Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Contents

1 General Considerations

Et_2O (Sigma-Aldrich), THF (Roth, 99%), *n*-hexane (Roth, 98%) were dried over sodium and distilled prior to use. $MgSO_4$ (Sigma-Aldrich, 99.5%), NaOH (Honeywell, 99%), *n*-BuLi (Sigma-Aldrich, 2.5 M in hexane), 1-bromo-3,5-di-tert-butylbenzene (98% ArkPharm, procured via ChemPur). $CDCl_3$ (Roth, 99.8%), $Li[N(SiMe_3)_2]$ (Sigma-Aldrich), $Na[N(SiMe_3)_2]$ (Sigma-Aldrich) and $K[N(SiMe_3)_2]$ (Sigma-Aldrich) were used as received. C_6D_6 (Roth, 99.5%) was dried over sodium and distilled prior to use. The protonated ligand (^{dtbp}Cbz)–H was prepared according to literature protocols.[1] $Rb[N(SiMe_3)_2]$ and $Cs[N(SiMe_3)_2]$ were prepared according to literature protocols.[2]

NMR spectra were acquired on a Bruker Advance 400 MHz spectrometer. Reported chemical shifts are referenced to the ^{1}H and ^{13}C NMR resonances of the deuterated solvent.[3] Coupling constants *J* are given in Hertz as positive values regardless of their real individual sign. ^{1}H and $^{13}C\{^1H\}$ NMR spectra were obtained at 400.1 and 100.6 MHz, respectively.

IR spectra were recorded on a Bruker Alpha FT-IR spectrometer using the ATR technique (attenuated total reflection) on powdered samples, and the data are quoted in wavenumbers (cm^{-1}). The intensities of the absorption bands are indicated as follows: vs = very strong, s = strong, m=medium, w = weak, vw = very weak.

Melting points were measured with a Thermo Fischer Scientific digital melting point apparatus of the IA9300 series and are not corrected. Pure samples of the compounds were sealed in a capillary tube under argon prior to measurement.

PL measurements in the solid state were performed with a PTI QuantaMaster™ 8075-22 fluorometer with double monochromator (Horiba Jobin Yvon GmbH). Solid samples (crystalline powders) were measured as dispersions in a thin layer of viscous polyfluoroether oil (ABCR GmbH) placed between two 1 mm thin quartz plates. The latter were mounted on the holder and emission was collected at ca. 30° angle relative to the excitation light beam. For detection a R928 photomultiplier (Horiba Jobin Yvon GmbH) was used. All emission spectra were corrected for the wavelength dependent response of the spectrometer and detector. Emission decay traces were recorded with a Delta Diode™ (HORIBA Jobin Yvon GmbH, Model DD-375L, λ_{Exc} = 375 nm, pulse width 70 ps, power 1.8 mW) or a PTI XenonFlash™ (before the emission monochromator, frequence 300 MHz, lifetime > 6 µs). Several thousand traces were acquired and averaged. PL quantum yields at ambient temperature were determined using an integrating sphere out of optical PTFE, which was installed into the sample chamber of the spectrometer, according to the method of de Mello et al.[4] The uncertainty of these measurements was estimated to be $\pm$ 10%.

PL measurements in solution were recorded with a resolution of ±1 nm using a photoluminescence spectrometer Horiba Jobin Yvon SpexFluorolog 3 (Horiba Jobin Yvon GmbH), equipped with a 450 W xenon lamp, double monochromators, Ulbricht sphere, and photomultiplier as the detector (90° angle between excitation source and detector). The determination of the absolute QY was performed as suggested by Friend.[4] The diffuse reflection of the sample was determined under excitation. Afterward, the emission was measured for the respective excitation wavelength. Integration over the reflected and emitted photons in the wavelength range of 390–700 nm using an Ulbricht sphere allowed

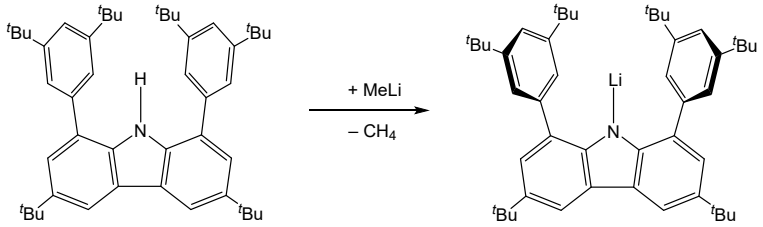
for the absolute QY calculation. Standard corrections were used for the spectral power of the excitation source, the reflection behavior of the Ulbricht sphere, and the sensitivity of the detector. The QY was obtained for samples in solution that were deposited in quartz-glass tubes. The sample holder for determining the absolute QY in an Ulbricht sphere was constructed according to Friend.[4]

Single crystals were mounted in perfluoropolyalkyl ether oil on a cryo loop and then brought into the cold nitrogen stream of a low-temperature device (Oxford Cryosystems Cryostream unit) so that the oil solidified. Diffraction data were collected using a Stoe IPDS II diffractometer and graphite-monochromated Mo-Kα (0.71073 Å) or Ga-Kα (1.34143 Å) radiation. The structures were solved by direct methods with SHELXS[5] intrinsic phasing with SHELXT[6] followed by full-matrix least-squares refinement using SHELXL-2014/7[7] and the ShelXle GUI.[8] All non-hydrogen atoms were refined anisotropically. The contribution of the hydrogen atoms, in their calculated positions, was included in the refinement using a riding model.

2 Syntheses

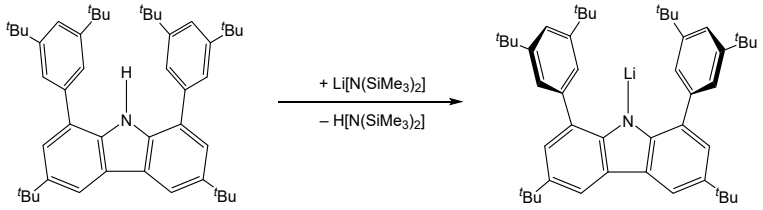
2.1 [(^{dtbp}Cbz)Li] (1a)

a)



To a solid mixture of (^{dtbp}Cbz)–H (203 mg, 0.301 mmol) and MeLi (7.0 mg, 0.318 mmol) 5 ml of toluene was added. The colourless mixture was sonicated for one hour and heated up to 125 °C over night. A yellow, luminescent solution formed. Volatiles were removed under reduced pressure and the residue was dried *in vacuo* for one hour at 100 °C. The residue was dissolved in *n*-hexane, dried *in vacuo* and dissolved again in *n*-hexane. The resulting yellow solution was filtered *via* a syringe filter. The solvent was evaporated to incipient crystallisation and left undisturbed until single crystals suitable for X-ray diffraction deposited.

b)



To a solid mixture of (^{dtbp}Cbz)–H (400.0 mg, 0.610 mmol) and Li[N(SiMe$_3$)$_2$] (112.3 mg. 0.671 mmol) 20 ml of *n*-hexane were added. The mixture was stirred for 3 days at 70 °C and a yellow, luminescent solution formed. Volatiles were removed under reduced pressure and the residue was dried in vacuo. The residue was redissolved in *n*-hexane and filtered via a syringe filter and dried again affording the product as a yellow crystalline solid (334.4 mg, 0.505 mmol, 83%).

^{1}H NMR (400 MHz, C_6D_6): δ (ppm) = 1.32 (s, 36 H, Ar-^{t}Bu); 1.63 (s, 18 H, Carb-^{t}Bu); 7.50 (br, 2 H, *p*-C*H*); 7.65 (d, J_{HH} = 2.0 Hz, 2 H, C^{2,7}*H*); 7.81 (br, 4 H, *o*-C*H*); 8.70 (br, 2 H, C^{4,5}*H*).
^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ (ppm) = 31.88 (s, Ar-C(*C*H$_3$)); 32.75 (s, Carb-C(*C*H$_3$)); 34.85 (s, Carb-*C*(CH$_3$)); 35.14 (s, Ar-*C*(CH$_3$)); 116.09 (s, *C*^{4,5}H); 120.91 (s, *p*-*C*H); 123.51 (s, *C*^{2,7}H); 123.67 (s, *o*-*C*H); 126.99 (s); 127.35 (s); 137.54 (s); 146.07 (s); 149.02 (s); 152.33 (s).
IR (ATR): ũ (cm^{-1}) = 3470 (vw), 2955 (vs), 2904 (w), 2868 (w), 1590 (m), 1492 (m), 1477 (m), 1463 (w), 1393 (w), 1362 (s), 1287 (s), 1245 (vs), 1202 (vw), 924 (vw), 900 (vw), 868 (s), 720 (m), 698 (w), 673 (vw), 654 (vw), 603 (w), 578 (w), 528 (m), 492 (s), 484 (s), 475 (m), 463 (s), 431 (s), 419 (m), 411 (m), 380 (vw).
PL ($\lambda_{max,emission}$ [nm], τ_{solid} [ns], Φ_{solid} [%]): 520 (14, 12%).
Mp.: 309 °C.

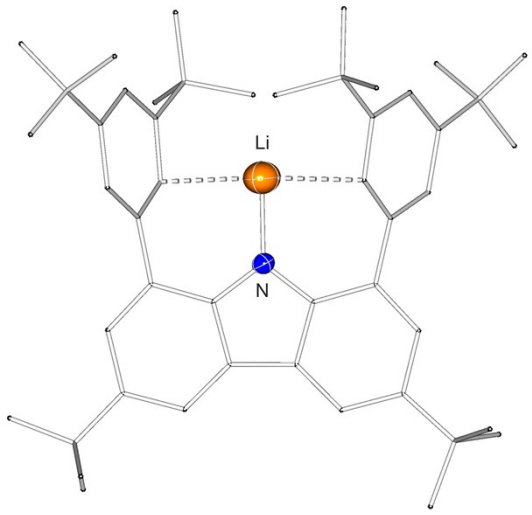


Figure S1: Molecular structure of **1a** (only one molecule of the asymmetric unit shown, disorder not displayed). Selected bond lengths [Å] and angles [°]: N1–C1 1.3742(14), N1–C12 1.3762(14), N1–Li1 1.877(3), Li1–C14 2.442(3), Li1–C40 2.419(3).

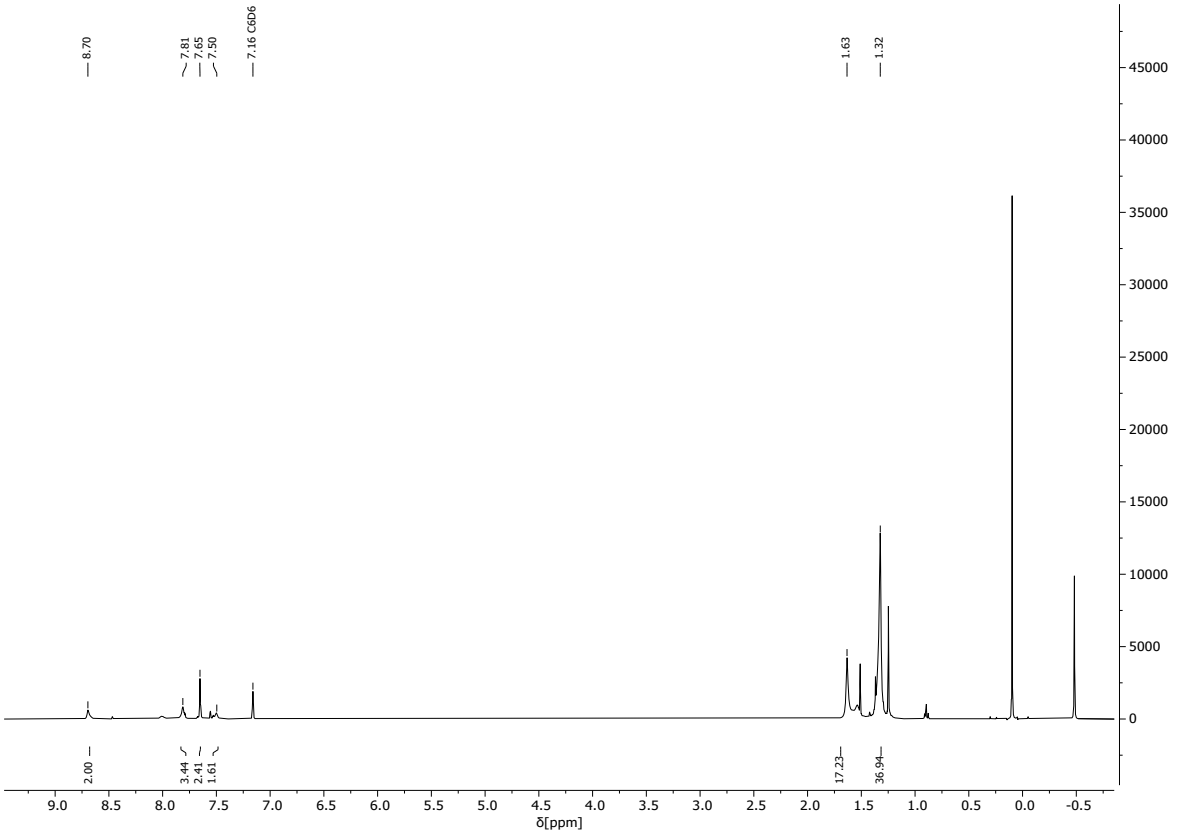


Figure S2: ^{1}H NMR spectrum of **1a**.

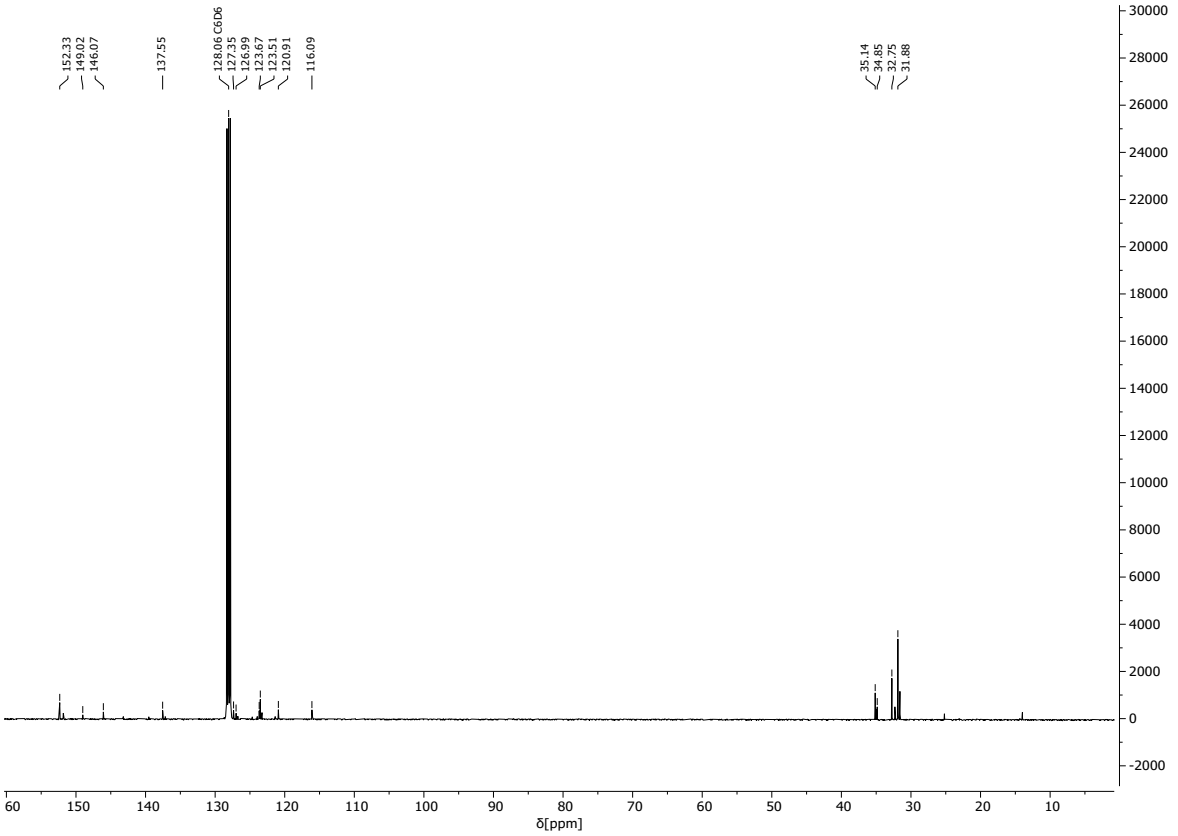


Figure S3: $^{13}C\{^{1}H\}$ NMR spectrum of **1a**.

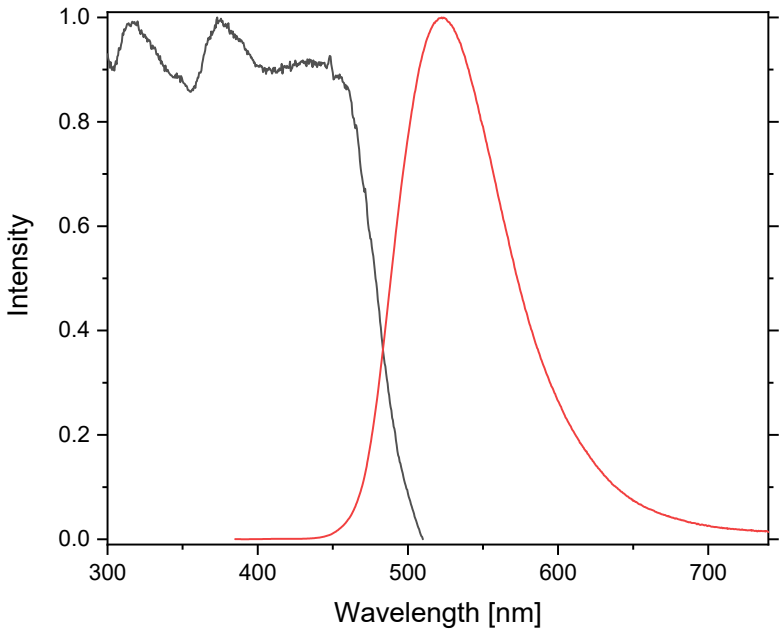


Figure S4: Photoluminescence emission (PL) and excitation (PLE) spectra of compound **1a** at 295 K.

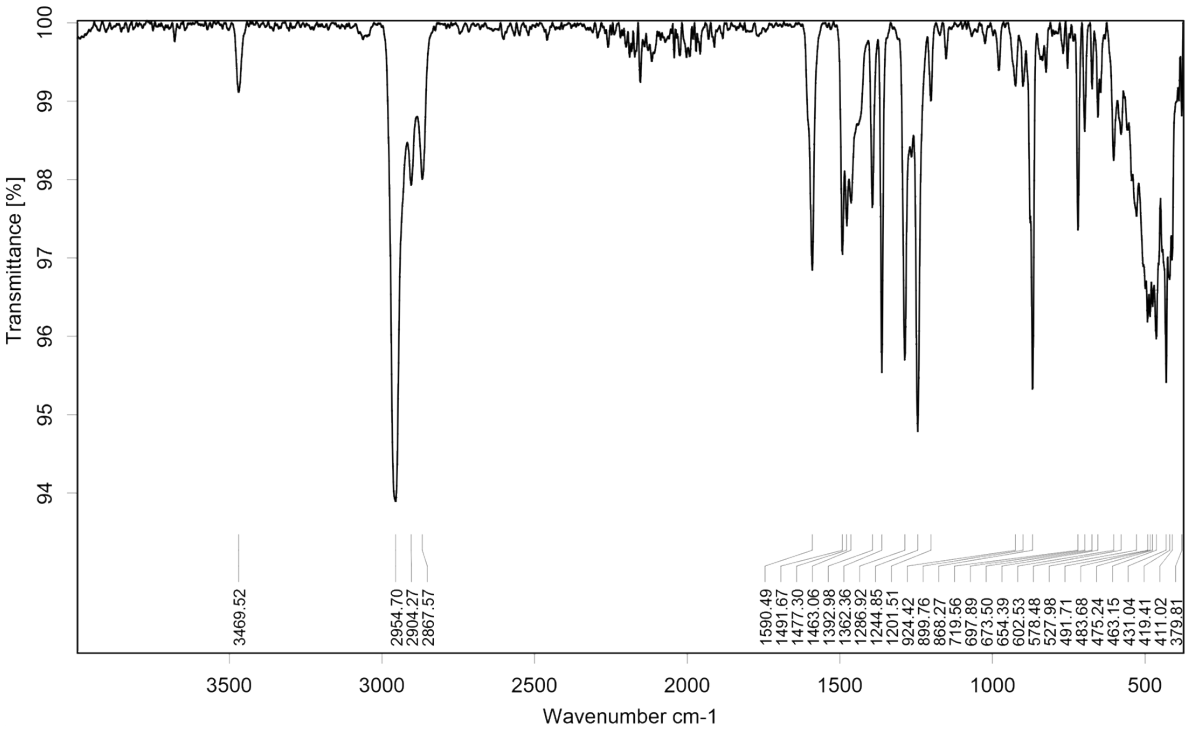
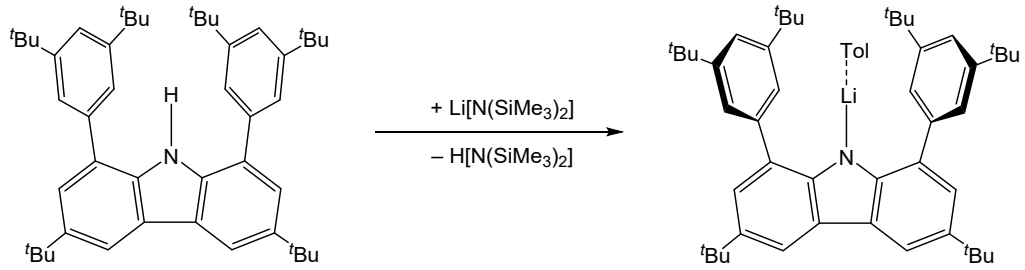


Figure S5: IR spectrum of **1a**.

2.2 [(^{dtbp}Cbz)Li(Tol)] (1b)



To a solid mixture of (^{dtbp}Cbz)–H (300 mg, 0.457 mmol) and Li[N(SiMe$_3$)$_2$] (90 mg, 0.534 mmol) 20 ml of toluene were added. The mixture was stirred for 3 days at 70 °C and a yellow, luminescent solution formed. Volatiles were removed under reduced pressure and the residue was dried *in vacuo*. The residue was redissolved in toluene. The solvent was evaporated to incipient crystallisation and left undisturbed until single crystals suitable for X-ray diffraction were obtained. Volatiles were removed under reduced pressure and the residue was dried *in vacuo* affording the product as a yellow crystalline solid (41.1 mg, 0.032 mmol, 23%).

^{1}H NMR (400 MHz, C_6D_6): δ (ppm) = 1.32 (s, 36 H, Ar-^{t}Bu); 1.64 (s, 18 H, Carb-^{t}Bu); 2.12 (s, Tol-CH_3), 7.05 (m, Ar-Tol), 7.50 (br, 2 H, *p*-C*H*); 7.65 (d, J_{HH} = 2.0 Hz, 2 H, C^{2,7}*H*); 7.81 (br, 4 H, *o*-C*H*); 8.70 (br, 2 H, C^{4,5}*H*).
^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ (ppm) = 21.44 (s, Tol-*C*H$_3$); 31.89 (s, Ar-C(*C*H$_3$)$_3$); 32.76 (s, Carb-C(*C*H$_3$)$_3$); 34.85 (s, Carb-*C*(CH$_3$)$_3$); 35.15 (s, Ar-*C*(CH$_3$)$_3$); 116.06 (s, *C*^{4,5}H); 120.93 (s, *p*-*C*H); 123.51 (s, C^{2,7}*H*); 123.68 (s, *o*-C*H*); 125.69 (s, Tol-*C*H(4)); 126.98 (s); 127.36 (s); 128.56 (s, Tol-*C*H(3,5)); 129.34 (s, Tol-*C*H(2,6)); 137.51 (s); 137.89 (s, Tol-*C*H(1)); 146.04 (s); 149.02 (s); 150.50 (s).
IR (ATR): ũ (cm^{-1}) = 2954 (vs), 2903 (w), 2866 (w), 1589 (s), 1492 (w), 1461 (m), 1393 (w), 1361 (s), 1286 (s), 1268 (m), 1235 (vs), 1202 (w), 1181 (w), 1028 (w), 932 (vw), 899 (vw), 865 (vs), 846 (m), 750 (m), 720 (s), 699 (m), 675 (vw), 645 (w), 516 (w), 467 (w).
PL ($\lambda_{max,emission}$ [nm], τ_{solid} [ns], Φ_{solid} [%]): 540, 580 (13, 8%).
Mp.: 286 °C.

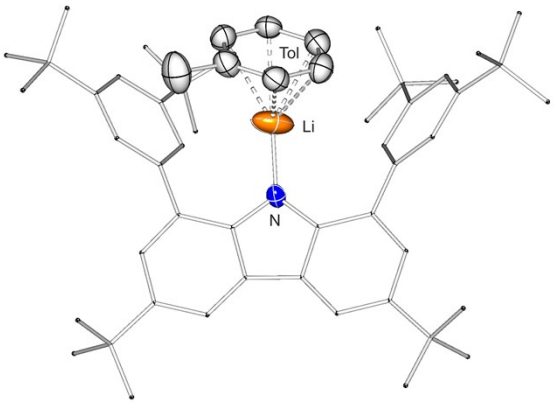


Figure S6: Molecular structure of **1b** (disorder of toluene not shown). Selected bond lengths [Å] and angles [°]: Li1–N1 1.879(3), Li1–C52 2.377(6), Li1–C53 2.425(5), Li1–C51 2.493(6), Li1–C54 2.585(5), Li1–C50 2.648(5), Li-centroid(Tol): 2.124(4).

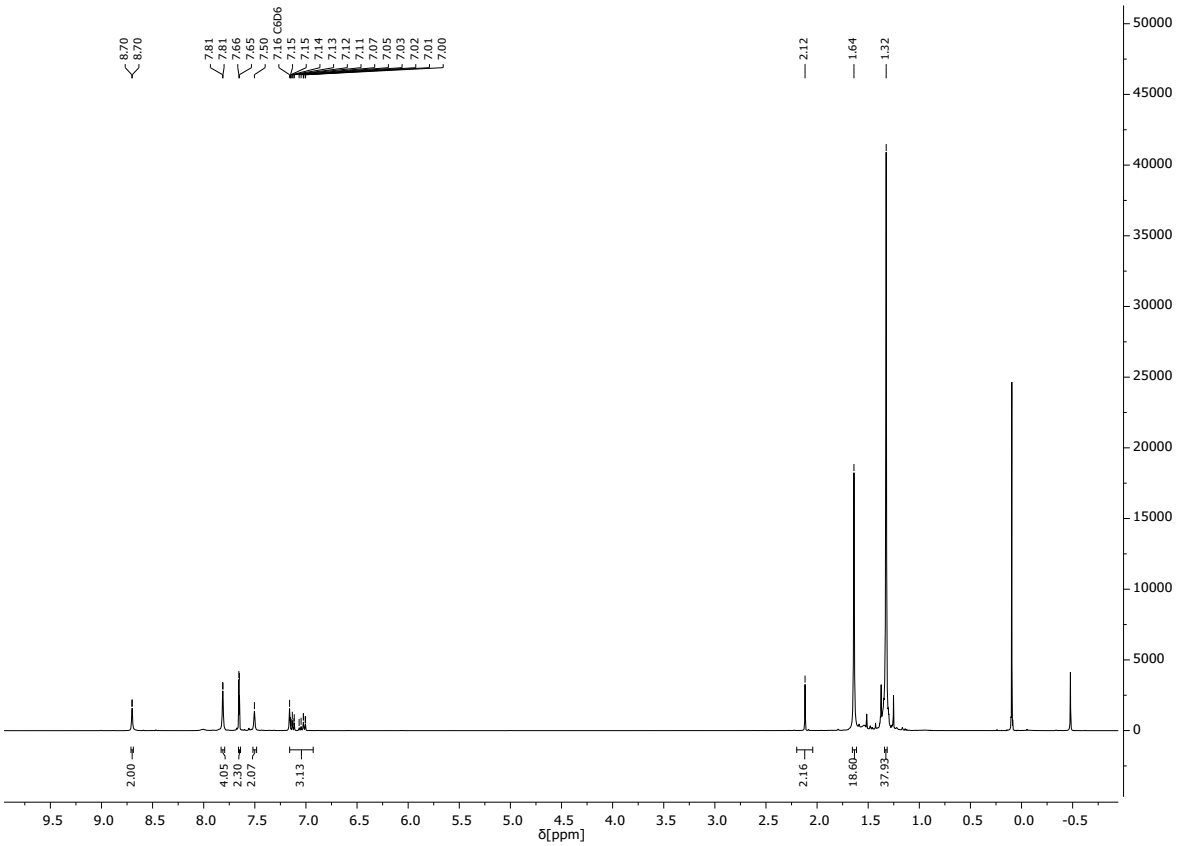


Figure S7: ^{1}H NMR spectrum of **1b**.

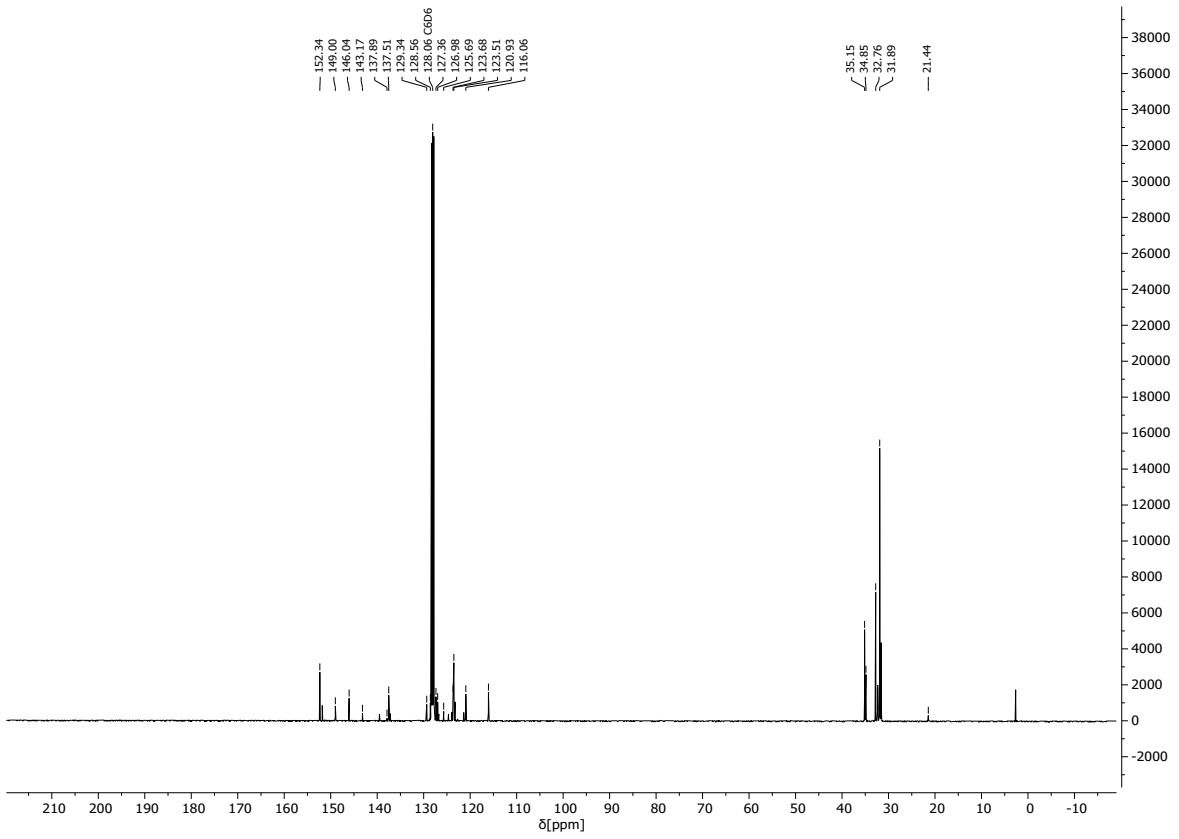


Figure S8: ^{13}C{^{1}H} NMR spectrum of **1b**.

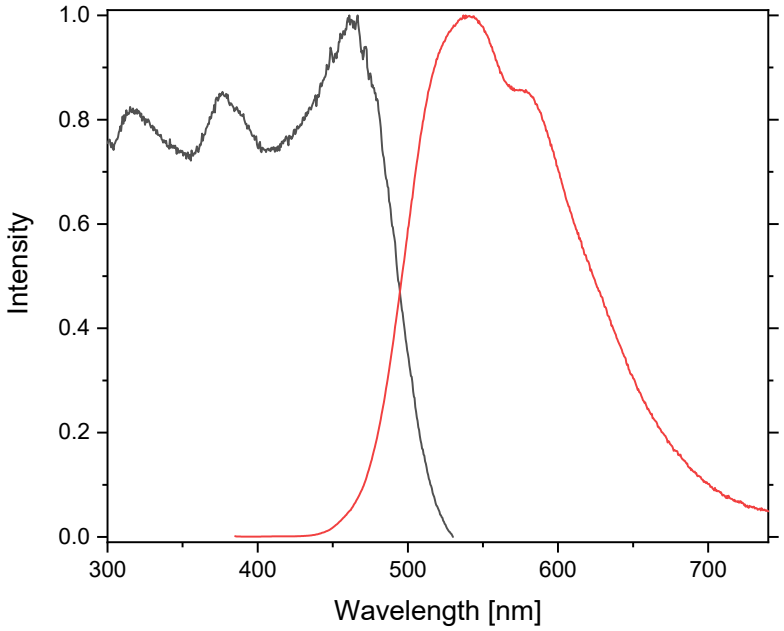


Figure S9: Photoluminescence emission (PL) and excitation (PLE) spectra of compound **1b** at 295 K.

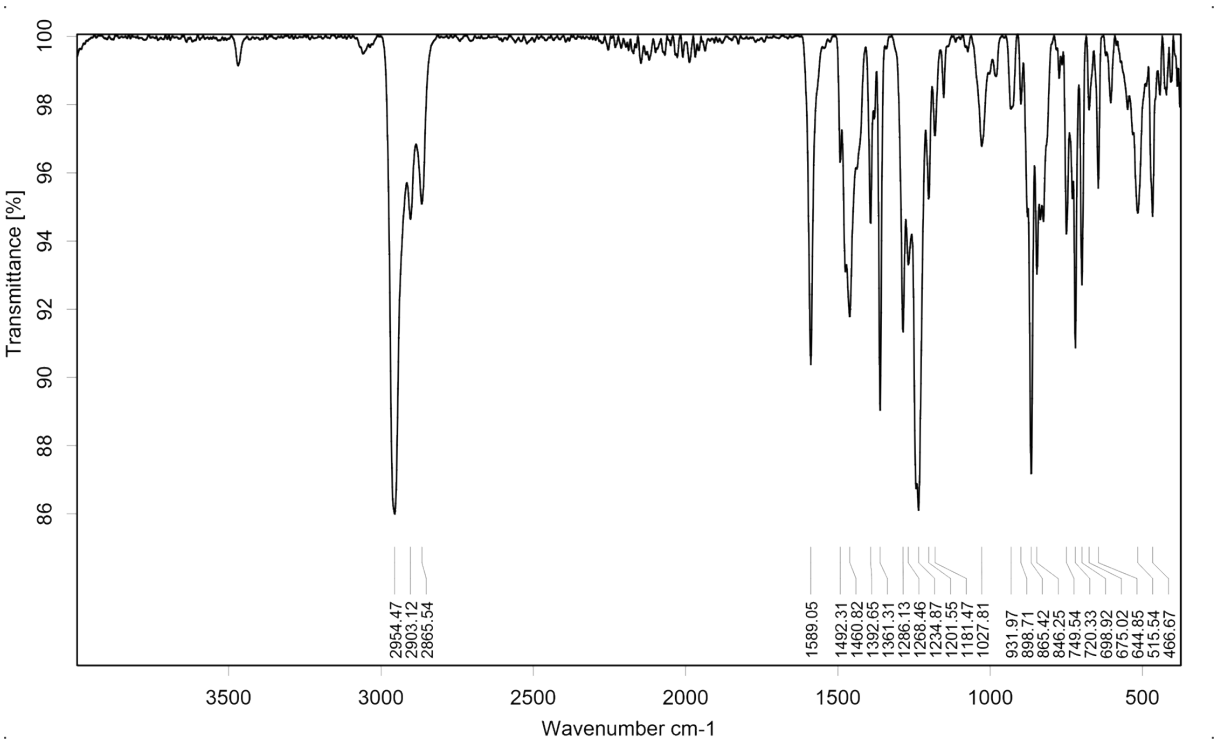
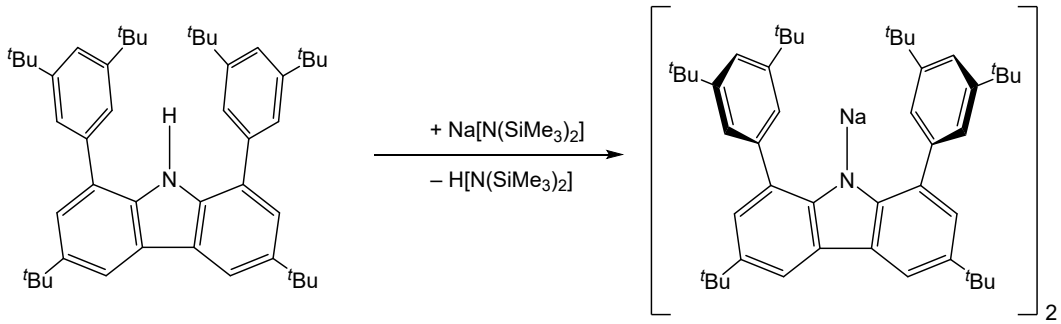


Figure S10: IR spectrum of **1b**.

2.3 [(^{dtbp}Cbz)Na] (2a)



To a solid mixture of (^{dtbp}Cbz)–H (400 mg, 0.610 mmol) and Na[N(SiMe$_3$)$_2$] (132 mg, 0.730 mmol) 20 ml of *n*-hexane was added. The colourless mixture was stirred for 3 days at 70 °C and a yellow, luminescent solution formed. Volatiles were removed under reduced pressure and the residue was dried *in vacuo*. The residue was dissolved in *n*-hexane and filtered *via* a syringe filter. The solvent was evaporated to incipient crystallisation and left undisturbed until single crystals suitable for X-ray diffraction deposited. The supernatant was removed with a syringe, volatiles were removed under reduced pressure and the residue was dried *in vacuo* affording the product as a yellow crystalline solid (373.0 mg, 0.550 mmol, 90 %).

^{1}H NMR (400 MHz, C_6D_6): δ (ppm) = 1.30 (s, 36 H, Ar-^{t}Bu); 1.66 (s, 18 H, Carb-^{t}Bu); 7.46 (br, 2 H, *p*-C*H*); 7.68 (d, J_{HH} = 2.2 Hz, 2 H, C^{2,7}*H*); 7.83 (br, 4 H, *o*-C*H*); 8.71 (br, 2 H, C^{4,5}*H*).
^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ (ppm) = 31.91 (s, Ar-C(*C*H$_3$)$_3$); 32.87 (s, Carb-C(*C*H$_3$)$_3$); 34.89 (s, Carb-*C*(CH$_3$)$_3$); 35.06 (s, Ar-*C*(CH$_3$)$_3$); 116.25 (s, *C*^{4,5}H); 120.38 (s, *p*-*C*H); 123.02 (s, *C*^{2,7}H); 123.75 (s, *o*-*C*H); 127.05 (s); 127.48 (s); 136.43 (s); 146.01 (s); 149.98 (s); 151.53 (s).
IR (ATR): ũ (cm^{-1}) = 3468 (vw), 2954 (vs), 2903 (w), 2866 (w), 1590 (m), 1491 (m), 1477 (m), 1462 (m), 1393 (m), 1362 (s), 1287 (s), 1245 (vs), 1201 (w), 1177 (w), 928 (m), 899 (vw), 868 (vs), 840 (s), 823 (m), 754 (vw), 719 (m), 697 (w), 674 (w), 654 (w), 603 (vw), 464 (w), 432 (vw), 417 (w), 382 (vw).
PL ($\lambda_{max,emission}$ [nm], τ_{solid} [ns], Φ_{solid} [%]): 515 (14, 9%).
Mp.: 173 °C.

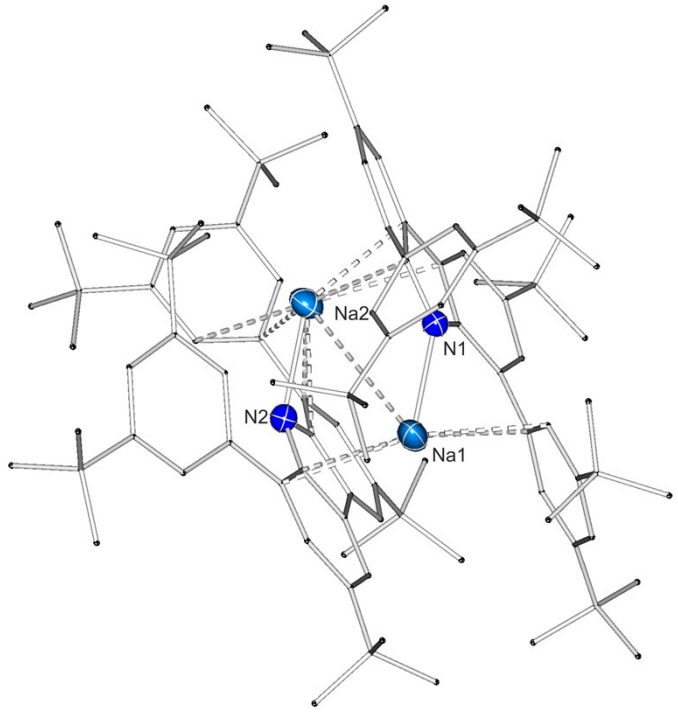


Figure S11: Molecular structure of **2a**. Selected bond lengths [Å] and angles [°]: Na1–N1 2.3377(16), Na1–C60 2.6921(19), Na1–C14 2.731(2), Na1–C59 2.7787(19), Na1–C13 2.9188(19), Na1–C55 2.953(2), Na1–C58 3.013(2), Na1–C1 3.0473(18), Na1–Na2 4.1004(12), Na2–N2 2.3308(16), Na2–C7 2.6115(17), Na2–C61 2.6662(19), Na2–C6 2.7780(18), Na2–C49 2.8335(18), Na2–C12 2.8777(17), Na2–C62 2.9473(19), Na2–C50 2.9930(19), Na2–C96 3.072(2), Na2–C1 3.0734(19), Na1-centroid: 2.640(9), Na2-centroid: 2.639(8).

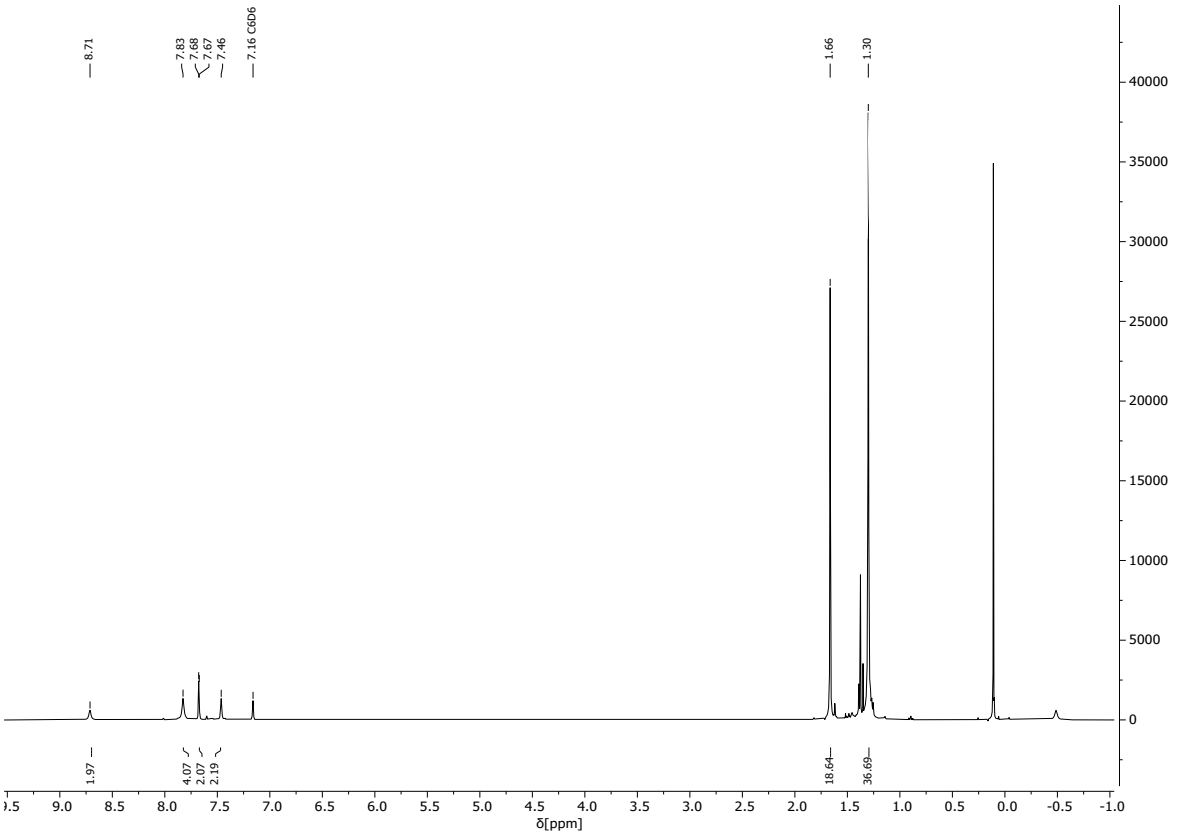


Figure S12: ^{1}H NMR spectrum of **2a**.

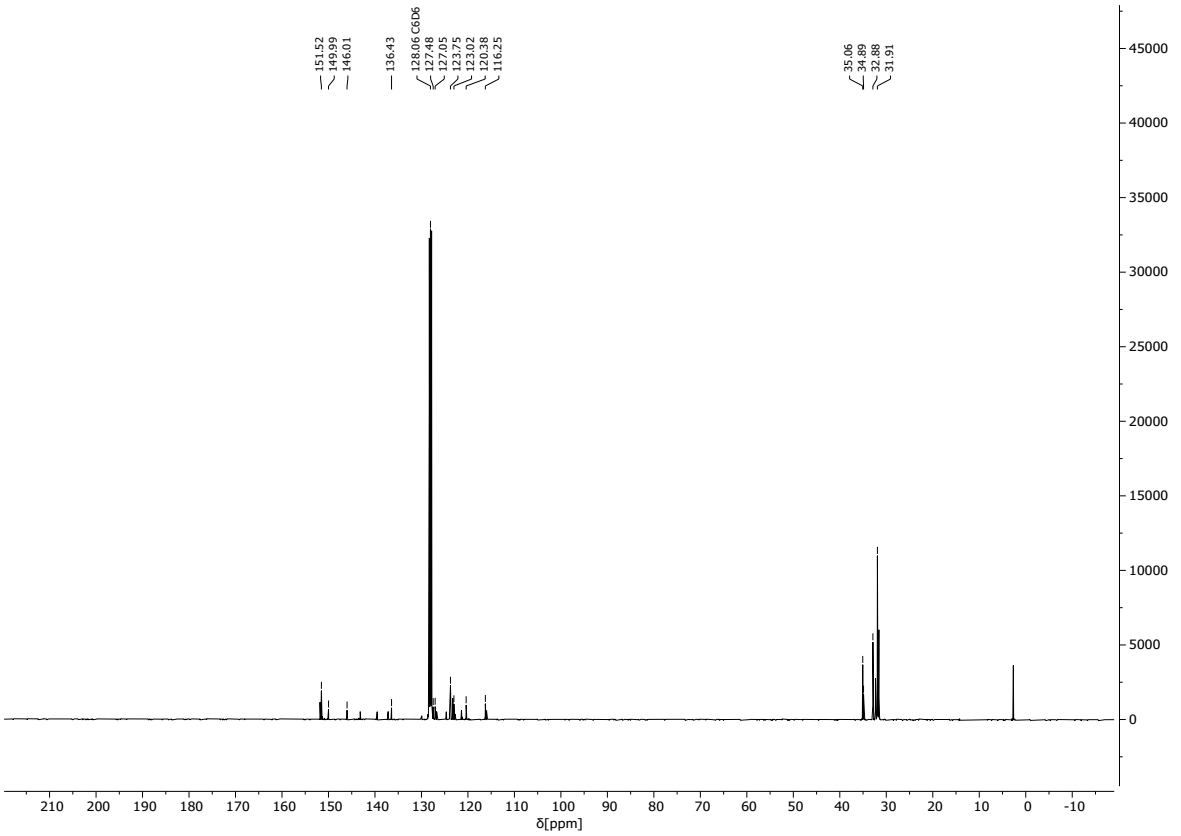


Figure S13: $^{13}C\{^{1}H\}$ NMR spectrum of **2a**.

