# Multi-Substituted Deep-Blue Emitting Carbazoles:

# Comparative Study on Photophysical and

# Electroluminescence Characteristics

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## Supplementary Information

**Fig. S1** (a) Absorption and (b) emission spectra of **1b** recorded in different solvents.
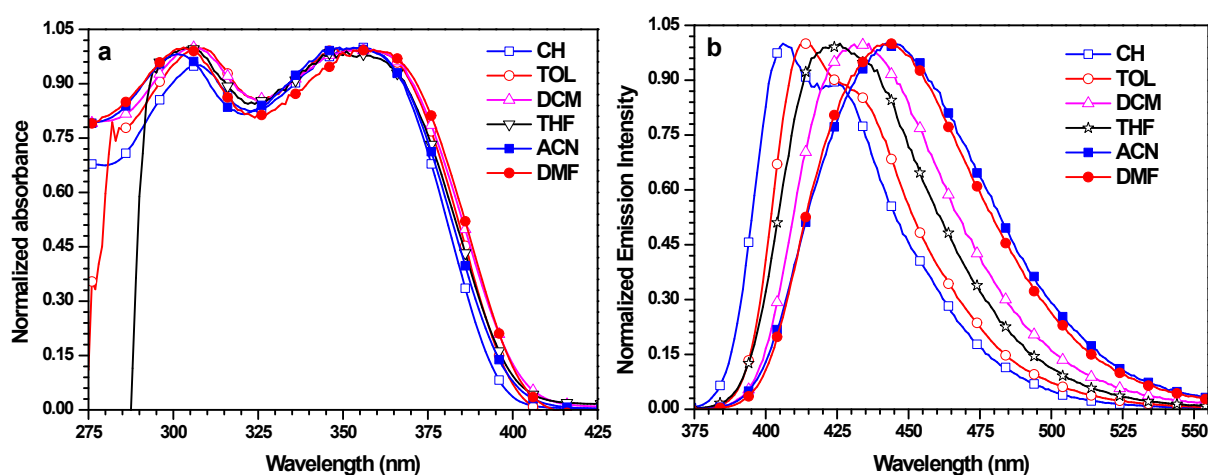


**Fig. S2** (a) Absorption and (b) emission spectra of **2a** recorded in different solvents.
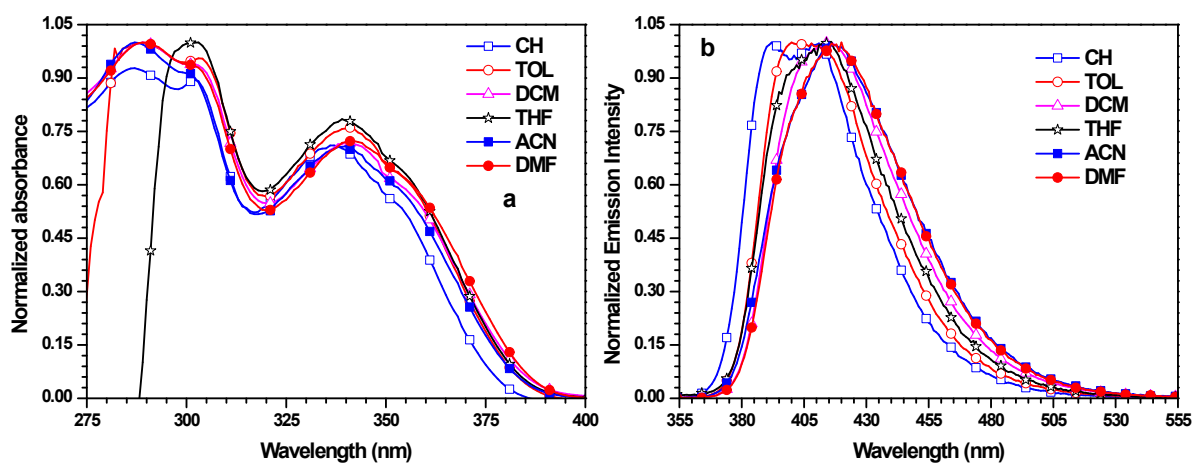


**Fig. S3** (a) Absorption and (b) emission spectra of **2b** recorded in different solvents.
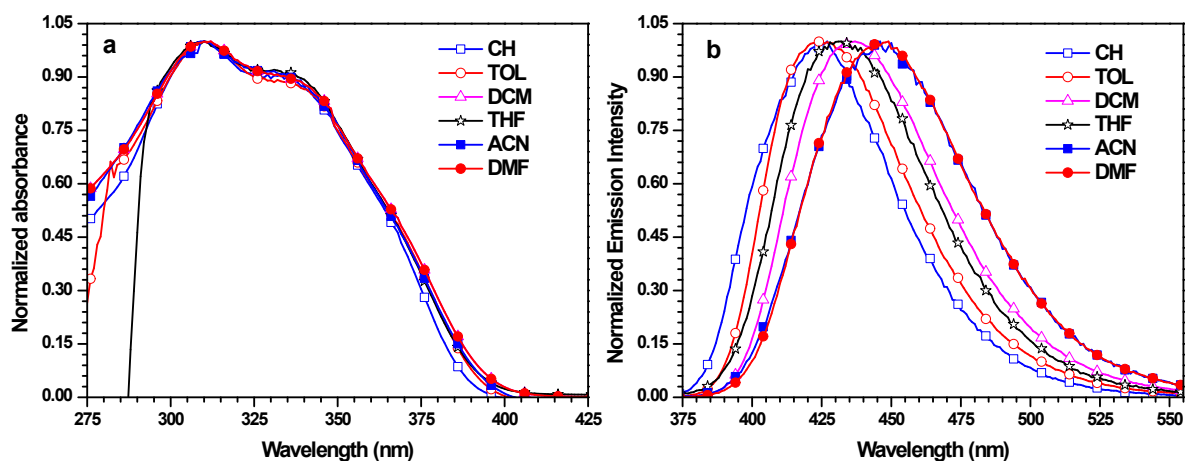
**Fig. S4** (a) Absorption and (b) emission spectra of **3a** recorded in different solvents.
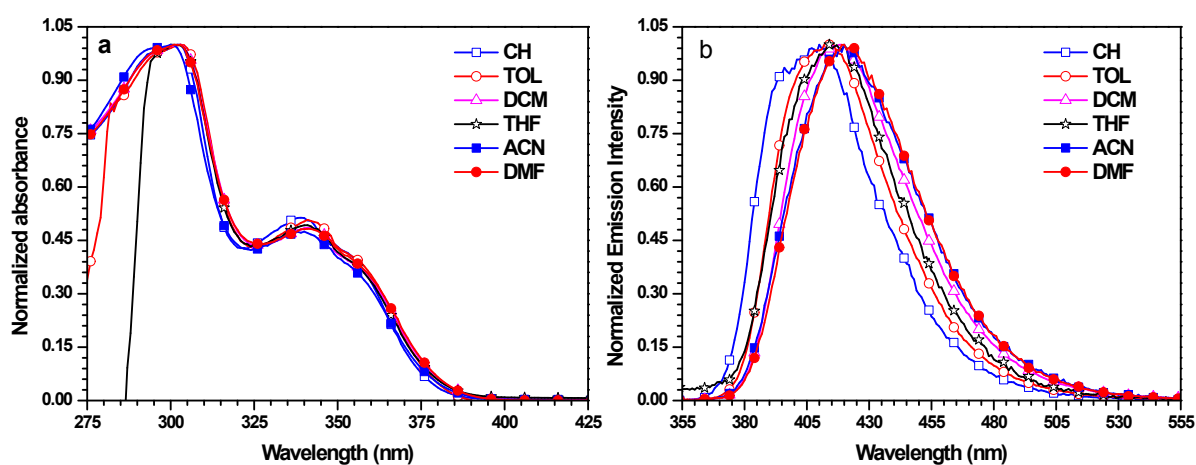


**Fig. S5** (a) Absorption and (b) emission spectra of **3b** recorded in different solvents.
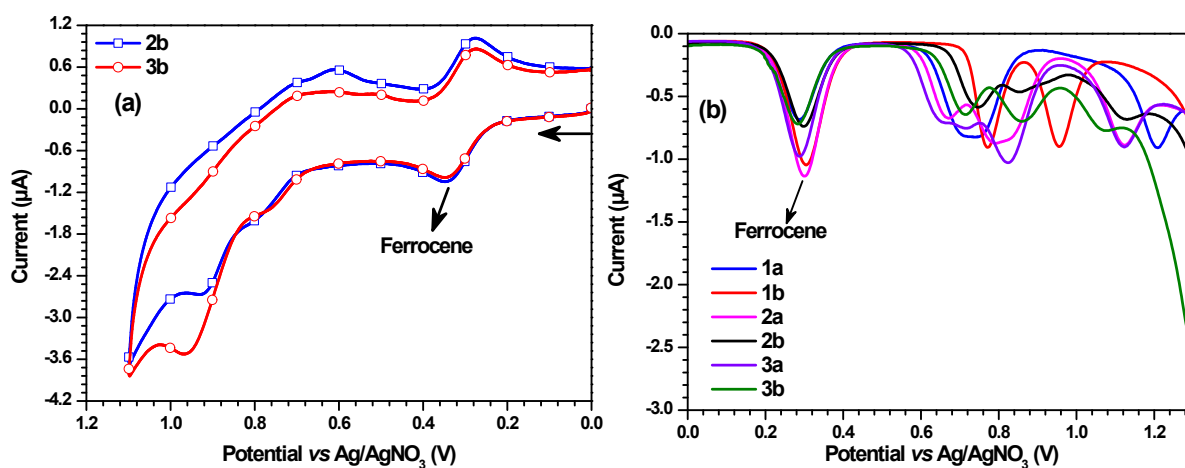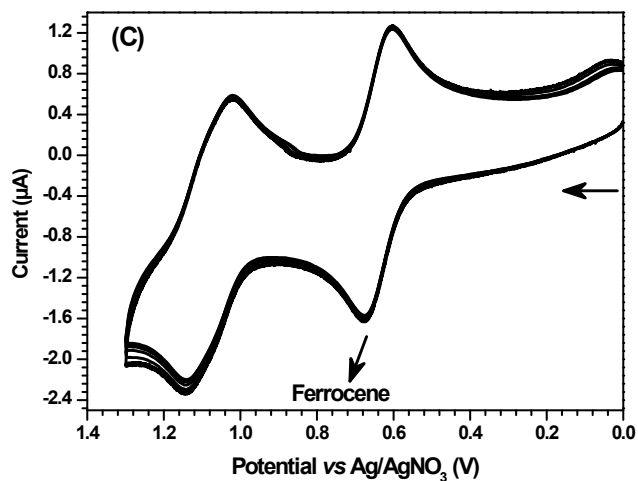
**Fig. S6** (a) Cyclic (**2b** and **3b**), (b) differential pulse voltammograms of the dyes and (c) repeated CV scans (7 times) of **1a** under similar electrochemical conditions.
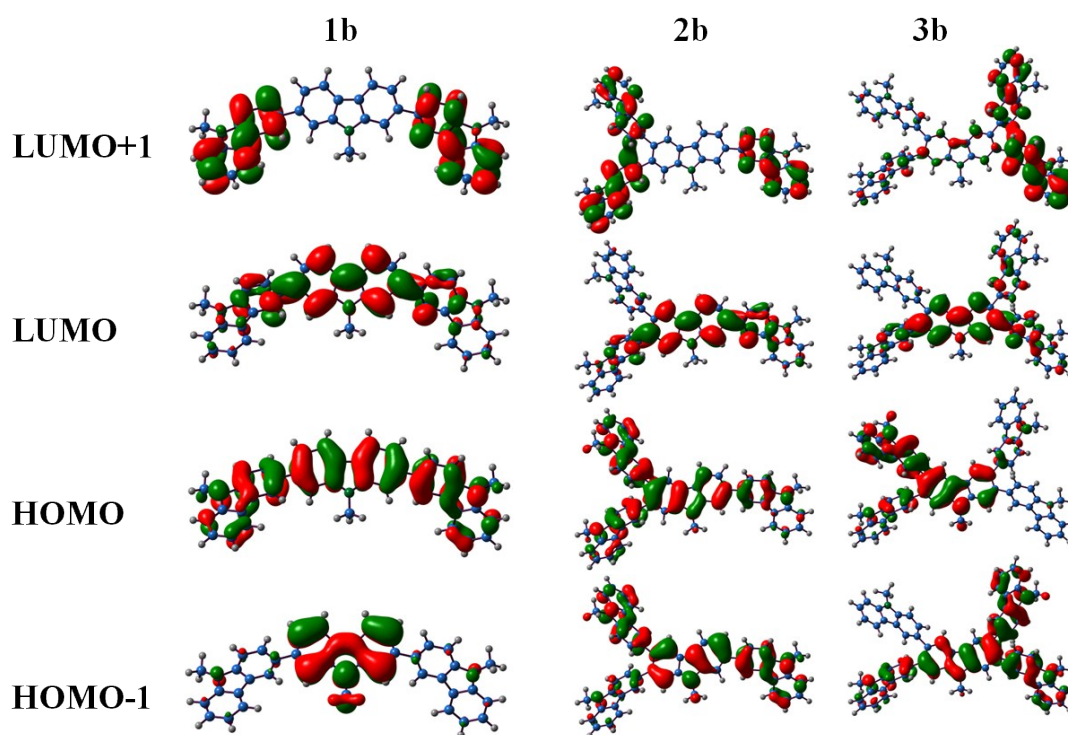


