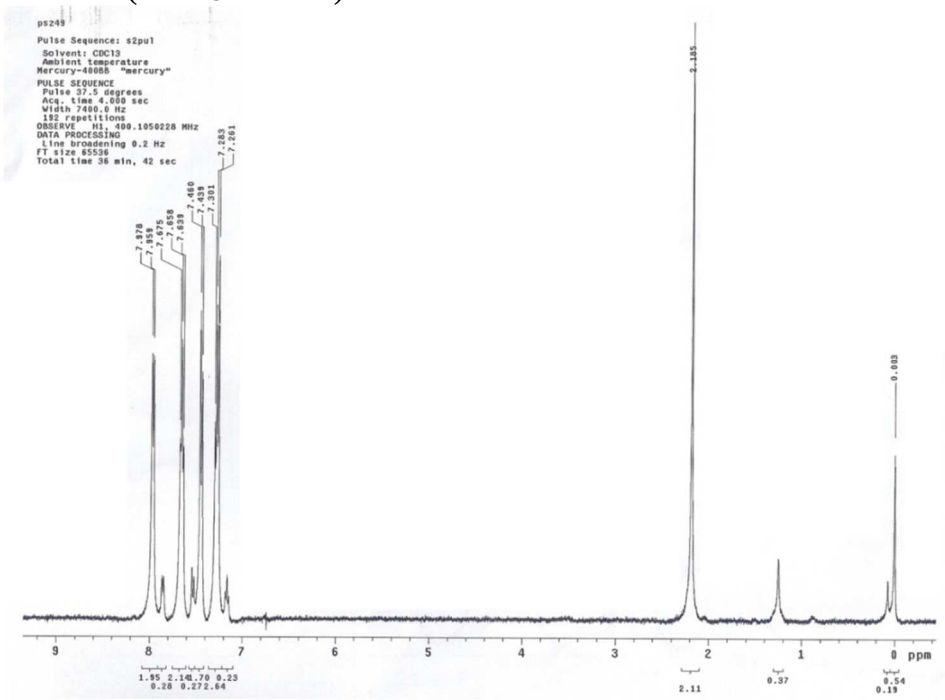
^{13}C NMR ($CDCl_3$ solution)



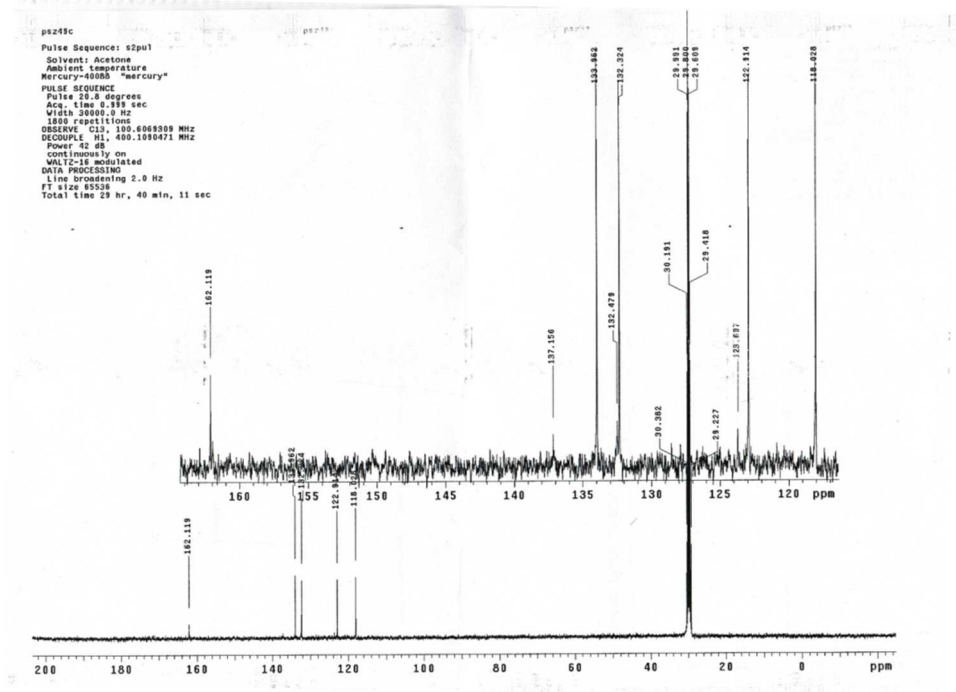


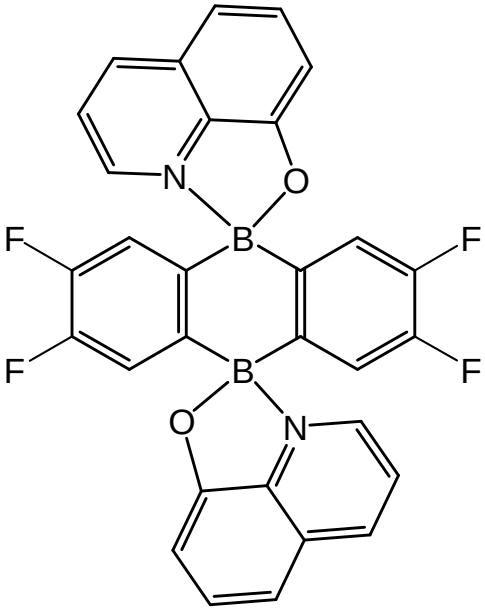
9b

^{1}H NMR ($CDCl_3$ solution)



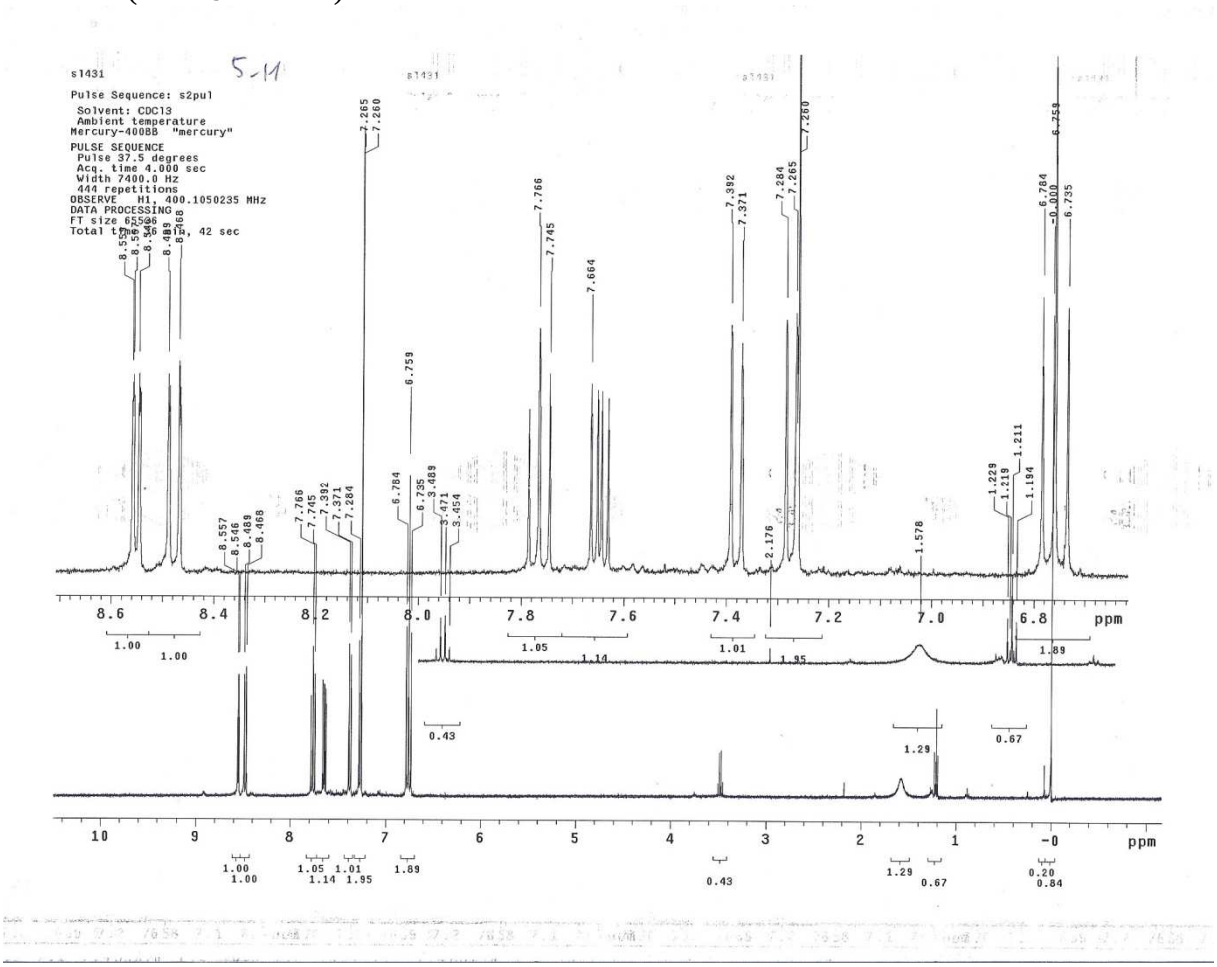
^{13}C NMR ($CDCl_3$ solution)



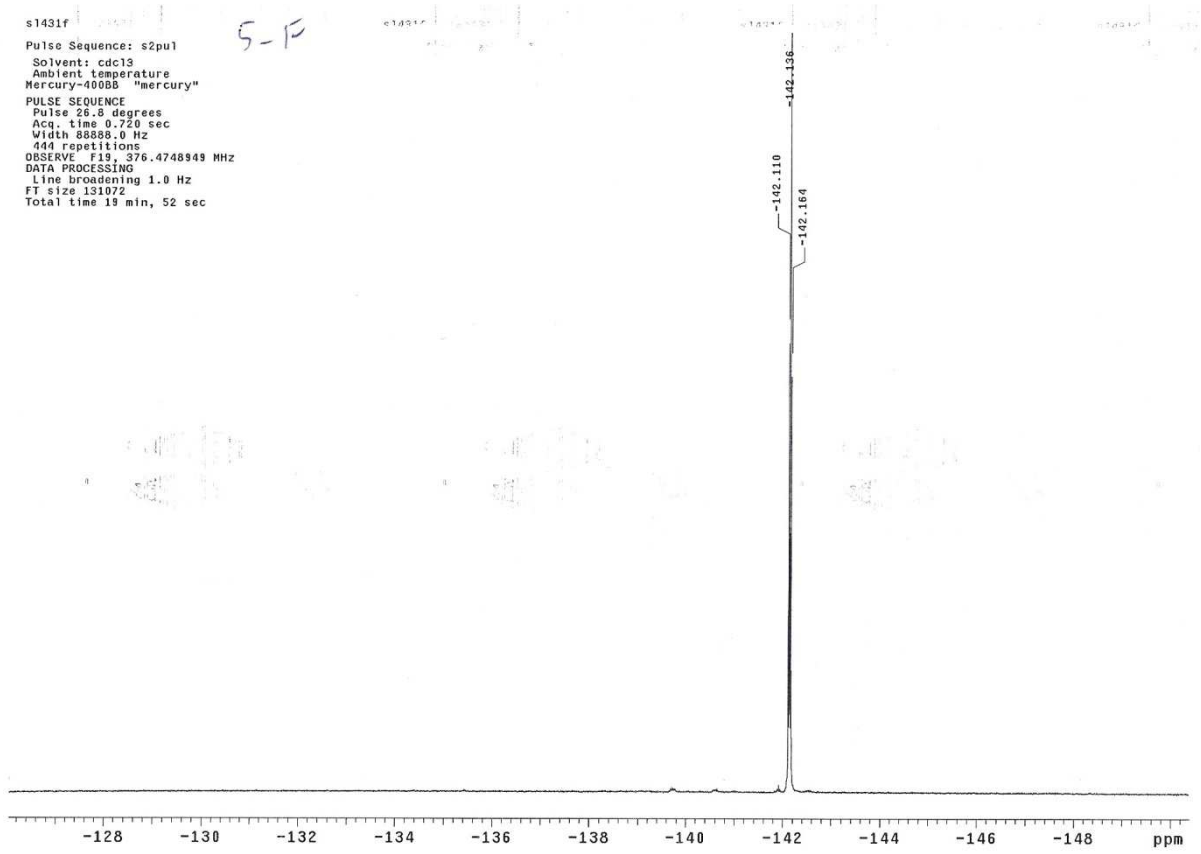


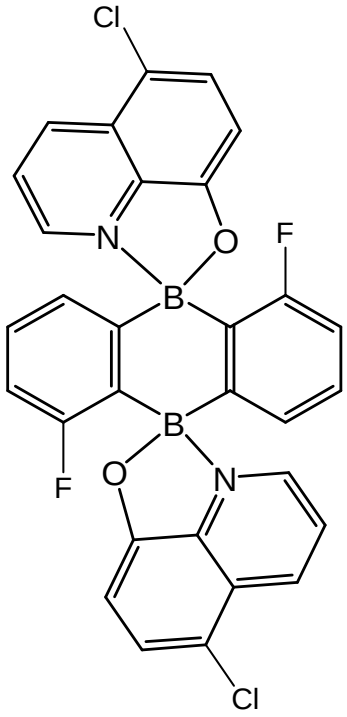
5

^{1}H NMR ($CDCl_3$ solution)



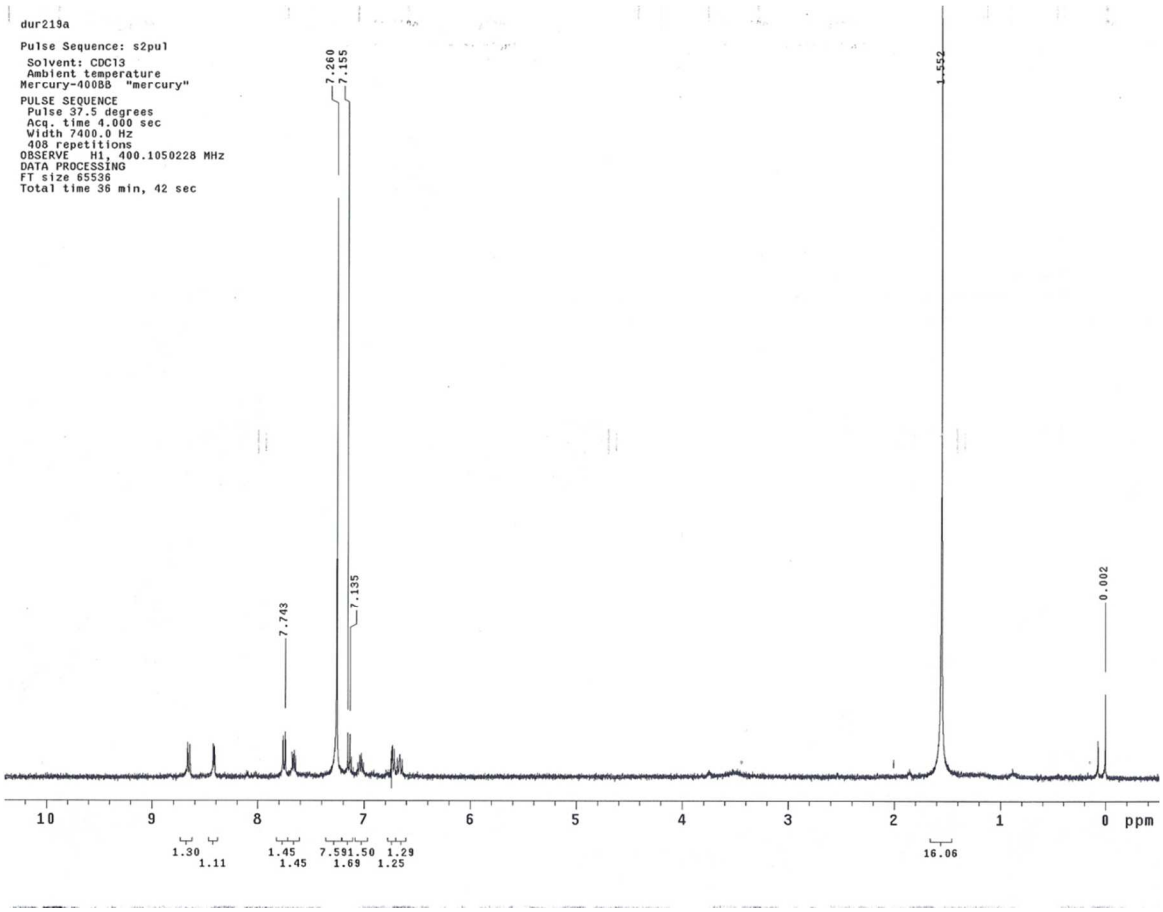
^{19}F NMR ($CDCl_3$ solution)

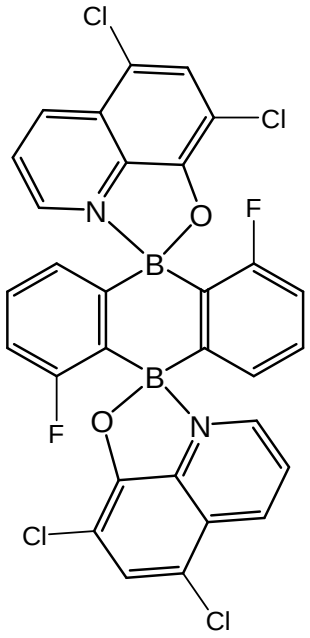




6

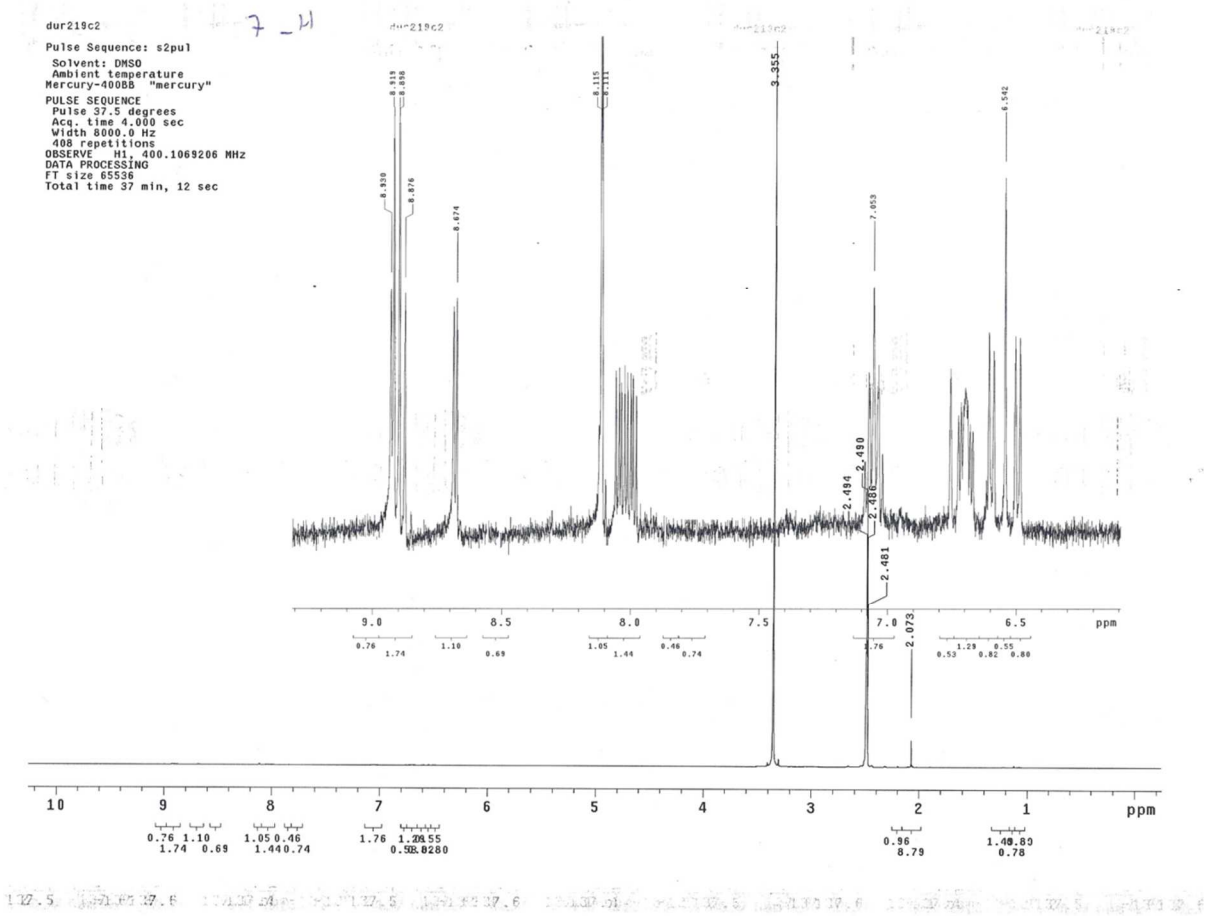
^{1}H NMR ($CDCl_3$ solution)

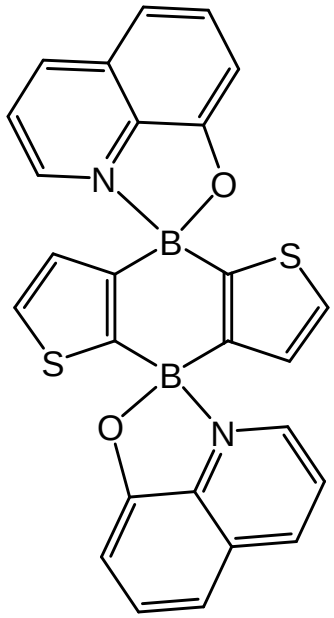




7

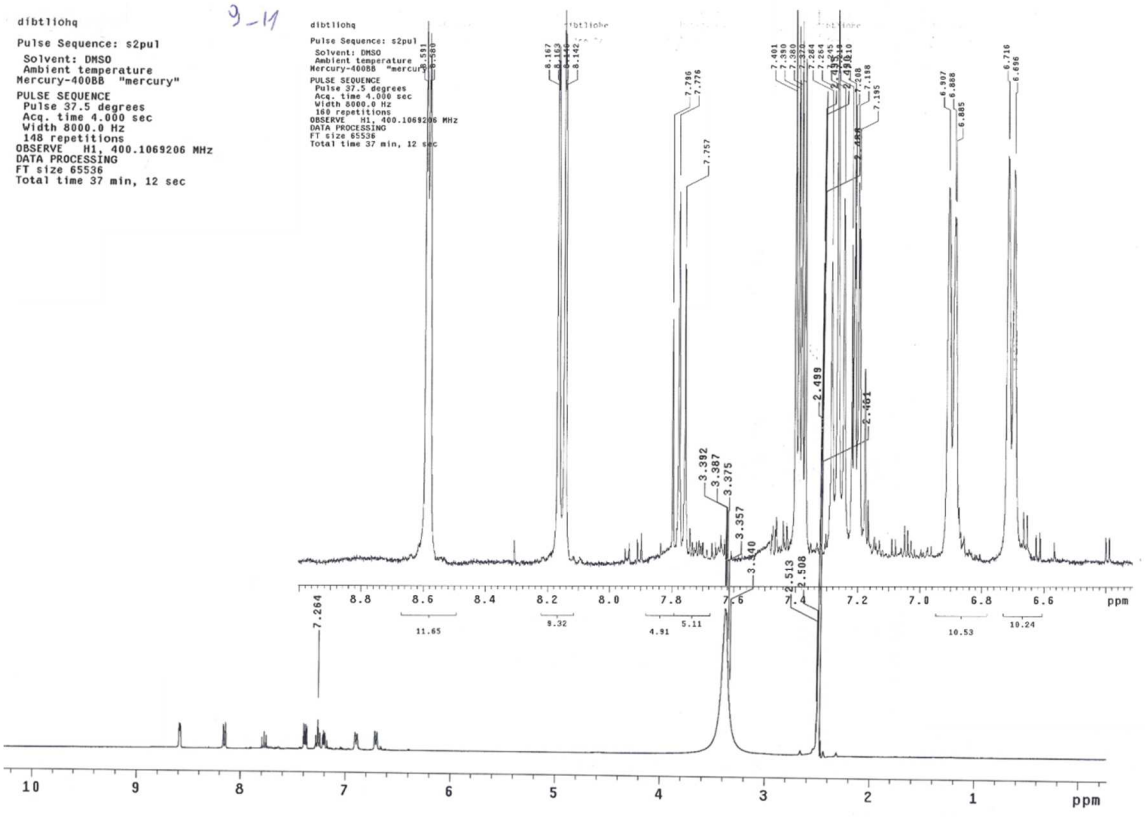
^{1}H NMR (DMSO-d_6 solution)



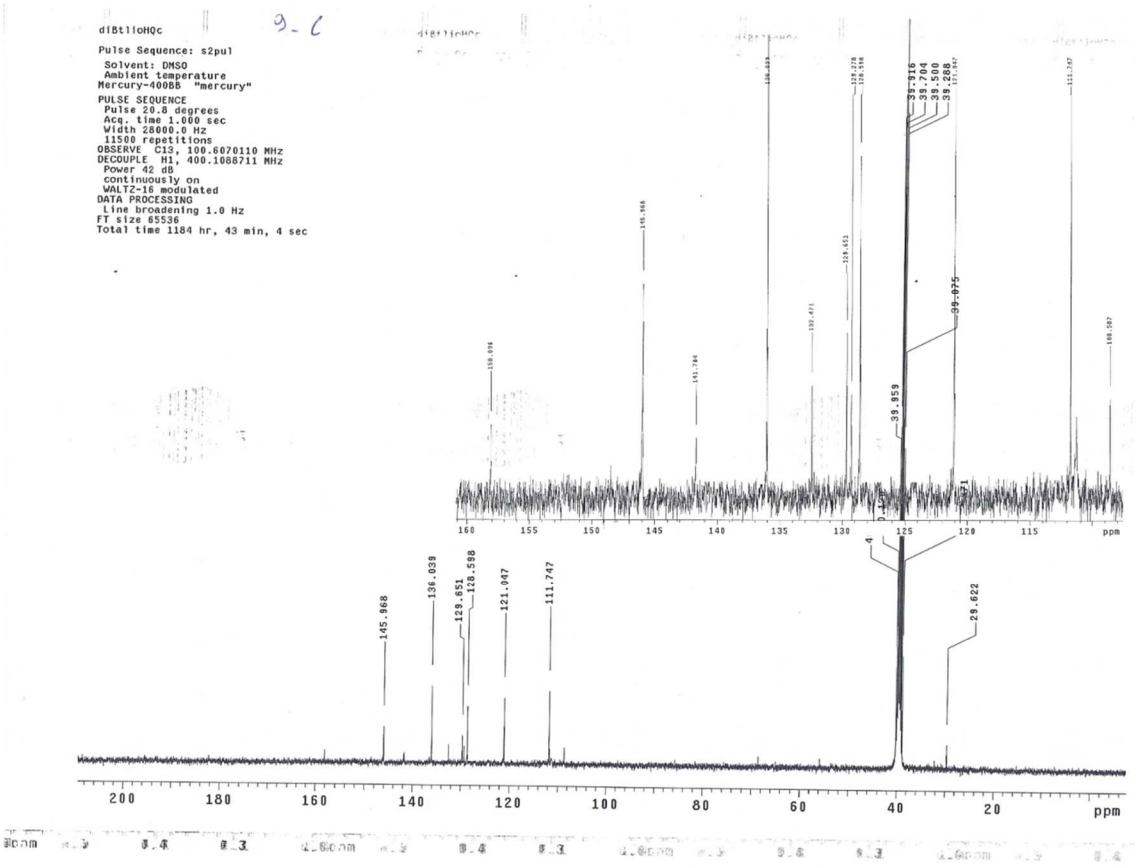


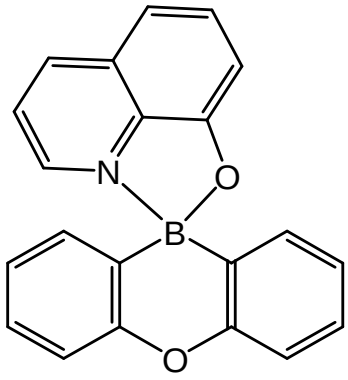
8

^{1}H NMR (DMSO-d_6 solution)



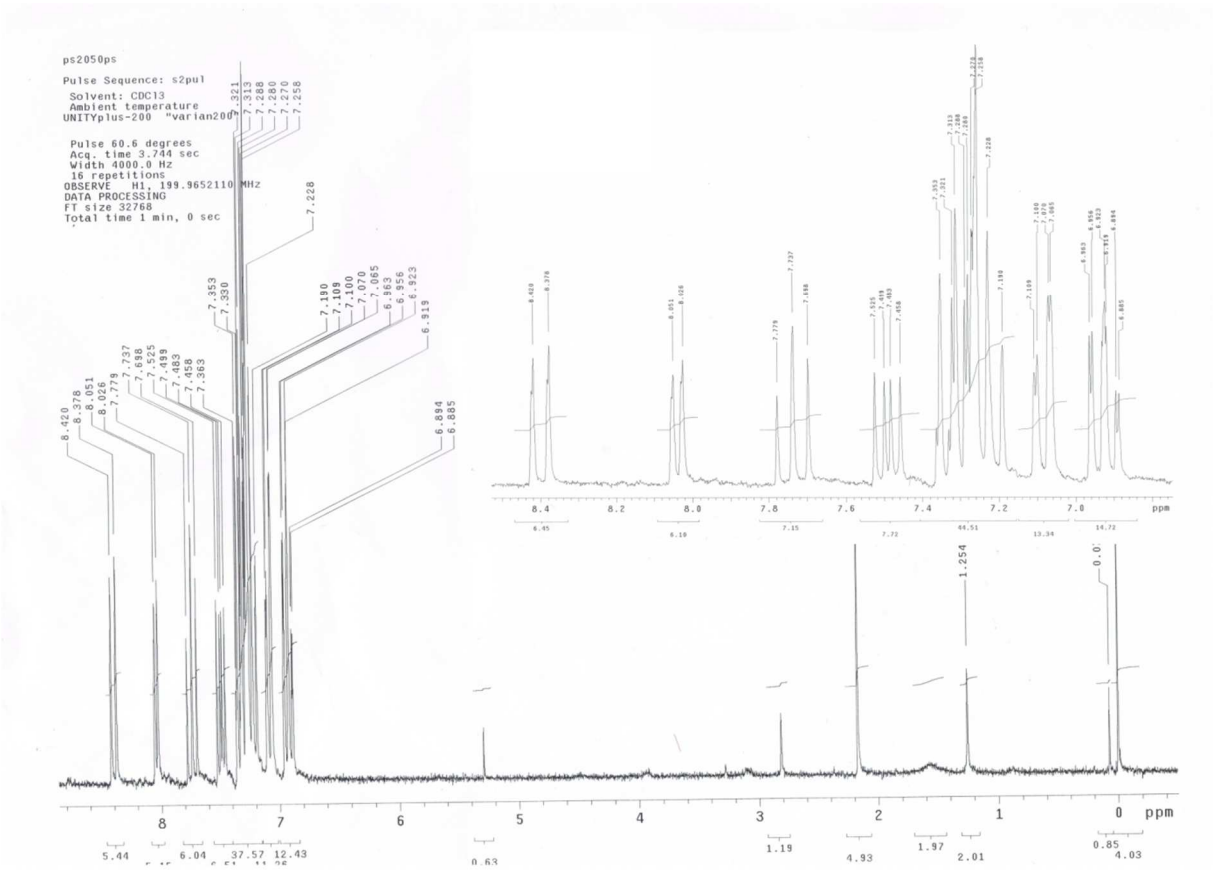
^{13}C NMR (DMSO-d_6 solution)



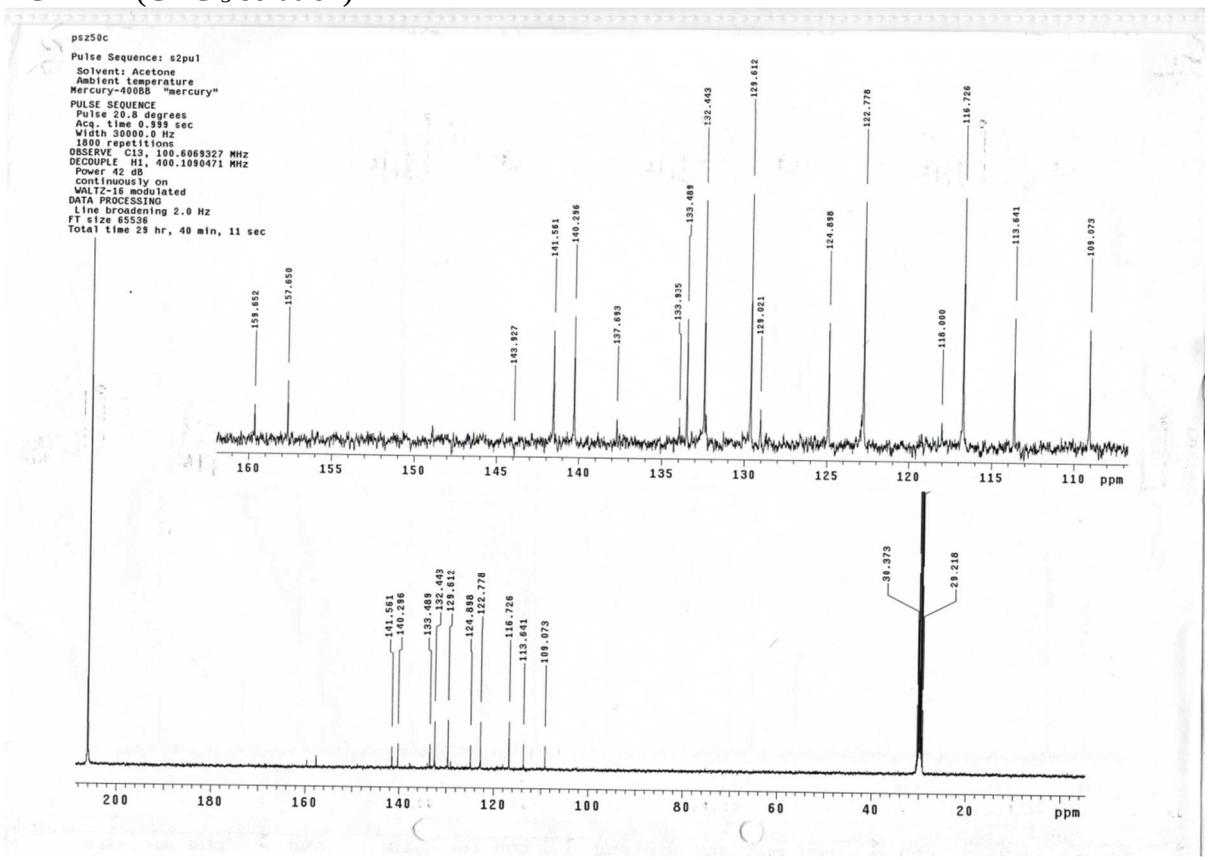


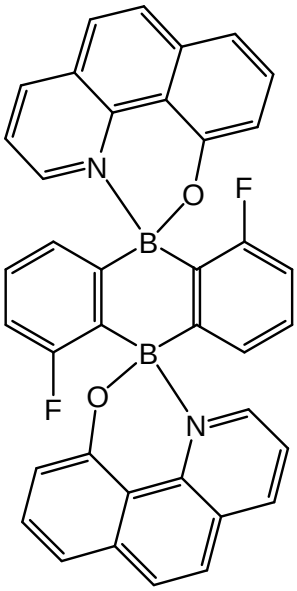
9

^{1}H NMR ($CDCl_3$ solution)



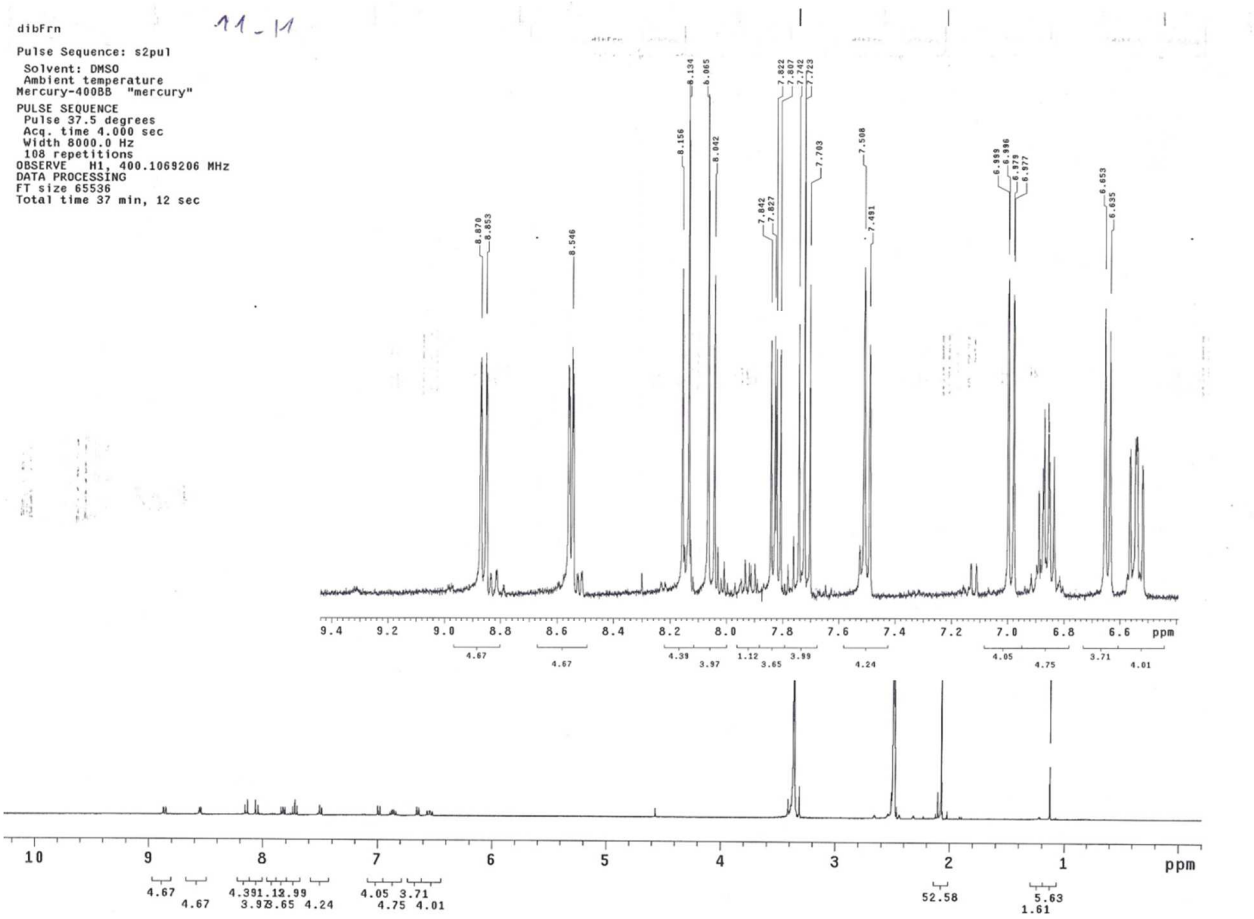
^{13}C NMR ($CDCl_3$ solution)





10

^{1}H NMR (DMSO-d_6 solution)



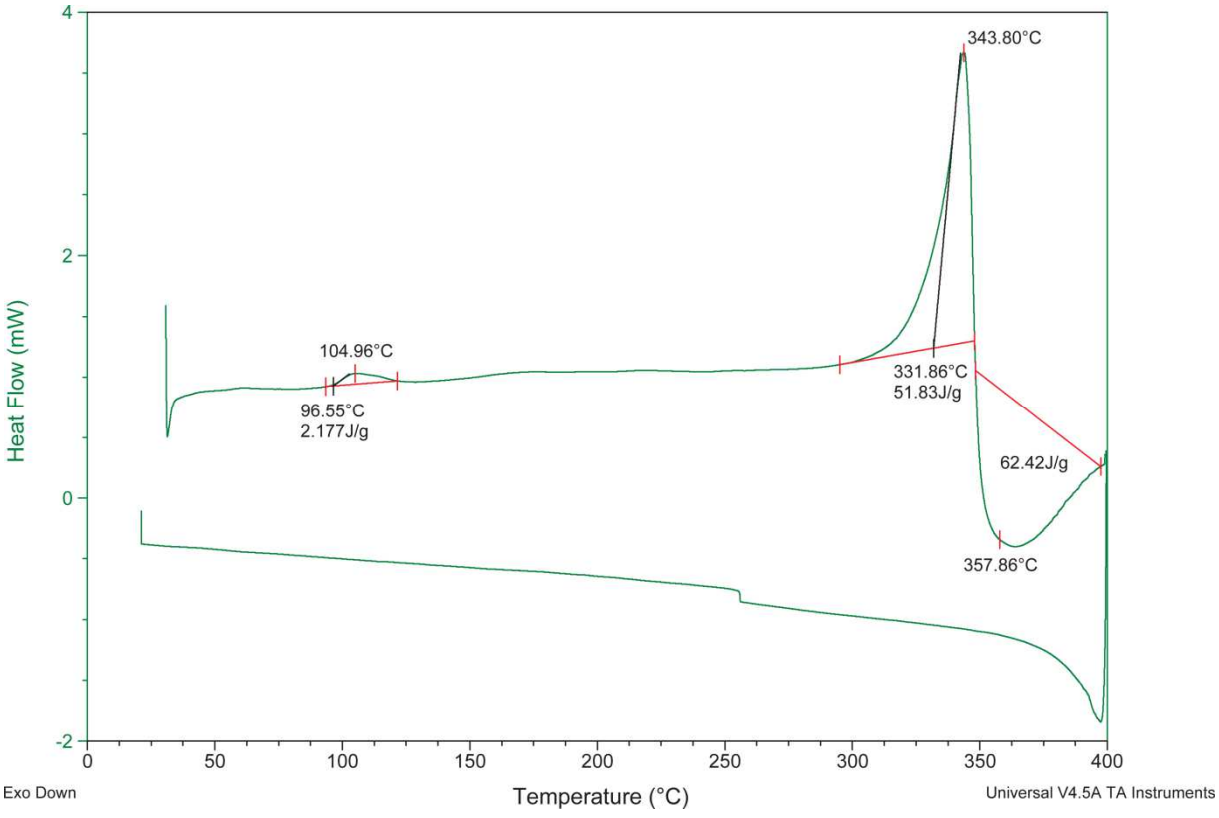
2. DSC curves of selected compounds

Table S1. The summary of DSC measurements for selected compounds. Melting points (T_m), glass transition temperatures (T_g), and crystallization temperatures (T_c). All the temperatures are provided in °C.

	m / mg	T_c	T_m	heating cycle
1	3.6860	--	344.0 (dec.)	first
2a	2.9060	278.4	367.4	first
		--	350.8 / 360.9	second
2b	2.0520	274.0	368.9	first
		--	345.2 / 361.4	second
3	2.9160	--	392.6	first
4	3.2680	--	361.5 (dec.)	first
8	2.9600	--	346.8 / 360.7 (dec.)	first