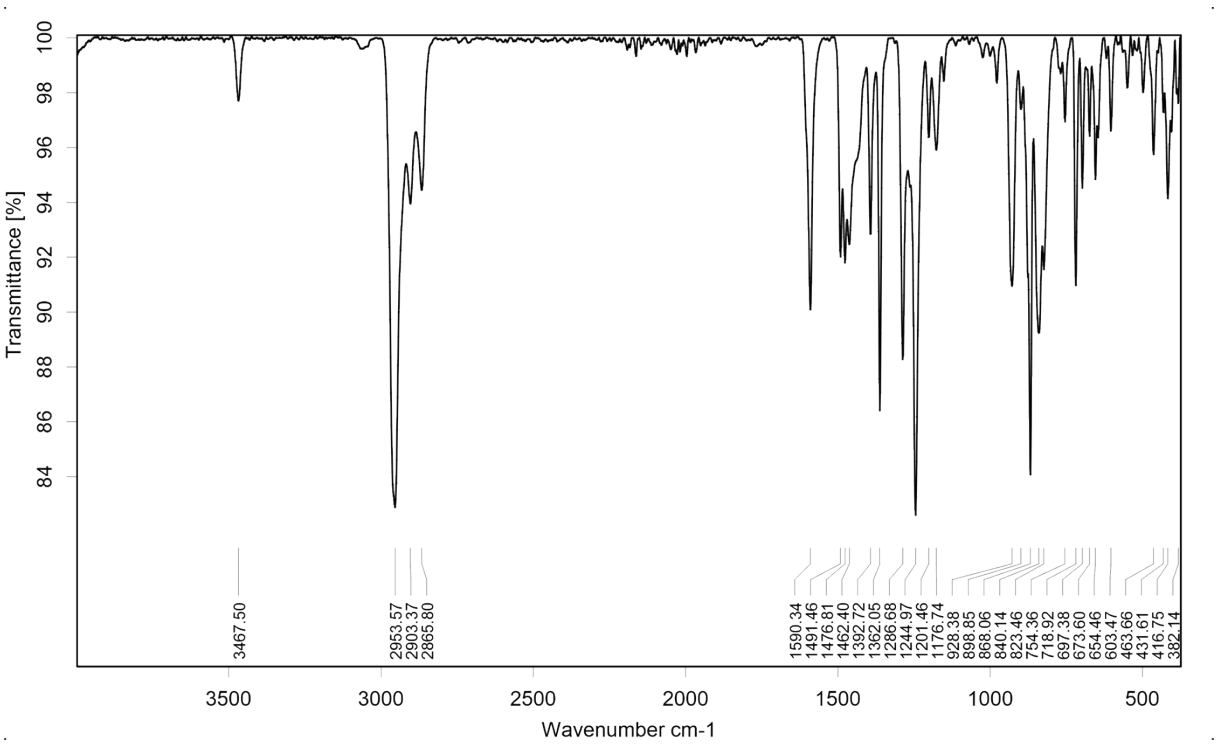


Figure S14: IR spectrum of **2a**.

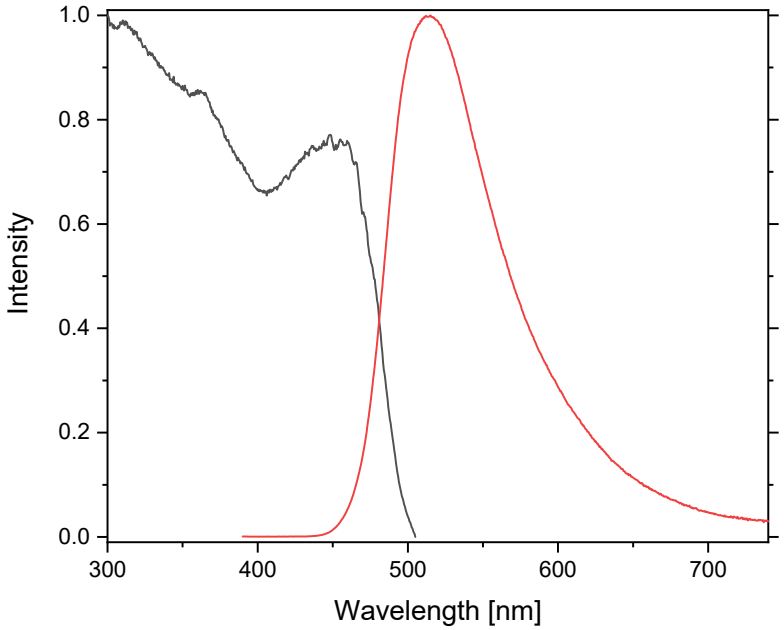
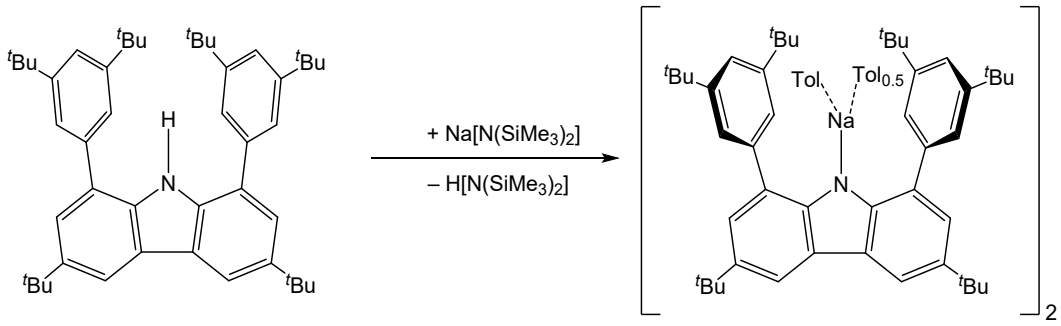


Figure S15: Photoluminescence emission (PL) and excitation (PLE) spectra of compound **2a** at 295 K.

2.4 [(^{dtbp}Cbz)Na(Tol)$_{1.5}$] (2b)



To a solid mixture of (^{dtbp}Cbz)–H (300 mg, 0.457 mmol) and Na[N(SiMe$_3$)$_2$] (100 mg, 0.545 mmol), 20 ml of toluene were added. The colourless mixture was stirred for 3 days at 70 °C and a yellow, luminescent solution formed. All volatiles were removed under reduced pressure and the residue was dried *in vacuo*. The residue was dissolved in hexane and filtered *via* a syringe filter. The solvent was evaporated to incipient crystallisation and left undisturbed overnight to allow single crystals suitable for X-ray diffraction to form. The supernatant was removed with a syringe and the residue was dried *in vacuo*, affording the product as a yellow crystalline solid (302.0 mg, 0.370 mmol, 81%).

^{1}H NMR (400 MHz, C_6D_6): δ (ppm) = 1.30 (s, 36 H, Ar-^{t}Bu); 1.60 (s, 18 H, Carb-^{t}Bu); 2.11 (s, Tol-CH_3), 7.06 (m, Ar-Tol), 7.46 (br, 2 H, *p*-C*H*); 7.68 (d, J_{HH} = 2.0 Hz, 2 H, C^{2,7}*H*); 7.84 (br, 4 H, *o*-C*H*); 8.72 (br, 2 H, C^{4,5}*H*).
^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ (ppm) = 21.43 (s, Tol-*C*H$_3$); 31.91 (s, Ar-C(*C*H$_3$)$_3$); 32.87 (s, Carb-C(*C*H$_3$)$_3$); 34.89 (s, Carb-*C*(CH$_3$)$_3$); 35.06 (s, Ar-*C*(CH$_3$)$_3$); 116.26 (s, *C*^{4,5}H); 120.39 (s, *p*-*C*H); 123.04 (s, *C*^{2,7}H); 123.75 (s, *o*-*C*H); 125.69 (s, Tol-*C*H(4)); 127.06 (s); 127.47(s); 128.57 (s, Tol-*C*H(3,5)); 129.34 (s, Tol-*C*H(2,6)); 136.46 (s); 137.89 (s, Tol-*C*H(1)); 146.01 (s); 149.98 (s); 151.53 (s).
IR (ATR): ũ (cm^{-1}) = 2954 (m), 2904 (w), 2866 (w), 1589 (m), 1461 (w), 1392 (vw), 1361 (m), 1274 (m), 1236 (vs), 1202 (m), 1179 (w), 1150 (m), 981 (m), 927 (vw), 899 (vw), 866 (m), 849 (w), 823 (vw), 739 (vw), 720 (m), 698 (w), 675 (vw), 643 (w), 553 (vw), 503 (m), 468 (vw), 416 (vw).
PL ($\lambda_{max,emission}$ [nm], τ_{solid} [ns], Φ_{solid} [%]): 490, 515 (13, 12%).
Mp.: 201 °C.

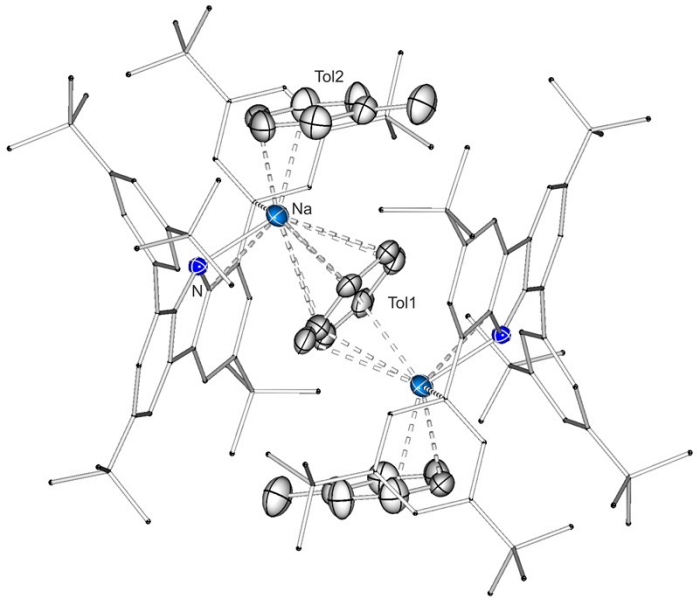


Figure S16: Molecular structure of **2b** (disorder not shown). Selected bond lengths [Å] and angles [°]: Na1–N1 2.2713(14), Na1–C52 2.6391(19), Na1–C51 2.836(2), Na1–C1 2.8794(15), Na1–C60 2.903(6), Na1–C13 2.9532(18), Na1–C61 2.959(5), Na1–C59 2.959(6), Na-centroid(Tol1): 2.639(2), Na-centroid(Tol2): 3.055(1).

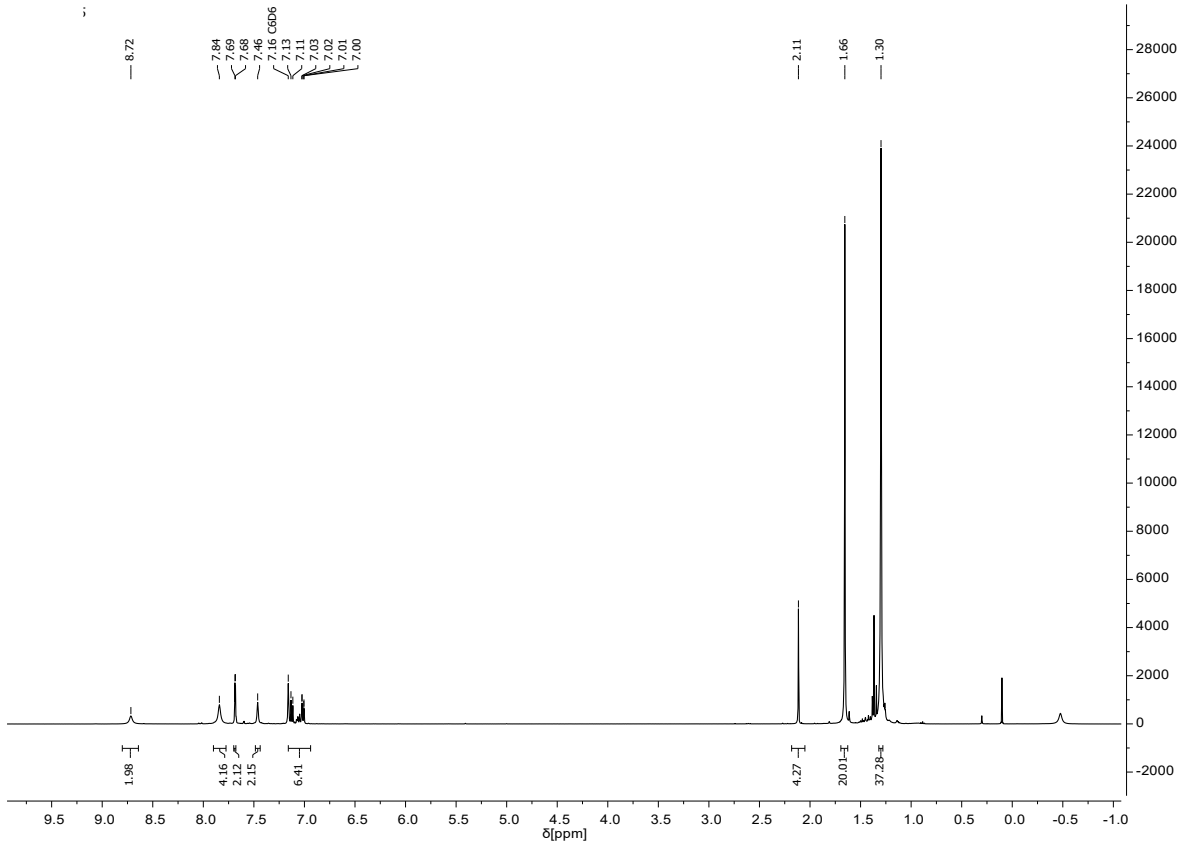


Figure S17: ^{1}H NMR spectrum of **2b**.

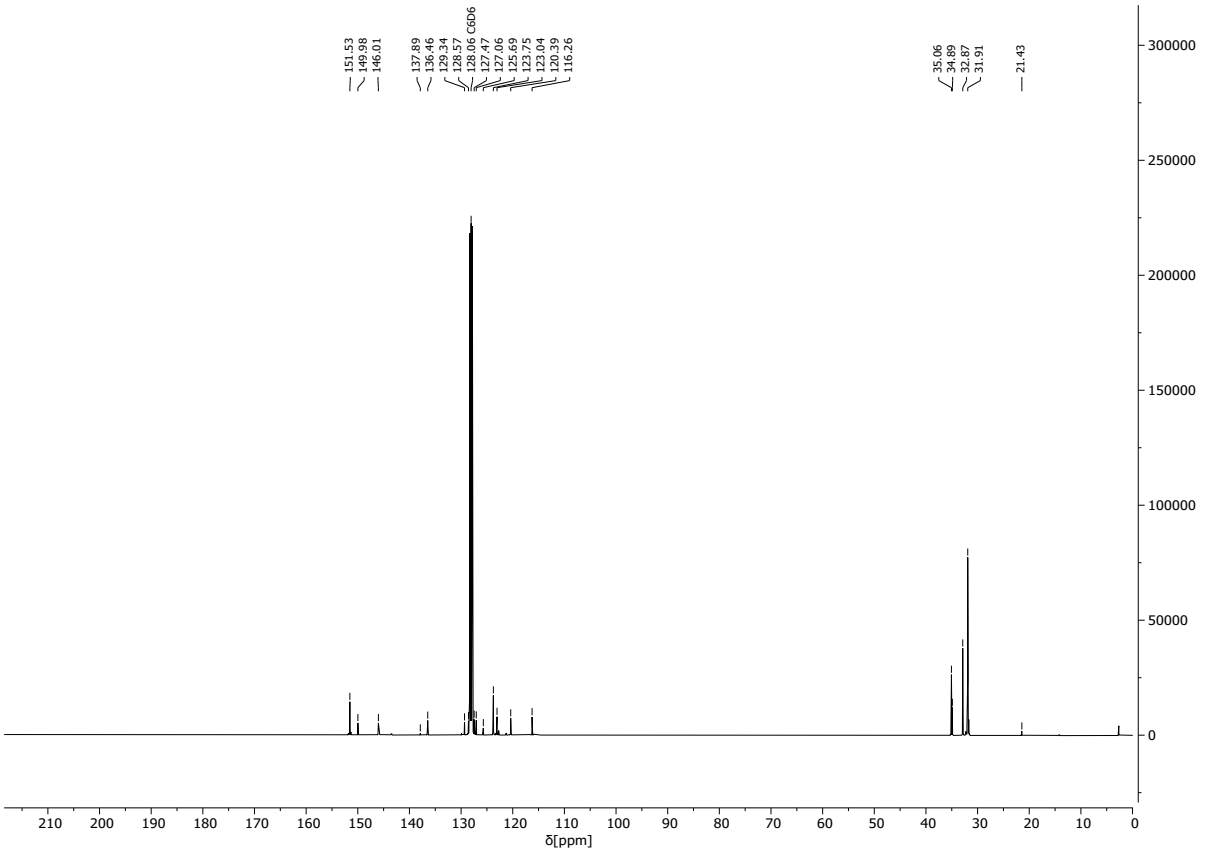


Figure S18: $^{13}C\{^{1}H\}$ NMR spectrum of **2b**.

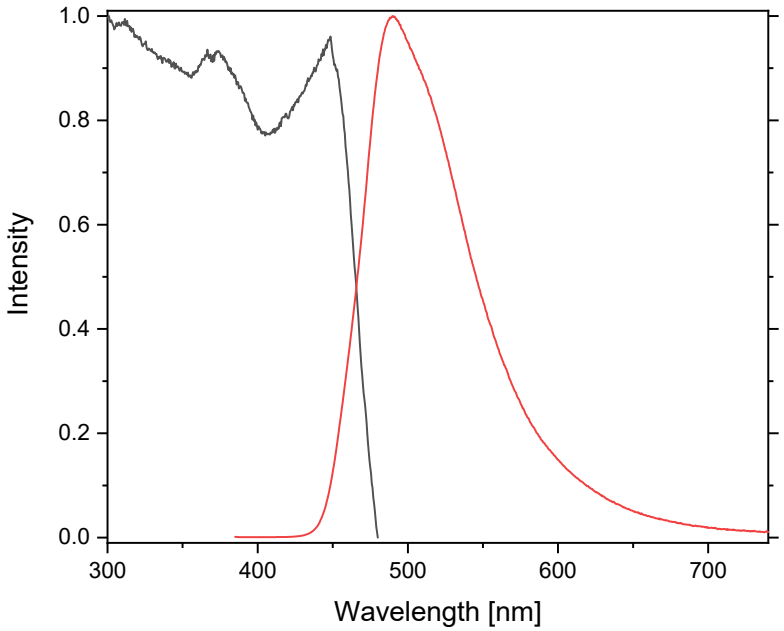


Figure S19: Photoluminescence emission (PL) and excitation (PLE) spectra of compound **2b** at 295 K.

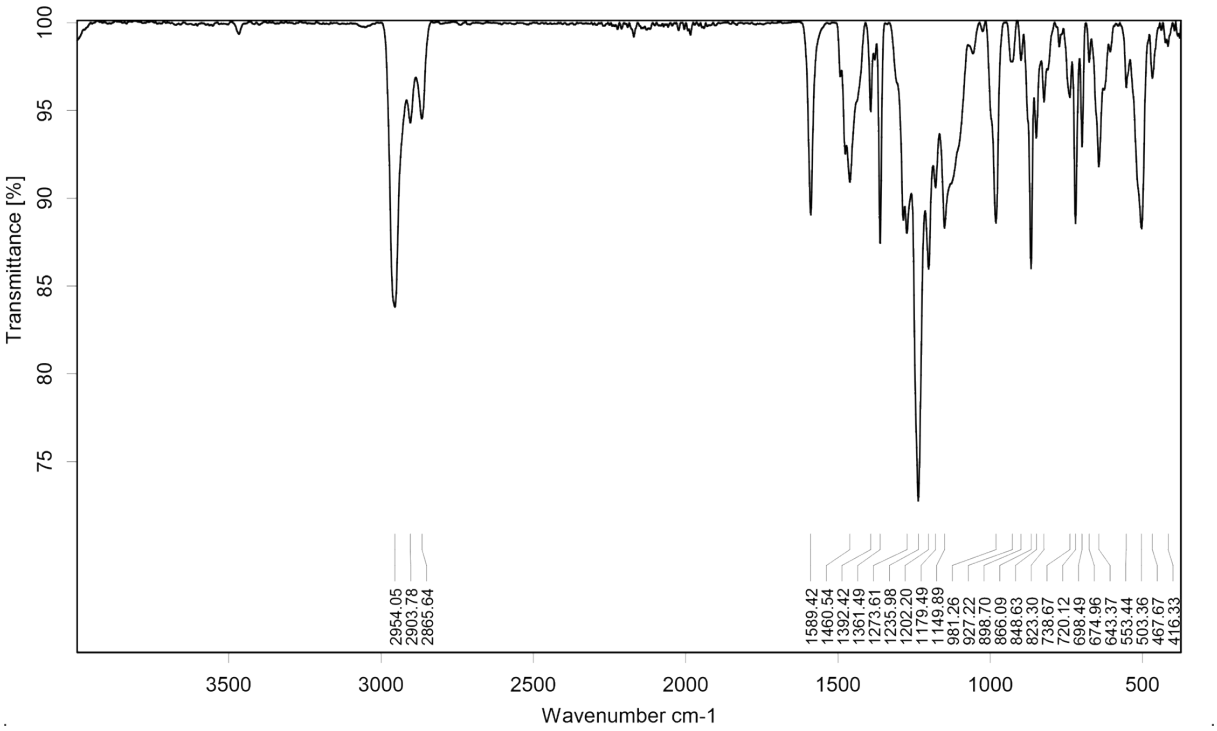
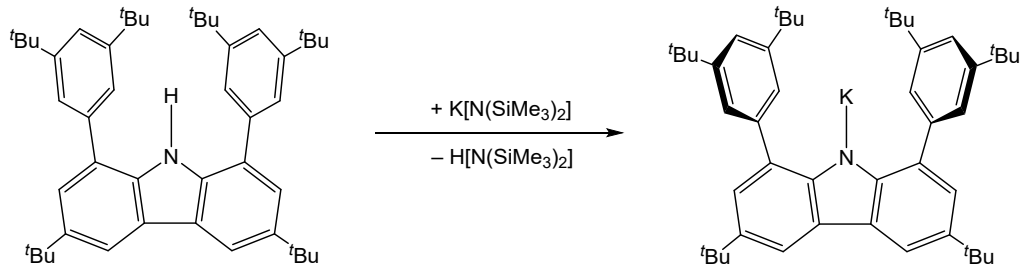


Figure S20: IR spectrum of **2b**.

2.5 [(^{dtbp}Cbz)K] (3a)

a) [(^{dtbp}Cbz)K] was prepared according to literature protocols, using benzyl potassium as base.[1]

b) Alternatively, K[N(SiMe$_3$)$_2$] can be used.



To a solid mixture of [(^{dtbp}Cbz)–H (300 mg, 0.457 mmol) and K[N(SiMe$_3$)$_2$] (110 mg, 0.551 mmol), 20 ml of *n*-hexane was added. The colourless mixture was stirred for 3 days at 70 °C and a yellow, luminescent solution formed. All volatiles were removed under reduced pressure and the residue was dried *in vacuo*. The residue was redissolved in *n*-hexane and filtered *via* a syringe filter. Again, the volatiles were removed under reduced pressure and the residue was dried in vacuo affording the product as a yellow solid (287 mg, 0.413 mmol, 90 %).

The NMR data correspond with those from the literature.[1]

IR (ATR): ũ (cm^{-1}) = 2957 (s), 2865 (w), 1585 (w), 1461 (m), 1430 (w), 1394 (w), 1361 (s), 1279 (vs), 1237 (vs), 1201 (vw), 1185 (vw), 933 (vw), 898 (vw), 880 (w), 858 (m), 821 (w), 776 (vw), 725 (m), 704 (w), 668 (vw), 645 (w), 496 (vw).
PL ($\lambda_{max,emission}$ [nm], τ_{solid} [ns], Φ_{solid} [%]): 500 (15, 18%).
Mp.: 377 °C.

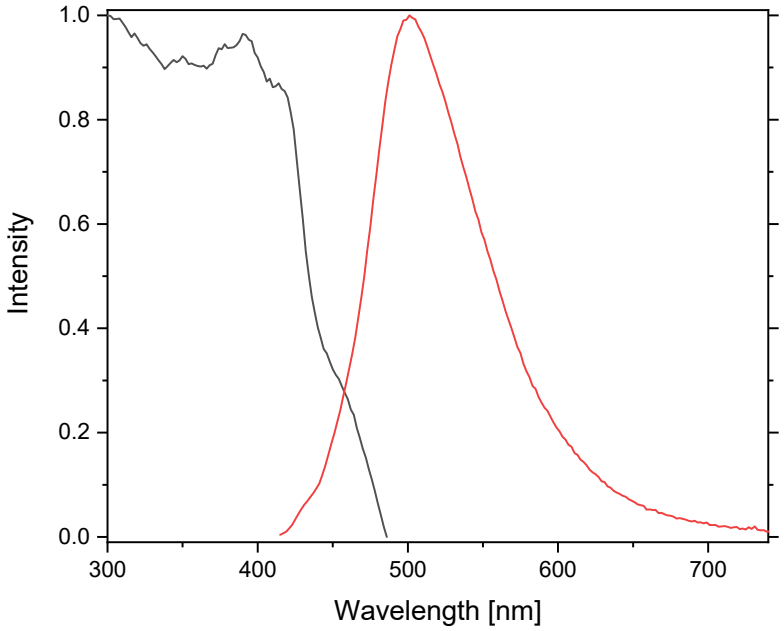


Figure S21: Photoluminescence emission (PL) and excitation (PLE) spectra of compound **3a** at 295 K.

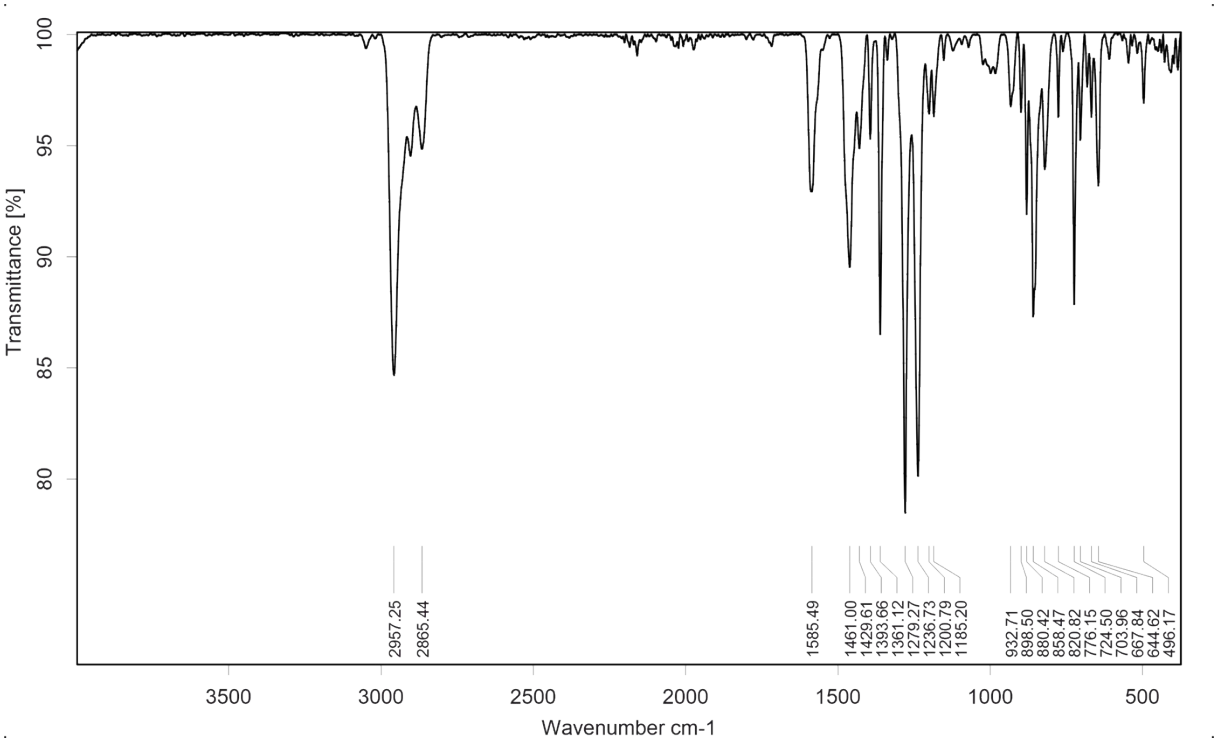
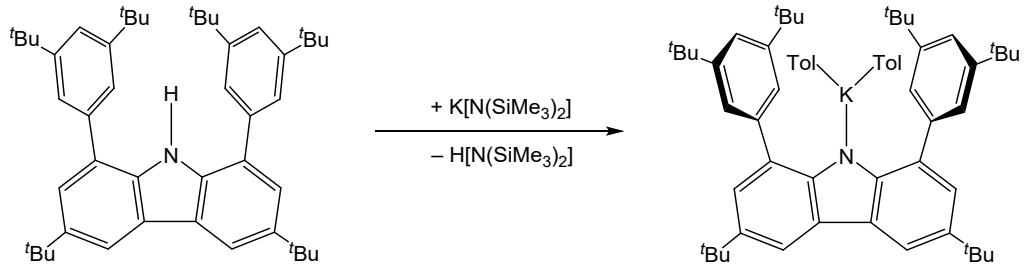


Figure S22: IR spectrum of **3a**.

2.6 [(^{dtbp}Cbz)K(Tol)$_2$] (3b)

a) [(^{dtbp}Cbz)K(Tol)$_2$] was prepared according to literature protocols.[1]

b) Alternatively, K[N(SiMe$_3$)$_2$] can be used.



To a solid mixture of (^{dtbp}Cbz)–H (300 mg, 0.457 mmol) and K[N(SiMe$_3$)$_2$] (110 mg, 0.545 mmol), 20 ml of toluene was added. The colourless mixture was stirred for 3 days at 70 °C and a yellow, luminescent solution formed. Volatiles were removed under reduces pressure and the residue was dried in vacuo. The residue was solved in toluene and filtered *via* a syringe filter. Volatiles were removed under reduces pressure until beginning crystallisation was observed. The solution was left undisturbed overnight, then the supernatant was removed via syringe and the residue was dried in vacuo affording the product as a yellow crystalline solid (330 mg, 0.376 mmol, 82 %).

IR (ATR): ũ (cm^{-1}) = 2958 (vs), 2903 (vs), 2866 (vs), 1588 (vs), 1494 (vs), 1458 (vs), 1393 (vs), 1380 (vs), 1361 (vs), 1286 (vs), 1271 (vs), 1235 (vs), 1202 (vs), 1177 (vs), 1151 (vs), 1083 (vs), 1002 (vs), 928 (vs), 900 (vs), 865 (vs), 847 (vs), 823 (vs), 775 (vs), 746 (vs), 738 (vs), 718 (vs), 698 (vs), 676 (vs), 645 (vs), 500 (vs), 469 (vs), 410 (vs), 381 (vs).
PL ($\lambda_{max,emission}$ [nm], τ_{solid} [ns], Φ_{solid} [%]): 550 (11, 14%).
Mp.: 350 °C.

The NMR data correspond with those from the literature.[1]

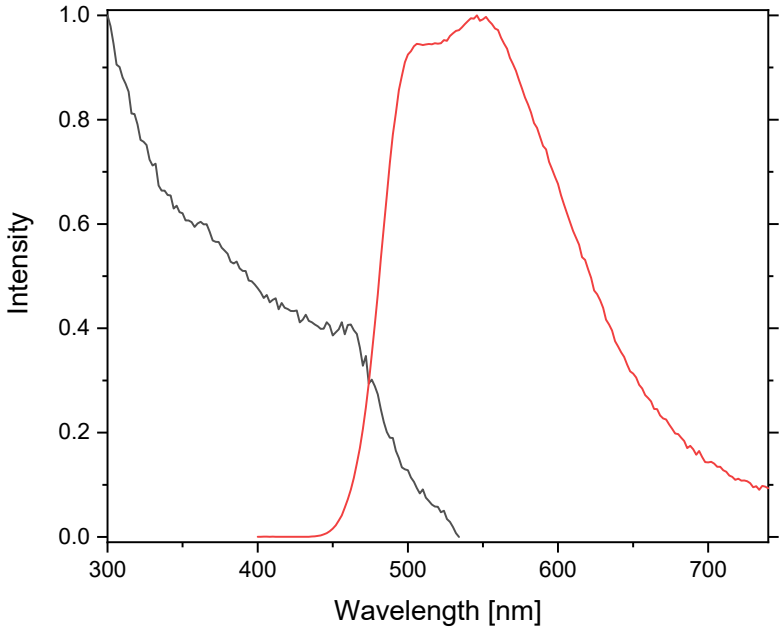


Figure S23: Photoluminescence emission (PL) and excitation (PLE) spectra of compound **3b** at 295 K.

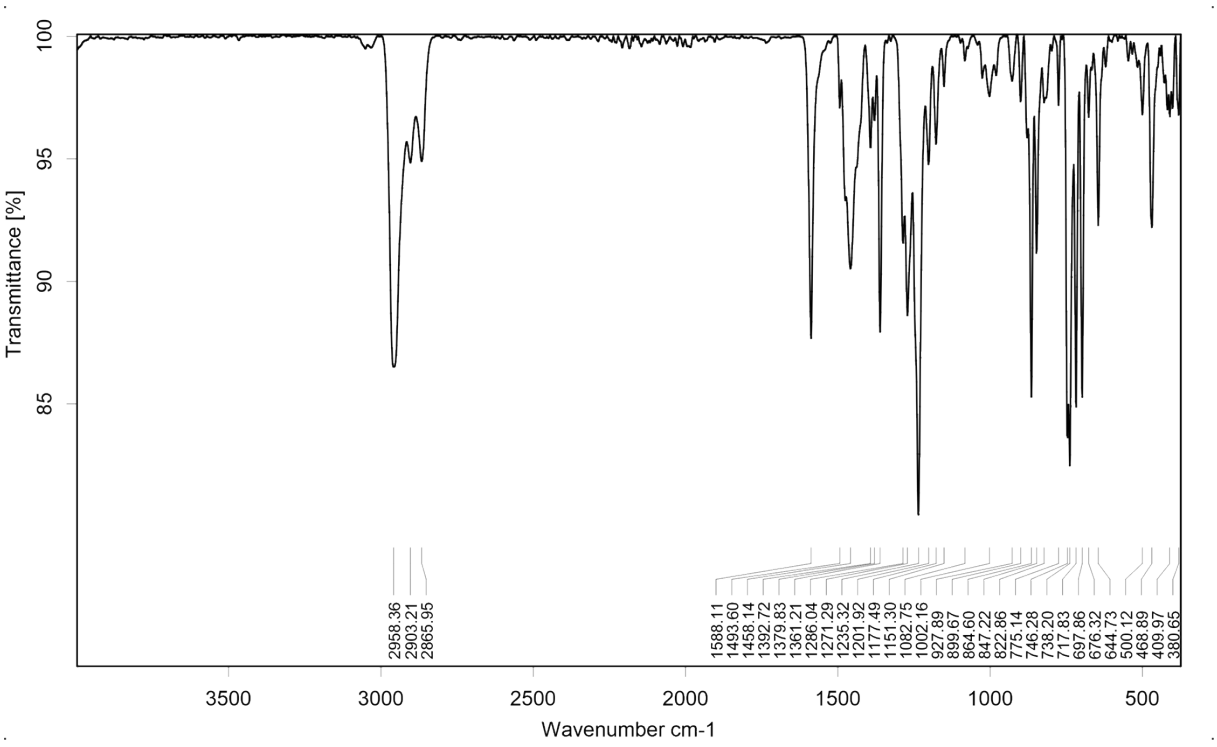
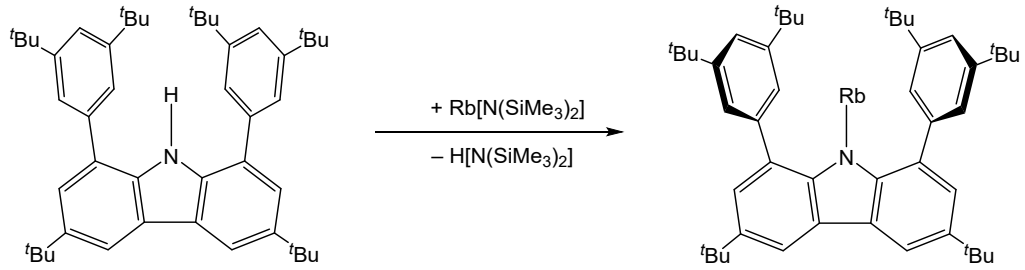


Figure S24: IR spectrum of **3b**.

2.7 [(^{dtbp}Cbz)Rb] (4a)



To a solid mixture of (^{dtbp}Cbz)–H (200 mg, 0.305 mmol) and Rb[N(SiMe$_3$)$_2$] (76 mg. 0.305 mmol) 5 ml of toluene was added. The mixture was sonicated for 30 minutes and heated to reflux overnight, forming a bright yellow solution. Volatiles were removed under reduced pressure and the residue was dried in vacuo at 100 °C.
The residue was redissolved in *n*-hexane and filtered *via* a syringe filter. Then, the solvent was evaporated to incipient crystallisation and left undisturbed overnight. The mother liquor was removed and the residue was dried in vacuo affording the product as a yellow crystalline solid (84 mg, 0.114 mmol, 38%).

^{1}H NMR (400 MHz, C_6D_6): δ (ppm) = 1.26 (s, 36 H, Ar-^{t}Bu); 1.70 (s, 18 H, Carb-^{t}Bu); 7.29 (t, J_{HH} = 1.9 Hz, 2 H, *p*-C*H*); 7.68 (d, J_{HH} = 2.1 Hz, 2 H, C^{2,7}*H*); 7.81 (d, J_{HH} = 1.9 Hz, 4 H, *o*-C*H*); 8.80 (d, J_{HH} = 2.0 Hz, 2 H, C^{4,5}*H*).
^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ (ppm) = 31.95(s, Ar-C(CH$_3$)$_3$); 33.00 (s, Carb-C(CH$_3$)$_3$); 34.95 (s, Carb-C(CH$_3$)$_3$); 34.99 (s, Ar-C(CH$_3$)$_3$); 116.21 (s, $C^{4,5}$H); 119.31 (s, *p*-*C*H); 121.62 (s, $C^{2,7}$H); 124.96 (s, *o*-*C*H); 126.58 (s); 135.64 (s); 146.65 (s); 150.53 (s); 150.75 (s).
IR (ATR): ũ (cm^{-1}) = 2957 (s), 2864 (w), 1583 (w), 1461 (m), 1429 (w), 1394 (w), 1361 (m), 1279 (vs), 1237 (s), 1185 (vw), 898 (vw), 880 (w), 859 (m), 776 (vw), 724 (m), 704 (vw), 668 (vw), 644 (w), 497 (vw).
PL ($\lambda_{max,emission}$ [nm], τ_{solid} [ns], Φ_{solid} [%]): 460 (9, 29%).
Mp.: >400 °C.

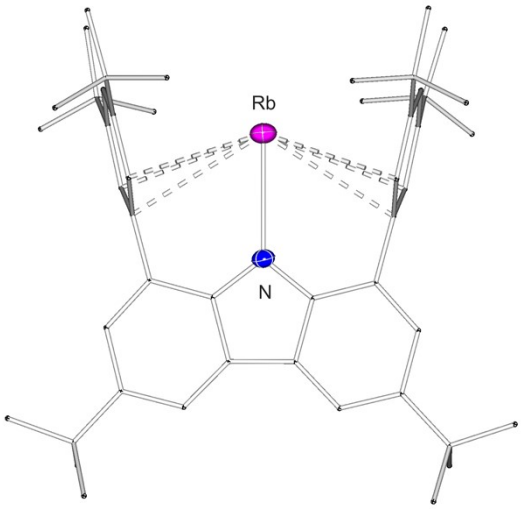


Figure S25: Molecular structure of **4a** (disorder not shown). Selected bond lengths [Å] and angles [°]: Rb1–N1 2.741(3), Rb1–C35 3.338(3), Rb1–C14 3.349(3), Rb1–C13 3.350(3), Rb1–C40 3.352(3), Rb1–C18 3.437(4), Rb1–C36 3.451(3), Rb1–C15 3.471(3), Rb1–C39 3.516(3), Rb1–C00S 3.536(4), Rb1–C16 3.539(4), Rb1–C33' 3.553(4).

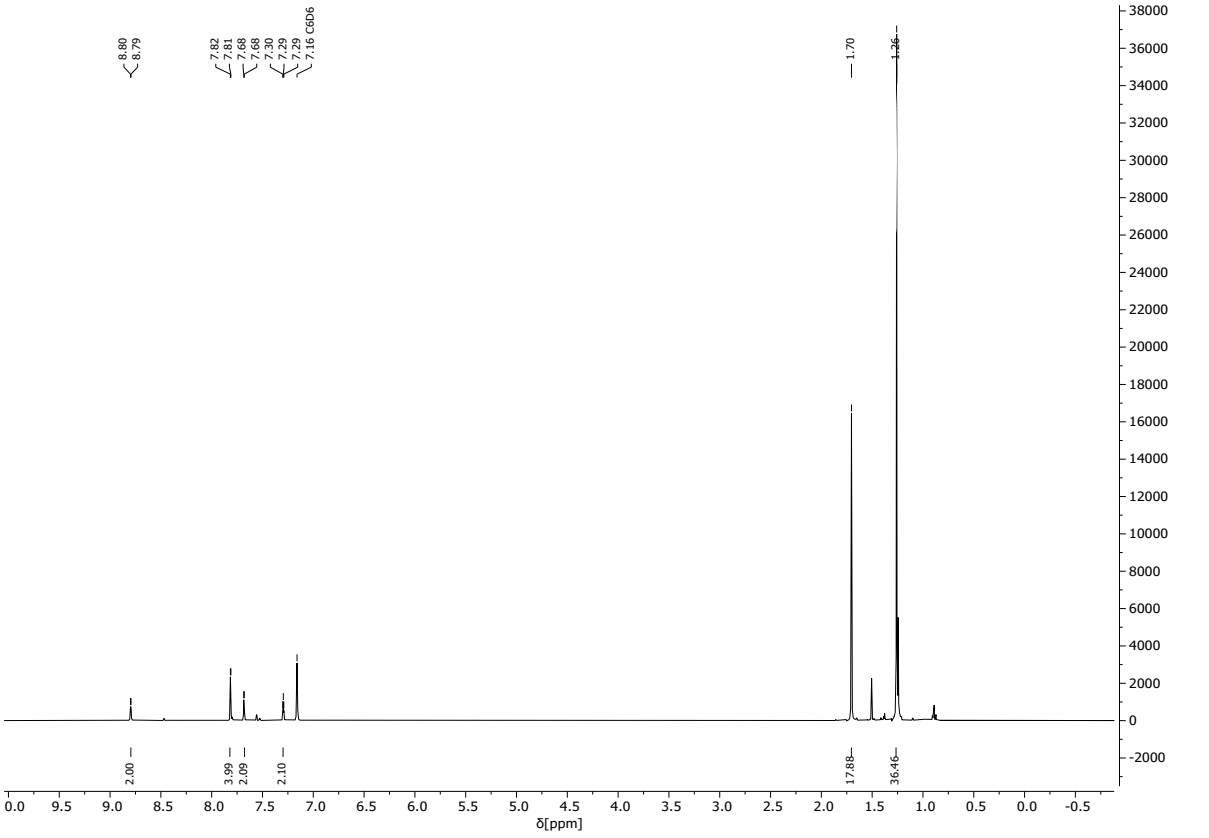


Figure S26: ^{1}H NMR spectrum of **4a**.

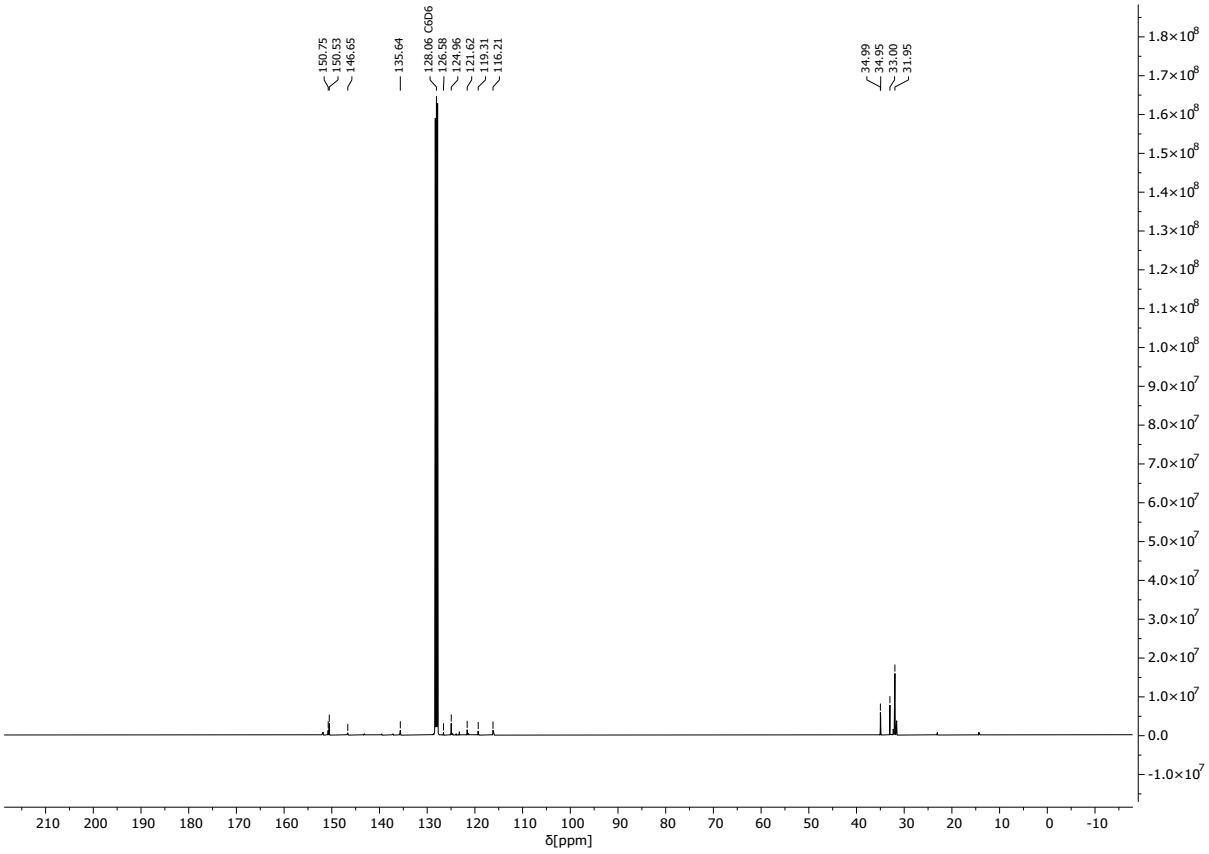


Figure S27: ^{13}C{^{1}H} NMR spectrum of **4a**.