**Fig. S7** Frontier molecular orbitals of the dyes **1b, 2b** and **3b**.
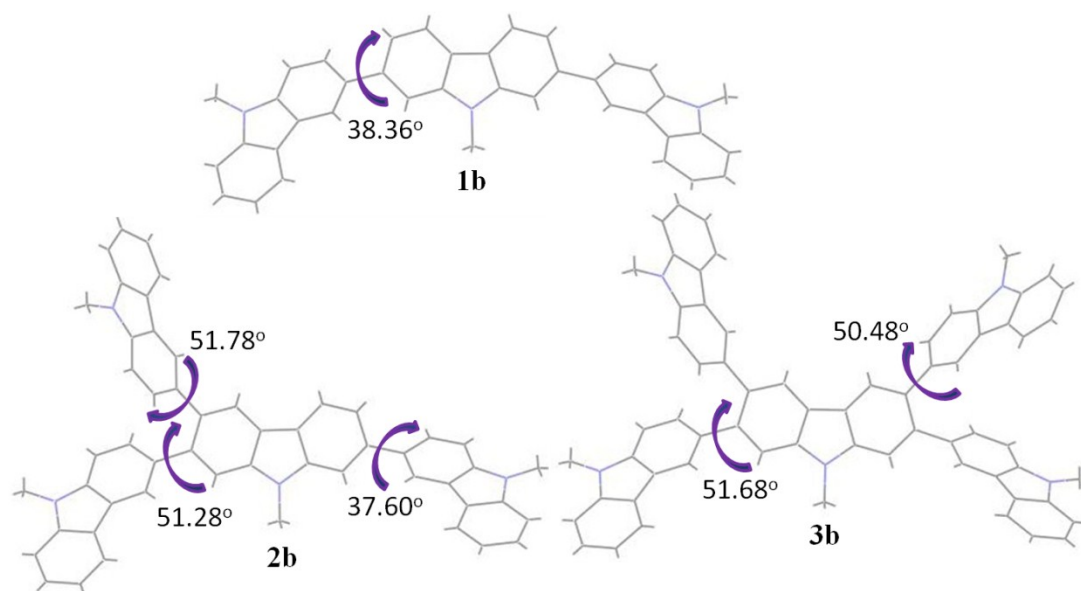
**Fig. S8.** Calculated dihedral angles in the B3LYP/6-31G(d,p) optimized geometries of **1b**, **2b** and **3b**.

**Table S1** Absorption data of the dyes recorded in various solvents

| Dye | $\lambda_{max}$ (nm) | | | | | |
|---|---|---|---|---|---|---|
| | CH | TOL | DCM | THF | ACN | DMF |
| **1a** | 367, 304 | 369, 303 | 371, 301 | 369, 300 | 367, 301 | 372, 296 |
| **1b** | 340, 284 | 341, 304 | 342, 303 | 343, 303 | 342, 302 | 349. 304 |
| **2a** | 356, 307 | 356, 307 | 357, 306 | 357, 305 | 354, 303 | 354, 304 |
| **2b** | 336, 289 | 341, 289 | 340, 289 | 340, 303 | 340, 290 | 341, 289 |
| **3a** | 335, 310 | 334, 309 | 334, 310 | 335, 309 | 334, 310 | 334, 309 |
| **3b** | 338, 302 | 341, 303 | 341, 303 | 340, 303 | 302, 340 | 341, 302 |

**Table S2** Emission properties of the dyes in different solvents with Stokes shift

| Dye | $\lambda_{em}$ (nm) | | | | | | | Stokes shift (cm$^{-1}$) | | | | | |
| | CH | TOL | DCM | THF | ACN | DMF | $\Delta f_{max,}$ (CH-DMF) | CH | TOL | DCM | THF | ACN | DMF |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **1a** | 408, 431 | 415, 436 (0.87) | 426 (0.60) | 417, 438 | 444 | 441 (0.39) | 33 | 2738 | 3004 | 3480 | 3119 | 4725 | 4206 |
| **1b** | 388, 409 | 394, 413 (0.67) | 397, 415 (0.69) | 393, 415 | 396, 412 | 398, 418 (0.65) | 10 | 3639 | 3945 | 3966 | 3709 | 3987 | 3528 |
| **2a** | 406,424 | 415, 432 (0.76) | 436 (0.37) | 426 | 442 | 444 (0.18) | 38 | 4505 | 4942 | 5075 | 4537 | 5465 | 5726 |
| **2b** | 392,411 | 400, 411 (0.51) | 415 (0.42) | 416 | 419 | 420 (0.24) | 9 | 5431 | 4995 | 5315 | 5373 | 5575 | 5516 |
| **3a** | 427 | 425 (0.59) | 438 (0.30) | 432 | 445 | 447 (0.19) | 20 | 6432 | 6411 | 7109 | 6703 | 7468 | 7519 |
| **3b** | 410 | 414 (0.43) | 419 (0.40) | 414 | 419 | 420 (0.36) | 10 | 5196 | 5171 | 5459 | 5257 | 5545 | 5516 |

**Table S3** Computed energies of the selected vertical transitions having oscillator strength higher than 0.1 and other related parameters for the dyes **1b, 2b** and **3b**

| Dye | B3LYP | | | | HOMO (eV) | LUMO (eV) | $E_g$ (eV) |
| | State | $\lambda_{max}$, nm | $f$ | Configuration | | | |
|---|---|---|---|---|---|---|---|
| **1b** | S1 | 344.7 | 1.29 | HOMO → LUMO (96%) | -4.90 | -0.87 | 4.02 |
| | S3 | 329.2 | 0.17 | HOMO → LUMO+2 (+81%), HOMO-2 → LUMO+1 (+10%) | | | |
| | S9 | 289.3 | 0.18 | HOMO-3 → LUMO (+70%), HOMO-4 → LUMO+1 (9%) | | | |
| **2b** | S1 | 350.7 | 0.45 | HOMO → LUMO (90%) | -4.82 | -0.82 | 3.99 |
| | S2 | 337.5 | 0.13 | HOMO → LUMO+1 (+46%); HOMO → LUMO+2 (+22%); HOMO-1 → LUMO (+18%); | | | |
| | S3 | 335.3 | 0.56 | HOMO-1 → LUMO (+62%); HOMO → LUMO+1 (+26%) | | | |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | S4 | 329.9 | 0.20 | HOMO → LUMO+2 (+50%); HOMO-1→ LUMO+2 (12%); | | | |
| **3b** | S1 | 342.8 | 0.69 | HOMO-1 → LUMO (+84%); HOMO → LUMO (8%) | -4.79 | -0.76 | 4.03 |
| | S3 | 335.4 | 0.14 | HOMO-1 → LUMO+1 (+73%); HOMO → LUMO+1 (+8%) | | | |
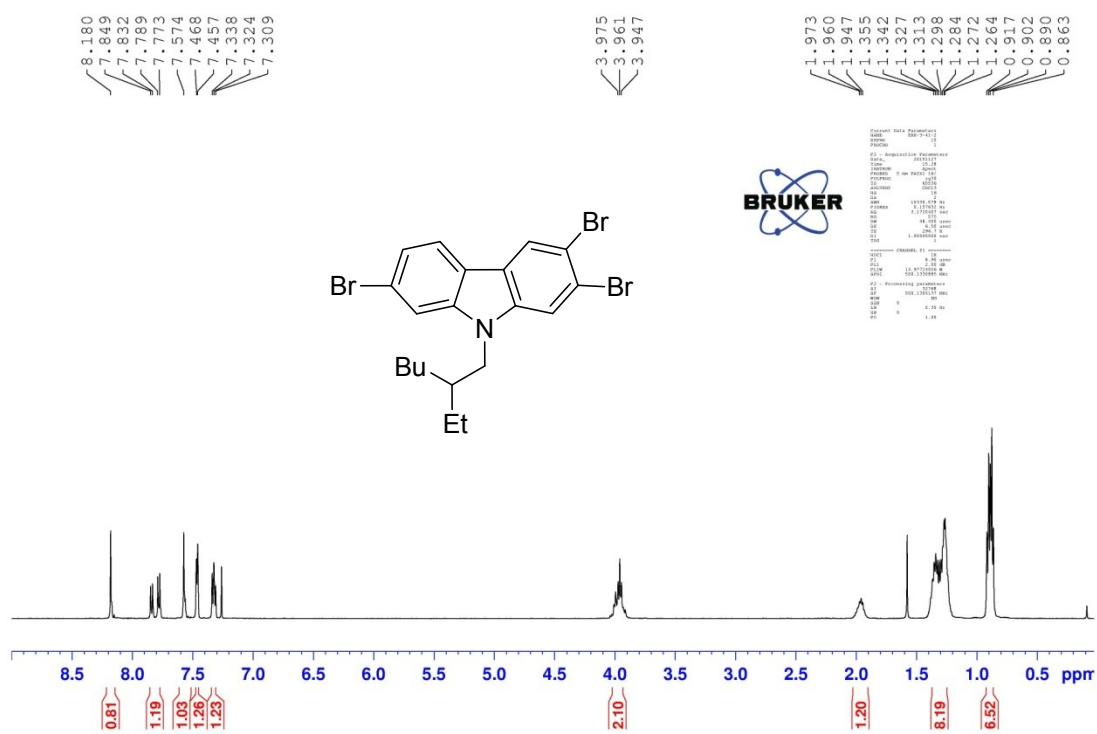
**Fig. S9** ^{1}H NMR spectrum of **2** recorded in CDCl$_3$.
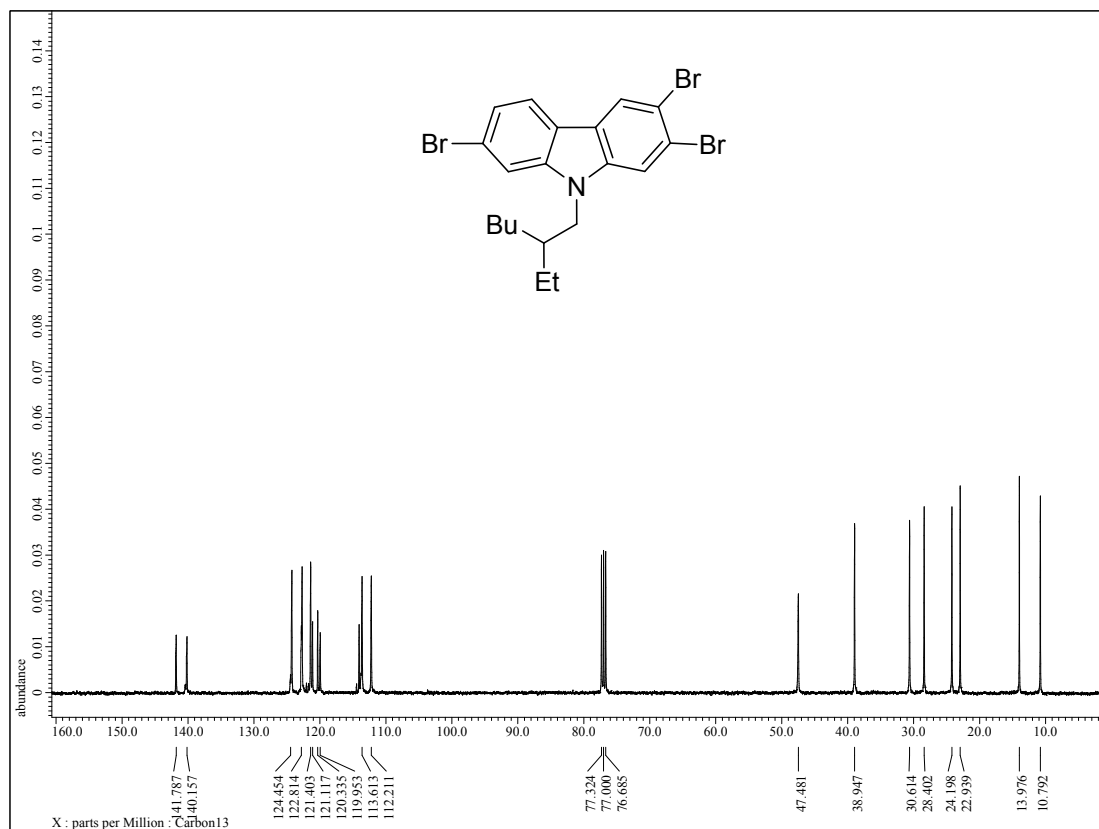