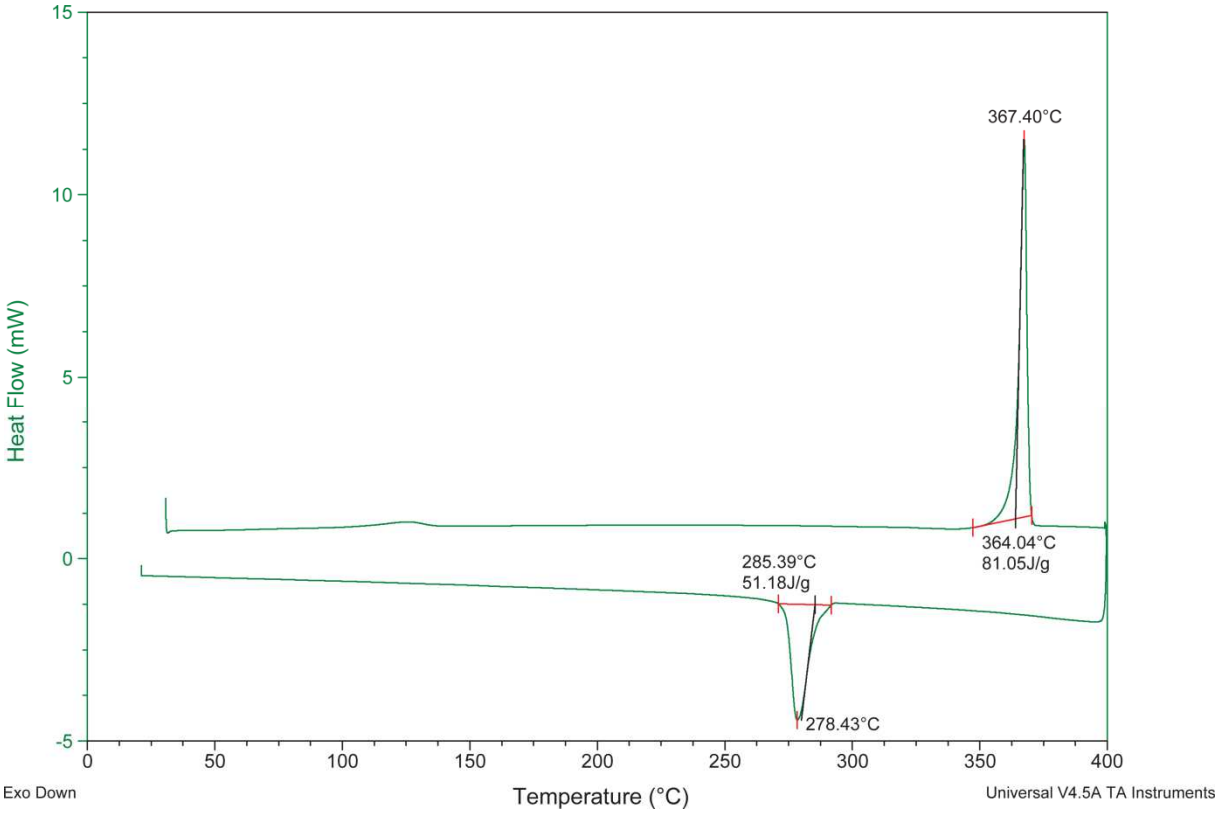
Compound **1**

cycle 1

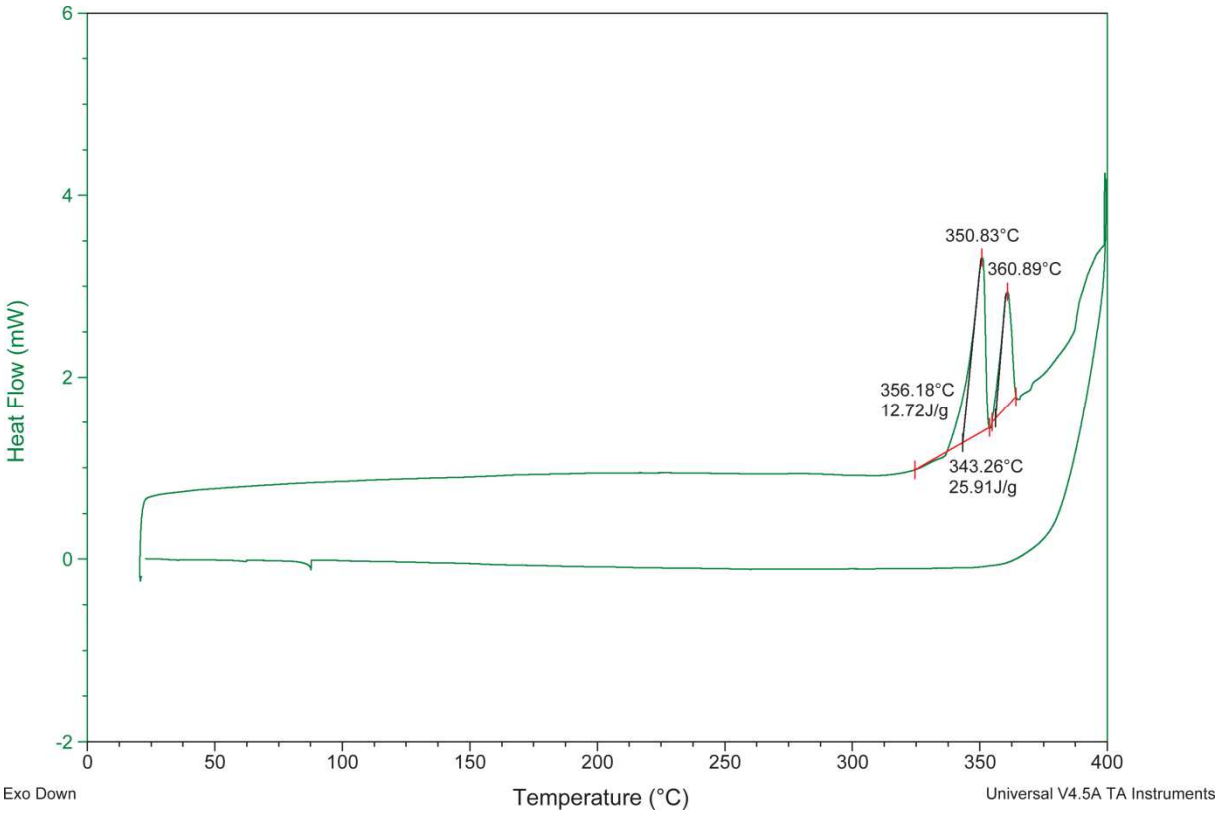


Compound **2a**

cycle 1

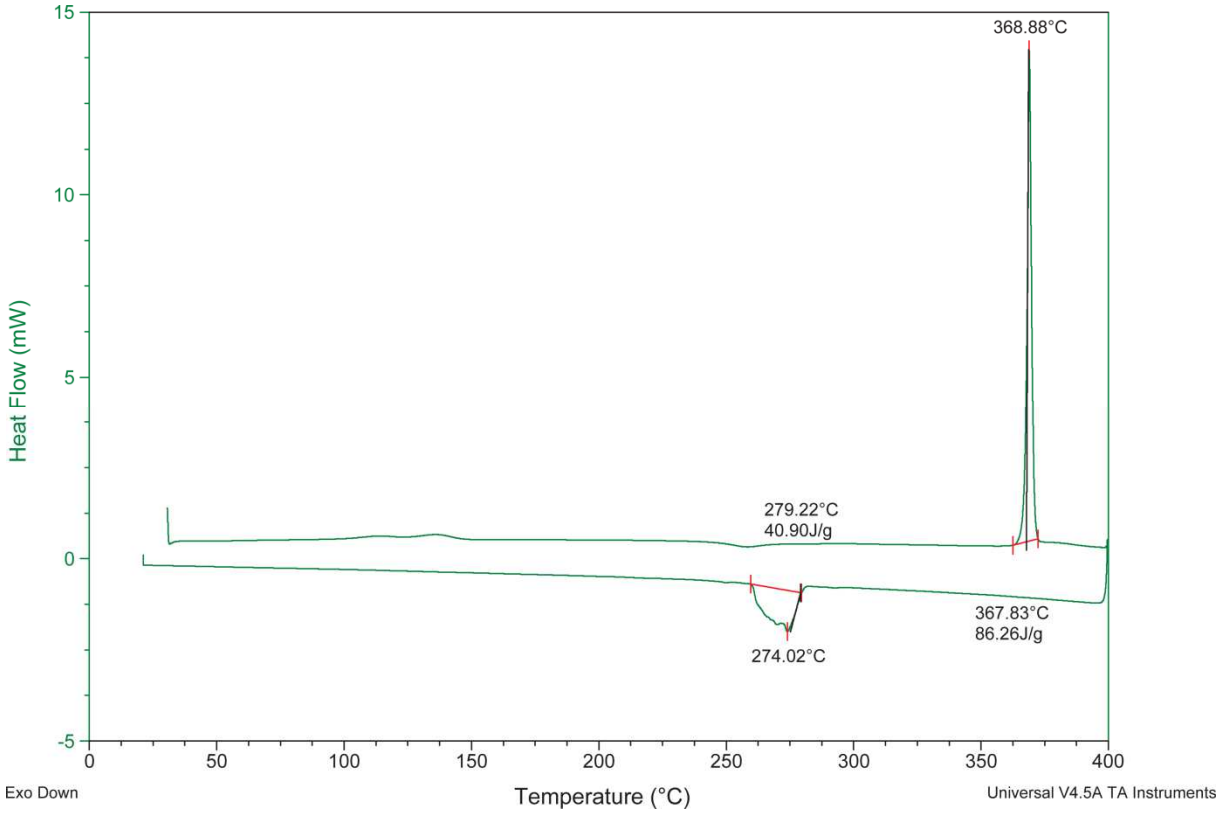


cycle 2

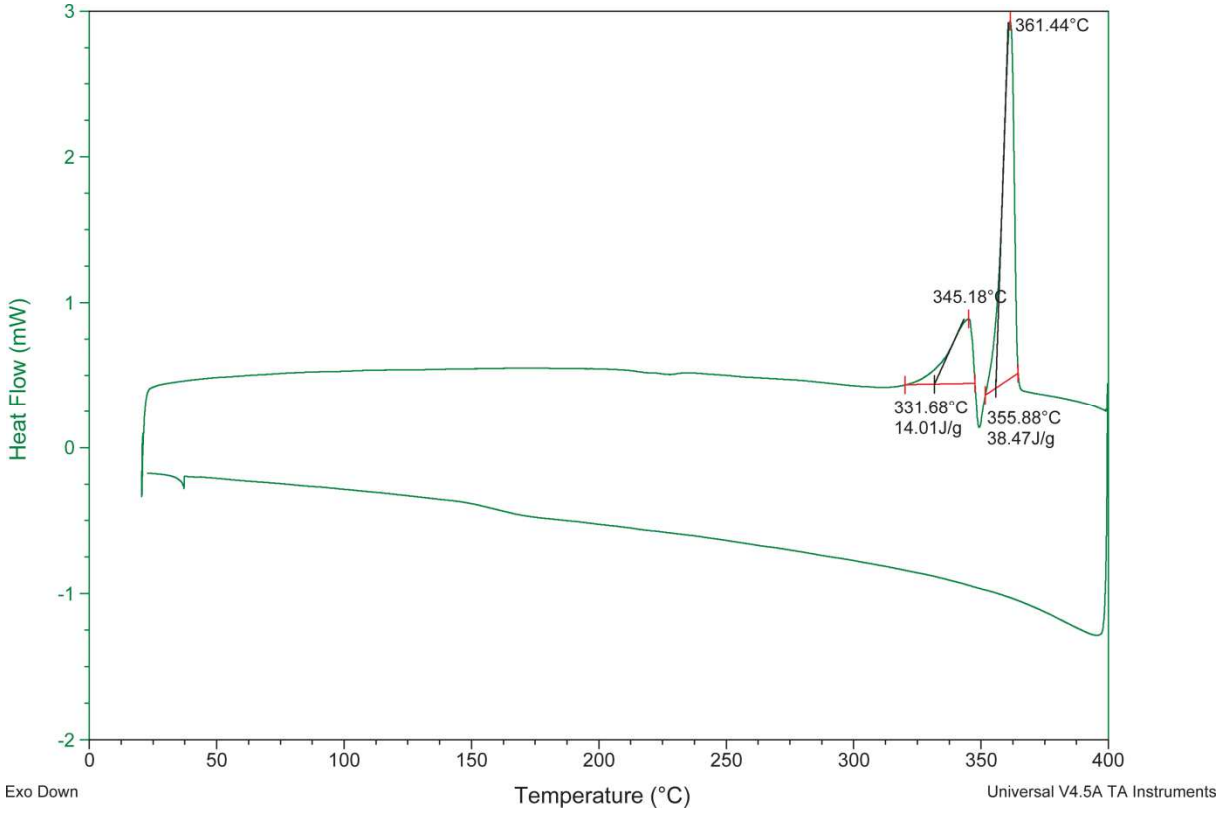


Compound **2b**

cycle 1

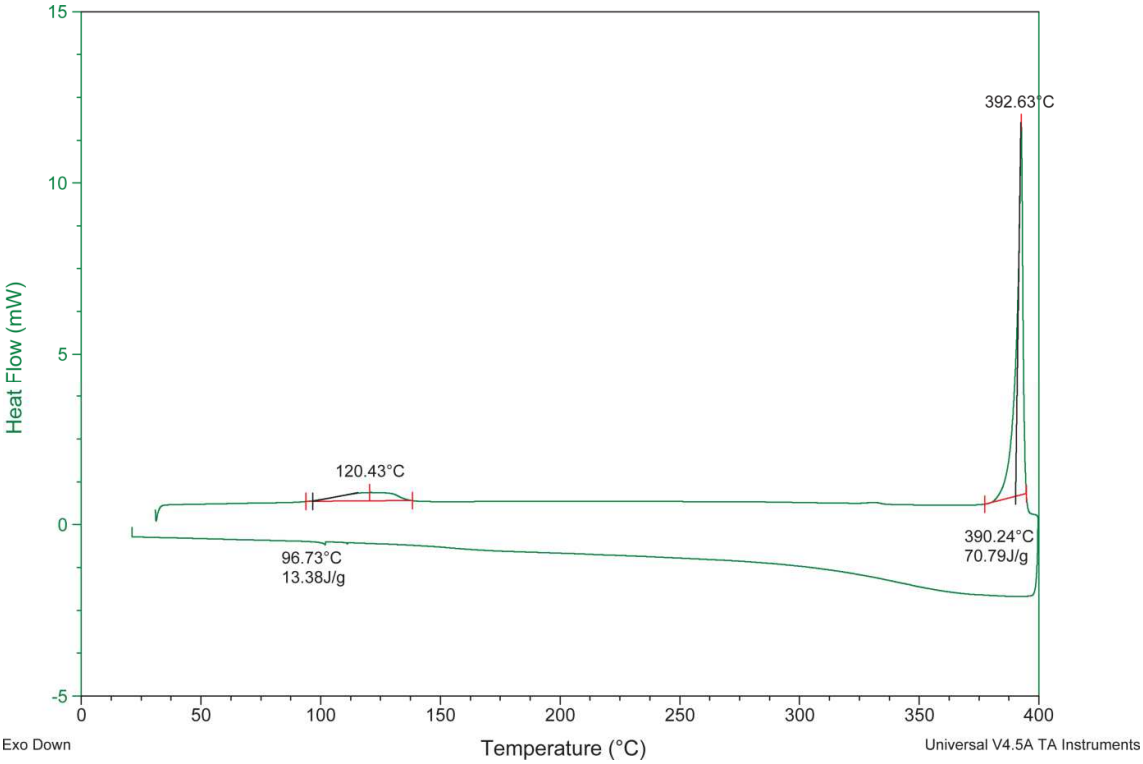


cycle 2



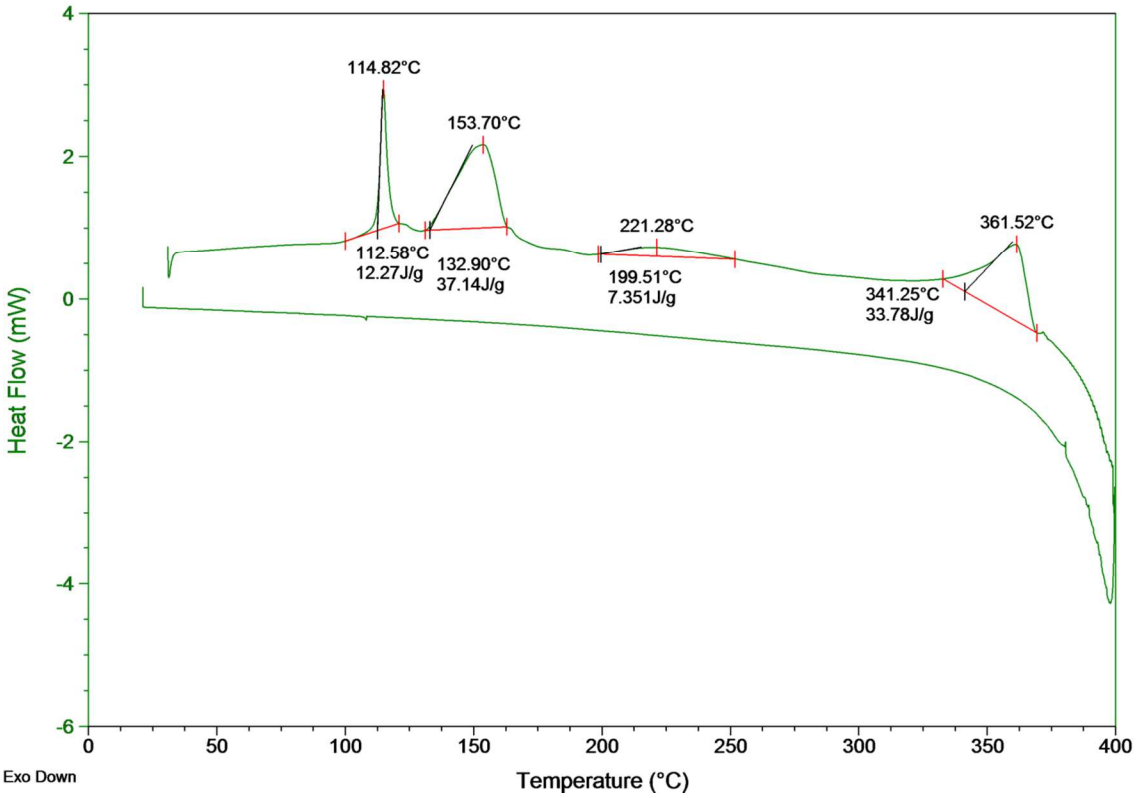
Compound **3**

cycle 1



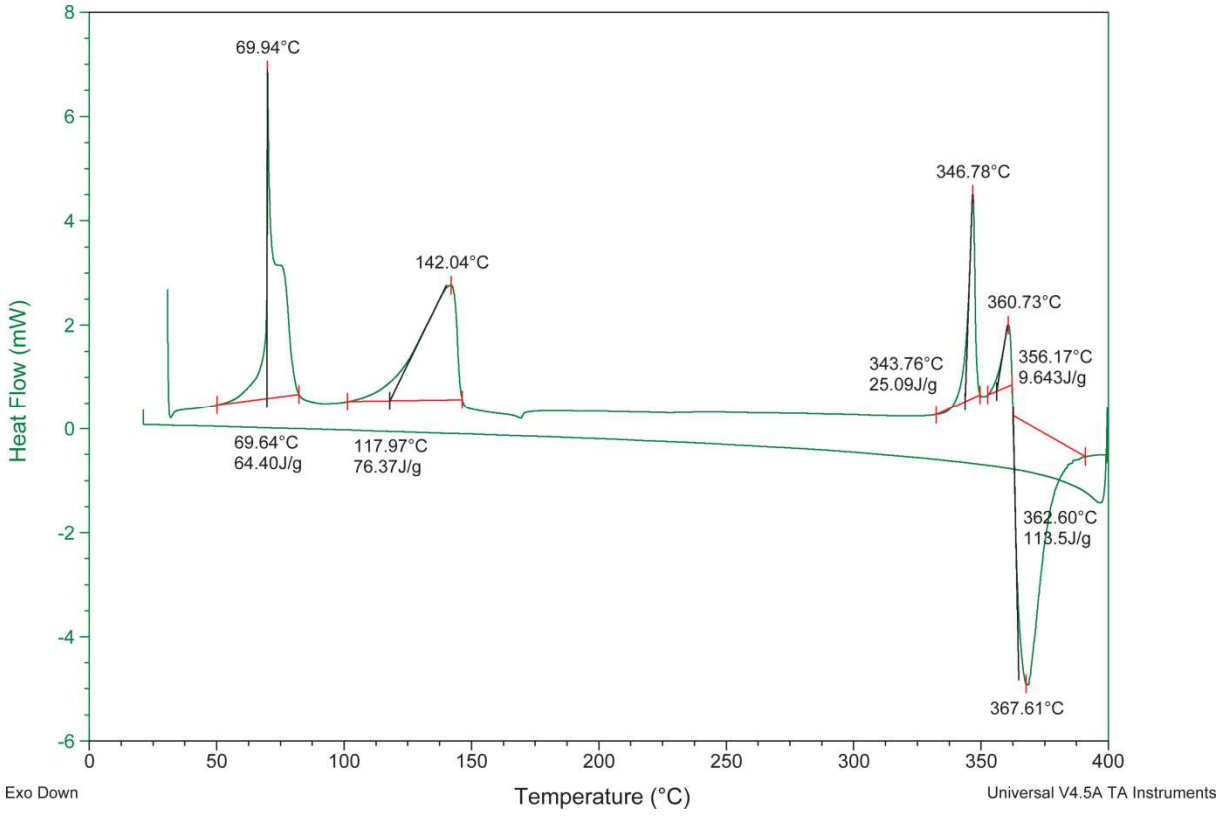
Compound **4**

cycle 1



Compound **8**

cycle 1



3. IR data

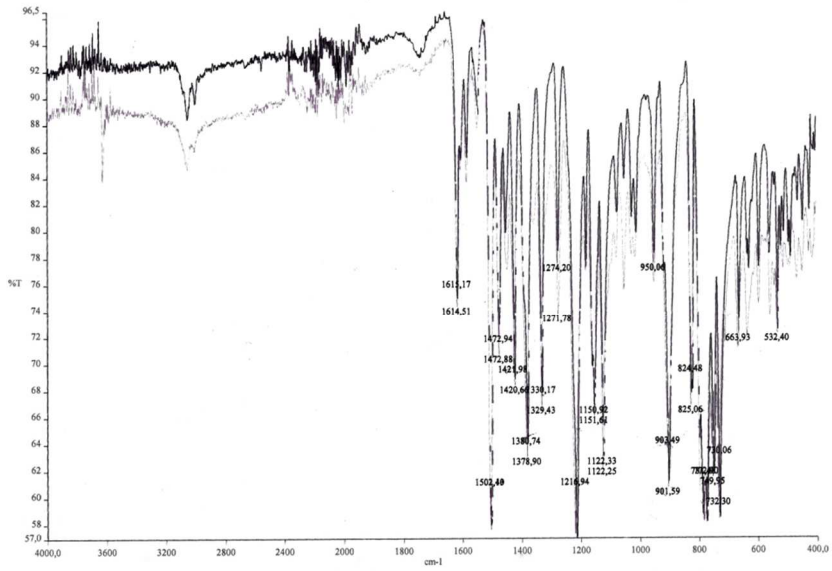


Figure S1. IR spectra of **2** synthesized using standard "wet" and mechanochemical methods (grey and black line, respectively).

4. Electrochemical data

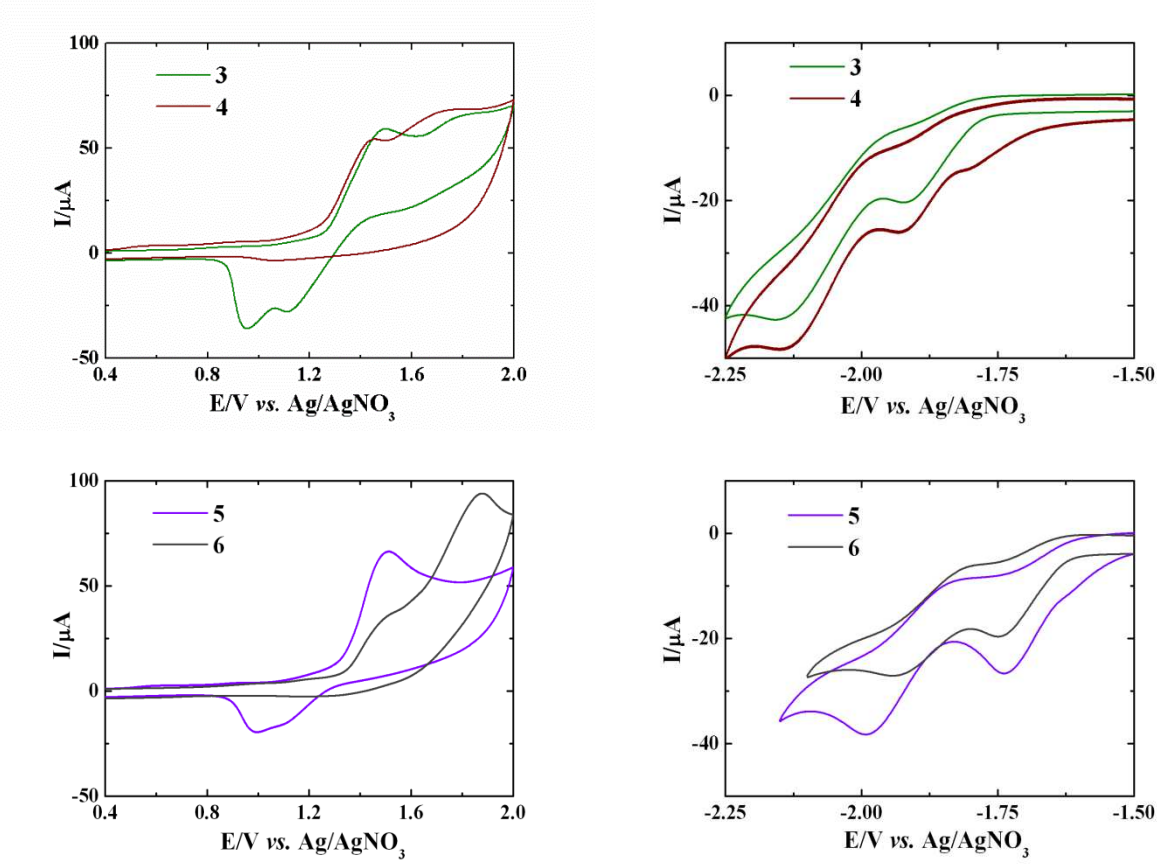


Figure S2. Cyclic voltammograms of **3-4** and **5-6** (1 mM) in Bu_4NPF_6/CH_2Cl_2, v = 0.1 V s^{-1}.

5. Crystallographic data

Crystallization, structural measurement and refinement details. The single crystals of **1**, **2a**, **2b**, **3**, **5**, **8** and **9** were obtained by the slow evaporation of corresponding acetone (**1**, **2a**, **3**, **8**) or chloroform (**2b**, **5**, **9**) solutions. In most cases the crystals possess well-defined faces (**Figure S3**). X-ray diffraction data sets for single crystals of **1**, **2a** and **8** were collected at 100 K on a Bruker AXS Kappa APEX II Ultra diffractometer with a TXS rotating anode (Mo-Kα radiation, λ = 0.71073 Å). The data collection strategy was optimized and monitored using the appropriate algorithms applied in the *APEX2* program package.[3] Data reduction and analysis were carried out with the *APEX2* suit of programs (integration was done with *SAINT*).[4] The multi-scan absorption correction, scaling and merging of reflection data were done with *SORTAV*.[5,6] Single crystals of **2b**, **5** and **9** were measured at 100 K on a Kuma KM4CCD κ-axis diffractometer with graphite-monochromated Mo-Kα radiation and equipped with an Oxford Cryosystems nitrogen gas-flow apparatus. In case of **3**, the measurement was performed on SuperNova diffractometer equipped with Eos CCD detector. Data reduction and analysis were carried out with the *CrysAlisPro* program.[7] All structures were solved by direct methods using *SHELXS-2013* and refined using *SHELXL-2013*.[8] All non-hydrogen atoms were refined anisotropically. Difference-Fourier maps from datasets collected from studied compounds are shown in **Figure 4S**. Selected crystal data is placed in **Table S2**. Labelling of atoms and estimation of atomic thermal motion as ADPs for **1**, **2a**, **2b**, **3**, **5**, **8** and **9** are shown in **Figure S6**, whereas selected geometrical parameters are placed in **Table S3**.

The crystal structure of **9** possess highly disordered solvent molecule, which could not be reliably modeled. The *Squeeze* routine from *PLATON*[9,10] was used to eliminate the contribution of the guest. The electron count and void volume is close to one acetone molecule (crystallization solvent) per one molecule of complex. The solvent molecules ($CHCl_3$) are also present in the structures **2a** and **9**. In the case of structure **2a** and **2b** the fluorine atoms were found to be disordered. The refinement leads to the occupancy ratio *ca.* 0.70:0.30 (**2a**) and 0.85:0.15 (**2b**). In the case of **8** difference-Fourier density map shows that sulfur and carbon atoms in thiophene moieties are slightly disordered. Such phenomenon is very often observed in the structures of compounds bearing thiophene rings. Since the contribution of the second component is very low (about 5%), the disorder has not been included in the final refinement. The disorder is also observed in case of **3** in the 9,10-dihydro-9,10-diboraanthracene ring. As in the previous case, the contribution of the second component is very small (approximately 7%) and therefore it was difficult to find stable

model describing all disordered atoms. We only managed to refine one half of the 9,10-dihydro-9,10-diboraanthracene moiety (**Figure S5**). In the case of **2a**, the relatively high residual density peaks near solvent molecule are observed (*ca.* 2 e·Å^{-3}), however we were unable to refine a more stable model with lower values of the residual densities. For **2b**, **3**, **8**, and **9** several reflection were omitted in the refinement procedure due to the fact that their intensities were substantially affected by the beamstop. The *CHECKCIF's* "Alert B" for **9** (*AddSymm* procedure detects additional pseudo-translation symmetry element) should be disproved, because disorder of one chloroform molecule was not taken into account in the test.

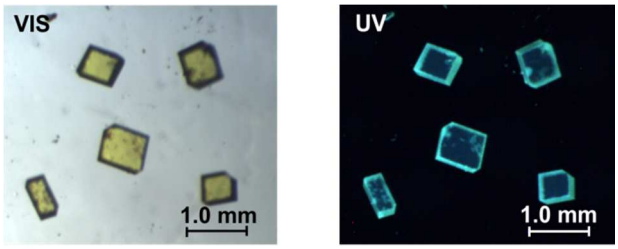
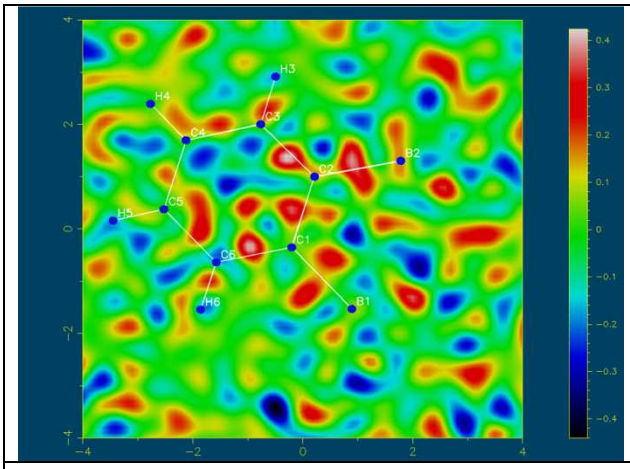


Figure S3. Single crystals of **2b** obtained from acetone solution viewed in (*a*) visible and (*b*) UV light.

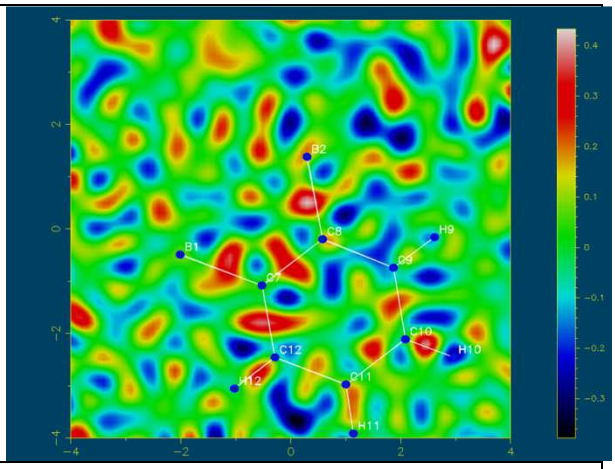
Table S2. Selected crystal data, data collection and refinement parameters for **1**, **2a**, **2b, 3**, **5**, **8** and **9**.

	1	**2a**	**2b**	**3**
chemical formula	$C_{30}H_{20}B_2N_2O_2$	$C_{30}H_{18}B_2F_2N_2O_2 \cdot 2(CHCl_3)$	$C_{30}H_{18}B_2F_2N_2O_2$	$C_{30}H_{18}B_2Cl_2N_2O_2$
molecular mass, M_r / a.u.	462.10	736.82	498.08	530.98
temperature, T / K	100(1)	100(1)	100(1)	100(1)
crystal system	monoclinic	monoclinic	triclinic	monoclinic
space group	$P2_1/c$	$P2_1/c$	$P-1$	$P2_1/c$
a / Å	9.595 (1)	9.531 (1)	10.372 (1)	9.940 (1)
b/ Å	20.393 (1)	14.069 (1)	10.655 (1)	12.561 (1)
c/ Å	11.840 (1)	12.309 (1)	11.367 (1)	19.659 (1)
α / °	90	90	90.03 (1)	90
β / °	98.68 (1)	107.30 (1)	96.60 (1)	91.60 (1)
γ / °	90	90	113.01	90
volume, V / Å^3	2290.2 (1)	1575.8 (1)	1147.2 (1)	2453.7 (2)
Z	4	2	2	4
D_{calcd} / g·cm^{-3}	1.340	1.553	1.442	1.437
θ_{max} / °	32.81	32.69	34.70	37.38
Absorption coefficient, μ / mm^{-1}	0.084	0.587	0.102	0.303
no. of meads / indep / and obsd [$F^2>2\sigma(F^2)$]	59124 / 8163 / 5101	37161 / 5560 / 4366	35016 / 9824 / 6804	61281 / 12402 / 7705
R_{int}	8.41%	3.10%	4.10%	5.50%
No. of parameters / restraints	325 / 0	218 / 1	362 / 0	343 / 0
$R[F]$ / $wR[F^2]$ ($I > 2\sigma(I)$)	5.66% / 11.00%	4.50% / 10.07%	5.57% / 13.28 %	7.50% / 22.40%
$\Delta\rho_{max}$, $\Delta\rho_{min}$ / e·Å^{-3}	+0.36 / −0.27	+1.29 / −1.36	+0.63 / −0.29	+2.33 / −0.51

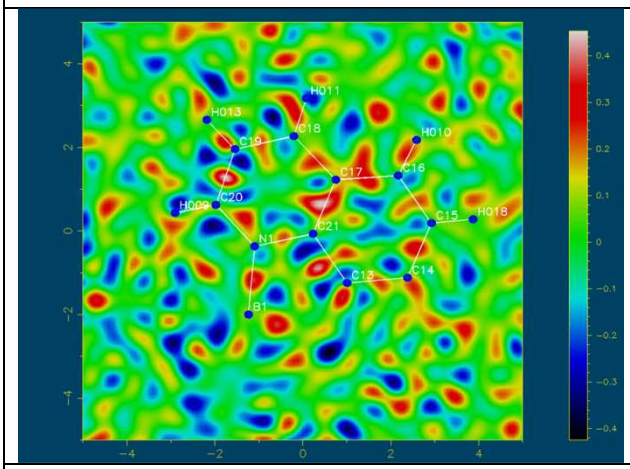
	5	**8**	**9**
chemical formula	$C_{30}H_{16}B_2F_4N_2O_2$	$C_{26}H_{16}B_2N_2O_2S_2$	$C_{21}H_{14}BNO_2 \cdot 2(CHCl_3)$
molecular mass, M_r / a.u.	534.07	474.15	561.94
temperature, T / K	100(1)	100(1)	100(1)
crystal system	triclinic	triclinic	monoclinic
space group	$P-1$	$P-1$	$P2_1/c$
a / Å	10.929 (1)	7.913 (1)	19.354 (1)
b/ Å	11.349 (1)	9.325 (1)	12.188 (1)
c/ Å	12.039 (1)	9.806 (1)	20.513 (1)
α / °	64.41 (1)	92.99 (2)	90
β / °	64.81 (1)	101.30 (1)	93.79 (1)
γ / °	84.20 (1)	113.32 (1)	90
volume, V / Å^3	1212.5 (1)	644.8 (1)	4828.0 (1)
Z	2	1	8
D_{calcd} / g·cm^{-3}	1.436	1.221	1.546
θ_{max} / °	32.29	27.16	34.60
Absorption coefficient, μ / mm^{-1}	0.112	0.231	0.735
no. of meads / indep / and obsd [$F^2>2\sigma(F^2)$]	45053 / 8202 / 6345	13958 / 2992 / 2948	135187 / 19819 / 14107
R_{int}	4.10%	2.67%	4.30%
No. of parameters / restraints	361 / 0	154 / 2	632 / 0
$R[F]$ / $wR[F^2]$ ($I > 2\sigma(I)$)	4.32% / 10.85 %	5.98% / 17.95%	4.29 % / 10.15%
$\Delta\rho_{max}$, $\Delta\rho_{min}$ / e·Å^{-3}	+0.46 / −0.25	+0.89 / −0.49	+1.13 / −0.97