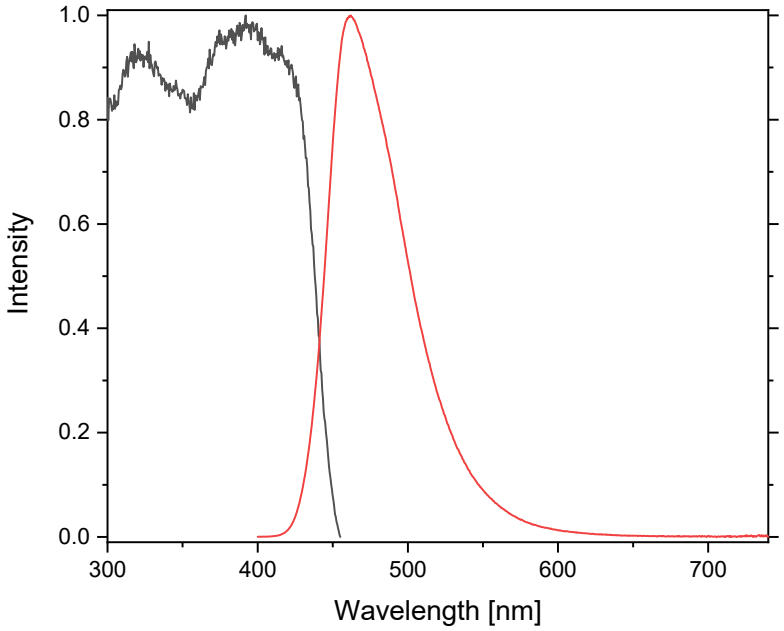


Figure S28: Photoluminescence emission (PL) and excitation (PLE) spectra of compound **4a** at 295 K.

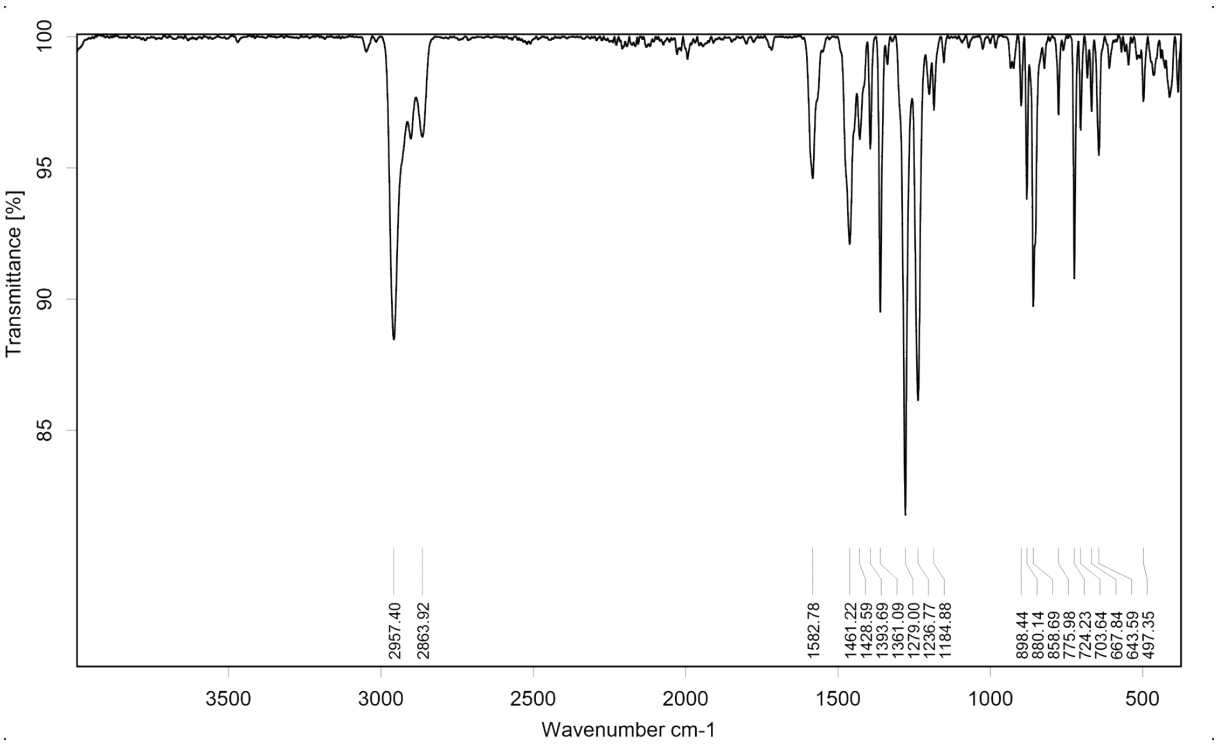
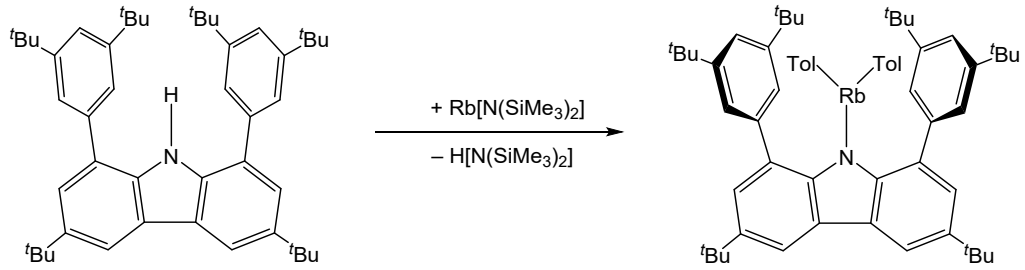


Figure S29: IR spectrum of **4a**.

2.8 [(^{dtbp}Cbz)Rb(Tol)$_2$] (4b)



To a solid mixture of (^{dtbp}Cbz)–H (200 mg, 0.305 mmol) and Rb[N(SiMe$_3$)$_2$] (76 mg. 0.305 mmol), 5 ml of toluene was added. The mixture was sonicated for 30 minutes and heated to refluxed overnight, affording a bright yellow solution. The solvent was slowly evaporated until crystallisation was observed. The mother liquor was removed and the residue was dried *in vacuo*, affording the product as a yellow crystalline solid (78.0 mg, 0.106 mmol, 35%).

^{1}H NMR (400 MHz, C_6D_6): δ (ppm) = 1.26 (s, 36 H, Ar-^{t}Bu); 1.70 (s, 18 H, Carb-^{t}Bu); 2.11 (s, CH_3-Tol), 7.06 (m, Ar-Tol), 7.30 (t, J_{HH} = 2.0 Hz, 2 H, *p*-C*H*); 7.68 (d, J_{HH} = 2.1 Hz, 2 H, C^{2,7}*H*); 7.81 (d, J_{HH} = 2.0 Hz, 4 H, *o*-C*H*); 8.79 (d, J_{HH} = 2.1 Hz, 2 H, C^{4,5}*H*).
^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ (ppm) = 21.43 (s, Tol-*C*H$_3$); 31.95 (s, Ar-C(*C*H$_3$)$_3$); 32.98 (s, Carb-C(*C*H$_3$)$_3$); 34.93 (s, Carb-*C*(CH$_3$)$_3$); 35.01 (s, Ar-*C*(CH$_3$)$_3$); 116.03 (s, *C*^{4,5}H); 119.51 (s, *p*-*C*H); 121.76 (s, *C*^{2,7}H); 124.87 (s, *o*-*C*H); 125.70 (s, Tol-*C*H(4)); 126.39 (s); 126.74(s) 128.57 (s, Tol-*C*H(3,5)); 129.34 (s, Tol-*C*H(2,6)); 135.75 (s); 137.89 (s, Tol-*C*H(1)); 146.35 (s); 150.59 (s); 150.68 (s).
IR (ATR): ũ (cm^{-1}) = 2953 (vs), 2903 (w), 2866 (w), 1589 (s), 1459 (m), 1392 (w), 1380 (vw), 1361 (s), 1273 (s), 1236 (vs), 1202 (w), 1177 (w), 1024 (vw), 925 (vw), 900 (vw), 865 (s), 847 (m), 746 (m), 738 (m), 718 (s), 698 (m), 644 (w), 502 (w), 469 (m), 452 (w), 433 (w), 408 (w), 389 (m).
PL ($\lambda_{max,emission}$ [nm], τ_{solid} [ns], Φ_{solid} [%]): 485 (8, 17%).
Mp.: 387 °C.

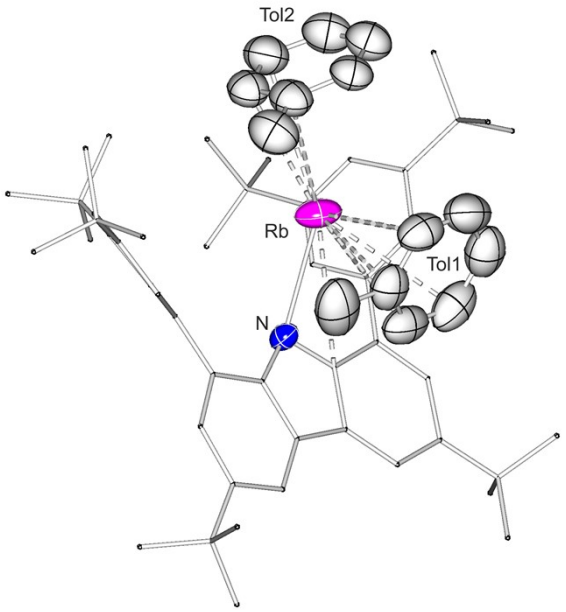


Figure S30: Molecular structure of **4b** (only one of the molecules of the asymmetric unit displayed, disorder not shown). Selected bond lengths [Å] and angles [°]: Rb1–N1 2.808(5), Rb1–C57 3.351(12), Rb1–C35 3.360(6), Rb1–C50 3.408(8), Rb1–C36 3.414(6), Rb1–C49 3.451(8), Rb1–C56 3.533(13), Rb1–C12 3.535(5), Rb1–C58 3.537(15), Rb-centroid(Tol1): 3.325(9), Rb-centroid(Tol2): 3.425(9).

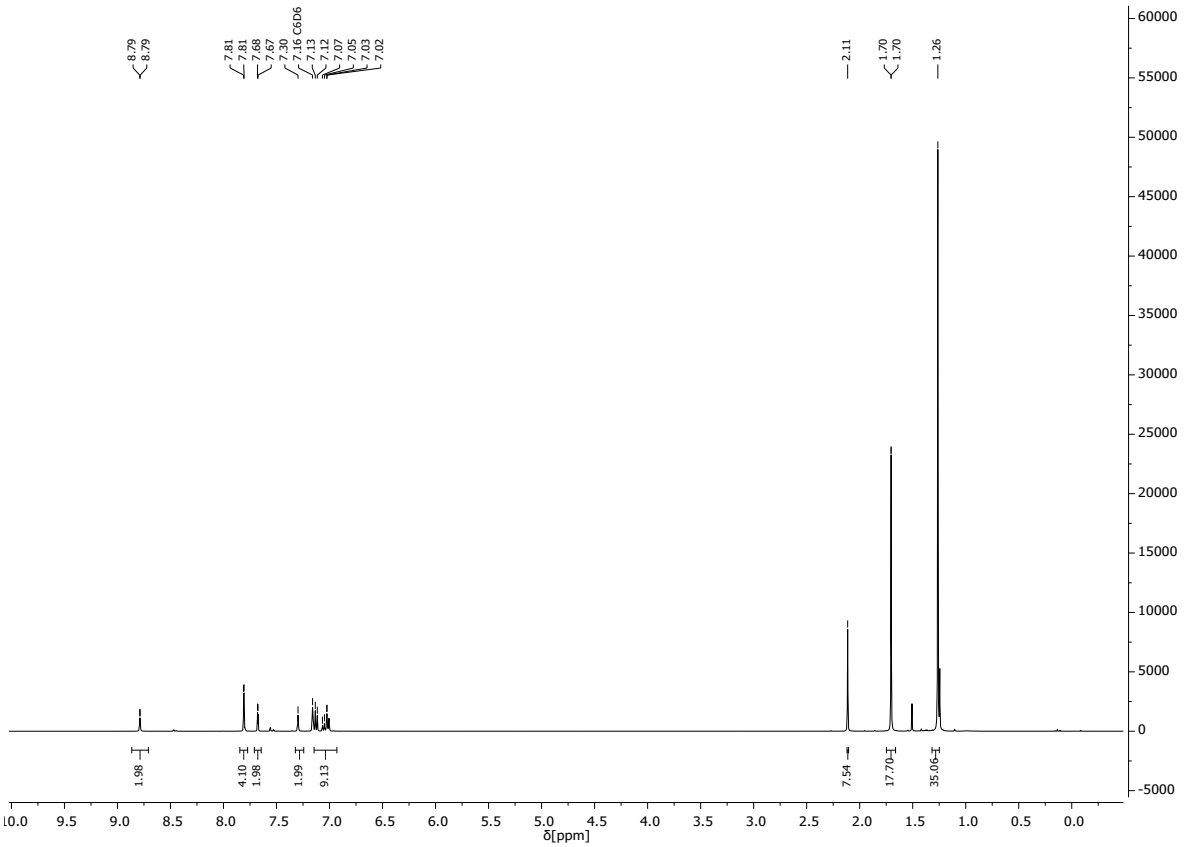


Figure S31: ^{1}H NMR spectrum of **4b**.

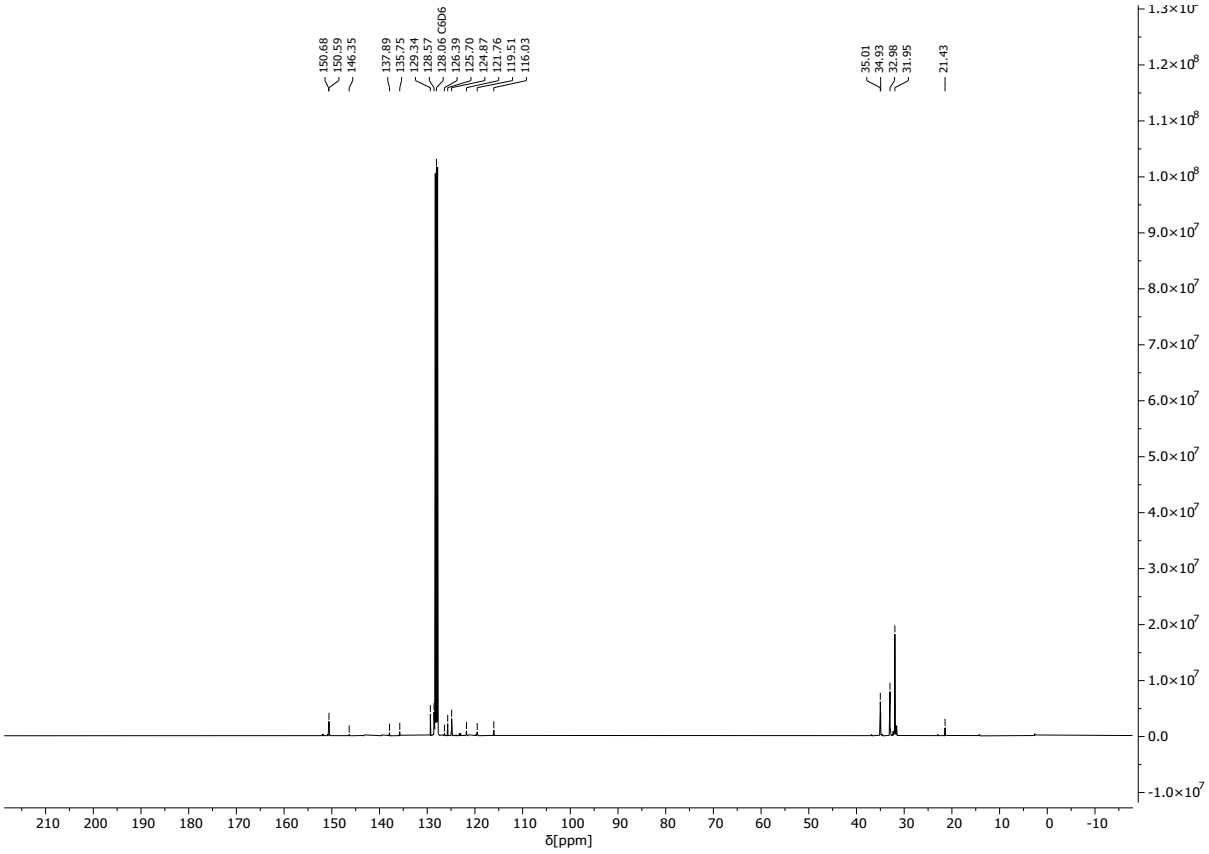


Figure S32: $^{13}C\{^{1}H\}$ NMR spectrum of **4b**.

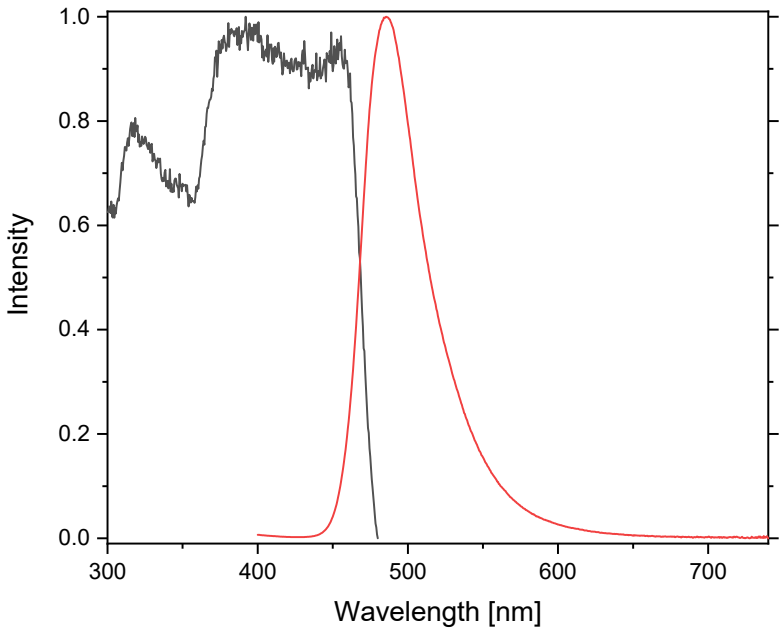


Figure S33: Photoluminescence emission (PL) and excitation (PLE) spectra of compound **4b** at 295 K.

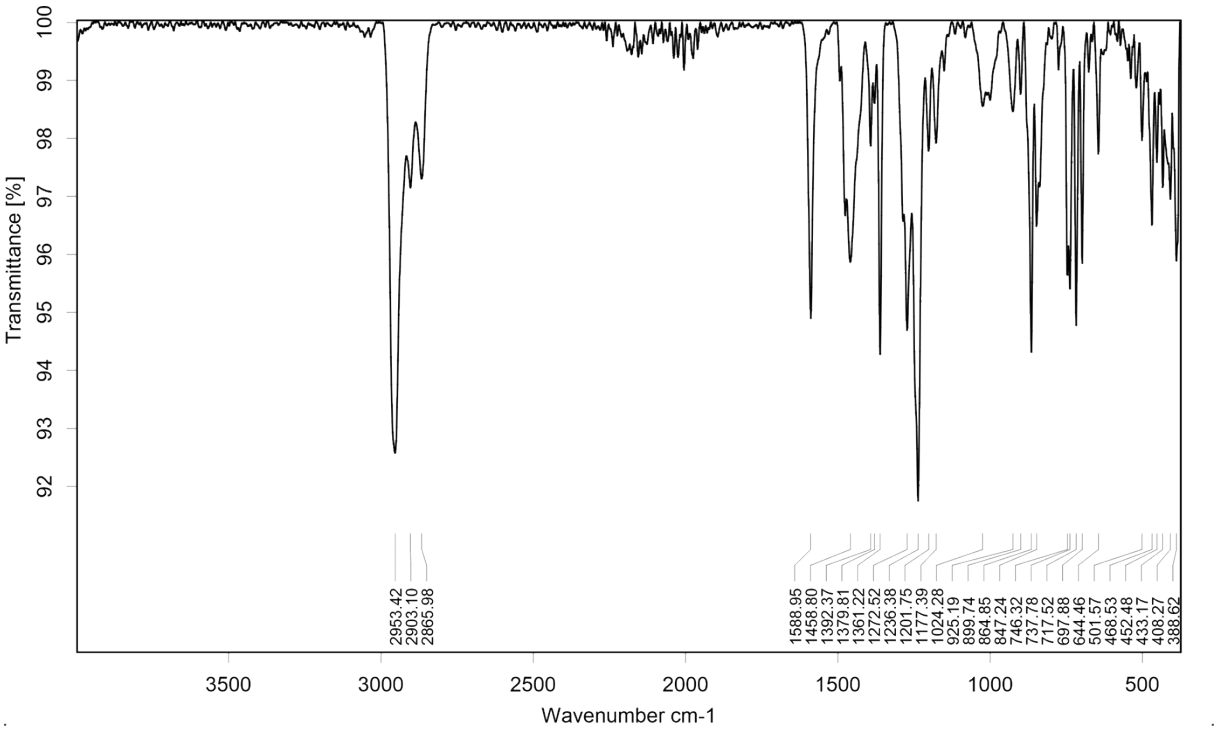
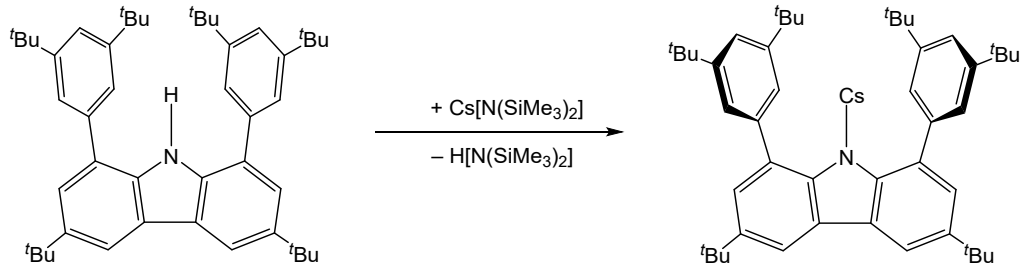


Figure S34: IR spectrum of **4b**.

2.9 [(^{dtbp}Cbz)Cs] (5a)



To a solid mixture of (^{dtbp}Cbz)–H (200 mg, 0.305 mmol) and Cs[N(SiMe$_3$)$_2$] (90 mg, 0.307 mmol), 5 ml of toluene was added. The mixture was sonicated for 30 minutes and heated to refluxed overnight, forming a bright yellow solution. Then, all volatiles were removed under reduced pressure and the residue was dried in vacuo at 100 °C. The residue was reddissolved in *n*-hexane and filtered *via* a syringe filter. Volatiles were removed under reduces pressure and the residue was dried in vacuo affording the product as a yellow solid (142.6 mg, 0.162 mmol, 71%).

^{1}H NMR (400 MHz, C_6D_6): δ (ppm) = 1.26 (s, 36 H, Ar-^{t}Bu); 1.71 (s, 18 H, Carb^{t}Bu); 7.26 (t, J_{HH} = 2.0 Hz, 2 H, p-C*H*); 7.67 (d, J_{HH} = 2.0 Hz, 2 H, C^{2,7}*H*); 7.79 (d, J_{HH} =2.0 Hz, 4 H, o-C*H*); 8.78 (br, 2 H, C^{4,5}*H*).
^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ (ppm) = 31.96 (s, Ar-C(*C*H$_3$)$_3$); 32.98 (s, Carb-C(*C*H$_3$)$_3$); 34.94 (s, Carb-*C*(CH$_3$)$_3$); 34.98 (s, Ar-*C*(CH$_3$)$_3$); 116.03 (s, *C*^{4,5}H); 119.52 (s, *p*-*C*H); 121.41 (s, *C*^{2,7}H); 125.36 (s, *o*-*C*H); 126.21 (s); 135.63 (s); 150.55 (s); 150.90 (s).
IR (ATR): ũ (cm^{-1}) = 2952 (s), 2903 (w), 2865 (w), 1592 (m), 1477 (w), 1458 (m), 1391 (w), 1361 (s), 1279 (s), 1239 (vs), 1202 (w), 1179 (vw), 996 (vw), 866 (s), 852 (m), 814 (vw), 778 (vw), 710 (s), 698 (w), 675 (vw), 653 (w), 642 (w), 402 (vw).
PL ($\lambda_{max,emission}$ [nm], τ_{solid} [ns], Φ_{solid} [%]): 505 (3, 3%).
Mp.: > 400 °C.

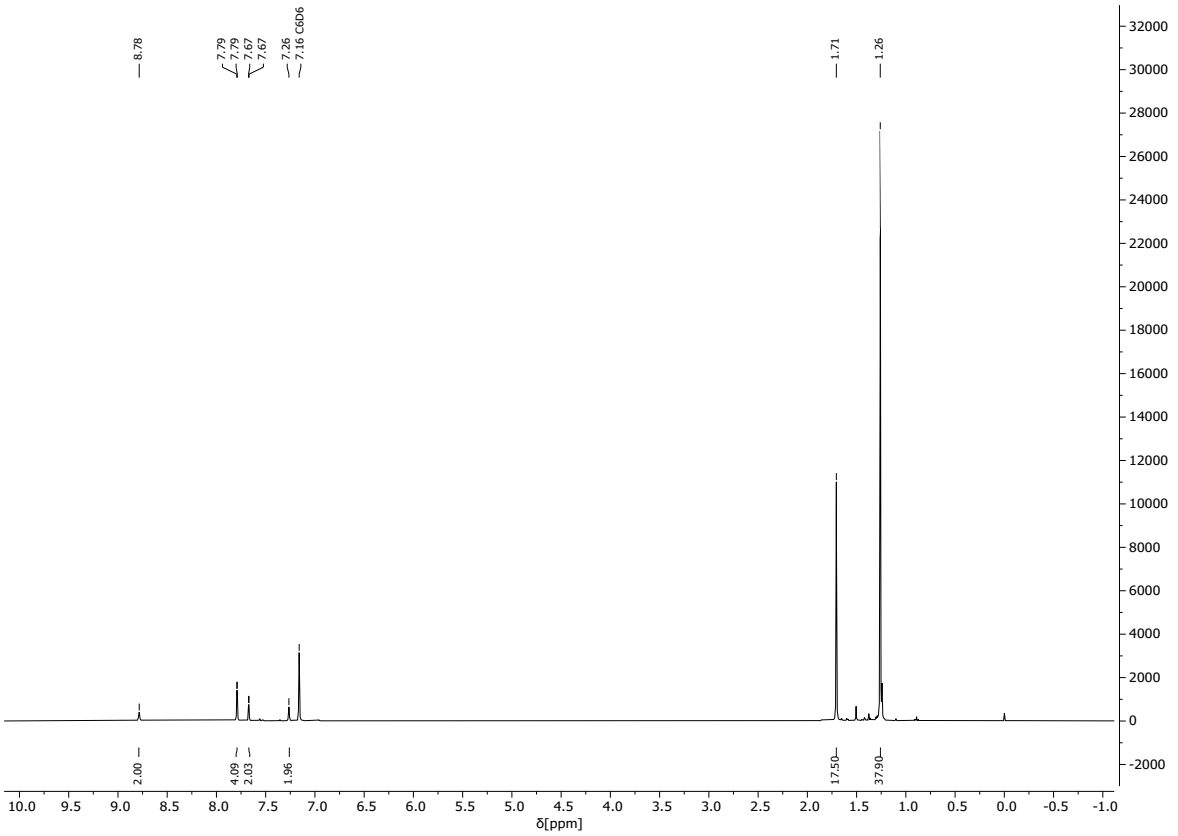


Figure S35: ^{1}H NMR spectrum of **5a**.

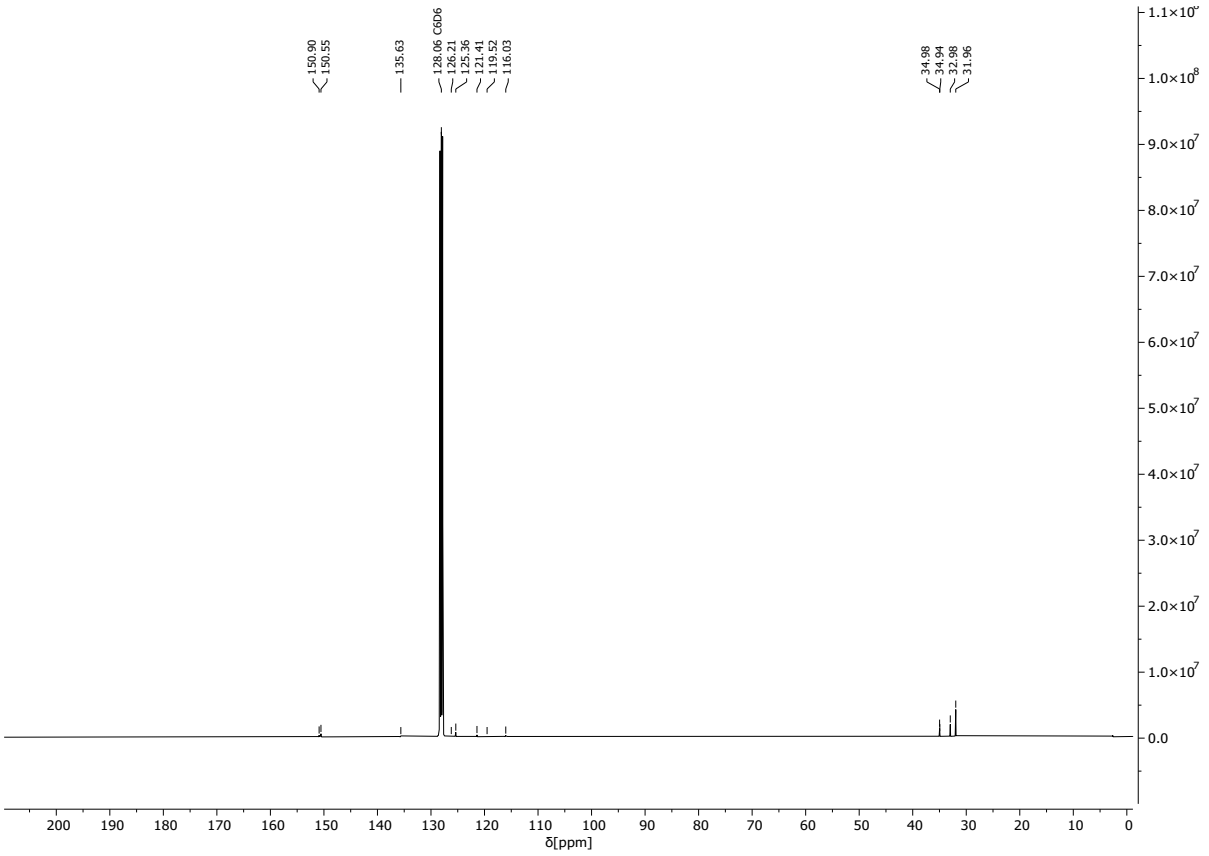


Figure S36: ^{13}C{^{1}H} NMR spectrum of **5a**.

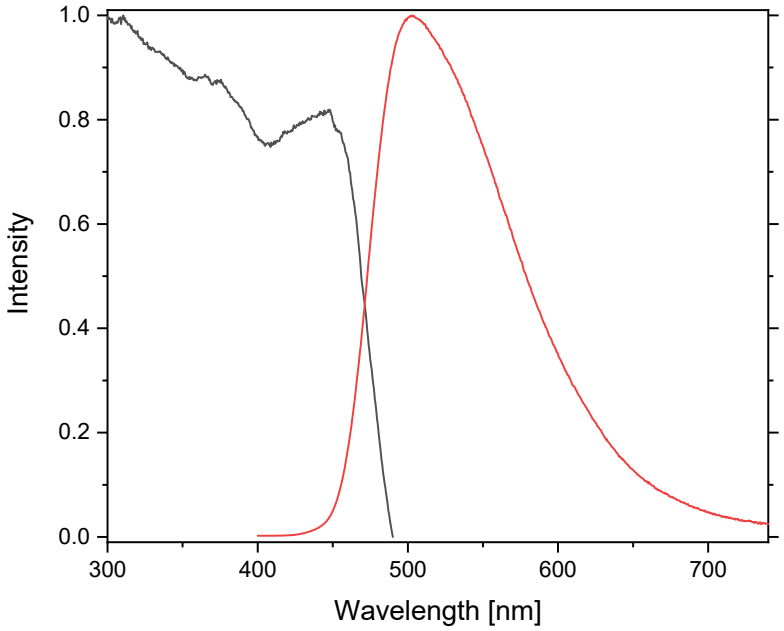


Figure S37: Photoluminescence emission (PL) and excitation (PLE) spectra of compound **5a** at 295 K.

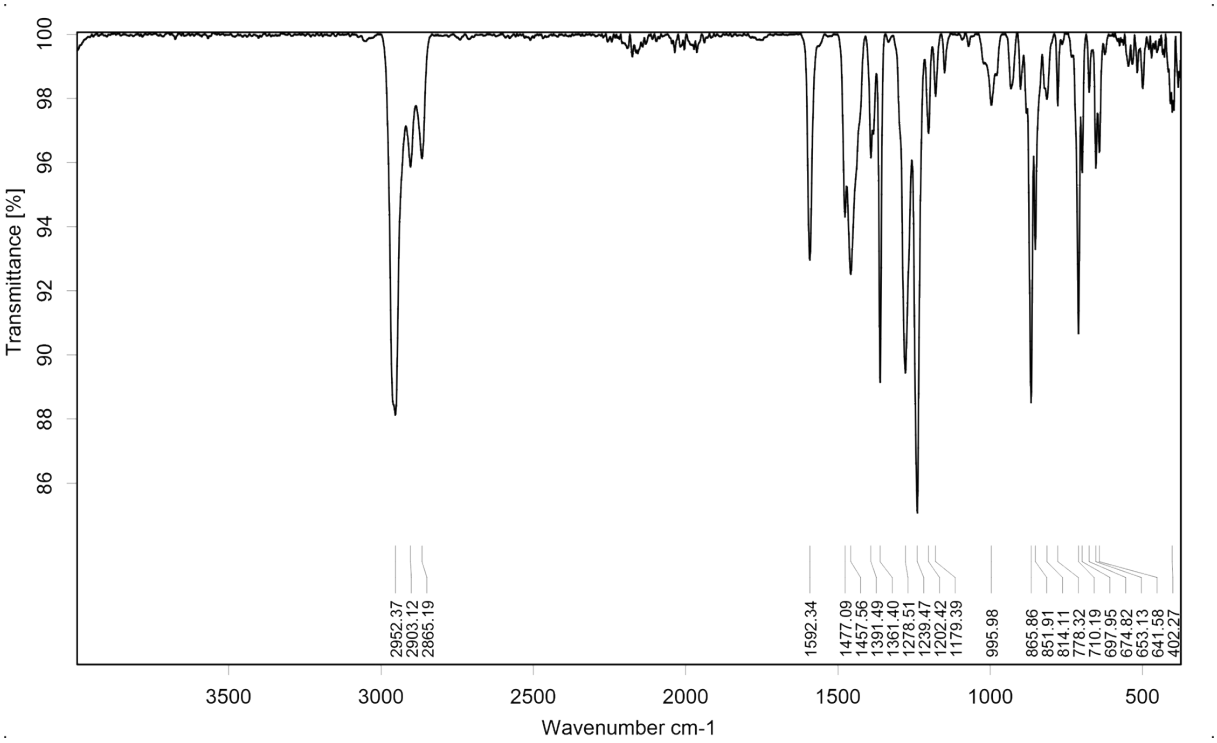
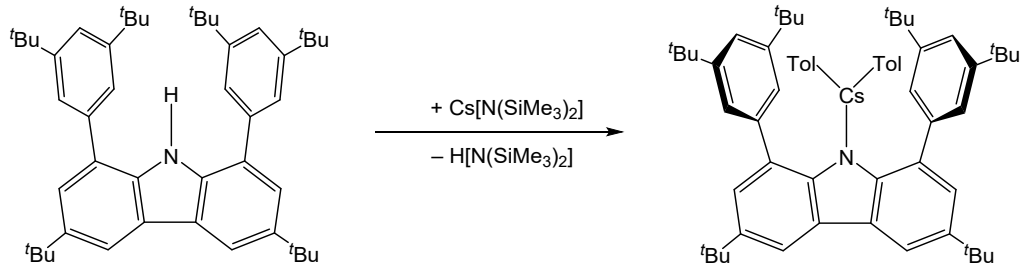


Figure S38: IR spectrum of **5a**.

2.10 [(^{dtbp}Cbz)Cs(Tol)$_2$] (5b)



To a solid mixture of [(^{dtbp}Cbz)–H (150 mg, 0.229 mmol) and Cs[N(SiMe$_3$)$_2$] (76 mg, 0.305 mmol), 5 ml of toluene was added. The mixture was sonicated for 30 minutes and heated to reflux overnight, resulting in a bright yellow solution. The solvent was evaporated to incipient crystallisation and left undisturbed overnight. The mother liquor was removed and the residue was dried in vacuo affording the product as a yellow crystalline solid (108.5 mg, 0.181 mmol, 59%).

^{1}H NMR (400 MHz, C_6D_6): δ (ppm) = 1.27 (s, 36 H, Ar-^{t}Bu); 1.68 (s, 18 H, Carb-^{t}Bu); 2.11 (s, Tol-CH_3), 7.04 (m, Ar-Tol), 7.30 (br, 2 H, *p*-C*H*); 7.64 (d, J_{HH} = 2.0 Hz, 2 H, C^{2,7}*H*); 7.76 (d, J_{HH} = 1.9 Hz, 4 H, *o*-C*H*); 8.72 (br, 2 H, C^{4,5}*H*).
^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ (ppm) = 21.43 (s, Tol-*C*H$_3$); 31.95 (s, Ar-C(*C*H$_3$)$_3$); 32.99 (s, Carb-C(*C*H$_3$)$_3$); 34.94 (s, Carb-*C*(CH$_3$)$_3$); 34.98 (s, Ar-*C*(CH$_3$)$_3$); 116.02 (s, *C*^{4,5}H); 119.45 (s, *p*-*C*H); 121.38 (s, *C*^{2,7}H); 125.39 (s, *o*-*C*H); 125.70 (s, Tol-*C*H(4)); 126.23 (s); 128.57 (s, Tol-*C*H(3,5)); 129.34 (s, Tol-*C*H(2,6)); 135.58 (s); 137.90 (s, Tol-*C*H(1)); 150.54(s); 150.90 (s).
IR (ATR): ũ (cm^{-1}) = 2953 (s), 2903 (w), 2865 (w), 1588 (s), 1493 (vw), 1459 (m), 1392 (w), 1361 (s), 1286 (m), 1273 (s), 1236 (vs), 1202 (w), 1177 (vw), 864 (s), 848 (m), 738 (vs), 718 (s), 698 (s), 675 (vw), 644 (w), 468 (m).
PL ($\lambda_{max,emission}$ [nm], τ_{solid} [ns], Φ_{solid} [%]): 510 (4, 3%).
Mp.: >400°C.

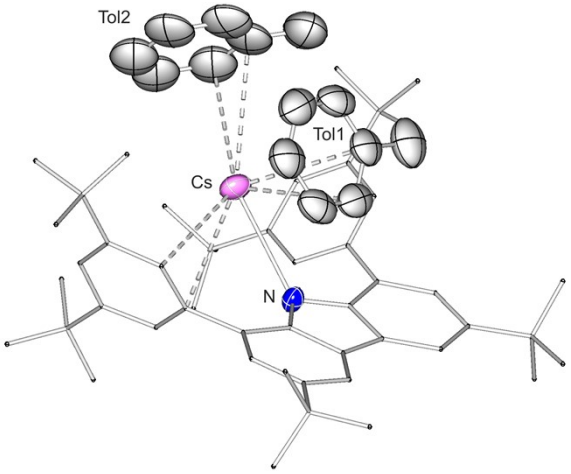


Figure S39: Molecular structure of **5b** (one of two molecules in the asymetric unit, disorder not shown). Selected bond lengths [Å] and angles [°]: Cs1–N1 2.948(4), Cs1–C13$_{arene}$ 3.503(5), Cs1–C54$_{toluene}$ 3.56(2), Cs1–C49$_{toluene}$ 3.585(9), Cs1–C18$_{arene}$ 3.588(5), Cs1–C57$_{toluene}$ 3.617(18), Cs1–C56$_{toluene}$ 3.694(18), Cs-centroid(Tol1): 3.493(7), Cs-centroid(Tol2): 3.541(7).

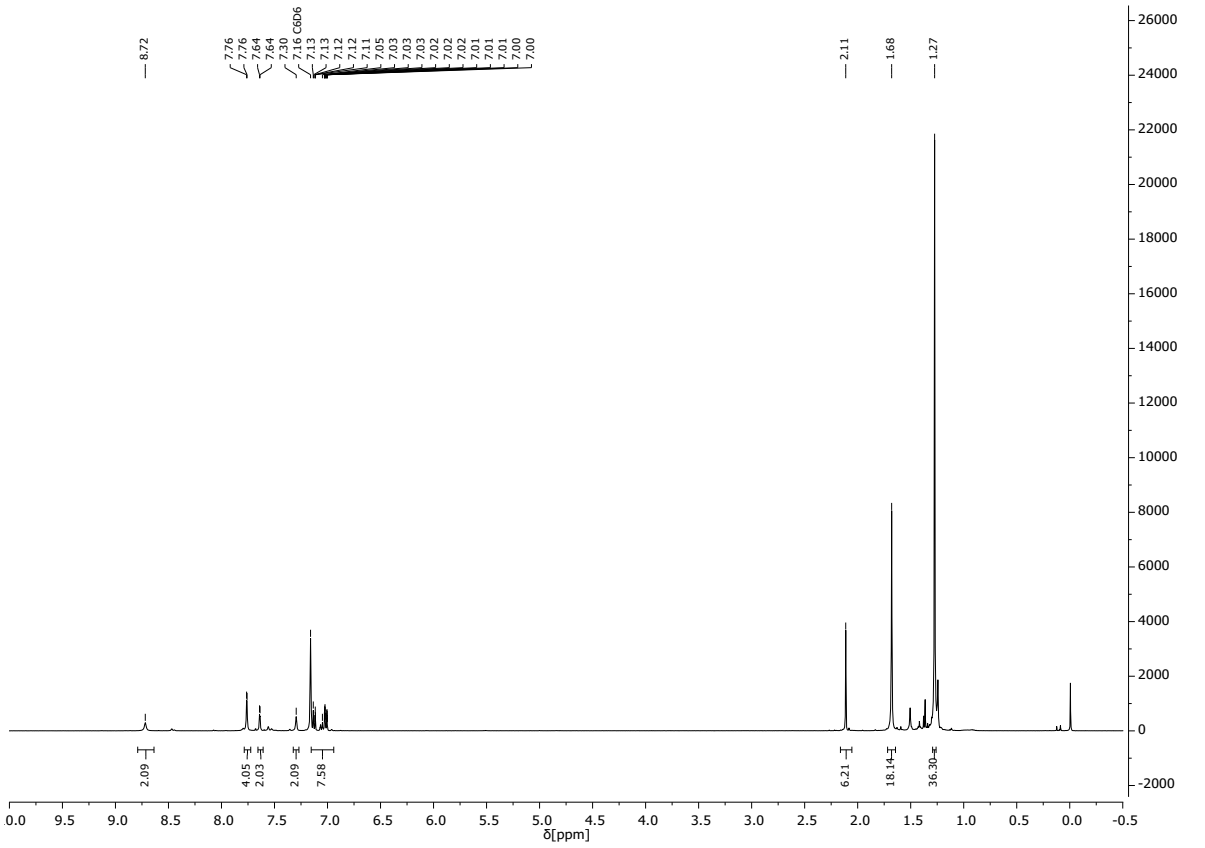


Figure S40: ^{1}H NMR spectrum of **5b**.

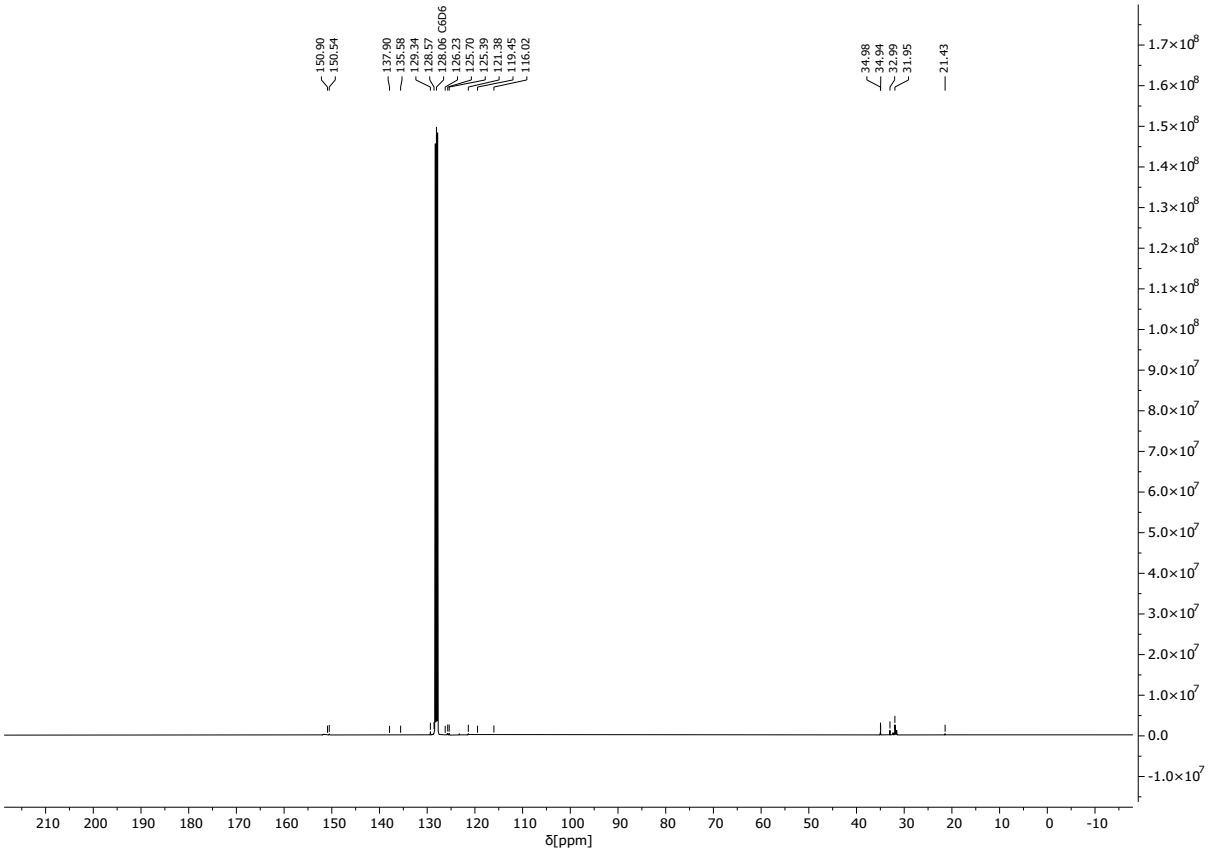


Figure S41: $^{13}C\{^{1}H\}$ NMR spectrum of **5b**.

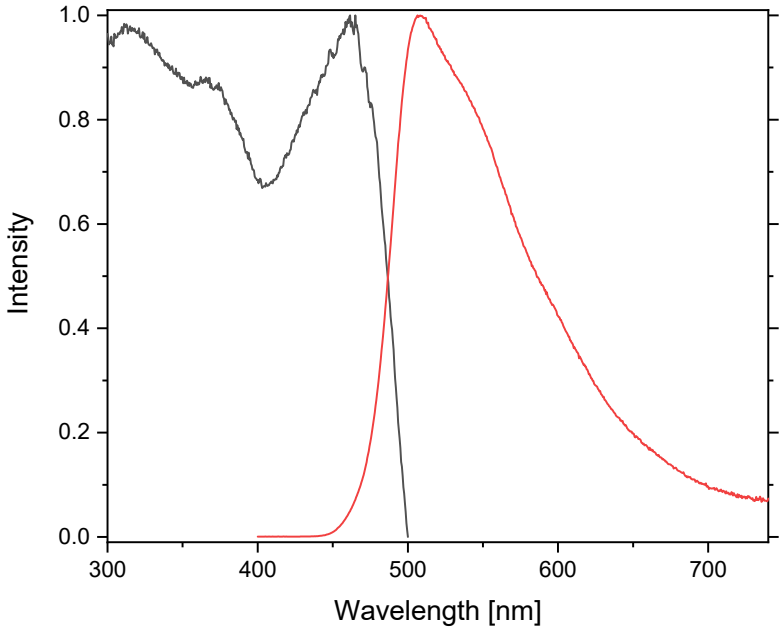


Figure S42: Photoluminescence emission (PL) and excitation (PLE) spectra of compound **5b** at 295 K.