**Fig. S10** ^{13}C NMR spectrum of **2** recorded in CDCl$_3$.
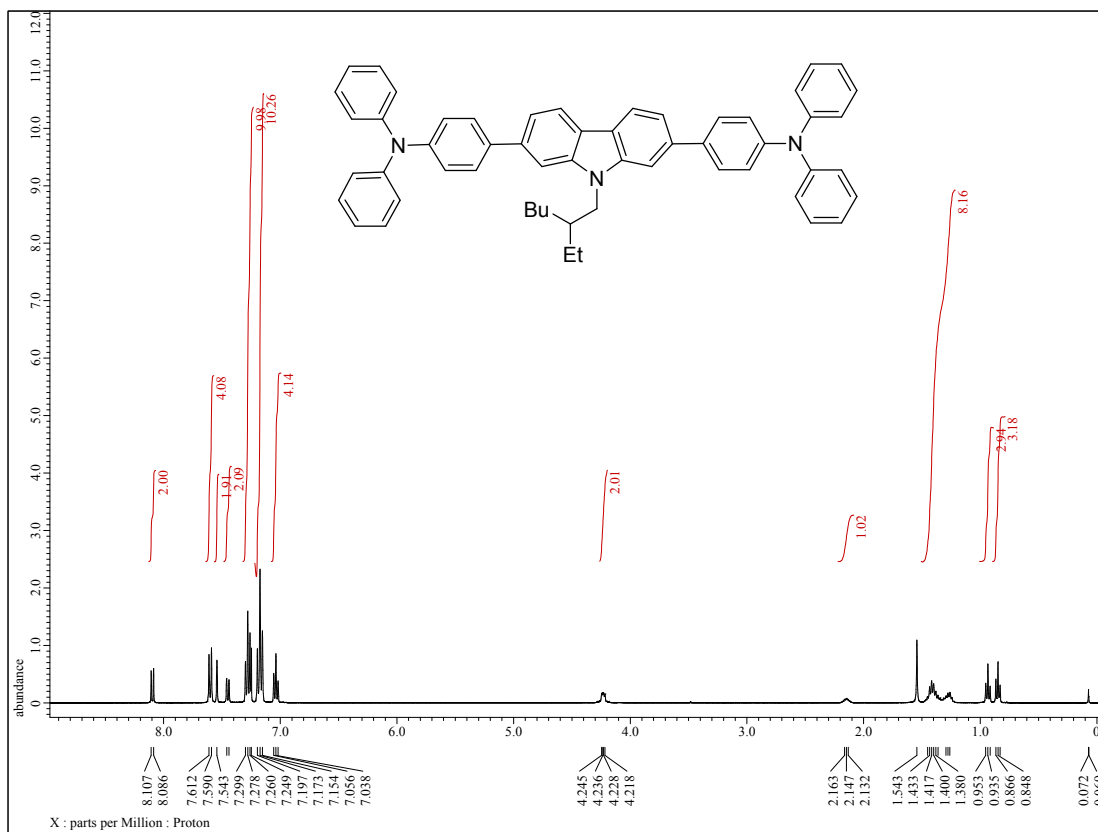
**Fig. S11** $^1$H NMR spectrum of **1a** recorded in CDCl$_3$.
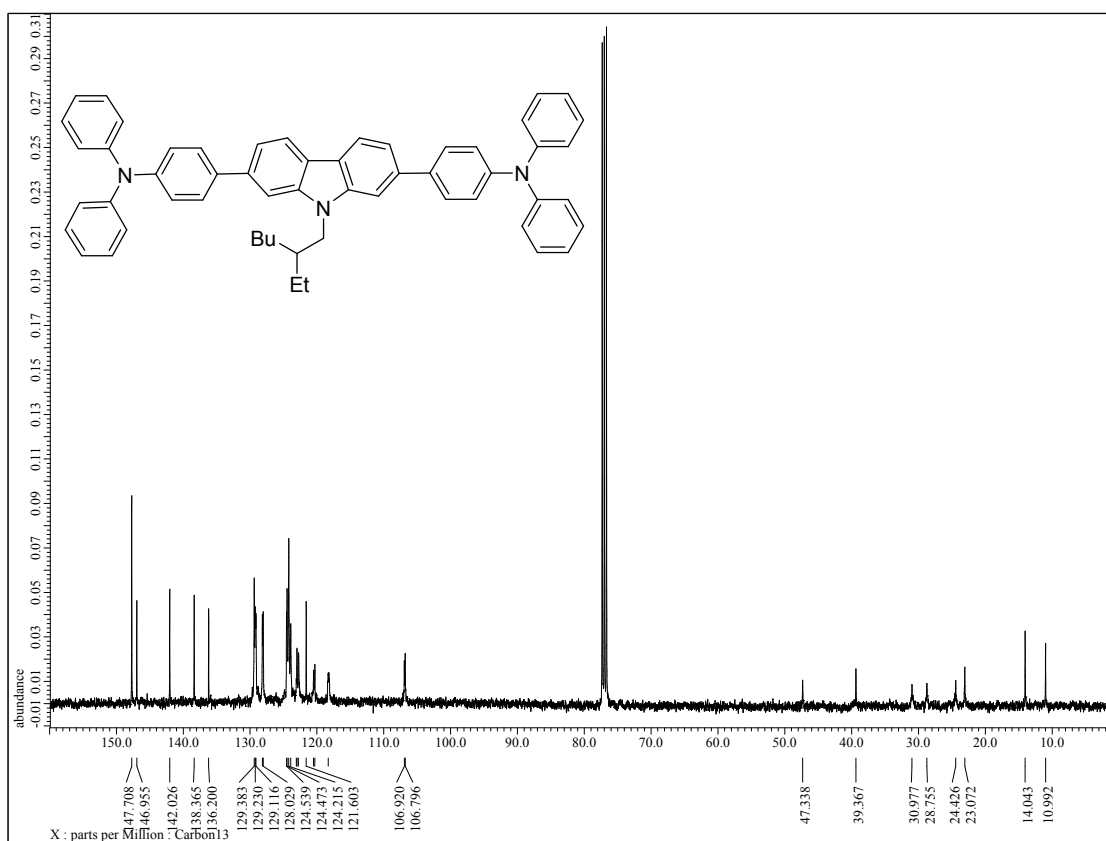


**Fig. S12** $^{13}$C NMR spectrum of **1a** recorded in CDCl$_3$.
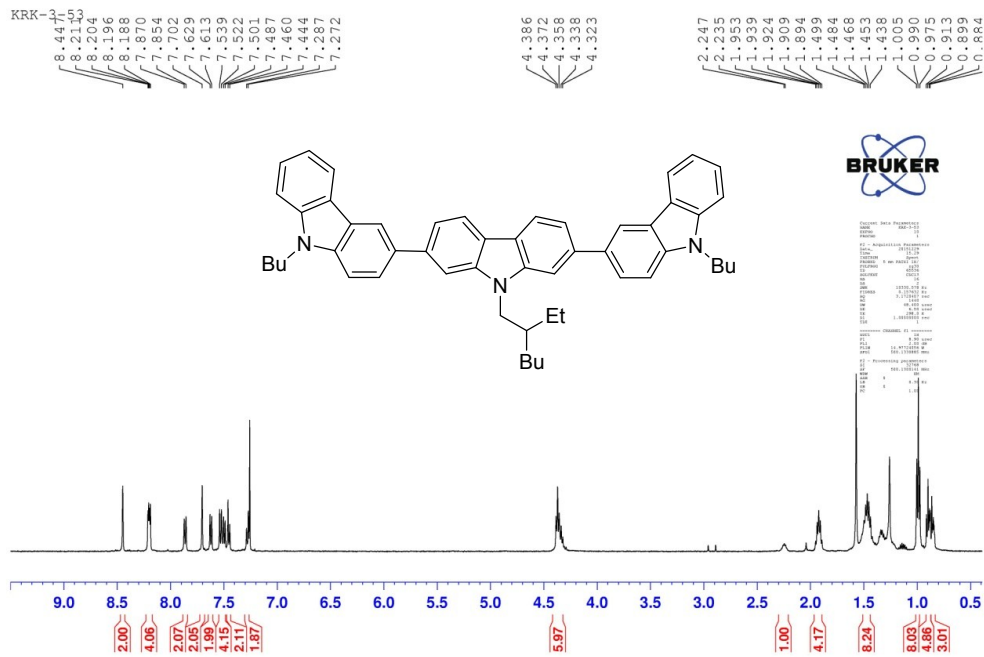
**Fig. S13** ^{1}H NMR spectrum of **1b** recorded in CDCl$_3$.
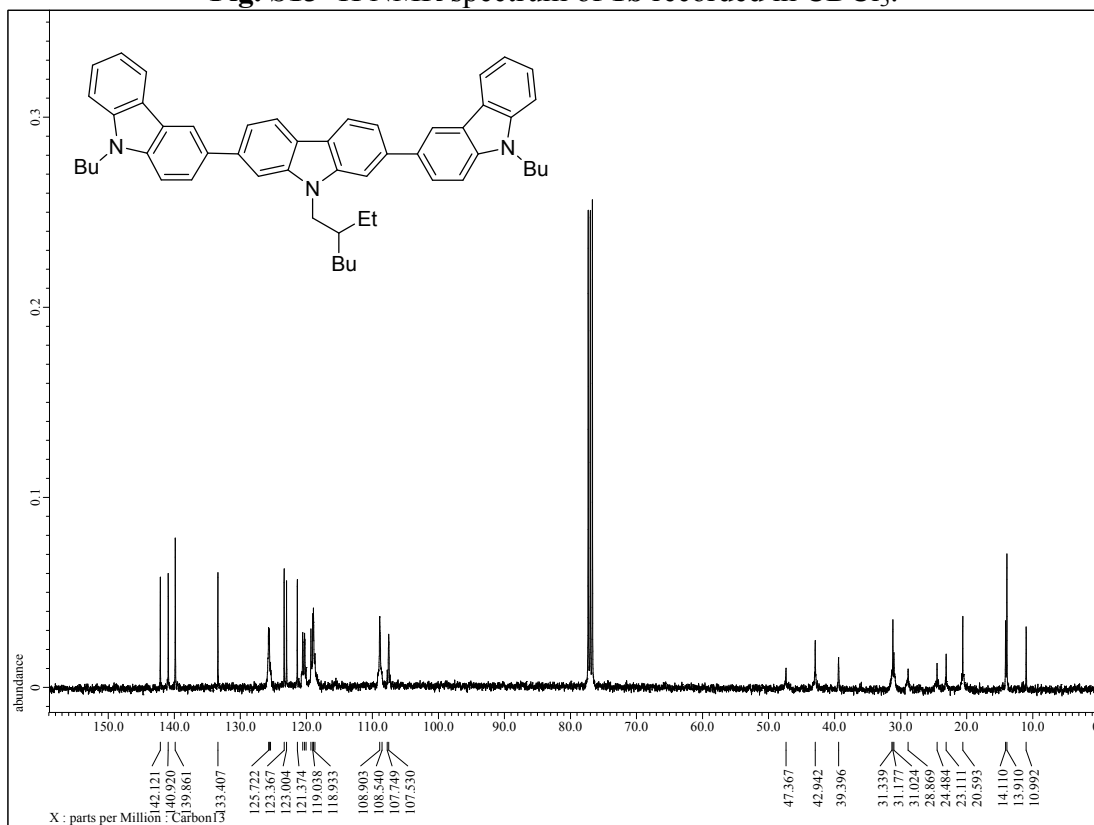