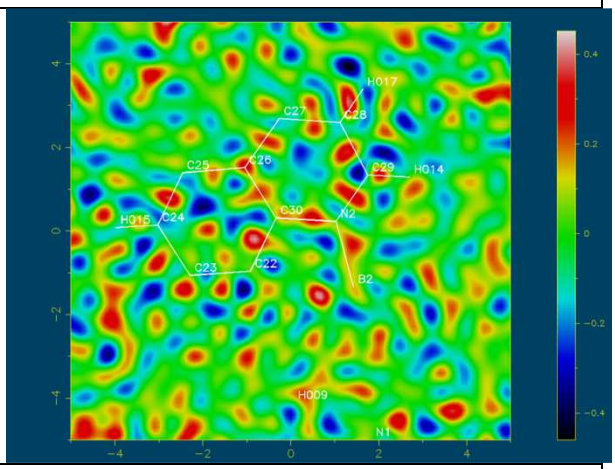
1 B1-C3-C5



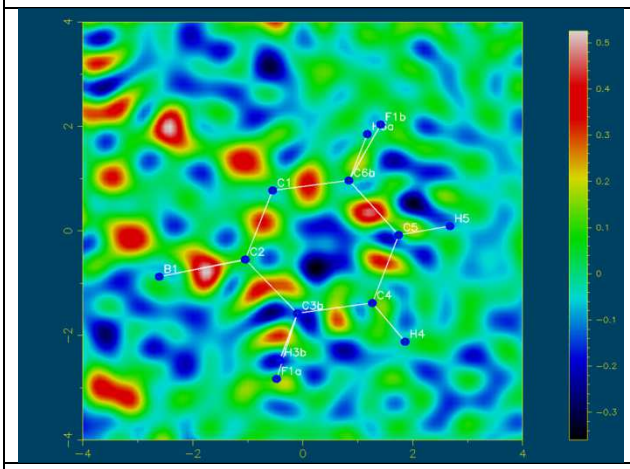
1 B2-C10-C12



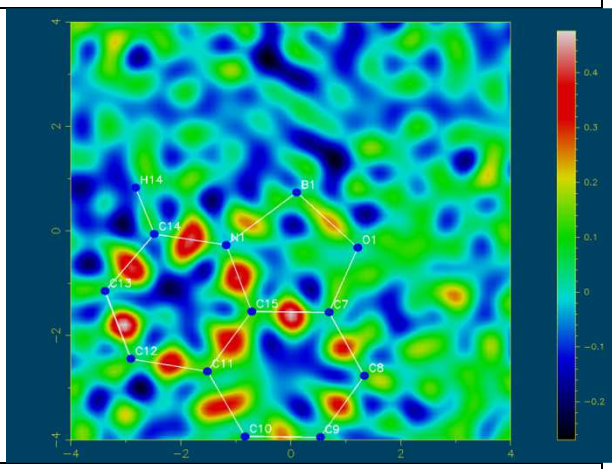
1 B1-C15-C19



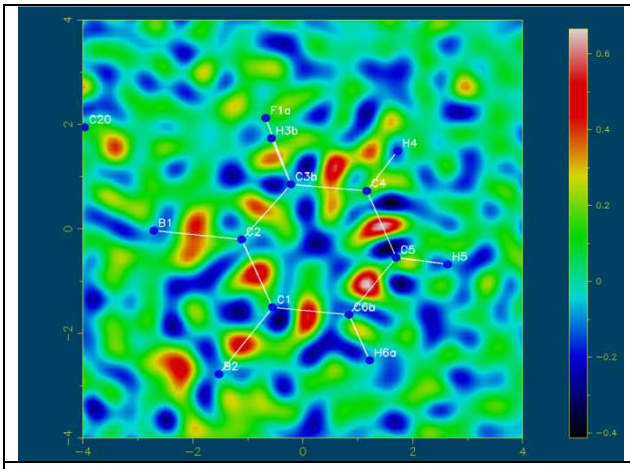
1 B2-C25-C27



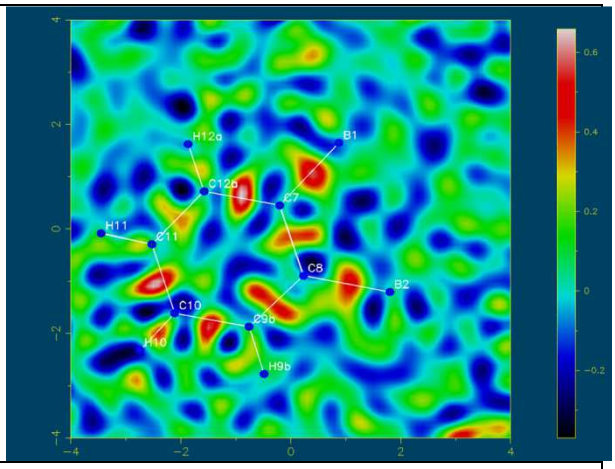
2a B1-C4-C5



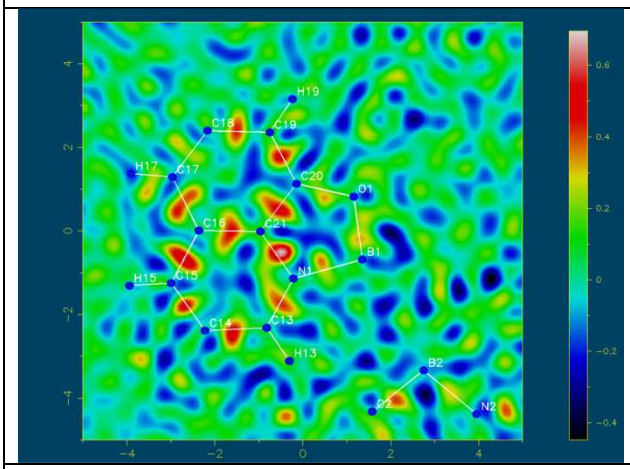
2a B1-C10-C13



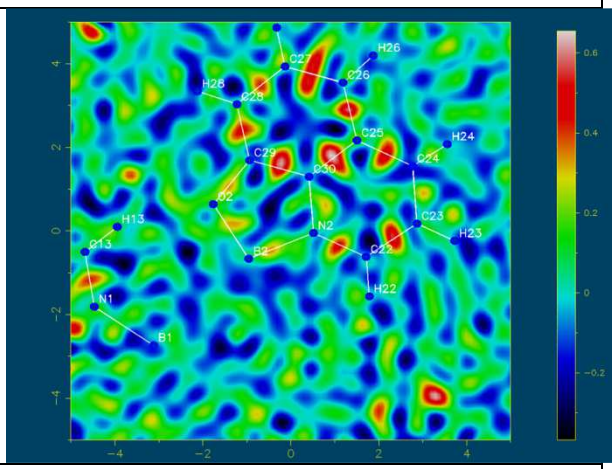
2b B1-C4-C5



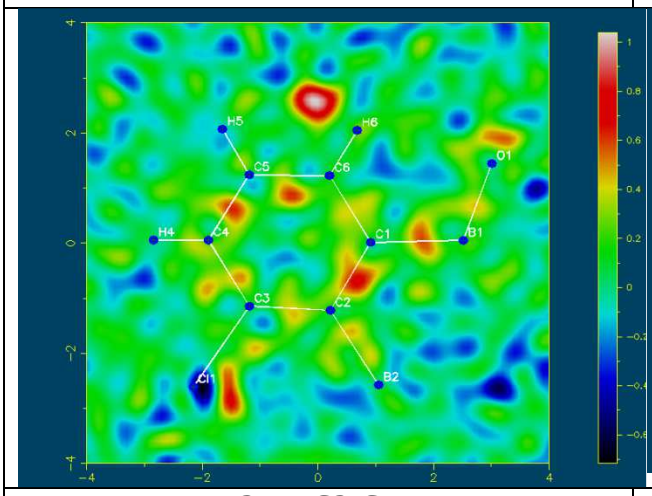
2b B2-C10-C11



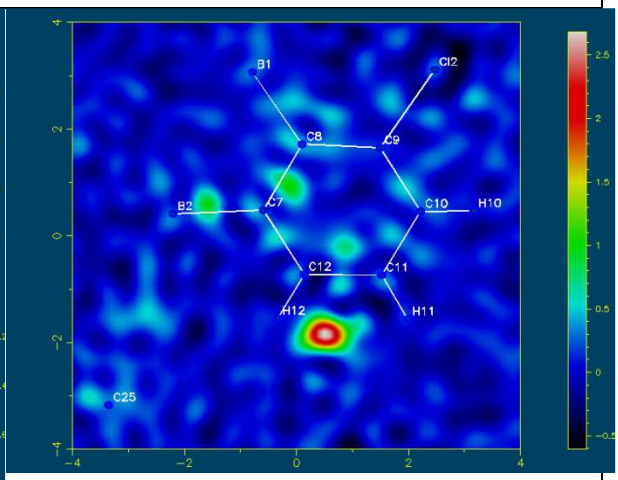
2b B1-C15-C17



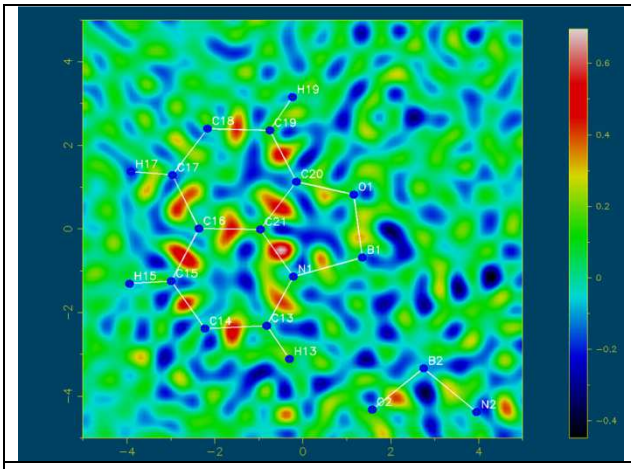
2b B2-C24-C26



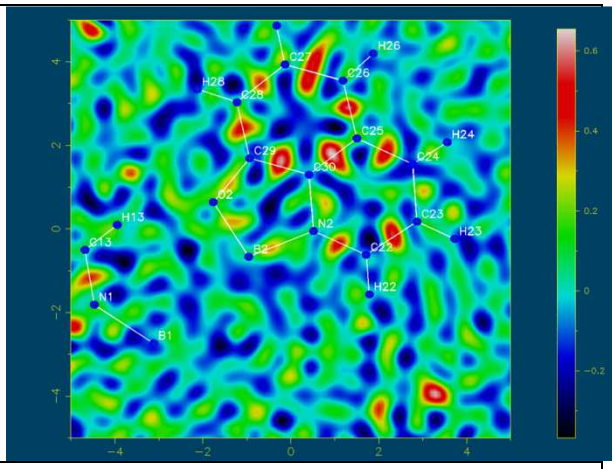
3 B1-C3-C5



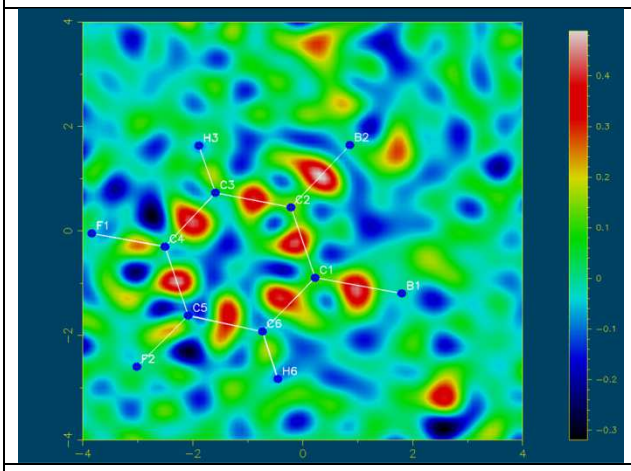
3 B2-C10-C12



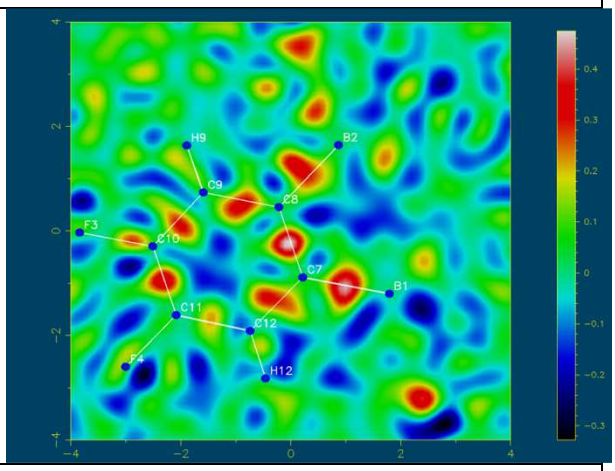
3 B1-C15-C19



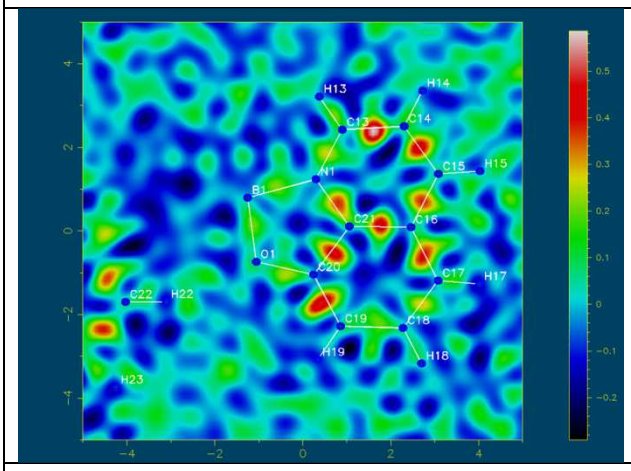
3 B2-C25-C27



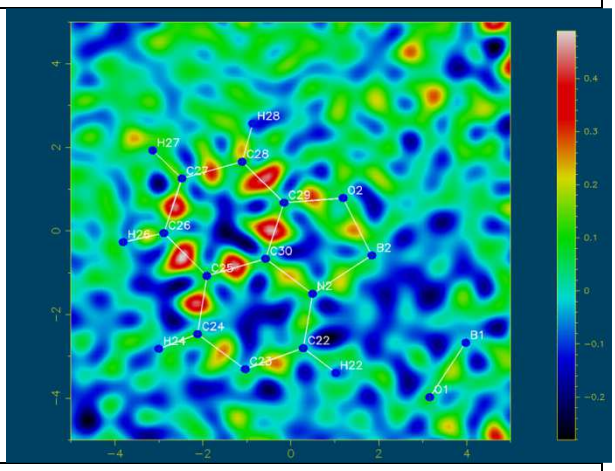
5 B1-C4-C5



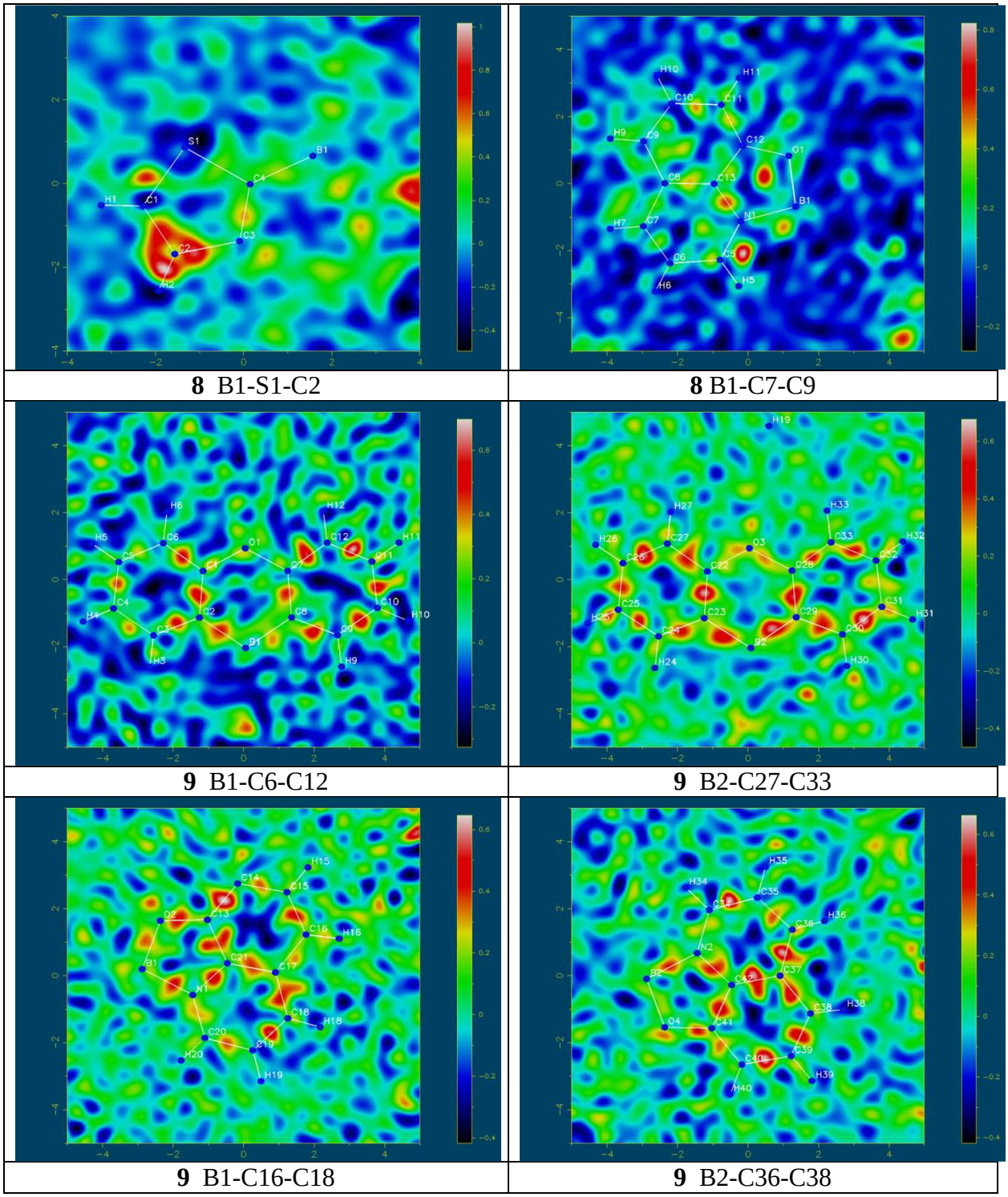
5 B2-C10-C11



5 B1-C15-C17



5 B2-C24-C26



8 B1-S1-C2	**8** B1-C7-C9
9 B1-C6-C12	**9** B2-C27-C33
9 B1-C16-C18	**9** B2-C36-C38

Figure S4. Difference-Fourier maps from datasets collected from studied compounds. All areas of negative electron density are represented in blue colour, whereas positive values of electron density in orange and red. Maps were generated with *MAPVIEW* program within *WinGX*.[11]

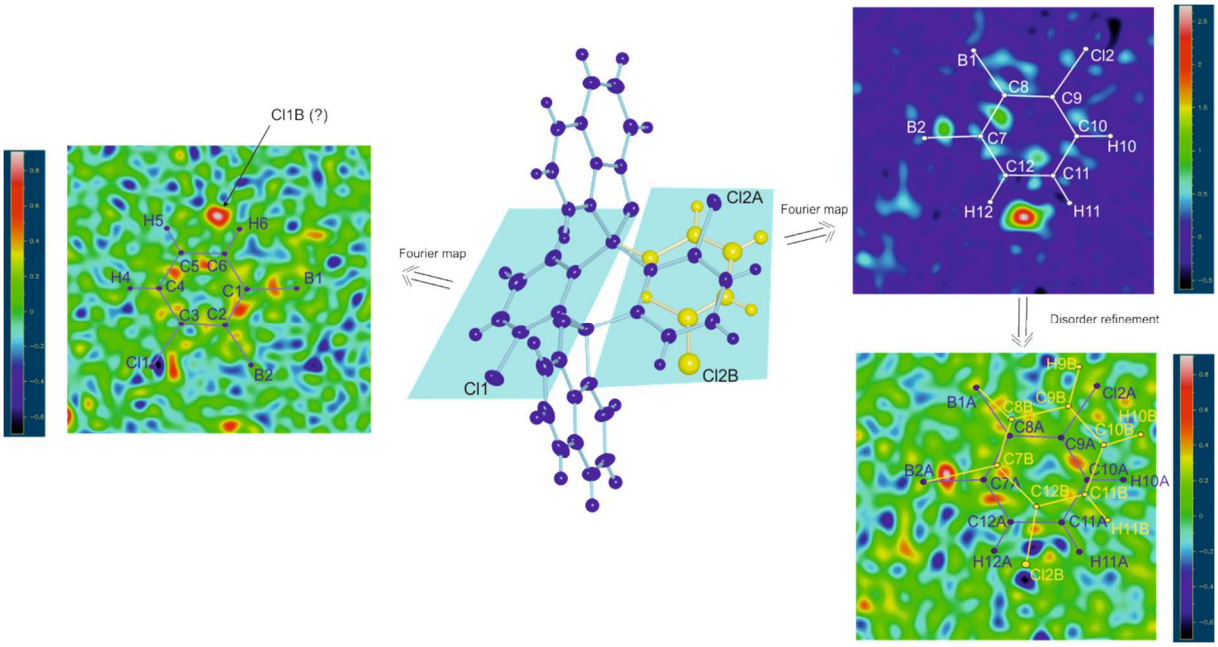


Figure S5. Difference-Fourier maps for the 9,10-dihydro-9,10-diboraanthracene ring region generated for molecule **3**. In the case of the C7-C12 ring the disorder was excluded (top, right) or included into the refinement (bottom, right).

Molecular geometry

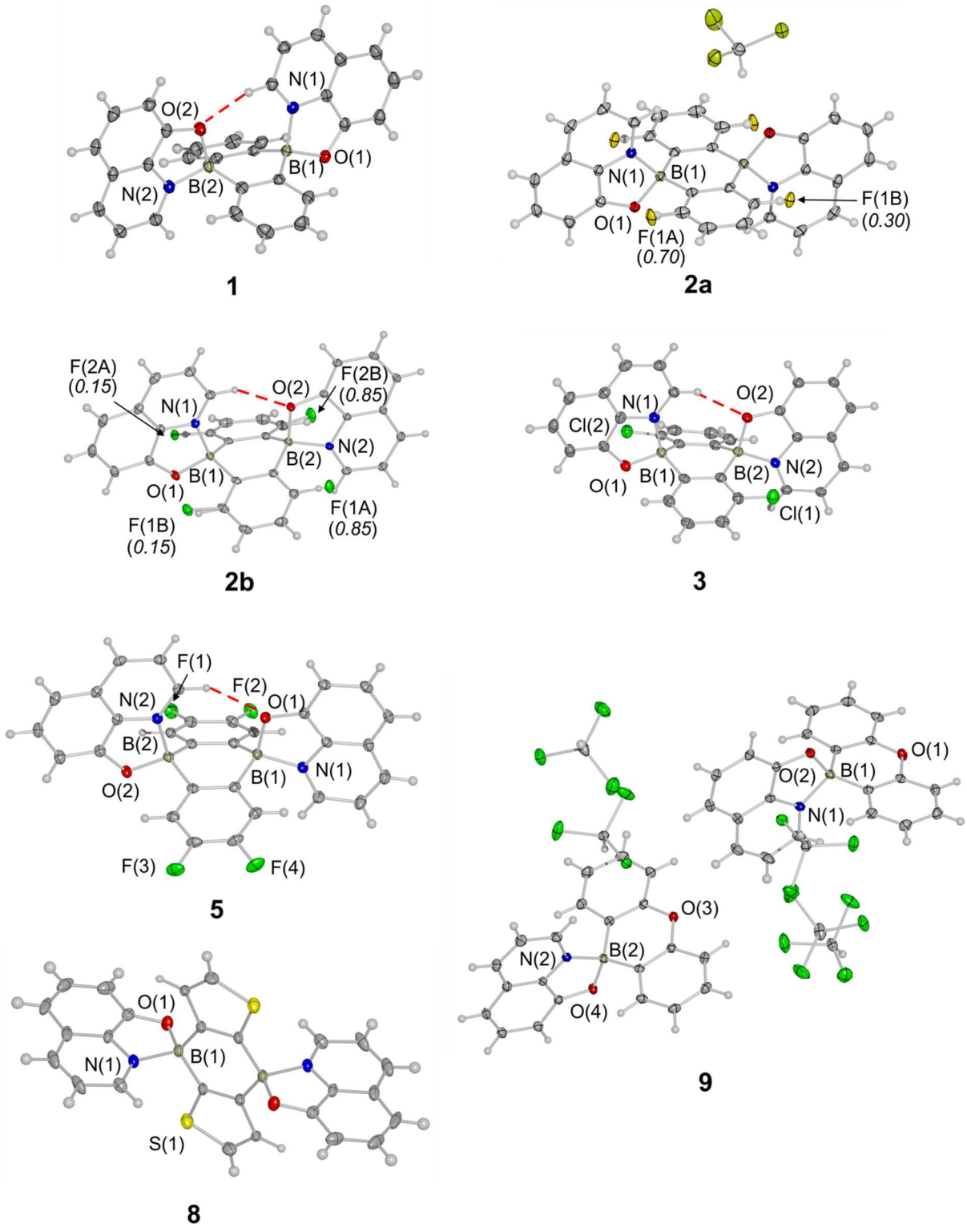


Figure S6. Labelling of atoms (only symmetrically non-equivalent heteroatoms) and estimation of atomic thermal motion as ADPs (50% probability level) for **1**, **2a**, **2b**, **3**, **5**, **8** and **9**. Intramolecular C−H…O contacts in **1**, **2b**, **3** and **5** are shown as dashed red lines. Site occupancy factors of disordered atoms (**2a**) are given in parentheses in *italics*.

Table S3. Selected bond lengths (Å) obtained from refinement and theoretical optimization for studied complexes. Calculated data are presented in *italics*. Calculations were done at the RB3LYP/6-31+g(d,p) level of theory.

	1	**2a**[a]	**2b**	**3**	**5**	**8**[a]	**9**[b]
B(1)−O(1)	1.535(2)	1.534(2)	1.518(1)	1.536(2)	1.545(1)	1.526(3)	1.534(2)
	1.523	*1.532*	*1.516*	*1.513*	*1.558*	*1.531*	*1.526*
B(2)−O(2)	1.546(2)	-	1.531(1)	1.547(2)	1.521(2)	-	1.532(2)
	1.565	*1.532*	*1.553*	*1.549*	*1.518*	*1.531*	-
B(1)−N(1)	1.637(2)	1.632(2)	1.637(1)	1.638(2)	1.618(2)	1.627(3)	1.628(2)
	1.669	*1.652*	*1.661*	*1.665*	*1.629*	*1.659*	*1.669*
B(2)−N(2)	1.614(2)	-	1.598(1)	1.614(2)	1.642(1)	-	1.629(2)
	1.630	*1.652*	*1.629*	*1.630*	*1.667*	*1.659*	-
B(1)−C(1)	1.607(2)	1.603(2)	1.609(2)	1.607(2)	1.606(2)	1.582(3)	1.588(2)
	1.605	1.60828	*1.611*	*1.615*	*1.610*	*1.596*	*1.592*
B(1)−C(7)	1.603(2)	-	1.609(2)	1.602(2)	1.606(2)	-	1.596(2)
	1.605	*1.611*	*1.609*	*1.615*	*1.610*	1.600	*1.592*
B(2)−C(2)	1.601(2)	1.602(2)	1.612(2)	1.600(2)	1.602(2)	1.599(3)	1.585(2)
	1.609	*1.611*	*1.614*	*1.624*	*1.606*	1.600	-
B(2)−C(8)	1.603(2)	-	1.602(2)	1.602(2)	1.607(2)	-	1.596(2)
	1.609	*1.608*	*1.609*	*1.614*	*1.606*	1.596	-

[a] *symmetrical* conformers, [b] two molecules in the asymmetric part of the unit cell.

Supramolecular patterns

The supramolecular structures of studied 8-oxyquinolinate (Q) complexes are dominated by the weak C–H…π and π-π interactions. The examples of supramolecular pattern are shown in **Figure S7**. In the case of the structures built up by a *bent* conformer (**1**, **2b**, **3**, and **5**), the π-stacking interactions occur between two neighbouring Q groups with the inter-planar separation distances equal to 3.487(3) Å (**1**), 3.276(3) Å (**2b**), 3.379(5) Å (**3**) and 3.243(3) Å (**5**). The π…π interactions were also found in the structure **8** with the separation distance of 3.459(3) Å between adjacent Q moieties. A different supramolecular assembly is found in the structure **2a** and **9**. The crystal packing of these compounds lacks π-stacking contacts, but is based on weak C–H…π interactions, supported by the intermolecular C–H…O and C–H…Cl contacts with solvent molecule. In the case of **1** and **2b**, the Q ligands are significantly displaced one to another, which results in less efficient stacking as compared to **8** (**Figure S7**). The geometry of intermolecular interactions is placed in **Table S4**.

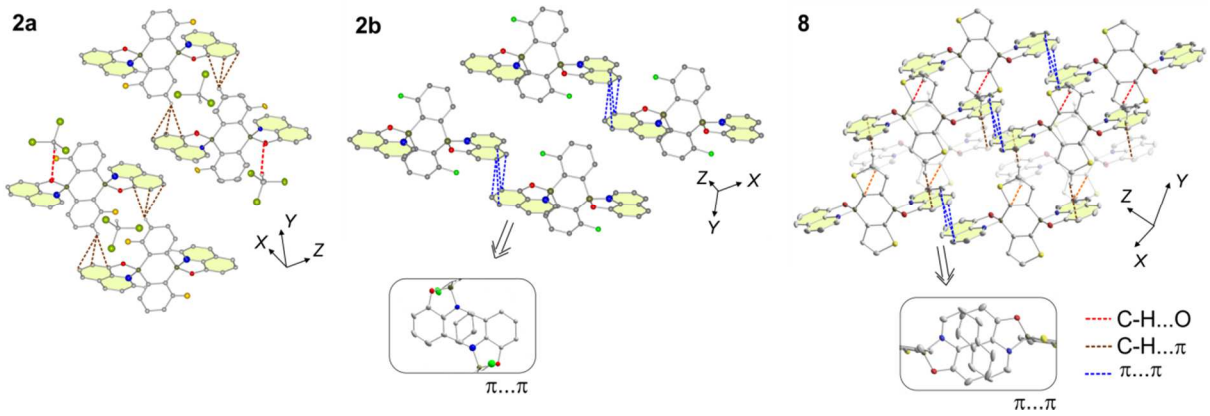


Figure S7. Stereo-views of crystal structures showing the molecular packing and weak interactions in **2a**, **2b** and **8**. The π-stacked Q ligands in **2b** and **8** are additionally shown in the direction perpendicular to their planes. Hydrogen atoms not involved in the C–H…π and C–H…O interactions are omitted for clarity.

Table S4. Geometry of weak intermolecular interactions (*d* and *θ* denote bond distances and angles, respectively, whereas $d_{p\text{-}p}$ denotes interplanar distance).

	Interaction	$d_{D–H}$ / Å	$d_{H\ldots A}$ / Å	$d_{D\ldots A}$ / Å	$\theta_{D–H\ldots A}$ / °
1	C20–H9….O2$^{\$}$	0.95	2.180	3.052(2)	152.1
	C28–H17….O1$^{\#1}$	0.95	2.375	3.290(2)	161.5
	C27–H8…C14(π)$^{\#2}$	0.95	2.887	3.765(2)	154.1
	C18–H11…C2(π) $^{\#3}$	0.95	2.824	3.635(2)	143.9
	C18–H11…C3(π) $^{\#3}$	0.95	2.754	3.695(2)	170.3
	C18–H11…C4(π) $^{\#3}$	0.95	2.734	3.643(2)	160.2
	C5–H5…C28(π)$^{\#4}$	0.95	2.838	3.642(2)	143.1
				$d_{c\ldots c}$ / Å	$d_{p\ldots p}$ / Å
	C20(π)–C23(π)$^{\#5}$			3.367(2)	3.331(2)
		$d_{D–H}$ / Å	$d_{H\ldots A}$ / Å	$d_{D\ldots A}$ / Å	$\theta_{D–H\ldots A}$ / °
2a	C19–H19….O1$^{\#6}$	1.00	2.515	3.251(2)	130.1
	C8–H8–Cl1$^{\#7}$	0.95	2.871	3.648(2)	139.7
	C9–H9–F1A$^{\#8}$	0.95	2.594	3.351(2)	137.0
	C5–H5…C8(π)$^{\#9}$	0.95	2.838	3.552(2)	143.3
	C12–H12…C3(π)$^{\#10}$	0.95	2.890	3.645(2)	127.8
	F1A–Cl$^{\#11}$			3.185(2)	
2b	C13–H13….O2$^{\$}$	0.95	2.267	3.140(1)	152.5
	C15–H15…C7(π) $^{\#12}$	0.95	2.826	3.526(2)	131.3
	C15–H15…C8(π)$^{\#12}$	0.95	2.894	3.722(2)	146.3
	C24–H24…F1A$^{\#13}$	0.95	2.342	3.148(1)	142.3
	C26–H26…F1A$^{\#13}$	0.95	2.506	3.261(1)	136.6
	C23–H23…O1$^{\#14}$	0.95	2.472	3.297(2)	145.1
	C23–H23…F1A$^{\#14}$	0.95	2.629	3.357(2)	136.7
	C22–H22…C2(π)$^{\#14}$	0.95	2.701	3.384(2)	137.6
	C22–H22…C3(π)$^{\#14}$	0.95	2.728	3.462(2)	124.4
	C27–H27….F1A$^{\#15}$	0.95	2.513	3.411(2)	157.7
				$d_{c\ldots c}$ / Å	$d_{p\ldots p}$ / Å
	C25(π)–C19(π)$^{\#13}$			3.330(2)	3.267(2)
	C26(π)–C19(π)$^{\#13}$			3.374(2)	

	C15(π)–C13(π)$^{\#12}$			3.315(2)	3.310(2)
		$d_{D–H}$ / Å	$d_{H...A}$ / Å	$d_{D...A}$ / Å	$\theta_{D–H...A}$ / º
3	C13–H13….O2$^{\$}$	0.95	2.466	3.357(2)	156.1
	C24–H24…O1$^{\#16}$	0.95	2.522	3.451(3)	166.1
	C26–H26…C1(π) $^{\#16}$	0.95	2.849	3.625(3)	139.7
	C28–H28…C9(π)$^{\#11}$	0.95	2.675	3.554(3)	154.3
	C22–H22…C27(π)$^{\#17}$	0.95	2.612	3.547(3)	167.8
	C15–H15…C3(π)$^{\#11}$	0.95	2.800	3.727(3)	165.8
	C10–H10…Cl2$^{\#5}$	0.95	2.8773	3.803(2)	165.4
	Cl1….C11(π) $^{\#16}$			3.411(2)	
				$d_{c...c}$ / Å	$d_{p...p}$ / Å
	C13(π)–C15(π)$^{\#5}$			3.329(3)	3.289(3)
		$d_{D–H}$ / Å	$d_{H...A}$ / Å	$d_{D...A}$ / Å	$\theta_{D–H...A}$ / º
5	C13–H13….O2$^{\$}$	0.95	2.260	3.129(2)	151.8
	C14–H14…O2$^{\#14}$	0.95	2.479	3.140(1)	154.0
	C13–H13…C2(π)$^{\#14}$	0.95	2.873	3.749(2)	126.7
	C17–H17…F1$^{\#18}$	0.95	2.504	3.198(2)	126.3
	C15–H15…F3$^{\#18}$	0.95	2.557	3.184(2)	123.7
	C27–H27…F2$^{\#19}$	0.95	2.548	3.204(2)	126.3
	C24–H24…C8(π) $^{\#20}$	0.95	2.821	3.549(1)	134.2
	C24–H24…C9(π) $^{\#20}$	0.95	2.821	3.529(1)	132.0
				$d_{c...c}$ / Å	$d_{p...p}$ / Å
	C22(π)–C24(π)$^{\#20}$			3.243(2)	3.221(2)
		$d_{D–H}$ / Å	$d_{H...A}$ / Å	$d_{D...A}$ / Å	$\theta_{D–H...A}$ / º
8	C4–H4…C11$^{\#21}$	0.95	2.943	3.853(3)	160.8
	C6–H6…C1$^{\#4}$	0.95	2.705	3.592(3)	155.7
	C6–H6…C2$^{\#4}$	0.95	2.812	3.707(3)	157.3
	C9–H9…S1$^{\#22}$	0.95	2.895	3.808(4)	161.7
				$d_{c...c}$ / Å	$d_{p...p}$ / Å
	C6…C10$^{\#23}$			3.402(3)	3.459(5)
	C8…C8$^{\#23}$			3.477(3)	
		$d_{D–H}$ / Å	$d_{H...A}$ / Å	$d_{D...A}$ / Å	$\theta_{D–H...A}$ / º
9	C14–H14…C9(π)$^{\#24}$	0.95	2.894	3.824(2)	166.3
	C14–H14…C10(π)$^{\#24}$	0.95	2.885	3.751(2)	152.0
	C4–H4…C14(π)$^{\#25}$	0.95	2.843	3.673(2)	146.4
	C20–H20…Cl1$^{\#26}$	0.95	2.872	3.735(2)	151.6
	C15–H15…C12(π)$^{\#24}$	0.95	2.883	3.588(2)	131.9
	C19–H19…C9(π)$^{\#26}$	0.95	2.824	3.618(2)	141.8
	C16–H16…Cl2	0.95	2.867	3.773(1)	160.0
	C32–H32…Cl3A	0.95	2.883	3.478(2)	121.9
	C33–H33…Cl3A	0.95	2.927	3.499(2)	120.0
	C38–H38…Cl1$^{\#17}$	0.95	2.890	3.812(1)	163.8
	C40–H40…C30(π)$^{\#17}$	0.95	2.836	3.780(2)	172.5
	C40–H40…C31(π)$^{\#17}$	0.95	2.827	3.698(2)	152.9
	C35–H35…C30(π)$^{\#16}$	0.95	2.896	3.699(2)	143.0
	C25–H25…C40(π)$^{\#27}$	0.95	2.833	3.699(2)	152.2
	C44–H44…O2$^{\#26}$	0.95	2.641	3.343(2)	127.3
	C44–H44…C2(π)$^{\#26}$	0.95	2.742	3.658(2)	152.4
	C44–H44…C3(π)$^{\#26}$	0.95	2.627	3.572(3)	157.5
	C45–H45…O4$^{\#19}$	0.95	2.350	3.227(2)	146.0

C45–H45…C23(π)[#19]	0.95	2.783	3.677(2)	149.2
C46–H46…C22(π)	0.95	2.678	3.470(2)	136.1
C46–H46…C23(π)	0.95	2.825	3.645(2)	139.6
C46–H46…C24(π)	0.95	2.807	3.719(2)	151.9
C46–H46…C25(π)	0.95	2.714	3.677(2)	161.6
C46–H46…C26(π)	0.95	2.596	3.528(2)	154.9
C46–H46…C27(π)	0.95	2.583	3.426(2)	141.8
C43–H43…C1(π) [#24]	0.95	2.681	3.502(2)	139.4
C43–H43…C2(π) [#24]	0.95	2.870	3.633(2)	133.6
C43–H43…C3(π) [#24]	0.95	2.855	3.675(2)	139.6
C43–H43…C4(π) [#24]	0.95	2.737	3.652(2)	152.2
C43–H43…C5(π) [#24]	0.95	2.593	3.566(2)	164.2
C43–H43…C6(π) [#24]	0.95	2.564	3.490(2)	153.8

$ Stands for intramolecular contact; Symmetry transformations: (#1) 1–x,1–y,2–z; (#2) 1–x,–1/2+y,1.5–z; (#3) –x,1–y,1–z; (#4) –1+x,y,z; (#5) 1–x,1–y,1–z; (#6) x,1/2–y,–1/2+z; (#7) 1–x,–y,–z; (#8) 1–x,–1/2+y,1.5–z; (#9) 1+x,y,z (#10) 1–x,–1/2+y,1.5–z; (#11) 1–x,–y,1–z; (#12) 1–x,1–y,–z; (#13) 1+x,1+y,z; (#14) 2–x,1–y,1–z; (#15) 2–x,1–y,–z; (#16) 1–x,–1/2+y,1/2–z; (#17) 1–x,1/2+y,1/2–z; (#18) x,y,1+z; (#19) x,–1+y,z; (#20) 1–x,–y,2–z; (#21) 1–x,3–y,1–z; (#22) 1+x,y,1+z; (#23) –x,2–y+2,–z; (#24) –x,–1/2+y,1/2–z; (#25) –x,1–y,–z; (#26) –x,1/2+y,1/2–z; (#27) 1–x,2–y,–z.

6. Photophysical properties and quantum-chemical calculations

Table S5. Experimental and theoretical UV-Vis absorption data for **1-10**.

IL - intraligand charge transfer
LLCT - ligand to ligand charge transfer
DBA - 9,10-dihydro-9,10-diboraanthracene

	Experimental results			Theoretical calculations	
	λ_{max} [nm]	ε [M^{-1} cm^{-1}]	λ_{bent} / $\lambda_{symmetrical}$ [nm]	oscillator strength, *f*	transition character
1	390	45800	427 / 427	0.0503 / 0.0506	*Bent:* HOMO -> LUMO | π (Q, DBA) -> π*(Q') | LLCT HOMO−1 -> LUMO | π (DBA, Q, Q') -> π*(Q') | IL / LLCT HOMO -> LUMO+1 | π (Q, DBA) -> π*(Q) | LLCT / IL *Symmetrical:* HOMO -> LUMO+1 | π (Q, Q'); n (O, O'); σ (B-C) -> π*(Q); n* (O); σ (B-C) | LLCT / IL HOMO -> LUMO | π (Q, Q', DBA); n (O, O'); σ (B-C) -> π*(Q'); n* (O'); σ (B-C) | LLCT / IL HOMO-1 -> LUMO | π (Q, Q', DBA); n (O, O'); σ (B-C) -> π*(Q'); n* (O'); σ (B-C) | LLCT / IL
2	397	8200	442 / --	0.085 / --	*Bent:* HOMO -> LUMO | π (Q) -> π*(Q') | LLCT HOMO−1 -> LUMO | π (Q',DBA) -> π*(Q') | IL / LLCT HOMO−1 -> LUMO+1 | π (Q',DBA) -> π*(Q) | LLCT
3	396	71000	442 / 439	0.0750 / 0.1155	*Bent:* HOMO -> LUMO | π (Q) -> π*(Q') | LLCT HOMO−1 -> LUMO | π (Q') -> π*(Q) | LLCT *Symmetrical:* HOMO -> LUMO | π (Q, Q'); n (O, O'); σ (B-C) -> π*(Q, Q'); n* (O, O') | LLCT / IL HOMO−1 -> LUMO+1 | π (Q, Q'); n (O, O'); σ (B-C) -> π*(Q, Q'); n* (O, O') | LLCT / IL
4	396	38000	442 / 440	0.0704 / 0.1148	*Bent:* HOMO−1 -> LUMO | π (Q) -> π*(Q) | IL HOMO -> LUMO | π (Q) -> π*(Q') | LLCT *Symmetrical:* HOMO -> LUMO | π (Q, Q'); n (O, O'); σ (B-C) -> π*(Q, Q'); n* (O, O') | LLCT / IL HOMO−1 -> LUMO+1 | π (Q, Q'); n (O, O'); σ (B-C) -> π*(Q, Q'); n* (O, O') | LLCT / IL
5	396	10000	421 / 435	0.0423 / 0.947	*Bent:* HOMO -> LUMO+1 | π (Q, Q'); n (O, O', F); σ (B-C, B'-C') -> π*(Q); n* (O); σ (B-C) | LLCT / IL HOMO -> LUMO | π (Q, Q'); n (O, O', F); σ (B-C, B'-C') -> π*(Q'); n* (O'); σ (B'-C') | LLCT / IL HOMO-1 -> LUMO | π (Q, Q'); n (O, O', F); σ (B-C, B'-C') -> π*(Q'); n* (O'); σ (B'-C') | LLCT / IL *Symmetrical:* HOMO -> LUMO | π (Q, Q'); n (O, O', F); σ (B-C) -> π*(Q, Q'); n*(O, O') | LLCT / IL HOMO-1 -> LUMO+1 | π (Q, Q'); n (O, O'); σ (B-C) -> π*(Q, Q'); n*(O, O') | LLCT / IL

6	414	9000	460 / 459	0.1063 / 0.1487	*Bent:* HOMO -> LUMO | π (Q); n (Cl, O); σ (B-C) -> π*(Q'); n* (O') | LLCT HOMO-1 -> LUMO | π (Q); n (Cl, O); σ (B-C) -> π*(Q'); n* (O') | LLCT HOMO -> LUMO+1 | π (Q', DBA); n (Cl, O); σ (B-C) -> π*(Q'); n* (O') | LLCT / IL *Symmetrical:* HOMO -> LUMO | π (Q, Q'); n (Cl, Cl', O, O'); σ (B-C) -> π*(Q, Q'); n* (O, O') | LLCT / IL HOMO−1 -> LUMO+1 | π (Q, Q'); n (Cl, Cl', O, O'); σ (B-C) -> π*(Q, Q'); n* (O, O') | LLCT / IL HOMO -> LUMO | π (Q); n (O); σ (B-C) -> π*(Q); n* (O); σ*(B-C) | IL
7	414	9400	467 / 464	0.0889 / 0.1411	*Bent:* HOMO -> LUMO | π (Q); n (Cl, O); σ (B-C) -> π*(Q'); n* (O') | LLCT HOMO-1 -> LUMO | π (Q); n (Cl, O); σ (B-C) -> π*(Q'); n* (O') | LLCT HOMO -> LUMO+1 | π (Q', DBA); n (Cl, O); σ (B-C) -> π*(Q'); n* (O') | LLCT / IL *Symmetrical:* HOMO -> LUMO | π (Q, Q'); n (Cl, Cl', O, O'); σ (B-C) -> π*(Q, Q'); n* (O, O') | LLCT / IL HOMO−1 -> LUMO+1 | π (Q, Q'); n (Cl, Cl', O, O'); σ (B-C) -> π*(Q, Q'); n* (O, O') | LLCT / IL
8	392	47800	-- / 426	-- / 0.1321	*Symmetrical:* HOMO−1 -> LUMO | π (Q, Q'); n (O, O'); σ (B-C) -> π*(Q, Q'); n*(O, O'); σ*(B-C) | LLCT / IL HOMO−2 -> LUMO+1 | π (Q, Q', DBA); n (O, O'); σ (B-C) -> π*(Q, Q'); n*(O, O'); σ*(B-C) | LLCT / IL
9	390	4200	430	0.0551	HOMO−1 -> LUMO | π (Q); n (O); σ (B-C) -> π*(Q); n*(O); σ*(B-C) | IL
10	427	12000	473	0.0805	*Symmetrical:* HOMO -> LUMO | π (BQ, BQ'); n (O); σ (B-C) -> π*(BQ, BQ') | LLCT / IL HOMO-1 -> LUMO+1 | π (BQ, BQ'); n (O); σ (B-C) -> π*(BQ, BQ') | LLCT / IL

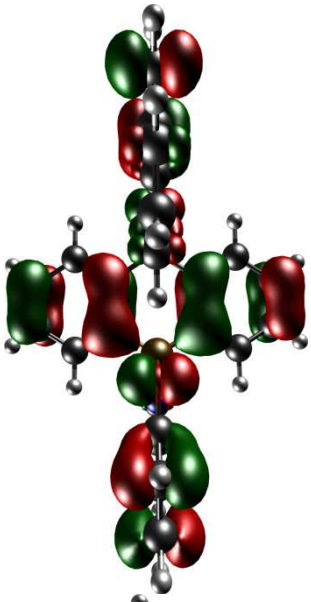
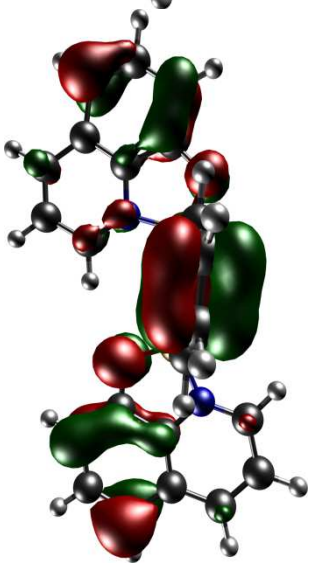
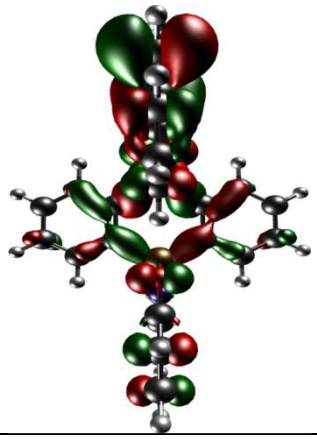
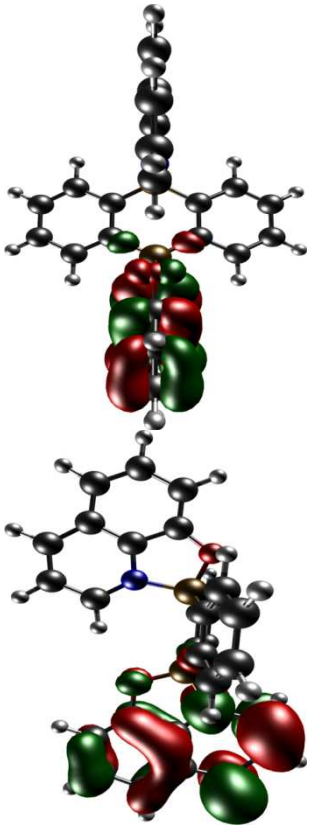
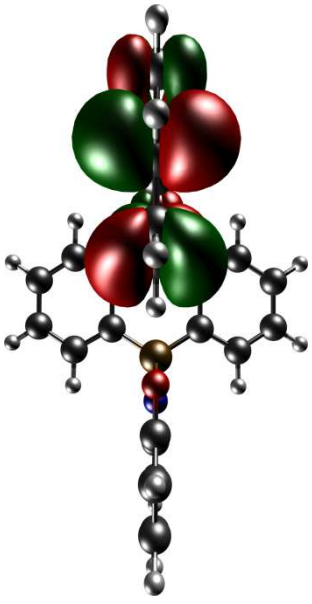
Table S6. Experimental and theoretical results regarding luminescence of **1**-**10**.