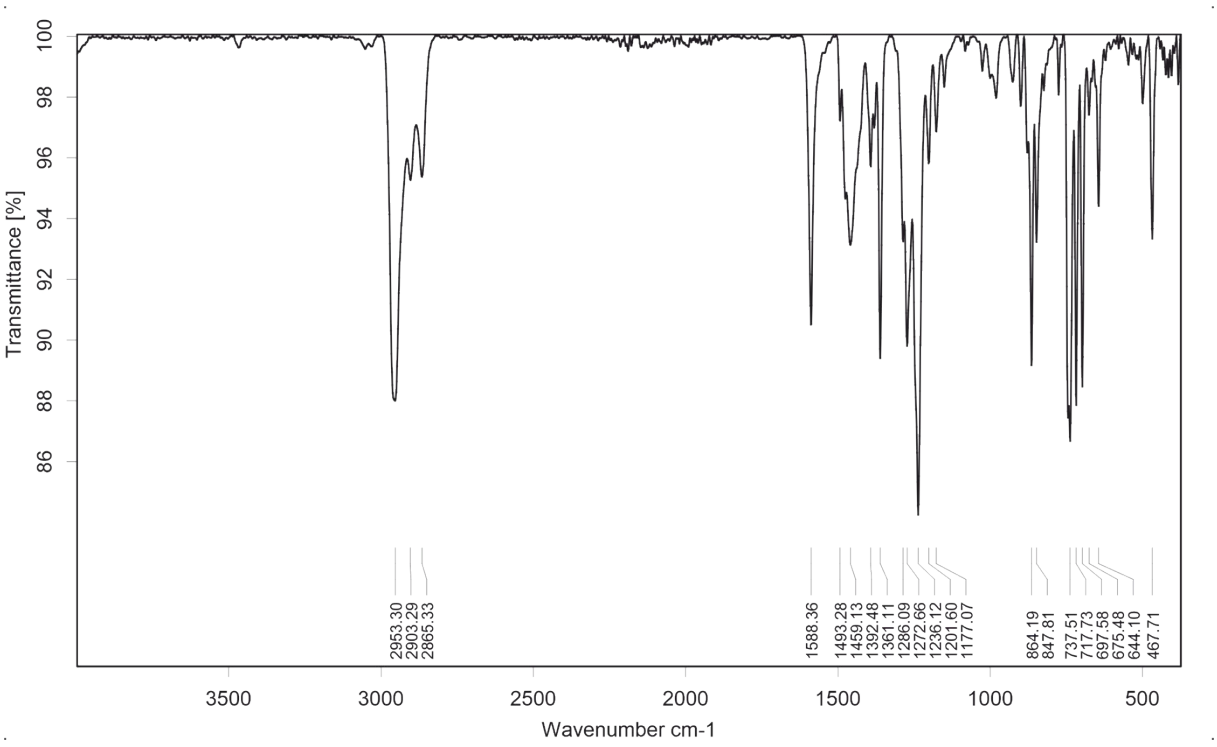
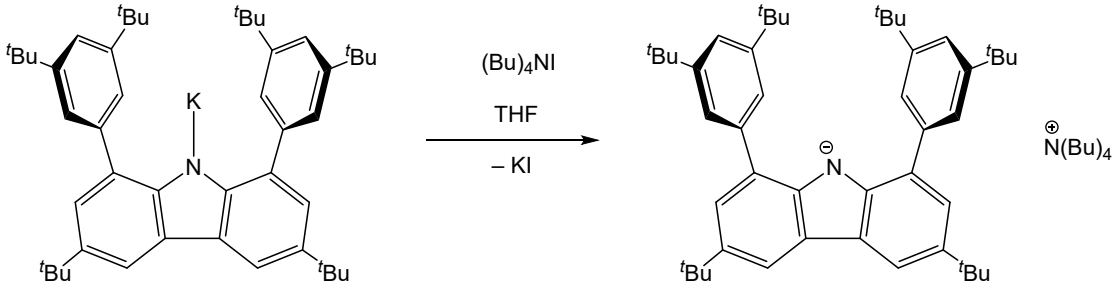


Figure S43: IR spectrum of **5b**.

2.11 $[N(Bu)_4][^{dtbp}Cbz]$ (6)



To a solid mixture of [(^{dtbp}Cbz)K] (300 mg, 0.428 mmol) and [$(Bu)_4N$]I (158 mg, 0.428 mmol), 20 ml of THF was added at ambient temperature. The mixture was stirred for 3 days at 70 °C. Then, volatiles were removed under reduced pressure and the residue was dried *in vacuo*. The residue was washed with *n*-hexane and filtered off. The residue was dried *in vacuo* affording the product as a yellow solid (299.8 mg, 0.334 mmol, 78%). Recrystallisation from hot THF afforded single crystals suitable for X-ray diffraction.

^{1}H NMR (400 MHz, THF-d_8): δ (ppm)= 0.76 (t, 12 H, N(butyl)$_4$-CH_3); 1.03 (br, 16 H, N(butyl)$_4$-CH_2); 1.37 (s, 36 H, Ar-^{t}Bu); 1.48 (s, 18 H, Carb^{t}Bu); 2.45 (br, 8 H, N(butyl)$_4$-CH_2); 7.26 (t, J_{HH} = 1.9 Hz, 2 H, *p*-C*H*); 7.27 (d, J_{HH} = 2.1 Hz, 2 H, C^{2,7}*H*); 7.97 (d, J_{HH} = 2.1 Hz, 2 H, C^{4,5}*H*); 8.06 (d, J_{HH} = 1.9 Hz, 4 H, *o*-C*H*).
^{13}C{^{1}H} NMR (101 MHz, THF-d_8): δ (ppm) = 14.23 (s, N(butyl)$_4$-*C*H$_3$); 20.47 (s, N(butyl)$_4$-*C*H$_2$); 24.72 (s, N(butyl)$_4$-*C*H$_2$); 32.05 (s, Ar-C(*C*H$_3$)$_3$); 32.59 (s, Carb-C(*C*H$_3$)$_3$); 33.34 (s, Carb-*C*(CH$_3$)$_3$); 35.69 (s, Ar-*C*(CH$_3$)$_3$); 58.68 (s, N(butyl)$_4$-*C*H$_2$), 114.72 (s, *C*^{4,5}H); 119.72 (s, *p*-*C*H); 121.55 (s, *C*^{2,7}H); 124.79 (s, *o*-*C*H); 127.00 (s); 129.18 (s); 133.80 (s); 145.05 (s); 150.55 (s); 150.90 (s).
IR (ATR): ũ (cm^{-1}) = 2960 (vs), 2902 (w), 2873 (m), 1593 (m), 1477 (vs), 1457 (s), 1390 (w), 1379 (m), 1360 (s), 1277 (vs), 1238 (vs), 1202 (w), 1177 (w), 1150 (vw), 900 (vw), 867 (vs), 850 (m), 776 (vw), 712 (s), 697 (w), 675 (vw), 647 (w).
PL ($\lambda_{max,emission}$ [nm], τ_{solid} [ns], Φ_{solid} [%]): 520 (21, 15%).
Mp.: 235 °C (Decomposition).

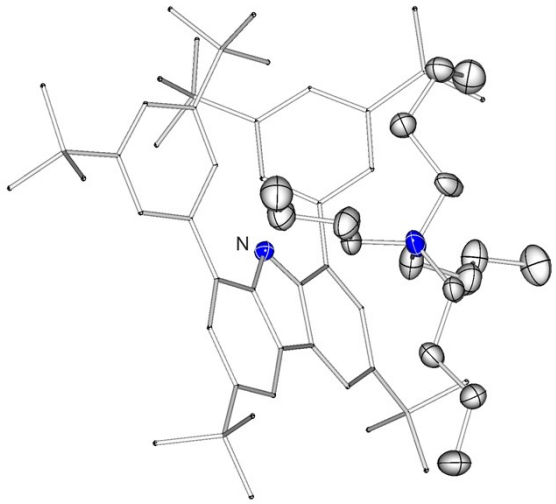


Figure S44: Molecular structure of **6**.

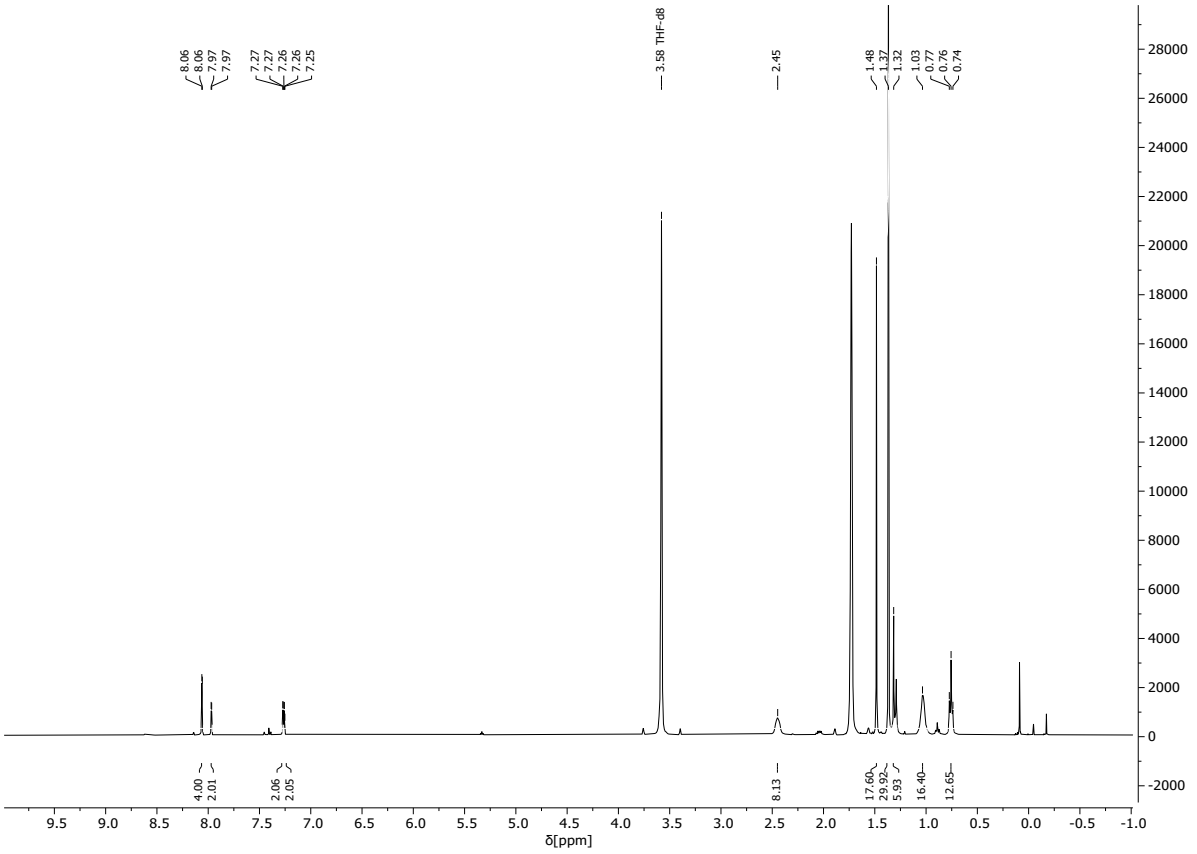


Figure S45: ^{1}H NMR spectrum of **6**.

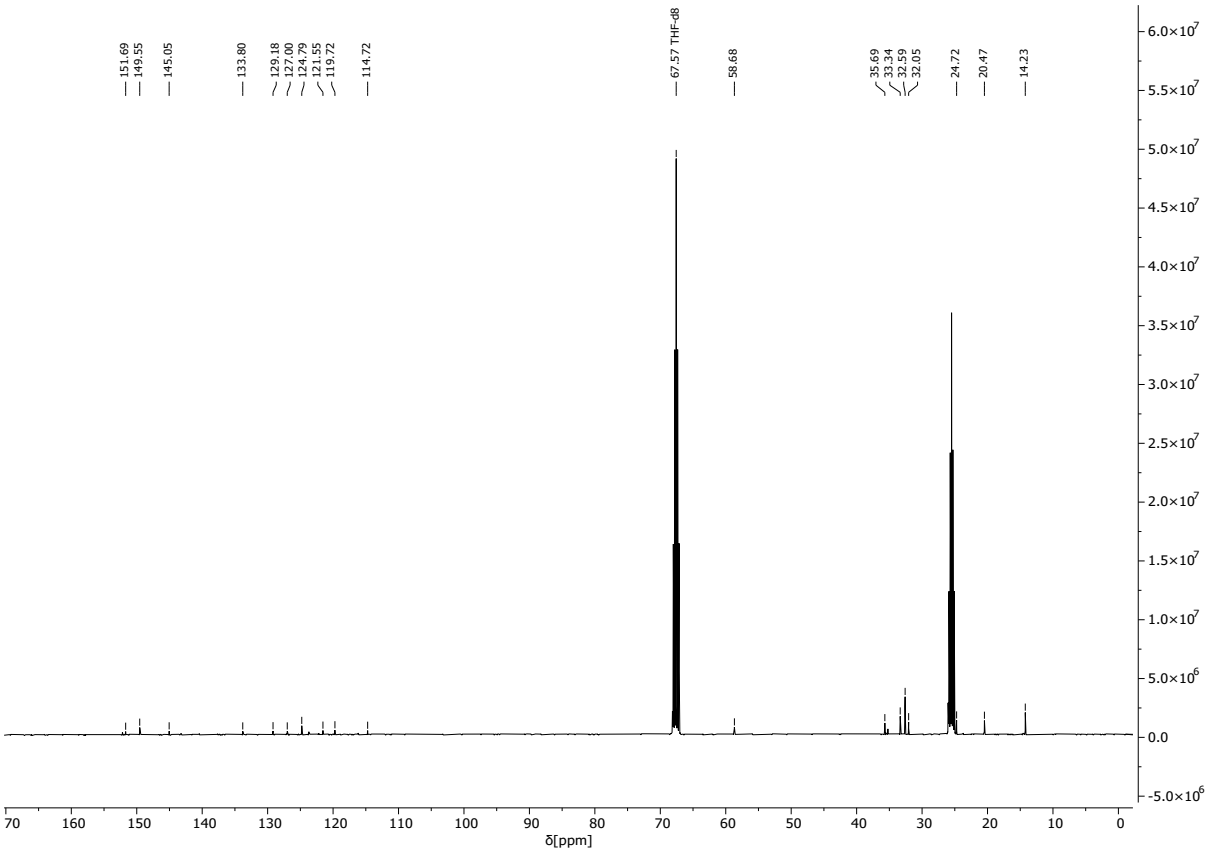


Figure S46: $^{13}C\{^{1}H\}$ NMR spectrum of **6**.

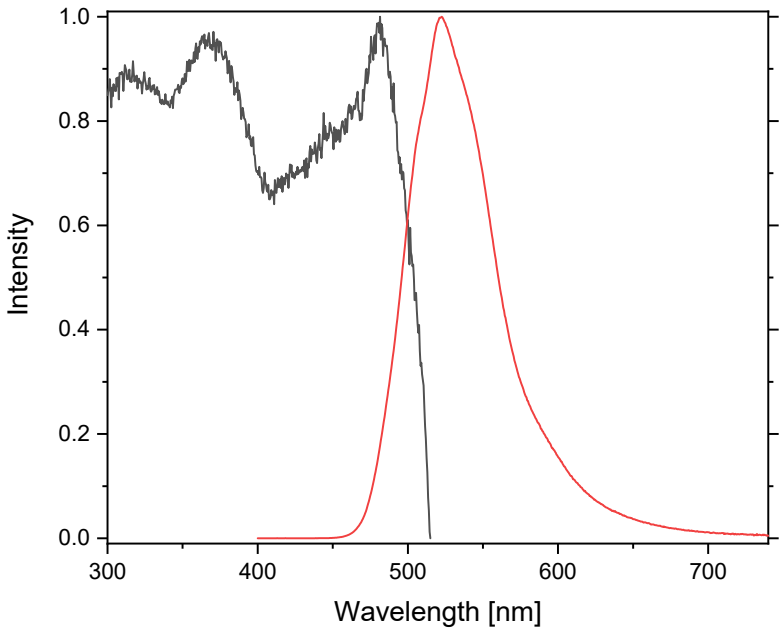


Figure S47: Photoluminescence emission (PL) and excitation (PLE) spectra of compound **6** at 295 K.

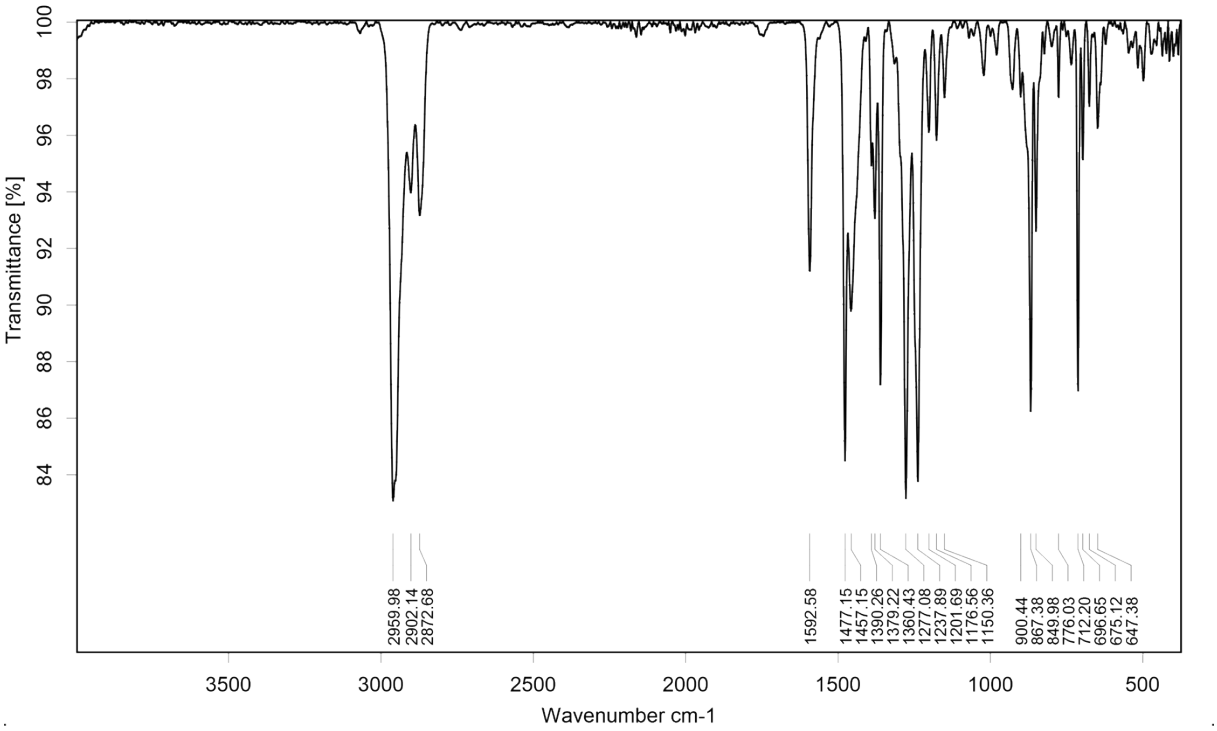


Figure S48: IR spectrum of **6**.

3 Photoluminescence properties

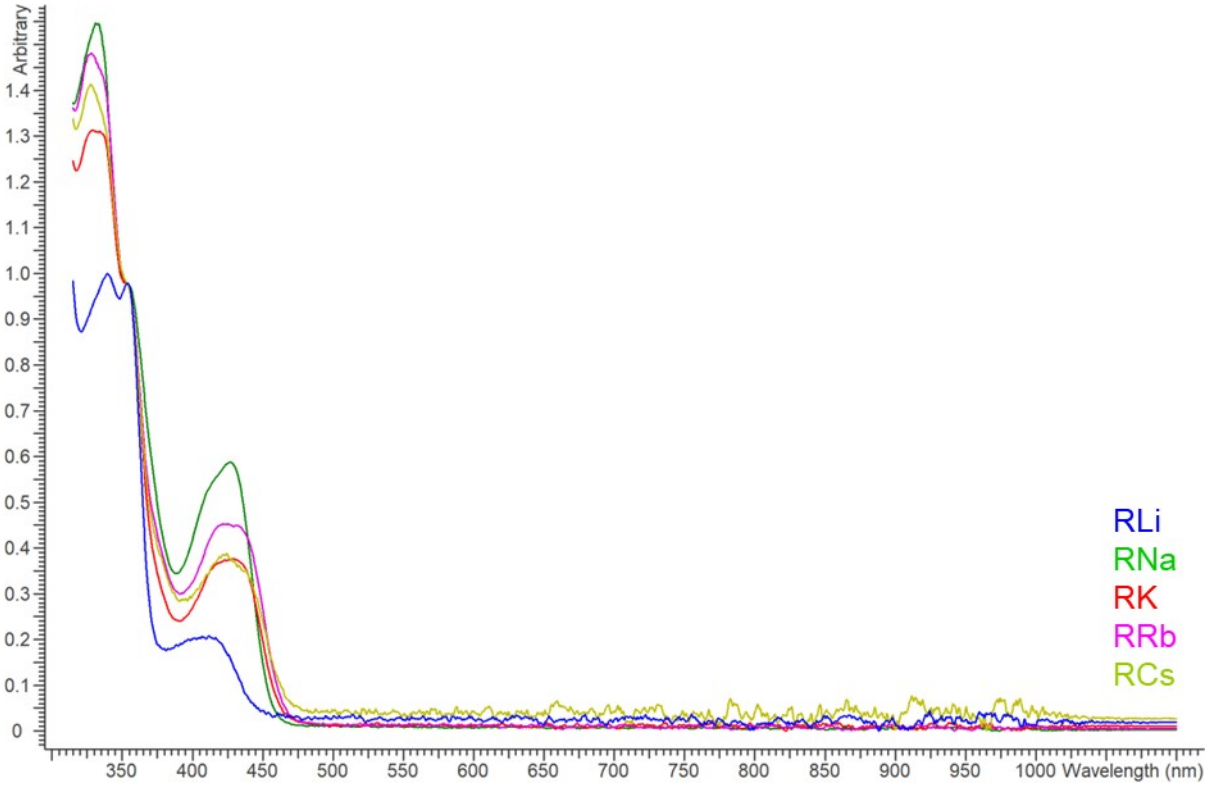


Figure S49: Absorption spectra of the alkali metal carbazolides in toluene solution, normalised to the peak at 354 nm.

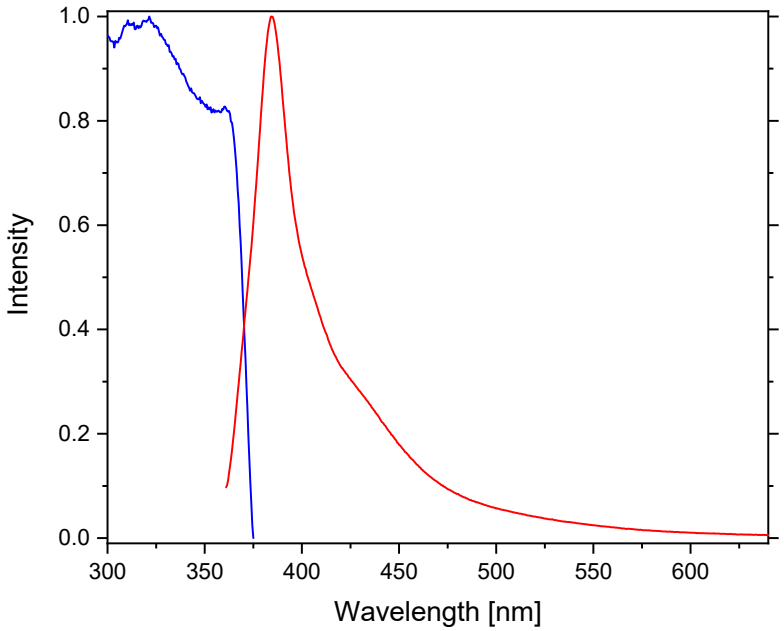


Figure S50: Photoluminescence emission (PL) and excitation (PLE) spectra of compound ^{dtbp}**Cbz–H** at 295 K in the solid state.

Table S1: Photoluminescence properties of (^{dtbp}Cbz)–H, the alkali metal-carbazolides **1a**/**b** – **5a**/**b** and **6** in the solid state.

	ϕ /%	**λ_{ex} /nm**	**$\lambda_{em,max}$ /nm**	**τ_{FL} /ns**
(^{dtbp}Cbz)–H	9	350	385	2
1a	12	375	520	14
1b	8	375	540/580	13
2a	9	375	515	14
2b	12	375	490/515	13
3a	18	400	500	15
3b	14	350	510/550	11
4a	29	375	460	9
4b	17	375	485	8
5a	3	375	505	3
5b	3	375	510	4
6	15	375	520	21

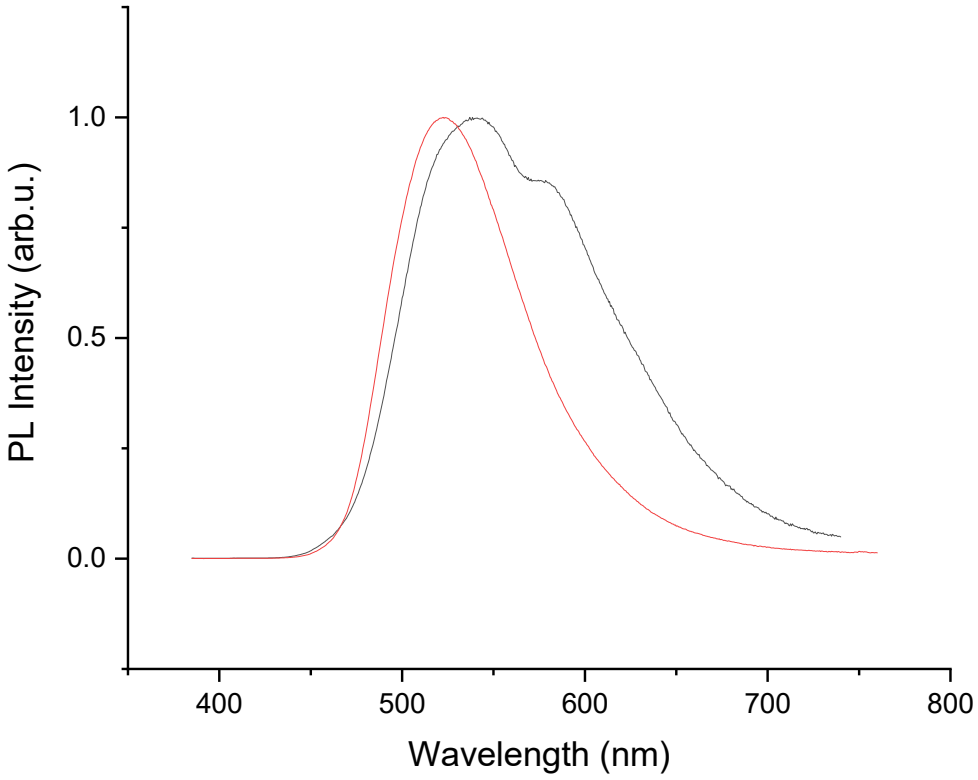


Figure S51: Photoluminescence emission spectra of compound [(^{dtbp}Cbz)Li] (**1a**, red) and [(^{dtbp}Cbz)Li(Tol)] (**1b**, black) at 295 K in the solid state.

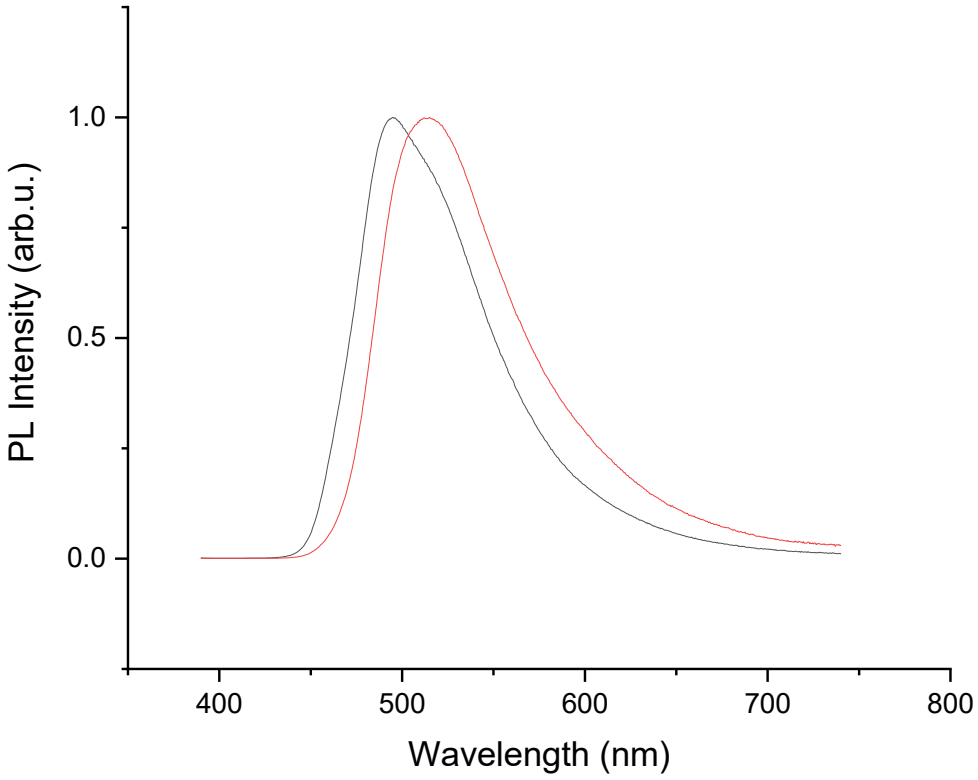


Figure S52: Photoluminescence emission spectra of compound [(^{dtbp}Cbz)Na] (**2a**, red) and [(^{dtbp}Cbz)Na(Tol)$_{1.5}$] (**2b**, black) at 295 K in the solid state.

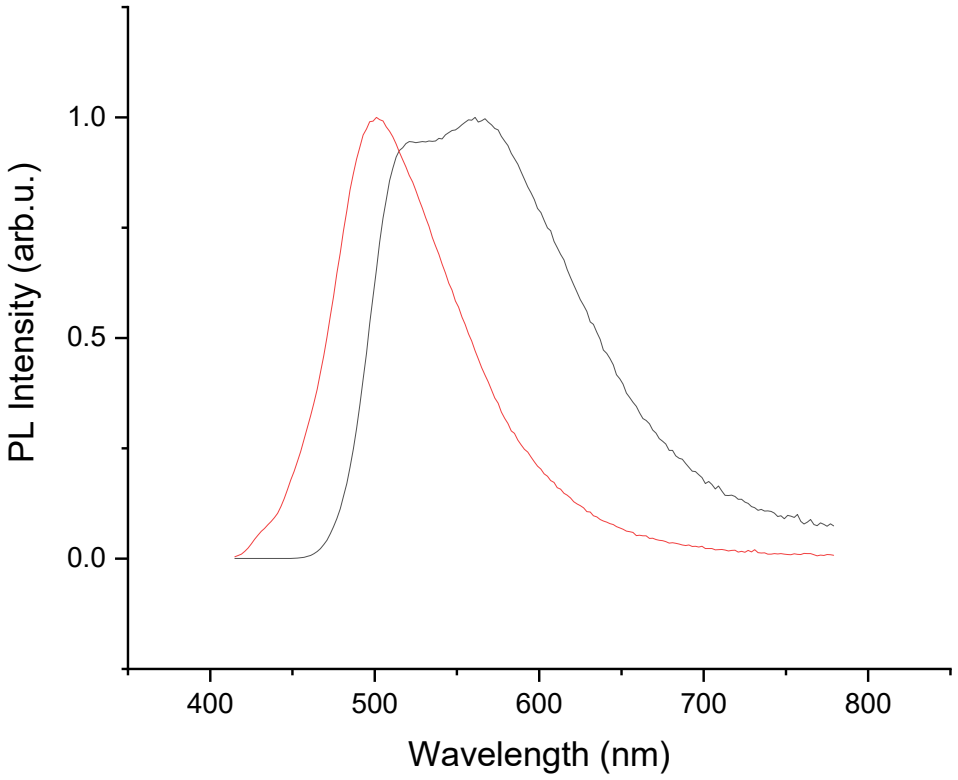


Figure S53: Photoluminescence emission spectra of compound [(^{dtbp}Cbz)K] (**3a**, red) and [(^{dtbp}Cbz)K(Tol)$_2$] (**3b**, black) at 295 K in the solid state.

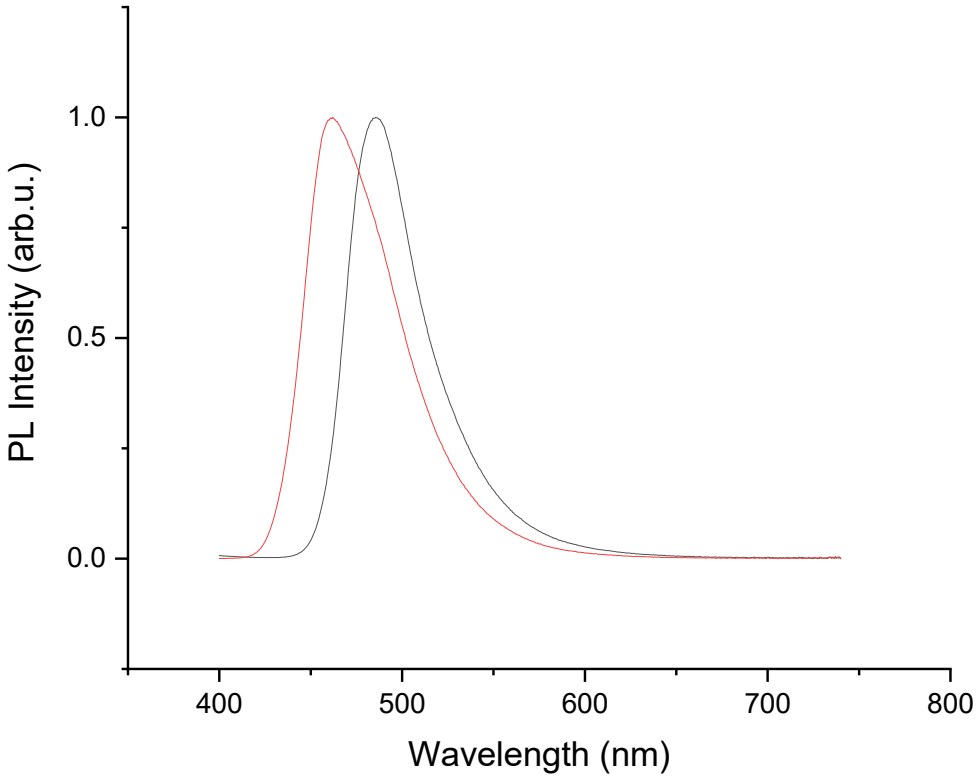


Figure S54: Photoluminescence emission spectra of compound [(^{dtbp}Cbz)Rb] (**4a**, red) and [(^{dtbp}Cbz)Rb(Tol)$_2$] (**4b**, black) at 295 K in the solid state.

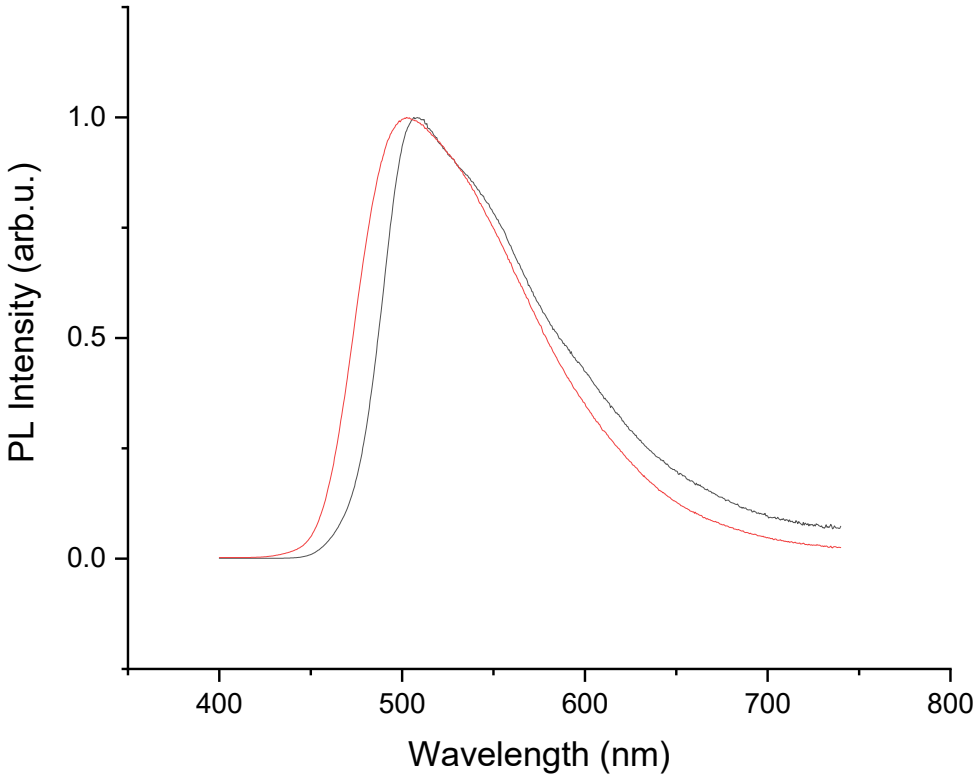


Figure S55: Photoluminescence emission spectra of compound [(^{dtbp}Cbz)Cs] (**5a**, red) and [(^{dtbp}Cbz)Cs(Tol)$_2$] (**5b**, black) at 295 K in the solid state.

4 Crystallography

Table S2: Crystallographic details for **1a**, **1b**, **2a** and **2b**.

	1a	**1b**	**2a**	**2b**
	[(^{dtbp}Cbz)Li]	[(^{dtbp}Cbz)Li(Tol)]	[(^{dtbp}Cbz)Na]	[(^{dtbp}Cbz)Na(Tol)$_{1.5}$]
CCDC #	2206682	2206683	2206684	2206685
Empirical formula	$C_{48}H_{64}NLi$	$C_{55}H_{72}LiN$	$C_{51}H_{71}NNa$	$C_{58.5}H_{76}NNa$
FW [g mol^{-1}]	661.94	800.14	721.07	816.19
Wavelength [Å]	1.34143	1.34143	0.71073	1.34143
Temperature [K]	150(2)	150(2)	200(2)	150(2)
Crystal system	triclinic	triclinic	triclinic	triclinic
Space group	*P*-1	*P*-1	*P*-1	*P*-1
a [Å]	10.2875(3)	11.4471(4)	14.7532(5)	12.9521(5)
b [Å]	12.9820(3)	13.5815(5)	15.1802(4)	14.6619(6)
c [Å]	31.9682(8)	17.3549(6)	22.6005(7)	15.9828(6)
α [°]	85.399(2)	81.887(3)	82.972(2)	62.724(3)
β [°]	87.100(2)	74.552(3)	84.666(2)	73.475(3)
γ [°]	82.983(2)	83.586(3)	66.072(2)	72.745(3)
V [Å^3]	4220.20(19)	2566.86(16)	4586.5(3)	2536.55(19)
Z	4	2	4	2
ρ_{calc} (g·cm^{-3})	1.042	1.035	1.044	1.069
μ	0.278	0.276	0.067	0.334
F(000)	1448.0	874.0	1580.0	890.0
reflections collected	54803	2867	26607	34399
independent reflections	19745	11244	18393	11961
reflectionsGT ($I > 2\sigma(I)$)	14457	9263	12907	
R_{int}	0.0194	0.0195	0.0371	0.0223
parameters	1211	633	1197	715
restraints	1332	702	984	722
GooF	1.068	1.031	1.033	1.084
R1	0.0477	0.0513	0.0573	0.0468
R1 (all)	0.0670	0.0602	0.0864	0.0640
wR2	0.1285	0.1434	0.1419	0.1316
wR2 (all)	0.1384	0.1490	0.1654	0.1394
Largest diff. peak/hole / e Å^{-3}	0.32/-0.32	0.23/-0.20	0.35/-0.35	0.50/-0.35

Table S3: Crystallographic details for **4a**, **4b**, **5b** and **6**.

	4a	**4b**	**5b**	**6**
	[(^{dtbp}Cbz)Rb	[(^{dtbp}Cbz)Rb(Tol)$_2$]	[(^{dtbp}Cbz)Cs(Tol)$_2$]	[(^{dtbp}Cbz)N(butyl)$_4$
CCDC #	2206686	2206687	2206688	2206689
Empirical formula	$C_{48}H_{64}NRb$	$C_{248}H_{320}N_4Rb_4$	$C_{62}H_{80}CsN$	$C_{64}H_{100}N_2$
FW [g mol^{-1}]	740.47	3698.94	972.18	897.45
Wavelength [Å]	1.34143	0.71073	0.71073	1.34143
Temperature [K]	150(2)	200(2)	200(2)	150(2)
Crystal system	triclinic	monoclinic	monoclinic	triclinic
Space group	*P*-1	*Cc*	*Cc*	*P*-1
a [Å]	11.9867(4)	23.0431(8)	23.0295(11)	13.7635(3)
b [Å]	12.3576(5)	24.7881(7)	24.6284(11)	16.7055(5)
c [Å]	14.2644(10)	19.6945(6)	19.9647(8)	26.5701(7)
α [°]	94.425(4)	90	90	94.652(2)
β [°]	95.090(4)	100.985(3)	101.290(3)	104.531(2)
γ [°]	94.840(3)	90	90	90.283(2)
V [Å^3]	2089.46(18)	11043.3(6)	11104.4(9)	5892.2(3)
Z	2	2	8	4
ρ_{calc} (g·cm^{-3})	1.177	1.112	1.163	1.012
μ	1.222	0.933	0.703	0.270
F(000)	792.0	3968.0	4112.0	1992.0
reflections collected	25027	41090	54595	68834
independent reflections	9206	20397	25870	25875
reflectionsGT (I > 2σ(I))	7988	13228	15048	19993
R_{int}	0.0198	0.0474	0.0406	0.0194
parameters	509	1562	1599	1402
restraints	168	1748	1900	721
GooF	1.148	1.041	1.013	1.065
R1	0.0643	0.0568	0.0472	0.0520
R1 (all)	0.0719	0.0999	0.1023	0.0679
wR2	0.1799	0.1325	0.1048	0.1401
wR2 (all)	0.1834	0.1577	0.1274	0.1488
Largest diff. peak/hole / e Å^{-3}	0.74/-0.84	1.16/-0.44	2.05/-0.56	0.51/-0.29

5 Computational Details

All computations were performed using Gaussian16[9] utilizing the PBE0 level of theory, Def2SVP basis sets and empirical dispersion correction (GD3). No solvent corrections were applied. All optimized molecular structures where checked to be minima on the energy hypersurface and possess no imaginary vibrational frequencies.

(^{dtbp}Cbz)H

Zero-point correction= 1.016236 (Hartree/Particle)

Thermal correction to Energy= 1.067693

Thermal correction to Enthalpy= 1.068637

Thermal correction to Gibbs Free Energy= 0.932168

Sum of electronic and zero-point Energies= -1918.533165

Sum of electronic and thermal Energies= -1918.481707

Sum of electronic and thermal Enthalpies= -1918.480763

Sum of electronic and thermal Free Energies= -1918.617233

[(^{dtbp}Cbz)]$^{-}$

Zero-point correction= 1.001519 (Hartree/Particle)

Thermal correction to Energy= 1.052757

Thermal correction to Enthalpy= 1.053702

Thermal correction to Gibbs Free Energy= 0.916966

Sum of electronic and zero-point Energies= -1917.983248

Sum of electronic and thermal Energies= -1917.932010

Sum of electronic and thermal Enthalpies= -1917.931065

Sum of electronic and thermal Free Energies= -1918.067801

[(^{dtbp}Cbz)Li]

Zero-point correction= 1.005559 (Hartree/Particle)

Thermal correction to Energy= 1.057794

Thermal correction to Enthalpy= 1.058738

Thermal correction to Gibbs Free Energy= 0.921691

Sum of electronic and zero-point Energies= -1925.493256

Sum of electronic and thermal Energies= -1925.441021

Sum of electronic and thermal Enthalpies= -1925.440077

Sum of electronic and thermal Free Energies= -1925.577124

[(^{dtbp}Cbz)Na]

Zero-point correction= 1.004050 (Hartree/Particle)

Thermal correction to Energy= 1.057006

Thermal correction to Enthalpy= 1.057950

Thermal correction to Gibbs Free Energy= 0.917958

Sum of electronic and zero-point Energies= -2080.122938

Sum of electronic and thermal Energies= -2080.069983

Sum of electronic and thermal Enthalpies= -2080.069039

Sum of electronic and thermal Free Energies= -2080.209030

[(^{dtbp}Cbz)K]

Zero-point correction= 1.002857 (Hartree/Particle)

Thermal correction to Energy= 1.056499

Thermal correction to Enthalpy= 1.057443

Thermal correction to Gibbs Free Energy= 0.912583

Sum of electronic and zero-point Energies= -2517.669468

Sum of electronic and thermal Energies= -2517.615826

Sum of electronic and thermal Enthalpies= -2517.614882

Sum of electronic and thermal Free Energies= -2517.759742

[(^{dtbp}Cbz)Rb]

Zero-point correction= 1.002794 (Hartree/Particle)

Thermal correction to Energy= 1.056506

Thermal correction to Enthalpy= 1.057450

Thermal correction to Gibbs Free Energy= 0.912949

Sum of electronic and zero-point Energies= -1942.085864

Sum of electronic and thermal Energies= -1942.032152

Sum of electronic and thermal Enthalpies= -1942.031208

Sum of electronic and thermal Free Energies= -1942.175708

[(^{dtbp}Cbz)Cs]

Zero-point correction= 1.002819 (Hartree/Particle)

Thermal correction to Energy= 1.056538

Thermal correction to Enthalpy= 1.057482

Thermal correction to Gibbs Free Energy= 0.912728

Sum of electronic and zero-point Energies= -1938.148198

Sum of electronic and thermal Energies= -1938.094479

Sum of electronic and thermal Enthalpies= -1938.093534

Sum of electronic and thermal Free Energies= -1938.238289

5.1 Orbitals

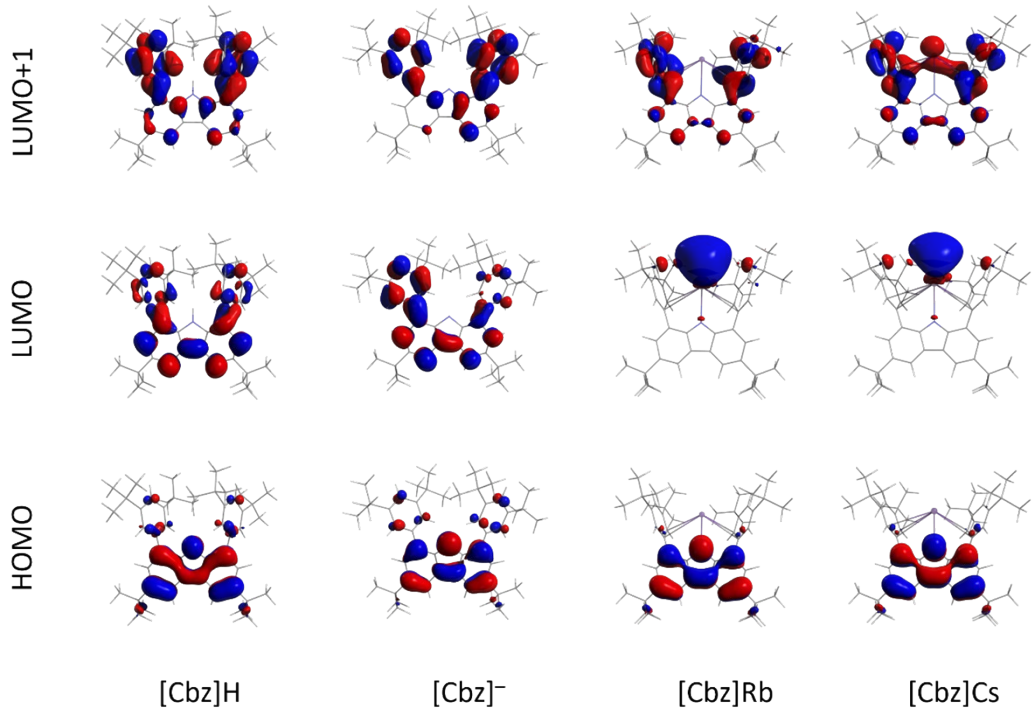


Figure S56: Selected orbitals of the carbazolides.