**Fig. S14** ^{13}C NMR spectrum of **1b** recorded in CDCl$_3$.
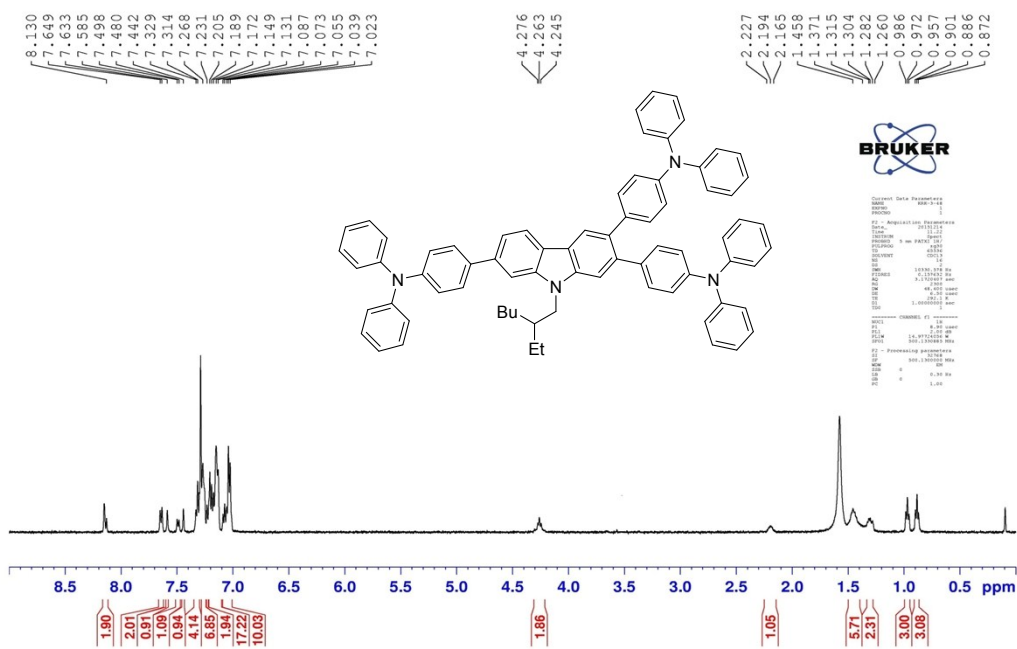
**Fig. S15** $^{1}$H NMR spectra of **2a** recorded in CDCl$_3$.
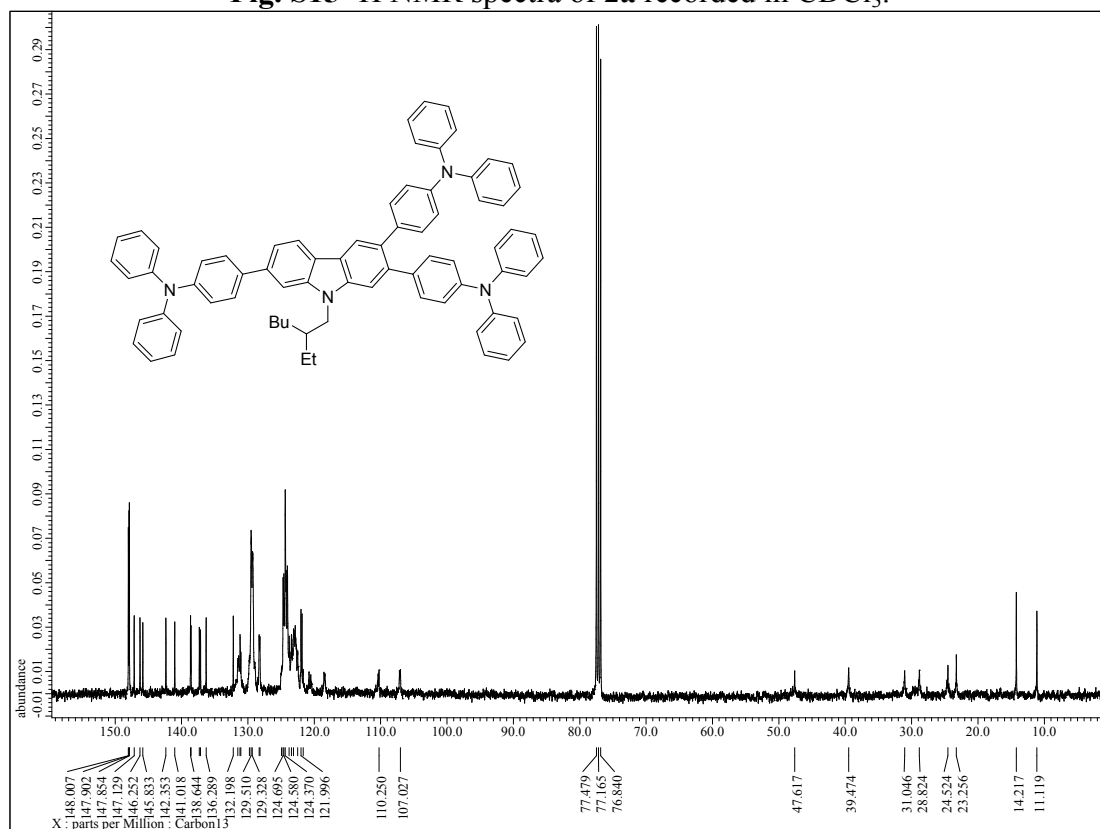


**Fig. S16** $^{13}$C NMR spectra of **2a** recorded in CDCl$_3$
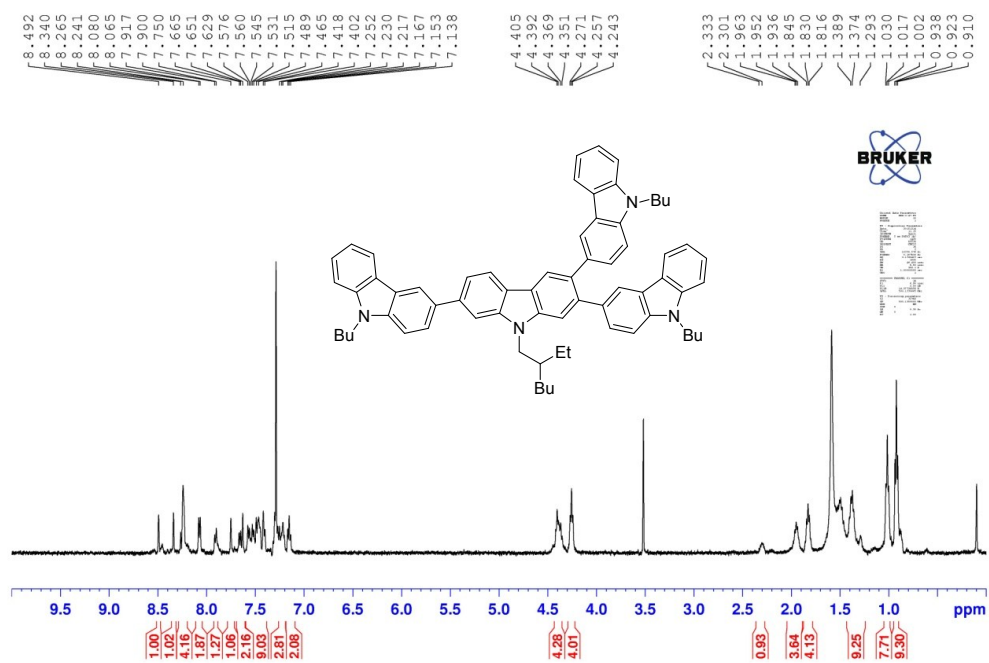
**Fig. S17** $^1$H NMR spectra of **2b** recorded in CDCl$_3$.
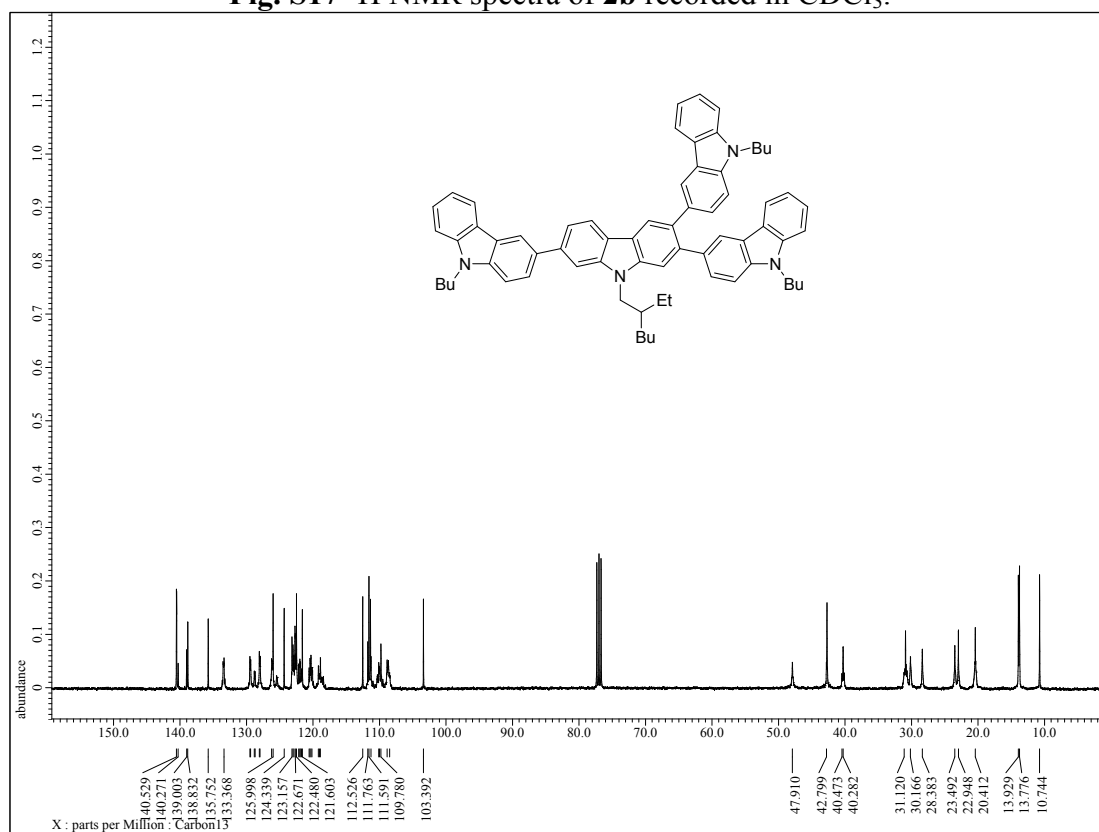


**Fig. S18** $^{13}$C NMR spectra of **2b** recorded in CDCl$_3$.
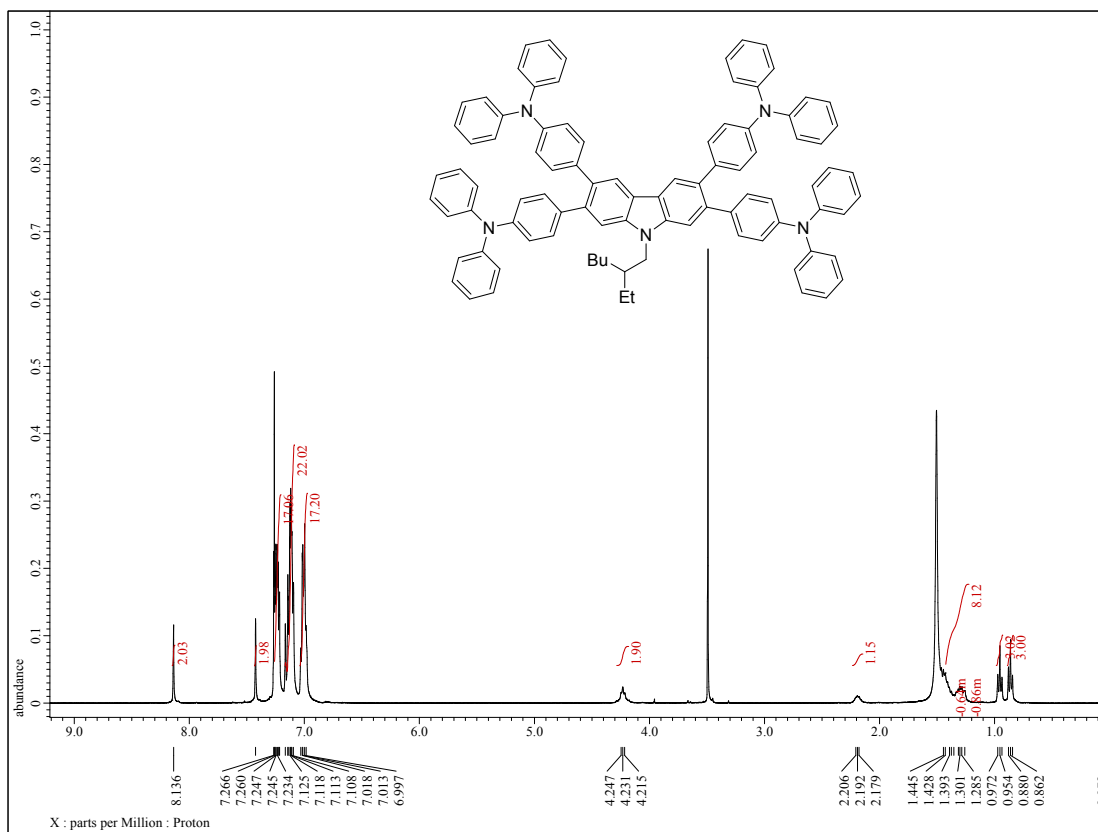
**Fig. S19**. $^1$H NMR spectra of **3a** recorded in CDCl$_3$.
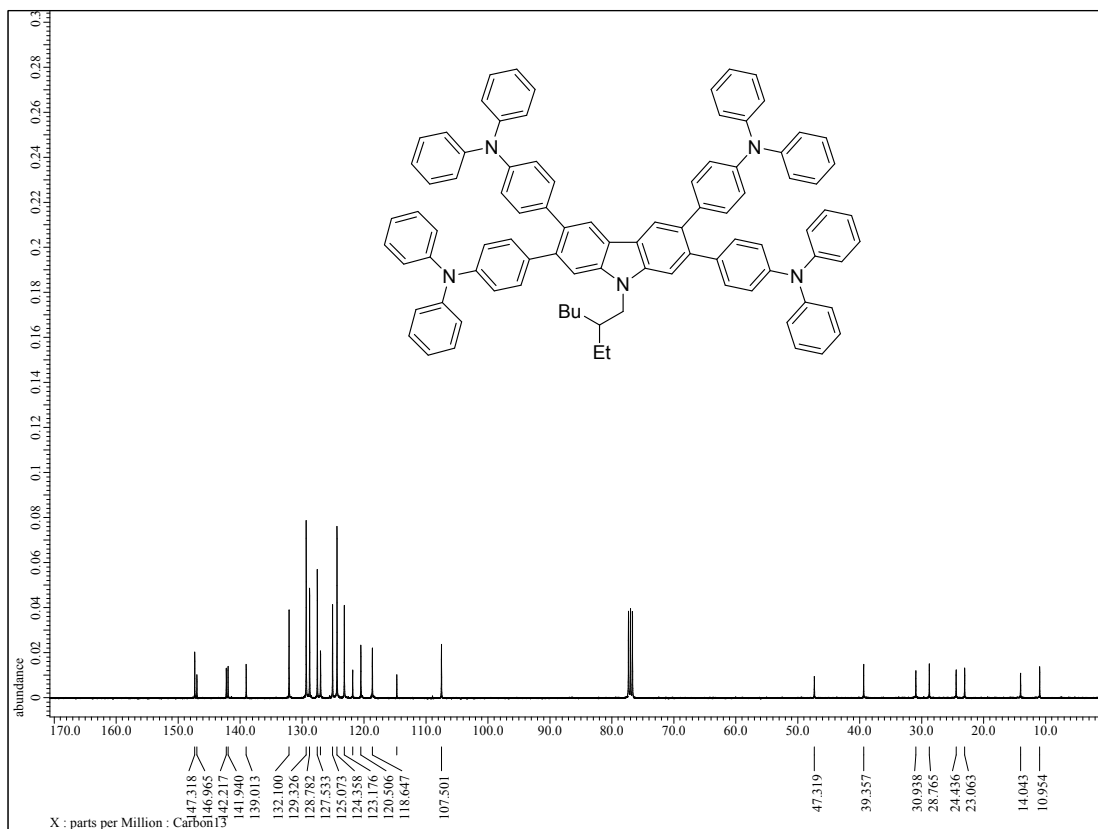