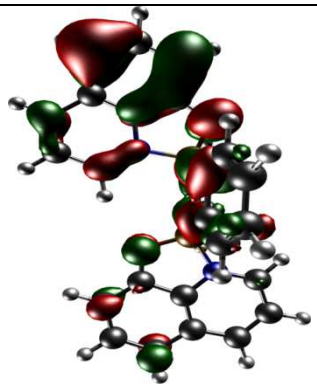
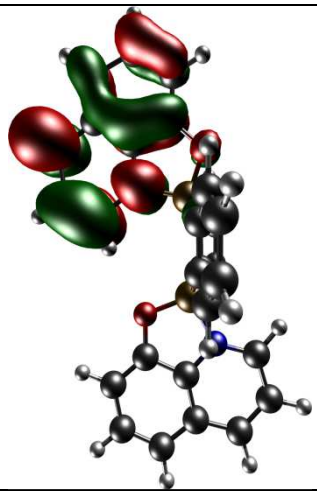
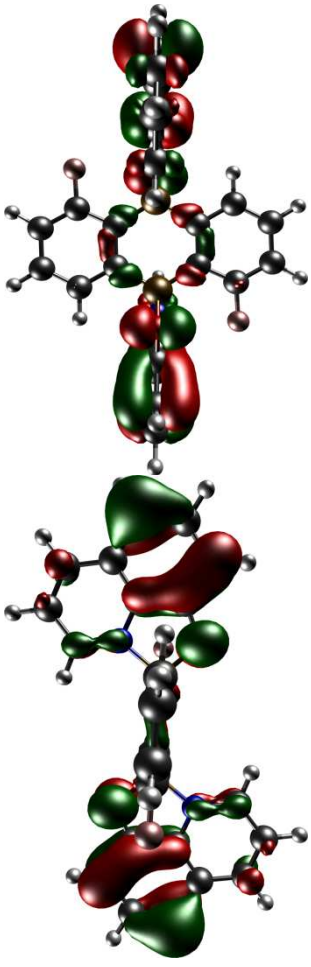
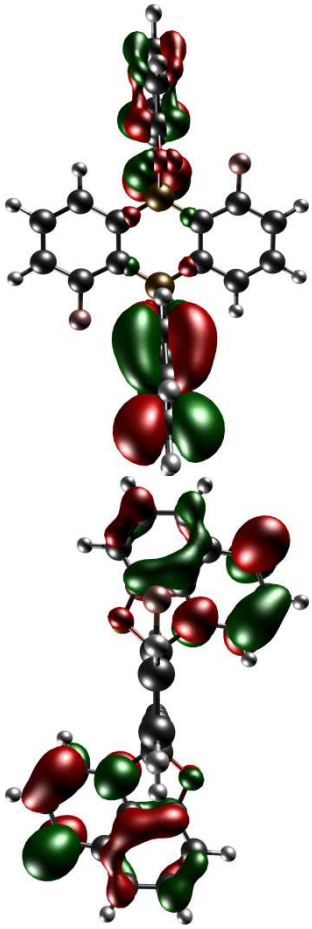
	λ_{em} [nm]	Φ [%]	λ_{bent} / $\lambda_{symmetrical}$ [nm]	oscillator strength, *f*	transition character
1	494	48	486 / --	0.0453 / --	*Bent:* HOMO−2 -> LUMO | π (Q', DBA); n (O'); σ (B-C) -> π*(Q'); n* (O'); σ* (B-C) | LLCT / IL
2	503	52	-- / 567	-- / 0.046	*Symmetrical:* HOMO -> LUMO | π (Q); n (O); σ (B-C) -> π*(Q); n* (O); σ* (B-C) | LLCT / IL
3	502	53	564 / --	0.048 / --	*Bent:* HOMO -> LUMO | π (Q,Q'); n (O,O'); σ (B-C) -> π*(Q); n* (O); σ* (B-C) | LLCT / IL HOMO-1 -> LUMO | π (Q,Q'); n (O,O'); σ (B-C) -> π*(Q); n* (O); σ* (B-C) | LLCT / IL

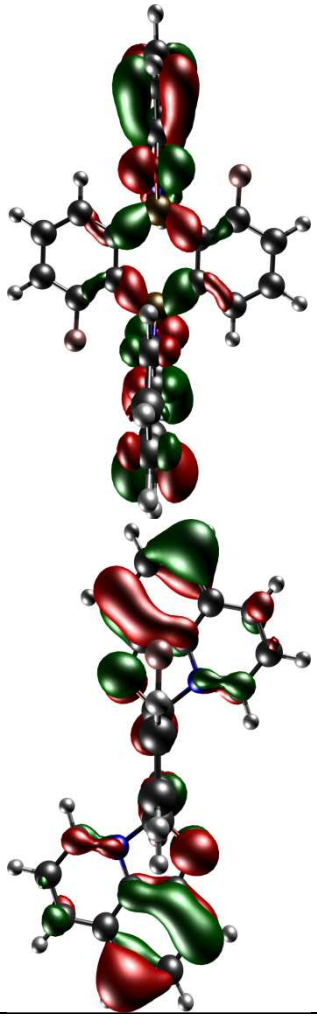
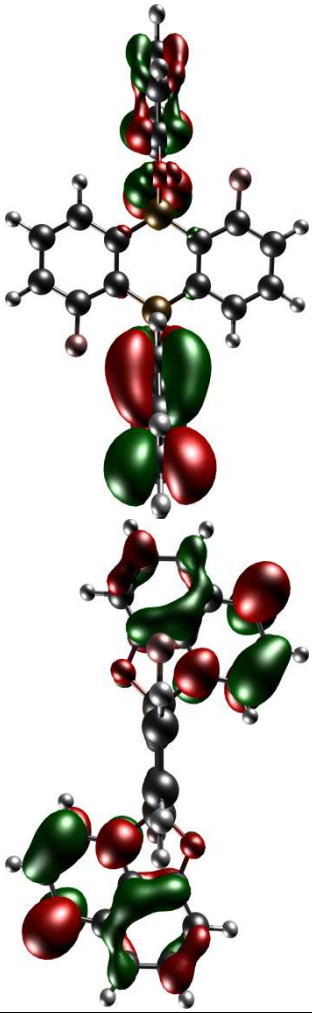
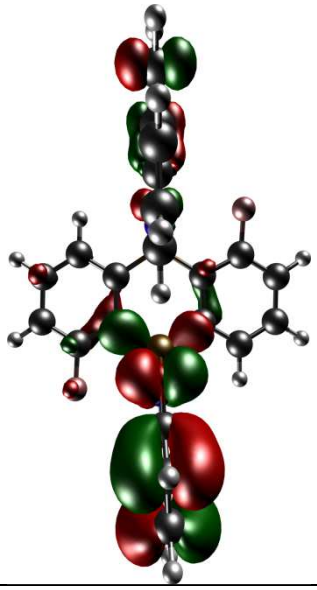
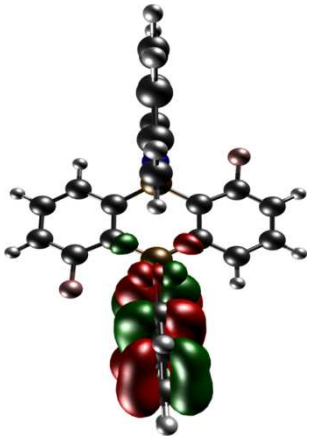
4	502	41	564 / 574	0.0458 / 0.0415	*Bent:* HOMO -> LUMO | π (Q,Q'); n (O, O'); σ (B-C) -> π*(Q); n* (O); σ* (B-C) | LLCT / IL HOMO-1 -> LUMO | π (Q,Q'); n (O, O'); σ (B-C) -> π*(Q); n* (O); σ* (B-C) | LLCT / IL *Symmetrical:* HOMO -> LUMO | π (Q); n (O); σ (B-C) -> π*(Q); n* (O); σ* (B-C) | IL
6	522	13	604 / --	0.0528 / --	*Bent:* HOMO -> LUMO | π (Q); n (Cl, O); σ (B-C) -> π*(Q); n* (Cl, O); σ*(B-C) | IL
7	516	26	528 / 604	0.0462 / 0.0517	*Bent:* HOMO-2 -> LUMO | π (DBA); n (F) -> π*(Q'); n* (O') | LLCT HOMO-1 -> LUMO | π (Q', DBA); n (Cl', O'); σ (B-C) -> π*(Q'); n* (O') | LLCT / IL *Symmetrical:* HOMO -> LUMO | π (Q); σ(B-C); n (O, Cl, Cl') -> π*(Q); n*(O); σ*(B-C)
8	506	22	482 / --	0.078 / --	*Bent:* HOMO-2 π (Q,Q', DBA); *n* (O,O') -> LUMO (Q) π*(Q); n* (O); σ* (B-C) | LLCT / IL HOMO-1 -> LUMO || π (Q, DBA); n (O)) -> (Q) π*(Q); n* (O); σ* (B-C) | LLCT / ILHOMO-1 (DBA;Q) -> LUMO (Q) HOMO-3 -> LUMO || π (Q,Q'); n (O,O',S); σ (B-C) -> (Q) π*(Q); n* (O); σ* (B-C) | LLCT / IL
10	520	19	487 / --	0.0631 / --	*Bent:* HOMO -> LUMO+1 | π (BQ); n (O,O'); σ (B-C) -> π*(BQ); n (O) | IL

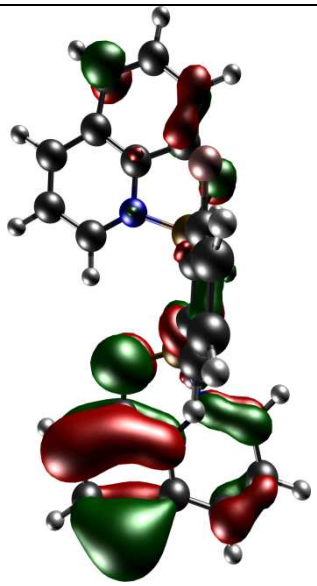
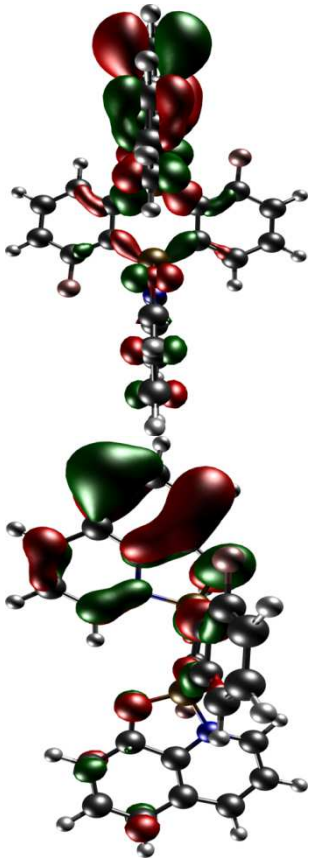
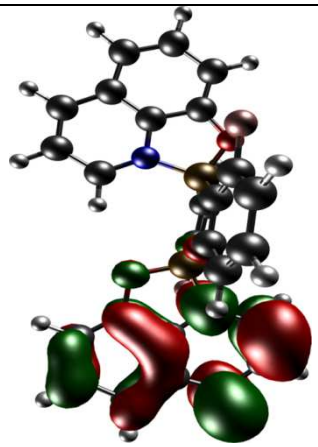
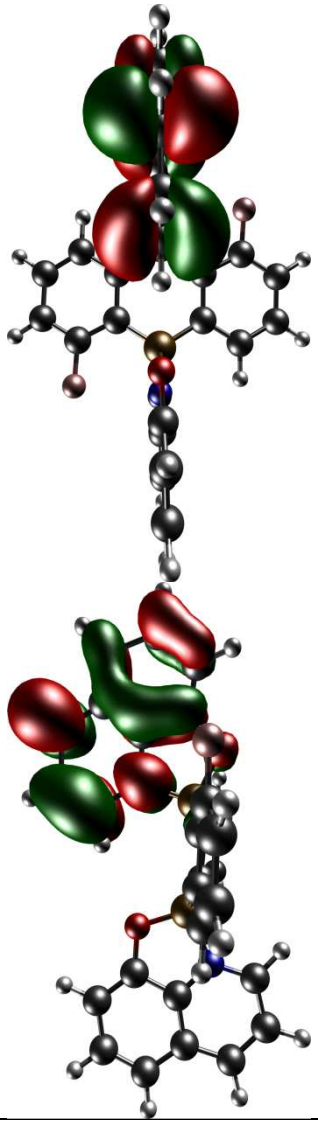
Table S7. HOMOs and LUMOs and their energies calculated for optimized ground state structures at TD-RB3LYP/6-31+g(d,p) level of theory.

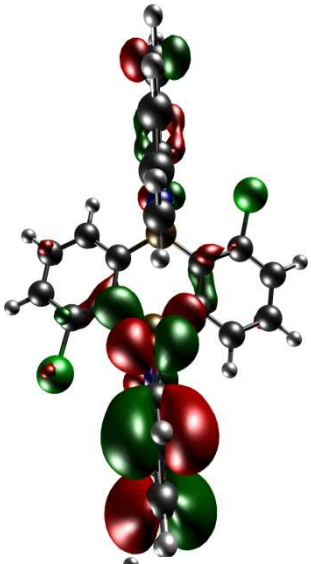
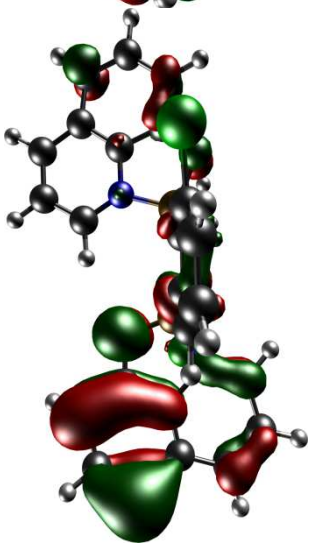
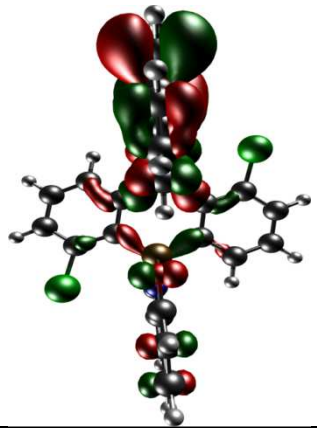
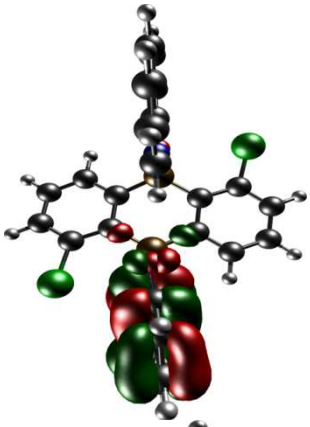
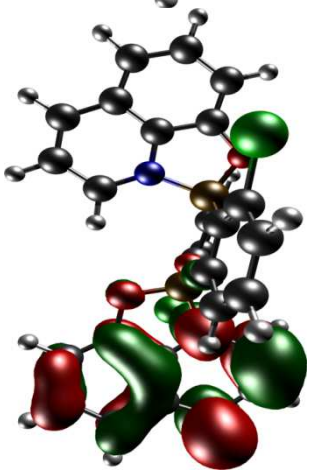
	E_{HOMO} (*bent*) / E_{HOMO} (*symmetrical*)	E_{LUMO} (*bent*) / E_{LUMO} (*symmetrical*)	ΔE
1	−5.65 / −5.65	−2.48 / −2.48	3.17 / 3.17
2	−5.72 / −5.72	−2.44 / −2.33	3.28 / 3.39
3	−5.78 / −5.79	−2.50 / −2.38	3.28 / 3.41
4	−5.80 / −5.80	−2.52 / −2.39	3.28 / 3.41
5	−6.01 / −6.03	−2.79 / −2.60	3.22 / 3.43
6	−5.87 / −5.88	−2.71 / −2.60	3.16 / 3.28
7	−6.00 / −6.02	−2.91 / −2.78	3.09 / 3.24
8	-- / −5.53	-- / −2.35	-- / 3.18
9	-- /−5.67	-- /−2.57	-- / 3.10
10	-- / −5.44	-- / −2.30	-- / 3.14

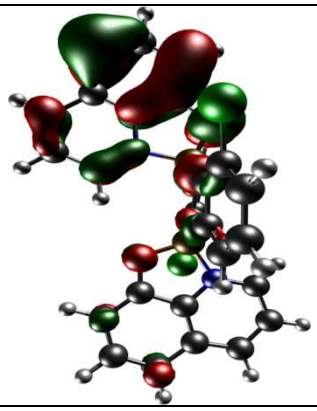
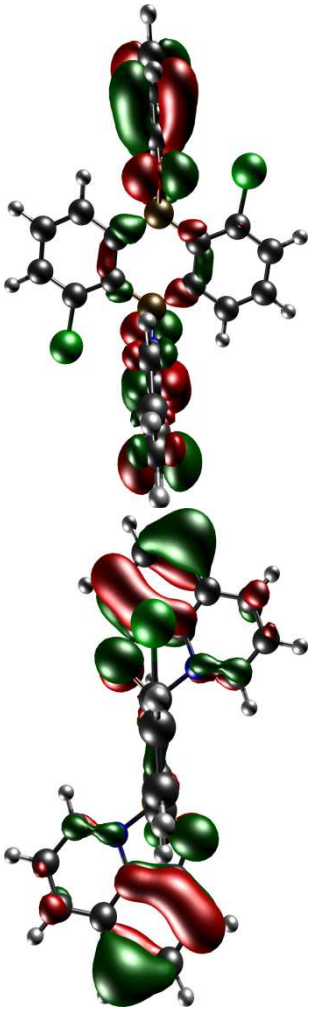
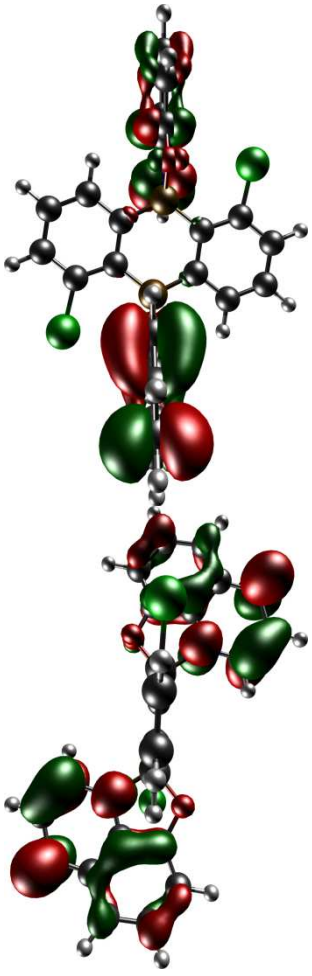
	HOMOs	LUMOs
1 – bent	HOMO−1   HOMO 	LUMO  LUMO+1 

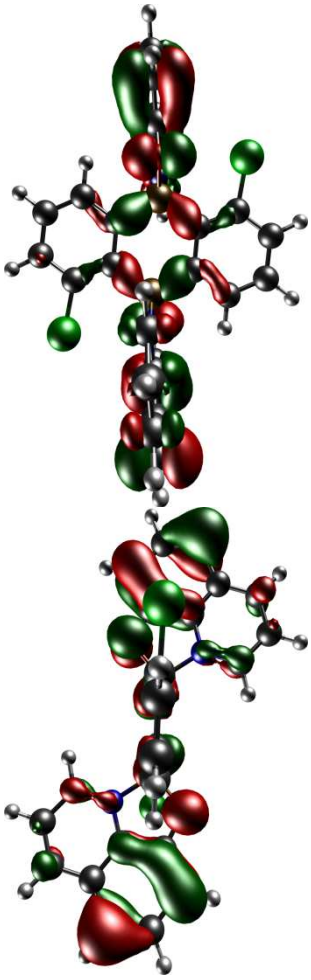
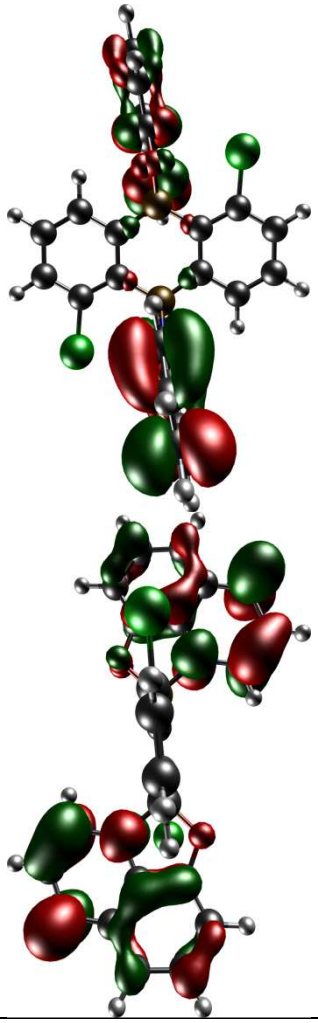
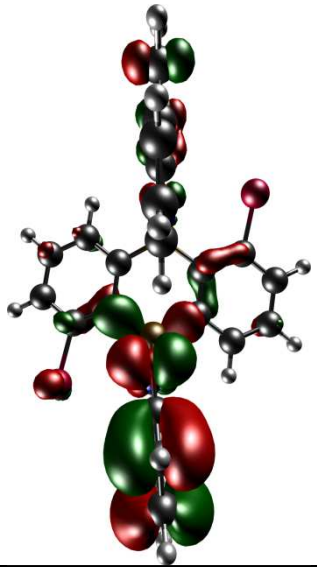
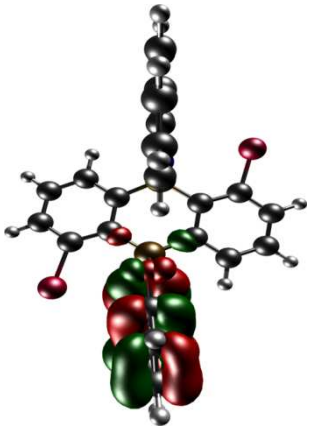
		
2 - symmetrical	HOMO−1 	LUMO+1 

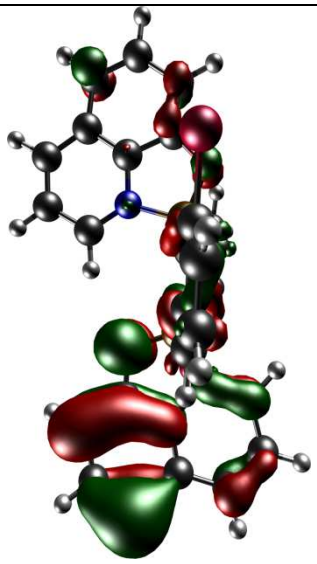
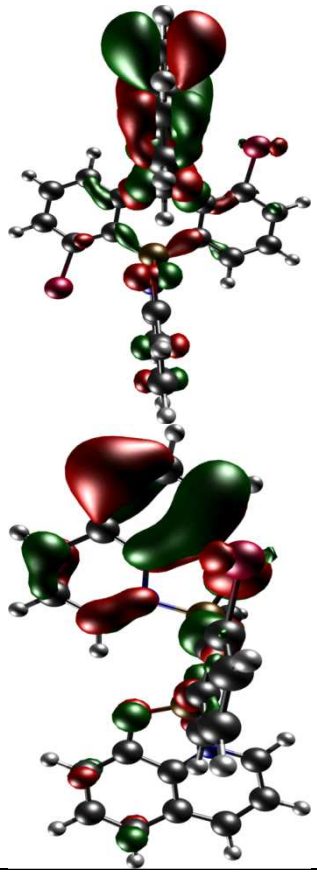
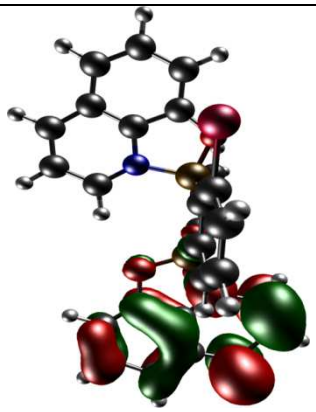
	HOMO 	LUMO 
2 –bent	HOMO−1 	LUMO 

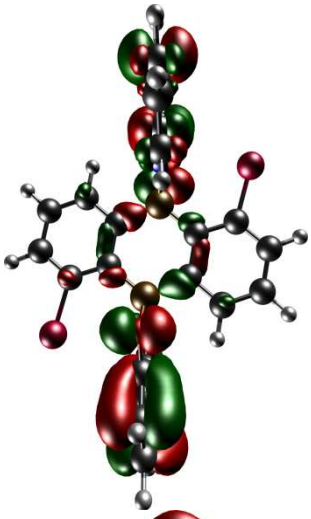
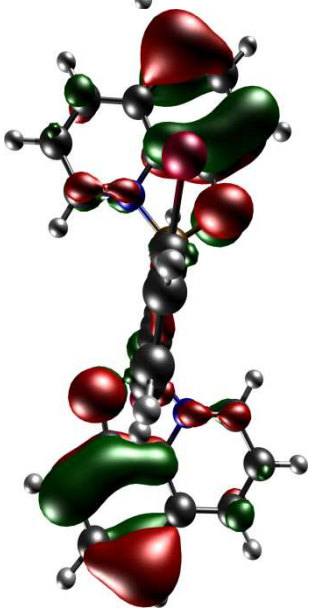
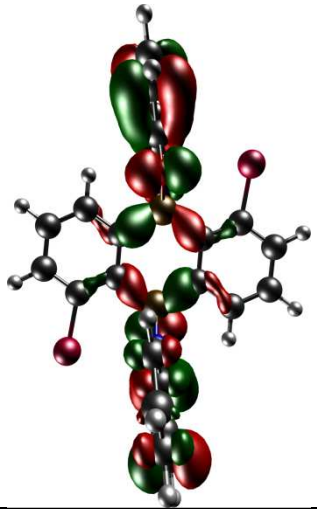
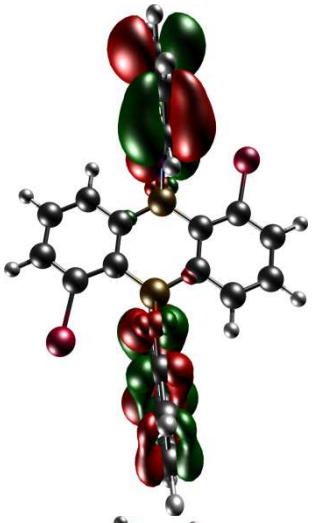
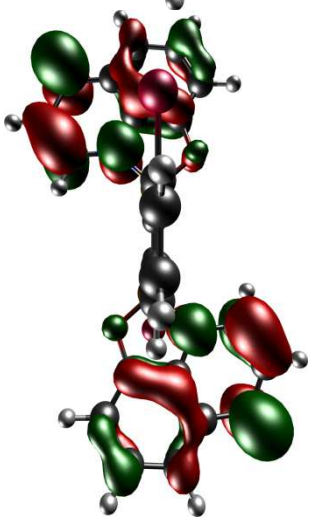
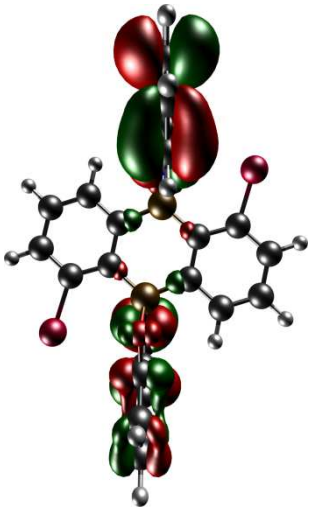
	 HOMO 	 LUMO+1 

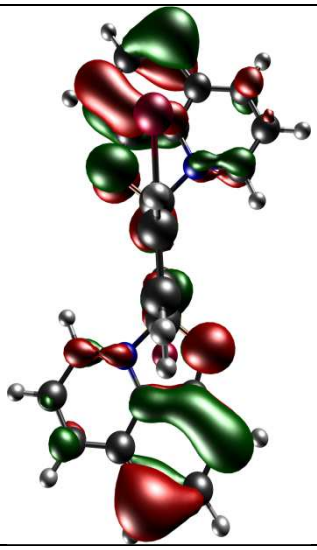
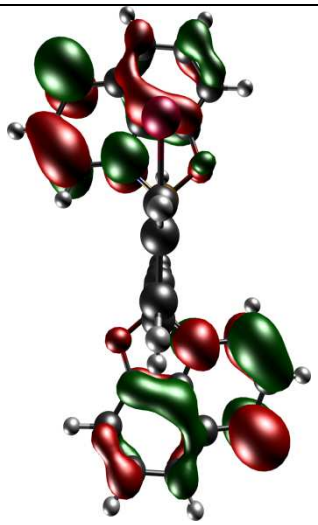
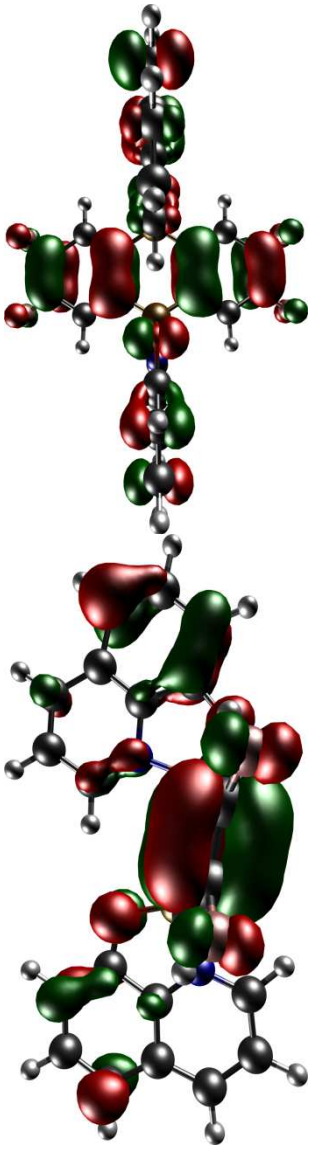
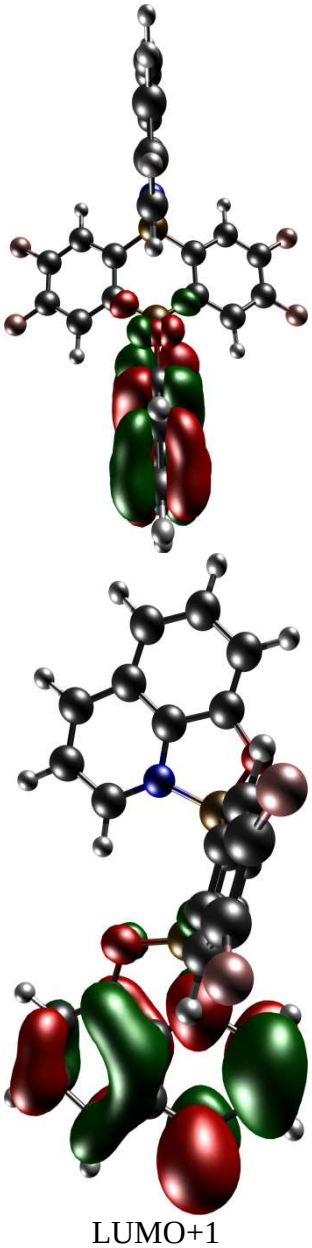
3 - bent	HOMO−1   HOMO 	LUMO  

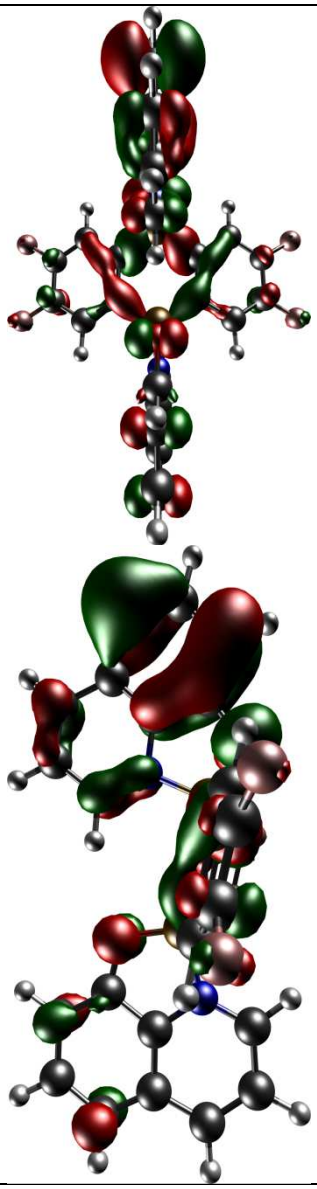
		
3 -symmetrical	HOMO−1 	LUMO 

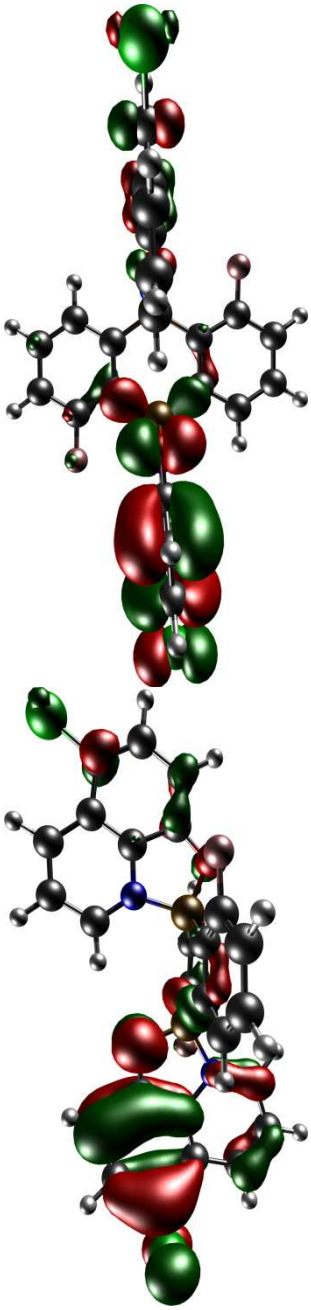
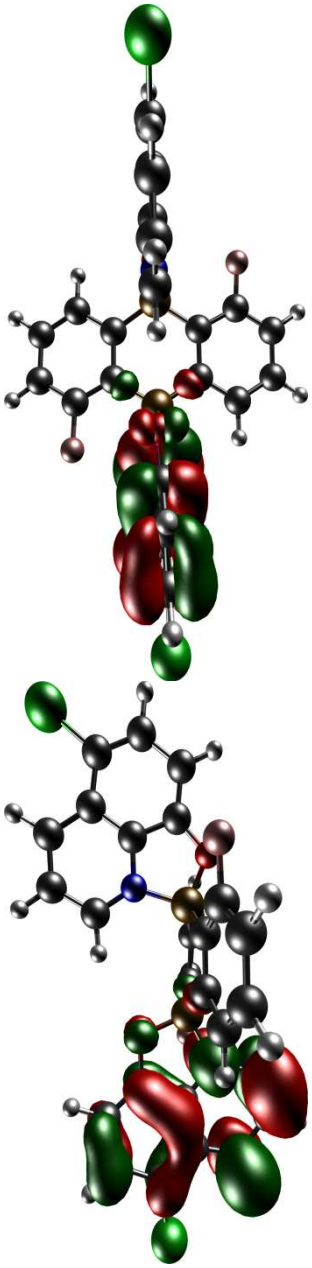
	HOMO 	LUMO+1 
4 -bent	HOMO−1 	LUMO 

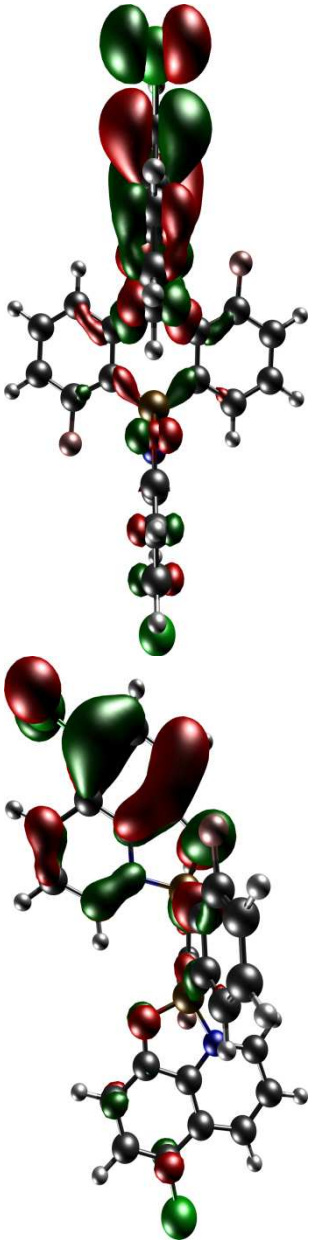
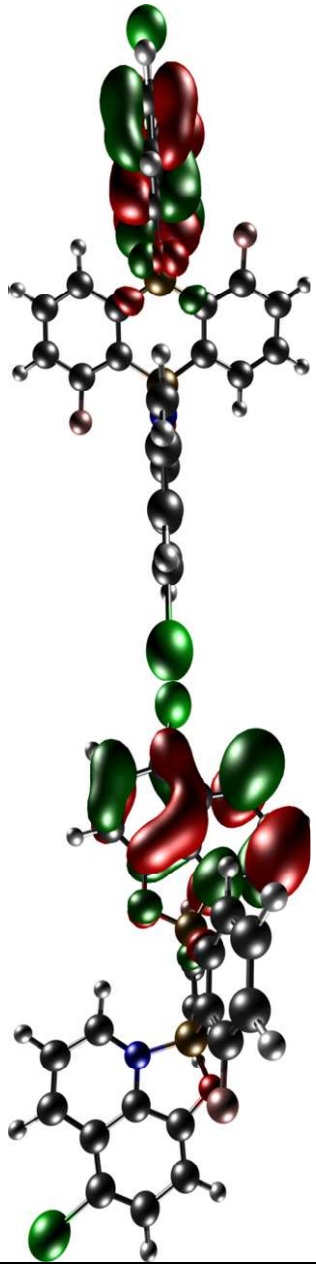
	 HOMO 	

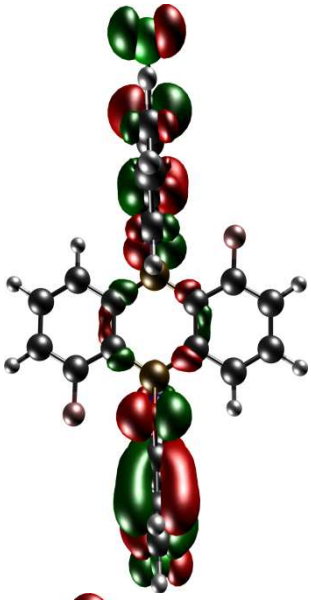
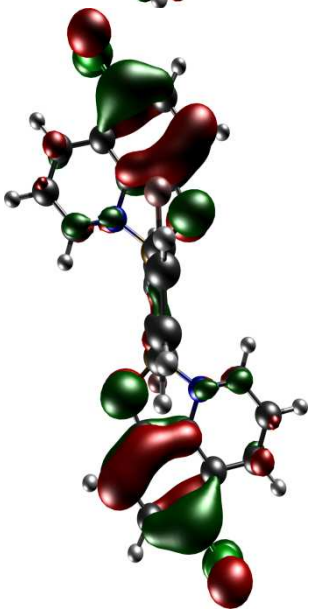
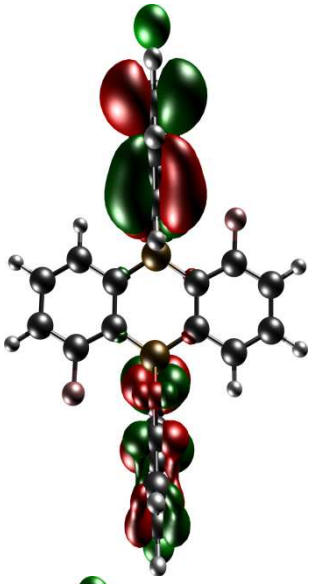
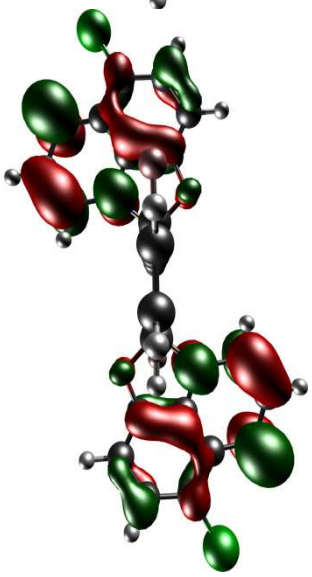
4 - symmetrical	HOMO−1   HOMO 	LUMO   LUMO+1 

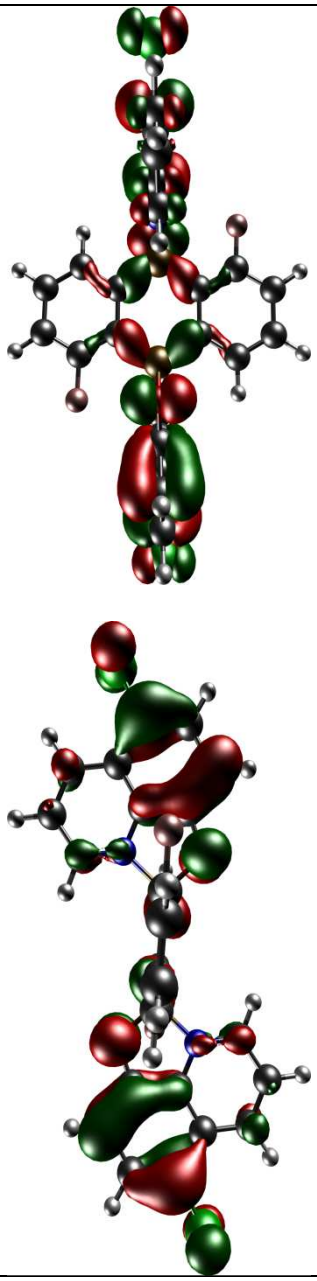
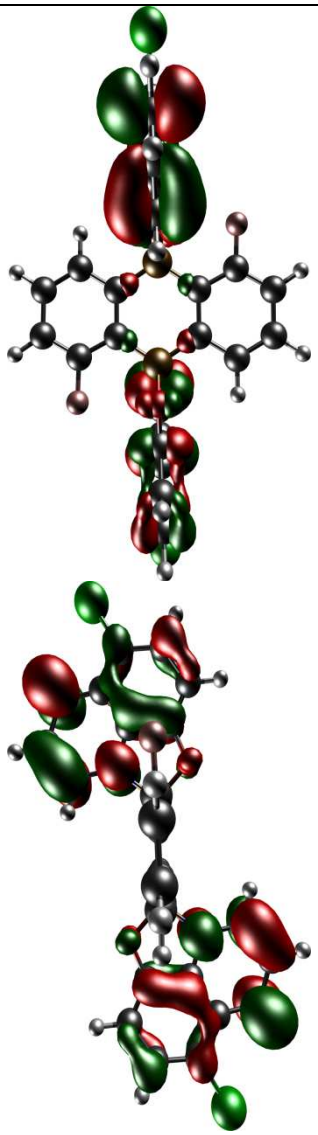
		
5 –bent	HOMO−1  HOMO	LUMO  LUMO+1

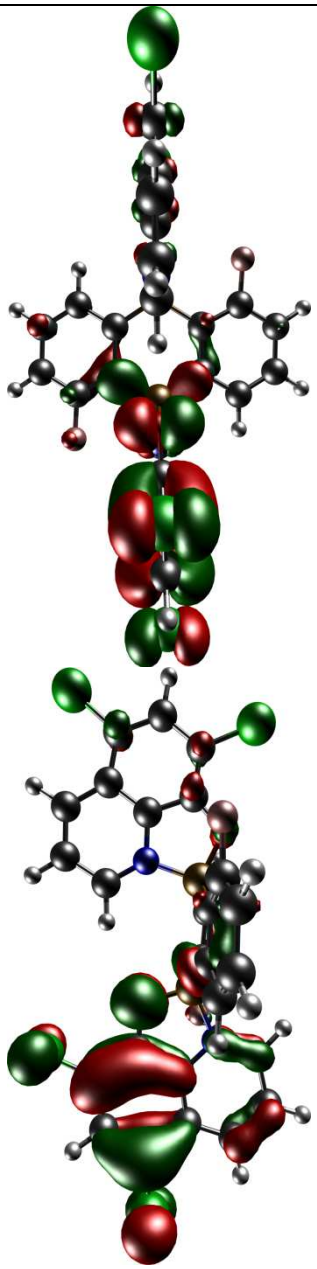
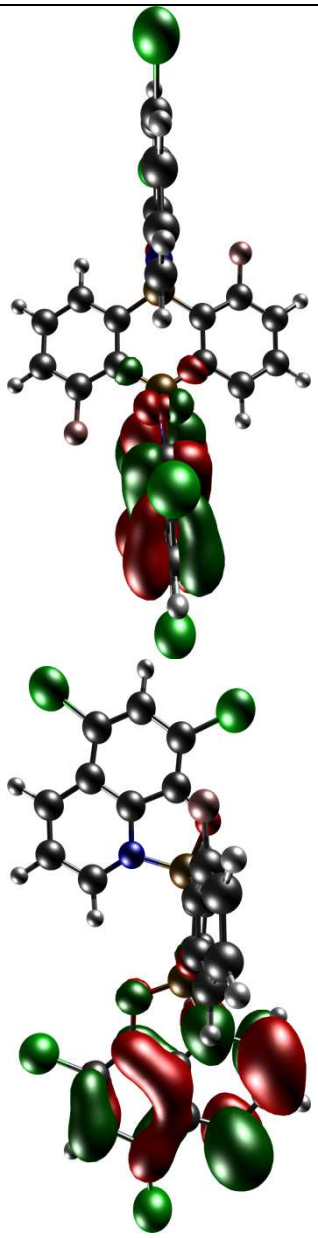
		

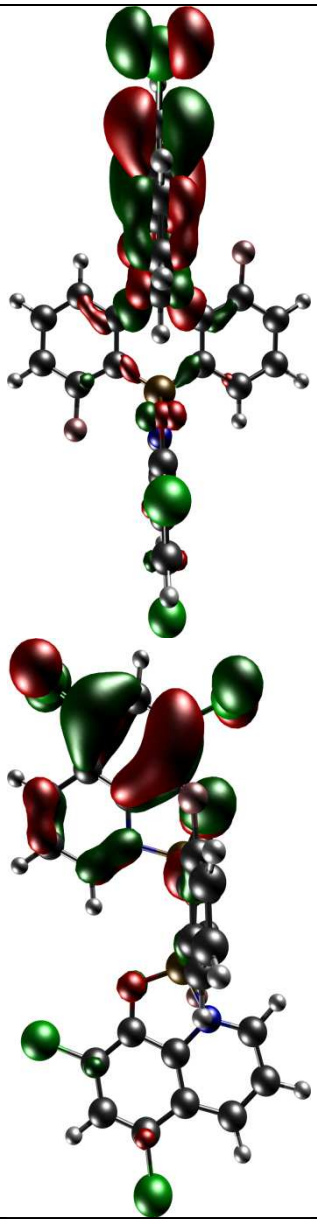
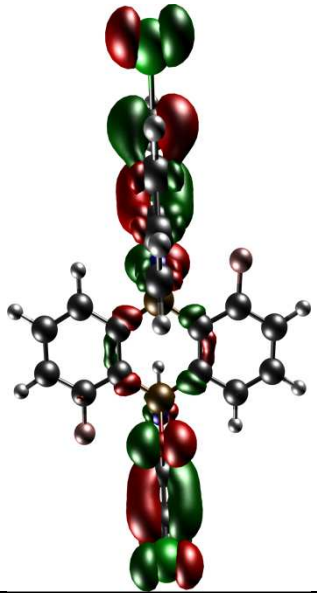
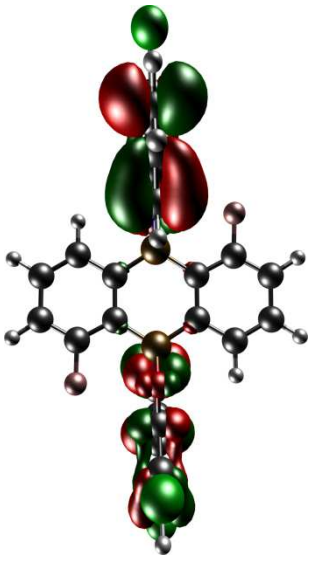
6 - bent	HOMO−1 	LUMO 

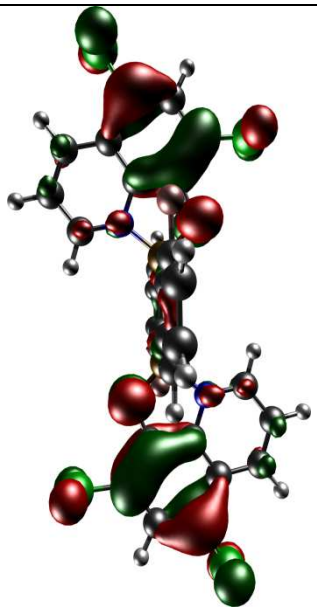
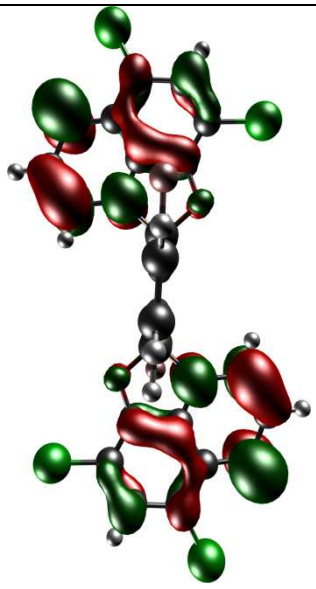
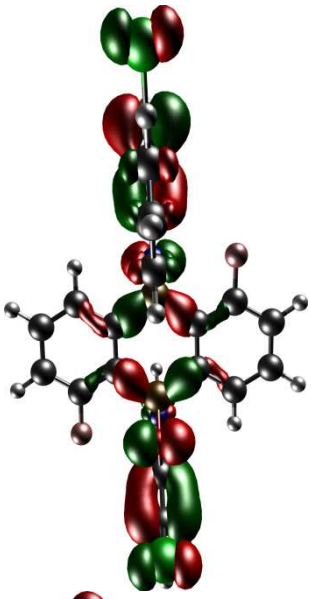
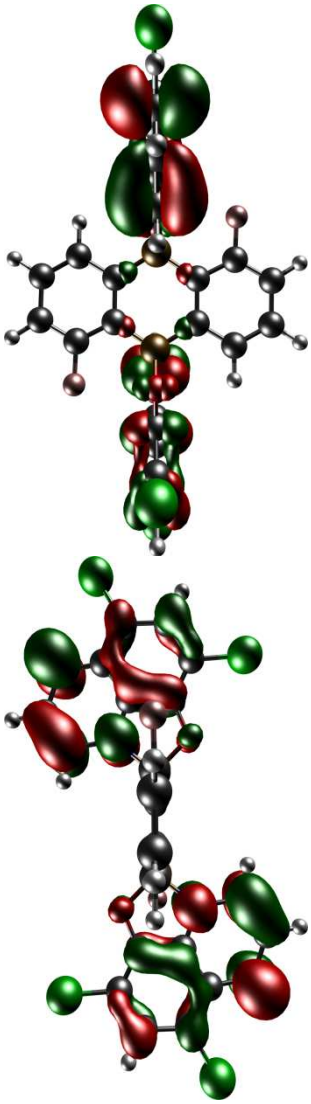
	HOMO 	LUMO+1 