Composition of HOMO, LUMO, LUMO+1 (Mulliken partitioning), only contributions of the N-bound atom (H, Li, Na, K, Rb, Cs) are shown

5.1.1 (^{dtbp}Cbz)–H

```
HOMO  Atom     2(H ) :    0.214971%
LUMO  Atom     2(H ) :    0.001735%
LUMO+1  Atom     2(H ) :    0.892676%
```

5.1.2 [(^{dtbp}Cbz)Li]

```
HOMO  Atom   114(Li) :    1.180950%
LUMO  Atom   114(Li) :    4.102392%
 Shell   490 Type: P    in atom  114(Li) :       0.66599%
 Shell   491 Type: P    in atom  114(Li) :       3.05070%
LUMO +1  Atom   114(Li) :    3.896592%
 Shell   488 Type: S    in atom  114(Li) :       0.64918%
 Shell   489 Type: S    in atom  114(Li) :       1.56616%
 Shell   491 Type: P    in atom  114(Li) :       1.22310%
```

5.1.3 [(^{dtbp}Cbz)Na] monomer

```
HOMO  Atom   114(Na) :    1.026812%
LUMO  Atom   114(Na) :    2.723261%
 Shell   490 Type: S    in atom  114(Na) :       1.02858%
 Shell   492 Type: P    in atom  114(Na) :       1.82573%
LUMO +1  Atom   114(Na) :    1.463017%
 Shell   492 Type: P    in atom  114(Na) :       0.54035%
 Shell   493 Type: D    in atom  114(Na) :       0.72651%
```

5.1.4 [(^{dtbp}Cbz)K]

```
HOMO  Atom   110(K ) :    0.894119%
LUMO  Atom   110(K ) :   64.771915%
 Shell   476 Type: S    in atom  110(K ) :      51.19542%
 Shell   479 Type: P    in atom  110(K ) :      12.65535%
 Shell   481 Type: D    in atom  110(K ) :       1.19664%
LUMO +1 Atom   110(K ) :   19.818257%
 Shell   476 Type: S    in atom  110(K ) :      14.99100%
 Shell   479 Type: P    in atom  110(K ) :       3.79751%
 Shell   481 Type: D    in atom  110(K ) :       1.18452%
```

5.1.5 [(^{dtbp}Cbz)Rb]

```
HOMO  Atom   114(Rb) :    0.408623%
LUMO Atom   114(Rb) :   94.161233%
 Shell   488 Type: S    in atom  114(Rb) :       0.62329%
 Shell   489 Type: S    in atom  114(Rb) :      -0.87644%
 Shell   490 Type: S    in atom  114(Rb) :       7.66271%
 Shell   491 Type: S    in atom  114(Rb) :      57.62618%
 Shell   492 Type: P    in atom  114(Rb) :       0.66118%
 Shell   494 Type: P    in atom  114(Rb) :      26.61720%
 Shell   496 Type: D    in atom  114(Rb) :       1.19056%
LUMO +1  Atom   114(Rb) :    7.313974%
 Shell   490 Type: S    in atom  114(Rb) :       0.61788%
 Shell   494 Type: P    in atom  114(Rb) :       1.11806%
```

```
 Shell   495 Type: D    in atom  114(Rb) :       0.68558%
 Shell   496 Type: D    in atom  114(Rb) :       4.57483%
```

5.1.6 [(^{dtbp}Cbz)Cs]

```
HOMO  Atom   114(Cs) :    0.904883%
LUMO  Atom   114(Cs) :   93.286924%
 Shell   489 Type: S    in atom  114(Cs) :      -0.58556%
 Shell   490 Type: S    in atom  114(Cs) :       1.44318%
 Shell   491 Type: S    in atom  114(Cs) :      -0.79924%
 Shell   492 Type: S    in atom  114(Cs) :       3.81754%
 Shell   493 Type: S    in atom  114(Cs) :      10.97123%
 Shell   494 Type: S    in atom  114(Cs) :      48.60679%
 Shell   498 Type: P    in atom  114(Cs) :       0.78694%
 Shell   499 Type: P    in atom  114(Cs) :      -0.61326%
 Shell   500 Type: P    in atom  114(Cs) :       3.69110%
 Shell   501 Type: P    in atom  114(Cs) :      15.71053%
 Shell   502 Type: P    in atom  114(Cs) :       7.78589%
 Shell   506 Type: D    in atom  114(Cs) :       2.00119%
LUMO+1  Atom   114(Cs) :   15.345293%
 Shell   492 Type: S    in atom  114(Cs) :       0.85155%
 Shell   493 Type: S    in atom  114(Cs) :      -1.03264%
 Shell   494 Type: S    in atom  114(Cs) :       1.05143%
 Shell   501 Type: P    in atom  114(Cs) :       2.77007%
 Shell   502 Type: P    in atom  114(Cs) :       2.27659%
 Shell   504 Type: D    in atom  114(Cs) :       0.84194%
 Shell   505 Type: D    in atom  114(Cs) :       1.91565%
 Shell   506 Type: D    in atom  114(Cs) :       4.70379%
 Shell   507 Type: D    in atom  114(Cs) :       2.19418%
```

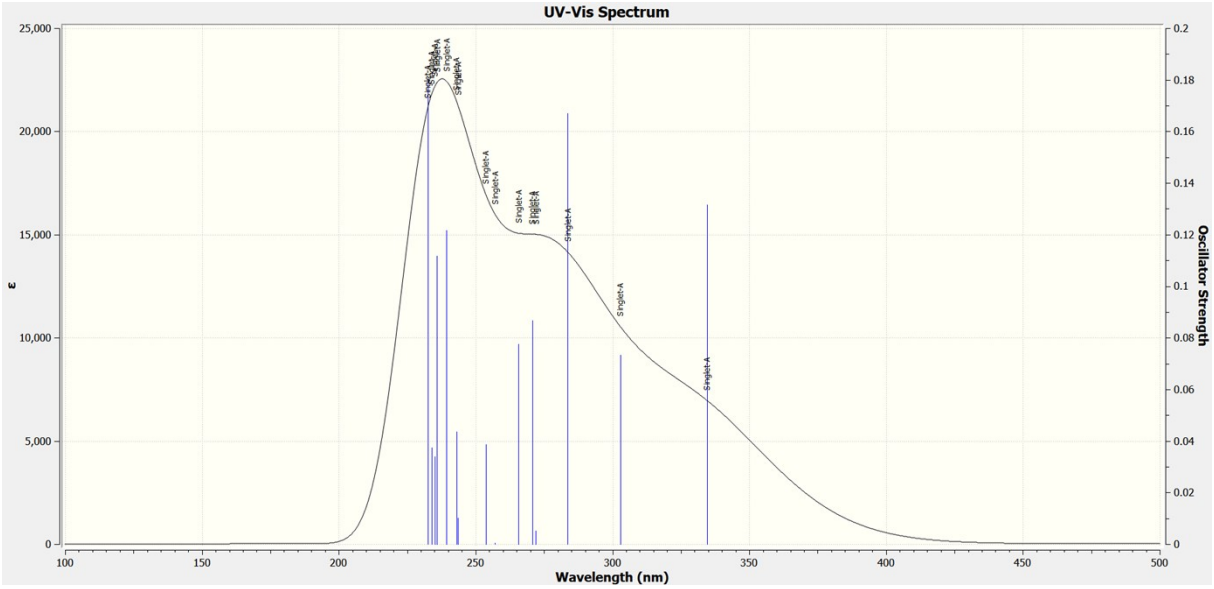
5.2 Absorptions

Table S4: Calculated absorption energies for selected compounds.

UV/Vis unsolvated	**1** λ_{abs} [nm]	oscillator strength	**2** λ_{abs} [nm]	oscillator strength	**3** λ_{abs} [nm]	oscillator strength
(dtbpCbz)–H	334.49	0.1315	302.83	0.0733	283.59	0.1671
[(dtbpCbz)Li]	422.82	0.0487	392.03	0.0350	379.19	0.0249
[(dtbpCbz)Na]	425.47	0.0308	410.30	0.0119	401.38	0.0212
[(dtbpCbz)K]	426.28	0.0060	419.99	0.0145	411.72	0.0086
[(dtbpCbz)Rb]	454.77	0.0005	422.11	0.0408	406.27	0.0283
[(dtbpCbz)Cs]	441.09	0.0006	423.82	0.0498	404.25	0.0467
$[(dtbpCbz)]^-$	436.34	0.1302	394.68	0.1819	351.99	0.0018
$[(dtbpCbz)Na]_2$	406.70	0.0471	389.43	0.1002	375.42	0.0165

Details on computed absorptions

5.2.1 (^{dtbp}Cbz)–H

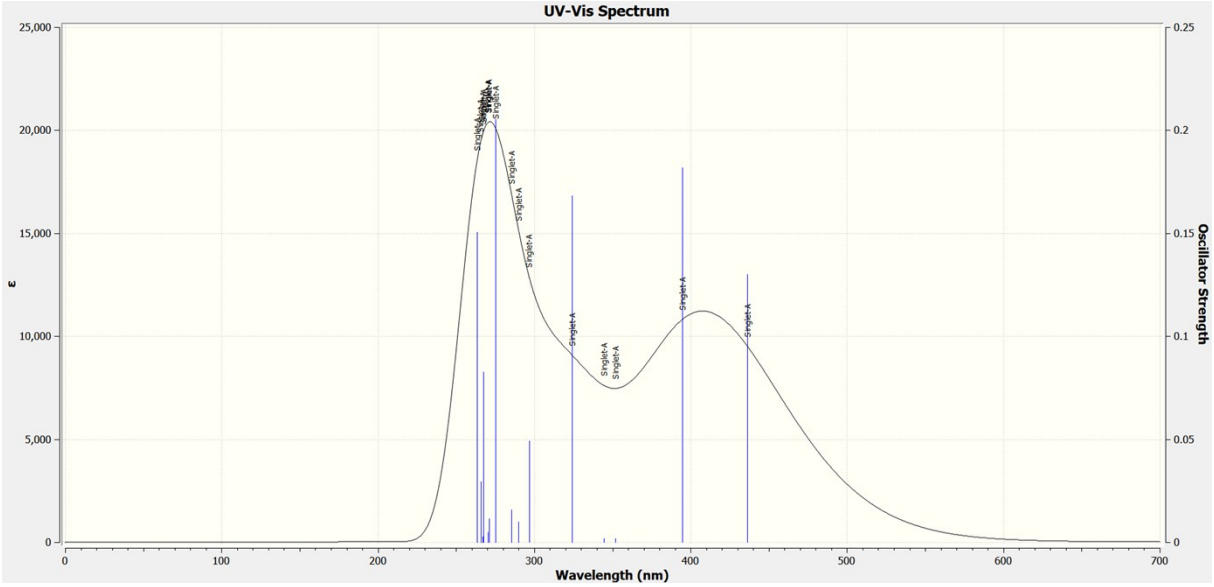



```
Excited State   1:       Singlet-A       3.7067 eV   334.49 nm   f=0.1315
<S**2>=0.000
     168 -> 181        0.01967
     173 -> 181       -0.01151
     173 -> 187        0.03460
     174 -> 182       -0.01053
     174 -> 186       -0.02395
     175 -> 181       -0.03483
     175 -> 187        0.02400
     178 -> 186        0.02322
     179 -> 182       -0.08490
     179 -> 183        0.03132
     179 -> 186       -0.09602
     179 -> 189       -0.02299
     180 -> 181        0.69027
     180 -> 185       -0.02534
     173 <- 187        0.01332
     178 <- 182        0.01230
     179 <- 182       -0.01125
     179 <- 186       -0.02247
     180 <- 181       -0.02129
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -1919.41318300
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:       Singlet-A       4.0942 eV   302.83 nm   f=0.0733
<S**2>=0.000
     158 -> 182        0.01278
     168 -> 182        0.02556
     170 -> 182       -0.01467
     173 -> 186       -0.02081
     174 -> 185        0.01033
     175 -> 182       -0.01008
     175 -> 186       -0.01912
     178 -> 181       -0.02109
     178 -> 184       -0.01334
     178 -> 185       -0.03540
```

```
     179 -> 181        0.08218
     179 -> 187        0.01950
     180 -> 182        0.69700
     180 -> 186        0.03430
     180 -> 207       -0.01025
     178 <- 181        0.01070
     180 <- 182       -0.01136
```

5.2.2 [(^{dtbp}Cbz)]$^{-}$

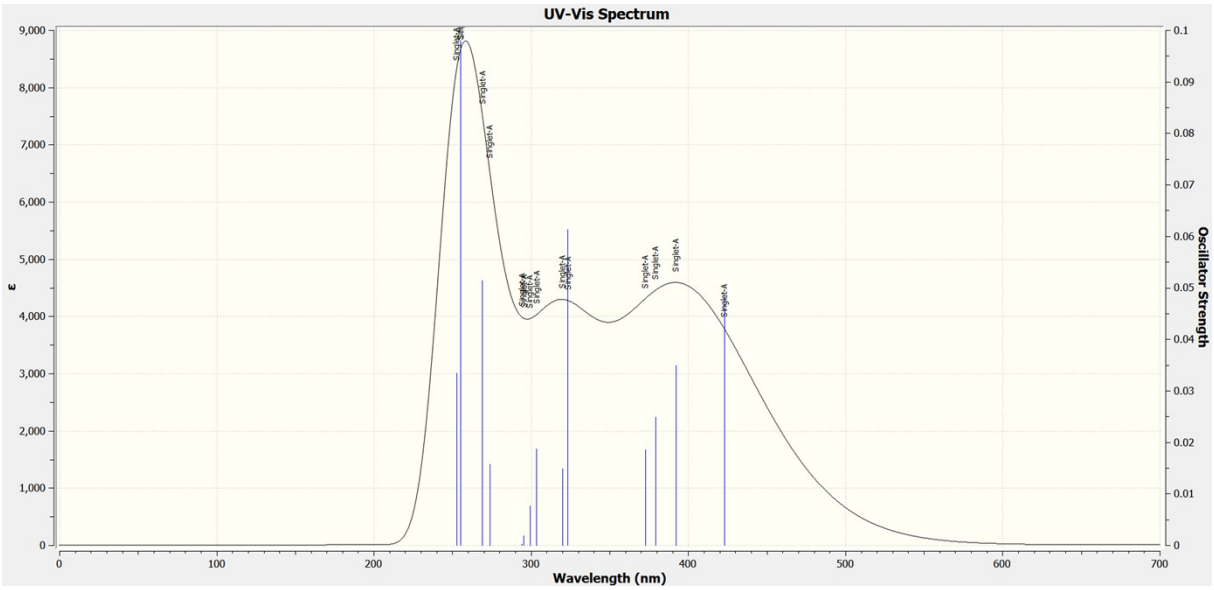



```
Excited State   1:       Singlet-A       2.8415 eV   436.34 nm   f=0.1302
<S**2>=0.000
     171 -> 181        0.02571
     172 -> 193       -0.01317
     173 -> 188        0.01243
     176 -> 181       -0.03570
     176 -> 185       -0.01260
     176 -> 193        0.01720
     177 -> 182        0.01055
     177 -> 183        0.01034
     178 -> 182        0.01794
     178 -> 188       -0.03066
     179 -> 182        0.02539
     179 -> 183        0.01213
     179 -> 186       -0.01095
     179 -> 188       -0.04876
     179 -> 194        0.01270
     179 -> 196       -0.01668
     180 -> 181        0.70065
     180 -> 185        0.03746
     178 <- 182        0.01783
     178 <- 188       -0.01042
     179 <- 188       -0.02102
     180 <- 181       -0.02771
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -1918.88034435
 Copying the excited state density for this state as the 1-particle RhoCI
density.
```

```
 Excited State    2:       Singlet-A       3.1414 eV   394.68 nm   f=0.1819
<S**2>=0.000
     171 -> 182        0.02485
     172 -> 188       -0.01066
     176 -> 182       -0.01654
     176 -> 188        0.01980
     178 -> 185        0.03051
     179 -> 181       -0.06138
     179 -> 185       -0.02170
     179 -> 193       -0.01720
     180 -> 182        0.69971
     180 -> 183        0.02125
     180 -> 184        0.01225
     180 -> 188       -0.03389
     180 -> 194       -0.01304
     180 -> 196        0.01672
     178 <- 181        0.01074
     180 <- 182       -0.01568

 Excited State    3:       Singlet-A       3.5224 eV   351.99 nm   f=0.0018
<S**2>=0.000
     171 -> 183        0.01894
     174 -> 181       -0.01488
     175 -> 181        0.02176
     175 -> 182        0.03417
     175 -> 185       -0.01366
     178 -> 181        0.01860
     178 -> 183       -0.04189
     178 -> 184        0.02306
     179 -> 181       -0.04939
     180 -> 182       -0.02678
     180 -> 183        0.70007
     180 -> 184        0.02080
     180 -> 188       -0.01410
```

5.2.3 [(^{dtbp}Cbz)Li]



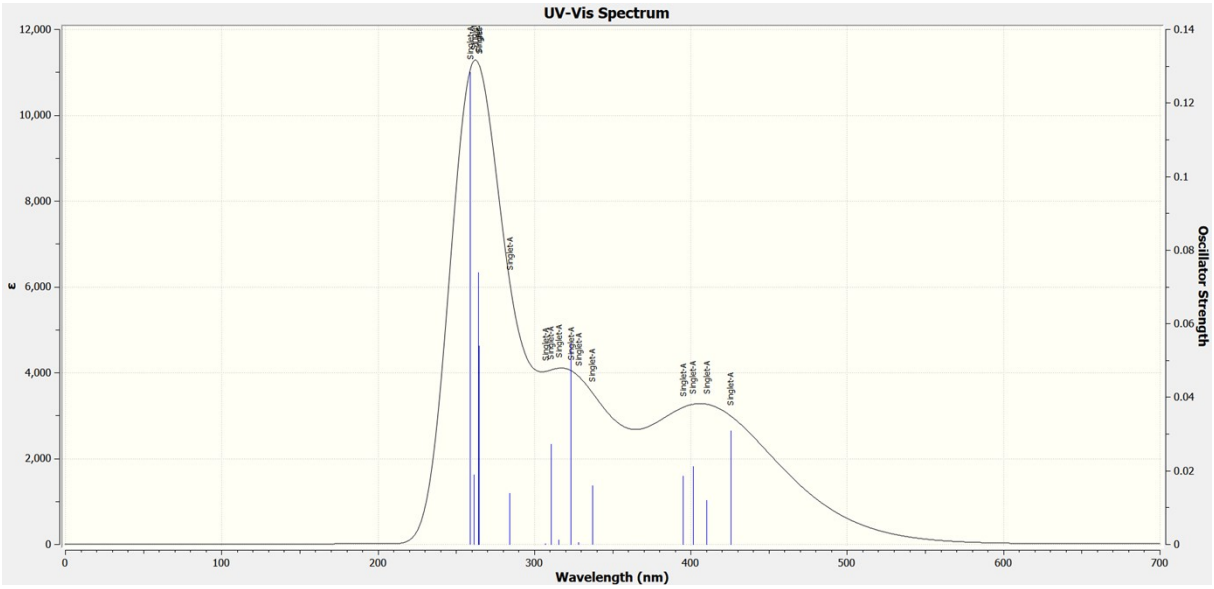

```
Excited State    1:       Singlet-A       2.9323 eV   422.82 nm   f=0.0487
<S**2>=0.000
     172 -> 182        0.03039
     178 -> 193       -0.01362
```

```
     179 -> 183       -0.01428
     179 -> 184        0.01343
     179 -> 185        0.01242
     179 -> 188       -0.02401
     180 -> 183       -0.01912
     180 -> 188        0.03391
     180 -> 194        0.01546
     181 -> 182        0.70258
     181 -> 183        0.01927
     181 -> 185        0.02159
     181 -> 189        0.01110
     181 -> 193        0.01296
     181 -> 204       -0.01036
     179 <- 188       -0.01203
     180 <- 188        0.01253
     181 <- 182       -0.01162
     181 <- 186       -0.01089
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -1926.39105563
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State    2:       Singlet-A       3.1626 eV   392.03 nm   f=0.0350
<S**2>=0.000
     172 -> 183        0.02690
     178 -> 188        0.01483
     179 -> 182       -0.03378
     179 -> 185        0.01664
     179 -> 186        0.02333
     181 -> 182       -0.01492
     181 -> 183        0.68891
     181 -> 185       -0.14020
     181 -> 188       -0.02436
     181 -> 213       -0.01452

 Excited State    3:       Singlet-A       3.2697 eV   379.19 nm   f=0.0249
<S**2>=0.000
     172 -> 184        0.02302
     176 -> 183        0.01159
     178 -> 182       -0.01343
     179 -> 182        0.02028
     179 -> 183        0.01144
     179 -> 184       -0.03511
     179 -> 188       -0.01541
     180 -> 182        0.02986
     180 -> 186        0.01113
     180 -> 188        0.01847
     181 -> 182       -0.01415
     181 -> 184        0.69765
     181 -> 185        0.08593
     181 -> 186        0.01268
```

5.2.4 [(^{dtbp}Cbz)Na] monomer

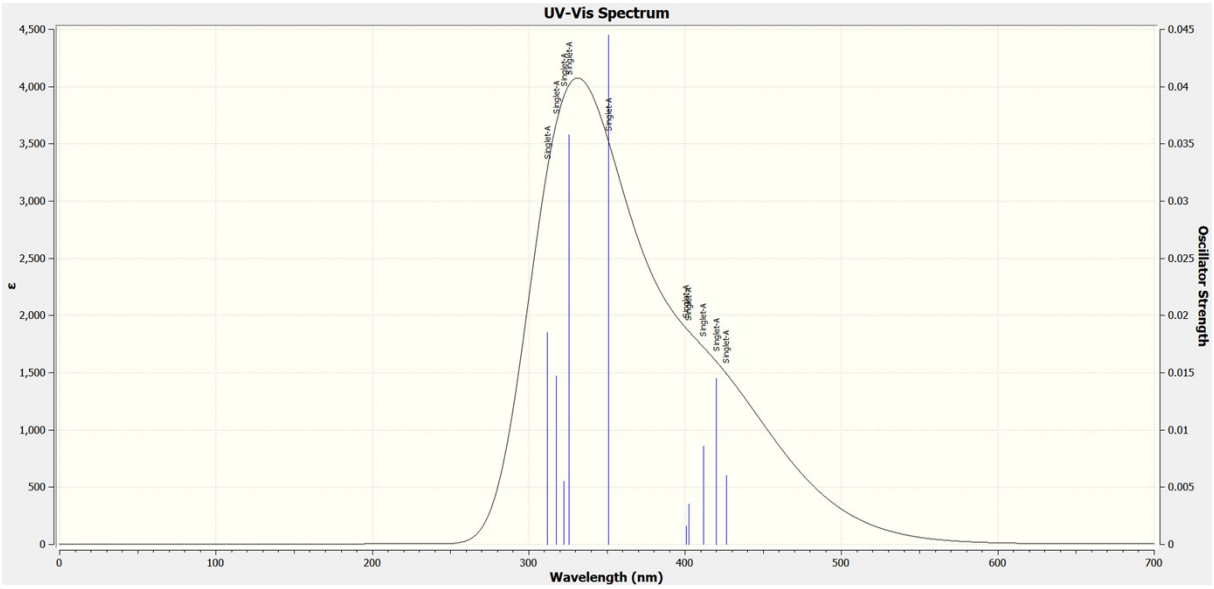



```
Excited State   1:       Singlet-A       2.9141 eV  425.47 nm  f=0.0308
<S**2>=0.000
     176 -> 186        0.02621
     182 -> 197       -0.01012
     183 -> 187        0.03293
     183 -> 189       -0.01054
     183 -> 192        0.01878
     184 -> 188       -0.01670
     184 -> 192        0.02906
     184 -> 199        0.01418
     185 -> 186        0.69030
     185 -> 187       -0.10555
     185 -> 188        0.08270
     185 -> 189       -0.01585
     185 -> 191        0.01083
     185 -> 197       -0.01331
     183 <- 192        0.01040
     184 <- 192        0.01032
     185 <- 191       -0.01078
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -2081.01989935
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:       Singlet-A       3.0218 eV  410.30 nm  f=0.0119
<S**2>=0.000
     176 -> 187        0.02254
     183 -> 186        0.03895
     183 -> 189       -0.01554
     183 -> 191       -0.01516
     184 -> 186       -0.01001
     185 -> 186        0.08366
     185 -> 187        0.65712
     185 -> 188        0.10644
     185 -> 189       -0.21113
     185 -> 190        0.02476
     185 -> 192       -0.01873
     185 -> 217       -0.01378
```

```
 Excited State    3:       Singlet-A       3.0889 eV   401.38 nm   f=0.0212
<S**2>=0.000
     176 -> 188        0.02174
     183 -> 186       -0.01354
     183 -> 187       -0.01997
     183 -> 188       -0.01477
     183 -> 189       -0.03155
     184 -> 186        0.02858
     184 -> 191        0.01799
     184 -> 192        0.01450
     185 -> 186       -0.10652
     185 -> 187       -0.14768
     185 -> 188        0.65779
     185 -> 189       -0.17069
```

5.2.5 [(^{dtbp}Cbz)K]



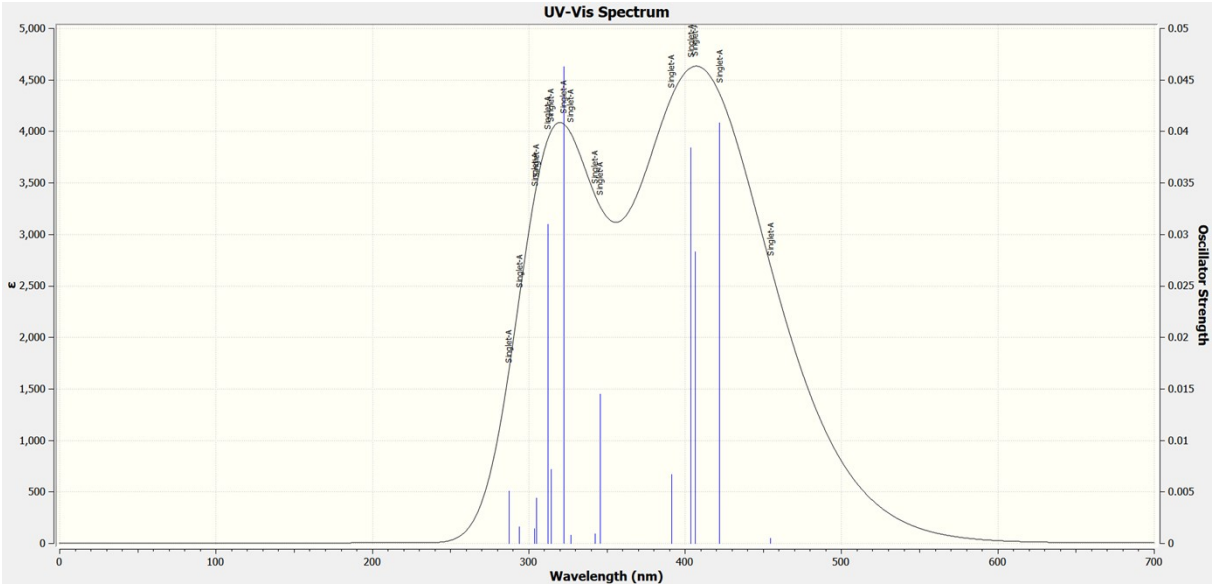

```
Excited State    1:       Singlet-A       2.9085 eV   426.28 nm   f=0.0060
<S**2>=0.000
     180 -> 190       -0.01210
     180 -> 191        0.01656
     187 -> 190       -0.01140
     187 -> 191        0.02933
     187 -> 193        0.02152
     187 -> 194       -0.01767
     188 -> 195       -0.01255
     188 -> 198        0.02149
     189 -> 190       -0.40702
     189 -> 191        0.53074
     189 -> 192       -0.18437
     189 -> 193       -0.11800
     189 -> 195       -0.02591
     189 -> 202        0.01139
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -2518.56543806
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State    2:       Singlet-A       2.9521 eV   419.99 nm   f=0.0145
<S**2>=0.000
     180 -> 192        0.02034
```

```
     185 -> 192       -0.01068
     187 -> 191        0.01334
     187 -> 192       -0.03638
     187 -> 194        0.02585
     189 -> 190       -0.12043
     189 -> 191        0.17296
     189 -> 192        0.64647
     189 -> 193        0.18073
     189 -> 194        0.01209
     189 -> 195       -0.01187
     189 -> 196        0.01181
     189 -> 212       -0.01046
     189 -> 222        0.01398

 Excited State    3:        Singlet-A        3.0114 eV   411.72 nm   f=0.0086
<S**2>=0.000
     180 -> 190        0.01058
     180 -> 193        0.01247
     187 -> 190       -0.01100
     187 -> 191        0.01856
     187 -> 192        0.01926
     187 -> 194        0.02424
     188 -> 191        0.01199
     188 -> 195       -0.01804
     189 -> 190        0.42230
     189 -> 191        0.36246
     189 -> 192       -0.12843
     189 -> 193        0.38404
     189 -> 194        0.14960
     189 -> 195        0.01134
     189 -> 200        0.02137
```

5.2.6 [(^{dtbp}Cbz)Rb]



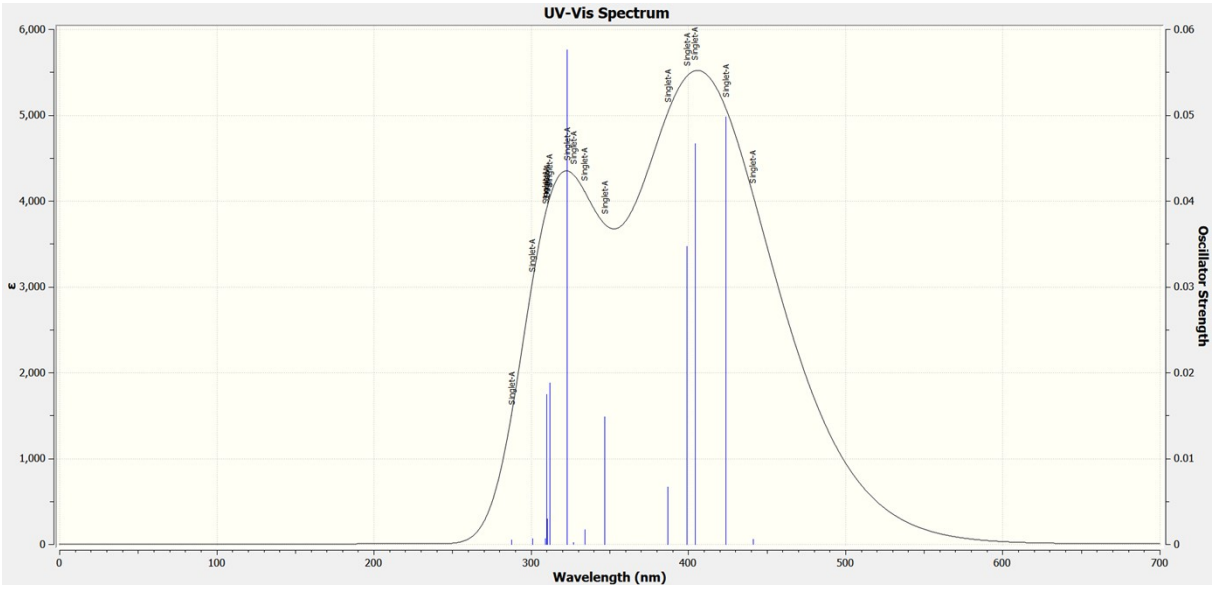

```
Excited State    1:        Singlet-A        2.7263 eV   454.77 nm   f=0.0005
<S**2>=0.000
     175 -> 185        0.01627
     184 -> 185        0.70129
     184 -> 186       -0.01773
     184 -> 187        0.05077
     184 -> 190        0.04226
```

```
     184 -> 194        0.04877
     184 -> 200        0.01231
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -1942.98846880
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:       Singlet-A       2.9373 eV  422.11 nm  f=0.0408
<S**2>=0.000
     175 -> 186        0.02513
     180 -> 202        0.01259
     182 -> 187       -0.01902
     182 -> 189        0.02606
     182 -> 195        0.02217
     183 -> 188        0.02516
     183 -> 195       -0.03165
     183 -> 201       -0.01708
     184 -> 185        0.01927
     184 -> 186        0.69861
     184 -> 187        0.02502
     184 -> 188        0.05754
     184 -> 190       -0.04641
     184 -> 200        0.01001
     184 -> 220       -0.01620
     182 <- 195        0.01100
     183 <- 195       -0.01140

 Excited State   3:       Singlet-A       3.0517 eV  406.27 nm  f=0.0283
<S**2>=0.000
     175 -> 187        0.01512
     175 -> 188       -0.01245
     182 -> 186       -0.03028
     182 -> 187       -0.01960
     182 -> 188        0.02245
     182 -> 189       -0.01503
     182 -> 191        0.01283
     184 -> 185       -0.04426
     184 -> 186        0.01767
     184 -> 187        0.53208
     184 -> 188       -0.42511
     184 -> 189       -0.16975
     184 -> 190        0.01747
     184 -> 193        0.01030
     184 -> 194       -0.01045
     184 -> 195        0.01197
```

5.2.7 [(^{dtbp}Cbz)Cs]



Excited State 1: Singlet-A 2.8109 eV 441.09 nm f=0.0006 <S**2>=0.000

175 -> 185	0.01473
184 -> 185	**0.69408**
184 -> 186	0.07460
184 -> 187	0.07007
184 -> 188	-0.01792
184 -> 190	-0.05895
184 -> 194	0.05169
184 -> 199	0.01296

This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -1939.04771868
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.9254 eV 423.82 nm f=0.0498 <S**2>=0.000

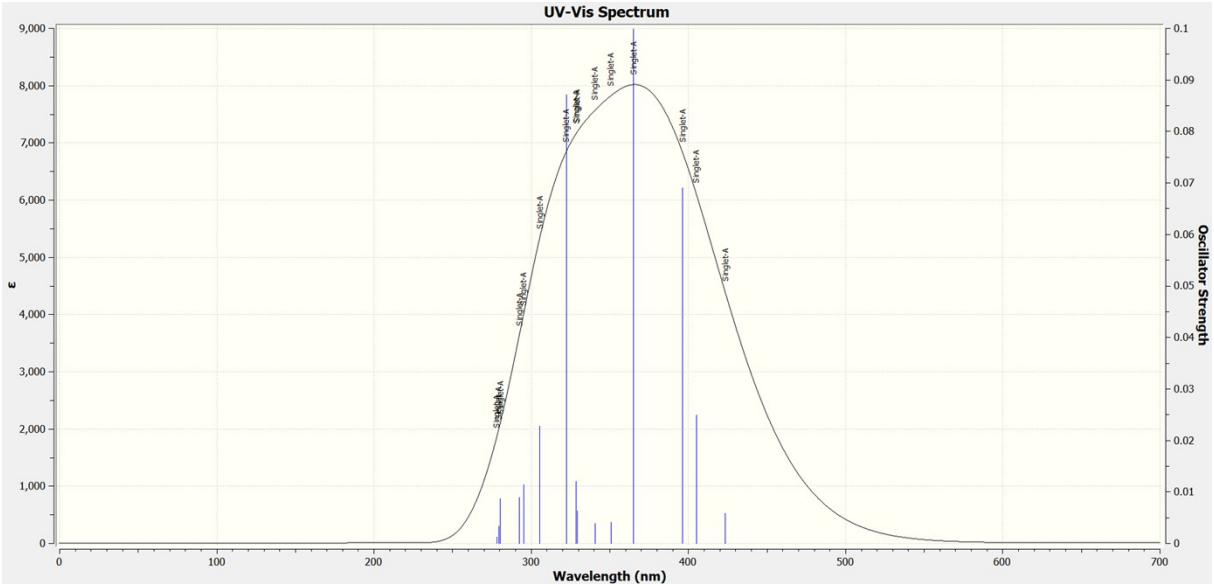
175 -> 186	0.02566
180 -> 202	0.01141
182 -> 187	-0.01226
182 -> 189	-0.02165
182 -> 195	-0.02421
183 -> 187	-0.01375
183 -> 188	-0.02144
183 -> 195	0.03333
183 -> 201	0.01514
184 -> 185	-0.07979
184 -> 186	**0.69663**
184 -> 187	0.01121
184 -> 188	0.01175
184 -> 190	-0.04921
184 -> 194	-0.01769
184 -> 221	-0.01048
182 <- 195	-0.01152
183 <- 195	0.01226
184 <- 186	-0.01024

Excited State 3: Singlet-A 3.0670 eV 404.25 nm f=0.0467 <S**2>=0.000

175 -> 187	0.01827

```
     182 -> 186       -0.02639
     182 -> 187        0.03028
     182 -> 189       -0.01385
     182 -> 192        0.01242
     183 -> 186        0.01264
     183 -> 192        0.01140
     184 -> 185       -0.05639
     184 -> 186       -0.02248
     184 -> 187        0.62787
     184 -> 188        0.27193
     184 -> 189        0.15131
     184 -> 190       -0.01234
     184 -> 192       -0.01083
     184 -> 195       -0.01372
     184 -> 225       -0.01085
```

5.2.8 [(^{dtbp}Cbz)Li(Tol)]




```
Excited State   1:       Singlet-A       2.9281 eV  423.43 nm  f=0.0058
<S**2>=0.000
     195 -> 207        0.01648
     196 -> 207        0.01538
     206 -> 207        0.70499
     206 -> 209        0.03892
     206 -> 210       -0.01039
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -2197.46555899
 Copying the excited state density for this state as the 1-particle RhoCI
density.

 Excited State   2:       Singlet-A       3.0614 eV  404.99 nm  f=0.0249
<S**2>=0.000
     195 -> 208        0.01443
     196 -> 208        0.01748
     203 -> 209       -0.01296
     204 -> 215        0.01084
     205 -> 210        0.01402
     205 -> 215        0.02058
     206 -> 208        0.70210
     206 -> 209        0.06669
     206 -> 211        0.01431
```

```
     206 -> 213        0.01445

 Excited State    3:       Singlet-A       3.1277 eV   396.41 nm   f=0.0690
<S**2>=0.000
     195 -> 209        0.01434
     196 -> 209        0.01952
     197 -> 209        0.01094
     203 -> 209       -0.01591
     203 -> 219        0.01492
     204 -> 215        0.02543
     205 -> 210        0.02957
     205 -> 215        0.04756
     205 -> 221        0.01571
     206 -> 207       -0.04053
     206 -> 208       -0.07120
     206 -> 209        0.69653
     206 -> 211        0.02741
     206 -> 213        0.01950
     206 -> 214       -0.01355
     204 <- 210        0.01031
     205 <- 215        0.01592
     206 <- 209       -0.01405

 Excited State    4:       Singlet-A       3.3962 eV   365.07 nm   f=0.0999
<S**2>=0.000
     195 -> 210        0.01489
     196 -> 210        0.01687
     197 -> 210        0.01022
     203 -> 215       -0.01721
     204 -> 209       -0.03191
     204 -> 213        0.02622
     205 -> 208       -0.01319
     205 -> 209       -0.02807
     205 -> 213       -0.01687
     205 -> 215       -0.01786
     205 -> 219       -0.01259
     206 -> 207        0.01047
     206 -> 210        0.69414
     206 -> 211        0.09646
     206 -> 212       -0.02096
     206 -> 213       -0.01065
     206 -> 215        0.03358
     206 -> 221       -0.01646

 Excited State    5:       Singlet-A       3.5345 eV   350.78 nm   f=0.0041
<S**2>=0.000
     195 -> 211        0.01188
     196 -> 211        0.01318
     201 -> 209       -0.02479
     201 -> 210       -0.01939
     203 -> 209        0.01013
     203 -> 211        0.01471
     204 -> 211       -0.05410
     205 -> 210       -0.01256
     205 -> 215       -0.01416
     206 -> 209       -0.02646
     206 -> 210       -0.09853
     206 -> 211        0.69444
     206 -> 213       -0.02350
```

5.3 Emissions & Excited States

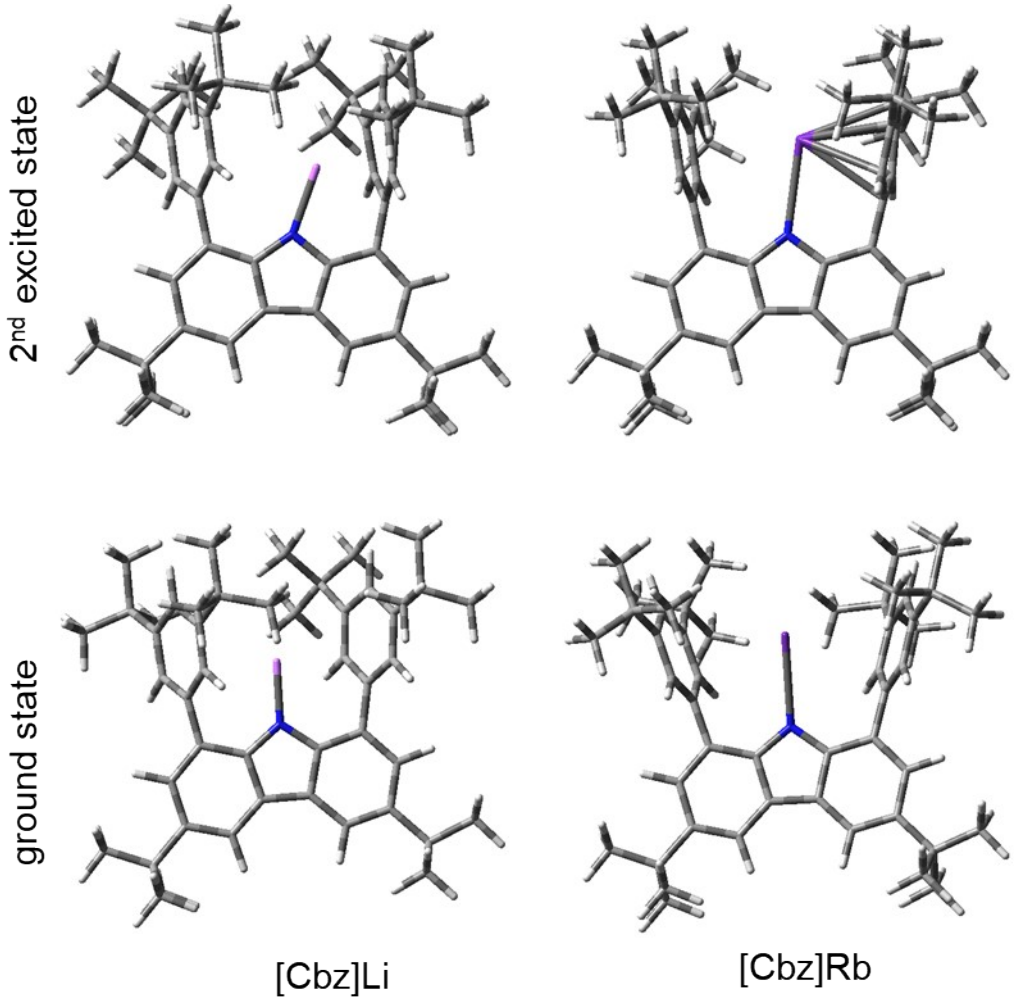


Figure S57: Optimised geometries of ground state and 2nd excited state of [Cbz]Li and [Cbz]Rb.

Table S5: Calculated emission energies for selected compounds. GS = ground state, ES = excited state, GS,distorted is based on the single-point ground state calculation with the geometry of the excited state. $\Delta G = G_{ES} - G_{GS,distorted}$.

	G_{GS} [a.u.]	G_{ES} [a.u.]	$G_{GS,distorted}$ [a.u.]	ΔG [a.u.]	λ_{em} [nm]
[(dtbpCbz)]$^-$	-1918.067801	-1917.974741	-1918.064339	0.089598	509
(dtbpCbz)–H	-1918.617233	-1918.490101	-1918.611267	0.121166	376
[(dtbpCbz)Li] 1st	-1925.577124	-1925.485851	-1925.551893	0.066042	690
[(dtbpCbz)Li] 2nd	-1925.577124	-1925.456067	-1925.551880	0.095813	476
[(dtbpCbz)Na] 1st	-2080.209030	-2080.122378	-2080.190783	0.068405	667
[(dtbpCbz)Na] 2nd	-2080.209030	-2080.098081	-2080.195354	0.097273	469
[(dtbpCbz)K] 1st	-2517.759742	-2517.672708	-2517.732712	0.060004	760
[(dtbpCbz)K] 2nd	-2517.759742	-2517.640422	-2517.734961	0.094539	482
[(dtbpCbz)Rb] 1st	-1942.175708	-1942.088424	-1942.152416	0.063992	713
[(dtbpCbz)Rb] 2nd	-1942.175708	-1942.053027	-1942.146546	0.093519	488
[(dtbpCbz)Cs] 1st	-1938.238289	-1938.933552	-1938.992594	0.059042	772
[(dtbpCbz)Cs] 2nd	-1938.238289	-1938.125836	-1938.222157	0.096321	473

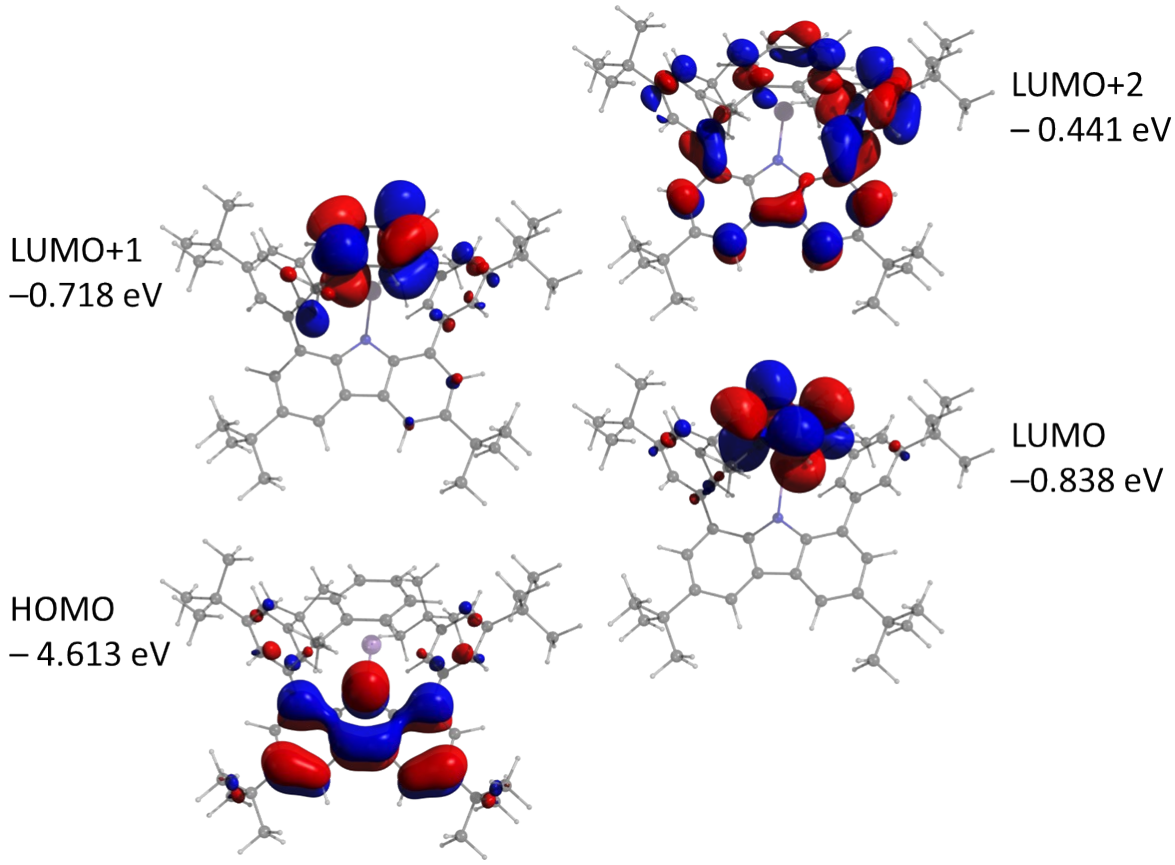


Figure S58: Selected orbitals of [(^{dtbp}Cbz)Li(Tol)] (**1b**).