**Fig. S20**. $^{13}$C NMR spectra of **3a** recorded in CDCl$_3$.

S14
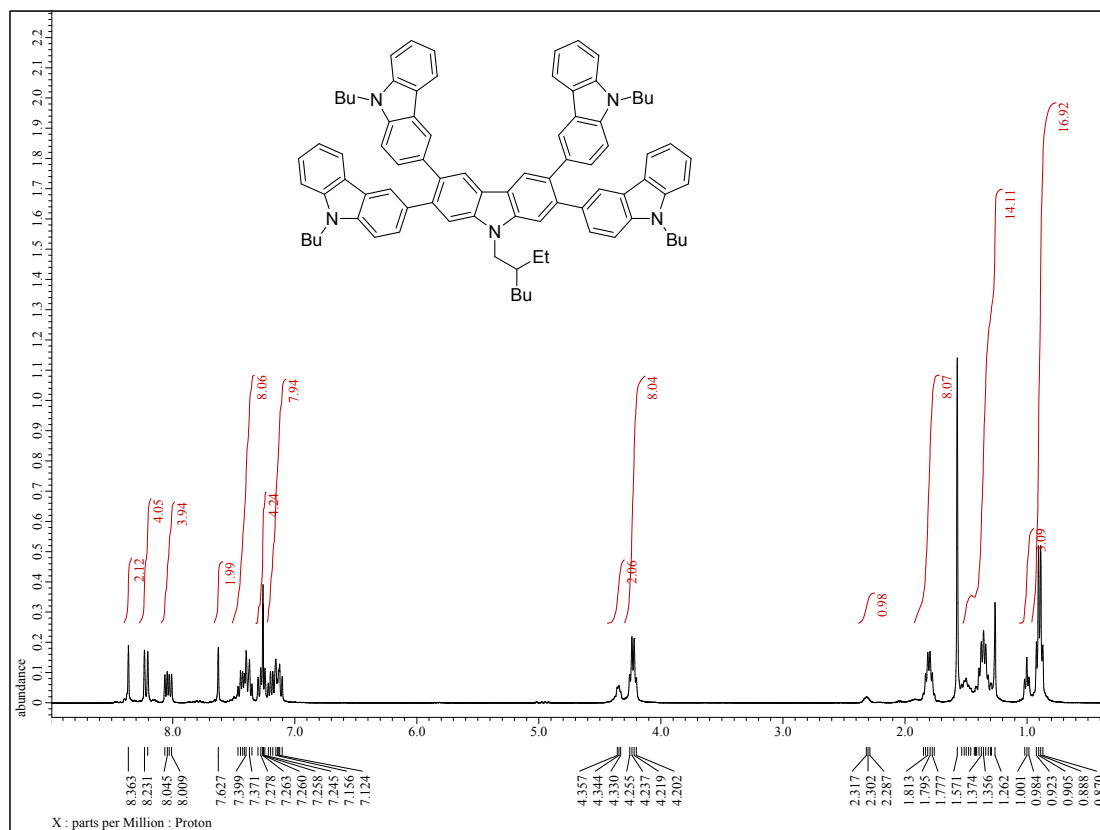
**Fig. S21** $^1$H NMR spectra of **3b** recorded in CDCl$_3$.
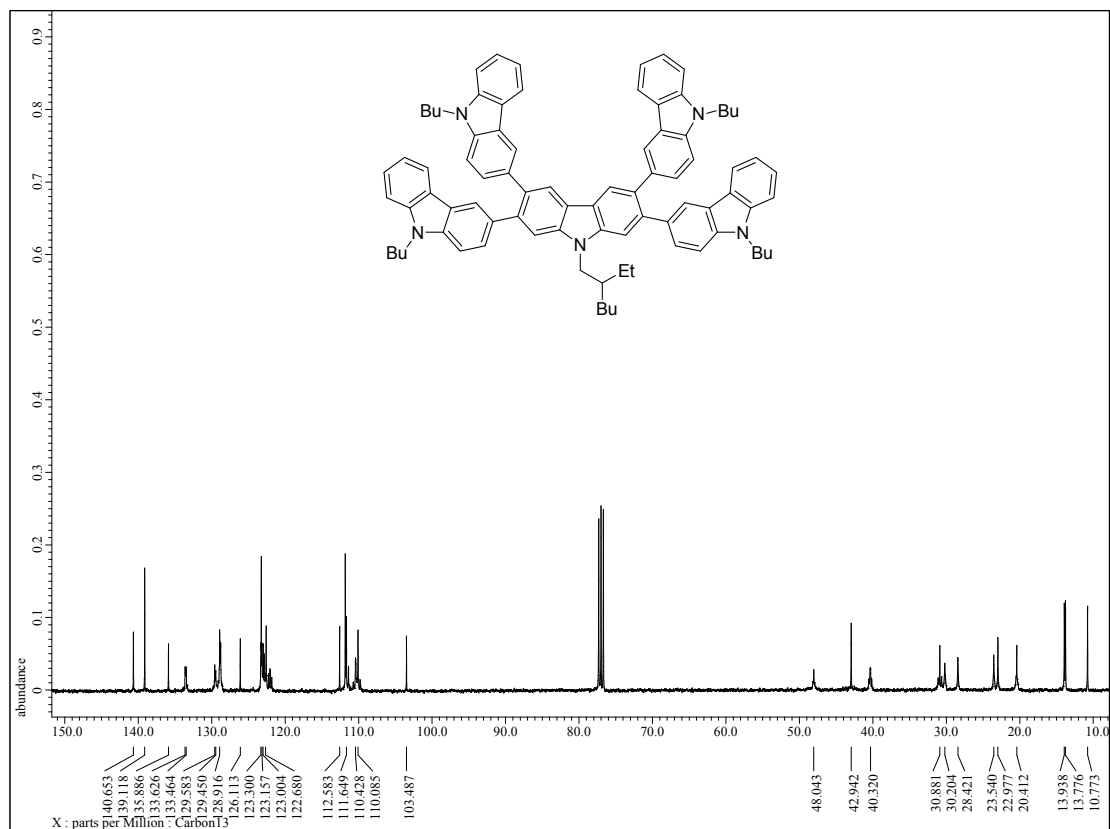


**Fig. S22** $^{13}$C NMR spectra of **3b** recorded in CDCl$_3$.

**Tabel S3** Cartesian coordinates for the optimized geometry of **1a**.

Energy = -2053.85292450 au

| At. NO | X | Y | Z |
|---|---|---|---|
| 6 | 3.042470000 | -0.040380000 | 2.357831000 |
| 6 | 3.449958000 | -0.041836000 | 1.002397000 |
| 6 | 2.476385000 | -0.049510000 | -0.008141000 |
| 6 | 1.129718000 | -0.062758000 | 0.355464000 |
| 6 | 0.721511000 | -0.049889000 | 1.716149000 |
| 6 | 1.700125000 | -0.042473000 | 2.715838000 |
| 1 | 1.416035000 | -0.045546000 | 3.764372000 |
| 6 | -1.130158000 | -0.045611000 | 0.354094000 |
| 6 | -2.476475000 | -0.032449000 | -0.010565000 |
| 6 | -3.450736000 | -0.026014000 | 0.999139000 |
| 6 | -3.044748000 | -0.028840000 | 2.355009000 |
| 6 | -1.702751000 | -0.036481000 | 2.714209000 |
| 6 | -0.723314000 | -0.042776000 | 1.715321000 |
| 1 | -1.419437000 | -0.025287000 | 3.762894000 |
| 7 | 0.000198000 | -0.077385000 | -0.455901000 |
| 6 | 0.002269000 | -0.052651000 | -1.902085000 |
| 1 | -0.882616000 | -0.570072000 | -2.279967000 |
| 1 | 0.882170000 | -0.580880000 | -2.276707000 |
| 1 | 2.776906000 | -0.008000000 | -1.049661000 |
| 1 | -2.777047000 | -0.051154000 | -1.052789000 |
| 1 | 0.009664000 | 0.969494000 | -2.301893000 |
| 1 | 3.800244000 | -0.064945000 | 3.134021000 |
| 1 | -3.803085000 | 0.008885000 | 3.130157000 |
| 6 | 4.891624000 | -0.032148000 | 0.653486000 |
| 6 | 5.383823000 | -0.744644000 | -0.453853000 |
| 6 | 5.824325000 | 0.690752000 | 1.417510000 |
| 6 | 6.732995000 | -0.730917000 | -0.789874000 |
| 1 | 4.698609000 | -1.332753000 | -1.057052000 |
| 6 | 7.178383000 | 0.695977000 | 1.102160000 |
| 1 | 5.481358000 | 1.269385000 | 2.269718000 |
| 6 | 7.655893000 | -0.013550000 | -0.011620000 |
| 1 | 7.081595000 | -1.288898000 | -1.652345000 |
| 1 | 7.874038000 | 1.260416000 | 1.713747000 |
| 7 | 9.036532000 | -0.006567000 | -0.341760000 |
| 6 | 9.671232000 | -1.198939000 | -0.785658000 |
| 6 | 9.792872000 | 1.191015000 | -0.211966000 |
| 6 | 10.596403000 | -1.161663000 | -1.841483000 |
| 6 | 9.385553000 | -2.431025000 | -0.175162000 |
| 6 | 11.079534000 | 1.164108000 | 0.349526000 |
| 6 | 9.264495000 | 2.418300000 | -0.643657000 |
| 6 | 11.225227000 | -2.329944000 | -2.266715000 |
| 1 | 10.817505000 | -0.214643000 | -2.322098000 |
| 6 | 10.005827000 | -3.596483000 | -0.620304000 |
| 1 | 8.677499000 | -2.467217000 | 0.645779000 |
| 6 | 11.819825000 | 2.338670000 | 0.466589000 |

| | | | |
|---|---|---|---|
| 1 | 11.491810000 | 0.220559000 | 0.690822000 |
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| 6 | 10.932290000 | -3.554892000 | -1.664095000 |
| 1 | 11.938356000 | -2.282162000 | -3.084801000 |
| 1 | 9.772820000 | -4.540594000 | -0.136121000 |
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| 1 | 9.580895000 | 4.530768000 | -0.844584000 |
| 1 | 11.418946000 | -4.464152000 | -2.003082000 |
| 1 | 11.865235000 | 4.473078000 | 0.145031000 |
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| 6 | -5.372945000 | 0.717641000 | -0.452949000 |
| 6 | -7.190224000 | -0.704032000 | 1.094536000 |
| 1 | -5.501983000 | -1.311846000 | 2.257930000 |
| 6 | -6.722389000 | 0.728087000 | -0.788189000 |
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| 6 | -9.810732000 | -1.149443000 | -0.228782000 |
| 6 | -9.653860000 | 1.246180000 | -0.771266000 |
| 6 | -11.097596000 | -1.111354000 | 0.331690000 |
| 6 | -9.298888000 | -2.378829000 | -0.674255000 |
| 6 | -10.583452000 | 1.236769000 | -1.823885000 |
| 6 | -9.345219000 | 2.466255000 | -0.147855000 |
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| 6 | -10.056207000 | -3.541816000 | -0.550810000 |
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| 6 | -11.194054000 | 2.420307000 | -2.233150000 |
| 1 | -10.822308000 | 0.299328000 | -2.314655000 |
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| 1 | -9.644218000 | -4.484183000 | -0.900469000 |
| 6 | -10.878308000 | 3.633159000 | -1.617702000 |
| 1 | -11.910907000 | 2.393937000 | -3.048953000 |
| 1 | -9.696626000 | 4.581415000 | -0.083083000 |
| 1 | -11.928845000 | -4.406502000 | 0.087201000 |
| 1 | -11.350841000 | 4.554321000 | -1.944301000 |