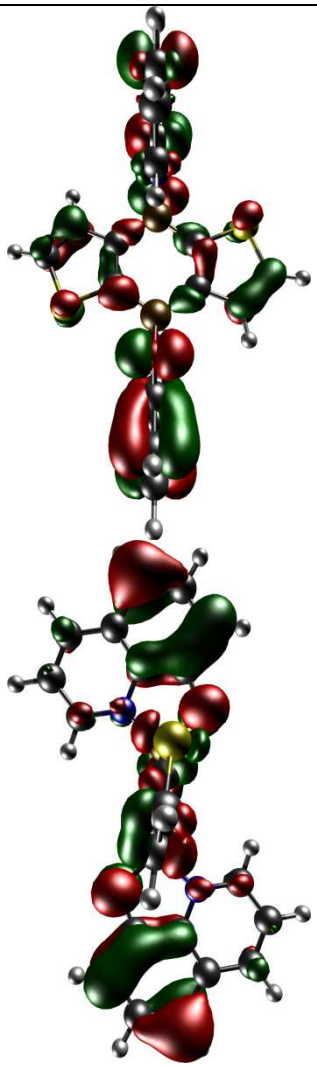
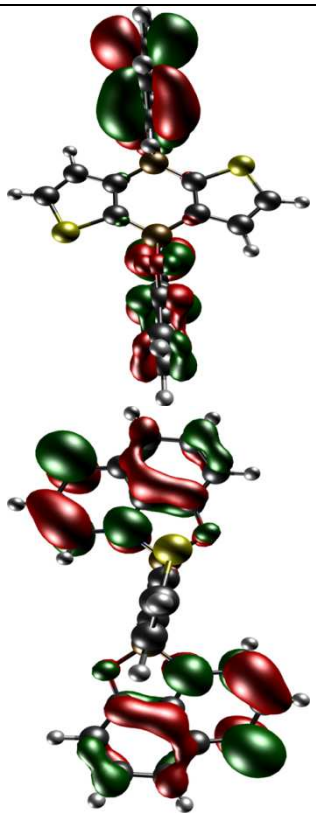
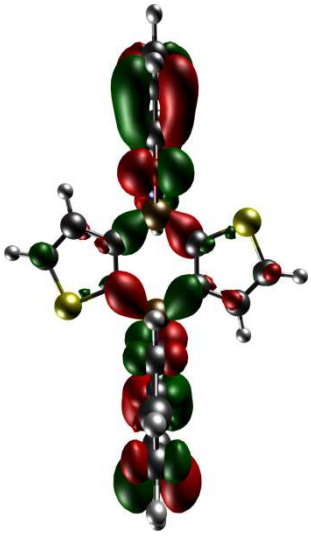
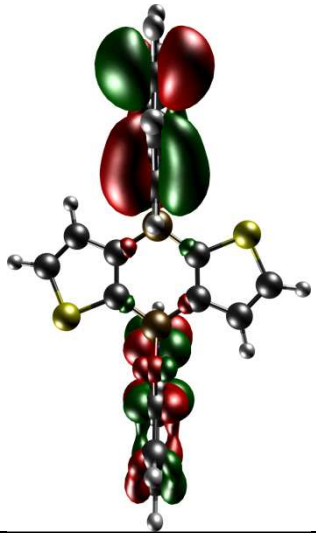
6 - symmetrical	HOMO-1   HOMO	LUMO   LUMO+1

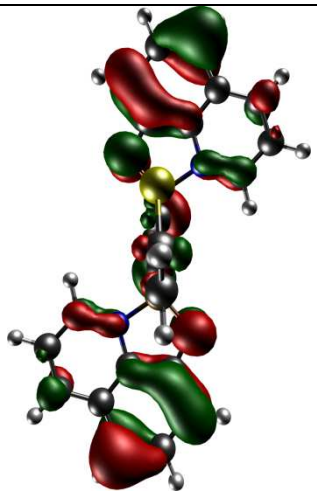
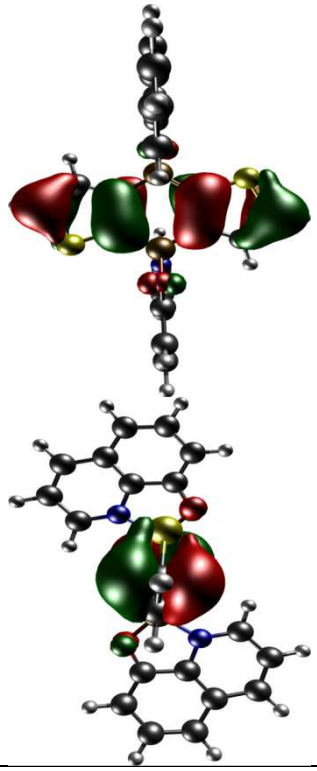
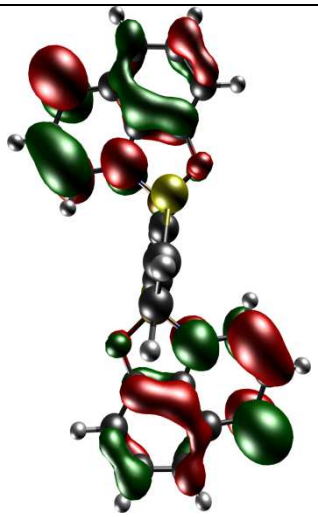
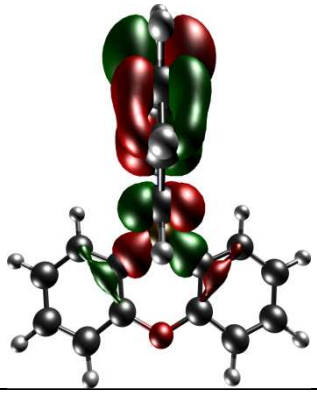
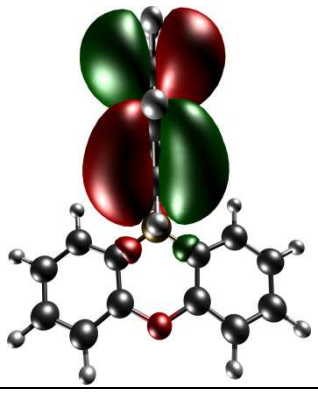
		
7 - bent	HOMO−1	LUMO

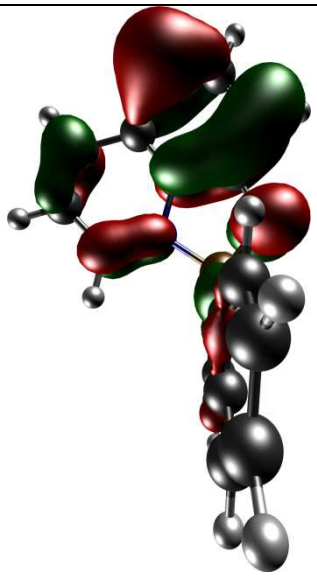
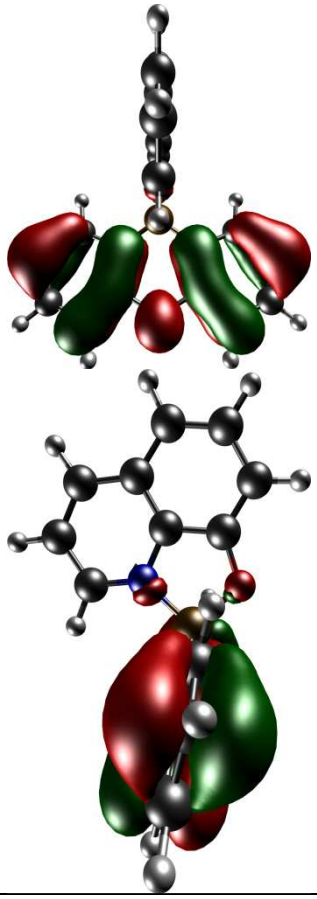
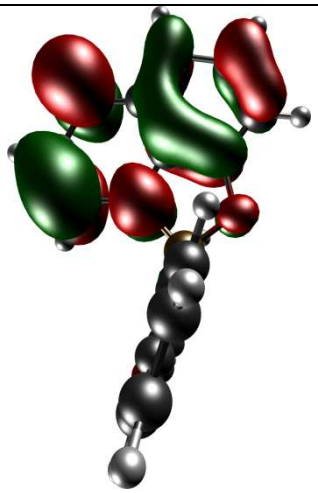
	 HOMO	

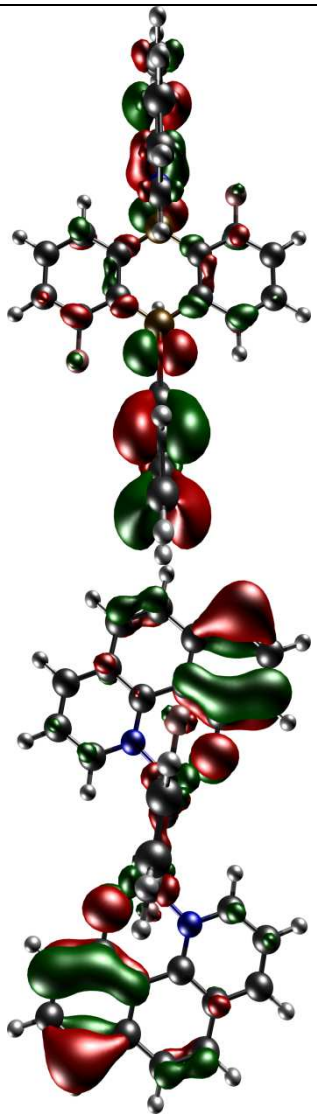
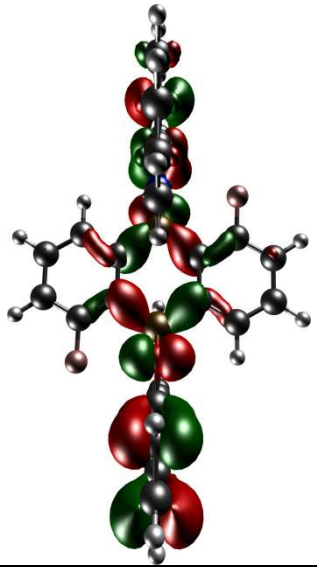
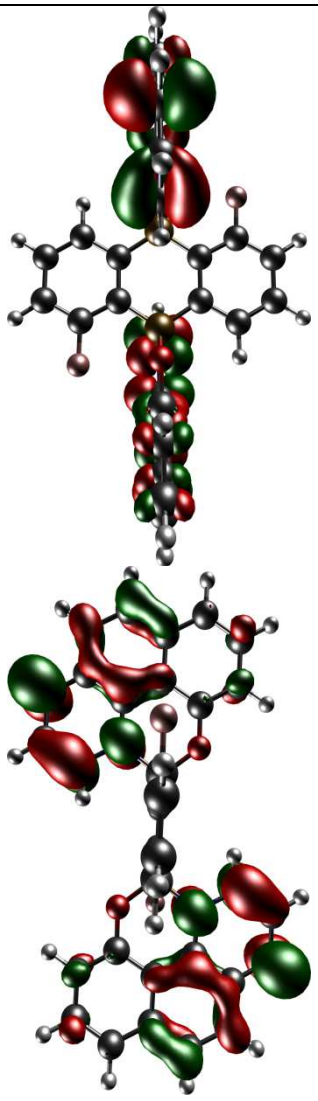
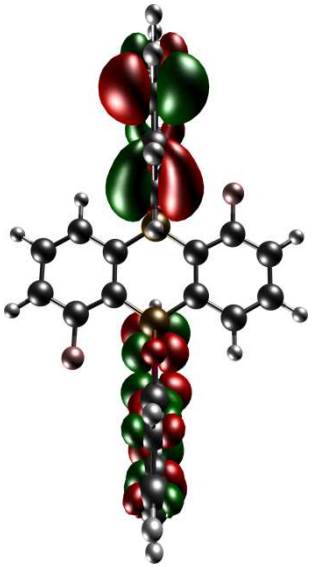
		
7 - symmetrical	HOMO-1 	LUMO 

	 HOMO	 LUMO+1
	 HOMO−2	 LUMO
8 - symmetrical		

		
	HOMO−1	LUMO+1
		

	 HOMO 	
9	HOMO−1 	LUMO 

	 HOMO 	
10 -symmetrical	HOMO−1	LUMO

	 HOMO 	 LUMO+1 

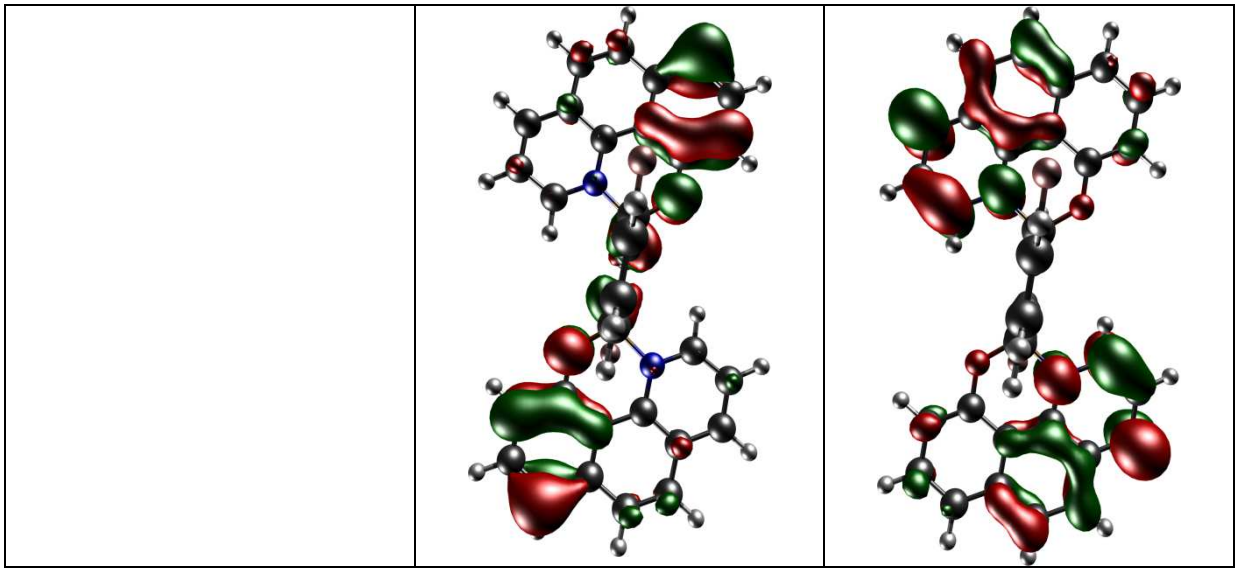


Table S8. Calculated energies (UB3LYP/6-31+g(d,p), in a.u.) for the optimized geometry of neutral state(A), the optimized geometry of cationic species (B), the optimized geometry of anionic state (C), cationic states with the optimized geometry of neutral species (D), anionic state with the optimized geometry of neutral species (E), neutral state with the optimized geometry of anionic species (F) and neutral state with the optimized geometry of cationic species (G) for *symmetrical* and *bent* forms.

bent form

	(A)	(B)	(C)	(D)	(E)	(F)	(G)
1	–39868.81	–39862.09	–39870.09	–39861.99	–39869.99	–39868.70	–39868.63
2	–45269.90	–45263.08	–45271.20	–45263.00	–45271.11	–45269.81	–45269.85
3	–64881.08	n.a.	–64882.44	–64874.12	–64882.34	–64880.98	n.a.
4	–179796.94	–179790.02	–179798.32	–179789.97	–179798.22	–179796.84	–179796.88
5	n.a.	–50663.46	–50672.14	–50663.37	–50672.03	–50670.43	–50670.41
6	–70282.19	–64881.08	–70283.79	–70275.17	–70283.69	–70282.09	n.a.
7	–95294.39	n.a.	–95296.18	–95287.25	–95296.08	–95294.28	n.a.
8	n.a.	–57318.86	n.a.	n.a.	n.a.	n.a.	n.a.
10	–53632.41	n.a.	n.a.	–53625.90	–53633.65	n.a.	n.a.

symmetrical form

	(A)	(B)	(C)	(D)	(E)	(F)	(G)
2	–45269.90	–45263.08	n.a.	–45263.03	–45271.09	–45269.81	–45269.85
3	–64881.06	–64874.19	n.a.	–64874.14	–64882.30	n.a.	–64881.01
4	–179796.90	–179790.02	–179798.25	–179789.97	–179798.17	–179796.84	–179796.85
6	–70282.19	–70275.27	–70283.74	–70275.21	–70283.67	–70282.08	n.a.
7	–95294.38	–95287.34	–95296.10	–95287.28	–95296.06	–95294.23	–95287.34
8	–57325.45	n.a.	–57326.74	–57318.67	–57326.65	–57325.37	–57325.16
9	–28269.06	–28262.02	–28270.28	–28261.90	–28270.08	–28268.86	–28268.95
10	n.a.	–53625.96	–53633.72	n.a.	n.a.	–53632.33	–53632.35

	(A)	(B)	(C)	(D)	(E)	(F)	(G)
AlQ_3_fac	–45509.11	–45502.51	–45510.06	–45502.44	–45509.99	–45509.05	–45509.04
AlQ_3_mer	–45509.35	–45502.87	–45510.31	–45502.78	–45510.2	–45509.18	–45509.21
Ph_2BQ	–26254.7	–26247.34	–26255.91	–26247.34	–26255.72	–26254.52	–26254.59

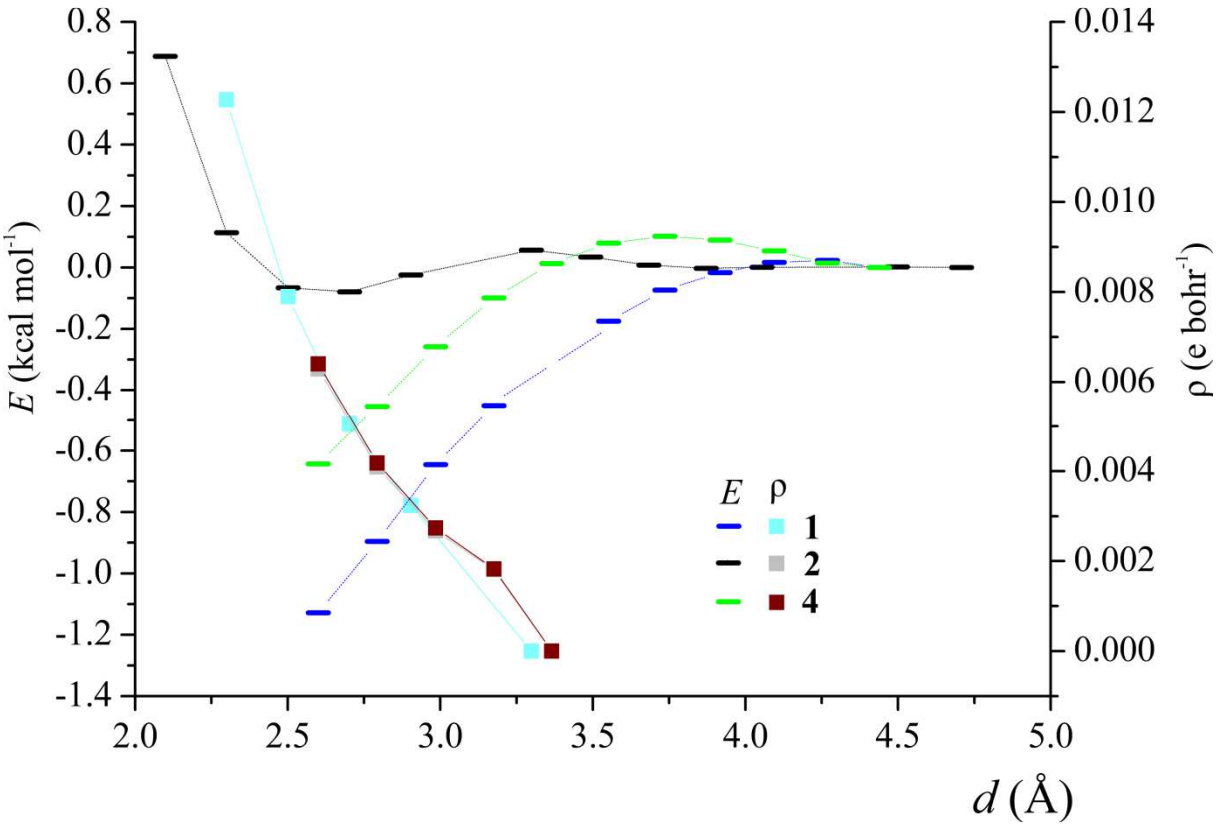
Table S9. Calculated inner reorganization energies (eV) for hole- and electron-acceptance. Calculation were done for *symmetrical* and *bent* forms. It was not possible to obtain the reorganization energies for all systems due to the conformational changes while optimizing charged (anionic or cationic) molecular structures.

bent form

	E_{hole}	$E_{electron}$	ΔE
1	0.27	0.20	0.07
2	0.14	0.19	0.06
3	n.a.	0.19	n.a.
4	0.11	0.19	0.09
6	n.a.	0.20	n.a.
7	n.a.	0.21	n.a.

symmetrical form

	E_{hole}	$E_{electron}$	ΔE
2	0.10	n.a	n.a
3	0.10	n.a	n.a
4	0.10	0.15	0.05
6	n.a	0.18	n.a
7	n.a	0.19	n.a
8	n.a	0.17	n.a
9	0.23	0.40	0.18



Figures S8. Energy scan over C–H...O bond with evaluation of charge density distribution at the BCP point for compounds **1**, **2** and **4.**

Tables S10. Integrated charges according to AIMs theory for selected atoms. Integration and energy calculations were done in *AimAll*[12] suit of programs. Values are obtained for the most stable conformations.

	QTAIM charges				
	C–H…O				
	C	H	O	C–X (X= H, Br, F)	
2	+0.591047	+0.092243	–1.277521	+0.404244	+0.431065
4	+0.591133	+0.095774	–1.281243	–0.098428	–0.106616
1	+0.593524	+0.096514	–1.276242	–0.022031	–0.030265

Table S11. Geometrical and topological parameters for the inner CH…O interaction present in the *bent* conformer of the selected DBA complexes. *d* donates to distance; θ, angle; ρ, electron density; $\nabla^2\rho$, Laplacian; *V*, potential energy density; E_{top}, interaction energy obtained via the Espinosa-Lecomte approximation.

Compound	$d_{X...A}$ / Å	d_{D-X} / Å	$d_{D...A}$ / Å	$\theta_{D-X...A}$ / °	$\rho(\mathbf{r}_{BCP})$ / e·Å^{-3}	$\nabla^2\rho$ ($\mathbf{r}_{BCP}$) / e·Å^{-5}	$V(\mathbf{r}_{BCP})$ / kJ·mol^{-1} · Å^{-3}	E_{top} / kJ·mol^{-1}
2	2.7031	1.0854	3.7146	154.9	0.03	0.47	−54.71	−27.36
4	2.6004	1.0846	3.6093	154.4	0.04	0.56	−73.32	−36.66
1	2.6004	1.0844	3.6215	156.7	0.04	0.56	−72.22	−36.11

Cartesian coordinates for the ground state geometry optimization (RB3LYP/6-31+g(d,p))

1 -bent

O	8.84453800	3.82670900	1.78354100
N	8.38634500	1.81664800	0.54245200
O	5.75733600	-0.52225800	2.21205200
N	4.87097800	0.27564200	4.29696000
C	5.43330600	2.06257600	2.40622300
C	6.38560400	2.96026400	1.86369800
C	9.30704400	2.59281200	-0.08078600
C	8.36598700	1.68588900	3.19470700
C	8.57946600	0.25627400	-1.23420800
H	8.25947400	-0.68773300	-1.66160300
C	9.92828800	2.27325400	-1.30655500
C	9.52095300	1.03999400	-1.88099200
H	9.94836000	0.71434600	-2.82546200
C	7.42461100	0.78088400	3.74400100
C	5.93613900	4.13001200	1.22600600
C	9.56132800	3.76996400	0.66696700
C	10.48456100	4.67410300	0.16272400
H	10.71491300	5.58968300	0.69615000
C	9.66466800	1.73060200	3.73174600
H	10.38197700	2.44116500	3.32782100
B	7.94866400	2.60547600	1.94715000
C	7.83454700	-0.05840100	4.79749000
C	3.53666800	0.24778600	6.25946500
H	3.24432700	0.74912200	7.17540900
C	4.33601900	-0.92043200	3.94889800
C	4.57569800	4.42255800	1.10808700
H	4.25276800	5.33821800	0.61862300
C	3.37519800	-1.61917400	4.71235800
C	4.87368900	-1.37138200	2.71571400
C	3.63260800	3.53077700	1.62604700
H	2.56975900	3.74215800	1.53674400
C	9.12930300	-0.00726300	5.31873300
H	9.41610000	-0.66476000	6.13589000
C	8.01445400	0.66584000	-0.00541000
H	7.27542600	0.07469100	0.52585000
C	4.06595900	2.36747500	2.26606500
H	3.31403300	1.68875700	2.66606700
C	10.04952400	0.89962100	4.78607900
H	11.05702300	0.95909400	5.19067900
C	11.12041300	4.36951400	-1.07022200
H	11.84224200	5.08342100	-1.45751900
C	2.98197600	-0.97518800	5.91536800
H	2.24653700	-1.44236300	6.56454000
B	5.93290400	0.72260600	3.14360000
C	4.49295500	0.86541700	5.42531100
H	4.94878400	1.82035600	5.66049700
C	3.45661000	-3.30562700	2.97606300
H	3.11112100	-4.25678100	2.58038400

C	10.87013800	3.21636000	-1.80099900
H	11.38424000	3.03178900	-2.73873500
C	4.42241100	-2.58863600	2.22269900
H	4.79781800	-2.98335600	1.28511700
C	2.93280000	-2.86088500	4.18297200
H	2.19547300	-3.44997200	4.71835000
H	6.66573900	4.83238800	0.82984600
H	7.13246300	-0.76949000	5.23047500

1-symmetrical

C	-0.67495300	3.73753100	-1.54195800
C	-1.39393600	2.54585600	-1.42671400
C	-0.77965700	1.35236400	-1.00819700
C	0.60418200	1.35984300	-0.70485700
C	1.30966000	2.57338900	-0.81376800
C	0.68627700	3.75324600	-1.22618500
C	0.60418200	-1.35984300	-0.70485800
C	-0.77965700	-1.35236300	-1.00819700
C	-1.39393600	-2.54585500	-1.42671500
C	-0.67495300	-3.73753000	-1.54196000
C	0.68627700	-3.75324500	-1.22618800
C	1.30966000	-2.57338900	-0.81377000
H	-1.17018000	4.64584000	-1.87664400
H	-2.45070100	2.53731500	-1.68313900
H	1.25793300	4.67478000	-1.30547400
H	-1.17018000	-4.64583900	-1.87664700
H	1.25793300	-4.67477900	-1.30547700
H	2.37213300	-2.60753900	-0.57706300
B	1.32203300	0.00000000	-0.23093800
B	-1.62475200	0.00000000	-0.82661000
O	1.54449000	0.00000000	1.31792400
O	-2.92388600	0.00000000	-1.62213700
C	-3.99022400	0.00000000	-0.83051400
C	-3.64440800	0.00000000	0.54420800
C	-5.33703700	0.00000000	-1.16242100
C	-4.57588000	0.00000000	1.60390700
C	-6.28969000	0.00000000	-0.10901200
H	-5.65431800	0.00000100	-2.19935300
C	-1.77621500	-0.00000100	1.92248500
C	-4.00425800	-0.00000100	2.90391800
C	-5.94921900	0.00000000	1.23652700
H	-7.34236400	0.00000000	-0.37841200
C	-2.62683900	-0.00000100	3.05092200
H	-0.69400400	-0.00000100	2.00423500
H	-4.64803300	-0.00000100	3.77930300
H	-6.71764700	-0.00000100	2.00284100
H	-2.17703200	-0.00000100	4.03777900
C	2.83639400	-0.00000100	1.61209800
C	3.65275500	0.00000000	0.45162000
C	3.47169800	-0.00000100	2.84691600
C	5.06492300	0.00000000	0.46015200

C	4.89071000	-0.00000100	2.87577800
H	2.89912400	-0.00000100	3.76775800
C	3.47450500	0.00000100	-1.86394800
C	5.67194400	0.00000000	-0.82361300
C	5.68640000	-0.00000100	1.73749400
H	5.37663400	-0.00000100	3.84763100
C	4.88231800	0.00000100	-1.96301300
H	2.82426200	0.00000100	-2.73122900
H	6.75497200	0.00000000	-0.91077700
H	6.76851200	-0.00000100	1.81712000
H	5.33429500	0.00000100	-2.94864300
N	2.89186400	0.00000000	-0.67042400
N	-2.29759700	0.00000000	0.70142500
H	-2.45070100	-2.53731400	-1.68314000
H	2.37213300	2.60753900	-0.57706100

2-bent

O	8.83778900	3.80263700	1.84388800
N	8.43533900	1.83548000	0.52208700
O	5.70949800	-0.56990500	2.26096900
N	4.87536900	0.28128200	4.34653400
C	5.43169500	2.00595800	2.41366600
C	6.37246400	2.87855900	1.80801900
C	9.35315200	2.64858400	-0.05570500
C	8.37046300	1.63963600	3.16769100
C	8.68849000	0.33548300	-1.29636200
H	8.39490200	-0.59975900	-1.76022400
C	10.00291100	2.37881400	-1.27879800
C	9.62831700	1.15746400	-1.89848000
H	10.07878500	0.86944300	-2.84445600
C	7.44434500	0.71582500	3.71390700
C	5.85001700	3.95009500	1.07786400
C	9.56967600	3.80374600	0.73635900
C	10.48371200	4.74048900	0.27970400
H	10.68208500	5.64496400	0.84370600
C	9.68464200	1.68756400	3.66655600
H	10.37988300	2.41581900	3.25945300
B	7.95049900	2.57595900	1.92813200
C	7.93401900	-0.13452900	4.70878000
C	3.56621200	0.32315800	6.32425500
H	3.30943400	0.84065200	7.24181300
C	4.28293000	-0.89056700	4.01077700
C	4.49720000	4.23765600	0.95200800
H	4.18122000	5.10191100	0.37696300
C	3.30224600	-1.54113500	4.78898000
C	4.78731500	-1.37421500	2.77771400
C	3.58687100	3.38082300	1.57135500
H	2.52022000	3.57207100	1.48975300
C	9.22524800	-0.10574600	5.21591400
H	9.51517400	-0.80009100	5.99777600
C	8.09278300	0.69606700	-0.06767900

H	7.35313900	0.07788400	0.43161200
C	4.05577300	2.27502100	2.28158500
H	3.32619600	1.60910900	2.73607800
C	10.11137600	0.83360300	4.68447000
H	11.12854300	0.89113500	5.06274400
C	11.14814200	4.48786000	-0.95005600
H	11.86131900	5.22878900	-1.30086200
C	2.95437800	-0.87593800	5.99388600
H	2.20919000	-1.30833900	6.65590300
B	5.93121400	0.66967200	3.16896500
C	4.53652800	0.89385300	5.47372800
H	5.03586500	1.82941100	5.69912700
C	3.28694300	-3.23918400	3.06219400
H	2.89498500	-4.17593300	2.67566100
C	10.93544600	3.35489300	-1.72352000
H	11.46991500	3.21238300	-2.65712600
C	4.27719900	-2.57013400	2.29489300
H	4.62675500	-2.98718000	1.35698800
C	2.79735800	-2.76430800	4.27107400
H	2.04055700	-3.31654000	4.81845200
F	6.70566000	4.78702100	0.40884600
F	7.09296200	-1.08464900	5.24866500

2-symmetrical

C	-0.74669200	-3.80567400	0.24452000
C	-1.37337300	-2.57406100	0.42443900
C	-0.69852100	-1.35590600	0.20785400
C	0.65843800	-1.37604000	-0.19594000
C	1.24185000	-2.63864200	-0.35131600
C	0.59227000	-3.84690400	-0.15396100
C	0.69829200	1.35583100	-0.20795800
C	-0.65866900	1.37596500	0.19583100
C	-1.24207900	2.63856700	0.35121200
C	-0.59249600	3.84682900	0.15386900
C	0.74646800	3.80559900	-0.24460400
C	1.37314700	2.57398700	-0.42453100
H	-1.28880400	-4.73167100	0.41660600
H	-2.41025900	-2.56224500	0.75160500
H	1.12542600	-4.78021800	-0.30264600
H	-1.12565100	4.78014300	0.30255900
H	1.28858300	4.73159600	-0.41668100
H	2.41003500	2.56217100	-0.75169200
B	1.49773900	-0.02488000	-0.43367100
B	-1.49797100	0.02480500	0.43355200
O	2.22506000	-0.00981000	-1.78145900
O	-2.22531500	0.00973700	1.78132900
C	-3.54237600	-0.01356600	1.62363200
C	-3.92265400	-0.00627800	0.25799700
C	-4.55057900	-0.04578300	2.57517600
C	-5.25480600	-0.02488500	-0.20707300
C	-5.89827100	-0.06801100	2.12743000

H	-4.31657600	-0.04908500	3.63387800
C	-2.97794900	0.04663800	-1.86138400
C	-5.39628600	-0.00450100	-1.61939900
C	-6.26768800	-0.05882300	0.78918300
H	-6.68084200	-0.09215600	2.88089700
C	-4.27051300	0.03130100	-2.42785900
H	-2.07530400	0.07409500	-2.46194800
H	-6.38720400	-0.01520400	-2.06505700
H	-7.31407100	-0.07500500	0.50232400
H	-4.36573400	0.04838900	-3.50789800
C	3.54212400	0.01349600	-1.62378400
C	3.92242400	0.00620300	-0.25815500
C	4.55031200	0.04571600	-2.57534400
C	5.25458300	0.02480900	0.20689400
C	5.89801100	0.06794500	-2.12761900
H	4.31629200	0.04902200	-3.63404100
C	2.97775300	-0.04672200	1.86124200
C	5.39608600	0.00441900	1.61921800
C	6.26745000	0.05875200	-0.78937800
H	6.68057000	0.09209300	-2.88109900
C	4.27032600	-0.03138600	2.42769600
H	2.07511800	-0.07418100	2.46182100
H	6.38701200	0.01512200	2.06486000
H	7.31383700	0.07493400	-0.50253600
H	4.36556500	-0.04847900	3.50773300
N	2.83001500	-0.02763400	0.54250600
N	-2.83023200	0.02755600	-0.54264600
F	2.56657500	-2.71122400	-0.71253500
F	-2.56680600	2.71114900	0.71242400

3-bent

Cl	6.65144000	5.11877700	0.13474100
Cl	7.22147900	-1.56118700	5.30395600
O	8.78018100	3.84926500	1.80324400
N	8.38704000	1.85078300	0.52765700
O	5.74902900	-0.57992300	2.25478100
N	4.93895100	0.25037700	4.35716700
C	5.43037500	1.98079300	2.44265400
C	6.30465100	2.90472100	1.80494100
C	9.35853900	2.61665400	-0.02709200
C	8.35930500	1.71951000	3.16323800
C	8.67363400	0.29515700	-1.23919700
H	8.36981100	-0.64208500	-1.69224800
C	10.05585500	2.29209500	-1.20963400
C	9.66905000	1.06813100	-1.81596100
H	10.15351800	0.73986100	-2.73151600
C	7.51529700	0.70814000	3.69588400
C	5.70079000	3.95459500	1.08752500
C	9.57505400	3.78705200	0.74051700
C	10.54021500	4.68059000	0.30512600
H	10.73901100	5.59545400	0.85200800

C	9.66911000	1.87273100	3.64933600
H	10.29101900	2.66924000	3.25383900
B	7.89183200	2.62939100	1.91299300
C	8.09873300	-0.15054300	4.64674000
C	3.61872100	0.29767900	6.32712000
H	3.38728100	0.79433500	7.26270900
C	4.27979700	-0.87055300	3.97393300
C	4.32135100	4.15504200	1.02889800
H	3.92060100	4.99532900	0.47239700
C	3.25554300	-1.48890200	4.72096600
C	4.76966800	-1.34212700	2.73103300
C	3.48270800	3.25472700	1.67955700
H	2.40516500	3.39074000	1.64087000
C	9.39833000	-0.00387800	5.13068500
H	9.78133700	-0.69473800	5.87394700
C	8.03457300	0.70761500	-0.04918400
H	7.25696000	0.12272600	0.43200900
C	4.03870100	2.17549000	2.36227600
H	3.36083000	1.47163100	2.83715000
C	10.18393600	1.03529100	4.63661700
H	11.19448300	1.17472500	5.01150400
C	11.25573800	4.37111500	-0.88290300
H	12.00964700	5.07810400	-1.21806400
C	2.93852400	-0.84900400	5.94803400
H	2.16385200	-1.26031300	6.58933000
B	5.98953400	0.64369100	3.17428100
C	4.62760800	0.84058500	5.50373200
H	5.17915900	1.73611800	5.76673100
C	3.15978100	-3.12363000	2.93671200
H	2.71802800	-4.02194000	2.51440300
C	11.04159300	3.22427000	-1.63430900
H	11.61486200	3.03740800	-2.53654900
C	4.19722300	-2.48900000	2.20286900
H	4.53464200	-2.89577500	1.25607700
C	2.68486200	-2.66141700	4.15621900
H	1.89054000	-3.18592400	4.67705100

3 –symmetrical

C	-0.93070800	-3.75768200	0.37428200
C	-1.46454500	-2.48414500	0.53763000
C	-0.72329500	-1.32031600	0.25408400
C	0.61833900	-1.43368700	-0.19570200
C	1.12166800	-2.74401300	-0.33869400
C	0.38195400	-3.89390900	-0.07487800
C	0.72305900	1.32025500	-0.25420700
C	-0.61857700	1.43362500	0.19557300
C	-1.12190200	2.74395200	0.33857600
C	-0.38218100	3.89384900	0.07477700
C	0.93048300	3.75762200	-0.37437600
C	1.46431500	2.48408400	-0.53773600
H	-1.52278100	-4.64153200	0.59645000
H	-2.48385200	-2.39746200	0.90320900

H	0.83126700	-4.87152200	-0.21202600
H	-0.83149100	4.87146200	0.21193400
H	1.52256000	4.64147100	-0.59653100
H	2.48362300	2.39740100	-0.90331000
B	1.48177400	-0.09675800	-0.45478000
B	-1.48201700	0.09669500	0.45463600
O	2.22525500	-0.08669800	-1.79009500
O	-2.22552900	0.08663400	1.78993300
C	-3.53671100	-0.03031900	1.61682800
C	-3.90099200	-0.03680000	0.24700200
C	-4.55041900	-0.13409200	2.55633900
C	-5.22367800	-0.13354600	-0.23357600
C	-5.88940700	-0.23956000	2.09284400
H	-4.32845900	-0.12749500	3.61759800
C	-2.93895800	0.10818700	-1.85996300
C	-5.35136200	-0.10138700	-1.64699100
C	-6.24345700	-0.24205400	0.75070700
H	-6.67701700	-0.32005200	2.83703100
C	-4.22185200	0.01978400	-2.44165500
H	-2.03376400	0.20126000	-2.45005900
H	-6.33479500	-0.16832800	-2.10414400
H	-7.28341600	-0.32204000	0.45146800
H	-4.30645300	0.04891200	-3.52228800
C	3.53644100	0.03024300	-1.61702200
C	3.90075600	0.03672100	-0.24720500
C	4.55012800	0.13400900	-2.55655600
C	5.22345400	0.13345700	0.23334200
C	5.88912800	0.23946500	-2.09309400
H	4.32814200	0.12741500	-3.61781100
C	2.93877000	-0.10825600	1.85978400
C	5.35117100	0.10129800	1.64675400
C	6.24321000	0.24195700	-0.75096600
H	6.67672000	0.31995200	-2.83729900
C	4.22167900	-0.01986200	2.44144500
H	2.03359000	-0.20132300	2.44990100
H	6.33461600	0.16823200	2.10388300
H	7.28317600	0.32193500	-0.45175100
H	4.30630500	-0.04899000	3.52207700
N	2.80381900	-0.07704200	0.54019400
N	-2.80403800	0.07697300	-0.54037000
Cl	-2.79631000	3.04892200	0.86474400
Cl	2.79607400	-3.04897800	-0.86487100

4-bent

O	8.81482700	3.83722500	1.81362300
N	8.37008200	1.84767900	0.54144200
O	5.80315700	-0.59503400	2.26767400
N	4.95407900	0.24479200	4.34943600
C	5.45577000	1.96384700	2.43488800
C	6.32482300	2.92183300	1.84079000
C	9.34046200	2.60250400	-0.03096600
C	8.38031000	1.72696500	3.18716800
C	8.59837800	0.29714000	-1.23877100

H	8.27441500	-0.63548500	-1.68739000
C	10.00288100	2.27741800	-1.23285600
C	9.59506200	1.05651500	-1.83086300
H	10.05923400	0.72371400	-2.75523100
C	7.53619700	0.72050500	3.72985500
C	5.71456800	3.98245600	1.14819200
C	9.58857900	3.76634600	0.73571400
C	10.55798800	4.64713400	0.28572100
H	10.78136600	5.55587700	0.83327800
C	9.68764700	1.89339000	3.67471400
H	10.30835700	2.68337600	3.26504200
B	7.91030500	2.63427600	1.93799700
C	8.11657200	-0.11221900	4.70308500
C	3.61202800	0.29158200	6.30411600
H	3.37168200	0.78595300	7.23860300
C	4.29398000	-0.87045500	3.95307600
C	4.33315700	4.14935200	1.05423100
H	3.92177400	5.00113700	0.52434000
C	3.25701600	-1.48439800	4.68438500
C	4.80536300	-1.34781900	2.72187600
C	3.49918400	3.20441400	1.64478100
H	2.42009200	3.31321100	1.57425300
C	9.41210900	0.04806800	5.19242700
H	9.79490400	-0.61972600	5.95600500
C	7.98890000	0.71309600	-0.03448700
H	7.21169100	0.13690500	0.45749900
C	4.06231000	2.12279700	2.31617700
H	3.39030200	1.38964100	2.75357400
C	10.20057800	1.07464900	4.67772000
H	11.20942900	1.22201900	5.05432400
C	11.24688500	4.33219100	-0.91651100
H	12.00742600	5.02732800	-1.26124400
C	2.92406100	-0.84422200	5.90695000
H	2.13186400	-1.24796000	6.53147200
B	6.01971100	0.63725200	3.18322800
C	4.64297400	0.82283900	5.50141300
H	5.20047900	1.71034600	5.77923300
C	3.16856900	-3.10842000	2.89038100
H	2.72172000	-3.99797100	2.45514500
C	10.99809200	3.19380500	-1.66970500
H	11.55146600	3.00149200	-2.58317400
C	4.23053600	-2.48666900	2.18032900
H	4.58224500	-2.89648500	1.24005200
C	2.67714900	-2.64404700	4.10239600
H	1.86656500	-3.15968200	4.60675600
Br	6.72478300	5.36810300	0.25370800
Br	7.17442500	-1.62180800	5.47654400

4-symmetrical

C	-1.01156500	-3.74277600	0.31210000
C	-1.54040800	-2.46180000	0.41589400

C	-0.75934100	-1.30957400	0.20057200
C	0.61500600	-1.44332600	-0.12878100
C	1.11200600	-2.76016000	-0.20186000
C	0.33753500	-3.89891400	-0.00128900
C	0.75911000	1.30950500	-0.20073000
C	-0.61524000	1.44325600	0.12860800
C	-1.11224100	2.76008900	0.20168400
C	-0.33776800	3.89884500	0.00112800
C	1.01133700	3.74270800	-0.31224200
C	1.54018100	2.46173100	-0.41603700
H	-1.63481800	-4.61750500	0.47822000
H	-2.58983300	-2.36220300	0.67808800
H	0.78035000	-4.88521000	-0.08339500
H	-0.78058300	4.88514000	0.08323000
H	1.63459200	4.61743700	-0.47835000
H	2.58960900	2.36213600	-0.67821900
B	1.49854100	-0.12089500	-0.38738300
B	-1.49877300	0.12082200	0.38721100
O	2.21217400	-0.12701600	-1.74425300
O	-2.21241500	0.12695400	1.74407800
C	-3.52328600	-0.02449100	1.59834400
C	-3.91436300	-0.04253800	0.23634200
C	-4.51520100	-0.15968100	2.55704900
C	-5.24415200	-0.15143500	-0.21799800
C	-5.85986300	-0.29731000	2.11942600
H	-4.27285700	-0.14842500	3.61379200
C	-3.00239000	0.15816600	-1.88807000
C	-5.40181200	-0.12358000	-1.62860600
C	-6.23999800	-0.30479700	0.78431400
H	-6.62932100	-0.40757400	2.87866400
C	-4.29228200	0.02729800	-2.44565900
H	-2.11346000	0.28858700	-2.49561400
H	-6.39221000	-0.21873300	-2.06525100
H	-7.28307800	-0.41125600	0.50486000
H	-4.39910200	0.05821500	-3.52422600
C	3.52304600	0.02443000	-1.59852500
C	3.91413000	0.04246200	-0.23652500
C	4.51495400	0.15963200	-2.55723500
C	5.24392200	0.15135400	0.21780800
C	5.85961900	0.29725700	-2.11961800
H	4.27260400	0.14839000	-3.61397700
C	3.00216900	-0.15826400	1.88788900
C	5.40159000	0.12348300	1.62841500
C	6.23976100	0.30472800	-0.78450900
H	6.62907200	0.40753100	-2.87885900
C	4.29206500	-0.02740400	2.44547200
H	2.11324200	-0.28868900	2.49543800
H	6.39199000	0.21863000	2.06505500
H	7.28284400	0.41118400	-0.50505900
H	4.39889000	-0.05833300	3.52403800