Table S6: Calculated emission energies for [(^{dtbp}Cbz)Li(Tol)] (**1b**). GS = ground state, ES = excited state, GS,distorted is based on the single-point ground state calculation with the geometry of the excited state. $\Delta G = G_{ES} - G_{GS,distorted}$.

	G_{GS} [a.u.]	G_{ES} [a.u.]	$G_{GS,distorted}$ [a.u.]	ΔG [a.u.]	λ_{em} [nm]
[(dtbpCbz)Li] ^{1st}	-2196.531322	-2196.45167	-2196.50507	0.053400	854
[(dtbpCbz)Li] ^{2nd}	-2196.531322	-2196.42047	-2196.50508	0.084610	539
[(dtbpCbz)Li] ^{3rd}	-2196.531322	-2196.40952	-2196.5017	0.092187	495

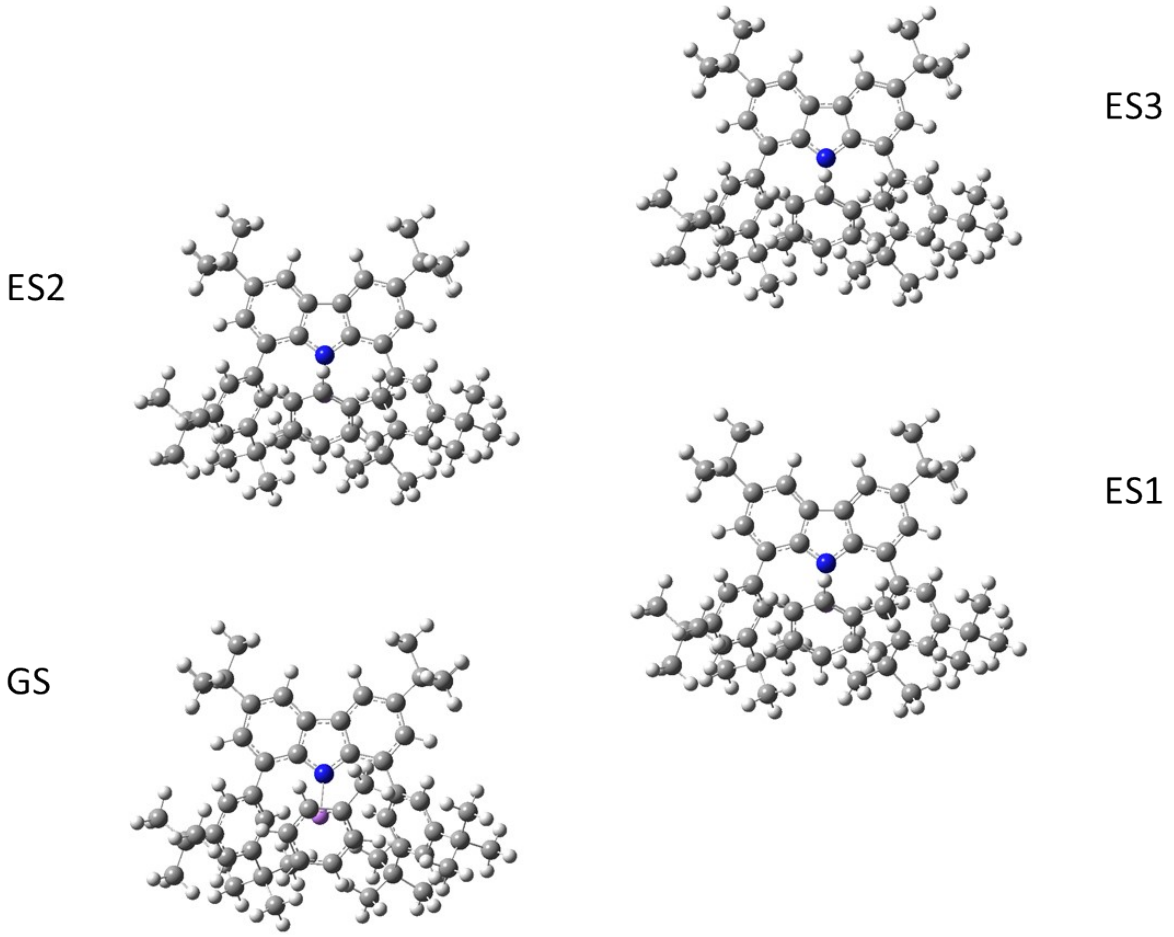


Figure S59: Optimised ground state (GS) and the first three excited states (ES) of [(^{dtbp}Cbz)Li(Tol)] (**1b**).

5.4 Optimised structures

5.4.1 (^{dtbp}Cbz)–H

```
0 1
 N                -0.00003800    0.87853800   -0.00013800
 H                -0.00001600   -0.13234400    0.00011800
 C                -0.71523000    3.03085900    0.12634200
 C                -1.10087400    1.67106500    0.20920000
 C                 1.98419600   -1.00125400   -1.32226800
 H                 1.24416700   -0.54428200   -1.98337200
 C                 2.74373100   -0.16483500   -0.49929300
 C                 1.10086400    1.67100900   -0.20934600
 C                -3.03119900    3.67113200    0.47249300
 C                 3.03130100    3.67098200   -0.47256200
 C                 2.42561500    1.28012800   -0.43546200
 C                 4.08267300    4.77995100   -0.61405100
 C                 2.14747800   -2.39184900   -1.31193100
 C                -2.42563200    1.28025200    0.43537700
 C                -1.98441300   -1.00107900    1.32240600
 H                -1.24451500   -0.54406600    1.98363100
 C                 0.71529200    3.03082200   -0.12648500
 C                 1.69074300    4.01980400   -0.26606300
 H                 1.39774300    5.07086000   -0.20418900
 C                -3.36879200    2.30451400    0.54887600
 H                -4.40395500    2.00863300    0.72359100
 C                 3.36883100    2.30435000   -0.54891300
 H                 4.40398600    2.00842300   -0.72359100
 C                -1.69063400    4.01988600    0.26593600
 H                -1.39759000    5.07092900    0.20406000
 C                 4.98219000   -2.77116900    1.25252500
 C                -4.08250900    4.78015300    0.61405800
 C                 3.12931300   -2.91856300   -0.47053600
 H                 3.27176100   -3.99877900   -0.43370700
 C                -2.14772100   -2.39167400    1.31213800
 C                 3.73095700   -0.73113800    0.31911300
 H                 4.30468900   -0.06523700    0.96448600
 C                 3.94020400   -2.11059200    0.34387100
 C                -2.74378500   -0.16470700    0.49923500
 C                 1.27321400   -3.26340600   -2.22058200
 C                -3.73083600   -0.73105300   -0.31935300
 H                -4.30442100   -0.06518200   -0.96489000
 C                -3.94008600   -2.11050800   -0.34406500
 C                -1.27365000   -3.26318800    2.22100600
 C                -3.12939000   -2.91843100    0.47058100
 H                -3.27185600   -3.99864700    0.43380000
 C                -5.49162000    4.22085000    0.82367700
 H                -5.81334100    3.59475800   -0.02286900
 H                -6.21104100    5.04923300    0.91508200
 H                -5.56121600    3.61923700    1.74296600
 C                 4.09372700    5.63708000    0.66129300
 H                 3.11659100    6.10747600    0.84665500
 H                 4.84198800    6.44235300    0.58030000
 H                 4.34177600    5.02502200    1.54226800
 C                 1.70859300   -3.03624200   -3.67672500
 H                 1.59922300   -1.98019700   -3.96670700
 H                 1.09555300   -3.64217300   -4.36358300
 H                 2.76397500   -3.31543600   -3.81952400
 C                 1.41003000   -4.75157100   -1.89012300
 H                 2.43292200   -5.12106700   -2.05885900
 H                 0.73943600   -5.34004100   -2.53484800
 H                 1.13718600   -4.95995400   -0.84335000
 C                 5.49175500    4.22058400   -0.82369000
 H                 5.81352200    3.59458600    0.02290600
 H                 6.21119400    5.04893700   -0.91522900
 H                 5.56126500    3.61885800   -1.74291300
 C                -4.98190700   -2.77113700   -1.25286600
 C                 0.20609100   -2.87656500    2.06640300
 H                 0.55508200   -3.00028000    1.02991800
 H                 0.83503500   -3.51419300    2.70763900
 H                 0.40150700   -1.83390700    2.35718200
 C                -3.73274300    5.66267900    1.82230800
 H                -3.71893100    5.06910800    2.74948600
 H                -4.47468500    6.46913600    1.94115000
 H                -2.74386200    6.13232600    1.71224000
```

C	-0.20649100	-2.87673100	-2.06574800
H	-0.55530300	-3.00037900	-1.02919700
H	-0.83557400	-3.51436900	-2.70684000
H	-0.40192300	-1.83407800	-2.35653000
C	-4.09355500	5.63737800	-0.66122000
H	-3.11642000	6.10778400	-0.84656200
H	-4.84179500	6.44266000	-0.58015100
H	-4.34163100	5.02539600	-1.54224100
C	3.73300000	5.66258800	-1.82224500
H	3.71918400	5.06909100	-2.74946900
H	4.47500100	6.46900300	-1.94099700
H	2.74415200	6.13231000	-1.71218800
C	-4.26154400	-3.68680800	-2.25549500
H	-3.55921300	-3.10961200	-2.87684800
H	-4.98905700	-4.17610300	-2.92307900
H	-3.68725800	-4.47680100	-1.74858300
C	-1.41044700	-4.75138100	1.89064200
H	-2.43336500	-5.12084800	2.05928000
H	-0.73994100	-5.33981200	2.53549500
H	-1.13747600	-4.95985300	0.84392000
C	-1.70927100	-3.03589000	3.67705200
H	-1.59994900	-1.97981500	3.96695000
H	-1.09634600	-3.64175800	4.36406800
H	-2.76467700	-3.31506900	3.81969700
C	-5.95162200	-3.60229400	-0.39890200
H	-5.43220600	-4.39495900	0.15976500
H	-6.70806600	-4.08595200	-1.03763300
H	-6.47559600	-2.96600600	0.33097600
C	-5.79669700	-1.74226100	-2.03940700
H	-6.33995500	-1.05598700	-1.37170800
H	-6.54160700	-2.25672400	-2.66574800
H	-5.16189800	-1.14094100	-2.70795200
C	5.79743300	-1.74223100	2.03852100
H	6.34061900	-1.05626100	1.37045100
H	6.54242900	-2.25666600	2.66478200
H	5.16297600	-1.14058700	2.70709700
C	5.95149200	-3.60276400	0.39852800
H	5.43178800	-4.39551400	-0.15974900
H	6.70802700	-4.08636800	1.03718800
H	6.47537700	-2.96679800	-0.33169400
C	4.26192900	-3.68639900	2.25564000
H	3.55995300	-3.10884500	2.87706200
H	4.98953200	-4.17570900	2.92311900
H	3.68727000	-4.47636300	1.74910200

5.4.2 [(^{dtbp}Cbz)Li]

0 1

C	0.75233800	-1.82681100	-0.15646300
N	0.71628000	-0.48323800	0.07757900
C	2.26594500	-3.73348000	-0.27527500
C	2.07304700	-2.36125400	-0.10358500
C	2.92025800	-1.21609500	0.15128600
C	4.29352400	-0.99180300	0.26787600
C	4.79442800	0.30121400	0.47210600
C	3.87893900	1.37221400	0.56832700
C	2.49963400	1.18743000	0.48374900
C	2.01807700	-0.11713400	0.25990500
C	-1.68630700	-2.02459700	-0.48539700
C	-1.86897400	-0.92433700	-1.35388800
C	-3.05923900	-0.19555100	-1.37991300
C	-4.09557700	-0.60333500	-0.51714000
C	-3.96931400	-1.70497700	0.32974600
C	-2.74915600	-2.40478300	0.33141800
C	-5.09377300	-2.15677500	1.26675700
C	-3.27183100	1.00034200	-2.31784200
C	1.42571500	-6.09355500	-0.66701600
C	6.31074100	0.51080900	0.58685100
C	1.48754900	2.26554900	0.55583000
C	0.43088400	2.14812400	1.47658500
C	-0.66229700	3.02214800	1.47000800
C	-0.66342700	4.05926400	0.52421500
C	0.38809300	4.23610800	-0.38362300
C	1.45594500	3.32716000	-0.35121600
C	-1.79973100	2.80865200	2.47840300
C	0.38128400	5.35189400	-1.43370800

C	1.17691500	-4.58902600	-0.49168600
C	-0.11843900	-4.03024400	-0.55234500
C	-0.35265800	-2.66282100	-0.40812200
C	2.33565900	-6.32571000	-1.88339600
H	3.30635500	-5.82108800	-1.76707400
H	2.53171200	-7.40156400	-2.02499500
H	1.86685100	-5.93750000	-2.80093300
C	2.10664700	-6.65023900	0.59318700
H	2.29952300	-7.73079400	0.48778000
H	3.07013400	-6.15592900	0.78737100
H	1.47088300	-6.49891900	1.47940200
C	0.12866300	-6.87543100	-0.88879500
H	-0.56208200	-6.77004000	-0.03782900
H	-0.39594000	-6.54768300	-1.79954900
H	0.35331600	-7.94745500	-1.00316400
C	-6.33673800	-1.27243000	1.15030600
H	-6.75847500	-1.28949400	0.13357200
H	-7.11648100	-1.63443600	1.83757800
H	-6.12121500	-0.22602800	1.41741300
C	-4.59579300	-2.09900300	2.71959300
H	-3.72460500	-2.75007900	2.88275600
H	-4.30344400	-1.07322600	2.99343800
H	-5.39007500	-2.42358100	3.41059300
C	-5.48855900	-3.59932600	0.91425100
H	-6.29316500	-3.95070100	1.57984200
H	-5.84892500	-3.66501600	-0.12394600
H	-4.64090900	-4.29242600	1.01916600
C	6.84991600	-0.29039300	1.78221300
H	6.65117700	-1.36692500	1.67248000
H	7.94025300	-0.15871600	1.88114000
H	6.37667100	0.04133000	2.71943700
C	6.68030700	1.98138300	0.79571600
H	6.34293300	2.61021800	-0.04279500
H	6.24596400	2.38439700	1.72361900
H	7.77422200	2.08516500	0.86904200
C	6.99473000	0.02729600	-0.70157400
H	8.08700500	0.16470300	-0.63884500
H	6.80231500	-1.03951600	-0.88922300
H	6.62652900	0.58984900	-1.57359400
C	1.63526100	6.22118700	-1.25541400
H	2.55922400	5.63560700	-1.37007300
H	1.65411500	7.02616600	-2.00737900
H	1.65338600	6.68446300	-0.25683300
C	-0.85135500	6.25127600	-1.31781000
H	-0.90799400	6.74525700	-0.33555700
H	-0.80815700	7.04065400	-2.08357400
H	-1.78525700	5.68963800	-1.47653900
C	-4.45918100	0.70169600	-3.24610100
H	-5.39055200	0.54561500	-2.68184300
H	-4.62444700	1.54077800	-3.94063400
H	-4.27109900	-0.20473000	-3.84142900
C	-3.57137700	2.26045100	-1.49032800
H	-4.44148300	2.12684000	-0.83004800
H	-2.70919400	2.54307000	-0.86354000
H	-3.78291000	3.11448400	-2.15362200
C	-2.04023900	1.28249600	-3.18226600
H	-1.15067000	1.52698300	-2.57902400
H	-1.78676800	0.42888500	-3.82820100
H	-2.23537600	2.14716400	-3.83497000
C	0.38499400	4.71955800	-2.83485200
H	1.27206400	4.09040100	-2.99924400
H	-0.50498300	4.08794300	-2.98233600
H	0.38090900	5.50271500	-3.60982300
C	-2.94553300	3.80281300	2.28065700
H	-3.74122500	3.60542800	3.01513600
H	-2.61255200	4.84148200	2.42583100
H	-3.39170200	3.72149100	1.27752100
C	-1.24604400	2.97160900	3.90173400
H	-0.83120400	3.98100400	4.04434400
H	-2.04379100	2.81941100	4.64630400
H	-0.44496800	2.24789900	4.11263500
C	-2.36491100	1.38697600	2.31094200
H	-2.80627300	1.23791200	1.30876900
H	-1.60656800	0.60719700	2.49477700
H	-3.17694900	1.20065400	3.03112300
H	-0.97957800	-4.67204300	-0.74614100
H	3.28043100	-4.14052900	-0.23399400
H	4.98240200	-1.83765800	0.18684900

H	4.24348600	2.38730500	0.73440200
H	2.27065200	3.40479900	-1.07516900
H	-1.50654800	4.74564900	0.49551100
H	0.49118800	1.33775000	2.20891300
H	-2.59833000	-3.25037300	1.00676500
H	-5.02868300	-0.03978200	-0.52250200
H	-1.04218000	-0.67305300	-2.02015800
Li	-0.81905500	0.56680100	0.19485800

5.4.3 [(^{dtbp}Cbz)Na]

0 1

C	1.72450200	-1.04439700	-0.19265800
N	0.87931400	0.00664300	0.00624900
C	4.09383600	-1.64504300	-0.26659000
C	3.10270400	-0.67218800	-0.12434400
C	3.08259300	0.75187800	0.11435500
C	4.04575100	1.75316100	0.25140500
C	3.66983300	3.08732000	0.45158300
C	2.29216800	3.39323000	0.52059400
C	1.30174500	2.41965400	0.40880700
C	1.69444300	1.08346700	0.19068900
C	-0.07753300	-2.70400600	-0.48382300
C	-0.86749300	-2.11370200	-1.49157400
C	-2.26080400	-2.20504100	-1.47718600
C	-2.86185900	-2.93646700	-0.43230500
C	-2.11246300	-3.57697200	0.55743300
C	-0.71286600	-3.44553500	0.51177300
C	-2.75686700	-4.38591900	1.68754100
C	-3.14532500	-1.52320600	-2.53004400
C	4.87182000	-4.03406800	-0.61085500
C	4.75473800	4.16417000	0.59055900
C	-0.15577700	2.69592100	0.45819400
C	-0.92682100	2.21174100	1.52693300
C	-2.32642500	2.29111900	1.52375100
C	-2.94686200	2.88933100	0.41510900
C	-2.21192700	3.41235100	-0.65767500
C	-0.81488300	3.30612100	-0.61334600
C	-3.12559200	1.70577300	2.69693700
C	-2.88245200	4.07031500	-1.86846300
C	3.75632100	-2.98975600	-0.46637900
C	2.38833600	-3.33502900	-0.53500900
C	1.36983800	-2.39069900	-0.42044100
C	5.74737500	-3.68593700	-1.82484800
H	6.20675800	-2.69155100	-1.72194300
H	6.56069400	-4.42104700	-1.94463100
H	5.14840100	-3.68126800	-2.74876400
C	5.73882500	-4.03809900	0.65800000
H	6.55170000	-4.77858100	0.57384000
H	6.19881000	-3.05531600	0.83924100
H	5.13379900	-4.28995800	1.54289100
C	4.32203200	-5.44823600	-0.81262600
H	3.70180900	-5.77009000	0.03831700
H	3.71466900	-5.52391400	-1.72778100
H	5.15425800	-6.16349300	-0.90650500
C	-4.28452700	-4.38408200	1.60419300
H	-4.64520100	-4.83084700	0.66498300
H	-4.70313600	-4.97517100	2.43288100
H	-4.69785000	-3.36619200	1.68364000
C	-2.34835900	-3.78544100	3.04197900
H	-1.25805100	-3.79351100	3.18512200
H	-2.69073400	-2.74231600	3.12840900
H	-2.79762400	-4.36010200	3.86752400
C	-2.26528200	-5.83911300	1.59976000
H	-2.70878500	-6.44430100	2.40657200
H	-2.54750500	-6.29143400	0.63657500
H	-1.17129400	-5.90524000	1.69318100
C	5.64609200	3.84179000	1.80015300
H	6.13380500	2.86124000	1.69490900
H	6.43820400	4.60032400	1.91599800
H	5.05212600	3.81972300	2.72706400
C	4.16454800	5.56148000	0.79560000
H	3.53267900	5.86621100	-0.05304700
H	3.55788800	5.61826900	1.71260400
H	4.97583400	6.30061500	0.88784000
C	5.61506900	4.19393200	-0.68248300

H	6.40613700	4.95810000	-0.60220400
H	6.10290500	3.22512900	-0.86613900
H	4.99853000	4.42780900	-1.56434000
C	-2.40221700	5.52610800	-1.97302200
H	-1.31096000	5.58738000	-2.09639300
H	-2.86671700	6.02272200	-2.83992900
H	-2.66987000	6.09367000	-1.06843300
C	-4.40880000	4.06955900	-1.75910700
H	-4.75839600	4.62832200	-0.87739000
H	-4.84490400	4.54980300	-2.64823300
H	-4.81552100	3.04742500	-1.70385200
C	-4.01294700	-2.58196500	-3.22714300
H	-4.67623900	-3.10117500	-2.51954700
H	-4.64594900	-2.11433500	-3.99803000
H	-3.38263000	-3.34078700	-3.71501500
C	-4.05772100	-0.49255200	-1.84184300
H	-4.67664800	-0.94699200	-1.05342700
H	-3.47900500	0.33170300	-1.38779100
H	-4.73799900	-0.02802100	-2.57342800
C	-2.31744300	-0.79802800	-3.59321700
H	-1.68472500	-0.00654400	-3.16173900
H	-1.66281400	-1.49178700	-4.14127300
H	-2.98618500	-0.32048900	-4.32567500
C	-2.49281000	3.30653500	-3.14386700
H	-1.40452200	3.29454400	-3.30183400
H	-2.83629800	2.26146400	-3.09745600
H	-2.95375500	3.77551400	-4.02778400
C	-4.62929500	1.95034700	2.55475300
H	-5.15984300	1.52596300	3.42074700
H	-4.86360800	3.02479800	2.51466900
H	-5.04144100	1.47532600	1.65068700
C	-2.64955100	2.34554100	4.00938000
H	-2.79380300	3.43626200	3.98428600
H	-3.21860300	1.94325000	4.86259100
H	-1.58336400	2.15362000	4.19780100
C	-2.89472800	0.18538800	2.75917100
H	-3.29331400	-0.31772400	1.85911100
H	-1.82886700	-0.07038100	2.87477800
H	-3.42304200	-0.25677600	3.61854600
H	2.09653600	-4.37294500	-0.70428800
H	5.14536800	-1.34740800	-0.21352800
H	5.10524800	1.48641100	0.19290000
H	1.97087100	4.42385000	0.68027800
H	-0.20470600	3.66885400	-1.44386600
H	-4.03216300	2.95602300	0.39145100
H	-0.39561400	1.74353000	2.36024400
H	-0.08973100	-3.89035000	1.29131500
H	-3.94934900	-3.01008200	-0.40734100
H	-0.34684900	-1.54847000	-2.26518100
Na	-1.34565900	-0.07911500	0.17574800

5.4.4 [(^{dtbp}Cbz)K]

0 1

C	-1.52206900	1.32153600	-0.11908800
N	-0.87144000	0.12312700	-0.07170400
C	-3.76289400	2.32197300	-0.12856300
C	-2.94727400	1.18967500	-0.11234200
C	-3.17872400	-0.23110900	-0.06216600
C	-4.31082600	-1.04638100	-0.02365000
C	-4.18861600	-2.43873100	0.04273100
C	-2.88903700	-2.99166200	0.07227900
C	-1.73703700	-2.20895600	0.03311100
C	-1.86902500	-0.80723900	-0.03730800
C	0.52761500	2.73289600	-0.13988700
C	1.26241000	2.48488200	-1.31326300
C	2.65931900	2.50847300	-1.31804300
C	3.31912900	2.78450500	-0.10421600
C	2.62596400	3.03221600	1.08427900
C	1.22076300	3.00644300	1.04053500
C	3.33537000	3.28873400	2.41819700
C	3.48550300	2.26721700	-2.58680800
C	-4.12775100	4.83217900	-0.15744500
C	-5.45150900	-3.30960500	0.08150400
C	-0.36783500	-2.78480000	0.06983500
C	0.28832000	-2.99393100	1.28903700

C	1.61686300	-3.43894900	1.34517200
C	2.28175600	-3.67886700	0.13242800
C	1.65748300	-3.48824300	-1.11059700
C	0.33035800	-3.03813400	-1.11665800
C	2.29806500	-3.61718100	2.70762400
C	2.37232700	-3.74574900	-2.44210800
C	-3.20581600	3.60556300	-0.14319900
C	-1.79804900	3.71899000	-0.14511200
C	-0.95223700	2.61121400	-0.14292400
C	-5.01191500	4.79523300	-1.41383100
H	-5.63134500	3.88659200	-1.44683600
H	-5.68920200	5.66523500	-1.44228400
H	-4.39429800	4.80937800	-2.32532300
C	-5.02058100	4.81867900	1.09331100
H	-5.69748500	5.68938400	1.10083200
H	-5.64117400	3.91143300	1.13922300
H	-4.40933800	4.84961100	2.00872100
C	-3.34553000	6.14778600	-0.16664300
H	-2.70840500	6.24989900	0.72553500
H	-2.70424600	6.23516500	-1.05732000
H	-4.04431500	6.99913700	-0.17532000
C	4.85697700	3.34321900	2.26739600
H	5.17037800	4.14737500	1.58412400
H	5.32178400	3.53877300	3.24574200
H	5.26916500	2.39326900	1.89243600
C	2.98524900	2.15064500	3.39142700
H	1.90008100	2.06866800	3.55357000
H	3.34679700	1.18076400	3.01002700
H	3.45949600	2.31746800	4.37181100
C	2.85917300	4.62752100	3.00220600
H	3.35974700	4.82654500	3.96315300
H	3.09047100	5.45730500	2.31689400
H	1.77461900	4.63508400	3.18318000
C	-6.29032700	-2.94438800	1.31629300
H	-6.59182300	-1.88640900	1.30361100
H	-7.20789800	-3.55466900	1.36107400
H	-5.71736400	-3.11540900	2.24095400
C	-5.12610800	-4.80345000	0.15492600
H	-4.54678500	-5.13829500	-0.71942300
H	-4.55287200	-5.05225400	1.06144900
H	-6.05855700	-5.38918700	0.18008600
C	1.60444600	-4.82392000	-3.22273900
H	0.57050700	-4.51551100	-3.43536100
H	2.09957600	-5.02758100	-4.18567500
H	1.56297500	-5.76454700	-2.65245200
C	3.81289300	-4.22336500	-2.24761700
H	3.85828900	-5.17152700	-1.69041000
H	4.28446400	-4.39303400	-3.22754900
H	4.42487600	-3.48035300	-1.71214100
C	4.20248700	3.57385700	-2.96168500
H	4.87480900	3.91187700	-2.15859700
H	4.80594000	3.43692000	-3.87346400
H	3.47418000	4.37733100	-3.14940300
C	4.53146600	1.17036800	-2.33390500
H	5.22667400	1.43212400	-1.52286500
H	4.05024400	0.21305400	-2.07363000
H	5.13245100	0.99575900	-3.24018400
C	2.61348300	1.82993500	-3.76596300
H	2.06209300	0.90189000	-3.54680500
H	1.88085600	2.60205600	-4.04315700
H	3.24492100	1.64203200	-4.64781000
C	2.40225200	-2.44526800	-3.26062800
H	1.39305100	-2.04870400	-3.44593600
H	2.98264600	-1.66583200	-2.74060000
H	2.88118400	-2.61273400	-4.23847700
C	3.71243200	-4.18739500	2.58177600
H	4.15572500	-4.30937300	3.58183300
H	3.71113600	-5.17499900	2.09586900
H	4.37729300	-3.52358500	2.00715800
C	1.46656700	-4.57590500	3.57341900
H	1.37423300	-5.55925300	3.08764000
H	1.94618100	-4.72138500	4.55446800
H	0.45101300	-4.19413400	3.75170700
C	2.38873800	-2.24891700	3.40412200
H	3.03323300	-1.55757100	2.83395700
H	1.39965800	-1.78077200	3.52280200
H	2.83243300	-2.34965600	4.40746300
H	-1.33221000	4.70589400	-0.15816500

H	-4.84985300	2.19563200	-0.12312100
H	-5.30197200	-0.58301100	-0.04407100
H	-2.75999200	-4.07394700	0.12700100
H	-0.19280700	-2.85970100	-2.05902000
H	3.31075500	-4.03179300	0.15616700
H	-0.26721900	-2.78089200	2.20569100
H	0.63314000	3.17891300	1.94548000
H	4.40903800	2.81244100	-0.09886700
H	0.69833800	2.26438600	-2.21992300
K	1.68738800	-0.27470500	0.20844600
C	-6.28239100	-3.06560200	-1.18804100
H	-7.20028600	-3.67700600	-1.17926900
H	-6.58256600	-2.01114900	-1.27965700
H	-5.70385900	-3.32555500	-2.08816200

5.4.5 [(dtbpCbz)Rb]

0 1

C	0.98042200	1.76942100	-0.29021400
N	-0.06271200	0.88793600	-0.26615400
C	1.48491100	4.17833900	-0.29467700
C	0.55656600	3.13759500	-0.31423900
C	-0.87985200	3.07381700	-0.29341600
C	-1.89650400	4.02722100	-0.23937000
C	-3.23658200	3.63835200	-0.13953500
C	-3.51974700	2.25706400	-0.10237800
C	-2.53213200	1.27345900	-0.17921400
C	-1.17999300	1.67369700	-0.26687300
C	2.85081600	0.09466900	-0.11742800
C	2.75535400	-0.79080400	-1.20676200
C	3.22413500	-2.10390000	-1.11908700
C	3.76155200	-2.53475700	0.10970600
C	3.86251900	-1.69160500	1.21866500
C	3.40793600	-0.36919000	1.07705200
C	4.43785900	-2.15318100	2.56195700
C	3.22551900	-3.06650500	-2.31251600
C	3.85892100	5.07158100	-0.21103300
C	-4.33644700	4.70586000	-0.07618700
C	-2.88562400	-0.16442100	-0.14056900
C	-3.46391100	-0.73758500	0.99893600
C	-3.77274900	-2.10408300	1.06193000
C	-3.50518300	-2.89161800	-0.06657400
C	-2.94480300	-2.35192100	-1.23578600
C	-2.62786000	-0.98874800	-1.24483100
C	-4.37806300	-2.68305800	2.34601400
C	-2.70243600	-3.19063900	-2.49609200
C	2.85622000	3.91074000	-0.23068400
C	3.26090000	2.56034600	-0.18050700
C	2.36338400	1.49182600	-0.21939100
C	3.70780200	5.90005500	-1.49644800
H	2.69165600	6.30984200	-1.59660300
H	4.41449100	6.74681800	-1.50279800
H	3.90476300	5.28005900	-2.38483000
C	3.58487700	5.96782700	1.00685000
H	4.29093300	6.81454400	1.03682700
H	2.56600600	6.38226800	0.98516400
H	3.69159000	5.39716600	1.94258800
C	5.30810300	4.58647800	-0.12601200
H	5.49063900	4.00551900	0.79137900
H	5.57930300	3.95837500	-0.98857500
H	5.99226400	5.44958800	-0.11453900
C	4.91137100	-3.60755900	2.52402800
H	5.70868900	-3.75748500	1.78014900
H	5.31688300	-3.89375500	3.50647700
H	4.08960600	-4.30302000	2.29128200
C	3.35160500	-2.02682200	3.64255700
H	2.98546200	-0.99340800	3.73641000
H	2.49100900	-2.67698700	3.41101800
H	3.74358500	-2.33316700	4.62562300
C	5.63480200	-1.26432800	2.93404300
H	6.06285400	-1.57952200	3.89907400
H	6.42414000	-1.33305400	2.16990300
H	5.34825800	-0.20645900	3.02445000
C	-4.10715300	5.60796900	1.14666000
H	-3.12957100	6.11072200	1.10285500
H	-4.88362200	6.38874700	1.20852600

H	-4.13631500	5.01882000	2.07654900
C	-5.73436200	4.09384300	0.04194300
H	-5.97535300	3.45663300	-0.82291300
H	-5.83777000	3.48621300	0.95439400
H	-6.49084200	4.89312300	0.08722600
C	-4.29603000	5.55993600	-1.35304200
H	-5.07457400	6.34072200	-1.32738100
H	-3.32340600	6.05946800	-1.47530800
H	-4.46317000	4.93570100	-2.24455900
C	-3.57459900	-2.63658900	-3.63398100
H	-3.33273000	-1.58696200	-3.85622100
H	-3.42385100	-3.22136500	-4.55571000
H	-4.64137800	-2.68487500	-3.36687800
C	-3.05067600	-4.66659800	-2.29293200
H	-4.11434900	-4.80706800	-2.04773800
H	-2.84890400	-5.22774400	-3.21812700
H	-2.45059500	-5.12462000	-1.49052800
C	4.68378600	-3.37684200	-2.68849900
H	5.22702900	-3.85077500	-1.85706500
H	4.72236500	-4.06154500	-3.55105800
H	5.22123400	-2.45487900	-2.95790400
C	2.51241300	-4.37442600	-1.93684900
H	2.99906200	-4.88592800	-1.09319400
H	1.46200200	-4.18902400	-1.66205000
H	2.51208700	-5.07129900	-2.78991000
C	2.52870900	-2.46812000	-3.53603100
H	1.48097800	-2.20767800	-3.32557100
H	3.03902200	-1.56140900	-3.89304900
H	2.53194400	-3.19658100	-4.36135300
C	-1.22394800	-3.09571800	-2.89606500
H	-0.90871000	-2.05630400	-3.06936000
H	-0.57776700	-3.52264200	-2.11190200
H	-1.02981600	-3.66182000	-3.82102500
C	-4.67605200	-4.17925200	2.22752700
H	-5.11026500	-4.54856600	3.16915400
H	-5.39909300	-4.38911900	1.42462200
H	-3.76566500	-4.76726600	2.03139300
C	-5.69259100	-1.95238900	2.66144100
H	-6.41603800	-2.07925400	1.84154000
H	-6.14435900	-2.35317000	3.58298400
H	-5.53748400	-0.87333200	2.80635500
C	-3.38894400	-2.47859500	3.50505000
H	-2.44311800	-3.01236100	3.31205200
H	-3.15546800	-1.41478700	3.66140600
H	-3.80630600	-2.87122300	4.44613100
H	4.32260700	2.31444300	-0.11780400
H	1.12597300	5.21191800	-0.31628700
H	-1.63185000	5.08884400	-0.26214700
H	-4.55454000	1.91696300	-0.02980900
H	-2.18338500	-0.52335400	-2.12747100
H	-3.75415700	-3.95047900	-0.04193500
H	-3.65764200	-0.08326200	1.85296200
H	3.47282900	0.33359700	1.91176800
H	4.12965700	-3.55825200	0.18503100
H	2.32227100	-0.40560400	-2.13025200
Rb	0.06093100	-1.69246700	0.72315700

5.4.6 [(^{dtbp}Cbz)Cs]

0 1

C	-0.97233800	1.82844600	0.33899100
N	0.06630300	0.94026200	0.33658100
C	-1.45592300	4.24408600	0.31434900
C	-0.53941200	3.19398500	0.35950100
C	0.89586600	3.12117600	0.36122400
C	1.91359000	4.07321900	0.31387300
C	3.25376800	3.68164100	0.23126000
C	3.53161800	2.30017500	0.20184500
C	2.54264600	1.31556500	0.27238900
C	1.18914300	1.71876400	0.34716400
C	-2.87662700	0.17801200	0.15913000
C	-2.78631500	-0.70514600	1.25048800
C	-3.31932400	-1.99435700	1.18683000
C	-3.90770200	-2.40979200	-0.02380600
C	-4.00114900	-1.57093300	-1.13610200
C	-3.48629200	-0.26887600	-1.01604400

C	-4.63574100	-2.01348000	-2.45911900
C	-3.34352200	-2.94370700	2.39060600
C	-3.81947800	5.15888500	0.17692200
C	4.35744100	4.74543300	0.17747200
C	2.91807500	-0.11522600	0.23501400
C	3.64351800	-0.63834000	-0.84358600
C	4.01159600	-1.98926500	-0.90169800
C	3.65238500	-2.81493500	0.17223100
C	2.93842700	-2.32759500	1.27844500
C	2.56340200	-0.97936900	1.28074100
C	4.77843000	-2.51126300	-2.12227300
C	2.57397400	-3.21328500	2.47586200
C	-2.82802900	3.98952000	0.22667600
C	-3.24276500	2.64258800	0.18200000
C	-2.35739700	1.56423800	0.24696500
C	-3.68561500	5.99814700	1.45721400
H	-2.66786100	6.39971800	1.57316400
H	-4.38449500	6.85124200	1.44193600
H	-3.90533400	5.38844400	2.34736200
C	-3.51346800	6.04096900	-1.04369300
H	-4.21100500	6.89366600	-1.09537600
H	-2.49144900	6.44642900	-1.00589500
H	-3.60721700	5.46243800	-1.97600500
C	-5.27103800	4.68586400	0.06801800
H	-5.44062700	4.09727500	-0.84701100
H	-5.56491500	4.06888000	0.93116300
H	-5.94698100	5.55485200	0.03442900
C	-5.17298200	-3.44471000	-2.39716700
H	-5.95472900	-3.55354900	-1.63003900
H	-5.61868800	-3.71873400	-3.36563000
H	-4.37691300	-4.17465800	-2.18160700
C	-3.57800200	-1.94322500	-3.57259000
H	-3.16349600	-0.92939700	-3.67987100
H	-2.74550800	-2.63698500	-3.36639200
H	-4.01473100	-2.22953600	-4.54278800
C	-5.80174800	-1.07346800	-2.80255100
H	-6.27304400	-1.37524500	-3.75163900
H	-6.56961600	-1.10089500	-2.01435700
H	-5.47044600	-0.03035100	-2.91002200
C	4.14472200	5.64460800	-1.05050500
H	3.16819300	6.15036500	-1.01935700
H	4.92408400	6.42298000	-1.10570300
H	4.18289400	5.05271800	-1.97835100
C	5.75466000	4.12868700	0.07708800
H	5.98379000	3.49340900	0.94655800
H	5.86644800	3.51780300	-0.83223800
H	6.51414300	4.92542600	0.03784200
C	4.30473600	5.60325500	1.45134100
H	5.08574100	6.38176500	1.43249500
H	3.33214000	6.10582500	1.56084400
H	4.45971100	4.98108800	2.34647000
C	3.16760600	-2.60344900	3.75522700
H	2.77790700	-1.59316400	3.94618600
H	2.92323100	-3.22903900	4.62874800
H	4.26336400	-2.53075900	3.68043500
C	3.10468500	-4.64104200	2.33197800
H	4.20257400	-4.66233100	2.25696800
H	2.82074600	-5.23474500	3.21439100
H	2.69080700	-5.14846300	1.44636200
C	-4.80821700	-3.20162500	2.78134800
H	-5.37376000	-3.66918400	1.96134500
H	-4.86122800	-3.87358600	3.65311100
H	-5.31382100	-2.25960800	3.04302400
C	-2.67575500	-4.27715000	2.02274400
H	-3.18364200	-4.77735700	1.18462800
H	-1.62207200	-4.12669300	1.74234600
H	-2.69619400	-4.96756000	2.88096800
C	-2.62038800	-2.35553400	3.60359600
H	-1.56472100	-2.13709500	3.38629100
H	-3.09562100	-1.42592700	3.95018900
H	-2.64699800	-3.07292400	4.43818500
C	1.04615700	-3.27644800	2.60263600
H	0.60308200	-2.27366100	2.69713500
H	0.60405500	-3.76878000	1.72053200
H	0.74425800	-3.86021700	3.48691200
C	5.12256600	-3.99747100	-2.00270500
H	5.67286800	-4.32604700	-2.89763200
H	5.76040100	-4.19975000	-1.12876400

H	4.22058600	-4.62414000	-1.92139300
C	6.08864100	-1.72309800	-2.27522100
H	6.72278900	-1.84326500	-1.38350800
H	6.65449600	-2.08232000	-3.14977000
H	5.90650200	-0.64732100	-2.41313600
C	3.91423800	-2.31590700	-3.37861300
H	2.97405400	-2.88692100	-3.29949500
H	3.65842500	-1.25773400	-3.53816800
H	4.44658000	-2.67060900	-4.27577700
H	-4.30557300	2.40546800	0.10563500
H	-1.08619800	5.27392100	0.33358200
H	1.64936000	5.13511400	0.32791000
H	4.56651300	1.95755200	0.14409100
H	1.99805700	-0.55610900	2.11407600
H	3.94729700	-3.86197100	0.15464400
H	3.90871600	0.04471300	-1.65476900
H	-3.54968500	0.43290200	-1.85181600
H	-4.32344600	-3.41615900	-0.08028800
H	-2.31198400	-0.33368800	2.15906400
Cs	-0.06603500	-1.67292300	-0.95638700

5.4.7 [(^{dtbp}Cbz)]$^{-}$

-1 1

C	1.12593400	1.46366700	-0.03478900
N	0.03466400	0.65729300	-0.01154300
C	1.76567800	3.85191900	0.00597200
C	0.78619900	2.86257400	-0.00511100
C	-0.64955500	2.88414700	0.01383000
C	-1.59905600	3.90229100	0.01459100
C	-2.96460300	3.59456300	0.03106400
C	-3.32935500	2.23474700	0.06712600
C	-2.41421500	1.17360300	0.07332900
C	-1.03105900	1.49574400	0.02424300
C	2.94366000	-0.29965800	-0.23325200
C	2.16942500	-1.22102700	-0.95386300
C	2.61861400	-2.51758400	-1.20969400
C	3.85926400	-2.91194200	-0.69113200
C	4.64474900	-2.03740100	0.07027500
C	4.17092400	-0.74032900	0.28401900
C	5.99106300	-2.45497100	0.67616300
C	1.73964800	-3.44956600	-2.05213500
C	4.19040400	4.60437800	-0.00624700
C	-4.00052400	4.72600200	0.03505400
C	-2.90568000	-0.21381000	0.20190600
C	-2.18068500	-1.16259300	0.94807200
C	-2.69540100	-2.43079600	1.20653700
C	-3.94559300	-2.77201700	0.66196100
C	-4.67162200	-1.87990200	-0.12863600
C	-4.13373000	-0.60482500	-0.34371500
C	-1.97193000	-3.42829800	2.11994600
C	-6.01886600	-2.24449300	-0.76441900
C	3.12147400	3.50415700	-0.01646200
C	3.44573900	2.13470400	-0.07050300
C	2.49957000	1.10167200	-0.08957500
C	4.01967000	5.50472400	-1.24015800
H	3.02342400	5.97119100	-1.26252200
H	4.77249500	6.31236600	-1.24930500
H	4.13018300	4.91745500	-2.16506900
C	4.04013600	5.45516600	1.26500400
H	4.79200200	6.26326500	1.29218300
H	3.04397300	5.91856200	1.32366500
H	4.16791700	4.83250900	2.16423500
C	5.61220600	4.03743300	-0.02809900
H	5.80475500	3.39326800	0.84386100
H	5.79934400	3.44375000	-0.93612900
H	6.34623300	4.85966500	-0.00778100
C	6.36501100	-3.89725700	0.32651300
H	6.45299200	-4.04247900	-0.76134400
H	7.33707000	-4.15264300	0.77829100
H	5.62111300	-4.61405400	0.70702400
C	5.91666300	-2.33692700	2.20629300
H	5.68556500	-1.30882300	2.52149100
H	5.12802700	-2.99155600	2.60870200
H	6.87619100	-2.62619200	2.66775600
C	7.09942100	-1.53223100	0.14594500

H	8.07730900	-1.81032900	0.57440400
H	7.17098100	-1.60052700	-0.95083300
H	6.90688100	-0.47963100	0.40058400
C	-3.80532400	5.60333300	1.28182900
H	-2.79561100	6.03940300	1.31218500
H	-4.53370400	6.43291900	1.30141400
H	-3.93500500	5.00660700	2.19815700
C	-5.43848700	4.20104700	0.04688500
H	-5.64816600	3.57477700	-0.83411900
H	-5.64487900	3.60071100	0.94631300
H	-6.14791600	5.04477700	0.03673200
C	-3.82290100	5.58984000	-1.22379800
H	-4.55038900	6.42023000	-1.24046700
H	-2.81334100	6.02424800	-1.27463700
H	-3.96757500	4.98406600	-2.13195600
C	-7.09783300	-1.26665200	-0.27394300
H	-6.85193900	-0.22684500	-0.53507800
H	-8.07571300	-1.50625300	-0.72497000
H	-7.20076300	-1.31826800	0.82125100
C	-6.46497800	-3.66431800	-0.40820500
H	-6.58941500	-3.79077900	0.67846500
H	-7.43435100	-3.88365500	-0.88400500
H	-5.74231300	-4.41725900	-0.75870600
C	2.38940200	-4.81582200	-2.28162300
H	2.57108400	-5.34523500	-1.33320300
H	1.72491600	-5.44780700	-2.89232500
H	3.34977200	-4.72736100	-2.81387100
C	0.40394400	-3.66328600	-1.32749700
H	0.57439500	-4.15891400	-0.36008100
H	-0.11516100	-2.71398800	-1.12677800
H	-0.27021700	-4.30023600	-1.92476400
C	1.48187300	-2.80329400	-3.42192200
H	0.97058500	-1.83550600	-3.31961400
H	2.42887000	-2.62836500	-3.95685000
H	0.84797700	-3.45686600	-4.04459300
C	-5.89882100	-2.14865200	-2.29316200
H	-5.61233800	-1.13614200	-2.61333300
H	-5.13097800	-2.84372500	-2.66692700
H	-6.85822200	-2.39929700	-2.77684700
C	-1.90686700	-4.81418400	1.46104000
H	-1.35716300	-5.51938400	2.10629300
H	-2.90818900	-5.23752200	1.29003600
H	-1.39333100	-4.76533000	0.49056500
C	-2.75978400	-3.53790700	3.43577800
H	-3.78945900	-3.88622200	3.25861800
H	-2.27197900	-4.24806300	4.12517600
H	-2.81914300	-2.55834900	3.93492500
C	-0.54550900	-2.97495500	2.44377100
H	0.05084100	-2.80979900	1.53477200
H	-0.53748200	-2.03510400	3.01490100
H	-0.03839100	-3.73954200	3.05415500
H	4.49450700	1.84476200	-0.14868800
H	1.46230700	4.90433400	0.02841000
H	-1.26453400	4.94542300	0.00632000
H	-4.38615300	1.97462700	0.14228200
H	-4.67497600	0.11432400	-0.96355400
H	-4.35182600	-3.76332200	0.86445200
H	-1.20124400	-0.85791500	1.31400600
H	4.75843900	-0.04134600	0.88456300
H	4.21636900	-3.92273700	-0.87831000
H	1.19294100	-0.88301600	-1.30395900

5.4.8 [(^{dtbp}Cbz)Na]$_2$

0 1

Na	14.32371	11.44888	6.99146
Na	15.21762	7.98179	4.98885
N	13.47561	9.28423	7.23371
N	15.92535	10.09542	4.31189
C	12.60114	9.06998	6.18422
C	11.70757	9.99547	5.58507
C	10.83548	9.50522	4.61911
H	10.23916	10.11979	4.20778
C	10.77698	8.16277	4.21078
C	11.66471	7.27013	4.78944
H	11.66126	6.35918	4.51993