**Tabel S4** Cartesian coordinates for the optimized geometry of **1b**

Energy = -1668.00741678 au

| At. No | X | Y | Z |
|---|---|---|---|
| 6 | 3.035187000 | -2.728844000 | -0.275158000 |
| 6 | 3.439278000 | -1.373581000 | -0.326223000 |
| 6 | 2.467484000 | -0.364302000 | -0.255020000 |
| 6 | 1.126073000 | -0.728518000 | -0.136410000 |
| 6 | 0.721519000 | -2.089073000 | -0.079377000 |
| 6 | 1.698156000 | -3.087820000 | -0.153929000 |
| 1 | 1.418089000 | -4.136360000 | -0.104606000 |
| 6 | -1.125757000 | -0.727710000 | 0.058886000 |
| 6 | -2.465113000 | -0.362068000 | 0.196133000 |
| 6 | -3.434237000 | -1.370436000 | 0.307139000 |
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| 6 | -1.692093000 | -3.086153000 | 0.162875000 |
| 6 | -0.718092000 | -2.088466000 | 0.049774000 |
| 1 | -1.409967000 | -4.135180000 | 0.146656000 |
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| 6 | -0.001681000 | 1.528295000 | -0.060693000 |
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| 1 | 0.828772000 | 1.900354000 | -0.665294000 |
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| 1 | -2.760951000 | 0.679973000 | 0.255315000 |
| 1 | 0.090575000 | 1.937863000 | 0.953509000 |
| 1 | 3.794661000 | -3.503559000 | -0.298678000 |
| 1 | -3.786043000 | -3.500923000 | 0.343649000 |
| 6 | 4.877229000 | -1.021763000 | -0.447522000 |
| 6 | 5.412339000 | 0.072453000 | 0.245590000 |
| 6 | 5.734143000 | -1.785411000 | -1.274752000 |
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| 1 | 4.776620000 | 0.654936000 | 0.905920000 |
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| 1 | 5.314927000 | -2.613747000 | -1.837066000 |
| 6 | 7.607675000 | 1.429653000 | 0.676413000 |
| 6 | 7.598737000 | -0.397212000 | -0.719064000 |
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| 1 | 6.390935000 | 2.667077000 | 1.965532000 |
| 6 | 9.976951000 | 2.062722000 | 0.483228000 |
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| | | | |
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| 6 | -8.916025000 | 1.211516000 | -0.123105000 |
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| 1 | -10.058890000 | 0.118525000 | 2.495863000 |
| 1 | -10.926434000 | -0.212406000 | 0.977657000 |
| 6 | 10.020649000 | -0.408791000 | -1.424818000 |
| 1 | 9.913642000 | -1.487765000 | -1.558548000 |
| 1 | 10.109912000 | 0.060723000 | -2.412912000 |
| 1 | 10.944105000 | -0.231930000 | -0.868373000 |

**Table S5** Cartesian coordinates for the optimized geometry of **2a**.

Energy = -2802.37261393 au

| At. No | X | Y | Z |
|---|---|---|---|
| 6 | -1.407156000 | 0.411875000 | 0.074557000 |
| 6 | -1.537188000 | -0.992234000 | -0.154186000 |
| 6 | -0.390318000 | -1.786109000 | -0.303491000 |
| 6 | 0.870702000 | -1.199306000 | -0.216205000 |
| 6 | 1.016376000 | 0.186261000 | 0.045711000 |
| 6 | -0.128086000 | 0.972977000 | 0.181421000 |
| 1 | -0.035932000 | 2.043677000 | 0.338226000 |
| 6 | 3.089521000 | -0.788925000 | -0.134683000 |
| 6 | 4.479970000 | -0.897264000 | -0.149562000 |
| 6 | 5.249980000 | 0.256928000 | 0.059841000 |
| 6 | 4.599128000 | 1.493467000 | 0.284607000 |
| 6 | 3.213626000 | 1.596241000 | 0.303190000 |
| 6 | 2.436943000 | 0.451883000 | 0.094687000 |
| 1 | 2.740839000 | 2.556248000 | 0.490016000 |
| 7 | 2.129799000 | -1.775198000 | -0.339611000 |
| 6 | 2.400622000 | -3.178149000 | -0.564710000 |
| 1 | 3.309592000 | -3.287703000 | -1.161579000 |
| 1 | 1.577024000 | -3.623564000 | -1.126781000 |
| 1 | -0.504327000 | -2.856424000 | -0.439083000 |

| | | | |
|---|---|---|---|
| 1 | 4.967393000 | -1.846630000 | -0.344284000 |
| 1 | 2.526954000 | -3.733823000 | 0.373302000 |
| 1 | 5.200703000 | 2.375465000 | 0.478248000 |
| 6 | -2.856150000 | -1.684469000 | -0.199201000 |
| 6 | -3.161969000 | -2.576245000 | -1.240217000 |
| 6 | -3.813660000 | -1.523971000 | 0.816625000 |
| 6 | -4.364742000 | -3.276155000 | -1.272205000 |
| 1 | -2.444895000 | -2.720520000 | -2.043415000 |
| 6 | -5.023288000 | -2.208058000 | 0.787795000 |
| 1 | -3.609540000 | -0.845768000 | 1.638503000 |
| 6 | -5.318953000 | -3.097076000 | -0.259197000 |
| 1 | -4.573373000 | -3.959254000 | -2.088701000 |
| 1 | -5.747315000 | -2.058918000 | 1.581722000 |
| 7 | -6.555513000 | -3.794873000 | -0.294658000 |
| 6 | -7.249698000 | -3.947272000 | -1.526309000 |
| 6 | -7.107556000 | -4.329063000 | 0.901495000 |
| 6 | -7.860041000 | -5.168654000 | -1.854380000 |
| 6 | -7.335047000 | -2.879023000 | -2.433724000 |
| 6 | -8.482745000 | -4.218649000 | 1.163928000 |
| 6 | -6.286763000 | -4.976857000 | 1.839038000 |
| 6 | -8.545486000 | -5.310449000 | -3.059154000 |
| 1 | -7.793090000 | -6.000386000 | -1.161194000 |
| 6 | -8.006601000 | -3.036847000 | -3.644205000 |
| 1 | -6.872269000 | -1.930432000 | -2.183335000 |
| 6 | -9.020628000 | -4.753164000 | 2.332688000 |
| 1 | -9.122511000 | -3.713922000 | 0.447990000 |
| 6 | -6.831544000 | -5.491723000 | 3.013469000 |
| 1 | -5.224541000 | -5.071938000 | 1.640684000 |
| 6 | -8.619877000 | -4.249781000 | -3.964067000 |
| 1 | -9.011538000 | -6.262587000 | -3.296562000 |
| 1 | -8.062631000 | -2.199544000 | -4.334023000 |
| 6 | -8.200630000 | -5.388595000 | 3.267218000 |
| 1 | -10.086666000 | -4.658284000 | 2.518849000 |
| 1 | -6.181360000 | -5.989528000 | 3.727317000 |
| 1 | -9.148573000 | -4.366644000 | -4.904985000 |
| 1 | -8.622428000 | -5.797421000 | 4.180154000 |
| 6 | 6.731490000 | 0.181371000 | 0.050119000 |
| 6 | 7.512184000 | 1.217930000 | -0.490481000 |
| 6 | 7.413993000 | -0.927664000 | 0.579428000 |
| 6 | 8.901237000 | 1.158311000 | -0.495402000 |
| 1 | 7.021927000 | 2.083476000 | -0.925450000 |
| 6 | 8.802097000 | -1.006470000 | 0.562382000 |
| 1 | 6.847548000 | -1.739425000 | 1.026051000 |
| 6 | 9.570555000 | 0.040459000 | 0.028325000 |
| 1 | 9.300237000 | -1.876771000 | 0.976046000 |
| 7 | 10.988481000 | -0.029170000 | 0.019370000 |
| 6 | 11.716848000 | 0.434619000 | -1.110735000 |
| 6 | 11.684025000 | -0.552555000 | 1.143740000 |
| 6 | 12.885016000 | 1.195325000 | -0.942541000 |
| 6 | 11.279506000 | 0.138005000 | -2.411694000 |

| 6 | 12.785337000 | -1.405624000 | 0.965989000 |
|---|---|---|---|
| 6 | 11.282773000 | -0.223294000 | 2.448638000 |
| 6 | 13.600703000 | 1.638698000 | -2.052694000 |
| 1 | 13.225319000 | 1.433643000 | 0.059511000 |
| 6 | 11.992204000 | 0.601593000 | -3.515533000 |
| 1 | 10.381226000 | -0.454514000 | -2.548864000 |
| 6 | 13.471290000 | -1.907199000 | 2.070053000 |
| 1 | 13.097931000 | -1.669241000 | -0.038761000 |
| 6 | 11.963959000 | -0.745199000 | 3.546277000 |
| 1 | 10.437675000 | 0.440984000 | 2.594340000 |
| 6 | 13.158566000 | 1.349988000 | -3.345241000 |
| 1 | 14.502241000 | 2.226233000 | -1.904031000 |
| 1 | 11.639287000 | 0.362758000 | -4.514767000 |
| 6 | 13.064249000 | -1.585714000 | 3.366371000 |
| 1 | 14.321268000 | -2.565343000 | 1.913571000 |
| 1 | 11.639616000 | -0.479395000 | 4.548381000 |
| 1 | 13.715011000 | 1.703529000 | -4.207722000 |
| 1 | 13.597023000 | -1.984367000 | 4.224107000 |
| 6 | -2.575720000 | 1.334215000 | 0.157326000 |
| 6 | -2.686426000 | 2.256441000 | 1.210693000 |
| 6 | -3.565832000 | 1.368891000 | -0.839259000 |
| 6 | -3.729840000 | 3.176542000 | 1.268569000 |
| 1 | -1.938845000 | 2.253104000 | 1.998855000 |
| 6 | -4.620357000 | 2.272987000 | -0.782876000 |
| 1 | -3.510275000 | 0.672038000 | -1.669101000 |
| 6 | -4.716309000 | 3.195500000 | 0.271672000 |
| 1 | -3.787717000 | 3.881756000 | 2.090927000 |
| 1 | -5.374145000 | 2.276479000 | -1.563039000 |
| 7 | -5.788579000 | 4.127570000 | 0.326276000 |
| 6 | -6.436909000 | 4.390838000 | 1.563226000 |
| 6 | -6.208389000 | 4.795604000 | -0.855526000 |
| 6 | -6.787471000 | 5.702866000 | 1.921305000 |
| 6 | -6.736191000 | 3.342251000 | 2.448428000 |
| 6 | -7.574039000 | 4.991913000 | -1.118745000 |
| 6 | -5.263750000 | 5.267941000 | -1.781430000 |
| 6 | -7.430709000 | 5.953440000 | 3.131481000 |
| 1 | -6.553659000 | 6.519405000 | 1.246542000 |
| 6 | -7.363330000 | 3.605599000 | 3.664307000 |
| 1 | -6.474669000 | 2.325303000 | 2.176123000 |
| 6 | -7.978991000 | 5.653881000 | -2.275856000 |
| 1 | -8.310588000 | 4.623125000 | -0.412958000 |
| 6 | -5.679878000 | 5.912200000 | -2.944511000 |
| 1 | -4.206901000 | 5.125055000 | -1.583160000 |
| 6 | -7.719294000 | 4.909907000 | 4.013124000 |
| 1 | -7.694236000 | 6.974742000 | 3.391649000 |
| 1 | -7.587462000 | 2.781727000 | 4.335983000 |
| 6 | -7.037798000 | 6.114554000 | -3.198640000 |
| 1 | -9.039672000 | 5.796318000 | -2.462620000 |
| 1 | -4.934542000 | 6.270551000 | -3.648939000 |
| 1 | -8.214230000 | 5.110220000 | 4.958344000 |

| 1 | -7.357946000 | 6.623386000 | -4.102580000 |
| 1 | 9.476513000 | 1.976359000 | -0.915522000 |