N	2.83709600	-0.10276800	0.57331500
N	-2.83732400	0.10268400	-0.57349400
Br	2.96655000	-3.13791300	-0.60558400
Br	-2.96679200	3.13784100	0.60538100

5 -bent

F	9.31413000	9.11983000	3.38036900
F	10.49048400	11.28773600	4.53191700
O	11.42174200	4.90228100	5.42209900
O	12.48591200	8.68851500	9.03331700
F	16.94233200	5.35583400	8.85037300
N	14.23353500	9.58263900	7.65017600
N	10.61942700	5.60049700	7.57992800
F	15.72576700	3.22479700	7.67214300
C	10.50859600	7.65909000	4.83481100
H	10.03000400	6.81465600	4.34760200
C	13.06538100	9.73724300	9.60639300
C	14.10115800	10.28113900	8.80578900
C	9.93811800	4.52297900	7.11606600
C	8.56356400	4.44803500	9.06606300
H	7.76601900	4.01743800	9.66526300
C	8.88683100	3.88189500	7.80464000
C	13.21767000	5.83016500	7.06466800
C	10.42465600	4.12772900	5.84611900
C	9.26686400	5.54840300	9.52863000
H	9.03022200	5.99053700	10.49013000
C	11.43678600	7.46752600	5.87270400
C	10.30658100	6.11994300	8.76141800
H	10.87570100	6.98149400	9.09584800
C	12.06576600	8.59197900	6.46056500
C	10.20025900	8.93591500	4.39061900
C	13.85655100	6.94552100	7.65914100
C	10.80373200	10.04387500	4.97643400
C	11.72540600	9.87734600	5.99921200
H	12.16958400	10.77586400	6.41998600
C	14.88997400	11.39774300	9.15923700
C	8.29526400	2.76556400	7.15299900
H	7.48155000	2.22696400	7.62760900
B	11.75465900	5.99338600	6.42378000
C	13.85836500	4.57923900	7.07692500
H	13.40431700	3.71210900	6.60638100
C	12.80592100	10.34441500	10.82646500
H	12.02544200	9.97152400	11.48030200
C	13.58845300	11.46891700	11.20015100
H	13.37662100	11.93648600	12.15759300
C	14.60215800	11.99898300	10.41355900
H	15.17008800	12.86091900	10.74756600
C	15.11295800	6.76283200	8.26652400
H	15.64463200	7.58096300	8.74577000
C	8.77107100	2.37756200	5.90876700
H	8.31172700	1.52313000	5.41972700

C	9.83192000	3.03676500	5.23106100
H	10.16809100	2.69466200	4.25857700
C	15.10195500	4.42917400	7.67157700
C	15.15629600	9.94107100	6.76366300
H	15.22491600	9.35354400	5.85519000
B	13.13128300	8.38260800	7.64893700
C	15.72558200	5.51865700	8.27080000
C	15.87053200	11.76686600	8.20096700
H	16.52189300	12.61522300	8.39155400
C	15.99572500	11.04497900	7.02394400
H	16.74068800	11.31733200	6.28482500

6 -bent

O	8.83148500	3.79761400	1.85509400
N	8.44674400	1.83953100	0.51450700
O	5.69268000	-0.58869700	2.26413000
N	4.87329700	0.28286600	4.34705500
C	5.42949800	1.98941000	2.39782100
C	6.37193200	2.86243400	1.79602400
C	9.36065700	2.66327500	-0.05320200
C	8.36844300	1.62142400	3.15857700
C	8.71099300	0.35310400	-1.31227500
H	8.42432200	-0.58024000	-1.78384600
C	10.01126500	2.39986400	-1.27812700
C	9.64727700	1.18234400	-1.90897700
H	10.10280300	0.90770900	-2.85441100
C	7.44063700	0.69684500	3.69992200
C	5.85193600	3.93042000	1.05884000
C	9.56541600	3.81244700	0.75096100
C	10.47359500	4.75899300	0.30433500
H	10.66706100	5.66153800	0.87247800
C	9.68338600	1.66188500	3.65612400
H	10.38096700	2.39060700	3.25385000
B	7.94943400	2.56622900	1.92643400
C	7.92878800	-0.16195300	4.68832500
C	3.57929800	0.35286900	6.33268200
H	3.33073600	0.88033200	7.24664400
C	4.27465000	-0.88930300	4.02511600
C	4.49959800	4.21460300	0.92314100
H	4.18525300	5.07610100	0.34320400
C	3.29617100	-1.52244300	4.82147800
C	4.77177700	-1.38388000	2.79325000
C	3.58728200	3.35753400	1.53931600
H	2.52086800	3.54603000	1.45008900
C	9.22056500	-0.14076600	5.19385900
H	9.50964900	-0.84124100	5.97046200
C	8.11136500	0.70247400	-0.08318700
H	7.37377000	0.07791000	0.41107000
C	4.05389100	2.25481400	2.25571600
H	3.32243700	1.58877500	2.70707100
C	10.10874900	0.79950200	4.66744800

H	11.12654100	0.85125400	5.04455400
C	11.14525700	4.52689200	-0.92350400
H	11.85516700	5.26850200	-1.27497800
C	2.95801000	-0.84601800	6.02163100
H	2.21590000	-1.27056900	6.68925800
B	5.92654800	0.65706200	3.15967200
C	4.54593800	0.90930600	5.46978300
H	5.05200200	1.84458300	5.68083200
C	3.26730600	-3.24400300	3.09845900
H	2.86334600	-4.18205800	2.73195800
C	10.93449200	3.39663100	-1.69646700
C	4.25493100	-2.58210200	2.32488900
H	4.59453600	-3.01285800	1.38992500
C	2.79481800	-2.74709600	4.30223100
F	6.71131500	4.76571200	0.39269400
F	7.08403400	-1.11184200	5.22202100
Cl	11.80922900	3.18586300	-3.20792200
Cl	1.56790900	-3.62973800	5.20010400

6-symmetrical

C	-0.74100300	-3.80688200	0.24005800
C	-1.37047800	-2.57662300	0.42006000
C	-0.69731300	-1.35718300	0.20640700
C	0.66026800	-1.37466100	-0.19508300
C	1.24641100	-2.63586200	-0.35060300
C	0.59877200	-3.84544000	-0.15568600
C	0.69708500	1.35710700	-0.20653200
C	-0.66049600	1.37458500	0.19495700
C	-1.24663900	2.63578600	0.35047800
C	-0.59899900	3.84536400	0.15556700
C	0.74077700	3.80680600	-0.24017600
C	1.37025100	2.57654800	-0.42018000
H	-1.28179200	-4.73393200	0.40991300
H	-2.40802400	-2.56773100	0.74524200
H	1.13372600	-4.77768100	-0.30417400
H	-1.13395200	4.77760600	0.30405600
H	1.28156700	4.73385600	-0.41002700
H	2.40779800	2.56765600	-0.74536100
B	1.49647500	-0.02251100	-0.43296600
B	-1.49670400	0.02243600	0.43283500
O	2.22409500	-0.00748000	-1.78067600
O	-2.22433400	0.00740500	1.78054000
C	-3.53991900	-0.01306000	1.62342200
C	-3.92344300	-0.00596800	0.25853300
C	-4.54740200	-0.04193400	2.57516400
C	-5.25342900	-0.02208900	-0.21486000
C	-5.89565500	-0.06158300	2.13469800
H	-4.31765000	-0.04476200	3.63445300
C	-2.97679900	0.04295700	-1.86158100
C	-5.39613100	-0.00278200	-1.62600100
C	-6.25240100	-0.05267500	0.79588900

H	-6.68457700	-0.08340700	2.87946600
C	-4.26770200	0.02972900	-2.43007100
H	-2.07258900	0.06807800	-2.45983200
H	-6.38664200	-0.01188100	-2.06820400
H	-4.36221900	0.04591900	-3.51003100
C	3.53968100	0.01298600	-1.62356700
C	3.92321400	0.00589300	-0.25868100
C	4.54715800	0.04186000	-2.57531600
C	5.25320400	0.02201400	0.21470300
C	5.89541400	0.06150900	-2.13486000
H	4.31739900	0.04468900	-3.63460300
C	2.97658600	-0.04303300	1.86144000
C	5.39591600	0.00270600	1.62584300
C	6.25216900	0.05260100	-0.79605300
H	6.68433100	0.08333400	-2.87963200
C	4.26749200	-0.02980500	2.42992100
H	2.07238000	-0.06815500	2.45969600
H	6.38642900	0.01180600	2.06803900
H	4.36201700	-0.04599600	3.50988000
N	2.83160200	-0.02501800	0.54260700
N	-2.83182500	0.02494200	-0.54274700
F	2.57193100	-2.70442300	-0.70942200
F	-2.57215900	2.70434700	0.70929500
Cl	7.94923000	0.07874100	-0.33489900
Cl	-7.94945900	-0.07881400	0.33472400

7–bent

O	8.84982800	3.79799500	1.84483100
N	8.43377200	1.82828700	0.53021200
O	5.72521300	-0.53960000	2.25874100
N	4.86590100	0.28240200	4.34625400
C	5.43378500	2.03225800	2.43610600
C	6.38049000	2.88796900	1.81656400
C	9.34670900	2.63941700	-0.06052800
C	8.37236800	1.64676400	3.18274300
C	8.66091100	0.31822100	-1.28396800
H	8.35950000	-0.61820200	-1.73948100
C	9.97591400	2.35431100	-1.29081900
C	9.59467900	1.13409900	-1.90298500
H	10.03508100	0.84631000	-2.85163700
C	7.43969800	0.73523600	3.73810200
C	5.86673600	3.95548800	1.07513800
C	9.56505000	3.79110200	0.73483300
C	10.48130000	4.71553100	0.25468300
C	9.68628700	1.69007100	3.68163700
H	10.38745300	2.41045100	3.27094800
B	7.95437500	2.57355900	1.93771800
C	7.92239200	-0.11059700	4.73981900
C	3.54598100	0.29938600	6.31725200
H	3.27806200	0.80790500	7.23628500
C	4.28926300	-0.89468000	3.99747300

C	4.51672200	4.25853500	0.95624300
H	4.20690400	5.11934600	0.37297100
C	3.31231500	-1.55404700	4.77275300
C	4.81487000	-1.35172400	2.76389500
C	3.60086400	3.42104600	1.59310600
H	2.53634700	3.62513700	1.51752900
C	9.21322900	-0.08596300	5.24746800
H	9.49847800	-0.77525800	6.03534100
C	8.08236100	0.68701400	-0.05092400
H	7.34675700	0.07271300	0.45910700
C	4.06062000	2.31609400	2.31113000
H	3.32515600	1.66416900	2.77629300
C	10.10574900	0.84246800	4.70800800
H	11.12268000	0.89702100	5.08673000
C	11.13816900	4.47379600	-0.97995000
H	11.84805600	5.21164400	-1.33620300
C	2.94842400	-0.90442800	5.97860800
H	2.20533200	-1.35250500	6.62950300
B	5.93130100	0.69625400	3.18686200
C	4.51364600	0.88394800	5.47518800
H	5.00275500	1.82319600	5.70763400
C	3.32753600	-3.25144500	3.02407300
H	2.95210900	-4.18759900	2.62660900
C	10.90238800	3.33855000	-1.73410200
C	4.31347400	-2.55250100	2.28147700
C	2.83653700	-2.77899000	4.22808700
F	6.72925600	4.76841900	0.38729600
F	7.07329200	-1.05067400	5.28542800
Cl	11.75305600	3.10786400	-3.25286400
Cl	1.61595300	-3.69665600	5.09257200
Cl	4.88738700	-3.21155000	0.77228800
Cl	10.83493800	6.16681400	1.15117900

7 –symmetrical

C	-0.72871800	-3.80927400	0.23506300
C	-1.36338200	-2.58156300	0.41442600
C	-0.69401100	-1.35981100	0.20351200
C	0.66451100	-1.37220300	-0.19428300
C	1.25595700	-2.63085900	-0.34909800
C	0.61215900	-3.84279300	-0.15711600
C	0.69378300	1.35973600	-0.20364100
C	-0.66473900	1.37212700	0.19415300
C	-1.25618400	2.63078400	0.34897000
C	-0.61238600	3.84271800	0.15699200
C	0.72849100	3.80919900	-0.23518600
C	1.36315500	2.58148800	-0.41455100
H	-1.26639300	-4.73830900	0.40329300
H	-2.40150400	-2.57747000	0.73785700
H	1.15058400	-4.77303000	-0.30520300
H	-1.15081000	4.77295400	0.30508000
H	1.26616800	4.73823400	-0.40341400

H	2.40127700	2.57739500	-0.73798100
B	1.49486100	-0.01732900	-0.42879700
B	-1.49509000	0.01725300	0.42866400
O	2.22141600	-0.00083100	-1.78195800
O	-2.22165300	0.00075600	1.78182100
C	-3.53129700	-0.01411800	1.62285500
C	-3.92605600	-0.00674400	0.26206400
C	-4.55001000	-0.03721200	2.56503100
C	-5.25450000	-0.01657800	-0.21369500
C	-5.90225100	-0.05036000	2.13513900
C	-2.98018400	0.03636000	-1.85918200
C	-5.39838600	0.00213100	-1.62328300
C	-6.25460100	-0.04073700	0.79738100
H	-6.68019700	-0.06778300	2.89001900
C	-4.27019000	0.02834900	-2.42853300
H	-2.07567700	0.05727600	-2.45729100
H	-6.38943900	-0.00250900	-2.06427900
H	-4.36445100	0.04391900	-3.50836500
C	3.53106200	0.01404300	-1.62299900
C	3.92582800	0.00666900	-0.26221000
C	4.54977000	0.03713800	-2.56518100
C	5.25427400	0.01650400	0.21354200
C	5.90201300	0.05028600	-2.13529600
C	2.97996700	-0.03643600	1.85904100
C	5.39816800	-0.00220600	1.62313000
C	6.25437000	0.04066300	-0.79753900
H	6.67995500	0.06771000	-2.89018000
C	4.26997600	-0.02842400	2.42838500
H	2.07546300	-0.05735200	2.45715500
H	6.38922300	0.00243400	2.06412000
H	4.36424300	-0.04399500	3.50821700
N	2.83343400	-0.01889500	0.54029200
N	-2.83365800	0.01882000	-0.54043200
F	2.58287100	-2.69303200	-0.70388900
F	-2.58309900	2.69295600	0.70376000
Cl	7.94962400	0.05856700	-0.34118900
Cl	-7.94985300	-0.05864100	0.34102200
Cl	4.18528600	0.04777100	-4.26907000
Cl	-4.18553600	-0.04784500	4.26892200

8 –symmetrical

S	-0.32046700	6.37216300	1.92481900
O	-0.75039600	9.68540900	2.48904200
N	-2.81632600	8.55793900	2.96755200
C	-0.55026900	7.24538300	3.42838900
C	-2.93826100	9.39201200	1.90743800
C	0.40814600	5.21278100	4.09845700
H	0.79583200	4.47168500	4.79122500
C	-0.10897200	6.49312300	4.50232300
B	-1.25649300	8.67333900	3.52048600
C	-4.12600900	9.57910900	1.16886900

C	-1.70838300	10.04702500	1.64359800
C	-3.85989800	7.84796600	3.37487200
H	-3.71044700	7.19472300	4.22770400
C	-1.66686900	10.93975700	0.58296900
H	-0.75267200	11.46736800	0.33497600
C	0.35842700	5.00230800	2.74654300
H	0.68469700	4.13374800	2.18942300
C	-5.09612500	7.96271400	2.70268200
H	-5.93564300	7.37224700	3.05256800
C	-5.23467900	8.81282800	1.61617400
H	-6.19045000	8.89341300	1.10564900
C	-4.05477500	10.49932600	0.08799600
H	-4.93073100	10.69202000	-0.52278500
C	-2.85260100	11.14303300	-0.17264000
H	-2.80908800	11.84374100	-1.00194000
S	-1.07085100	9.36839300	7.59075600
O	-0.64091500	6.05514800	7.02653400
N	1.42501300	7.18262100	6.54801900
C	-0.84104800	8.49517300	6.08718600
C	1.54695100	6.34854900	7.60813300
C	-1.79946300	10.52777500	5.41711800
H	-2.18714800	11.26887100	4.72435000
C	-1.28234400	9.24743300	5.01325200
B	-0.13482200	7.06721800	5.99508800
C	2.73470100	6.16145400	8.34670000
C	0.31707400	5.69353400	7.87197700
C	2.46858200	7.89259500	6.14069700
H	2.31912900	8.54583800	5.28786500
C	0.27556500	4.80080300	8.93260700
H	-0.63863200	4.27319100	9.18060100
C	-1.74974900	10.73824500	6.76903300
H	-2.07602300	11.60680400	7.32615300
C	3.70481100	7.77785000	6.81288400
H	4.54432700	8.36831900	6.46299600
C	3.84336900	6.92773700	7.89939200
H	4.79914100	6.84715400	8.40991600
C	2.66347000	5.24123800	9.42757400
H	3.53942800	5.04854600	10.03835300
C	1.46129800	4.59752900	9.68821300
H	1.41778800	3.89682200	10.51751300

9

C	-2.14867400	6.71770600	5.00793500
O	-3.90626500	7.79750900	3.69085000
C	1.21167100	6.68529100	3.85579300
C	2.55176800	7.11708100	3.95917700
C	-2.01843400	6.93297200	2.39527000
C	-3.40112100	7.33789400	4.88823300
O	-0.51278300	5.20455200	3.64648700
C	0.80656300	5.33290800	3.72419500
C	-3.28162500	7.53539500	2.49031600

C	3.14982000	4.77543500	3.79743500
H	3.91682100	4.00631100	3.77331000
C	-3.83903400	7.10719700	7.24848400
H	-4.49076500	7.25837500	8.10449300
C	1.79508100	4.36067500	3.69459300
H	1.54064700	3.31136700	3.59552800
C	-4.01344700	7.92212800	1.35780500
H	-4.98742500	8.38217400	1.49192700
C	2.71991000	8.52147300	4.08290500
H	3.71778600	8.94276400	4.16813500
C	-1.52130200	6.71160900	1.09591700
H	-0.55465600	6.22531800	0.98381800
C	0.30874800	8.81727700	3.98477800
H	-0.58035200	9.43831400	3.99059800
N	0.13470400	7.50715500	3.86858600
C	-1.78062100	6.28295500	6.29634300
H	-0.82591000	5.77692200	6.42247000
C	-3.48230400	7.69685100	0.09251400
H	-4.04747800	7.99108900	-0.78746600
C	3.54410000	6.10037200	3.92615300
H	4.59463100	6.36142000	4.00091600
C	-4.24434000	7.54049300	5.99078600
H	-5.20399000	8.02423300	5.83803400
C	1.61048900	9.35271000	4.09472200
H	1.72581400	10.42683400	4.18863300
C	-2.22904000	7.08264900	-0.04505300
H	-1.81689300	6.89516400	-1.03233900
C	-2.60061800	6.46842800	7.40700800
H	-2.28658100	6.11876100	8.38622100
B	-1.22522100	6.55149800	3.72181500

10 –symmetrical

C	-0.77106300	0.90737600	3.70571500
C	-1.42712900	0.72534200	2.48963800
C	-0.73324200	0.38528000	1.30982900
C	0.67344200	0.23159300	1.35401600
C	1.28193500	0.43342900	2.59761800
C	0.61802600	0.75834300	3.76977100
C	0.70538000	-0.33084400	-1.31661900
C	-0.70130400	-0.17714700	-1.36080900
C	-1.30979500	-0.37896900	-2.60441400
C	-0.64588600	-0.70388100	-3.77656700
C	0.74320200	-0.85292900	-3.71250800
C	1.39926600	-0.67090700	-2.49642800
H	-1.32888500	1.16784100	4.60139600
H	-2.50629000	0.85961700	2.45640700
H	1.17480400	0.89389100	4.69131100
H	-1.20266200	-0.83941700	-4.69810900
H	1.30102400	-1.11339500	-4.60818800
H	2.47842600	-0.80519200	-2.46319500
B	1.55050200	-0.15278600	0.05148400

B	-1.57836600	0.20721500	-0.05827200
O	2.33954200	-1.39443000	0.30041700
F	2.65168100	0.31958900	2.68092300
F	-2.67953900	-0.26512000	-2.68772100
C	-4.00379700	-0.84496200	0.16701600
C	-2.13080600	-2.23513600	0.43942500
C	-4.54432100	0.45523500	-0.09749300
C	-4.87331800	-1.95280400	0.39913700
C	-2.92375700	-3.35635600	0.67112000
H	-1.04845400	-2.28960100	0.44505800
C	-5.96097000	0.63267700	-0.12795900
C	-6.29296900	-1.73971800	0.36351300
C	-4.30313900	-3.21129800	0.65078000
H	-2.45251600	-4.31340400	0.86203100
C	-6.49671400	1.90716100	-0.39128000
C	-6.80775800	-0.50458900	0.11165300
C	-4.25206000	2.81987100	-0.59424000
H	-6.94601700	-2.58937900	0.54112300
H	-4.95295600	-4.06419400	0.82739500
C	-5.64044700	2.97988900	-0.62082000
H	-7.57379900	2.04080000	-0.41467000
H	-7.88385600	-0.35649000	0.08575300
H	-3.58436500	3.65561200	-0.77433900
H	-6.05472400	3.96324500	-0.82565600
C	3.65698800	-1.51079500	0.32749300
C	4.51645400	-0.40084300	0.09070400
C	4.22416200	-2.76546600	0.58749400
C	3.97594800	0.89935800	-0.17381900
C	5.93310000	-0.57830400	0.12117000
C	5.61254700	-2.92550300	0.61407400
H	3.55645700	-3.60119400	0.76761000
C	4.84548400	2.00718500	-0.40595800
C	6.77990400	0.55894600	-0.11846400
C	6.46882800	-1.85279100	0.38451200
H	6.02681000	-3.90886000	0.81892900
C	4.27532100	3.26568500	-0.65760700
C	6.26513100	1.79407900	-0.37034000
C	2.10297600	2.28955700	-0.44622500
H	7.85600000	0.41083100	-0.09256800
H	7.54591100	-1.98644400	0.40790000
C	2.89594100	3.41076400	-0.67793600
H	4.92515000	4.11857000	-0.83423600
H	6.91819100	2.64372700	-0.54796600
H	1.02062500	2.34403800	-0.45185100
H	2.42471400	4.36781700	-0.86885100
N	2.62205300	1.07795300	-0.20305000
N	-2.64989900	-1.02353700	0.19625300
C	-3.68486900	1.56520200	-0.33426300
O	-2.36742300	1.44885300	-0.30719300

Cartesian coordinates for ground state geometry optimization (UB3LYP/6-31+g(d,p))

1 -bent

O	8.84453800	3.82670900	1.78354100
N	8.38634500	1.81664800	0.54245200
O	5.75733600	-0.52225800	2.21205200
N	4.87097800	0.27564200	4.29696000
C	5.43330600	2.06257600	2.40622300
C	6.38560400	2.96026400	1.86369800
C	9.30704400	2.59281200	-0.08078600
C	8.36598700	1.68588900	3.19470700
C	8.57946600	0.25627400	-1.23420800
H	8.25947400	-0.68773300	-1.66160300
C	9.92828800	2.27325400	-1.30655500
C	9.52095300	1.03999400	-1.88099200
H	9.94836000	0.71434600	-2.82546200
C	7.42461100	0.78088400	3.74400100
C	5.93613900	4.13001200	1.22600600
C	9.56132800	3.76996400	0.66696700
C	10.48456100	4.67410300	0.16272400
H	10.71491300	5.58968300	0.69615000
C	9.66466800	1.73060200	3.73174600
H	10.38197700	2.44116500	3.32782100
B	7.94866400	2.60547600	1.94715000
C	7.83454700	-0.05840100	4.79749000
C	3.53666800	0.24778600	6.25946500
H	3.24432700	0.74912200	7.17540900
C	4.33601900	-0.92043200	3.94889800
C	4.57569800	4.42255800	1.10808700
H	4.25276800	5.33821800	0.61862300
C	3.37519800	-1.61917400	4.71235800
C	4.87368900	-1.37138200	2.71571400
C	3.63260800	3.53077700	1.62604700
H	2.56975900	3.74215800	1.53674400
C	9.12930300	-0.00726300	5.31873300
H	9.41610000	-0.66476000	6.13589000
C	8.01445400	0.66584000	-0.00541000
H	7.27542600	0.07469100	0.52585000
C	4.06595900	2.36747500	2.26606500
H	3.31403300	1.68875700	2.66606700
C	10.04952400	0.89962100	4.78607900
H	11.05702300	0.95909400	5.19067900
C	11.12041300	4.36951400	-1.07022200
H	11.84224200	5.08342100	-1.45751900
C	2.98197600	-0.97518800	5.91536800
H	2.24653700	-1.44236300	6.56454000
B	5.93290400	0.72260600	3.14360000
C	4.49295500	0.86541700	5.42531100
H	4.94878400	1.82035600	5.66049700
C	3.45661000	-3.30562700	2.97606300
H	3.11112100	-4.25678100	2.58038400
C	10.87013800	3.21636000	-1.80099900

H	11.38424000	3.03178900	-2.73873500
C	4.42241100	-2.58863600	2.22269900
H	4.79781800	-2.98335600	1.28511700
C	2.93280000	-2.86088500	4.18297200
H	2.19547300	-3.44997200	4.71835000
H	6.66573900	4.83238800	0.82984600
H	7.13246300	-0.76949000	5.23047500

2-bent

O	8.83778900	3.80263700	1.84388800
N	8.43533900	1.83548000	0.52208700
O	5.70949800	-0.56990500	2.26096900
N	4.87536900	0.28128200	4.34653400
C	5.43169500	2.00595800	2.41366600
C	6.37246400	2.87855900	1.80801900
C	9.35315200	2.64858400	-0.05570500
C	8.37046300	1.63963600	3.16769100
C	8.68849000	0.33548300	-1.29636200
H	8.39490200	-0.59975900	-1.76022400
C	10.00291100	2.37881400	-1.27879800
C	9.62831700	1.15746400	-1.89848000
H	10.07878500	0.86944300	-2.84445600
C	7.44434500	0.71582500	3.71390700
C	5.85001700	3.95009500	1.07786400
C	9.56967600	3.80374600	0.73635900
C	10.48371200	4.74048900	0.27970400
H	10.68208500	5.64496400	0.84370600
C	9.68464200	1.68756400	3.66655600
H	10.37988300	2.41581900	3.25945300
B	7.95049900	2.57595900	1.92813200
C	7.93401900	-0.13452900	4.70878000
C	3.56621200	0.32315800	6.32425500
H	3.30943400	0.84065200	7.24181300
C	4.28293000	-0.89056700	4.01077700
C	4.49720000	4.23765600	0.95200800
H	4.18122000	5.10191100	0.37696300
C	3.30224600	-1.54113500	4.78898000
C	4.78731500	-1.37421500	2.77771400
C	3.58687100	3.38082300	1.57135500
H	2.52022000	3.57207100	1.48975300
C	9.22524800	-0.10574600	5.21591400
H	9.51517400	-0.80009100	5.99777600
C	8.09278300	0.69606700	-0.06767900
H	7.35313900	0.07788400	0.43161200
C	4.05577300	2.27502100	2.28158500
H	3.32619600	1.60910900	2.73607800
C	10.11137600	0.83360300	4.68447000
H	11.12854300	0.89113500	5.06274400
C	11.14814200	4.48786000	-0.95005600
H	11.86131900	5.22878900	-1.30086200
C	2.95437800	-0.87593800	5.99388600

H	2.20919000	-1.30833900	6.65590300
B	5.93121400	0.66967200	3.16896500
C	4.53652800	0.89385300	5.47372800
H	5.03586500	1.82941100	5.69912700
C	3.28694300	-3.23918400	3.06219400
H	2.89498500	-4.17593300	2.67566100
C	10.93544600	3.35489300	-1.72352000
H	11.46991500	3.21238300	-2.65712600
C	4.27719900	-2.57013400	2.29489300
H	4.62675500	-2.98718000	1.35698800
C	2.79735800	-2.76430800	4.27107400
H	2.04055700	-3.31654000	4.81845200
F	6.70566000	4.78702100	0.40884600
F	7.09296200	-1.08464900	5.24866500

2-symmetrical

C	-0.74669200	-3.80567400	0.24452000
C	-1.37337300	-2.57406100	0.42443900
C	-0.69852100	-1.35590600	0.20785400
C	0.65843800	-1.37604000	-0.19594000
C	1.24185000	-2.63864200	-0.35131600
C	0.59227000	-3.84690400	-0.15396100
C	0.69829200	1.35583100	-0.20795800
C	-0.65866900	1.37596500	0.19583100
C	-1.24207900	2.63856700	0.35121200
C	-0.59249600	3.84682900	0.15386900
C	0.74646800	3.80559900	-0.24460400
C	1.37314700	2.57398700	-0.42453100
H	-1.28880400	-4.73167100	0.41660600
H	-2.41025900	-2.56224500	0.75160500
H	1.12542600	-4.78021800	-0.30264600
H	-1.12565100	4.78014300	0.30255900
H	1.28858300	4.73159600	-0.41668100
H	2.41003500	2.56217100	-0.75169200
B	1.49773900	-0.02488000	-0.43367100
B	-1.49797100	0.02480500	0.43355200
O	2.22506000	-0.00981000	-1.78145900
O	-2.22531500	0.00973700	1.78132900
C	-3.54237600	-0.01356600	1.62363200
C	-3.92265400	-0.00627800	0.25799700
C	-4.55057900	-0.04578300	2.57517600
C	-5.25480600	-0.02488500	-0.20707300
C	-5.89827100	-0.06801100	2.12743000
H	-4.31657600	-0.04908500	3.63387800
C	-2.97794900	0.04663800	-1.86138400
C	-5.39628600	-0.00450100	-1.61939900
C	-6.26768800	-0.05882300	0.78918300
H	-6.68084200	-0.09215600	2.88089700
C	-4.27051300	0.03130100	-2.42785900
H	-2.07530400	0.07409500	-2.46194800
H	-6.38720400	-0.01520400	-2.06505700

H	-7.31407100	-0.07500500	0.50232400
H	-4.36573400	0.04838900	-3.50789800
C	3.54212400	0.01349600	-1.62378400
C	3.92242400	0.00620300	-0.25815500
C	4.55031200	0.04571600	-2.57534400
C	5.25458300	0.02480900	0.20689400
C	5.89801100	0.06794500	-2.12761900
H	4.31629200	0.04902200	-3.63404100
C	2.97775300	-0.04672200	1.86124200
C	5.39608600	0.00441900	1.61921800
C	6.26745000	0.05875200	-0.78937800
H	6.68057000	0.09209300	-2.88109900
C	4.27032600	-0.03138600	2.42769600
H	2.07511800	-0.07418100	2.46182100
H	6.38701200	0.01512200	2.06486000
H	7.31383700	0.07493400	-0.50253600
H	4.36556500	-0.04847900	3.50773300
N	2.83001500	-0.02763400	0.54250600
N	-2.83023200	0.02755600	-0.54264600
F	2.56657500	-2.71122400	-0.71253500
F	-2.56680600	2.71114900	0.71242400

3-bent

Cl	6.65144000	5.11877700	0.13474100
Cl	7.22147900	-1.56118700	5.30395600
O	8.78018100	3.84926500	1.80324400
N	8.38704000	1.85078300	0.52765700
O	5.74902900	-0.57992300	2.25478100
N	4.93895100	0.25037700	4.35716700
C	5.43037500	1.98079300	2.44265400
C	6.30465100	2.90472100	1.80494100
C	9.35853900	2.61665400	-0.02709200
C	8.35930500	1.71951000	3.16323800
C	8.67363400	0.29515700	-1.23919700
H	8.36981100	-0.64208500	-1.69224800
C	10.05585500	2.29209500	-1.20963400
C	9.66905000	1.06813100	-1.81596100
H	10.15351800	0.73986100	-2.73151600
C	7.51529700	0.70814000	3.69588400
C	5.70079000	3.95459500	1.08752500
C	9.57505400	3.78705200	0.74051700
C	10.54021500	4.68059000	0.30512600
H	10.73901100	5.59545400	0.85200800
C	9.66911000	1.87273100	3.64933600
H	10.29101900	2.66924000	3.25383900
B	7.89183200	2.62939100	1.91299300
C	8.09873300	-0.15054300	4.64674000
C	3.61872100	0.29767900	6.32712000
H	3.38728100	0.79433500	7.26270900
C	4.27979700	-0.87055300	3.97393300
C	4.32135100	4.15504200	1.02889800

H	3.92060100	4.99532900	0.47239700
C	3.25554300	-1.48890200	4.72096600
C	4.76966800	-1.34212700	2.73103300
C	3.48270800	3.25472700	1.67955700
H	2.40516500	3.39074000	1.64087000
C	9.39833000	-0.00387800	5.13068500
H	9.78133700	-0.69473800	5.87394700
C	8.03457300	0.70761500	-0.04918400
H	7.25696000	0.12272600	0.43200900
C	4.03870100	2.17549000	2.36227600
H	3.36083000	1.47163100	2.83715000
C	10.18393600	1.03529100	4.63661700
H	11.19448300	1.17472500	5.01150400
C	11.25573800	4.37111500	-0.88290300
H	12.00964700	5.07810400	-1.21806400
C	2.93852400	-0.84900400	5.94803400
H	2.16385200	-1.26031300	6.58933000
B	5.98953400	0.64369100	3.17428100
C	4.62760800	0.84058500	5.50373200
H	5.17915900	1.73611800	5.76673100
C	3.15978100	-3.12363000	2.93671200
H	2.71802800	-4.02194000	2.51440300
C	11.04159300	3.22427000	-1.63430900
H	11.61486200	3.03740800	-2.53654900
C	4.19722300	-2.48900000	2.20286900
H	4.53464200	-2.89577500	1.25607700
C	2.68486200	-2.66141700	4.15621900
H	1.89054000	-3.18592400	4.67705100

3-symmetrical

C	-0.93070800	-3.75768200	0.37428200
C	-1.46454500	-2.48414500	0.53763000
C	-0.72329500	-1.32031600	0.25408400
C	0.61833900	-1.43368700	-0.19570200
C	1.12166800	-2.74401300	-0.33869400
C	0.38195400	-3.89390900	-0.07487800
C	0.72305900	1.32025500	-0.25420700
C	-0.61857700	1.43362500	0.19557300
C	-1.12190200	2.74395200	0.33857600
C	-0.38218100	3.89384900	0.07477700
C	0.93048300	3.75762200	-0.37437600
C	1.46431500	2.48408400	-0.53773600
H	-1.52278100	-4.64153200	0.59645000
H	-2.48385200	-2.39746200	0.90320900
H	0.83126700	-4.87152200	-0.21202600
H	-0.83149100	4.87146200	0.21193400
H	1.52256000	4.64147100	-0.59653100
H	2.48362300	2.39740100	-0.90331000
B	1.48177400	-0.09675800	-0.45478000
B	-1.48201700	0.09669500	0.45463600
O	2.22525500	-0.08669800	-1.79009500

O	-2.22552900	0.08663400	1.78993300
C	-3.53671100	-0.03031900	1.61682800
C	-3.90099200	-0.03680000	0.24700200
C	-4.55041900	-0.13409200	2.55633900
C	-5.22367800	-0.13354600	-0.23357600
C	-5.88940700	-0.23956000	2.09284400
H	-4.32845900	-0.12749500	3.61759800
C	-2.93895800	0.10818700	-1.85996300
C	-5.35136200	-0.10138700	-1.64699100
C	-6.24345700	-0.24205400	0.75070700
H	-6.67701700	-0.32005200	2.83703100
C	-4.22185200	0.01978400	-2.44165500
H	-2.03376400	0.20126000	-2.45005900
H	-6.33479500	-0.16832800	-2.10414400
H	-7.28341600	-0.32204000	0.45146800
H	-4.30645300	0.04891200	-3.52228800
C	3.53644100	0.03024300	-1.61702200
C	3.90075600	0.03672100	-0.24720500
C	4.55012800	0.13400900	-2.55655600
C	5.22345400	0.13345700	0.23334200
C	5.88912800	0.23946500	-2.09309400
H	4.32814200	0.12741500	-3.61781100
C	2.93877000	-0.10825600	1.85978400
C	5.35117100	0.10129800	1.64675400
C	6.24321000	0.24195700	-0.75096600
H	6.67672000	0.31995200	-2.83729900
C	4.22167900	-0.01986200	2.44144500
H	2.03359000	-0.20132300	2.44990100
H	6.33461600	0.16823200	2.10388300
H	7.28317600	0.32193500	-0.45175100
H	4.30630500	-0.04899000	3.52207700
N	2.80381900	-0.07704200	0.54019400
N	-2.80403800	0.07697300	-0.54037000
Cl	-2.79631000	3.04892200	0.86474400
Cl	2.79607400	-3.04897800	-0.86487100

4-bent

O	8.81482700	3.83722500	1.81362300
N	8.37008200	1.84767900	0.54144200
O	5.80315700	-0.59503400	2.26767400
N	4.95407900	0.24479200	4.34943600
C	5.45577000	1.96384700	2.43488800
C	6.32482300	2.92183300	1.84079000
C	9.34046200	2.60250400	-0.03096600
C	8.38031000	1.72696500	3.18716800
C	8.59837800	0.29714000	-1.23877100
H	8.27441500	-0.63548500	-1.68739000
C	10.00288100	2.27741800	-1.23285600
C	9.59506200	1.05651500	-1.83086300
H	10.05923400	0.72371400	-2.75523100
C	7.53619700	0.72050500	3.72985500

C	5.71456800	3.98245600	1.14819200
C	9.58857900	3.76634600	0.73571400
C	10.55798800	4.64713400	0.28572100
H	10.78136600	5.55587700	0.83327800
C	9.68764700	1.89339000	3.67471400
H	10.30835700	2.68337600	3.26504200
B	7.91030500	2.63427600	1.93799700
C	8.11657200	-0.11221900	4.70308500
C	3.61202800	0.29158200	6.30411600
H	3.37168200	0.78595300	7.23860300
C	4.29398000	-0.87045500	3.95307600
C	4.33315700	4.14935200	1.05423100
H	3.92177400	5.00113700	0.52434000
C	3.25701600	-1.48439800	4.68438500
C	4.80536300	-1.34781900	2.72187600
C	3.49918400	3.20441400	1.64478100
H	2.42009200	3.31321100	1.57425300
C	9.41210900	0.04806800	5.19242700
H	9.79490400	-0.61972600	5.95600500
C	7.98890000	0.71309600	-0.03448700
H	7.21169100	0.13690500	0.45749900
C	4.06231000	2.12279700	2.31617700
H	3.39030200	1.38964100	2.75357400
C	10.20057800	1.07464900	4.67772000
H	11.20942900	1.22201900	5.05432400
C	11.24688500	4.33219100	-0.91651100
H	12.00742600	5.02732800	-1.26124400
C	2.92406100	-0.84422200	5.90695000
H	2.13186400	-1.24796000	6.53147200
B	6.01971100	0.63725200	3.18322800
C	4.64297400	0.82283900	5.50141300
H	5.20047900	1.71034600	5.77923300
C	3.16856900	-3.10842000	2.89038100
H	2.72172000	-3.99797100	2.45514500
C	10.99809200	3.19380500	-1.66970500
H	11.55146600	3.00149200	-2.58317400
C	4.23053600	-2.48666900	2.18032900
H	4.58224500	-2.89648500	1.24005200
C	2.67714900	-2.64404700	4.10239600
H	1.86656500	-3.15968200	4.60675600
Br	6.72478300	5.36810300	0.25370800
Br	7.17442500	-1.62180800	5.47654400

4-symmetrical

C	-1.01156500	-3.74277600	0.31210000
C	-1.54040800	-2.46180000	0.41589400
C	-0.75934100	-1.30957400	0.20057200
C	0.61500600	-1.44332600	-0.12878100
C	1.11200600	-2.76016000	-0.20186000
C	0.33753500	-3.89891400	-0.00128900
C	0.75911000	1.30950500	-0.20073000

C	-0.61524000	1.44325600	0.12860800
C	-1.11224100	2.76008900	0.20168400
C	-0.33776800	3.89884500	0.00112800
C	1.01133700	3.74270800	-0.31224200
C	1.54018100	2.46173100	-0.41603700
H	-1.63481800	-4.61750500	0.47822000
H	-2.58983300	-2.36220300	0.67808800
H	0.78035000	-4.88521000	-0.08339500
H	-0.78058300	4.88514000	0.08323000
H	1.63459200	4.61743700	-0.47835000
H	2.58960900	2.36213600	-0.67821900
B	1.49854100	-0.12089500	-0.38738300
B	-1.49877300	0.12082200	0.38721100
O	2.21217400	-0.12701600	-1.74425300
O	-2.21241500	0.12695400	1.74407800
C	-3.52328600	-0.02449100	1.59834400
C	-3.91436300	-0.04253800	0.23634200
C	-4.51520100	-0.15968100	2.55704900
C	-5.24415200	-0.15143500	-0.21799800
C	-5.85986300	-0.29731000	2.11942600
H	-4.27285700	-0.14842500	3.61379200
C	-3.00239000	0.15816600	-1.88807000
C	-5.40181200	-0.12358000	-1.62860600
C	-6.23999800	-0.30479700	0.78431400
H	-6.62932100	-0.40757400	2.87866400
C	-4.29228200	0.02729800	-2.44565900
H	-2.11346000	0.28858700	-2.49561400
H	-6.39221000	-0.21873300	-2.06525100
H	-7.28307800	-0.41125600	0.50486000
H	-4.39910200	0.05821500	-3.52422600
C	3.52304600	0.02443000	-1.59852500
C	3.91413000	0.04246200	-0.23652500
C	4.51495400	0.15963200	-2.55723500
C	5.24392200	0.15135400	0.21780800
C	5.85961900	0.29725700	-2.11961800
H	4.27260400	0.14839000	-3.61397700
C	3.00216900	-0.15826400	1.88788900
C	5.40159000	0.12348300	1.62841500
C	6.23976100	0.30472800	-0.78450900
H	6.62907200	0.40753100	-2.87885900
C	4.29206500	-0.02740400	2.44547200
H	2.11324200	-0.28868900	2.49543800
H	6.39199000	0.21863000	2.06505500
H	7.28284400	0.41118400	-0.50505900
H	4.39889000	-0.05833300	3.52403800
N	2.83709600	-0.10276800	0.57331500
N	-2.83732400	0.10268400	-0.57349400
Br	2.96655000	-3.13791300	-0.60558400
Br	-2.96679200	3.13784100	0.60538100

5 -bent

F	9.31413000	9.11983000	3.38036900
F	10.49048400	11.28773600	4.53191700
O	11.42174200	4.90228100	5.42209900
O	12.48591200	8.68851500	9.03331700
F	16.94233200	5.35583400	8.85037300
N	14.23353500	9.58263900	7.65017600
N	10.61942700	5.60049700	7.57992800
F	15.72576700	3.22479700	7.67214300
C	10.50859600	7.65909000	4.83481100
H	10.03000400	6.81465600	4.34760200
C	13.06538100	9.73724300	9.60639300
C	14.10115800	10.28113900	8.80578900
C	9.93811800	4.52297900	7.11606600
C	8.56356400	4.44803500	9.06606300
H	7.76601900	4.01743800	9.66526300
C	8.88683100	3.88189500	7.80464000
C	13.21767000	5.83016500	7.06466800
C	10.42465600	4.12772900	5.84611900
C	9.26686400	5.54840300	9.52863000
H	9.03022200	5.99053700	10.49013000
C	11.43678600	7.46752600	5.87270400
C	10.30658100	6.11994300	8.76141800
H	10.87570100	6.98149400	9.09584800
C	12.06576600	8.59197900	6.46056500
C	10.20025900	8.93591500	4.39061900
C	13.85655100	6.94552100	7.65914100
C	10.80373200	10.04387500	4.97643400
C	11.72540600	9.87734600	5.99921200
H	12.16958400	10.77586400	6.41998600
C	14.88997400	11.39774300	9.15923700
C	8.29526400	2.76556400	7.15299900
H	7.48155000	2.22696400	7.62760900
B	11.75465900	5.99338600	6.42378000
C	13.85836500	4.57923900	7.07692500
H	13.40431700	3.71210900	6.60638100
C	12.80592100	10.34441500	10.82646500
H	12.02544200	9.97152400	11.48030200
C	13.58845300	11.46891700	11.20015100
H	13.37662100	11.93648600	12.15759300
C	14.60215800	11.99898300	10.41355900
H	15.17008800	12.86091900	10.74756600
C	15.11295800	6.76283200	8.26652400
H	15.64463200	7.58096300	8.74577000
C	8.77107100	2.37756200	5.90876700
H	8.31172700	1.52313000	5.41972700
C	9.83192000	3.03676500	5.23106100
H	10.16809100	2.69466200	4.25857700
C	15.10195500	4.42917400	7.67157700
C	15.15629600	9.94107100	6.76366300
H	15.22491600	9.35354400	5.85519000

B	13.13128300	8.38260800	7.64893700
C	15.72558200	5.51865700	8.27080000
C	15.87053200	11.76686600	8.20096700
H	16.52189300	12.61522300	8.39155400
C	15.99572500	11.04497900	7.02394400
H	16.74068800	11.31733200	6.28482500