C	12.56481	7.70161	5.76677
C	13.46231	7.01449	6.66417
C	13.80124	5.66474	6.84513
H	13.52479	5.01698	6.20758
C	14.53599	5.27617	7.94831
C	14.87695	6.26779	8.89538
H	15.32118	5.99239	9.68865
C	14.60341	7.61713	8.73856
C	13.92907	8.02216	7.56218
C	11.55315	11.39054	6.07587
C	11.64413	11.66661	7.44536
H	11.86613	10.96458	8.04568
C	11.41722	12.94500	7.94952
C	11.04504	13.94494	7.04089
H	10.88086	14.82113	7.36927
C	10.90731	13.70787	5.68696
C	11.20635	12.43138	5.21046
H	11.17344	12.26578	4.27557
C	11.57997	13.27274	9.43433
C	11.76032	12.02160	10.29058
H	10.98493	11.43321	10.17663
H	11.83926	12.27918	11.23282
H	12.57253	11.54933	10.01187
C	12.82941	14.15927	9.57992
H	13.61515	13.67239	9.25443
H	12.95687	14.39174	10.52339
H	12.71186	14.97824	9.05468
C	10.36402	14.04177	9.96625
H	10.25609	14.87342	9.45920
H	10.49946	14.25212	10.91378
H	9.55963	13.49109	9.86562
C	10.34318	14.74150	4.63577
C	11.39620	15.06476	3.58294
H	11.66184	14.24120	3.12298
H	12.17932	15.46417	4.01608
H	11.02469	15.69684	2.93267
C	9.95909	16.04914	5.33331
H	9.62886	16.68915	4.66868
H	10.74542	16.42233	5.78367
H	9.25714	15.87294	5.99409
C	9.10348	14.17392	3.93918
H	8.74744	14.83861	3.31322
H	8.42190	13.95858	4.60960
H	9.34760	13.36129	3.44883
C	9.72747	7.66316	3.20431
C	8.74317	8.75983	2.79426
H	8.08937	8.39270	2.16325
H	9.23178	9.49458	2.36786
H	8.27772	9.09483	3.58894
C	8.90758	6.53051	3.81922
H	8.45458	6.85545	4.62521
H	9.50193	5.78798	4.05545
H	8.24022	6.22143	3.17154
C	10.43755	7.15206	1.95306
H	9.77164	6.89462	1.28172
H	10.98647	6.37373	2.18390
H	11.01031	7.85976	1.59042
C	14.89333	3.79552	8.19059
C	14.80386	2.96842	6.91071
H	15.34303	3.39133	6.21011
H	13.86974	2.91853	6.61864
H	15.14139	2.06441	7.08171
C	13.92397	3.24948	9.22956
H	13.00521	3.34948	8.90353
H	14.02914	3.74655	10.06756
H	14.11348	2.30085	9.38645
C	16.31191	3.63905	8.73183
H	16.95260	3.97590	8.07119
H	16.49175	2.69192	8.90788
H	16.40216	4.14885	9.56389
C	14.81132	8.54905	9.88637
C	14.05281	8.33305	11.03594
H	13.44635	7.60212	11.05721
C	14.15704	9.15364	12.15004
C	15.10750	10.18080	12.10204
H	15.20986	10.74287	12.86106
C	15.90620	10.41107	10.99027
C	15.71874	9.60235	9.86393

H	16.21763	9.77505	9.07414
C	13.21629	8.96110	13.34812
C	12.16117	10.06507	13.31406
H	12.60241	10.93965	13.34280
H	11.56721	9.97327	14.08812
H	11.63696	9.99061	12.48941
C	12.48276	7.61572	13.34242
H	11.91153	7.55847	12.54819
H	11.93009	7.54157	14.14832
H	13.13754	6.88673	13.32713
C	13.99197	9.04293	14.66512
H	14.66889	8.33471	14.69010
H	13.37295	8.92978	15.41641
H	14.43071	9.91667	14.73211
C	16.97263	11.51427	10.96337
C	17.20953	12.10750	12.35649
H	17.95645	12.74086	12.31914
H	17.42294	11.38753	12.98617
H	16.40073	12.57347	12.65499
C	18.30554	10.94482	10.46764
H	18.19935	10.61579	9.55064
H	18.58200	10.20645	11.04966
H	18.98798	11.64794	10.48541
C	16.52373	12.62591	10.02730
H	16.36725	12.25670	9.13308
H	17.22010	13.31379	9.97943
H	15.69458	13.02347	10.36624
C	15.02256	10.22866	3.27220
C	14.66641	9.24162	2.32874
C	13.73501	9.58189	1.35406
H	13.47249	8.91542	0.73003
C	13.15814	10.86809	1.24316
C	13.52954	11.82399	2.17628
H	13.15950	12.69743	2.12463
C	14.44083	11.52060	3.19198
C	15.06504	12.26806	4.25268
C	14.96933	13.59766	4.67098
H	14.34942	14.18246	4.25120
C	15.77811	14.06800	5.69947
C	16.69659	13.16280	6.27735
H	17.25132	13.48447	6.97827
C	16.84678	11.83080	5.89200
C	15.97919	11.34911	4.87167
C	15.33073	7.90580	2.32280
C	16.72691	7.82897	2.45922
H	17.22337	8.62939	2.58312
C	17.40092	6.61736	2.41810
C	16.63902	5.45505	2.24616
H	17.08474	4.61685	2.21044
C	15.25131	5.48284	2.12552
C	14.61033	6.72625	2.17695
H	13.66340	6.76458	2.11077
C	18.93898	6.54755	2.46337
C	19.53562	7.82375	3.06411
H	19.35226	8.58121	2.46993
H	20.50429	7.71517	3.16553
H	19.13210	7.99151	3.94127
C	19.40810	5.35095	3.29127
H	19.13051	4.52039	2.85138
H	19.00956	5.39600	4.18545
H	20.38494	5.36943	3.36772
C	19.45716	6.38087	1.03756
H	19.07330	5.57000	0.64318
H	20.43421	6.30627	1.05169
H	19.19668	7.15933	0.50224
C	14.42338	4.20647	1.91004
C	15.27085	2.95337	1.87020
H	15.92889	3.02689	1.14773
H	14.69647	2.17548	1.71101
H	15.73602	2.84628	2.72609
C	13.67517	4.32938	0.57014
H	14.32382	4.38179	-0.16260
H	13.12388	5.13958	0.57696
H	13.10155	3.54499	0.44314
C	13.37912	4.07300	3.01741
H	12.82570	4.88136	3.04369
H	13.83031	3.95784	3.87973
H	12.81159	3.29421	2.83910

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 C   12.28865   11.21573    0.05730
 C   11.41679   10.06039   -0.37898
 H   10.82310   10.35377   -1.10139
 H   10.87956    9.75165    0.38028
 H   11.98249    9.32679   -0.69867
 C   13.18730   11.61915   -1.09755
 H   13.71524   10.84565   -1.38630
 H   13.78956   12.33594   -0.80787
 H   12.63733   11.93634   -1.84408
 C   11.32243   12.35807    0.38411
 H   10.67771   12.45982   -0.34688
 H   11.82668   13.19126    0.49329
 H   10.84464   12.15413    1.21509
 C   15.78325   15.54907    6.12510
 C   14.44939   16.22723    5.83774
 H   14.29887   16.25497    4.86977
 H   14.46428   17.14072    6.19233
 H   13.72714   15.72220    6.26631
 C   16.87581   16.25101    5.32609
 H   16.67977   16.17608    4.36883
 H   17.74059   15.83105    5.51629
 H   16.90929   17.19706    5.57962
 C   16.05799   15.71732    7.61186
 H   16.96381   15.40283    7.81432
 H   15.40799   15.19373    8.12546
 H   15.97914   16.66375    7.85360
 C   17.95979   11.01676    6.45727
 C   19.17857   11.62143    6.78243
 H   19.27818   12.55820    6.65982
 C   20.24784   10.88541    7.28063
 C   20.08711    9.51119    7.43059
 H   20.81540    8.99740    7.75942
 C   18.89784    8.86465    7.11586
 C   17.84093    9.64198    6.64503
 H   17.01316    9.22050    6.44586
 C   21.60529   11.52140    7.61699
 C   21.55449   13.04608    7.54243
 H   21.28081   13.32018    6.64222
 H   22.44167   13.41253    7.73991
 H   20.90838   13.38382    8.19731
 C   22.03440   11.11497    9.03374
 H   22.06742   10.13759    9.09730
 H   21.38825   11.46291    9.68322
 H   22.92147   11.48494    9.22515
 C   22.65074   11.02653    6.60956
 H   22.36966   11.26743    5.70218
 H   22.73473   10.05252    6.67780
 H   23.51579   11.44350    6.80509
 C   18.75709    7.35418    7.33594
 C   18.51519    7.10490    8.83090
 H   17.72108    7.60085    9.12048
 H   19.29408    7.40766    9.34280
 H   18.37589    6.14700    8.98399
 C   20.03385    6.61408    6.90178
 H   20.25883    6.86332    5.98109
 H   19.88352    5.64693    6.95095
 H   20.77259    6.86052    7.49672
 C   17.57974    6.77368    6.53769
 H   17.65409    7.04804    5.59982
 H   16.73672    7.10725    6.90979
 H   17.59741    5.79548    6.59427
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5.4.9 [(^{dtbp}Cbz)]$^{-}$ – 1st excited state

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-1 1
 C                  1.09413500    1.53824800   -0.03635000
 N                  0.01680100    0.71883200    0.01549300
 C                  1.66409300    3.92989000    0.00265500
 C                  0.70610600    2.92387800   -0.00350700
 C                 -0.73409500    2.91188700    0.03849900
 C                 -1.70436600    3.92615900    0.02230600
 C                 -3.06476100    3.55084500    0.03432800
 C                 -3.40757300    2.19619500    0.07999700
 C                 -2.44916500    1.13202200    0.11762600
 C                 -1.09521300    1.53876900    0.07089200
 C                  2.91675100   -0.21950600   -0.21099400
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C	2.13579000	-1.19702400	-0.86192700
C	2.60892000	-2.48863600	-1.06715500
C	3.88989400	-2.81994300	-0.58491400
C	4.68254100	-1.89398900	0.09498500
C	4.18109400	-0.59899000	0.26733300
C	6.06593000	-2.24440500	0.65721300
C	1.80244500	-3.53743000	-1.84157900
C	4.08085100	4.70547000	-0.02406600
C	-4.13329200	4.65117700	0.00833000
C	-2.89003500	-0.25586000	0.21242500
C	-2.08360100	-1.26751800	0.79180300
C	-2.55253500	-2.55756100	0.99282100
C	-3.86950700	-2.87805700	0.58316900
C	-4.68943400	-1.92267000	-0.02354800
C	-4.19369600	-0.62781200	-0.19580400
C	-1.71067300	-3.63227400	1.68999300
C	-6.10911300	-2.24921100	-0.50880400
C	3.03732700	3.58387500	-0.02883900
C	3.40199300	2.23403900	-0.07863400
C	2.45824100	1.17231200	-0.09798100
C	3.87400300	5.59954800	-1.25726200
H	2.86733300	6.04231400	-1.27293600
H	4.60835600	6.42312900	-1.26930600
H	3.99406300	5.01575900	-2.18309300
C	3.91240100	5.54743600	1.25119600
H	4.64797000	6.36967000	1.27489300
H	2.90751800	5.98961800	1.31633400
H	4.05990600	4.92570400	2.14793800
C	5.51634000	4.17560900	-0.05562100
H	5.73056800	3.53616700	0.81446500
H	5.71296500	3.58892200	-0.96596800
H	6.22719300	5.01750100	-0.03859600
C	6.46703100	-3.68980900	0.35448700
H	6.51240400	-3.88064100	-0.72892600
H	7.46461900	-3.89784800	0.77342700
H	5.76142500	-4.40875800	0.79848800
C	6.05304600	-2.05927800	2.18241800
H	5.80550200	-1.02475700	2.46242400
H	5.30230800	-2.71692900	2.64739100
H	7.03955800	-2.30080400	2.61307500
C	7.12066700	-1.31484600	0.03748300
H	8.12414400	-1.54542000	0.43334600
H	7.14652800	-1.43073300	-1.05731200
H	6.90785700	-0.25762200	0.25417800
C	-3.96435200	5.55489400	1.23978700
H	-2.96588300	6.01534700	1.26899200
H	-4.71493800	6.36433100	1.23796100
H	-4.08689200	4.97148600	2.16563000
C	-5.55854100	4.09347300	0.02029800
H	-5.74423600	3.44419300	-0.84893000
H	-5.75628300	3.50639000	0.93007100
H	-6.28622100	4.92086000	-0.01240400
C	-3.96395300	5.49091800	-1.26791800
H	-4.71686500	6.29717000	-1.30904900
H	-2.96702300	5.95261100	-1.31947600
H	-4.08331400	4.86022500	-2.16269900
C	-7.11666400	-1.32662600	0.19391200
H	-6.90402400	-0.26683300	-0.00901500
H	-8.14528900	-1.53884900	-0.14524300
H	-7.07615000	-1.46882400	1.28521900
C	-6.50663900	-3.69771100	-0.21537500
H	-6.48566500	-3.91213200	0.86433400
H	-7.53021700	-3.88817600	-0.57716300
H	-5.83461900	-4.41110300	-0.71681800
C	2.52195800	-3.82928600	-3.16862500
H	3.54258000	-4.20696700	-3.00006800
H	1.97047400	-4.58631000	-3.75143000
H	2.59924100	-2.91524000	-3.77770600
C	1.70971400	-4.83607700	-1.02583500
H	2.70056700	-5.28146900	-0.84927300
H	1.24357500	-4.65450200	-0.04729900
H	1.10038900	-5.58346100	-1.56015200
C	0.38482700	-3.05200200	-2.15677600
H	-0.17480500	-2.77068200	-1.25230000
H	0.39449300	-2.17453300	-2.82028100
H	-0.17940800	-3.84820900	-2.66799000
C	-6.18918800	-2.03071000	-2.02744000
H	-5.94837300	-0.99224700	-2.29817500

H	-5.47284300	-2.68344200	-2.55039800
H	-7.20220300	-2.25594800	-2.40344900
C	-1.63153300	-4.88689200	0.80589400
H	-1.00604800	-5.66112000	1.28177000
H	-2.62628500	-5.32280700	0.62898500
H	-1.19459700	-4.64881100	-0.17446000
C	-2.37826600	-4.00333700	3.02457000
H	-3.40235500	-4.37749700	2.87243200
H	-1.80225000	-4.78666400	3.54676800
H	-2.43955100	-3.12288200	3.68300400
C	-0.28830500	-3.15003200	1.98640000
H	0.24143300	-2.82561000	1.07872600
H	-0.28753200	-2.29879900	2.68336800
H	0.29706900	-3.96157500	2.44874300
H	4.45449800	1.96942900	-0.16581100
H	1.35365700	4.97756700	0.03651900
H	-1.40390300	4.97584200	-0.01847200
H	-4.45727800	1.91941500	0.15558400
H	-4.81526200	0.12048800	-0.69222300
H	-4.24453300	-3.88717400	0.75385300
H	-1.07688400	-0.98746900	1.09437900
H	4.77329000	0.14030300	0.81120100
H	4.26627200	-3.82928600	-0.75249700
H	1.14680000	-0.89903600	-1.20421800

5.4.10 (^{dtbp}Cbz)–H – 1st excited state

0 1

N	-0.00001100	0.93064300	-0.00004200
H	0.00000100	-0.08635100	-0.00004200
C	-0.71596200	3.06714000	0.10258600
C	-1.11015800	1.70380800	0.19724400
C	1.89103100	-0.98148700	-1.28677300
H	1.11898100	-0.51078300	-1.89920100
C	2.72236900	-0.15596400	-0.50402200
C	1.11013400	1.70381800	-0.19733800
C	-3.07618100	3.65405800	0.29333300
C	3.07615700	3.65406800	-0.29336000
C	2.43127900	1.26993200	-0.37621900
C	4.14030400	4.75245900	-0.33683700
C	2.06401200	-2.36673100	-1.33906900
C	-2.43129700	1.26993300	0.37615900
C	-1.89104700	-0.98145800	1.28676600
H	-1.11897800	-0.51073400	1.89915300
C	0.71593700	3.06714400	-0.10268300
C	1.71189800	4.04593100	-0.17025800
H	1.44496800	5.10141200	-0.10057800
C	-3.41510400	2.29952600	0.38361100
H	-4.45294000	1.99957700	0.51971000
C	3.41508500	2.29953800	-0.38363100
H	4.45292700	1.99959400	-0.51969400
C	-1.71192500	4.04591500	0.17018800
H	-1.44499700	5.10139800	0.10051200
C	5.12942600	-2.80794000	0.93686400
C	-4.14032400	4.75245100	0.33685200
C	3.12072700	-2.91672100	-0.60649800
H	3.27323500	-3.99567100	-0.62201300
C	-2.06402200	-2.36670100	1.33910300
C	3.80239300	-0.74823100	0.18174700
H	4.44036900	-0.10273900	0.78602300
C	4.00711600	-2.12379200	0.15007500
C	-2.72238500	-0.15597100	0.50399100
C	1.14353100	-3.21794300	-2.22241900
C	-3.80239000	-0.74825400	-0.18178200
H	-4.44035800	-0.10278000	-0.78608500
C	-4.00710700	-2.12381900	-0.15007500
C	-1.14351600	-3.21787400	2.22245900
C	-3.12072700	-2.91671500	0.60653500
H	-3.27322800	-3.99566500	0.62207800
C	-5.55836800	4.19300900	0.46786600
H	-5.81857800	3.54054600	-0.37952900
H	-6.28391400	5.02070500	0.48605200
H	-5.68636500	3.61846400	1.39781000
C	4.06718600	5.57411600	0.96147100
H	3.08387100	6.04810500	1.09531100
H	4.82633300	6.37299800	0.94994600

H	4.25367100	4.93567700	1.83874000
C	1.56623600	-3.01882200	-3.68655500
H	1.48456300	-1.96191600	-3.98297700
H	0.92686300	-3.61289800	-4.35985500
H	2.61121800	-3.32995200	-3.83938600
C	1.24100400	-4.70638000	-1.87596700
H	2.24253000	-5.11489200	-2.07812700
H	0.52677000	-5.27956500	-2.48672300
H	1.00308100	-4.88994000	-0.81628500
C	5.55835200	4.19301700	-0.46780900
H	5.81853300	3.54055000	0.37959200
H	6.28390000	5.02071300	-0.48596700
H	5.68637800	3.61847500	-1.39775000
C	-5.12940500	-2.80799500	-0.93685700
C	0.32196600	-2.78768100	2.05517000
H	0.65779700	-2.87035900	1.01047900
H	0.97782600	-3.42770000	2.66630400
H	0.49662200	-1.75105300	2.37894600
C	-3.87098000	5.66910700	1.54185300
H	-3.91745800	5.10027400	2.48321500
H	-4.62535000	6.47133300	1.58709800
H	-2.88015800	6.14319300	1.48574600
C	-0.32198300	-2.78788300	-2.05506700
H	-0.65775600	-2.87058400	-1.01035900
H	-0.97781300	-3.42796900	-2.66616300
H	-0.49675200	-1.75127500	-2.37884400
C	-4.06724700	5.57411500	-0.96145500
H	-3.08393500	6.04810300	-1.09532400
H	-4.82639100	6.37299800	-0.94990000
H	-4.25376200	4.93568200	-1.83872200
C	3.87100200	5.66912300	-1.54184200
H	3.91751100	5.10029400	-2.48320600
H	4.62537500	6.47134900	-1.58705900
H	2.88017900	6.14320800	-1.48576700
C	-4.50539200	-3.75988100	-1.96993700
H	-3.86161900	-3.20663900	-2.67149500
H	-5.29159800	-4.26768100	-2.55170100
H	-3.88828500	-4.53504100	-1.49147100
C	-1.24085400	-4.70631200	1.87596200
H	-2.24235300	-5.11491500	2.07807200
H	-0.52659600	-5.27945300	2.48673000
H	-1.00287200	-4.88982300	0.81628500
C	-1.56629100	-3.01882200	3.68658400
H	-1.48471700	-1.96191500	3.98303300
H	-0.92689000	-3.61285700	4.35989300
H	-2.61125200	-3.33004400	3.83937200
C	-6.01802200	-3.60586500	0.02996700
H	-5.45035700	-4.38045700	0.56652800
H	-6.82991700	-4.10827100	-0.52016200
H	-6.47264200	-2.94242200	0.78185500
C	-6.01175700	-1.80259000	-1.67935000
H	-6.49193700	-1.09333600	-0.98770500
H	-6.81064300	-2.33446700	-2.21862400
H	-5.43942000	-1.22533600	-2.42152500
C	6.01173400	-1.80251500	1.67938400
H	6.49188700	-1.09322600	0.98775600
H	6.81064000	-2.33437000	2.21865000
H	5.43936900	-1.22530000	2.42156800
C	6.01808900	-3.60576800	-0.02995300
H	5.45046200	-4.38038000	-0.56652700
H	6.82999700	-4.10814500	0.52018200
H	6.47269000	-2.94230100	-0.78183100
C	4.50543100	-3.75986000	1.96992400
H	3.86163600	-3.20664600	2.67148500
H	5.29164400	-4.26764900	2.55168700
H	3.88834800	-4.53502700	1.49143800

5.4.11 [(^{dtbp}Cbz)]Li – 1st excited state

0 1

C	1.31214400	1.37254200	-0.42098800
N	0.92082900	0.09273500	-0.18594100
C	3.30711900	2.76620600	-0.51768000
C	2.73444800	1.52175100	-0.36252000
C	3.23150800	0.18378300	-0.04553000
C	4.46407900	-0.38883100	0.20307800

C	4.54352600	-1.75580100	0.56751600
C	3.35700400	-2.51165200	0.68051200
C	2.09803400	-1.97404800	0.42556200
C	2.05769300	-0.61498400	0.05434700
C	-0.99298000	2.32712400	-0.51714500
C	-1.70597600	3.00084100	0.48439000
C	-3.07165300	2.78413500	0.66416100
C	-3.71665100	1.89765900	-0.21251800
C	-3.04761000	1.22937100	-1.23900000
C	-1.66782300	1.44944900	-1.36859800
C	-3.76573600	0.29695100	-2.21955200
C	-3.87164300	3.43784500	1.79453500
C	3.14910000	5.27291500	-0.89421800
C	5.92224800	-2.36447000	0.83193400
C	0.78635300	-2.68191500	0.49902000
C	0.29369500	-3.32202600	-0.69208900
C	-1.03594300	-3.86324200	-0.68261400
C	-1.88905900	-3.51181100	0.34259700
C	-1.48703900	-2.61254300	1.41718400
C	-0.08401200	-2.38431700	1.53795700
C	-1.44165900	-4.83414600	-1.79506000
C	-2.48989700	-2.25927800	2.50970500
C	2.48548300	3.90633400	-0.71712400
C	1.09338900	3.74076600	-0.73366400
C	0.47495500	2.48985400	-0.59586200
C	3.98100300	5.59677600	0.35786300
H	4.77080700	4.85149500	0.53373700
H	4.46881700	6.57837500	0.24763700
H	3.34402100	5.62922400	1.25509700
C	4.06839600	5.22914000	-2.12607300
H	4.56058000	6.20427900	-2.26951300
H	4.85778000	4.46954700	-2.02478100
H	3.49439500	4.99752900	-3.03638000
C	2.12820500	6.39448500	-1.09581300
H	1.51304400	6.23158800	-1.99384400
H	1.45575200	6.49689300	-0.23040500
H	2.65207300	7.35404000	-1.22245300
C	-5.23228300	0.07944400	-1.84070800
H	-5.80735100	1.01771800	-1.86343200
H	-5.70180700	-0.61071800	-2.55801600
H	-5.33077100	-0.36486100	-0.83816300
C	-3.07341100	-1.07190700	-2.23697900
H	-2.02541700	-1.00604500	-2.56940400
H	-3.09507600	-1.55131600	-1.24524100
H	-3.58267300	-1.75184800	-2.93787800
C	-3.70622900	0.92082600	-3.62262400
H	-4.21208900	0.27095700	-4.35463800
H	-4.20066400	1.90439500	-3.63675400
H	-2.66804300	1.06212700	-3.95917700
C	6.77892100	-2.24006500	-0.43919300
H	6.91812300	-1.19185500	-0.74278500
H	7.77742900	-2.67339600	-0.26893200
H	6.31234200	-2.77461000	-1.28079900
C	5.84455800	-3.84374700	1.21530700
H	5.26482600	-3.99828600	2.13780900
H	5.39031000	-4.45044600	0.41748400
H	6.85862900	-4.23350200	1.39193800
C	-2.86049300	-3.51779300	3.31512800
H	-1.96608000	-3.94366800	3.79584800
H	-3.60138200	-3.29267400	4.10093300
H	-3.28649800	-4.29544000	2.66227200
C	-3.76411600	-1.67314100	1.87837800
H	-4.22608600	-2.37050100	1.16292000
H	-4.51790300	-1.44349300	2.64998700
H	-3.53448500	-0.74014900	1.33773600
C	-5.04865400	4.22714600	1.20160800
H	-5.73066700	3.58156100	0.62866600
H	-5.63592900	4.69969600	2.00506800
H	-4.69063100	5.02032800	0.52705000
C	-4.40286300	2.33465100	2.72422100
H	-5.06414600	1.63418400	2.19270400
H	-3.57530200	1.74771200	3.15165400
H	-4.97795500	2.77537500	3.55435200
C	-3.01710200	4.39859500	2.62372800
H	-2.17783900	3.88134000	3.11325400
H	-2.60836900	5.21600100	2.00962500
H	-3.63116400	4.85341900	3.41595000
C	-1.92993900	-1.21082100	3.47499300

H	-1.06954400	-1.59243700	4.04543000
H	-1.60712000	-0.30501600	2.93568300
H	-2.70044900	-0.91499500	4.20478400
C	-2.93124600	-5.18174700	-1.75553000
H	-3.18028300	-5.86430800	-2.58299800
H	-3.20702800	-5.68485500	-0.81659000
H	-3.55848100	-4.28247100	-1.85827200
C	-0.63445800	-6.13074900	-1.61502200
H	-0.85301200	-6.58950500	-0.63847200
H	-0.88422000	-6.85892600	-2.40433500
H	0.44718200	-5.93461700	-1.65708900
C	-1.12878200	-4.23714200	-3.17530600
H	-1.69569400	-3.30918000	-3.34188400
H	-0.06134400	-4.00295800	-3.29258100
H	-1.40310000	-4.94970100	-3.97002000
H	0.44406200	4.60640100	-0.86447800
H	4.39301700	2.87708500	-0.47058100
H	5.37452500	0.21040700	0.12788500
H	3.40558300	-3.55983800	0.97305200
H	0.30419400	-1.82175100	2.38918600
H	-2.90904000	-3.89643700	0.34834500
H	0.99433100	-3.57005300	-1.48800000
H	-1.09976400	0.95602500	-2.16141800
H	-4.78346400	1.72198100	-0.07685700
H	-1.15297300	3.66554100	1.14857400
Li	-0.67704300	-1.17197800	-0.18579900
C	6.59751300	-1.60268500	1.98476800
H	7.59245400	-2.02875700	2.19049700
H	6.73417100	-0.53616600	1.75213000
H	5.99800900	-1.67204100	2.90537600

5.4.12 [(^{dtbp}Cbz)]Na – 1st excited state

0 1

C	-1.58257700	1.21026000	-0.32569000
N	-0.94836300	0.02250200	-0.14628000
C	-3.80200800	2.20528900	-0.36838600
C	-3.00495700	1.08458700	-0.26015400
C	-3.23190000	-0.33967800	-0.01774000
C	-4.34144300	-1.14695600	0.14385700
C	-4.16729800	-2.53032200	0.39027100
C	-2.86130800	-3.05189300	0.48375400
C	-1.71030400	-2.27547000	0.32087000
C	-1.92645900	-0.90627300	0.05387400
C	0.50593000	2.55883900	-0.47673100
C	1.26849100	1.85349700	-1.42523800
C	2.66318800	1.84492500	-1.36577700
C	3.27921400	2.55593600	-0.31965400
C	2.55603600	3.27570700	0.63073700
C	1.15593000	3.27335200	0.52550600
C	3.22419700	4.02772100	1.78509700
C	3.53501600	1.10900100	-2.39011700
C	-4.12026300	4.70883900	-0.64855400
C	-5.40948100	-3.40890200	0.55509500
C	-0.31811000	-2.78754600	0.42024500
C	0.48272700	-2.45864300	1.58746500
C	1.86847000	-2.60144400	1.55902200
C	2.50265300	-3.04803400	0.37399700
C	1.70866300	-3.51617200	-0.76384400
C	0.33038800	-3.34582100	-0.70136500
C	2.69210700	-2.18255400	2.79064800
C	2.40819800	-4.28342100	-1.88151800
C	-3.21061900	3.48432700	-0.53078700
C	-1.81090700	3.58473500	-0.57507700
C	-0.97223900	2.46685700	-0.48615300
C	-5.03163300	4.54226200	-1.87570500
H	-5.66381600	3.64511300	-1.80064300
H	-5.69884800	5.41310800	-1.97665500
H	-4.43665500	4.45733800	-2.79799400
C	-4.98098800	4.82276100	0.62054500
H	-5.64461300	5.69956100	0.55354800
H	-5.61529400	3.93668100	0.77067900
H	-4.34918000	4.93845000	1.51458800
C	-3.33007100	6.00908700	-0.81012100
H	-2.67440900	6.19999000	0.05321900
H	-2.71030000	6.00164700	-1.71968200

H	-4.02587900	6.85796400	-0.89074300
C	4.74996100	3.92753300	1.73389900
H	5.15863900	4.35674600	0.80600300
H	5.18684300	4.48466200	2.57647700
H	5.09461300	2.88510600	1.81483700
C	2.74428700	3.42513500	3.11547500
H	1.65389700	3.50887800	3.23457500
H	3.00608700	2.35792100	3.18158900
H	3.21441700	3.94740900	3.96394900
C	2.83199500	5.51153800	1.71666400
H	3.29810300	6.06911500	2.54456800
H	3.16479100	5.96337200	0.76935400
H	1.74357700	5.65267900	1.79243200
C	-6.23976500	-2.89151700	1.74157200
H	-6.57105700	-1.85304000	1.59260100
H	-7.13995100	-3.51245400	1.87621400
H	-5.65586700	-2.92755100	2.67405600
C	-5.05805300	-4.87458400	0.81846600
H	-4.48031000	-5.31195600	-0.00965200
H	-4.47636100	-4.99621300	1.74455700
H	-5.98207700	-5.46296700	0.92659400
C	2.93584800	-5.61390100	-1.31406100
H	2.10252600	-6.23053600	-0.94363200
H	3.47927800	-6.18879100	-2.08299300
H	3.61979300	-5.44051100	-0.46941700
C	3.59435400	-3.47941700	-2.43705000
H	4.32219800	-3.22436800	-1.65292000
H	4.12794300	-4.05409300	-3.21186400
H	3.24883800	-2.53850900	-2.89225500
C	4.38497800	2.14297500	-3.14629000
H	5.04182300	2.70501800	-2.46575400
H	5.02296600	1.64291200	-3.89218100
H	3.74544100	2.86852700	-3.67207300
C	4.46247300	0.11891400	-1.66684200
H	5.12894500	0.62566700	-0.95360900
H	3.90140400	-0.64946900	-1.10833700
H	5.09619300	-0.41165900	-2.39416000
C	2.69716800	0.33897300	-3.41373400
H	2.06454000	-0.43502100	-2.94949400
H	2.04462600	1.00665200	-3.99599300
H	3.35991500	-0.17914600	-4.12266900
C	1.46988500	-4.59751000	-3.04825600
H	0.63383800	-5.24198900	-2.73719300
H	1.04714600	-3.67786800	-3.48384100
H	2.01750500	-5.12661100	-3.84414700
C	4.17973900	-2.51094500	2.64066700
H	4.72325400	-2.21437700	3.55160700
H	4.34039000	-3.58821100	2.48526600
H	4.63142500	-1.97390100	1.79247000
C	2.16956800	-2.90609900	4.03903700
H	2.23955500	-3.99707900	3.91047900
H	2.76047300	-2.62516800	4.92673000
H	1.11722000	-2.66328900	4.24358200
C	2.56089300	-0.66269000	2.98809600
H	2.96182800	-0.11831900	2.11448900
H	1.51219600	-0.36009300	3.12709700
H	3.13179500	-0.32628800	3.86990700
H	-1.33805900	4.55963900	-0.69365700
H	-4.88915500	2.10956000	-0.31612800
H	-5.34603300	-0.72193600	0.08007600
H	-2.71290800	-4.11084700	0.69285500
H	-0.29056500	-3.63688600	-1.55231100
H	3.57752800	-3.21202100	0.36422400
H	-0.02068100	-2.09000800	2.48263300
H	0.54675300	3.80155200	1.26268300
H	4.36704700	2.54307600	-0.25796200
H	0.73563000	1.32556200	-2.21778900
Na	1.27130700	-0.78108400	-0.21053100
C	-6.25017800	-3.33834800	-0.73066200
H	-7.15082000	-3.96542100	-0.63225600
H	-6.58082300	-2.31263500	-0.95205600
H	-5.67393100	-3.69975500	-1.59619800

5.4.13 [(^{dtbp}Cbz)]K – 1st excited state

0 1

C	2.07640600	-0.45021500	-0.02697600
N	0.92409400	0.27403300	-0.01542400
C	4.49794400	-0.20512600	0.00171800
C	3.24412600	0.37115600	-0.00897800
C	2.72203400	1.73543400	-0.00301500
C	3.28669900	2.99390900	-0.02464600
C	2.44818500	4.13475800	-0.04411500
C	1.05180800	3.95379500	-0.02871500
C	0.43776600	2.70000600	0.00638500
C	1.29982400	1.58000300	0.00427700
C	0.94045900	-2.66292600	-0.10094600
C	0.27844800	-2.83819400	-1.32616600
C	-0.94437400	-3.50836200	-1.39489200
C	-1.49078600	-4.00325300	-0.19581100
C	-0.85776600	-3.85081900	1.04034200
C	0.37301700	-3.17243200	1.06493400
C	-1.46318500	-4.36460300	2.35085100
C	-1.70638200	-3.70726800	-2.70995500
C	6.03246700	-2.22814900	0.01699700
C	3.09154500	5.52207800	-0.07620100
C	-1.04171500	2.52580100	0.06098100
C	-1.66699500	2.30122600	1.34324500
C	-3.07933700	2.08898200	1.38104700
C	-3.78180200	1.96110400	0.19501900
C	-3.14956700	2.04950900	-1.11114400
C	-1.77619600	2.43136400	-1.10538100
C	-3.76476600	1.98008700	2.74914700
C	-4.01979600	2.09867100	-2.36086300
C	4.63005300	-1.61610200	-0.00238600
C	3.46793000	-2.40502500	-0.02779500
C	2.18369200	-1.84985600	-0.04774600
C	6.80667000	-1.75667000	-1.22493500
H	6.90685900	-0.66164600	-1.25705000
H	7.82195900	-2.18446500	-1.22752200
H	6.29834900	-2.07415300	-2.14835300
C	6.76676900	-1.76666600	1.28664700
H	7.78144600	-2.19475700	1.31813900
H	6.86583000	-0.67196000	1.33066300
H	6.22935700	-2.09128800	2.19091900
C	6.00112500	-3.75788100	0.01054200
H	5.47946700	-4.16050300	0.89223400
H	5.51031900	-4.15377400	-0.89163900
H	7.02941100	-4.14995100	0.02675100
C	-2.77140100	-5.12553800	2.12584900
H	-2.62726500	-6.00407700	1.47828600
H	-3.16315400	-5.48413700	3.08971000
H	-3.54721500	-4.48778800	1.67450900
C	-1.75096600	-3.16717300	3.27068300
H	-0.84435900	-2.58134200	3.48347500
H	-2.49144400	-2.48857300	2.81782500
H	-2.16219500	-3.50875600	4.23377400
C	-0.46517600	-5.31130100	3.03526900
H	-0.88606500	-5.69332900	3.97878200
H	-0.23498000	-6.17253800	2.38930700
H	0.48278300	-4.80757900	3.27463800
C	3.97455700	5.69694900	1.17057800
H	4.77774100	4.94648900	1.21687800
H	4.44775600	6.69192400	1.16542100
H	3.37657400	5.60654300	2.09034700
C	2.05453800	6.64695000	-0.09218100
H	1.40347900	6.59090500	-0.97750800
H	1.41687400	6.62879200	0.80437000
H	2.56606300	7.62132100	-0.11679100
C	-4.83792700	3.40471900	-2.37621900
H	-4.16500200	4.27617300	-2.38600200
H	-5.49886800	3.46660400	-3.25824200
H	-5.46491200	3.48332900	-1.47433100
C	-4.99514600	0.91033600	-2.39137900
H	-5.64173900	0.88471100	-1.50154300
H	-5.65300400	0.95852800	-3.27529200
H	-4.44357100	-0.04366100	-2.43183200
C	-1.88807900	-5.21203700	-2.96325200
H	-2.46215200	-5.69782300	-2.16012900
H	-2.42919600	-5.37890700	-3.90809900
H	-0.91294700	-5.71811800	-3.03288300
C	-3.08353200	-3.03282200	-2.60797100
H	-3.68039200	-3.42921600	-1.77271300
H	-2.98348000	-1.94372900	-2.47196700

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H                -3.66102500   -3.19210200   -3.53211700
C                -0.96516800   -3.10029800   -3.90303200
H                -0.82717200   -2.01360400   -3.79144600
H                 0.02419600   -3.56037200   -4.04730600
H                -1.54525500   -3.26512200   -4.82359600
C                -3.18214500    2.03963400   -3.64116400
H                -2.53267900    2.92132200   -3.74870700
H                -2.54006100    1.14312000   -3.65515100
H                -3.83605500    2.00441600   -4.52724800
C                -5.27489000    1.76071600    2.64145200
H                -5.71882200    1.69354200    3.64722900
H                -5.76535500    2.59068400    2.11093400
H                -5.51406100    0.82803400    2.10674500
C                -3.52844100    3.27692000    3.53880900
H                -3.94596600    4.13782800    2.99434300
H                -4.01219700    3.22591100    4.52837300
H                -2.45704500    3.46978300    3.69156500
C                -3.16869900    0.79683400    3.52838800
H                -3.38477300   -0.15510200    3.01277700
H                -2.07738700    0.88570900    3.63323900
H                -3.60558300    0.72712700    4.53826500
H                 3.54774600   -3.49192200   -0.04078800
H                 5.38946200    0.42662700    0.01709100
H                 4.37331600    3.10891000   -0.03397000
H                 0.39293000    4.82121600   -0.03318100
H                -1.25253500    2.58707600   -2.05165900
H                -4.85873400    1.79613900    0.23324300
H                -1.09356200    2.46100200    2.25565900
H                 0.89635200   -3.01056800    2.01014900
H                -2.44607400   -4.52685800   -0.24007000
H                 0.73887500   -2.41913300   -2.22106100
K                -1.80051700   -0.34835600    0.09443900
C                 3.95716700    5.64553600   -1.34131600
H                 4.43047300    6.63959600   -1.38321700
H                 4.75943800    4.89317400   -1.36820000
H                 3.34644800    5.51826500   -2.24828600
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5.4.14 [(^{dtbp}Cbz)]Rb – 1st excited state

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0 1
C                -1.96765100    0.95633500   -0.06320800
N                -0.61201400    0.82446300   -0.05846000
C                -3.72843300    2.64416300   -0.06731700
C                -2.38717300    2.32210200   -0.07662000
C                -1.14122400    3.08133200   -0.07803600
C                -0.82947900    4.42492500   -0.05229900
C                 0.52728400    4.82400200   -0.01298900
C                 1.52474100    3.83130100   -0.00541700
C                 1.25437000    2.46047400   -0.03780200
C                -0.10975600    2.09016800   -0.07108500
C                -2.47517300   -1.49636600   -0.01713300
C                -2.33375100   -2.17068800    1.20485500
C                -1.85819500   -3.48308400    1.25191600
C                -1.54227900   -4.11234200    0.03386700
C                -1.68206400   -3.47576400   -1.20211800
C                -2.14864000   -2.15048100   -1.20405400
C                -1.33937300   -4.15852600   -2.53099200
C                -1.66230000   -4.24590300    2.56695400
C                -6.18456400    1.99901100   -0.03408900
C                 0.85848900    6.31683400    0.01982900
C                 2.34479300    1.44473000   -0.03066500
C                 2.73037200    0.81449700   -1.26932100
C                 3.80928500   -0.12397800   -1.24272000
C                 4.32589300   -0.53176100   -0.02604800
C                 3.84241800   -0.02664200    1.24693500
C                 2.91154600    1.04908200    1.16657000
C                 4.34751400   -0.65569100   -2.57694600
C                 4.58180300   -0.39917800    2.52562500
C                -4.70311000    1.61676100   -0.04233400
C                -4.27229900    0.28046300   -0.02603900
C                -2.91887600   -0.07758400   -0.03884600
C                -6.47872400    2.85361900    1.20976100
H                -5.88278400    3.77811400    1.22508800
H                -7.54180400    3.14199200    1.23247900
H                -6.25503600    2.29509100    2.13168000
C                -6.50334900    2.80874500   -1.30163400
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H	-7.56654000	3.09740800	-1.31349200
H	-5.90704900	3.73120800	-1.36190400
H	-6.29836800	2.21720700	-2.20714900
C	-7.10237500	0.77512500	-0.00304100
H	-6.95884800	0.13300500	-0.88545000
H	-6.94039400	0.16441700	0.89830700
H	-8.15390900	1.10016200	0.00211000
C	-0.89778400	-5.61096800	-2.33962900
H	-1.68475500	-6.21932600	-1.86793300
H	-0.67075700	-6.06208700	-3.31738200
H	0.01256700	-5.68792700	-1.72470200
C	-0.19603800	-3.39174400	-3.21340000
H	-0.44576300	-2.33353000	-3.38175700
H	0.72286200	-3.42935800	-2.60722700
H	0.04014500	-3.83835500	-4.19222400
C	-2.57937800	-4.14666400	-3.43865700
H	-2.35624900	-4.64121200	-4.39730300
H	-3.41765800	-4.68009900	-2.96458100
H	-2.91537700	-3.12365300	-3.66269500
C	0.28376100	6.98715000	-1.23912500
H	-0.80900800	6.87682600	-1.30340500
H	0.51061900	8.06532900	-1.23395700
H	0.71995100	6.54940700	-2.15010200
C	2.36512400	6.58021000	0.05955500
H	2.83339200	6.14413500	0.95474400
H	2.87508000	6.17378200	-0.82672900
H	2.55069800	7.66499900	0.08209300
C	6.01858300	0.15739000	2.48329200
H	5.99921700	1.25510900	2.39952900
H	6.58996800	-0.11132100	3.38863300
H	6.56565500	-0.22949000	1.60955000
C	4.65375600	-1.92833900	2.68162600
H	5.13226600	-2.40589300	1.81301700
H	5.23306900	-2.21260900	3.57646900
H	3.64113200	-2.35490000	2.78514500
C	-2.51172600	-5.52635100	2.54224900
H	-2.22500200	-6.19548300	1.71737400
H	-2.38908700	-6.08603700	3.48307800
H	-3.57933500	-5.28550000	2.42380800
C	-0.17853400	-4.61776200	2.72086500
H	0.18129600	-5.23549700	1.88405200
H	0.45206900	-3.71531900	2.77696700
H	-0.01810300	-5.18961600	3.64854300
C	-2.07730300	-3.41556700	3.78327600
H	-1.48217100	-2.49383800	3.87515400
H	-3.14084700	-3.13526200	3.74269500
H	-1.92306400	-4.00012500	4.70291200
C	3.89048600	0.16057800	3.77134800
H	3.89541900	1.26091100	3.78331200
H	2.84112700	-0.17319400	3.83037500
H	4.40692500	-0.18056000	4.68283400
C	5.49343600	-1.65385500	-2.40118500
H	5.84507000	-2.00126200	-3.38550000
H	6.34838200	-1.19802400	-1.87956100
H	5.17891500	-2.53939500	-1.82649400
C	4.86989300	0.52286200	-3.41372100
H	5.67930700	1.04279900	-2.87845200
H	5.26474800	0.17145300	-4.38148400
H	4.07872600	1.25945400	-3.61403400
C	3.21992700	-1.36114100	-3.34642700
H	2.87325500	-2.25208900	-2.79533900
H	2.35444000	-0.70010400	-3.50085200
H	3.56999700	-1.70326200	-4.33444700
H	-5.00446200	-0.52674000	-0.00627700
H	-4.03780700	3.69221200	-0.07590000
H	-1.62551400	5.17359700	-0.05292200
H	2.57501300	4.11896300	0.02275800
H	2.57758300	1.54969200	2.07881600
H	5.14498000	-1.25180400	-0.01315400
H	2.34455000	1.20449000	-2.21081300
H	-2.25792200	-1.60354300	-2.14337100
H	-1.17852800	-5.13980000	0.06139900
H	-2.59179300	-1.63452800	2.11862800
Rb	1.26188800	-1.47347400	0.17202100
C	0.22500800	6.94546700	1.27217200
H	0.45187700	8.02285700	1.31388000
H	-0.86958200	6.83489900	1.28128500
H	0.61787000	6.47688200	2.18754100