**Table S6** Cartesian coordinates for the optimized geometry of **2b**.

Energy = -2223.60469586 au

| At. No | X | Y | Z |
|---|---|---|---|
| 6 | 1.924141000 | 0.616282000 | -0.185806000 |
| 6 | 1.969622000 | -0.783110000 | 0.097867000 |
| 6 | 0.778267000 | -1.519100000 | 0.180696000 |
| 6 | -0.444673000 | -0.874439000 | 0.006387000 |
| 6 | -0.507794000 | 0.516787000 | -0.256535000 |
| 6 | 0.681333000 | 1.241398000 | -0.350708000 |
| 1 | 0.655458000 | 2.299953000 | -0.591996000 |
| 6 | -2.633634000 | -0.355006000 | -0.189830000 |
| 6 | -4.025464000 | -0.399411000 | -0.273011000 |
| 6 | -4.725908000 | 0.787562000 | -0.535818000 |
| 6 | -4.004141000 | 1.990932000 | -0.719184000 |
| 6 | -2.616538000 | 2.028477000 | -0.649516000 |
| 6 | -1.909141000 | 0.851101000 | -0.386006000 |
| 1 | -2.089075000 | 2.967499000 | -0.791696000 |
| 7 | -1.736130000 | -1.387242000 | 0.063442000 |
| 6 | -2.087683000 | -2.775211000 | 0.266225000 |
| 1 | -3.045442000 | -2.839269000 | 0.788560000 |
| 1 | -1.333431000 | -3.257522000 | 0.891956000 |
| 1 | 0.828484000 | -2.577197000 | 0.415147000 |
| 1 | -4.565015000 | -1.335466000 | -0.175541000 |
| 1 | -2.166042000 | -3.328092000 | -0.678806000 |
| 6 | 3.243561000 | -1.517227000 | 0.353055000 |
| 6 | 3.508618000 | -2.721516000 | -0.310120000 |
| 6 | 4.169490000 | -1.050278000 | 1.315014000 |
| 6 | 4.674382000 | -3.438881000 | -0.024853000 |
| 1 | 2.809792000 | -3.087938000 | -1.056819000 |
| 6 | 5.334113000 | -1.744771000 | 1.621598000 |
| 1 | 3.956031000 | -0.124502000 | 1.837875000 |
| 6 | 5.233563000 | -4.680416000 | -0.518414000 |
| 6 | 5.586538000 | -2.939205000 | 0.940020000 |
| 1 | 6.013155000 | -1.365083000 | 2.378296000 |
| 6 | 4.817371000 | -5.626419000 | -1.461291000 |
| 6 | 6.459519000 | -4.876117000 | 0.173680000 |
| 7 | 6.668079000 | -3.807066000 | 1.037948000 |
| 6 | 5.611913000 | -6.745259000 | -1.697585000 |
| 1 | 3.884432000 | -5.490365000 | -2.001118000 |
| 6 | 7.256602000 | -6.001680000 | -0.054581000 |
| 6 | 6.817184000 | -6.927703000 | -0.998806000 |
| 1 | 5.298040000 | -7.486468000 | -2.426090000 |
| 1 | 8.184261000 | -6.160635000 | 0.485829000 |
| 1 | 7.419165000 | -7.810475000 | -1.193674000 |
| 6 | -6.208566000 | 0.778296000 | -0.622789000 |
| 6 | -6.974952000 | -0.026974000 | 0.230681000 |

| | | | |
|---|---|---|---|
| 6 | -6.876243000 | 1.580889000 | -1.577850000 |
| 6 | -8.367815000 | -0.031129000 | 0.130366000 |
| 1 | -6.482998000 | -0.630098000 | 0.988023000 |
| 6 | -8.261710000 | 1.599514000 | -1.698030000 |
| 1 | -6.283852000 | 2.180945000 | -2.261233000 |
| 6 | -9.421126000 | -0.728404000 | 0.839637000 |
| 6 | -9.006333000 | 0.792467000 | -0.833562000 |
| 1 | -8.736847000 | 2.213688000 | -2.456285000 |
| 6 | -9.437085000 | -1.662044000 | 1.881221000 |
| 6 | -10.648756000 | -0.297201000 | 0.268417000 |
| 7 | -10.382814000 | 0.635336000 | -0.728654000 |
| 6 | -10.658500000 | -2.154420000 | 2.333430000 |
| 1 | -8.507329000 | -1.999751000 | 2.330380000 |
| 6 | -11.876973000 | -0.794382000 | 0.713807000 |
| 6 | -11.862966000 | -1.723379000 | 1.752420000 |
| 1 | -10.682965000 | -2.880025000 | 3.140545000 |
| 1 | -12.814388000 | -0.478598000 | 0.267367000 |
| 1 | -12.804634000 | -2.124225000 | 2.115985000 |
| 6 | -11.370090000 | 1.277568000 | -1.567996000 |
| 1 | -11.011409000 | 2.265514000 | -1.866258000 |
| 1 | -11.590426000 | 0.696003000 | -2.472428000 |
| 1 | -12.296680000 | 1.415231000 | -1.005807000 |
| 6 | 7.783153000 | -3.665352000 | 1.947871000 |
| 1 | 7.978359000 | -2.605398000 | 2.125769000 |
| 1 | 7.599075000 | -4.155205000 | 2.912754000 |
| 1 | 8.680770000 | -4.099494000 | 1.500785000 |
| 6 | 3.148868000 | 1.450994000 | -0.364813000 |
| 6 | 3.278273000 | 2.666745000 | 0.317603000 |
| 6 | 4.165518000 | 1.067435000 | -1.270327000 |
| 6 | 4.396482000 | 3.478665000 | 0.102412000 |
| 1 | 2.511373000 | 2.967945000 | 1.025738000 |
| 6 | 5.286901000 | 1.855062000 | -1.505293000 |
| 1 | 4.063326000 | 0.127625000 | -1.802042000 |
| 6 | 4.830134000 | 4.751377000 | 0.640987000 |
| 6 | 5.394624000 | 3.067574000 | -0.817894000 |
| 1 | 6.048601000 | 1.526292000 | -2.204990000 |
| 6 | 4.294193000 | 5.644440000 | 1.575012000 |
| 6 | 6.071386000 | 5.053603000 | 0.017763000 |
| 7 | 6.390710000 | 4.036360000 | -0.874330000 |
| 6 | 4.992581000 | 6.810187000 | 1.879089000 |
| 1 | 3.345821000 | 5.428745000 | 2.059082000 |
| 6 | 6.779193000 | 6.219350000 | 0.324743000 |
| 6 | 6.221836000 | 7.090447000 | 1.259001000 |
| 1 | 4.586741000 | 7.509337000 | 2.603758000 |
| 1 | 7.734523000 | 6.443698000 | -0.139172000 |
| 1 | 6.753023000 | 8.002808000 | 1.514234000 |
| 6 | 7.599111000 | 3.959160000 | -1.664689000 |
| 1 | 7.913185000 | 4.964418000 | -1.956354000 |
| 1 | 8.422990000 | 3.477580000 | -1.122036000 |
| 1 | 7.404183000 | 3.392650000 | -2.578042000 |

| | | | |
|---|---|---|---|
| 1 | -4.553442000 | 2.910522000 | -0.892728000 |

**Table S7** Cartesian coordinates for the optimized geometry of **3a**.

Energy = -3550.89231642 au

| At. NO | X | Y | Z |
|---|---|---|---|
| 6 | -3.064127000 | -0.300488000 | -0.060569000 |
| 6 | -3.454813000 | -1.674367000 | -0.036800000 |
| 6 | -2.477629000 | -2.680700000 | -0.044760000 |
| 6 | -1.128842000 | -2.331258000 | -0.059848000 |
| 6 | -0.724490000 | -0.972794000 | -0.044556000 |
| 6 | -1.700855000 | 0.023631000 | -0.053218000 |
| 1 | -1.409169000 | 1.069130000 | -0.088985000 |
| 6 | 1.126647000 | -2.332012000 | -0.044140000 |
| 6 | 2.475251000 | -2.681798000 | -0.035637000 |
| 6 | 3.452766000 | -1.675883000 | -0.025738000 |
| 6 | 3.062561000 | -0.302047000 | 0.002424000 |
| 6 | 1.699457000 | 0.022663000 | -0.012653000 |
| 6 | 0.722882000 | -0.973203000 | -0.038135000 |
| 1 | 1.407879000 | 1.067741000 | 0.034419000 |
| 7 | -0.001305000 | -3.144442000 | -0.076612000 |
| 6 | -0.002868000 | -4.590797000 | -0.048840000 |
| 1 | 0.880264000 | -4.969349000 | -0.568760000 |
| 1 | -0.885213000 | -4.966351000 | -0.572225000 |
| 1 | -2.789084000 | -3.718554000 | 0.008604000 |
| 1 | 2.787485000 | -3.720227000 | -0.072086000 |
| 1 | -0.005733000 | -4.987773000 | 0.974356000 |
| 6 | -4.877757000 | -2.110094000 | 0.047662000 |
| 6 | -5.378390000 | -3.093619000 | -0.820780000 |
| 6 | -5.749320000 | -1.609729000 | 1.029734000 |
| 6 | -6.685183000 | -3.562105000 | -0.717134000 |
| 1 | -4.731622000 | -3.497581000 | -1.594489000 |
| 6 | -7.059426000 | -2.062074000 | 1.134470000 |
| 1 | -5.395611000 | -0.849286000 | 1.718063000 |
| 6 | -7.548602000 | -3.049196000 | 0.262557000 |
| 1 | -7.044131000 | -4.324656000 | -1.400132000 |
| 1 | -7.712687000 | -1.654452000 | 1.898632000 |
| 7 | -8.886002000 | -3.515480000 | 0.369891000 |
| 6 | -9.653575000 | -3.749691000 | -0.803942000 |
| 6 | -9.455694000 | -3.753364000 | 1.650309000 |
| 6 | -10.471541000 | -4.886645000 | -0.906205000 |
| 6 | -9.604952000 | -2.847937000 | -1.879346000 |
| 6 | -10.779902000 | -3.373796000 | 1.923529000 |
| 6 | -8.703679000 | -4.371808000 | 2.662304000 |
| 6 | -11.227577000 | -5.107469000 | -2.055504000 |
| 1 | -10.509878000 | -5.590877000 | -0.082021000 |
| 6 | -10.350727000 | -3.087421000 | -3.031565000 |
| 1 | -8.980880000 | -1.963922000 | -1.804338000 |
| 6 | -11.337017000 | -3.617708000 | 3.176981000 |

| | | | |
|---|---|---|---|
| 1 | -11.365160000 | -2.888928000 | 1.149522000 |
| 6 | -9.264135000 | -4.594549000 | 3.918265000 |
| 1 | -7.682082000 | -4.673559000 | 2.457346000 |
| 6 | -11.169770000 | -4.214230000 | -3.126996000 |
| 1 | -11.854808000 | -5.992276000 | -2.117306000 |
| 1 | -10.301207000 | -2.378884000 | -3.853503000 |
| 6 | -10.583962000 | -4.224694000 | 4.184024000 |
| 1 | -12.362810000 | -3.316801000 | 3.370113000 |
| 1 | -8.667244000 | -5.074023000 | 4.688966000 |
| 1 | -11.755033000 | -4.393356000 | -4.023602000 |
| 1 | -11.019162000 | -4.406552000 | 5.161781000 |
| 6 | 4.876910000 | -2.111707000 | -0.088012000 |
| 6 | 5.762629000 | -1.611513000 | -1.057331000 |
| 6 | 5.364996000 | -3.093846000 | 0.789077000 |
| 6 | 7.074806000 | -2.062351000 | -1.141366000 |
| 1 | 5.418519000 | -0.852212000 | -1.751808000 |
| 6 | 6.673930000 | -3.560563000 | 0.706163000 |
| 1 | 4.706947000 | -3.497650000 | 1.553312000 |
| 6 | 7.551722000 | -3.047355000 | -0.260464000 |
| 1 | 7.023548000 | -4.321593000 | 1.395704000 |
| 7 | 8.891756000 | -3.511154000 | -0.345419000 |
| 6 | 9.481026000 | -3.753345000 | -1.616054000 |
| 6 | 9.642766000 | -3.734501000 | 0.841115000 |
| 6 | 10.808082000 | -3.371436000 | -1.871694000 |
| 6 | 8.745487000 | -4.378362000 | -2.636116000 |
| 6 | 10.465846000 | -4.865937000 | 0.962074000 |
| 6 | 9.572243000 | -2.827320000 | 1.910761000 |
| 6 | 11.384061000 | -3.619668000 | -3.115743000 |
| 1 | 11.380775000 | -2.881429000 | -1.091562000 |
| 6 | 9.324819000 | -4.605440000 | -3.882707000 |
| 1 | 7.721770000 | -4.681821000 | -2.444671000 |
| 6 | 11.205538000 | -5.075922000 | 2.123963000 |
| 1 | 10.520913000 | -5.574301000 | 0.142409000 |
| 6 | 10.301696000 | -3.056075000 | 3.075521000 |
| 1 | 8.944084000 | -1.947576000 | 1.821378000 |
| 6 | 10.647420000 | -4.233320000 | -4.130852000 |
| 1 | 12.411775000 | -3.316901000 | -3.295294000 |
| 1 | 8.740505000 | -5.090038000 | -4.659816000 |
| 6 | 11.125954000 | -4.177312000 | 3.189588000 |
| 1 | 11.837047000 | -5.956551000 | 2.200190000 |
| 1 | 10.235345000 | -2.343469000 | 3.892744000 |
| 1 | 11.097364000 | -4.418546000 | -5.101276000 |
| 1 | 11.698478000 | -4.348081000 | 4.095996000 |
| 6 | -4.042130000 | 0.821514000 | -0.143414000 |
| 6 | -3.935918000 | 1.928965000 | 0.713844000 |
| 6 | -5.056113000 | 0.852843000 | -1.115816000 |
| 6 | -4.793180000 | 3.020661000 | 0.606450000 |
| 1 | -3.165218000 | 1.935046000 | 1.479370000 |
| 6 | -5.928607000 | 1.929891000 | -1.220414000 |
| 1 | -5.165736000 | 0.016175000 | -1.797866000 |