8 -symmetrical

S	-0.32046700	6.37216300	1.92481900
O	-0.75039600	9.68540900	2.48904200
N	-2.81632600	8.55793900	2.96755200
C	-0.55026900	7.24538300	3.42838900
C	-2.93826100	9.39201200	1.90743800
C	0.40814600	5.21278100	4.09845700
H	0.79583200	4.47168500	4.79122500
C	-0.10897200	6.49312300	4.50232300
B	-1.25649300	8.67333900	3.52048600
C	-4.12600900	9.57910900	1.16886900
C	-1.70838300	10.04702500	1.64359800
C	-3.85989800	7.84796600	3.37487200
H	-3.71044700	7.19472300	4.22770400
C	-1.66686900	10.93975700	0.58296900
H	-0.75267200	11.46736800	0.33497600
C	0.35842700	5.00230800	2.74654300
H	0.68469700	4.13374800	2.18942300
C	-5.09612500	7.96271400	2.70268200
H	-5.93564300	7.37224700	3.05256800
C	-5.23467900	8.81282800	1.61617400
H	-6.19045000	8.89341300	1.10564900
C	-4.05477500	10.49932600	0.08799600
H	-4.93073100	10.69202000	-0.52278500
C	-2.85260100	11.14303300	-0.17264000
H	-2.80908800	11.84374100	-1.00194000
S	-1.07085100	9.36839300	7.59075600
O	-0.64091500	6.05514800	7.02653400
N	1.42501300	7.18262100	6.54801900
C	-0.84104800	8.49517300	6.08718600
C	1.54695100	6.34854900	7.60813300
C	-1.79946300	10.52777500	5.41711800
H	-2.18714800	11.26887100	4.72435000
C	-1.28234400	9.24743300	5.01325200
B	-0.13482200	7.06721800	5.99508800
C	2.73470100	6.16145400	8.34670000
C	0.31707400	5.69353400	7.87197700
C	2.46858200	7.89259500	6.14069700
H	2.31912900	8.54583800	5.28786500
C	0.27556500	4.80080300	8.93260700
H	-0.63863200	4.27319100	9.18060100
C	-1.74974900	10.73824500	6.76903300
H	-2.07602300	11.60680400	7.32615300
C	3.70481100	7.77785000	6.81288400

H	4.54432700	8.36831900	6.46299600
C	3.84336900	6.92773700	7.89939200
H	4.79914100	6.84715400	8.40991600
C	2.66347000	5.24123800	9.42757400
H	3.53942800	5.04854600	10.03835300
C	1.46129800	4.59752900	9.68821300
H	1.41778800	3.89682200	10.51751300

Cartesian coordinates for ground state optimized geometry of the cationic species (UB3LYP/6-31+g(d,p))

1 -bent

O	8.85338800	3.78157200	1.72833600
N	8.37346100	1.77797100	0.52610400
O	5.77081300	-0.49498100	2.22014300
N	4.86461300	0.26530100	4.29751400
C	5.44828400	2.06659300	2.41032000
C	6.40464800	2.98326600	1.92394200
C	9.29629800	2.53579100	-0.11954800
C	8.33806100	1.73938800	3.22365500
C	8.54122500	0.19390000	-1.23576900
H	8.21146400	-0.75207100	-1.64988100
C	9.90307800	2.19784700	-1.34260900
C	9.48531800	0.96348700	-1.90180600
H	9.90147100	0.62233300	-2.84521300
C	7.42431400	0.79506300	3.73810800
C	5.99067800	4.22865000	1.40559100
C	9.56945900	3.71829900	0.60499200
C	10.49356600	4.61843300	0.09404200
H	10.73134000	5.53685000	0.61889900
C	9.60024100	1.90621300	3.83199800
H	10.27772000	2.67081900	3.46612000
B	7.97647900	2.58516500	1.88774000
C	7.86086900	-0.06888300	4.75838800
C	3.51241400	0.20144100	6.25011800
H	3.20820200	0.68837200	7.16954700
C	4.33917500	-0.93212700	3.93301600
C	4.63660800	4.51556500	1.26184100
H	4.32373500	5.46136900	0.82889600
C	3.37990500	-1.64554300	4.67851000
C	4.88442600	-1.36871600	2.70291100
C	3.67858900	3.57337200	1.66399100
H	2.62023600	3.79833700	1.56700100
C	9.12875900	0.06588700	5.32629700
H	9.43007900	-0.58434100	6.14271400
C	7.98951600	0.61968700	-0.01019200
H	7.25073900	0.03793700	0.53096600
C	4.08590500	2.36057700	2.22208100
H	3.32549800	1.65749100	2.55346000
C	9.99926100	1.06469600	4.86599000
H	10.98602100	1.17418500	5.30666400
C	11.11787900	4.29729800	-1.13894000

H	11.84138700	4.99903600	-1.54169700
C	2.96954300	-1.02341600	5.88558300
H	2.23278500	-1.50381000	6.52284300
B	5.91875100	0.71248500	3.15646400
C	4.46919300	0.83698300	5.43389700
H	4.91186400	1.79288100	5.69021200
C	3.48749200	-3.31622400	2.91812200
H	3.15229400	-4.26433100	2.50928500
C	10.84884700	3.13456300	-1.85074200
H	11.35484500	2.93712100	-2.78987300
C	4.45427200	-2.58007100	2.18324400
H	4.84192100	-2.95798800	1.24393600
C	2.95362000	-2.88591900	4.12547200
H	2.21676200	-3.48746900	4.64690000
H	6.73297200	4.95135400	1.08283900
H	7.19198400	-0.83114200	5.15070300

2 -bent

O	8.42642900	3.45552400	2.04723500
N	8.67902800	1.95252200	0.20754300
O	5.17378000	-1.12216600	2.51760900
N	4.92110200	0.38078400	4.35733700
C	5.31742500	1.36782900	1.91383300
C	6.26157800	2.22722800	1.31871200
C	9.49400900	3.02472600	0.09144000
C	8.28273400	0.96555600	2.65108700
C	9.54208100	1.15105300	-1.85553800
H	9.53022800	0.37774400	-2.61505400
C	10.37919400	3.25073900	-0.97580400
C	10.38243900	2.25126800	-1.98046300
H	11.03492700	2.34427200	-2.84361700
C	7.33858100	0.10615600	3.24620600
C	5.76059100	3.20148100	0.44745200
C	9.32524700	3.90326100	1.19404700
C	10.08646700	5.07194000	1.23941700
H	9.98514200	5.77096400	2.06170900
C	9.64717300	0.83382200	2.97491900
H	10.37776900	1.50733100	2.53489200
B	7.84292300	2.11360900	1.60186900
C	7.83956900	-0.86808200	4.11748300
C	4.05797800	1.18217500	6.42042100
H	4.06979100	1.95546700	7.17995500
C	4.10615200	-0.69144900	4.47339600
C	4.42260700	3.36118700	0.12681400
H	4.11988400	4.13708300	-0.56813200
C	3.22095200	-0.91751700	5.54061700
C	4.27496000	-1.56995200	3.37077200
C	3.50460800	2.48700900	0.71520100
H	2.44711300	2.58067300	0.48693500
C	9.17755000	-1.02777700	4.43813100
H	9.48027000	-1.80366300	5.13309100

C	8.68924500	1.01840700	-0.74323900
H	8.02187000	0.17311000	-0.61708900
C	3.95298600	1.49957000	1.59000400
H	3.22238900	0.82605600	2.03002400
C	10.09555000	-0.15360600	3.84973600
H	11.15304400	-0.24726600	4.07800700
C	10.98587200	5.31525800	0.17675700
H	11.57919100	6.22364100	0.20675600
C	3.21765400	0.08192900	6.54530100
H	2.56515200	-0.01111900	7.40844000
B	5.75724200	0.21975600	2.96302500
C	4.91083300	1.31487400	5.30814100
H	5.57818300	2.16019700	5.18202800
C	2.61435700	-2.98202500	4.38799400
H	2.02106500	-3.89042400	4.35795900
C	11.14628700	4.45115900	-0.90545200
H	11.85084600	4.68997100	-1.69515000
C	3.51377500	-2.73865100	3.32535700
H	3.61513400	-3.43764900	2.50304700
C	2.45389700	-2.11795800	5.47022200
H	1.74933200	-2.35681100	6.25990200
F	6.64992400	4.04919300	-0.16054200
F	6.95023400	-1.71579000	4.72548200

2 -symmetrical

C	-0.74071200	-3.80317300	0.21678200
C	-1.38016100	-2.57710300	0.38763700
C	-0.70213400	-1.35917600	0.18547300
C	0.66233900	-1.37030100	-0.16414000
C	1.25827100	-2.62678400	-0.32346500
C	0.60828400	-3.83708600	-0.14682900
C	0.70190700	1.35910100	-0.18561400
C	-0.66256600	1.37022600	0.16400000
C	-1.25849800	2.62670900	0.32332500
C	-0.60851100	3.83701100	0.14668900
C	0.74048500	3.80309800	-0.21692200
C	1.37993400	2.57702700	-0.38777700
H	-1.28333800	-4.73193500	0.36554500
H	-2.42739700	-2.57452000	0.67794100
H	1.14892700	-4.76800900	-0.27985900
H	-1.14915500	4.76793300	0.27971900
H	1.28311100	4.73186000	-0.36568500
H	2.42717000	2.57444400	-0.67808000
B	1.51999500	-0.02268700	-0.36933900
B	-1.52022300	0.02261200	0.36919900
O	2.22789700	-0.01421000	-1.72514300
O	-2.22812400	0.01413500	1.72500200
C	-3.53867500	-0.01048100	1.59029200
C	-3.93187900	-0.00809200	0.22594800
C	-4.53086800	-0.03466900	2.57123400
C	-5.26525200	-0.02251700	-0.21627100

C	-5.87861200	-0.05362300	2.14624600
H	-4.27313200	-0.03360400	3.62415400
C	-3.01978800	0.03888400	-1.90374500
C	-5.43575400	-0.00463700	-1.62300600
C	-6.26020500	-0.04826900	0.80538400
H	-6.65406500	-0.07102600	2.90549300
C	-4.31787900	0.02607800	-2.44864800
H	-2.12816500	0.06352700	-2.52037100
H	-6.43248400	-0.01254800	-2.05415400
H	-7.31125100	-0.06124200	0.53670000
H	-4.42947000	0.04170700	-3.52675400
C	3.53844800	0.01040600	-1.59043200
C	3.93165200	0.00801700	-0.22608900
C	4.53064100	0.03459400	-2.57137500
C	5.26502500	0.02244100	0.21613000
C	5.87838500	0.05354800	-2.14638700
H	4.27290400	0.03352900	-3.62429400
C	3.01956100	-0.03895900	1.90360500
C	5.43552700	0.00456200	1.62286500
C	6.25997800	0.04819400	-0.80552400
H	6.65383800	0.07095000	-2.90563400
C	4.31765300	-0.02615300	2.44850800
H	2.12793800	-0.06360300	2.52023000
H	6.43225700	0.01247200	2.05401300
H	7.31102400	0.06116700	-0.53684100
H	4.42924300	-0.04178200	3.52661400
N	2.84829900	-0.02160200	0.58186300
N	-2.84852600	0.02152700	-0.58200300
F	2.58809900	-2.67862400	-0.65218400
F	-2.58832600	2.67854900	0.65204400

3-symmetrical

Cl	6.56738500	4.46920000	-0.31688200
Cl	7.03329100	-2.13824800	4.87921700
O	8.39174900	3.49125000	2.04158700
N	8.61994900	1.98047600	0.20455400
O	5.20888200	-1.16028800	2.52083800
N	4.98076800	0.35057800	4.35780400
C	5.32190300	1.30888000	1.91580000
C	6.19435800	2.25086400	1.32823800
C	9.50841800	2.99688100	0.12765600
C	8.27878100	1.02204800	2.64650400
C	9.49026600	1.14704400	-1.84261100
H	9.44814100	0.38635100	-2.61368800
C	10.44131600	3.17301300	-0.90754500
C	10.40871700	2.18668800	-1.92508400
H	11.09344900	2.24452400	-2.76605100
C	7.40632400	0.08007400	3.23407800
C	5.60214500	3.22100800	0.49079300
C	9.35635900	3.87915700	1.22950800
C	10.18859300	4.99498000	1.31161400

H	10.10049000	5.69646300	2.13334700
C	9.65513100	0.99318300	2.94532100
H	10.32226300	1.73553500	2.51797300
B	7.78325900	2.16306400	1.59934400
C	7.99853600	-0.89008200	4.07150900
C	4.11052900	1.18412800	6.40495400
H	4.15269500	1.94485500	7.17599500
C	4.09227400	-0.66580000	4.43477400
C	4.23720100	3.26752600	0.21648100
H	3.84450500	4.03193500	-0.44484100
C	3.15939900	-0.84185900	5.47000800
C	4.24428200	-1.54813100	3.33295900
C	3.40026000	2.30934000	0.78646500
H	2.33507200	2.32515000	0.57578700
C	9.36348600	-0.93662700	4.34578800
H	9.75618300	-1.70104500	5.00710000
C	8.59525800	1.06055500	-0.75876800
H	7.86780400	0.26179100	-0.66565100
C	3.94555900	1.33771800	1.61695200
H	3.27843200	0.59535600	2.04429100
C	10.20043300	0.02154500	3.77578700
H	11.26562600	0.00571100	3.98644000
C	11.14087000	5.18492700	0.28395000
H	11.79056000	6.05240900	0.34289100
C	3.19205200	0.14451200	6.48750000
H	2.50734200	0.08673400	7.32848900
B	5.81741800	0.16789700	2.96300100
C	5.00551000	1.27054200	5.32108300
H	5.73298300	2.06928300	5.22791000
C	2.45976200	-2.85381100	4.27862600
H	1.81004900	-3.72128000	4.21974200
C	11.28295300	4.31932400	-0.79936500
H	12.02918500	4.51660400	-1.56179100
C	3.41201800	-2.66393700	3.25092800
H	3.50008200	-3.36546200	2.42922700
C	2.31773000	-1.98815400	5.36190300
H	1.57151400	-2.18537800	6.12435900

4-bent

O	8.76763600	3.82207500	1.77167000
N	8.35892900	1.84440500	0.49704100
O	5.74838700	-0.57212700	2.27763100
N	4.93966100	0.26152700	4.36633700
C	5.42670800	1.95863300	2.40945300
C	6.29439200	2.90195100	1.81475700
C	9.34795300	2.59060600	-0.04398600
C	8.35702400	1.72525100	3.15362100
C	8.63218200	0.30460900	-1.29042300
H	8.31717500	-0.62115900	-1.75821000
C	10.04429200	2.27353800	-1.22176100
C	9.65484800	1.06306800	-1.84733200

H	10.14550300	0.73418900	-2.75862600
C	7.51660900	0.72839800	3.70088000
C	5.69850100	3.98491800	1.13857800
C	9.57980400	3.75284400	0.73450600
C	10.57211600	4.64508500	0.32976500
H	10.77395900	5.54784200	0.89499100
C	9.66418600	1.90964000	3.63784200
H	10.28472800	2.70081100	3.23258100
B	7.88226900	2.60682500	1.87670000
C	8.10513000	-0.12235300	4.65654300
C	3.63471600	0.29112600	6.34957400
H	3.40830100	0.78005700	7.29004600
C	4.27862900	-0.85645100	3.98518400
C	4.31667900	4.15138700	1.04938000
H	3.90499300	5.00517100	0.52349100
C	3.26632800	-1.48044700	4.73257700
C	4.77010300	-1.33573700	2.74610100
C	3.47689200	3.19950100	1.62489200
H	2.39937800	3.31698400	1.55695200
C	9.40326700	0.04759200	5.13721900
H	9.79368600	-0.61902500	5.89773000
C	7.98979600	0.71289800	-0.10508300
H	7.19427600	0.13802600	0.35758500
C	4.03161300	2.10683100	2.28016000
H	3.35908700	1.37378500	2.71509600
C	10.18359800	1.08409100	4.63022400
H	11.19299700	1.23331400	5.00226700
C	11.29670100	4.33582900	-0.84303900
H	12.07279900	5.02410500	-1.16217300
C	2.94592900	-0.85132200	5.96206300
H	2.16952000	-1.26291700	6.60032600
B	5.98251900	0.64564300	3.19575800
C	4.64518200	0.83183800	5.53224600
H	5.20164900	1.72095500	5.80713600
C	3.16074600	-3.11476000	2.92890700
H	2.71270000	-4.00822900	2.50572800
C	11.05929400	3.19630800	-1.61124300
H	11.64423400	3.01069200	-2.50601800
C	4.20145100	-2.48413100	2.20431800
H	4.54599300	-2.88739900	1.25887300
C	2.68981200	-2.64812600	4.15232500
H	1.89311900	-3.17272600	4.66903500
Br	6.71329900	5.36490100	0.26591600
Br	7.17723100	-1.63356600	5.41630300

4-symmetrical

C	-1.00744000	-3.74416200	0.28308600
C	-1.54519400	-2.46707800	0.38011600
C	-0.75935400	-1.31632000	0.18100400
C	0.62068700	-1.43861100	-0.09649400
C	1.12923900	-2.75233800	-0.17456900

C	0.34993800	-3.89168500	0.00359800
C	0.75912300	1.31624500	-0.18118300
C	-0.62091900	1.43853600	0.09631500
C	-1.12947100	2.75226200	0.17438900
C	-0.35017000	3.89161000	-0.00377700
C	1.00720800	3.74408700	-0.28326600
C	1.54496200	2.46700300	-0.38029500
H	-1.63021400	-4.62205200	0.42755500
H	-2.60264800	-2.37553600	0.60927200
H	0.79791800	-4.87657500	-0.06376400
H	-0.79815000	4.87649900	0.06358500
H	1.62998200	4.62197700	-0.42773400
H	2.60241600	2.37546100	-0.60945100
B	1.51485200	-0.11655300	-0.32449600
B	-1.51508400	0.11647800	0.32431800
O	2.21186100	-0.11331900	-1.69204300
O	-2.21209100	0.11324500	1.69186600
C	-3.51548600	-0.02883600	1.56713600
C	-3.91889300	-0.04840700	0.20549800
C	-4.49351600	-0.15545700	2.55473000
C	-5.25044300	-0.14666800	-0.22639800
C	-5.83774300	-0.28529100	2.13901600
H	-4.22801200	-0.14171700	3.60561600
C	-3.03831200	0.14843100	-1.92811400
C	-5.43672500	-0.11862500	-1.63131900
C	-6.22936400	-0.29205400	0.80057800
H	-6.60157200	-0.38866200	2.90321800
C	-4.33433400	0.02632400	-2.46480800
H	-2.15978500	0.27614600	-2.55086100
H	-6.43345900	-0.20583800	-2.05361700
H	-7.27741900	-0.39311800	0.53890200
H	-4.45711000	0.05947400	-3.54125400
C	3.51525600	0.02876200	-1.56731200
C	3.91866100	0.04833400	-0.20567300
C	4.49328700	0.15538400	-2.55490500
C	5.25021100	0.14659500	0.22622400
C	5.83751400	0.28521900	-2.13918900
H	4.22778400	0.14164400	-3.60579100
C	3.03807800	-0.14850600	1.92793700
C	5.43649100	0.11855100	1.63114600
C	6.22913300	0.29198300	-0.80075000
H	6.60134300	0.38859100	-2.90339000
C	4.33410000	-0.02639800	2.46463300
H	2.15955000	-0.27622200	2.55068400
H	6.43322500	0.20576600	2.05344400
H	7.27718800	0.39304700	-0.53907300
H	4.45687400	-0.05954900	3.54108000
N	2.85026100	-0.09075000	0.61090700
N	-2.85049400	0.09067500	-0.61108400
Br	2.98704400	-3.11977800	-0.53546600

Br	-2.98727600	3.11970100	0.53528800

5 –bent

F	9.46837200	9.04321900	3.24961400
F	10.55674500	11.22045500	4.42255100
O	11.37805000	4.90468700	5.49034200
O	12.49650800	8.66046300	8.97872800
F	16.96061000	5.33283400	8.70943800
N	14.25068500	9.60059600	7.64908500
N	10.60243300	5.62172500	7.63475000
F	15.76031700	3.25818000	7.46217400
C	10.61055500	7.60666200	4.74929300
H	10.15699200	6.75142200	4.26009800
C	13.05026900	9.70913700	9.59047500
C	14.08996800	10.27633800	8.81604700
C	9.90926800	4.54383400	7.18782900
C	8.54641100	4.48586400	9.14397900
H	7.75121000	4.06383000	9.75146200
C	8.86271000	3.91432500	7.88522200
C	13.22037700	5.84224800	7.02839700
C	10.38030600	4.13246300	5.91860800
C	9.25980300	5.58817400	9.59443700
H	9.03053500	6.03689700	10.55421400
C	11.46803500	7.45333200	5.85548700
C	10.29531700	6.14950200	8.81941400
H	10.86915200	7.01041400	9.14603500
C	12.09475000	8.58876800	6.43011800
C	10.30768600	8.87289100	4.28253100
C	13.87543500	6.95166700	7.62195700
C	10.86618400	10.00417300	4.89603000
C	11.74479000	9.86558100	5.95976700
H	12.16913100	10.77248700	6.38030900
C	14.85494100	11.39317300	9.20543000
C	8.26489500	2.79444200	7.23763800
H	7.45180900	2.26179100	7.71941400
B	11.70702400	5.98263500	6.48029800
C	13.87929300	4.60128300	6.93760000
H	13.42101200	3.75022000	6.44552400
C	12.75309600	10.28128100	10.81892700
H	11.96548100	9.88291700	11.44846500
C	13.51159900	11.40775500	11.23130700
H	13.27780200	11.85419800	12.19266300
C	14.53176100	11.96296500	10.46953000
H	15.08130500	12.82527900	10.83154300
C	15.12900000	6.75431100	8.22492800
H	15.66497000	7.55870800	8.71999800
C	8.72737700	2.38992300	5.99030200
H	8.25902200	1.53480500	5.51346400
C	9.78463900	3.03891900	5.30402400
H	10.11682600	2.69278200	4.33173100
C	15.12821800	4.44079100	7.50975600

C	15.18881300	9.99401400	6.78731600
H	15.28725300	9.43017400	5.86643700
B	13.16861200	8.40059600	7.61776500
C	15.74861800	5.51532100	8.16441400
C	15.84840000	11.79867000	8.27761000
H	16.48406400	12.65137200	8.49763100
C	16.00583500	11.10196000	7.08668900
H	16.76059100	11.40006200	6.36807700

6-symmetrical

C	-0.73256200	-3.80678700	0.20442100
C	-1.37698200	-2.58215200	0.36947500
C	-0.70104600	-1.36149600	0.17912900
C	0.66701100	-1.36910900	-0.16194700
C	1.26733100	-2.62406100	-0.31425000
C	0.61990400	-3.83674700	-0.14546400
C	0.70081900	1.36142100	-0.17927000
C	-0.66723800	1.36903400	0.16180600
C	-1.26755800	2.62398600	0.31410900
C	-0.62013200	3.83667100	0.14532300
C	0.73233500	3.80671100	-0.20456200
C	1.37675500	2.58207700	-0.36961600
H	-1.27391900	-4.73714700	0.34746100
H	-2.42693300	-2.58402000	0.65059200
H	1.16388200	-4.76602900	-0.27616400
H	-1.16410900	4.76595400	0.27602200
H	1.27369200	4.73707200	-0.34760200
H	2.42670600	2.58394500	-0.65073300
B	1.51530200	-0.01829800	-0.36793800
B	-1.51552900	0.01822300	0.36779700
O	2.22837200	-0.00983500	-1.72627300
O	-2.22859800	0.00975900	1.72613300
C	-3.53545100	-0.00980700	1.59045900
C	-3.93315800	-0.00814100	0.22635300
C	-4.52872300	-0.02857100	2.57137100
C	-5.26390900	-0.01872400	-0.22422200
C	-5.87413200	-0.04313700	2.15486900
H	-4.27458500	-0.02683700	3.62499300
C	-3.01742900	0.03113600	-1.90356600
C	-5.43393700	-0.00304300	-1.62967100
C	-6.25187600	-0.03885000	0.81054700
H	-6.65522300	-0.05635900	2.90738600
C	-4.31384000	0.02170000	-2.45135500
H	-2.12363800	0.05140300	-2.51721600
H	-6.43005700	-0.00829400	-2.05904200
H	-4.42466300	0.03532400	-3.52950300
C	3.53522400	0.00973200	-1.59060000
C	3.93293100	0.00806600	-0.22649400
C	4.52849600	0.02849600	-2.57151200
C	5.26368200	0.01864900	0.22408100
C	5.87390600	0.04306200	-2.15500900

H	4.27435900	0.02676200	-3.62513300
C	3.01720200	-0.03121100	1.90342500
C	5.43371000	0.00296800	1.62953100
C	6.25164900	0.03877500	-0.81068700
H	6.65499700	0.05628400	-2.90752600
C	4.31361300	-0.02177500	2.45121500
H	2.12341100	-0.05147800	2.51707500
H	6.42983000	0.00821900	2.05890100
H	4.42443500	-0.03539900	3.52936200
N	2.84999900	-0.01638700	0.58199200
N	-2.85022600	0.01631200	-0.58213200
F	2.60097400	-2.67169300	-0.63254900
F	-2.60120200	2.67161800	0.63240800
Cl	7.93385400	0.05643800	-0.38724500
Cl	-7.93408100	-0.05651300	0.38710500

7 -symmetrical

C	-0.72413800	-3.80861400	0.19817200
C	-1.37249100	-2.58581600	0.36166200
C	-0.69894200	-1.36338700	0.17509000
C	0.67048200	-1.36745100	-0.16049500
C	1.27462500	-2.62058600	-0.31184600
C	0.62969700	-3.83497100	-0.14658300
C	0.69871500	1.36331200	-0.17523200
C	-0.67070900	1.36737600	0.16035300
C	-1.27485200	2.62051000	0.31170400
C	-0.62992400	3.83489600	0.14644100
C	0.72391100	3.80853900	-0.19831400
C	1.37226400	2.58574100	-0.36180400
H	-1.26364800	-4.74042000	0.33842700
H	-2.42350500	-2.59107700	0.63878100
H	1.17626400	-4.76283100	-0.27641800
H	-1.17649200	4.76275600	0.27627600
H	1.26342100	4.74034500	-0.33857000
H	2.42327800	2.59100200	-0.63892400
B	1.51457800	-0.01439600	-0.36251700
B	-1.51480500	0.01432100	0.36237500
O	2.22577300	-0.00541700	-1.72666800
O	-2.22600000	0.00534200	1.72652700
C	-3.52758000	-0.01056600	1.58889300
C	-3.93595700	-0.00912800	0.22945400
C	-4.53126700	-0.02438800	2.56601700
C	-5.26559900	-0.01537000	-0.22217600
C	-5.88369300	-0.03441100	2.15397900
C	-3.02153000	0.02559000	-1.90209200
C	-5.43713400	-0.00040900	-1.62552100
C	-6.25488900	-0.03028900	0.81427500
H	-6.65499600	-0.04413400	2.91585700
C	-4.31738200	0.01961700	-2.44924300
H	-2.12783300	0.04274500	-2.51604900
H	-6.43390300	-0.00254300	-2.05339200

H	-4.42913200	0.03247600	-3.52723000
C	3.52735400	0.01049100	-1.58903300
C	3.93572900	0.00905300	-0.22959400
C	4.53104100	0.02431300	-2.56615700
C	5.26537100	0.01529500	0.22203700
C	5.88346700	0.03433600	-2.15411800
C	3.02130200	-0.02566500	1.90195100
C	5.43690600	0.00033400	1.62538200
C	6.25466200	0.03021400	-0.81441400
H	6.65477000	0.04405900	-2.91599600
C	4.31715400	-0.01969200	2.44910300
H	2.12760500	-0.04282000	2.51590800
H	6.43367400	0.00246900	2.05325300
H	4.42890300	-0.03255000	3.52709000
N	2.85224000	-0.01155100	0.58051200
N	-2.85246700	0.01147600	-0.58065300
F	2.60960500	-2.66384800	-0.62561700
F	-2.60983200	2.66377300	0.62547500
Cl	7.93660800	0.04244500	-0.39073900
Cl	-7.93683500	-0.04251900	0.39060100
Cl	4.12525900	0.02535700	-4.24172800
Cl	-4.12548400	-0.02543200	4.24158800

8-bent

S	-1.71264500	5.54776400	2.54734700
O	-0.69175700	9.02832900	3.34852900
N	-3.00515900	8.56605700	2.92079300
C	-1.43500400	6.61210500	3.88797200
C	-2.49945700	9.45928200	2.02705400
C	-0.65748900	4.53436700	4.68704300
H	-0.23699300	3.82633100	5.39149200
C	-0.82187100	5.92054900	4.96055300
B	-1.81079500	8.17091900	3.93427500
C	-3.24007300	10.04402300	0.97877100
C	-1.13647100	9.72165400	2.28816500
C	-4.28234700	8.19711600	2.83232800
H	-4.64788300	7.48332400	3.56207900
C	-0.47009000	10.61027400	1.46530200
H	0.57656700	10.84573600	1.62179900
C	-1.07503100	4.18063000	3.42668400
H	-1.03215500	3.20581700	2.95723200
C	-5.10365400	8.72805500	1.81769800
H	-6.13856700	8.40975900	1.76738000
C	-4.59745600	9.63800100	0.90018200
H	-5.23997300	10.03926900	0.12174800
C	-2.53501100	10.95529100	0.14570900
H	-3.04342700	11.44087900	-0.68023800
C	-1.19666200	11.21263200	0.40073800
H	-0.66826700	11.90975200	-0.24221000
S	-2.07419200	8.36405300	8.05945500
O	-0.32868900	5.77109900	7.49755500

N	1.11637200	7.24890200	6.28499900
C	-1.50056900	7.84554100	6.50666500
C	1.76911700	6.64962400	7.31776800
C	-3.01700700	9.55034100	5.95260300
H	-3.58911700	10.23063000	5.33103500
C	-2.13260500	8.55938600	5.45573200
B	-0.41406900	6.68109900	6.31510300
C	3.12437200	6.86557400	7.63906100
C	0.90903900	5.78256700	8.02472200
C	1.76730800	8.10419100	5.49998300
H	1.21099200	8.56078400	4.68757200
C	1.41282400	5.09132400	9.10854300
H	0.78958400	4.41551500	9.68327600
C	-3.09441200	9.56923300	7.33082200
H	-3.68864800	10.22889900	7.95114200
C	3.12822900	8.38498200	5.74349000
H	3.63721000	9.08535300	5.09115000
C	3.80397000	7.78021800	6.79325300
H	4.85195300	8.00598000	6.96833100
C	3.62526200	6.14450400	8.75841500
H	4.65983400	6.26356600	9.06200600
C	2.77950400	5.29360400	9.45259100
H	3.17260700	4.74911700	10.30560300

9

C	-2.11570800	6.76300900	5.02180700
O	-3.94746600	7.61357200	3.67362600
C	1.23783600	6.67716400	3.85642100
C	2.58684400	7.08146900	3.95698900
C	-1.98386400	6.97917800	2.39379700
C	-3.42895700	7.26765100	4.88015100
O	-0.52825100	5.24667700	3.65044700
C	0.81111700	5.33852600	3.72494400
C	-3.30866800	7.46494400	2.48449300
C	3.13557800	4.72739000	3.79058800
H	3.88420200	3.94158700	3.76325000
C	-3.91138000	7.09090800	7.22969800
H	-4.57913300	7.20898400	8.07618700
C	1.76816300	4.34347300	3.69076300
H	1.49041500	3.30022900	3.59098700
C	-4.09775800	7.82216200	1.36503500
H	-5.10661100	8.18850600	1.52246300
C	2.78789100	8.48022800	4.08215300
H	3.79480200	8.87903300	4.16526100
C	-1.48361100	6.84134100	1.09976200
H	-0.48040600	6.44987400	0.95716300
C	0.38506400	8.83716800	3.99150700
H	-0.48288100	9.48733400	4.00162700
N	0.17516000	7.52757600	3.87331600
C	-1.74546700	6.41212700	6.31933600
H	-0.75815900	5.99466700	6.49529200

C	-3.55355100	7.67759500	0.10139300
H	-4.13468700	7.93770400	-0.77667600
C	3.55581500	6.04235700	3.91980600
H	4.61141400	6.28094500	3.99211000
C	-4.32843400	7.44383500	5.95873100
H	-5.31968000	7.83894600	5.76355700
C	1.69755700	9.33911700	4.09837100
H	1.83873900	10.40965400	4.19351600
C	-2.24444600	7.18114800	-0.03436200
H	-1.81734500	7.05526100	-1.02450600
C	-2.61812000	6.56863200	7.41229800
H	-2.29055000	6.27965900	8.40619900
B	-1.16579000	6.59962900	3.72982300

10 -symmetrical

C	-0.76091800	0.88728300	3.70566900
C	-1.42660600	0.70455100	2.49590000
C	-0.73346600	0.36856300	1.31486300
C	0.67194700	0.25148700	1.34392100
C	1.29197100	0.43893300	2.58550300
C	0.63104200	0.75362400	3.76031300
C	0.70560900	-0.31415600	-1.32165500
C	-0.69980400	-0.19708100	-1.35071300
C	-1.31982900	-0.38452800	-2.59229500
C	-0.65890000	-0.69922000	-3.76710400
C	0.73306100	-0.83287800	-3.71246000
C	1.39874800	-0.65014600	-2.50269200
H	-1.31475600	1.12988200	4.60785300
H	-2.50820400	0.81409600	2.47556900
H	1.19053800	0.89768500	4.67844400
H	-1.21839600	-0.84328200	-4.68523500
H	1.28689800	-1.07547800	-4.61464400
H	2.48034700	-0.75969000	-2.48236100
B	1.56157800	-0.09317500	0.03705100
B	-1.58943600	0.14758200	-0.04384300
O	2.33121200	-1.34329300	0.29676800
F	2.65927500	0.33855900	2.64655700
F	-2.68713300	-0.28415500	-2.65334800
C	-4.00668600	-0.87409800	0.17422500
C	-2.14755000	-2.27957300	0.45587700
C	-4.53525400	0.42540300	-0.09319300
C	-4.89002800	-1.97031600	0.40362500
C	-2.95642600	-3.39296800	0.68605500
H	-1.06618200	-2.34913500	0.46672500
C	-5.94319900	0.61848600	-0.12992000
C	-6.30402000	-1.74335400	0.36218200
C	-4.33214600	-3.23741600	0.66007100
H	-2.49585800	-4.35436500	0.88029900
C	-6.45698800	1.90797600	-0.40086900
C	-6.80811700	-0.50110800	0.10629100
C	-4.21144700	2.80359900	-0.59913500

H	-6.96748400	-2.58443100	0.53813400
H	-4.98914400	-4.08436200	0.83524400
C	-5.59403700	2.97889800	-0.63139800
H	-7.53194300	2.05476700	-0.42935300
H	-7.88174600	-0.34228300	0.07596000
H	-3.52902700	3.62704400	-0.77826400
H	-6.00247000	3.96262700	-0.83967400
C	3.63949600	-1.47822700	0.32499300
C	4.50739600	-0.37099300	0.08640000
C	4.18359200	-2.74918900	0.59234200
C	3.97882800	0.92850700	-0.18101700
C	5.91534200	-0.56407500	0.12312600
C	5.56618200	-2.92448700	0.62460500
H	3.50117300	-3.57263500	0.77147200
C	4.86216800	2.02472700	-0.41041900
C	6.78025900	0.55552000	-0.11308500
C	6.42913200	-1.85356400	0.39407500
H	5.97461500	-3.90821600	0.83288100
C	4.30428500	3.29182600	-0.66686500
C	6.27616100	1.79776600	-0.36897600
C	2.11969000	2.33398100	-0.46267000
H	7.85388800	0.39669600	-0.08275400
H	7.50408700	-2.00035400	0.42255900
C	2.92856600	3.44737600	-0.69284700
H	4.96128200	4.13877200	-0.84203700
H	6.93962400	2.63884300	-0.54492800
H	1.03832200	2.40354200	-0.47351700
H	2.46799600	4.40877300	-0.88709200
N	2.62336200	1.11748800	-0.21529400
N	-2.65122100	-1.06308000	0.20850200
C	-3.66735300	1.53263600	-0.33178500
O	-2.35906900	1.39770100	-0.30356000

Cartesian coordinates for ground state optimized geometry of the anionic species (UB3LYP/6-31+g(d,p))

1 -bent

O	8.87315500	3.81991100	1.73663500
N	8.36474700	1.79503800	0.55556200
O	5.79745500	-0.45169500	2.22106300
N	4.86426400	0.26947400	4.30041800
C	5.44081500	2.12509500	2.46939200
C	6.39730400	2.99168900	1.88508800
C	9.29196900	2.54361900	-0.10577100
C	8.37208200	1.72051400	3.21303800
C	8.50902100	0.19103200	-1.19123200
H	8.16824800	-0.75822700	-1.59222300
C	9.89000600	2.18896900	-1.33253800
C	9.45950600	0.94717900	-1.88020500
H	9.86790500	0.59480200	-2.82339500
C	7.42183400	0.84968600	3.80118200
C	5.96087900	4.16919600	1.25177700

C	9.57397000	3.72964100	0.60953800
C	10.50476500	4.61802200	0.07713800
H	10.75098100	5.54000700	0.59326500
C	9.67186700	1.78022400	3.74696400
H	10.39442900	2.46560400	3.30821700
B	7.95909600	2.60032500	1.92864200
C	7.82440000	0.06311100	4.89710100
C	3.48126000	0.14671800	6.24335600
H	3.15837700	0.61238600	7.17006600
C	4.34868000	-0.94207700	3.90903900
C	4.60556700	4.50264100	1.17924400
H	4.29228200	5.42364200	0.69056700
C	3.38971300	-1.68382600	4.62808800
C	4.91303100	-1.34383600	2.68440900
C	3.65697500	3.64474500	1.74412300
H	2.59712000	3.88843500	1.69497700
C	9.12044300	0.12704100	5.41676400
H	9.39985500	-0.49173700	6.26772500
C	7.96793700	0.62651900	0.02849800
H	7.22844100	0.05858800	0.58429500
C	4.07993200	2.47407000	2.38009900
H	3.33158300	1.82084000	2.82507400
C	10.05122700	0.99664700	4.84030500
H	11.06105700	1.06578800	5.24112600
C	11.11841300	4.28214600	-1.15487700
H	11.84538900	4.97642100	-1.57012600
C	2.94396100	-1.09605500	5.85468600
H	2.20621100	-1.60007200	6.47178400
B	5.91427800	0.75924200	3.20699300
C	4.42802800	0.81214100	5.46958700
H	4.85226900	1.76807400	5.75247200
C	3.54913100	-3.32137800	2.82403800
H	3.22984800	-4.26817300	2.39386000
C	10.83743000	3.11258900	-1.85594200
H	11.33569700	2.90084600	-2.79777300
C	4.50986800	-2.55687600	2.12436700
H	4.92293300	-2.89981100	1.18112900
C	2.99402200	-2.91505700	4.03966100
H	2.25763200	-3.53819600	4.54059400
H	6.69810900	4.84495600	0.82261900
H	7.10686900	-0.61005300	5.36264700

2-bent

O	8.86479000	3.81452200	1.79201400
N	8.39812400	1.82171300	0.54827000
O	5.76040300	-0.50188600	2.25561700
N	4.87560900	0.27456700	4.33591700
C	5.44171700	2.06982900	2.47455400
C	6.37564800	2.93288300	1.84468200
C	9.33373900	2.59434500	-0.07467100
C	8.37434600	1.69980500	3.19515400

C	8.59738900	0.25499800	-1.22649200
H	8.27642200	-0.68876200	-1.65597400
C	9.96376800	2.27059000	-1.29335300
C	9.55819700	1.03533700	-1.87712500
H	9.99168800	0.70631400	-2.81741600
C	7.45538300	0.78151400	3.76377000
C	5.84734400	4.01931300	1.14302000
C	9.58603200	3.76488600	0.67397100
C	10.51966100	4.67402500	0.18525500
H	10.73950400	5.58900500	0.72495100
C	9.68690600	1.78349800	3.69575000
H	10.37073600	2.50914600	3.26424600
B	7.95578900	2.59473400	1.91557000
C	7.95732800	-0.03419900	4.78169800
C	3.51270700	0.22910100	6.29243100
H	3.22444700	0.71366200	7.22065300
C	4.30197200	-0.91177700	3.95765600
C	4.49535700	4.32997000	1.06170400
H	4.17615500	5.20459300	0.50295300
C	3.31520700	-1.60146000	4.68941100
C	4.83442800	-1.34719600	2.73030800
C	3.59151900	3.48211800	1.70464400
H	2.52481900	3.69096100	1.66031600
C	9.24834100	0.03003200	5.29232400
H	9.54413300	-0.64089700	6.09320000
C	8.02326000	0.65866600	-0.01317500
H	7.27669100	0.07267700	0.51325200
C	4.06679400	2.36446800	2.39217300
H	3.35019100	1.70643700	2.87637100
C	10.12398100	0.96741400	4.74017600
H	11.13988800	1.05098600	5.12039200
C	11.16586200	4.37162500	-1.03832400
H	11.89398800	5.08282800	-1.42169600
C	2.91190400	-0.98506600	5.91515500
H	2.15825000	-1.45009500	6.54364900
B	5.92603200	0.70538000	3.22044400
C	4.48253300	0.84359300	5.50290700
H	4.95633500	1.77891800	5.77656600
C	3.37493100	-3.25211400	2.89308600
H	3.00570300	-4.18389500	2.47041200
C	10.91377500	3.21459500	-1.77209700
H	11.43623900	3.02983900	-2.70653500
C	4.36595900	-2.53887200	2.17972600
H	4.75269500	-2.90661100	1.23480200
C	2.85239000	-2.81424400	4.11112500
H	2.09146300	-3.39808900	4.62236300
F	6.69122000	4.86103400	0.45395800
F	7.14465400	-0.99213500	5.34649000

3-bent

Cl	6.64485400	5.17725800	0.16699500

Cl	7.26124200	-1.48367800	5.38230000
O	8.80441900	3.85872000	1.75512300
N	8.35763700	1.83949200	0.54916000
O	5.79341400	-0.52349500	2.25254300
N	4.94595000	0.24029700	4.35075000
C	5.44101200	2.03641900	2.49718500
C	6.31054500	2.94877700	1.83575500
C	9.34192100	2.57193900	-0.04634800
C	8.36528500	1.76965100	3.18464300
C	8.60153800	0.22448900	-1.17648100
H	8.27770600	-0.72217600	-1.59711800
C	10.02069200	2.20229800	-1.22491300
C	9.61103700	0.96411400	-1.79830900
H	10.07977600	0.60135200	-2.70879900
C	7.52590300	0.76398500	3.73692400
C	5.70195500	4.01117100	1.14510200
C	9.58723100	3.75569100	0.68220300
C	10.56469800	4.62937800	0.21763200
H	10.77911500	5.55397700	0.74284000
C	9.67042100	1.95185400	3.67447000
H	10.28378800	2.74530800	3.25866700
B	7.90046200	2.64166800	1.89851500
C	8.11756800	-0.06601500	4.70621900
C	3.56735200	0.22119500	6.29702300
H	3.30307100	0.69431300	7.23816100
C	4.29929100	-0.89467700	3.93156200
C	4.32523300	4.23782000	1.12566700
H	3.92372300	5.08766900	0.58333000
C	3.26909500	-1.54519900	4.63801600
C	4.81034900	-1.32337200	2.69388600
C	3.49226200	3.34883100	1.80058200
H	2.41546900	3.50343500	1.79711700
C	9.41326600	0.10693400	5.19600900
H	9.79900000	-0.56594400	5.95506500
C	7.98172600	0.67199300	-0.00096600
H	7.20324000	0.11149400	0.50648300
C	4.05159000	2.25853700	2.46406900
H	3.38630000	1.56509200	2.96941900
C	10.18992300	1.14523900	4.68563300
H	11.19724400	1.30623800	5.06388000
C	11.26248600	4.27913700	-0.96476200
H	12.02602400	4.96227000	-1.32955600
C	2.89733600	-0.94359800	5.88148000
H	2.11381600	-1.38115000	6.49284800
B	5.98264300	0.67126800	3.22265200
C	4.57614000	0.80032400	5.53069100
H	5.10179200	1.69796400	5.83395200
C	3.23832500	-3.13998600	2.79093600
H	2.81524600	-4.03373400	2.33783300
C	11.01657800	3.11008400	-1.68024000

H	11.57842300	2.88797500	-2.58310000
C	4.27495400	-2.46666800	2.10424500
H	4.64517600	-2.82839200	1.15047200
C	2.73642200	-2.70860600	4.01998500
H	1.93783600	-3.25996200	4.50937100

4-bent

O	8.83561700	3.84709900	1.77976600
N	8.35069200	1.84591500	0.55998800
O	5.83190200	-0.56663500	2.26775100
N	4.96405200	0.23830100	4.34077400
C	5.46552100	1.99745900	2.46277600
C	6.33190800	2.95459500	1.86270600
C	9.33228200	2.57557000	-0.04380900
C	8.38548900	1.76188600	3.20115700
C	8.54571600	0.25258500	-1.19206200
H	8.20590800	-0.68626300	-1.61755400
C	9.97992300	2.21826300	-1.24312700
C	9.55566300	0.98659800	-1.81927600
H	10.00744000	0.62897600	-2.74027400
C	7.54549000	0.75448000	3.74949600
C	5.71696300	4.02730900	1.19786600
C	9.60119800	3.74778700	0.69378300
C	10.57927600	4.61698400	0.22391200
H	10.81199700	5.53249100	0.75708600
C	9.68732900	1.95034700	3.69650400
H	10.30076500	2.74199500	3.27770500
B	7.92040400	2.64258100	1.92379600
C	8.13238900	-0.06301800	4.72926300
C	3.57848400	0.25140800	6.28130800
H	3.31678100	0.73377000	7.21837700
C	4.30647900	-0.89164700	3.92698100
C	4.33641500	4.21005600	1.12484200
H	3.92542900	5.07290800	0.61189000
C	3.26384600	-1.52163600	4.63216600
C	4.82878100	-1.34530300	2.70360300
C	3.50524400	3.26294100	1.71832300
H	2.42492500	3.38022300	1.66696400
C	9.42278900	0.11590700	5.22867000
H	9.80643600	-0.54451200	5.99897300
C	7.95066700	0.69134000	-0.00051400
H	7.17318100	0.13256700	0.51014700
C	4.07178300	2.17088900	2.37071200
H	3.41024200	1.43853800	2.82354800
C	10.20305700	1.14868300	4.71288200
H	11.20805400	1.31253900	5.09625200
C	11.25487400	4.27388800	-0.97338300
H	12.02176000	4.95181600	-1.34069400
C	2.88888800	-0.90183200	5.86554300
H	2.09011000	-1.31936100	6.47116500
B	6.01021300	0.64741800	3.21488500

C	4.60703800	0.80301700	5.52172800
H	5.14618100	1.69299600	5.82438000
C	3.22033800	-3.12969300	2.79726800
H	2.78427800	-4.01795900	2.34577600
C	10.98199400	3.11817900	-1.70031400
H	11.52686900	2.90091000	-2.61468700
C	4.28100900	-2.48494800	2.11943200
H	4.65742700	-2.86428300	1.17496900
C	2.71152700	-2.67675900	4.01561100
H	1.89640800	-3.20769000	4.50024000
Br	6.72709200	5.43196000	0.30727400
Br	7.20198900	-1.58486200	5.49987200

4-symmetrical

C	-1.03220200	-3.73929300	0.29503000
C	-1.55600700	-2.45520100	0.38769100
C	-0.76496600	-1.30589900	0.18843300
C	0.61404500	-1.44494800	-0.11733300
C	1.10172500	-2.76412800	-0.18327300
C	0.32221800	-3.90167000	0.00460100
C	0.76473200	1.30583300	-0.18858900
C	-0.61427900	1.44488200	0.11717600
C	-1.10195700	2.76406400	0.18312200
C	-0.32244800	3.90160500	-0.00474400
C	1.03197200	3.73922800	-0.29517300
C	1.55577500	2.45513500	-0.38783900
H	-1.66384400	-4.61147200	0.44928100
H	-2.61060300	-2.34545600	0.62316500
H	0.76457800	-4.88917100	-0.07152900
H	-0.76480600	4.88910700	0.07139000
H	1.66361600	4.61140600	-0.44941700
H	2.61037100	2.34539000	-0.62331200
B	1.52493500	-0.12601300	-0.36030100
B	-1.52517100	0.12594700	0.36013700
O	2.22225000	-0.13626600	-1.73426200
O	-2.22250000	0.13619900	1.73409100
C	-3.54131200	-0.01861500	1.59178200
C	-3.93055000	-0.03778900	0.23712500
C	-4.52468200	-0.16084900	2.56723200
C	-5.25861400	-0.15708000	-0.21404800
C	-5.86648100	-0.30610500	2.14042000
H	-4.26792800	-0.14994300	3.62126000
C	-3.02231100	0.15940300	-1.90997200
C	-5.42997600	-0.13839200	-1.63152800
C	-6.24415500	-0.31530800	0.79788300
H	-6.63644300	-0.42231000	2.89980700
C	-4.30330000	0.01964200	-2.45047400
H	-2.13787100	0.29124400	-2.52260700
H	-6.41999200	-0.24127900	-2.06611400
H	-7.28870200	-0.42964900	0.52134400
H	-4.41217600	0.04792200	-3.53026500

C	3.54106400	0.01853800	-1.59196600
C	3.93031600	0.03771200	-0.23731200
C	4.52442600	0.16076700	-2.56742500
C	5.25838500	0.15699700	0.21384700
C	5.86623000	0.30601400	-2.14062700
H	4.26766100	0.14986100	-3.62145100
C	3.02209700	-0.15947200	1.90979400
C	5.42976100	0.13831000	1.63132600
C	6.24391700	0.31521700	-0.79809400
H	6.63618600	0.42221400	-2.90002100
C	4.30309200	-0.01971600	2.45028300
H	2.13766200	-0.29130700	2.52243700
H	6.41978100	0.24119200	2.06590200
H	7.28846700	0.42955200	-0.52156500
H	4.41197800	-0.04799500	3.53007300
N	2.84000500	-0.11092600	0.57406700
N	-2.84023200	0.11085600	-0.57424400
Br	2.96688400	-3.15005100	-0.56327400
Br	-2.96711500	3.14999000	0.56312400

5-bent

F	9.37435900	9.07395100	3.27678800
F	10.61780100	11.24926900	4.34583000
O	11.38061600	4.87399400	5.44383900
O	12.48038300	8.63737800	8.97116500
F	17.03589600	5.34694800	8.64185000
N	14.23409000	9.58716200	7.65646700
N	10.63507900	5.62849000	7.59437700
F	15.75639700	3.20494800	7.54839600
C	10.53000600	7.63157900	4.79260100
H	10.02828600	6.78200500	4.33752000
C	13.03028100	9.69086500	9.59491000
C	14.06614800	10.26724100	8.83938900
C	9.92439500	4.54567100	7.16799400
C	8.58070300	4.52567400	9.14766600
H	7.78906000	4.11800000	9.76999200
C	8.87852000	3.93281700	7.88787000
C	13.22757400	5.82040600	7.02755700
C	10.38004700	4.11926900	5.90130600
C	9.31661000	5.63384700	9.57117200
H	9.10442500	6.09956200	10.52813500
C	11.45182900	7.45343100	5.83899100
C	10.34366200	6.17761600	8.78409900
H	10.93046600	7.03814300	9.08971300
C	12.11215800	8.57952100	6.38854400
C	10.26004900	8.90019800	4.30214700
C	13.89429200	6.94052700	7.58160200
C	10.89692900	10.00921500	4.84537200
C	11.81327800	9.85521100	5.87529700
H	12.29721200	10.74716300	6.26427100
C	14.82218900	11.38541000	9.24367600

C	8.26454500	2.81162300	7.26370400
H	7.45201400	2.29248000	7.76374900
B	11.73864900	5.98417600	6.43442100
C	13.86314200	4.56642300	7.02340600
H	13.38323100	3.69680500	6.58290300
C	12.71048400	10.24611500	10.83321800
H	11.91701900	9.82831100	11.44436400
C	13.45286900	11.36899200	11.26450800
H	13.21007400	11.80852800	12.22921300
C	14.48045900	11.93567100	10.50789700
H	15.02303000	12.79964100	10.88229500
C	15.17849500	6.76038300	8.12795500
H	15.72863000	7.59141600	8.56134300
C	8.71078400	2.38842900	6.01523800
H	8.22969900	1.52971200	5.55324800
C	9.76496600	3.02082100	5.31000100
H	10.08430600	2.66071200	4.33782800
C	15.13202700	4.41983600	7.56306800
C	15.20071600	10.01218300	6.79579000
H	15.31104300	9.45826700	5.87121600
B	13.17999200	8.39911800	7.59906900
C	15.78575800	5.51326800	8.11775600
C	15.83228600	11.81549100	8.32527800
H	16.46094100	12.66958800	8.55746200
C	15.99351200	11.11027500	7.11761500
H	16.75344300	11.41874000	6.40579200

6 -bent

O	8.86305700	3.81201700	1.79928300
N	8.40438300	1.82347400	0.54611000
O	5.75387700	-0.50838300	2.25581300
N	4.87437500	0.27545500	4.33533600
C	5.44109300	2.06410800	2.46797200
C	6.37667300	2.92617300	1.84014000
C	9.33618300	2.60154600	-0.07309700
C	8.37387300	1.69142200	3.19298100
C	8.60399100	0.26094000	-1.23014500
H	8.28603400	-0.68225000	-1.66239500
C	9.96243300	2.27569600	-1.29534500
C	9.56200100	1.04286200	-1.88270600
H	9.99613500	0.72066000	-2.82224200
C	7.45316100	0.77362600	3.75848700
C	5.85090200	4.01077200	1.13376500
C	9.58272100	3.76954000	0.68192000
C	10.51148000	4.68451800	0.19661100
H	10.73043400	5.59932300	0.73596400
C	9.68663400	1.76978400	3.69356300
H	10.37290700	2.49498800	3.26527700
B	7.95617100	2.59089400	1.91765500
C	7.95266300	-0.04744200	4.77324300
C	3.52270200	0.24735100	6.29675400

H	3.23840100	0.73663900	7.22325700
C	4.29982000	-0.91035100	3.96382800
C	4.49932900	4.32082700	1.04697500
H	4.18167700	5.19380600	0.48501900
C	3.31331600	-1.58926700	4.71051900
C	4.82991800	-1.34976600	2.73649900
C	3.59359500	3.47417100	1.68859900
H	2.52717600	3.68251900	1.63993600
C	9.24359100	0.01161700	5.28400500
H	9.53794200	-0.66280700	6.08230900
C	8.03095500	0.66065000	-0.01654300
H	7.28605300	0.07310600	0.51033600
C	4.06644900	2.35782800	2.37985000
H	3.34740200	1.70092300	2.86199800
C	10.12143600	0.94862700	4.73491700
H	11.13748700	1.02803200	5.11511000
C	11.16108900	4.39604300	-1.02629400
H	11.88638900	5.10267400	-1.41697700
C	2.91619100	-0.96750200	5.93205800
H	2.16571700	-1.42815800	6.56312200
B	5.92505200	0.70204000	3.21532900
C	4.48931100	0.85391400	5.49962200
H	4.96760400	1.78970100	5.76312900
C	3.37070900	-3.25624200	2.90603900
H	2.99176700	-4.18857000	2.49987900
C	10.90261000	3.23847100	-1.74998300
C	4.35927700	-2.54303300	2.19313000
H	4.73985500	-2.91925900	1.24966700
C	2.86448600	-2.79860600	4.11948800
F	6.69808200	4.84945800	0.44586400
F	7.13609600	-1.00443400	5.33346100
Cl	11.76182700	2.95495800	-3.27303100
Cl	1.62146400	-3.75460100	4.95007800

7 -bent

O	8.87794700	3.80901800	1.79473400
N	8.39379300	1.81175600	0.56205000
O	5.78530600	-0.46302800	2.25768500
N	4.86664700	0.27472800	4.33671700
C	5.44614900	2.10057400	2.50639700
C	6.38522400	2.94410100	1.85935700
C	9.32007200	2.57943500	-0.07646000
C	8.37876900	1.70938400	3.21651200
C	8.55783200	0.23269500	-1.20380000
H	8.22649000	-0.71199400	-1.62136600
C	9.92477800	2.23761500	-1.30412400
C	9.50875400	1.00355800	-1.87463700
H	9.92781400	0.67231700	-2.81790200
C	7.45230200	0.80724300	3.79815900
C	5.86696600	4.02461100	1.14219400
C	9.57730500	3.75003800	0.67450200

C	10.51114000	4.63962600	0.15308400
C	9.69257100	1.78773900	3.71330000
H	10.38320600	2.50279100	3.27535200
B	7.95882400	2.59299800	1.93353900
C	7.94756100	-0.00030700	4.82547200
C	3.48952300	0.19900600	6.28146000
H	3.18684600	0.66962900	7.21169100
C	4.31233200	-0.91339600	3.94030200
C	4.51893600	4.35266600	1.06836500
H	4.20616100	5.22191700	0.49818900
C	3.32580400	-1.61508600	4.66409800
C	4.87056900	-1.31843300	2.71314000
C	3.61024500	3.52787800	1.73347100
H	2.54653400	3.75123400	1.69588400
C	9.23964900	0.05957000	5.33339200
H	9.53070500	-0.60312600	6.14255200
C	8.00562500	0.64768600	0.01572900
H	7.26430500	0.06817100	0.55671800
C	4.07516700	2.41216700	2.43168400
H	3.35293200	1.77025100	2.92877300
C	10.12286700	0.98113200	4.76792900
H	11.13943900	1.06106300	5.14608100
C	11.14622000	4.34845900	-1.07580400
H	11.86912400	5.05412900	-1.46840600
C	2.90313500	-1.01865600	5.88984100
H	2.15079200	-1.49963700	6.50288300
B	5.92801100	0.73592500	3.24699200
C	4.45727300	0.82967500	5.50808100
H	4.92101000	1.76651000	5.79232600
C	3.42480600	-3.25922800	2.83677900
H	3.07353200	-4.18700200	2.40097000
C	10.86532400	3.18865600	-1.78328100
C	4.41040800	-2.51192700	2.16190100
C	2.90089100	-2.82117400	4.04979200
F	6.71861900	4.83657200	0.42899300
F	7.12657100	-0.94319200	5.40188400
Cl	11.69811300	2.89052400	-3.31285100
Cl	1.66295400	-3.80671600	4.84502100
Cl	5.05227800	-3.09273100	0.63182200
Cl	10.91126000	6.11695800	1.00609000

8 -symmetrical

S	-0.35934000	6.33809600	1.93468100
O	-0.77078100	9.67274500	2.48084500
N	-2.82938800	8.55537700	2.96134800
C	-0.57182100	7.23184000	3.43456000
C	-2.95665800	9.39727400	1.89296300
C	0.44478500	5.22843700	4.10740400
H	0.86759500	4.51164200	4.80587400
C	-0.09113900	6.50390800	4.50574900
B	-1.30614400	8.65765300	3.50859200

C	-4.14222700	9.59315200	1.15599000
C	-1.73093000	10.04443100	1.63074800
C	-3.90168500	7.84283500	3.36423500
H	-3.76036300	7.18605800	4.21481200
C	-1.67052400	10.94707100	0.57088200
H	-0.74727800	11.46526700	0.33369400
C	0.37008100	4.99341400	2.76041100
H	0.70406600	4.12242200	2.21048100
C	-5.12060100	7.97095900	2.69342800
H	-5.96419200	7.38318300	3.04214900
C	-5.26732600	8.83251100	1.59556300
H	-6.22222400	8.91983600	1.08541100
C	-4.05578500	10.51853900	0.07997600
H	-4.93129900	10.71906300	-0.53156800
C	-2.84752400	11.16293100	-0.18525900
H	-2.80307700	11.86633400	-1.01373300
S	-1.03197400	9.40246000	7.58089400
O	-0.62052900	6.06780900	7.03473300
N	1.43807400	7.18518300	6.55422300
C	-0.81949900	8.50871300	6.08101600
C	1.56534900	6.34328800	7.62260800
C	-1.83610900	10.51211500	5.40817300
H	-2.25892200	11.22890800	4.70970400
C	-1.30018000	9.23664600	5.00982700
B	-0.08517200	7.08290200	6.00698300
C	2.75092100	6.14741500	8.35957800
C	0.33962400	5.69612700	7.88482800
C	2.51036800	7.89772800	6.15133200
H	2.36904000	8.55450400	5.30075500
C	0.27922500	4.79348800	8.94469500
H	-0.64401900	4.27529000	9.18188700
C	-1.76141000	10.74713500	6.75516700
H	-2.09540100	11.61812400	7.30509700
C	3.72928600	7.76960800	6.82213600
H	4.57287400	8.35738700	6.47341100
C	3.87601700	6.90805800	7.92000100
H	4.83091700	6.82073600	8.43015000
C	2.66448500	5.22202800	9.43559300
H	3.54000200	5.02150700	10.04713400
C	1.45622700	4.57763200	9.70083200
H	1.41178500	3.87423000	10.52930700

9

C	-2.14589000	6.82715200	5.01846200
O	-4.09211000	7.41392800	3.64995000
C	1.23299300	6.65602700	3.85435200
C	2.58753100	7.02738500	3.95260100
C	-2.01479400	7.04229200	2.40437800
C	-3.49866300	7.16499400	4.87227700
O	-0.56704400	5.27269900	3.65064200
C	0.77947300	5.33717800	3.72326200

C	-3.37813000	7.36270900	2.46849800
C	3.07471400	4.63227200	3.78004500
H	3.81218000	3.83250400	3.75119200
C	-3.89353900	7.05361700	7.25201600
H	-4.56656200	7.14149700	8.10194900
C	1.70762700	4.29378500	3.68387000
H	1.38421200	3.26236900	3.58293200
C	-4.14037900	7.66167300	1.32782200
H	-5.19357100	7.90118600	1.44587300
C	2.84413700	8.43562400	4.08123100
H	3.85992700	8.81036900	4.16277400
C	-1.44184300	7.03855800	1.11833000
H	-0.38512100	6.79574200	1.03056300
C	0.42883800	8.87338800	3.99652200
H	-0.42400900	9.54231700	4.00895100
N	0.16208200	7.52910900	3.87266500
C	-1.70363900	6.60880100	6.33714500
H	-0.65896500	6.34607100	6.48868200
C	-3.53360100	7.64424000	0.07516000
H	-4.11952300	7.87502100	-0.81169200
C	3.51761300	5.95434900	3.91087100
H	4.58222600	6.16611500	3.98150700
C	-4.37289500	7.28026800	5.96496700
H	-5.41102900	7.54457900	5.78348500
C	1.73606500	9.32012600	4.09857900
H	1.90257300	10.39021800	4.19486100
C	-2.17141300	7.33045100	-0.03451700
H	-1.68909300	7.31547000	-1.00899400
C	-2.54653800	6.71473800	7.44386100
H	-2.16342300	6.53687200	8.44588300
B	-1.17074700	6.68356800	3.73637300

10-symmetrical

C	-0.83099300	0.91642600	3.69239900
C	-1.46603800	0.72066100	2.46782300
C	-0.75136900	0.38357900	1.29857500
C	0.65606500	0.24415000	1.36284000
C	1.24312800	0.45446500	2.61554600
C	0.55912400	0.77960800	3.77681200
C	0.72351100	-0.32917200	-1.30536700
C	-0.68392200	-0.18974200	-1.36963300
C	-1.27098600	-0.40006100	-2.62233800
C	-0.58698200	-0.72520500	-3.78360400
C	0.80313400	-0.86202100	-3.69919100
C	1.43818100	-0.66625500	-2.47461500
H	-1.40545000	1.17502000	4.57922900
H	-2.54675600	0.83586000	2.41664800
H	1.10283500	0.92242000	4.70572700
H	-1.13069400	-0.86802000	-4.71251800
H	1.37759200	-1.12061700	-4.58602000
H	2.51889900	-0.78145300	-2.42344000

B	1.56497200	-0.12428800	0.06952800
B	-1.59282900	0.17869600	-0.07632000
O	2.34127700	-1.37799300	0.34185700
F	2.61253600	0.34620400	2.72987600
F	-2.64039400	-0.29180300	-2.73666700
C	-4.00656500	-0.85071000	0.16256500
C	-2.12363300	-2.26348800	0.40925700
C	-4.55050800	0.44804400	-0.09271800
C	-4.87587400	-1.95420900	0.40849900
C	-2.91911700	-3.36884500	0.64986600
H	-1.04250700	-2.32372900	0.39986500
C	-5.96985800	0.64095500	-0.09920000
C	-6.28784400	-1.72616800	0.39564800
C	-4.30992400	-3.22891400	0.65390000
H	-2.44633300	-4.32802800	0.83314500
C	-6.49768300	1.92852700	-0.35543900
C	-6.81345200	-0.48369400	0.15337900
C	-4.24645100	2.81605400	-0.59767500
H	-6.94319900	-2.57332000	0.58437400
H	-4.96056200	-4.07843400	0.84051600
C	-5.63982000	2.99056900	-0.60005400
H	-7.57531700	2.06917000	-0.35939500
H	-7.89073600	-0.33578100	0.14797400
H	-3.57308700	3.64491900	-0.79034400
H	-6.04791900	3.97906600	-0.79821600
C	3.65909400	-1.50423400	0.34053700
C	4.52265100	-0.39363400	0.08592500
C	4.21859500	-2.76164400	0.59088400
C	3.97870700	0.90512000	-0.16935800
C	5.94200100	-0.58654400	0.09240800
C	5.61196500	-2.93615800	0.59326300
H	3.54523200	-3.59051000	0.78355200
C	4.84801500	2.00861900	-0.41529200
C	6.78559400	0.53810500	-0.16017200
C	6.46982700	-1.87411600	0.34864700
H	6.02006400	-3.92465500	0.79142500
C	4.28206400	3.28332400	-0.66069400
C	6.25998500	1.78057900	-0.40244200
C	2.09577400	2.31789600	-0.41605000
H	7.86287800	0.39019400	-0.15476700
H	7.54746000	-2.01475800	0.35260300
C	2.89125700	3.42325400	-0.65666000
H	4.93270200	4.13284400	-0.84731000
H	6.91534000	2.62773200	-0.59116800
H	1.01464800	2.37813700	-0.40665800
H	2.41847300	4.38243600	-0.83994000
N	2.61572100	1.08152700	-0.17738200
N	-2.64358000	-1.02711800	0.17058900
C	-3.68695100	1.55864400	-0.34732900
O	-2.36913400	1.43240100	-0.34865000

Cartesian coordinates for the first singlet excited state geometry optimization (RB3LYP/6-31+g(d,p))

1 -bent

O	8.91744006	3.78928196	1.64496890
N	8.32553247	1.73897402	0.56348932
O	5.85386414	-0.41154987	2.18082924
N	4.87319139	0.24018066	4.26156800
C	5.48109950	2.14543602	2.48071580
C	6.45298210	3.07791851	2.00640512
C	9.25195803	2.43352537	-0.15159558
C	8.34242740	1.86215680	3.27777448
C	8.38013756	0.06629347	-1.11863732
H	8.00233614	-0.88762348	-1.46885877
C	9.80323525	2.01222565	-1.37602169
C	9.32288336	0.76514868	-1.85418430
H	9.69447770	0.36307881	-2.79259285
C	7.42706831	0.89328225	3.79010595
C	6.07100607	4.37408210	1.59105414
C	9.58956822	3.64007805	0.50086889
C	10.52275421	4.47430985	-0.09013929
H	10.81135854	5.40980912	0.37592281
C	9.56246515	2.12760833	3.94077801
H	10.21146056	2.91747147	3.57654955
B	8.00064626	2.62702100	1.89633205
C	7.87182949	0.09384400	4.85693267
C	3.44993336	0.03098026	6.17778719
H	3.10077841	0.46237632	7.11048646
C	4.37833464	-0.98174526	3.82707297
C	4.72585776	4.70223462	1.48931021
H	4.42650178	5.67814455	1.11692906
C	3.42352983	-1.75293885	4.50814841
C	4.96029543	-1.34732619	2.61246613
C	3.74943147	3.75502793	1.85621661
H	2.69639597	4.01689561	1.79438491
C	9.11015934	0.30584514	5.46388546
H	9.41031404	-0.30292771	6.31275839
C	7.88304758	0.57047752	0.10426211
H	7.14227186	0.04146327	0.70081357
C	4.12919801	2.50199806	2.33839836
H	3.36253111	1.80617873	2.66428037
C	9.95787833	1.33592131	5.01050738
H	10.92028526	1.50009302	5.48748030
C	11.09240386	4.06803341	-1.32772988
H	11.82432750	4.72389735	-1.78987939
C	2.93825550	-1.21726982	5.74277410
H	2.19993032	-1.75202357	6.32870691
B	5.92509046	0.75121132	3.18701804
C	4.39291289	0.73467717	5.44953394
H	4.78548463	1.68845289	5.77955241
C	3.63873012	-3.34640710	2.66278946

H	3.34358702	-4.28530619	2.20258239
C	10.76081597	2.88368314	-1.96799636
H	11.22395389	2.61772577	-2.91254042
C	4.60036549	-2.54229192	2.00348368
H	5.03752657	-2.84993417	1.05940550
C	3.06141686	-2.97680231	3.87466525
H	2.32725365	-3.62360654	4.34669616
H	6.83181074	5.09195070	1.30197423
H	7.21193545	-0.67069724	5.25463798

2 -symmetrical

O	8.56962408	3.63326796	1.98844723
N	8.61753879	1.93819458	0.28881297
O	5.28080086	-0.92792127	2.45318386
N	4.86586428	0.38855590	4.39619159
C	5.33781991	1.63783560	2.10453746
C	6.28985458	2.46676698	1.46423396
C	9.48983905	2.93962162	0.02071551
C	8.29707671	1.20158680	2.81389861
C	9.30157775	0.87040758	-1.71653069
H	9.19486932	0.02434895	-2.38639285
C	10.32596934	2.98991829	-1.11506067
C	10.19887349	1.88845439	-2.00137335
H	10.80394737	1.84532468	-2.90284688
C	7.35191015	0.32601013	3.40036966
C	5.78261217	3.44044553	0.59756896
C	9.44212673	3.92940869	1.03421114
C	10.27893661	5.02767391	0.90601575
H	10.27972357	5.81620924	1.65015017
C	9.65488837	1.09556505	3.17322634
H	10.37720382	1.78703276	2.74691586
B	7.86974069	2.30350223	1.71880337
C	7.85889712	-0.63553866	4.28275250
C	3.82806281	0.88059651	6.50460404
H	3.74313110	1.56591921	7.34186708
C	4.11361703	-0.76676695	4.38651358
C	4.43663329	3.65589107	0.34241625
H	4.13432557	4.43988087	-0.34418060
C	3.22216562	-1.16501180	5.35193941
C	4.40002402	-1.51231543	3.21285307
C	3.51204094	2.83427179	0.99234112
H	2.44822466	2.97484044	0.82090827
C	9.19183915	-0.76408486	4.63957494
H	9.49385844	-1.53654317	5.33922774
C	8.50915132	0.91499012	-0.54960969
H	7.79771793	0.13721248	-0.29446499
C	3.96516673	1.83861466	1.85573884
H	3.23209278	1.21055009	2.35588622
C	10.10396981	0.13078025	4.07376742
H	11.15676456	0.06792585	4.33574946
C	11.12997127	5.09592640	-0.22890328

H	11.78101575	5.96096113	-0.32112916
C	3.04742521	-0.30437139	6.48629875
H	2.36530540	-0.54995791	7.28991496
B	5.77157766	0.45096738	3.10801452
C	4.70914687	1.21171334	5.49048237
H	5.30366923	2.11681282	5.50783714
C	2.82980583	-3.18277036	3.94294043
H	2.31131657	-4.12500127	3.79900501
C	11.17369685	4.12555939	-1.22102139
H	11.84269425	4.22908770	-2.06907132
C	3.74775652	-2.74847001	2.97681758
H	3.96456100	-3.32224748	2.08299667
C	2.56576264	-2.43001374	5.09348336
H	1.84884930	-2.80451270	5.81831635
F	6.66627620	4.24701346	-0.07805673
F	6.98703693	-1.53149782	4.85533808

3-bent

Cl	6.66392948	5.01986833	-0.00939012
Cl	7.17340335	-1.54394305	5.31048576
O	8.76024621	3.84355652	1.79386459
N	8.39406844	1.85776921	0.49434928
O	5.66445116	-0.53984066	2.30468572
N	4.90444623	0.31173165	4.39963665
C	5.40819090	2.02476756	2.45933941
C	6.29301314	2.89567596	1.76758759
C	9.37498527	2.62855967	-0.03537781
C	8.34302094	1.69373864	3.12559575
C	8.71097607	0.31991381	-1.28348802
H	8.41489393	-0.61201887	-1.75235260
C	10.09329688	2.31572220	-1.20862021
C	9.71736218	1.09830444	-1.83420098
H	10.21788827	0.77903618	-2.74422748
C	7.48412561	0.71696055	3.69638661
C	5.70097697	3.92412341	1.01006881
C	9.57559854	3.79220934	0.74681052
C	10.54759332	4.69086779	0.33725878
H	10.73490003	5.60113836	0.89568114
C	9.67048237	1.80968209	3.57282104
H	10.30523718	2.58647523	3.15899177
B	7.87828989	2.61569743	1.88094084
C	8.07167046	-0.16618572	4.62443291
C	3.56094708	0.30176592	6.38939557
H	3.31487141	0.79016464	7.32676154
C	4.24701003	-0.84676323	4.04393351
C	4.32508198	4.14758932	0.95773922
H	3.93336020	4.96668400	0.36432107
C	3.26947880	-1.48198799	4.77206015
C	4.74014581	-1.31619343	2.79934002
C	3.47650910	3.29881220	1.66483539
H	2.40224791	3.46110100	1.63958889

C	9.39068579	-0.05958747	5.06287764
H	9.77661151	-0.76177739	5.79395943
C	8.05201072	0.72150520	-0.10127796
H	7.26514488	0.13478110	0.36081769
C	4.01888414	2.24157119	2.39008199
H	3.34394431	1.58179898	2.92663334
C	10.19056075	0.95635882	4.54369328
H	11.21693151	1.06438865	4.88440180
C	11.28492519	4.39270421	-0.84005054
H	12.04416587	5.10327393	-1.15484475
C	2.88332234	-0.88835048	6.01968643
H	2.12330276	-1.33053845	6.65073773
B	5.92130113	0.72054293	3.27687427
C	4.53885645	0.88091687	5.60094640
H	5.05461046	1.78934675	5.88596978
C	3.22363961	-3.17747199	2.94822256
H	2.80320632	-4.09315425	2.54564908
C	11.08571559	3.25261363	-1.60618000
H	11.67557103	3.07503520	-2.49951398
C	4.22424601	-2.50732572	2.23180333
H	4.59892945	-2.87230185	1.28227054
C	2.75237826	-2.69418901	4.17517009
H	1.97785379	-3.24612435	4.69961655

4- bent

O	8.80140724	3.83494409	1.80305364
N	8.36742404	1.85784160	0.51116504
O	5.73324718	-0.54552471	2.31977478
N	4.91374662	0.30925043	4.39003731
C	5.43266795	2.01353995	2.45275396
C	6.31346719	2.92641969	1.81093592
C	9.35021757	2.61074857	-0.04104609
C	8.36504029	1.70932282	3.15308319
C	8.61276770	0.31906026	-1.27749439
H	8.28943346	-0.60725069	-1.73946932
C	10.03094912	2.28936883	-1.23380729
C	9.62387473	1.07654601	-1.84810616
H	10.09996475	0.74761609	-2.76772881
C	7.50417589	0.74612184	3.74433075
C	5.71453028	3.97172434	1.08543149
C	9.59218019	3.76783190	0.73792455
C	10.57540834	4.64516121	0.31111804
H	10.79545805	5.54836518	0.86904467
C	9.69407250	1.83171557	3.59266228
H	10.32949289	2.59557091	3.15694203
B	7.89646386	2.62927085	1.90993769
C	8.08810541	-0.10530233	4.70169530
C	3.54847379	0.27953379	6.36400694
H	3.29613409	0.75420806	7.30669641
C	4.26404371	-0.84676978	4.01542882
C	4.33512759	4.15623803	0.99639036

H	3.93287951	4.99212923	0.43500750
C	3.27058614	-1.48314286	4.72062170
C	4.79245705	-1.32038280	2.78780257
C	3.48961678	3.25088440	1.63338465
H	2.41221240	3.38035597	1.57358983
C	9.40778850	0.00822723	5.13572660
H	9.79427152	-0.66731357	5.89065263
C	7.98853930	0.73069918	-0.07992978
H	7.20015176	0.15848323	0.39720946
C	4.04007915	2.18711101	2.34099374
H	3.36931565	1.48976592	2.83349314
C	10.21351605	1.00035832	4.58218698
H	11.24174103	1.11099856	4.91663863
C	11.28173524	4.33431308	-0.88178878
H	12.05251874	5.02672810	-1.20866153
C	2.85902101	-0.89288907	5.96211901
H	2.07991857	-1.33252713	6.57135893
B	5.95095001	0.72316747	3.29075852
C	4.55080297	0.85321380	5.60333727
H	5.07604707	1.74796459	5.91357353
C	3.25328491	-3.16538474	2.88530169
H	2.83229172	-4.07274610	2.46487354
C	11.03872722	3.20265587	-1.64740031
H	11.60611810	3.01365970	-2.55287511
C	4.28334021	-2.50501349	2.20245127
H	4.68197771	-2.87133138	1.26323276
C	2.75231608	-2.68198475	4.10084557
H	1.95516661	-3.22600938	4.59902889
Br	6.73967523	5.30285449	0.12810844
Br	7.11358734	-1.55362539	5.53601258

4 - symmetrical

C	-1.00739340	-3.77670916	-0.29420458
C	-1.54206244	-2.49934017	-0.16941580
C	-0.73950478	-1.34468480	-0.24617929
C	0.65854636	-1.46905864	-0.45764478
C	1.15965205	-2.78156835	-0.54597570
C	0.36603572	-3.92429187	-0.47828355
C	0.77651777	1.28195038	-0.55167578
C	-0.61368750	1.40811230	-0.29116866
C	-1.12712165	2.72093000	-0.27141491
C	-0.36128212	3.86018564	-0.50312004
C	0.99691649	3.70944328	-0.77443375
C	1.54846479	2.43319550	-0.79647815
H	-1.64594184	-4.65476689	-0.24528407
H	-2.61382408	-2.40107929	-0.02282792
H	0.81382291	-4.90778958	-0.56733633
H	-0.81908135	4.84264957	-0.47642458
H	1.61209502	4.58460704	-0.96640560
H	2.60664604	2.33542459	-1.01972354
B	1.55700234	-0.13839845	-0.59405087

B	-1.48804695	0.07625600	-0.02638360
O	2.48499687	-0.14975395	-1.80723844
O	-1.93669996	0.06906223	1.52239070
C	-3.23024567	-0.02444920	1.62241110
C	-3.87257141	-0.04802513	0.35607793
C	-3.99662369	-0.11619909	2.81209557
C	-5.23240313	-0.12297403	0.18584721
C	-5.38618083	-0.22158110	2.67116528
H	-3.51052175	-0.10096724	3.78086085
C	-3.41383716	0.13481007	-1.93366424
C	-5.73395726	-0.11023747	-1.15914183
C	-5.99648689	-0.23203961	1.41004565
H	-6.00680644	-0.30044694	3.55768184
C	-4.77027716	0.04102497	-2.18846782
H	-2.68207787	0.25653582	-2.72272913
H	-6.79258165	-0.17710843	-1.37410998
H	-7.07751019	-0.31488348	1.34595994
H	-5.09357477	0.09258720	-3.22315522
C	3.75240194	0.01400340	-1.44823649
C	3.91284563	0.04976922	-0.04081554
C	4.88643046	0.15443094	-2.23240333
C	5.14885073	0.17602033	0.62527863
C	6.14007551	0.30348451	-1.58068884
H	4.82066353	0.13273481	-3.31438511
C	2.66258485	-0.13079381	1.90566197
C	5.07181254	0.15977899	2.04259447
C	6.29527683	0.32603467	-0.20135611
H	7.02339810	0.41276968	-2.20393046
C	3.84282726	0.01016549	2.66651113
H	1.68547132	-0.25724577	2.35907180
H	5.97608980	0.26344684	2.63596857
H	7.27772504	0.44149631	0.24462894
H	3.77063240	-0.01093596	3.74824218
N	2.71710054	-0.09261433	0.58085220
N	-2.93123993	0.06039373	-0.64526659
Br	3.04328134	-3.14630441	-0.78432177
Br	-2.99311335	3.10086861	0.08006348

6 - symmetrical

O	8.55060084	3.60925824	1.99898905
N	8.62524420	1.93768510	0.27685288
O	5.25216066	-0.95890052	2.45773131
N	4.86392806	0.38608431	4.38489897
C	5.33017211	1.60527980	2.07734213
C	6.28434421	2.43465005	1.44052387
C	9.49042480	2.94964689	0.02825193
C	8.28949170	1.16398598	2.78975329
C	9.32759674	0.89806495	-1.73571543
H	9.23169683	0.05965113	-2.41649892
C	10.33051510	3.01396674	-1.10477981
C	10.21923755	1.92430955	-2.00598339

H	10.83059491	1.90045718	-2.90175278
C	7.34076336	0.29246775	3.37684867
C	5.78127017	3.40488373	0.56761875
C	9.42564491	3.92426776	1.05585008
C	10.25334454	5.03112617	0.94709332
H	10.24575611	5.81216439	1.69859710
C	9.64848890	1.04611430	3.14093093
H	10.37461327	1.73280558	2.71304345
B	7.86164032	2.27670802	1.70741508
C	7.84530209	-0.67236965	4.25660114
C	3.85942283	0.92784375	6.49174698
H	3.78656895	1.62757743	7.31771861
C	4.10529356	-0.76590678	4.40094706
C	4.43708807	3.61738211	0.30234604
H	4.13779561	4.39896445	-0.38822984
C	3.22364922	-1.13377795	5.39135541
C	4.37840780	-1.52662965	3.23392789
C	3.50998896	2.79604402	0.94906764
H	2.44714580	2.93390513	0.76987146
C	9.17898701	-0.81234165	4.60614215
H	9.47870669	-1.58815507	5.30302600
C	8.52885624	0.92347472	-0.57338672
H	7.82138851	0.13827201	-0.33039390
C	3.95918300	1.80435155	1.81922096
H	3.22325907	1.17653303	2.31568759
C	10.09522813	0.07584707	4.03665346
H	11.14882142	0.00430376	4.29278705
C	11.11227926	5.12688173	-0.17753807
H	11.75973957	5.99345188	-0.26366141
C	3.07048429	-0.25405168	6.50667770
H	2.39866544	-0.47734564	7.32270839
B	5.76141275	0.42354335	3.08606070
C	4.72780718	1.23205756	5.46182885
H	5.32916010	2.13278344	5.45167897
C	2.81190536	-3.18256789	3.99540487
H	2.28286933	-4.12154221	3.87990550
C	11.16185590	4.16480376	-1.17359858
C	3.71825024	-2.76254792	3.02217192
H	3.91988491	-3.35295905	2.13609123
C	2.56535326	-2.40625545	5.14055352
F	6.66953825	4.21153507	-0.10289936
F	6.96865633	-1.56131074	4.83405163
Cl	12.25692213	4.36092422	-2.53601271
Cl	1.42854748	-2.99691482	6.30061537

7 -bent

O	8.92898478	3.77711727	1.71623113
N	8.32406374	1.72184412	0.62885789
O	5.93527352	-0.26241855	2.31129345
N	4.84294876	0.28522745	4.36812549
C	5.47403150	2.24303954	2.67447264

C	6.41597026	3.01334197	1.94295603
C	9.22002413	2.42664827	-0.08271439
C	8.41646852	1.77545776	3.30662408
C	8.36906530	0.07411552	-1.07413685
H	7.99907360	-0.87846593	-1.43402134
C	9.75046495	2.03732067	-1.31091884
C	9.29332501	0.79869946	-1.81644208
H	9.65726071	0.42324160	-2.76634350
C	7.46195522	0.96512241	3.97942820
C	5.93653709	4.07972228	1.18554938
C	9.54595022	3.64165038	0.61075802
C	10.48637594	4.52349789	-0.00091102
C	9.74970148	1.84328174	3.74645508
H	10.46682846	2.48235755	3.23805989
B	7.93994052	2.56399955	2.00687495
C	7.96105833	0.24374969	5.06713576
C	3.34072743	-0.01150579	6.20575693
H	2.95478073	0.36639730	7.14666624
C	4.37175882	-0.90488811	3.84806145
C	4.61204948	4.48737457	1.15309652
H	4.31818271	5.34231821	0.55353301
C	3.37664293	-1.69993319	4.44502399
C	5.02001541	-1.19926731	2.64515005
C	3.69837802	3.75094853	1.90957591
H	2.65034731	4.03817959	1.91311678
C	9.27267031	0.30251191	5.53132668
H	9.55827439	-0.28768268	6.39597334
C	7.88326424	0.55009500	0.15841216
H	7.15154523	0.01790062	0.77002006
C	4.12658715	2.64083165	2.64221546
H	3.39431382	2.06594549	3.19921928
C	10.17889808	1.12038873	4.86155891
H	11.20659752	1.19330292	5.20619440
C	11.03462486	4.16091859	-1.23721691
H	11.74634607	4.82766514	-1.70957668
C	2.83523209	-1.22574559	5.67969101
H	2.06899071	-1.78528782	6.19794980
B	5.94035585	0.86226026	3.39960620
C	4.31989497	0.71921226	5.56323679
H	4.71600782	1.64375809	5.96275335
C	3.67662625	-3.20415140	2.51133948
H	3.40038163	-4.11075165	1.98764214
C	10.69295713	2.96769485	-1.88332162
C	4.66522537	-2.36041067	1.97257808
C	3.05541653	-2.87561487	3.71342174
F	6.82272413	4.78873089	0.38807266
F	7.13646264	-0.60043545	5.75116599
Cl	11.42121006	2.60543040	-3.40175338
Cl	1.82004920	-3.96772282	4.34564492
Cl	5.44863397	-2.78205586	0.44762599

Cl	10.91593410	5.98940857	0.77216127

8-bent

S	0.65535316	7.30789316	1.53102602
O	-1.04740932	9.91437937	2.04009985
N	-2.58188366	8.48903530	3.18157507
C	0.03107221	7.81341035	3.06561625
C	-3.19046756	9.13018672	2.11173653
C	1.56113702	6.11391588	3.64982845
H	2.12190041	5.43439247	4.28327217
C	0.65472853	7.09252567	4.12707985
B	-1.08292743	8.98819449	3.22028567
C	-4.53624685	8.97821561	1.74003232
C	-2.28369491	9.95871958	1.45344499
C	-3.35264621	7.64773532	3.95023116
H	-2.86990007	7.16215869	4.78794264
C	-2.68962693	10.69747180	0.35023707
H	-2.00053986	11.34760492	-0.17791934
C	1.67025908	6.10185345	2.27292554
H	2.27649267	5.44041558	1.66663254
C	-4.68645692	7.44780886	3.64185473
H	-5.25786649	6.77354022	4.27218202
C	-5.31651902	8.08848588	2.54653037
H	-6.36368906	7.91509135	2.32734125
C	-4.94358450	9.73769151	0.60786227
H	-5.97132084	9.66894140	0.26221282
C	-4.03895145	10.56585889	-0.05586324
H	-4.37939590	11.13354489	-0.91754013
S	0.23439623	10.11499315	7.02120867
O	-0.71164509	6.59367075	6.29679711
N	1.59555219	7.15976209	6.62489675
C	-0.05240579	9.04515188	5.67367858
C	1.16619191	6.25774583	7.54456024
C	-0.79391200	11.12421504	4.87009414
H	-1.21021925	11.82609273	4.15736660
C	-0.64489305	9.73285150	4.59257278
B	0.33350220	7.49591445	5.64279150
C	1.97133666	5.71744352	8.57036549
C	-0.19689799	5.93748412	7.33377175
C	2.85313775	7.58966228	6.65827355
H	3.15156260	8.31291421	5.90786252
C	-0.78933703	5.02701608	8.19391252
H	-1.83031885	4.74752232	8.07861675
C	-0.38593256	11.48296976	6.12876229
H	-0.43193007	12.45826099	6.59642903
C	3.73803690	7.10818795	7.64587409
H	4.75809755	7.47521294	7.65330050
C	3.31088169	6.18687288	8.59037973
H	4.00077605	5.82448489	9.34735681
C	1.34001616	4.78623742	9.43759108
H	1.89901024	4.33175649	10.24870217

C	0.00369908	4.47045877	9.23291360
H	-0.46932162	3.75804662	9.90259387

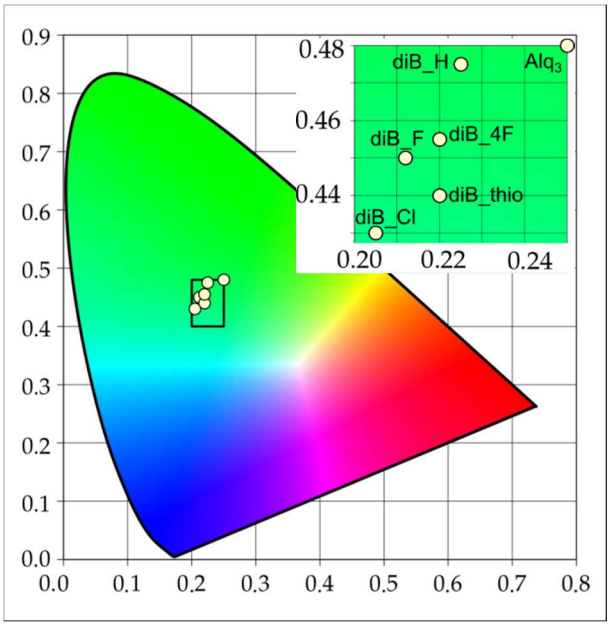


Figure S9. Colour coordinates for OLEDs. The measurements were performed according to CIE1931 diagram. Inset: enlarged part of the CIE 1931diagram showing precisely colour coordinates of investigated emitters.

7. References for Supporting Information

1. K. Durka, S. Luliński, K. N. Jarzembska, J. Smętek, J. Serwatowski and K. Woźniak, *Acta Crystallogr. Sect. B*, 2014, **70**, 157–171.
2. S. Luliński, J. Smętek, K. Durka and J. Serwatowski, *Eur. J. Org. Chem.*, 2013, **2013**, 8315–8322.
3. Bruker AXS Inc., *APEX2*, Bruker AXS Inc., Madison, Wisconsin, USA., 2010.
4. Bruker AXS Inc., *SAINT*, Bruker–Nonius, Madison, Wisconsin, USA, 2010.
5. R. H. Blessing, *Acta Crystallogr. Sect. A*, 1995, **51**, 33–38.
6. R. H. Blessing, *J. Appl. Crystallogr.*, 1989, **22**, 396–397.
7. *CrysAlis Pro Software*, Agilent Technologies, 2010.
8. G. M. Sheldrick, *Acta Crystallogr. Sect. A*, 2008, **64**, 112–122.
9. A. L. Spek, *PLATON, A Multipurpose Crystallographic Tool*, Utrecht University: Utrecht, The Netherlands, 2001.
10. P. van der Sluis and A. L. Spek, *Acta Crystallogr. Sect. A*, 1990, **46**, 194–201.
11. L. J. Farrugia, *J. Appl. Crystallogr.*, 1999, **32**, 837–838.
12. T. A. Keith, *AIMAll*, TK Gristmill Software, Overland Park KS, USA, 2012.