| | | | |
|---|---|---|---|
| 6 | -5.808073000 | 3.035119000 | -0.361936000 |
| 1 | -4.683694000 | 3.865057000 | 1.278604000 |
| 1 | -6.706354000 | 1.924910000 | -1.976630000 |
| 7 | -6.694074000 | 4.140840000 | -0.471387000 |
| 6 | -7.206361000 | 4.759477000 | 0.701437000 |
| 6 | -7.070367000 | 4.626996000 | -1.752793000 |
| 6 | -7.294580000 | 6.158286000 | 0.789618000 |
| 6 | -7.631692000 | 3.981796000 | 1.790764000 |
| 6 | -8.397389000 | 5.008880000 | -2.009607000 |
| 6 | -6.122029000 | 4.731978000 | -2.783501000 |
| 6 | -7.805675000 | 6.759673000 | 1.937776000 |
| 1 | -6.961735000 | 6.766166000 | -0.044932000 |
| 6 | -8.123976000 | 4.593524000 | 2.941651000 |
| 1 | -7.573009000 | 2.900461000 | 1.727521000 |
| 6 | -8.759867000 | 5.491999000 | -3.265078000 |
| 1 | -9.137506000 | 4.924889000 | -1.221031000 |
| 6 | -6.498840000 | 5.198811000 | -4.040917000 |
| 1 | -5.093652000 | 4.444740000 | -2.592214000 |
| 6 | -8.219249000 | 5.984189000 | 3.022714000 |
| 1 | -7.866267000 | 7.843160000 | 1.988126000 |
| 1 | -8.448673000 | 3.975966000 | 3.774326000 |
| 6 | -7.816859000 | 5.586096000 | -4.290446000 |
| 1 | -9.791034000 | 5.782641000 | -3.445044000 |
| 1 | -5.751517000 | 5.272825000 | -4.825893000 |
| 1 | -8.610023000 | 6.456741000 | 3.918543000 |
| 1 | -8.104832000 | 5.955948000 | -5.269637000 |
| 1 | 7.739398000 | -1.654882000 | -1.895794000 |
| 6 | 4.039936000 | 0.819182000 | 0.102679000 |
| 6 | 3.942002000 | 1.931646000 | -0.749063000 |
| 6 | 5.044323000 | 0.844841000 | 1.085159000 |
| 6 | 4.798188000 | 3.022661000 | -0.627023000 |
| 1 | 3.178607000 | 1.942144000 | -1.521821000 |
| 6 | 5.915803000 | 1.921212000 | 1.204403000 |
| 1 | 5.147390000 | 0.004368000 | 1.763516000 |
| 6 | 5.803659000 | 3.031356000 | 0.351174000 |
| 1 | 4.695382000 | 3.870930000 | -1.295339000 |
| 1 | 6.686180000 | 1.911814000 | 1.968088000 |
| 7 | 6.688736000 | 4.136326000 | 0.475394000 |
| 6 | 7.212692000 | 4.761049000 | -0.689040000 |
| 6 | 7.052501000 | 4.615414000 | 1.763055000 |
| 6 | 7.302175000 | 6.160272000 | -0.768869000 |
| 6 | 7.648509000 | 3.989053000 | -1.778272000 |
| 6 | 8.376745000 | 4.996709000 | 2.034679000 |
| 6 | 6.094335000 | 4.713793000 | 2.785281000 |
| 6 | 7.824764000 | 6.767610000 | -1.908686000 |
| 1 | 6.961299000 | 6.763771000 | 0.065612000 |
| 6 | 8.152331000 | 4.606753000 | -2.920945000 |
| 1 | 7.588868000 | 2.907420000 | -1.721395000 |
| 6 | 8.726898000 | 5.472769000 | 3.296323000 |
| 1 | 9.124349000 | 4.917856000 | 1.252670000 |

| 6 | 6.458818000 | 5.173559000 | 4.048915000 |
|---|---|---|---|
| 1 | 5.068069000 | 4.426919000 | 2.582496000 |
| 6 | 8.248830000 | 5.997795000 | -2.993613000 |
| 1 | 7.886168000 | 7.851330000 | -1.952644000 |
| 1 | 8.485055000 | 3.993547000 | -3.753669000 |
| 6 | 7.774121000 | 5.560270000 | 4.313217000 |
| 1 | 9.756094000 | 5.763062000 | 3.487773000 |
| 1 | 5.704000000 | 5.242520000 | 4.827151000 |
| 1 | 8.648589000 | 6.474995000 | -3.882990000 |
| 1 | 8.052511000 | 5.924630000 | 5.297224000 |

**Table S7** Cartesian coordinates for the optimized geometry of **3b**.

Energy = -2779.20173492 au

| At. NO | X | Y | Z |
|---|---|---|---|
| 6 | 3.300853000 | 0.239996000 | -0.111976000 |
| 6 | 3.680013000 | -1.114793000 | 0.134802000 |
| 6 | 2.698055000 | -2.114630000 | 0.200614000 |
| 6 | 1.355888000 | -1.774799000 | 0.043232000 |
| 6 | 0.962448000 | -0.432970000 | -0.188734000 |
| 6 | 1.944271000 | 0.555652000 | -0.263312000 |
| 1 | 1.666332000 | 1.583542000 | -0.476924000 |
| 6 | -0.892757000 | -1.785360000 | -0.141304000 |
| 6 | -2.237213000 | -2.141206000 | -0.227283000 |
| 6 | -3.203639000 | -1.153436000 | -0.469012000 |
| 6 | -2.806727000 | 0.211230000 | -0.615553000 |
| 6 | -1.446344000 | 0.539244000 | -0.541060000 |
| 6 | -0.479702000 | -0.440820000 | -0.313123000 |
| 1 | -1.151687000 | 1.580425000 | -0.634108000 |
| 7 | 0.223710000 | -2.581435000 | 0.090882000 |
| 6 | 0.214459000 | -4.017469000 | 0.260706000 |
| 1 | -0.710208000 | -4.322124000 | 0.756620000 |
| 1 | 1.049901000 | -4.317776000 | 0.897417000 |
| 1 | 2.999139000 | -3.136017000 | 0.408455000 |
| 1 | -2.550944000 | -3.177341000 | -0.156735000 |
| 1 | 0.291535000 | -4.550995000 | -0.695528000 |
| 6 | 5.094359000 | -1.531081000 | 0.365702000 |
| 6 | 5.630087000 | -2.621904000 | -0.329739000 |
| 6 | 5.893893000 | -0.880874000 | 1.334669000 |
| 6 | 6.935552000 | -3.049318000 | -0.068825000 |
| 1 | 5.029755000 | -3.125287000 | -1.082312000 |
| 6 | 7.192872000 | -1.287198000 | 1.617929000 |
| 1 | 5.473728000 | -0.044491000 | 1.882316000 |
| 6 | 7.767786000 | -4.110395000 | -0.597271000 |
| 6 | 7.713418000 | -2.371378000 | 0.904841000 |
| 1 | 7.770980000 | -0.775812000 | 2.380878000 |
| 6 | 7.578096000 | -5.104424000 | -1.563273000 |
| 6 | 9.012185000 | -4.026991000 | 0.084516000 |
| 7 | 8.970564000 | -2.960452000 | 0.975608000 |

| | | | |
|---|---|---|---|
| 6 | 8.612575000 | -5.996956000 | -1.831969000 |
| 1 | 6.634042000 | -5.179785000 | -2.095616000 |
| 6 | 10.050653000 | -4.925747000 | -0.176176000 |
| 6 | 9.833634000 | -5.905921000 | -1.142816000 |
| 1 | 8.475863000 | -6.773234000 | -2.578539000 |
| 1 | 10.995065000 | -4.873816000 | 0.356085000 |
| 1 | 10.625466000 | -6.615878000 | -1.363296000 |
| 6 | -4.619377000 | -1.606969000 | -0.600614000 |
| 6 | -5.184861000 | -2.436414000 | 0.375273000 |
| 6 | -5.390057000 | -1.267338000 | -1.736887000 |
| 6 | -6.492660000 | -2.907895000 | 0.225212000 |
| 1 | -4.606250000 | -2.699285000 | 1.256369000 |
| 6 | -6.690489000 | -1.725203000 | -1.914491000 |
| 1 | -4.945610000 | -0.636651000 | -2.499063000 |
| 6 | -7.352398000 | -3.752607000 | 1.028141000 |
| 6 | -7.242307000 | -2.541010000 | -0.921952000 |
| 1 | -7.247063000 | -1.457223000 | -2.806801000 |
| 6 | -7.196773000 | -4.415120000 | 2.250515000 |
| 6 | -8.584330000 | -3.859247000 | 0.327251000 |
| 7 | -8.508346000 | -3.108568000 | -0.840490000 |
| 6 | -8.252523000 | -5.171652000 | 2.752499000 |
| 1 | -6.262703000 | -4.341002000 | 2.800383000 |
| 6 | -9.644145000 | -4.623941000 | 0.823486000 |
| 6 | -9.461057000 | -5.273132000 | 2.042977000 |
| 1 | -8.142585000 | -5.690916000 | 3.699558000 |
| 1 | -10.579484000 | -4.719160000 | 0.281280000 |
| 1 | -10.270183000 | -5.872907000 | 2.449482000 |
| 6 | -9.551606000 | -2.990393000 | -1.835042000 |
| 1 | -9.468134000 | -2.025674000 | -2.340585000 |
| 1 | -9.502467000 | -3.787755000 | -2.587783000 |
| 1 | -10.529343000 | -3.028128000 | -1.348627000 |
| 6 | 10.029559000 | -2.581069000 | 1.884425000 |
| 1 | 9.973192000 | -1.508875000 | 2.085699000 |
| 1 | 9.973965000 | -3.120997000 | 2.838486000 |
| 1 | 10.999696000 | -2.783682000 | 1.424217000 |
| 6 | 4.290314000 | 1.347729000 | -0.262975000 |
| 6 | 4.137908000 | 2.530776000 | 0.470001000 |
| 6 | 5.355294000 | 1.252461000 | -1.188708000 |
| 6 | 5.029728000 | 3.592123000 | 0.285257000 |
| 1 | 3.331105000 | 2.612679000 | 1.192948000 |
| 6 | 6.255549000 | 2.292090000 | -1.394551000 |
| 1 | 5.470404000 | 0.337047000 | -1.759052000 |
| 6 | 5.158502000 | 4.908011000 | 0.876666000 |
| 6 | 6.083668000 | 3.466441000 | -0.655792000 |
| 1 | 7.063732000 | 2.181680000 | -2.110509000 |
| 6 | 4.439826000 | 5.609941000 | 1.850302000 |
| 6 | 6.285242000 | 5.519913000 | 0.263006000 |
| 7 | 6.822656000 | 4.644358000 | -0.673763000 |
| 6 | 4.847916000 | 6.893906000 | 2.202309000 |
| 1 | 3.575571000 | 5.156964000 | 2.327871000 |

| | | | |
|---|---|---|---|
| 6 | 6.702698000 | 6.805898000 | 0.618313000 |
| 6 | 5.968274000 | 7.481575000 | 1.591128000 |
| 1 | 4.298474000 | 7.446947000 | 2.957891000 |
| 1 | 7.572220000 | 7.268222000 | 0.162090000 |
| 1 | 6.273111000 | 8.482084000 | 1.883999000 |
| 6 | 8.006964000 | 4.884045000 | -1.467893000 |
| 1 | 8.080097000 | 5.947506000 | -1.707991000 |
| 1 | 8.925575000 | 4.576692000 | -0.951265000 |
| 1 | 7.935285000 | 4.334168000 | -2.409119000 |
| 6 | -3.779862000 | 1.326619000 | -0.809977000 |
| 6 | -4.877659000 | 1.498209000 | 0.042960000 |
| 6 | -3.562777000 | 2.274182000 | -1.836592000 |
| 6 | -5.736758000 | 2.584723000 | -0.132895000 |
| 1 | -5.053826000 | 0.788312000 | 0.844373000 |
| 6 | -4.400450000 | 3.369240000 | -2.032931000 |
| 1 | -2.714904000 | 2.134924000 | -2.500659000 |
| 6 | -6.923967000 | 3.042690000 | 0.560363000 |
| 6 | -5.493812000 | 3.516148000 | -1.176769000 |
| 1 | -4.197693000 | 4.078702000 | -2.828991000 |
| 6 | -7.655059000 | 2.564157000 | 1.652617000 |
| 6 | -7.345048000 | 4.230115000 | -0.096762000 |
| 7 | -6.483064000 | 4.493160000 | -1.156219000 |
| 6 | -8.778496000 | 3.268540000 | 2.078531000 |
| 1 | -7.348550000 | 1.655013000 | 2.161970000 |
| 6 | -8.467105000 | 4.944986000 | 0.332108000 |
| 6 | -9.175687000 | 4.446420000 | 1.423885000 |
| 1 | -9.352470000 | 2.907376000 | 2.926318000 |
| 1 | -8.779599000 | 5.861582000 | -0.158030000 |
| 1 | -10.051098000 | 4.984193000 | 1.776371000 |
| 6 | -6.549231000 | 5.644165000 | -2.028437000 |
| 1 | -7.592531000 | 5.932198000 | -2.178999000 |
| 1 | -6.001703000 | 6.506104000 | -1.625368000 |
| 1 | -6.129816000 | 5.389600000 | -3.004552000 |