5.4.15 [(^{dtbp}Cbz)]Cs – 1st excited state

```
0 1
 C                 -1.01016600    1.84371100    0.31435300
 N                  0.06110900    0.95303900    0.30317000
 C                 -1.47731900    4.25985800    0.28923000
 C                 -0.57451700    3.21186900    0.33990500
 C                  0.88435300    3.14982500    0.36271400
 C                  1.87280800    4.11824700    0.34651900
 C                  3.23611100    3.72432200    0.30774000
 C                  3.53566400    2.34871400    0.28540800
 C                  2.55387900    1.33778700    0.30588100
 C                  1.20341600    1.74942400    0.34529000
 C                 -2.93911600    0.16719000    0.21656900
 C                 -2.71756400   -0.71420600    1.29292500
 C                 -3.33957100   -1.97046200    1.32706200
 C                 -4.14482100   -2.34498000    0.22941300
 C                 -4.37105400   -1.49916100   -0.86474900
 C                 -3.76732500   -0.22560400   -0.84245100
 C                 -5.26147600   -1.89518200   -2.05179100
 C                 -3.21757700   -2.92708500    2.52309900
 C                 -3.86143900    5.14661700    0.14198800
 C                  4.32697900    4.80074300    0.28991200
 C                  2.98427300   -0.08321300    0.28071300
 C                  3.91901700   -0.50159500   -0.68078000
 C                  4.40444400   -1.81965400   -0.70226400
 C                  3.95069300   -2.70265600    0.29360600
 C                  3.02405300   -2.31498400    1.27800900
 C                  2.52970300   -0.99795700    1.24380600
 C                  5.39539000   -2.24431700   -1.79595600
 C                  2.53909900   -3.27998900    2.37076700
 C                 -2.86671200    3.98215300    0.20447100
 C                 -3.28063000    2.63586700    0.17845000
 C                 -2.38801200    1.54763800    0.23787300
 C                 -3.71144200    6.01276300    1.41546600
 H                 -2.69899400    6.42026100    1.51437200
 H                 -4.41130600    6.85695000    1.37963700
 H                 -3.92727300    5.42305700    2.31428500
 C                 -3.55459000    6.01054200   -1.10478600
 H                 -4.25522500    6.85310200   -1.15860900
 H                 -2.53875600    6.42053200   -1.07747400
 H                 -3.65516500    5.41883500   -2.02238600
 C                 -5.32268700    4.67300000    0.05089200
 H                 -5.50034100    4.07517900   -0.85131000
 H                 -5.61228500    4.07783800    0.92530500
 H                 -5.98608100    5.54471600    0.00760300
 C                 -5.81201300   -3.32620400   -1.91908900
 H                 -6.44358100   -3.43965600   -1.02883300
 H                 -6.42782700   -3.56270800   -2.79491800
 H                 -5.00315700   -4.06585000   -1.87318400
 C                 -4.44746400   -1.81320800   -3.36344400
 H                 -4.04240400   -0.80876200   -3.53417600
 H                 -3.60469900   -2.51650600   -3.34800100
 H                 -5.08450600   -2.06716700   -4.22035800
 C                 -6.45862500   -0.91797600   -2.12868700
 H                 -7.10870100   -1.18354100   -2.97195500
 H                 -7.05304600   -0.95783400   -1.20762900
 H                 -6.12677600    0.11667400   -2.27361900
 C                  4.13787900    5.69517000   -0.95880400
 H                  3.16019200    6.19002700   -0.96247400
 H                  4.90885100    6.47541500   -0.98115600
 H                  4.21965000    5.10266800   -1.87775900
 C                  5.74554600    4.20616300    0.24482100
 H                  5.95339900    3.58335500    1.12322500
 H                  5.90399800    3.60123300   -0.65627600
 H                  6.48089800    5.01915000    0.23239600
 C                  4.20595800    5.66858200    1.56533300
 H                  4.97511600    6.45095900    1.56112900
 H                  3.22846600    6.15929200    1.63319700
 H                  4.34001600    5.05720800    2.46558100
 C                  2.76046000   -2.64174300    3.76165700
 H                  2.19832500   -1.70853800    3.87742700
 H                  2.42926400   -3.33147000    4.54840000
 H                  3.82219400   -2.41891200    3.92193200
 C                  3.27847600   -4.62947900    2.33969000
 H                  4.35847400   -4.50220300    2.48473500
 H                  2.90431000   -5.26868900    3.14848600
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H	3.11299700	-5.16284000	1.39581100
C	-4.62841000	-3.18140500	3.10687500
H	-5.29647000	-3.63950900	2.36903900
H	-4.56272000	-3.85924100	3.96761000
H	-5.08610200	-2.24218200	3.44043400
C	-2.61256000	-4.27114600	2.05787800
H	-3.23387300	-4.75282800	1.29467800
H	-1.61477100	-4.12699700	1.63065400
H	-2.52678000	-4.96213900	2.90654100
C	-2.34065300	-2.34934800	3.64795800
H	-1.31880700	-2.14856500	3.30902700
H	-2.76175400	-1.41854400	4.04740600
H	-2.28047100	-3.07002300	4.47243800
C	1.03330400	-3.54944600	2.16545100
H	0.46279400	-2.61428600	2.13010600
H	0.86281600	-4.08989900	1.22517100
H	0.63340400	-4.16052000	2.98475700
C	5.80974500	-3.72122100	-1.67109000
H	6.51113000	-3.97230600	-2.47566600
H	6.31171600	-3.92497000	-0.71678700
H	4.94611600	-4.39117200	-1.76343200
C	6.66893100	-1.37205000	-1.69682800
H	7.15383700	-1.50071600	-0.72134400
H	7.38377000	-1.65805400	-2.47880900
H	6.44121000	-0.30738400	-1.82420800
C	4.74099600	-2.04346900	-3.18287000
H	3.83287400	-2.65250000	-3.27951900
H	4.46172200	-0.99742700	-3.35506200
H	5.43835900	-2.34029100	-3.97673300
H	-4.33778700	2.40249100	0.12664700
H	-1.12490400	5.28748000	0.30072500
H	1.60784700	5.17183700	0.35228200
H	4.57125600	2.02955400	0.27100800
H	1.80093700	-0.66004100	1.97422000
H	4.32588800	-3.71713200	0.30095900
H	4.24905700	0.21402500	-1.42913900
H	-3.92966600	0.47079700	-1.66100700
H	-4.61211500	-3.32307100	0.24073700
H	-2.08083900	-0.38503500	2.10616500
Cs	-0.05425600	-2.01634700	-1.67224200

5.4.16 [(^{dtbp}Cbz)]Li – 2nd excited state

0 1

C	1.31281700	1.37200700	-0.42073100
N	0.92082700	0.09240000	-0.18562600
C	3.30851000	2.76461200	-0.51766800
C	2.73518200	1.52049300	-0.36221400
C	3.23154600	0.18229700	-0.04512400
C	4.46379900	-0.39095000	0.20354400
C	4.54254000	-1.75796700	0.56797500
C	3.35563300	-2.51324000	0.68086000
C	2.09696700	-1.97498600	0.42584600
C	2.05729600	-0.61587800	0.05471500
C	-0.99180600	2.32772300	-0.51729400
C	-1.70446000	3.00182000	0.48421800
C	-3.07021600	2.78568200	0.66411500
C	-3.71565500	1.89948800	-0.21251000
C	-3.04695600	1.23087400	-1.23900800
C	-1.66706600	1.45027900	-1.36866100
C	-3.76558300	0.29876300	-2.21948800
C	-3.86970200	3.43946600	1.79479300
C	3.15180400	5.27131600	-0.89481100
C	5.92094200	-2.36731600	0.83248900
C	0.78489800	-2.68217100	0.49904200
C	0.29202300	-3.32163100	-0.69228100
C	-1.03784300	-3.86239900	-0.68292600
C	-1.89080900	-3.51087900	0.34234800
C	-1.48854100	-2.61191600	1.41705500
C	-0.08536800	-2.38441700	1.53800300
C	-1.44392600	-4.83296100	-1.79552800
C	-2.49128600	-2.25839000	2.50957500
C	2.48747600	3.90512300	-0.71738900
C	1.09529400	3.74027500	-0.73393500
C	0.47623000	2.48969900	-0.59589900
C	3.98410300	5.59494000	0.35706500

H	4.77352300	4.84925400	0.53294400
H	4.47244900	6.57624500	0.24657900
H	3.34729600	5.62790800	1.25440500
C	4.07085800	5.22682400	-2.12682400
H	4.56352600	6.20167500	-2.27054900
H	4.85986100	4.46683600	-2.02552200
H	3.49657100	4.99533000	-3.03698100
C	2.13148400	6.39340400	-1.09641400
H	1.51609600	6.23071500	-1.99432700
H	1.45922100	6.49630000	-0.23091700
H	2.65585300	7.35265600	-1.22328200
C	-5.23228300	0.08222500	-1.84069500
H	-5.80676000	1.02085900	-1.86355200
H	-5.70220600	-0.60772300	-2.55794600
H	-5.33109600	-0.36190000	-0.83810100
C	-3.07412900	-1.07053300	-2.23670500
H	-2.02605100	-1.00539700	-2.56901600
H	-3.09617300	-1.54985400	-1.24493400
H	-3.58376700	-1.75019900	-2.93759200
C	-3.70561300	0.92241800	-3.62264500
H	-4.21183200	0.27276100	-4.35459700
H	-4.19944700	1.90628700	-3.63692600
H	-2.66732100	1.06303600	-3.95915600
C	6.77778600	-2.24329600	-0.43855800
H	6.91751700	-1.19514800	-0.74212300
H	7.77606900	-2.67710600	-0.26820900
H	6.31102800	-2.77760600	-1.28021400
C	5.84250600	-3.84656400	1.21582300
H	5.26262500	-4.00084800	2.13827400
H	5.38803300	-4.45302600	0.41794800
H	6.85637400	-4.23681300	1.39253000
C	-2.86201600	-3.51678200	3.31511600
H	-1.96764900	-3.94270700	3.79588200
H	-3.60290600	-3.29155800	4.10089400
H	-3.28806900	-4.29443700	2.66229400
C	-3.76545500	-1.67213500	1.87828800
H	-4.22773100	-2.36952500	1.16306700
H	-4.51904200	-1.44210700	2.64997700
H	-3.53569600	-0.73932300	1.33738800
C	-5.04756000	4.22804100	1.20263200
H	-5.72974100	3.58204500	0.63035500
H	-5.63444300	4.70041100	2.00648100
H	-4.69049200	5.02130900	0.52766700
C	-4.39965000	2.33620200	2.72515500
H	-5.06102000	1.63534900	2.19425700
H	-3.57145400	1.74971500	3.15198000
H	-4.97424500	2.77680300	3.55569700
C	-3.01498900	4.40086700	2.62305900
H	-2.17526000	3.88412500	3.11233100
H	-2.60689600	5.21812600	2.00833500
H	-3.62872700	4.85580400	3.41546500
C	-1.93114100	-1.20988300	3.47472100
H	-1.07081400	-1.59153200	4.04523000
H	-1.60818700	-0.30419900	2.93528300
H	-2.70161500	-0.91382300	4.20445900
C	-2.93365400	-5.17995200	-1.75612200
H	-3.18294000	-5.86218200	-2.58378900
H	-3.20967100	-5.68323500	-0.81734300
H	-3.56050500	-4.28038400	-1.85862400
C	-0.63723600	-6.12992600	-1.61562400
H	-0.85598900	-6.58867900	-0.63911700
H	-0.88728800	-6.85792100	-2.40501300
H	0.44447600	-5.93419600	-1.65765800
C	-1.13073600	-4.23595400	-3.17570300
H	-1.69731000	-3.30778800	-3.34231500
H	-0.06319900	-4.00214600	-3.29287100
H	-1.40519900	-4.94837900	-3.97048700
H	0.44641400	4.60621300	-0.86494200
H	4.39446700	2.87491200	-0.47060600
H	5.37455900	0.20781800	0.12841100
H	3.40367800	-3.56146700	0.97333600
H	0.30307800	-1.82230900	2.38942400
H	-2.91088800	-3.89525000	0.34804300
H	0.99249700	-3.56950100	-1.48837300
H	-1.09924900	0.95649900	-2.16143300
H	-4.78254300	1.72428500	-0.07682500
H	-1.15113000	3.66634700	1.14830100
Li	-0.67769400	-1.17143700	-0.18565000

C	6.59647100	-1.60588000	1.98540000
H	7.59118600	-2.03244200	2.19120800
H	6.73366800	-0.53942300	1.75279800
H	5.99685100	-1.67496500	2.90595300

5.4.17 [(^{dtbp}Cbz)]Na – 2nd excited state

0 1

C	-1.60994300	1.18173800	-0.32731000
N	-0.94913000	0.00897600	-0.15088400
C	-3.85043800	2.12805300	-0.36149300
C	-3.02904000	1.02518500	-0.25408900
C	-3.22314100	-0.40390700	-0.01000000
C	-4.31334000	-1.23709700	0.15195300
C	-4.10699000	-2.61748600	0.39073600
C	-2.78943300	-3.11030100	0.47673900
C	-1.65833000	-2.30535800	0.31717100
C	-1.90499700	-0.94077100	0.05597700
C	0.44863100	2.57447800	-0.48468200
C	1.22678100	1.87271200	-1.42349300
C	2.62117700	1.89186800	-1.36134500
C	3.22125100	2.62861600	-0.32370600
C	2.48244100	3.34557000	0.61661100
C	1.08283600	3.31379000	0.50963400
C	3.13370400	4.12172700	1.76461500
C	3.51015300	1.15675700	-2.37164900
C	-4.22373600	4.62366400	-0.64500600
C	-5.32837300	-3.52487000	0.55487200
C	-0.25273300	-2.78335500	0.41417900
C	0.53250300	-2.43264200	1.58942100
C	1.93071900	-2.57324000	1.55977600
C	2.56148100	-3.02930800	0.39383700
C	1.79095700	-3.45700200	-0.77569800
C	0.39896500	-3.30821300	-0.70557400
C	2.74523100	-2.14659800	2.79368600
C	2.49813500	-4.22106100	-1.88913800
C	-3.28731200	3.41939500	-0.52927400
C	-1.89036900	3.55014200	-0.57969600
C	-1.02717600	2.45089500	-0.49231300
C	-5.13840900	4.43417500	-1.86639900
H	-5.75110000	3.52412100	-1.78518100
H	-5.82449100	5.29039800	-1.96588400
H	-4.54709000	4.35917500	-2.79189100
C	-5.07942600	4.72249500	0.62877800
H	-5.76235900	5.58445000	0.56321500
H	-5.69339200	3.82324500	0.78502900
H	-4.44515700	4.85447700	1.51880800
C	-3.46271900	5.94018500	-0.81463400
H	-2.80659300	6.14779300	0.04449000
H	-2.84794600	5.94345200	-1.72760600
H	-4.17713700	6.77359600	-0.89373500
C	4.66147800	4.06387300	1.70802800
H	5.05409600	4.49758700	0.77530400
H	5.08582000	4.63896300	2.54493000
H	5.03587900	3.03227000	1.79510300
C	2.67499400	3.51128000	3.09898600
H	1.58294800	3.56462100	3.22056300
H	2.96693200	2.45203200	3.16848600
H	3.13266500	4.04980800	3.94412900
C	2.70071500	5.59388200	1.69191600
H	3.15508200	6.16723100	2.51553600
H	3.01691700	6.05086900	0.74140200
H	1.60927800	5.70602200	1.77230600
C	-6.16711300	-3.03221200	1.74587500
H	-6.52241300	-2.00087200	1.60276700
H	-7.05255300	-3.67414400	1.87970800
H	-5.58017600	-3.05937700	2.67674600
C	-4.94290800	-4.98338100	0.81027700
H	-4.35802400	-5.40375000	-0.02163600
H	-4.35579900	-5.09603400	1.73408200
H	-5.85297700	-5.59311300	0.91836100
C	2.97724700	-5.57801100	-1.33903200
H	2.11921600	-6.17776800	-0.99822200
H	3.52253000	-6.15474900	-2.10564300
H	3.64624400	-5.43910700	-0.47590300
C	3.71874300	-3.44129900	-2.40290300
H	4.43429500	-3.21889500	-1.59742100

H	4.25685100	-4.01737500	-3.17361100
H	3.40913400	-2.48413600	-2.84966000
C	4.34538900	2.19394200	-3.13957200
H	4.98878900	2.77846200	-2.46511400
H	4.99585400	1.69383900	-3.87454800
H	3.69550100	2.89944600	-3.67970400
C	4.45204400	0.19506800	-1.62892300
H	5.10232000	0.72362600	-0.91663600
H	3.90252800	-0.57785800	-1.06568300
H	5.10180300	-0.33245000	-2.34412800
C	2.69206100	0.35474700	-3.38669600
H	2.07722400	-0.42859400	-2.91385200
H	2.02593300	0.99969800	-3.97906900
H	3.36823700	-0.15722700	-4.08736400
C	1.57852200	-4.48435000	-3.08333400
H	0.72108700	-5.11633000	-2.80677100
H	1.18681400	-3.54376400	-3.50371000
H	2.13000500	-5.00657200	-3.88115100
C	4.24306200	-2.41735500	2.63467200
H	4.77863900	-2.11155400	3.54717600
H	4.44369500	-3.48597200	2.46650300
H	4.67125900	-1.85413900	1.79097000
C	2.25035200	-2.91606800	4.02644200
H	2.36283200	-4.00044300	3.87394300
H	2.82960000	-2.63188100	4.92059500
H	1.18886300	-2.71864100	4.23242900
C	2.55980300	-0.63728700	3.02376900
H	2.94605600	-0.05980000	2.16480700
H	1.50120700	-0.37259300	3.16261000
H	3.11475000	-0.30239900	3.91602300
H	-1.43946700	4.53496200	-0.70172000
H	-4.93505000	2.00929300	-0.30417300
H	-5.32765100	-0.83515200	0.09308400
H	-2.61629200	-4.16676500	0.67904600
H	-0.21543000	-3.57346100	-1.56998300
H	3.64256000	-3.14963800	0.37752300
H	0.02091700	-2.08324600	2.48622700
H	0.46220200	3.83738100	1.24051300
H	4.30902900	2.63781900	-0.26005600
H	0.70607500	1.32406300	-2.21000600
Na	1.28680000	-0.74844700	-0.19772200
C	-6.17376700	-3.46734900	-0.72850300
H	-7.05950900	-4.11538800	-0.63085100
H	-6.52841200	-2.44843800	-0.94407000
H	-5.59164300	-3.81132000	-1.59720100

5.4.18 [(^{dtbp}Cbz)]K – 2nd excited state

0 1

C	2.04898100	-0.54358800	-0.08544200
N	0.93352800	0.23440100	-0.04550800
C	4.47867400	-0.41729900	-0.06691400
C	3.25462700	0.22020000	-0.06445500
C	2.79852400	1.60766700	-0.02811400
C	3.42076700	2.83905900	-0.02392300
C	2.63717100	4.01790900	-0.00330000
C	1.23299900	3.90363700	0.02361600
C	0.56352500	2.68004900	0.03428400
C	1.37002500	1.51941500	-0.00701800
C	0.80338200	-2.69481600	-0.16977500
C	0.04873700	-2.70155900	-1.35416200
C	-1.21018100	-3.30309300	-1.40444000
C	-1.70009200	-3.89961800	-0.22732300
C	-0.97816000	-3.91050700	0.96858300
C	0.28966600	-3.30355600	0.97308100
C	-1.52847700	-4.51864000	2.26271700
C	-2.06587800	-3.32742900	-2.67635400
C	5.91323500	-2.51172200	-0.07752100
C	3.34530500	5.37382800	-0.00517900
C	-0.92391700	2.56764900	0.10064000
C	-1.54274100	2.40079300	1.38220100
C	-2.97172700	2.22786400	1.42990300
C	-3.67470500	2.10186800	0.24509600
C	-3.05370100	2.12205300	-1.05600600
C	-1.65622400	2.47013300	-1.06365900
C	-3.64982000	2.14527200	2.80070900
C	-3.88482000	2.22588500	-2.33056200

C	4.54182400	-1.83300200	-0.08371300
C	3.34258700	-2.56440300	-0.10920200
C	2.08669200	-1.94715700	-0.12158900
C	6.70117600	-2.07003300	-1.32176600
H	6.85351800	-0.98086600	-1.34780000
H	7.69473200	-2.54598900	-1.33398400
H	6.17211100	-2.35666400	-2.24361200
C	6.67746200	-2.09484900	1.18991500
H	7.67038100	-2.57178100	1.21165600
H	6.83001100	-1.00659400	1.24035200
H	6.13098600	-2.39899000	2.09588200
C	5.80853100	-4.03820000	-0.09321000
H	5.27336200	-4.42108800	0.78921400
H	5.29420400	-4.40458700	-0.99476600
H	6.81697200	-4.47906800	-0.08561700
C	-2.89316500	-5.17957600	2.05813500
H	-2.84576900	-5.99601000	1.32116000
H	-3.24355900	-5.61009300	3.00837200
H	-3.65520300	-4.45798100	1.72523700
C	-1.68194200	-3.40231100	3.30897200
H	-0.72537700	-2.90191500	3.52107400
H	-2.39496100	-2.63427600	2.96774600
H	-2.06300900	-3.81188400	4.25789500
C	-0.54955200	-5.58195000	2.78361500
H	-0.93070200	-6.02903600	3.71535300
H	-0.41733600	-6.38842700	2.04596600
H	0.44215900	-5.15845900	3.00023300
C	4.24557700	5.47381600	1.23746600
H	5.01195400	4.68475400	1.25711700
H	4.76599000	6.44478900	1.25335100
H	3.65129300	5.38832300	2.16010500
C	2.36244700	6.54620500	0.01811700
H	1.70205400	6.54430600	-0.86205200
H	1.73239800	6.53421900	0.92013500
H	2.91918500	7.49575700	0.01407900
C	-4.19031200	3.70631400	-2.63077900
H	-3.25450000	4.27373200	-2.75407400
H	-4.79183500	3.82959000	-3.54853900
H	-4.74270400	4.15980000	-1.79277400
C	-5.21394600	1.47209700	-2.19949900
H	-5.87080800	1.91687100	-1.43720700
H	-5.76532200	1.49243000	-3.15345200
H	-5.04444800	0.41750600	-1.92474600
C	-2.28500000	-4.78889500	-3.09813400
H	-2.80716200	-5.36550600	-2.31979500
H	-2.89316600	-4.83644700	-4.01536500
H	-1.32390500	-5.28719500	-3.29775300
C	-3.42543500	-2.66524200	-2.39999100
H	-3.97246200	-3.15905300	-1.58291100
H	-3.30894900	-1.59984300	-2.14215700
H	-4.06254500	-2.70893300	-3.29708500
C	-1.39911100	-2.57970900	-3.83305100
H	-1.22610400	-1.51934200	-3.59170900
H	-0.43537200	-3.03177200	-4.11236800
H	-2.04949000	-2.61204300	-4.72013500
C	-3.13647000	1.62866300	-3.53104700
H	-2.19412300	2.15669700	-3.73786100
H	-2.89392700	0.56771600	-3.35386500
H	-3.75096300	1.68977900	-4.44440900
C	-5.16697700	1.97691600	2.70323800
H	-5.60783200	1.93259200	3.71168500
H	-5.63149100	2.81938200	2.16880000
H	-5.44220500	1.04905000	2.17736800
C	-3.36471900	3.43321100	3.58972100
H	-3.76303700	4.30697900	3.05140800
H	-3.83598400	3.39584900	4.58595200
H	-2.28607000	3.59392300	3.72906000
C	-3.08792300	0.94355500	3.57960300
H	-3.34419500	-0.00349900	3.07206300
H	-1.99270300	0.99517200	3.67074300
H	-3.51326600	0.89317900	4.59556500
H	3.36939100	-3.65380300	-0.13274300
H	5.39981700	0.17034300	-0.04885500
H	4.51142000	2.90400000	-0.04121200
H	0.61675600	4.80142800	0.04906800
H	-1.12854800	2.58192300	-2.01378700
H	-4.75358100	1.95612100	0.29420500
H	-0.95936200	2.56361200	2.28763900

H	0.88311000	-3.26996000	1.88976200
H	-2.68382200	-4.36864300	-0.25569100
H	0.46799000	-2.20661700	-2.23023100
K	-1.79306000	-0.27929100	0.21359900
C	4.20518900	5.49018000	-1.27485400
H	4.72444500	6.46169500	-1.29502200
H	4.97076200	4.70197500	-1.32934100
H	3.58157500	5.41609100	-2.17893400

5.4.19 [(^{dtbp}Cbz)]Rb – 2nd excited state

0 1

C	-2.14040500	-0.51527500	0.02923100
N	-1.01614900	0.25181600	0.01866500
C	-4.56942100	-0.36147700	-0.00190100
C	-3.33818500	0.26157500	0.00991200
C	-2.86779000	1.64453100	0.00418100
C	-3.47942700	2.88087200	0.02499400
C	-2.68445200	4.05246600	0.04505300
C	-1.28224100	3.92416900	0.03106700
C	-0.62142300	2.69436600	-0.00316800
C	-1.44073200	1.54272000	-0.00167700
C	-0.92208200	-2.68366500	0.10478000
C	-0.25516200	-2.83369100	1.33068800
C	0.99194200	-3.45736200	1.40075800
C	1.55777800	-3.93154700	0.20231900
C	0.92069800	-3.80325000	-1.03448900
C	-0.33471300	-3.17165700	-1.06043500
C	1.54632100	-4.29411300	-2.34429400
C	1.75958800	-3.62723200	2.71661300
C	-6.02672200	-2.44080900	-0.01827300
C	-3.37958800	5.41460200	0.07621700
C	0.86361800	2.57594300	-0.05626900
C	1.49817800	2.37483600	-1.33786900
C	2.91754300	2.21587600	-1.37423500
C	3.62314400	2.11472100	-0.18748900
C	2.98673400	2.17949700	1.11803200
C	1.59997400	2.50940700	1.11083600
C	3.60794200	2.13261600	-2.74163600
C	3.85325500	2.26158100	2.36859800
C	-4.64835000	-1.77642400	0.00236500
C	-3.45739300	-2.52105800	0.02908400
C	-2.19497300	-1.91795800	0.05018500
C	-6.81935000	-1.99858200	1.22279700
H	-6.96070100	-0.90809800	1.25458600
H	-7.81782600	-2.46427600	1.22447200
H	-6.30036000	-2.29655800	2.14678200
C	-6.77660700	-2.00749700	-1.28874200
H	-7.77442600	-2.47346900	-1.32114600
H	-6.91674400	-0.91730100	-1.33308300
H	-6.22646400	-2.31182300	-2.19241700
C	-5.93785200	-3.96827700	-0.01147000
H	-5.40053900	-4.35113600	-0.89256400
H	-5.43339300	-4.34526900	0.89127600
H	-6.95064100	-4.39876200	-0.02861200
C	2.88201800	-5.00524800	-2.11784500
H	2.77039700	-5.88847900	-1.47024200
H	3.28794300	-5.34901700	-3.08124500
H	3.63283800	-4.33868200	-1.66587200
C	1.78975700	-3.08685900	-3.26409000
H	0.86196100	-2.53559200	-3.47789700
H	2.50372700	-2.38080200	-2.81064300
H	2.21450300	-3.41289200	-4.22670400
C	0.58532000	-5.27780900	-3.02949900
H	1.02122200	-5.64389000	-3.97251800
H	0.38705100	-6.14698700	-2.38358600
H	-0.38068300	-4.81015200	-3.26990700
C	-4.26731600	5.55591300	-1.17146800
H	-5.04164800	4.77575500	-1.21840400
H	-4.77762100	6.53237900	-1.16698400
H	-3.66544200	5.48791400	-2.09062800
C	-2.38565500	6.57769800	0.09298600
H	-1.73382800	6.54634100	0.97896600
H	-1.74687000	6.58339400	-0.80293200
H	-2.93350400	7.53213800	0.11689000
C	4.62165000	3.59749000	2.38449000
H	3.91640200	4.44300900	2.39342900

H	5.27891800	3.68435000	3.26715100
H	5.24612800	3.69948200	1.48320400
C	4.87259600	1.11079100	2.40032200
H	5.52057800	1.10936200	1.51112900
H	5.52729700	1.18385200	3.28487300
H	4.35726700	0.13672300	2.44042900
C	1.99752400	-5.12405600	2.97040100
H	2.59026600	-5.58803500	2.16794500
H	2.54359800	-5.27028800	3.91581600
H	1.04205500	-5.66645800	3.03917600
C	3.11048700	-2.90146500	2.61584700
H	3.72266800	-3.27526300	1.78126000
H	2.96966300	-1.81693100	2.47951900
H	3.69264600	-3.03874600	3.54059500
C	0.99487700	-3.04837800	3.90883300
H	0.81620200	-1.96766500	3.79688600
H	0.02338100	-3.54532800	4.05222700
H	1.57984000	-3.19110300	4.83000200
C	3.01714800	2.17128500	3.64808500
H	2.33486100	3.02793000	3.75480500
H	2.40923700	1.25124900	3.66162500
H	3.67104000	2.16084700	4.53482100
C	5.12514200	1.97023900	-2.63240700
H	5.57228600	1.91964500	-3.63773200
H	5.58350500	2.81816400	-2.10157800
H	5.39870600	1.04730700	-2.09727100
C	3.32377300	3.41950400	-3.53179900
H	3.70806900	4.29560500	-2.98710100
H	3.81008800	3.38656500	-4.52087500
H	2.24603200	3.57189200	-3.68565200
C	3.05759100	0.92764000	-3.52121900
H	3.30881800	-0.01540400	-3.00519800
H	1.96381300	0.97537300	-3.62716400
H	3.49779100	0.87424900	-4.53065000
H	-3.49626900	-3.61018600	0.04222300
H	-5.48406200	0.23628100	-0.01828400
H	-4.56961000	2.95490700	0.03322300
H	-0.65647200	4.81576700	0.03600300
H	1.06988500	2.64546600	2.05656500
H	4.70555700	1.99038800	-0.22461700
H	0.92004600	2.51276700	-2.25088100
H	-0.86282900	-3.02976000	-2.00619900
H	2.53204600	-4.41883100	0.24762800
H	-0.73191900	-2.43209900	2.22504200
Rb	1.73005800	-0.26763400	-0.08838300
C	-4.25049800	5.50561800	1.34045300
H	-4.76091200	6.48117200	1.38168100
H	-5.02391900	4.72360600	1.36670200
H	-3.63632400	5.40157000	2.24805100

5.4.20 [(^{dtbp}Cbz)]Cs – 2nd excited state

0 1

C	-1.01016600	1.84371100	0.31435300
N	0.06110900	0.95303900	0.30317000
C	-1.47731900	4.25985800	0.28923000
C	-0.57451700	3.21186900	0.33990500
C	0.88435300	3.14982500	0.36271400
C	1.87280800	4.11824700	0.34651900
C	3.23611100	3.72432200	0.30774000
C	3.53566400	2.34871400	0.28540800
C	2.55387900	1.33778700	0.30588100
C	1.20341600	1.74942400	0.34529000
C	-2.93911600	0.16719000	0.21656900
C	-2.71756400	-0.71420600	1.29292500
C	-3.33957100	-1.97046200	1.32706200
C	-4.14482100	-2.34498000	0.22941300
C	-4.37105400	-1.49916100	-0.86474900
C	-3.76732500	-0.22560400	-0.84245100
C	-5.26147600	-1.89518200	-2.05179100
C	-3.21757700	-2.92708500	2.52309900
C	-3.86143900	5.14661700	0.14198800
C	4.32697900	4.80074300	0.28991200
C	2.98427300	-0.08321300	0.28071300
C	3.91901700	-0.50159500	-0.68078000
C	4.40444400	-1.81965400	-0.70226400

C	3.95069300	-2.70265600	0.29360600
C	3.02405300	-2.31498400	1.27800900
C	2.52970300	-0.99795700	1.24380600
C	5.39539000	-2.24431700	-1.79595600
C	2.53909900	-3.27998900	2.37076700
C	-2.86671200	3.98215300	0.20447100
C	-3.28063000	2.63586700	0.17845000
C	-2.38801200	1.54763800	0.23787300
C	-3.71144200	6.01276300	1.41546600
H	-2.69899400	6.42026100	1.51437200
H	-4.41130600	6.85695000	1.37963700
H	-3.92727300	5.42305700	2.31428500
C	-3.55459000	6.01054200	-1.10478600
H	-4.25522500	6.85310200	-1.15860900
H	-2.53875600	6.42053200	-1.07747400
H	-3.65516500	5.41883500	-2.02238600
C	-5.32268700	4.67300000	0.05089200
H	-5.50034100	4.07517900	-0.85131000
H	-5.61228500	4.07783800	0.92530500
H	-5.98608100	5.54471600	0.00760300
C	-5.81201300	-3.32620400	-1.91908900
H	-6.44358100	-3.43965600	-1.02883300
H	-6.42782700	-3.56270800	-2.79491800
H	-5.00315700	-4.06585000	-1.87318400
C	-4.44746400	-1.81320800	-3.36344400
H	-4.04240400	-0.80876200	-3.53417600
H	-3.60469900	-2.51650600	-3.34800100
H	-5.08450600	-2.06716700	-4.22035800
C	-6.45862500	-0.91797600	-2.12868700
H	-7.10870100	-1.18354100	-2.97195500
H	-7.05304600	-0.95783400	-1.20762900
H	-6.12677600	0.11667400	-2.27361900
C	4.13787900	5.69517000	-0.95880400
H	3.16019200	6.19002700	-0.96247400
H	4.90885100	6.47541500	-0.98115600
H	4.21965000	5.10266800	-1.87775900
C	5.74554600	4.20616300	0.24482100
H	5.95339900	3.58335500	1.12322500
H	5.90399800	3.60123300	-0.65627600
H	6.48089800	5.01915000	0.23239600
C	4.20595800	5.66858200	1.56533300
H	4.97511600	6.45095900	1.56112900
H	3.22846600	6.15929200	1.63319700
H	4.34001600	5.05720800	2.46558100
C	2.76046000	-2.64174300	3.76165700
H	2.19832500	-1.70853800	3.87742700
H	2.42926400	-3.33147000	4.54840000
H	3.82219400	-2.41891200	3.92193200
C	3.27847600	-4.62947900	2.33969000
H	4.35847400	-4.50220300	2.48473500
H	2.90431000	-5.26868900	3.14848600
H	3.11299700	-5.16284000	1.39581100
C	-4.62841000	-3.18140500	3.10687500
H	-5.29647000	-3.63950900	2.36903900
H	-4.56272000	-3.85924100	3.96761000
H	-5.08610200	-2.24218200	3.44043400
C	-2.61256000	-4.27114600	2.05787800
H	-3.23387300	-4.75282800	1.29467800
H	-1.61477100	-4.12699700	1.63065400
H	-2.52678000	-4.96213900	2.90654100
C	-2.34065300	-2.34934800	3.64795800
H	-1.31880700	-2.14856500	3.30902700
H	-2.76175400	-1.41854400	4.04740600
H	-2.28047100	-3.07002300	4.47243800
C	1.03330400	-3.54944600	2.16545100
H	0.46279400	-2.61428600	2.13010600
H	0.86281600	-4.08989900	1.22517100
H	0.63340400	-4.16052000	2.98475700
C	5.80974500	-3.72122100	-1.67109000
H	6.51113000	-3.97230600	-2.47566600
H	6.31171600	-3.92497000	-0.71678700
H	4.94611600	-4.39117200	-1.76343200
C	6.66893100	-1.37205000	-1.69682800
H	7.15383700	-1.50071600	-0.72134400
H	7.38377000	-1.65805400	-2.47880900
H	6.44121000	-0.30738400	-1.82420800
C	4.74099600	-2.04346900	-3.18287000
H	3.83287400	-2.65250000	-3.27951900

H	4.46172200	-0.99742700	-3.35506200
H	5.43835900	-2.34029100	-3.97673300
H	-4.33778700	2.40249100	0.12664700
H	-1.12490400	5.28748000	0.30072500
H	1.60784700	5.17183700	0.35228200
H	4.57125600	2.02955400	0.27100800
H	1.80093700	-0.66004100	1.97422000
H	4.32588800	-3.71713200	0.30095900
H	4.24905700	0.21402500	-1.42913900
H	-3.92966600	0.47079700	-1.66100700
H	-4.61211500	-3.32307100	0.24073700
H	-2.08083900	-0.38503500	2.10616500
Cs	-0.05425600	-2.01634700	-1.67224200

5.4.21 [(^{dtbp}Cbz)Li(Tol)]

0 1

Li	-0.20674300	-0.91694700	0.28279200
N	-0.03745500	0.83543700	-0.39624600
C	-1.05787300	-2.78752700	1.92000000
C	0.31546600	-2.90900600	1.68424200
C	-1.54121200	-1.63736600	2.55017900
C	1.19169300	-1.88864700	2.07202700
C	-0.66438600	-0.62280400	2.93588300
C	-1.13698400	1.66027000	-0.42621600
C	1.04885000	1.67646400	-0.44413700
C	2.43317300	1.37130600	-0.39173700
C	0.65994500	3.04880900	-0.49396900
C	3.33343200	2.43956900	-0.38476800
C	2.97712100	-0.00420000	-0.32646700
C	2.95784400	3.79841700	-0.43862400
C	1.59680400	4.08674400	-0.49520200
C	4.04625900	4.87645500	-0.43925500
C	-0.77449900	3.03765200	-0.48463600
C	-1.73309900	4.05530000	-0.48153200
C	-3.08802300	3.73861800	-0.41401600
C	-3.43656200	2.37326500	-0.34789600
C	-4.19835900	4.79446600	-0.42081200
C	-2.51344600	1.32490200	-0.35291900
C	-3.01103000	-0.06622700	-0.28247500
C	2.58502200	-0.99723500	-1.23562200
C	3.97551900	-0.30596000	0.61293400
C	3.19174700	-2.26106700	-1.23711600
C	4.15177400	-2.52904700	-0.25463700
C	2.84242500	-3.33532900	-2.27568700
C	4.56646600	-1.56842000	0.67722900
C	5.64125000	-1.92823400	1.70896100
C	2.21577500	-2.71908600	-3.53035500
C	1.85837800	-4.32777000	-1.64015000
C	4.10109200	-4.09595000	-2.71886600
C	5.96978300	-0.75374100	2.63297800
C	6.92746000	-2.33953600	0.97573200
C	5.14583800	-3.09836100	2.57304000
C	4.89841400	4.74718200	0.83320100
C	3.45379100	6.28662900	-0.47522100
C	4.94344800	4.70020900	-1.67437100
C	-5.04887600	4.65638300	0.85178000
C	-3.63477600	6.21623500	-0.46510800
C	-5.09118400	4.59255400	-1.65521000
C	-4.05602400	-0.39602600	0.58716100
C	-2.50733400	-1.07078900	-1.13312500
C	-4.62088800	-1.67767300	0.62087800
C	-4.09251300	-2.64334600	-0.23729600
C	-5.80308300	-1.95999300	1.55575300
C	-3.04635400	-2.36059400	-1.13099600
C	-2.58758900	-3.45218700	-2.10349700
C	-6.30067500	-3.40238800	1.44186500
C	-6.96003800	-1.01838700	1.18414200
C	-5.38995600	-1.70866900	3.01362800
C	-1.47134700	-2.95918600	-3.02155600
C	-2.07404900	-4.66537900	-1.31344200
C	-3.77605900	-3.87977100	-2.97927600
C	0.71673300	-0.72719700	2.70675000
C	1.64125900	0.39131100	3.07956900
H	4.39754100	2.18923100	-0.36409300
H	1.23994500	5.11753100	-0.53279800

H	-1.39919100	5.09333800	-0.52913200
H	-4.49576600	2.10337600	-0.32353000
H	1.84067800	-0.72871300	-1.98690600
H	4.61532300	-3.51650500	-0.22708100
H	4.26999400	0.48019600	1.30763900
H	1.99991700	-3.50675000	-4.26873600
H	2.89817000	-1.99184200	-3.99601100
H	1.26944400	-2.20340700	-3.32218000
H	1.56931500	-5.11445000	-2.35605200
H	0.94093300	-3.81760700	-1.31359100
H	2.30471300	-4.81464900	-0.75870400
H	3.84613600	-4.80915900	-3.51833500
H	4.55329400	-4.67671900	-1.90191000
H	4.86477200	-3.40482400	-3.10706600
H	5.91240900	-3.38489900	3.31084100
H	4.91738700	-3.98769700	1.96670600
H	4.23256600	-2.82421100	3.12459600
H	7.71720400	-2.59878600	1.69913100
H	7.29713200	-1.51726500	0.34401000
H	6.76811100	-3.21377600	0.32713000
H	6.74434600	-1.05264100	3.35577800
H	5.09005700	-0.42612900	3.20823000
H	6.35339900	0.11279700	2.07339000
H	5.73704600	5.46553300	-1.69265000
H	4.35441200	4.79290100	-2.59989400
H	5.42959500	3.71310500	-1.68696900
H	5.69014900	5.51429400	0.85214900
H	5.38667300	3.76304800	0.89890900
H	4.27653500	4.87272300	1.73328200
H	4.26236800	7.03429100	-0.46945300
H	2.81321000	6.48110900	0.39878700
H	2.85384100	6.45251400	-1.38311900
H	-4.45842000	6.94727400	-0.46228300
H	-3.03952700	6.38960300	-1.37466800
H	-2.99717300	6.42830600	0.40698200
H	-5.85521800	5.40822300	0.86546200
H	-4.43046200	4.79898500	1.75165800
H	-5.51871900	3.66363500	0.92276800
H	-5.90020900	5.34143000	-1.67863100
H	-5.55721700	3.59568000	-1.66188000
H	-4.50365300	4.69140100	-2.58104100
H	-4.43298000	0.38539700	1.25113500
H	-4.51925000	-3.64633400	-0.23806500
H	-1.73339700	-0.78407100	-1.84802000
H	-6.24995300	-1.85258900	3.68687600
H	-5.01809000	-0.68421800	3.16526000
H	-4.60095200	-2.41005000	3.32779600
H	-7.83277600	-1.20773300	1.82960200
H	-7.26711600	-1.16981400	0.13790400
H	-6.68029300	0.03906700	1.30084800
H	-7.14642100	-3.56023400	2.12846800
H	-5.51745200	-4.12849700	1.70993800
H	-6.65235700	-3.63467800	0.42502500
H	-3.46127300	-4.64912900	-3.70255700
H	-4.17513400	-3.02219200	-3.54216200
H	-4.59763400	-4.29995100	-2.38050200
H	-1.74711000	-5.46328400	-1.99907700
H	-2.85113600	-5.08624000	-0.65784900
H	-1.21449800	-4.39120300	-0.68326100
H	-1.12985600	-3.77349900	-3.67848100
H	-0.59916700	-2.61551800	-2.44833300
H	-1.80298000	-2.12780700	-3.66140600
H	-1.06108300	0.28136300	3.40437700
H	-2.61132400	-1.52222300	2.71978100
H	-1.75115000	-3.56974700	1.60576200
H	0.71545900	-3.79866100	1.19212300
H	2.25842400	-1.98845100	1.85971500
H	2.63993000	0.01582000	3.34067400
H	1.24718100	0.96765200	3.92817600
H	1.76048300	1.08525700	2.23041700

5.4.22 [(^{dtbp}Cbz)Li(Tol)] – 1st excited state

0 1

Li	-0.01828000	-0.78171900	1.10488500
N	-0.00682800	0.87910400	-0.18278200

C	-1.36956200	-2.30197400	2.10181500
C	-0.19469200	-2.94257200	1.75936600
C	-1.35633700	-1.10349600	2.87463300
C	1.08318900	-2.41322800	2.18517500
C	-0.09182100	-0.67722000	3.43665500
C	-1.10248000	1.69793300	-0.26144000
C	1.09205500	1.68941400	-0.31775200
C	2.46523200	1.33922300	-0.34008100
C	0.72298400	3.06432900	-0.40732400
C	3.38188600	2.39570200	-0.41871500
C	2.99255400	-0.04342300	-0.33245800
C	3.02772400	3.75266700	-0.47937500
C	1.65816700	4.07906700	-0.47632200
C	4.12771200	4.81161500	-0.56178900
C	-0.72638200	3.07081900	-0.36507800
C	-1.65451900	4.09402100	-0.36857500
C	-3.02486300	3.78003600	-0.28775500
C	-3.38818900	2.42507800	-0.22348800
C	-4.11711200	4.84975000	-0.28960500
C	-2.47899400	1.36047600	-0.21632200
C	-3.02534900	-0.01500200	-0.22734900
C	2.47143900	-1.02604500	-1.17527900
C	4.11451500	-0.33842700	0.45794200
C	3.07952000	-2.28621500	-1.27565500
C	4.19049100	-2.53900800	-0.47179200
C	2.50247700	-3.35576300	-2.20727400
C	4.72018200	-1.59021100	0.41561600
C	5.91884500	-1.96265000	1.29298300
C	2.09960000	-2.73805000	-3.55350000
C	1.27149500	-3.95824400	-1.51788500
C	3.50607200	-4.47796400	-2.48985600
C	6.37897500	-0.79337000	2.16643800
C	7.09350000	-2.38772100	0.39865700
C	5.51989200	-3.12792900	2.21250400
C	5.04541700	4.68294000	0.66487300
C	3.55867100	6.23182100	-0.59158200
C	4.94620100	4.58932400	-1.84416300
C	-4.96306600	4.70960600	0.98638000
C	-3.53716800	6.26523500	-0.33116600
C	-5.01111000	4.65441700	-1.52526200
C	-4.06292000	-0.34283700	0.64638300
C	-2.61414900	-0.94848200	-1.19021000
C	-4.70431900	-1.58373300	0.58831400
C	-4.29052600	-2.47536200	-0.40288800
C	-5.82340700	-1.90585400	1.58332400
C	-3.25965700	-2.18090800	-1.30733500
C	-2.90443600	-3.20807400	-2.38650100
C	-6.37220500	-3.32146200	1.39412200
C	-6.97410400	-0.90750100	1.38080600
C	-5.28324800	-1.78434800	3.01644400
C	-1.80665600	-2.69900800	-3.32121900
C	-2.42420800	-4.50013200	-1.70753700
C	-4.15021500	-3.50630800	-3.23553500
C	1.08937700	-1.31795900	3.11534500
C	2.39137900	-0.89790400	3.73054600
H	4.43894800	2.12860800	-0.46535800
H	1.32675200	5.11673000	-0.52283400
H	-1.31710700	5.12918700	-0.42633000
H	-4.44834900	2.16588200	-0.21271300
H	1.60217800	-0.77868700	-1.78652700
H	4.66864200	-3.51684800	-0.52765400
H	4.49219500	0.43536700	1.12600100
H	1.69546500	-3.51553900	-4.22060700
H	2.96641600	-2.27573600	-4.05080900
H	1.32243100	-1.96823400	-3.44876900
H	0.77243000	-4.69092000	-2.17208200
H	0.54290900	-3.17962200	-1.25138500
H	1.55621200	-4.46349400	-0.58308500
H	3.07219700	-5.19070600	-3.20788000
H	3.75781100	-5.04877300	-1.58366800
H	4.44043100	-4.08730200	-2.92241500
H	6.36604400	-3.41580000	2.85692200
H	5.22004200	-4.01669900	1.63734500
H	4.67458600	-2.84780000	2.85844800
H	7.96431600	-2.66216400	1.01536100
H	7.39369600	-1.56824300	-0.27281500
H	6.84209300	-3.25786900	-0.22580100
H	7.24166800	-1.10202400	2.77637800

H	5.58881500	-0.46241000	2.85722800
H	6.69345300	0.07074000	1.56062000
H	5.74478700	5.34421100	-1.92163500
H	4.30829500	4.67214500	-2.73754300
H	5.42055400	3.59712500	-1.86144000
H	5.84356500	5.44104300	0.62435400
H	5.52635000	3.69505800	0.71683400
H	4.47935200	4.83041000	1.59741500
H	4.38177600	6.96043900	-0.64253000
H	2.97314500	6.45725000	0.31300900
H	2.91688900	6.39820600	-1.47038000
H	-4.35479500	7.00167100	-0.32069000
H	-2.94812500	6.44065100	-1.24445700
H	-2.89589600	6.47050100	0.53980300
H	-5.75487500	5.47518300	1.00385700
H	-4.34239300	4.83749200	1.88649600
H	-5.44973200	3.72530700	1.05093200
H	-5.80516000	5.41775300	-1.54480500
H	-5.49554900	3.66697500	-1.52925000
H	-4.42553400	4.74512800	-2.45305900
H	-4.35520600	0.38848900	1.40282000
H	-4.78608700	-3.44271100	-0.48314100
H	-1.81371400	-0.66739300	-1.87452700
H	-6.07581500	-2.02090400	3.74428700
H	-4.92442100	-0.76799700	3.23542700
H	-4.44271800	-2.47356300	3.18589200
H	-7.79304300	-1.11513000	2.08827900
H	-7.37828000	-0.97444100	0.35866000
H	-6.64646800	0.13013300	1.54588500
H	-7.16506100	-3.51463800	2.13279700
H	-5.59093700	-4.08326700	1.53962800
H	-6.81136200	-3.46261400	0.39437500
H	-3.91016000	-4.24172900	-4.02020400
H	-4.52102300	-2.59212000	-3.72454000
H	-4.97106700	-3.92086300	-2.63179400
H	-2.12751500	-5.24629900	-2.46225600
H	-3.21382500	-4.94932300	-1.08690700
H	-1.56039500	-4.30457700	-1.05665500
H	-1.56880100	-3.46581500	-4.07440900
H	-0.87856800	-2.47594100	-2.77845000
H	-2.11925800	-1.78998500	-3.85780300
H	-0.06969400	0.16560500	4.13194200
H	-2.28148200	-0.59877200	3.14111200
H	-2.32092400	-2.69959800	1.74247500
H	-0.23118400	-3.85359600	1.15946400
H	2.01250900	-2.91591600	1.92240500
H	2.77364200	-1.68758800	4.40004700
H	2.29165100	0.02690400	4.31687300
H	3.15776800	-0.73965000	2.95715300

5.4.23 [(^{dtbp}Cbz)Li(Tol)] – 2nd excited state

0 1

Li	-0.01888400	-0.78135400	1.10472300
N	-0.00674900	0.87903200	-0.18329300
C	-1.36910300	-2.30198400	2.10231400
C	-0.19398700	-2.94209000	1.75976500
C	-1.35634400	-1.10339100	2.87489600
C	1.08370400	-2.41207600	2.18539800
C	-0.09194800	-0.67639300	3.43670200
C	-1.10235800	1.69789800	-0.26193600
C	1.09218100	1.68930600	-0.31821700
C	2.46536100	1.33909200	-0.34041600
C	0.72313900	3.06423500	-0.40775000
C	3.38203200	2.39559200	-0.41876200
C	2.99262400	-0.04354800	-0.33292900
C	3.02789900	3.75255200	-0.47933600
C	1.65834000	4.07897300	-0.47649600
C	4.12790100	4.81152000	-0.56145500
C	-0.72622800	3.07077000	-0.36558300
C	-1.65435000	4.09399200	-0.36907300
C	-3.02469900	3.78002000	-0.28826300
C	-3.38805700	2.42506500	-0.22397100
C	-4.11693400	4.84974500	-0.29011700
C	-2.47887200	1.36046600	-0.21675700
C	-3.02522300	-0.01501400	-0.22754700

C	2.47140300	-1.02615300	-1.17571600
C	4.11451900	-0.33867500	0.45751100
C	3.07935300	-2.28639200	-1.27602500
C	4.19017500	-2.53934900	-0.47201400
C	2.50224700	-3.35588300	-2.20765300
C	4.71992100	-1.59058700	0.41538900
C	5.91818800	-1.96327300	1.29317800
C	2.09939000	-2.73808900	-3.55384700
C	1.27127400	-3.95835800	-1.51829300
C	3.50577400	-4.47813400	-2.49025200
C	6.37867300	-0.79389300	2.16630700
C	7.09286100	-2.38932400	0.39936900
C	5.51830100	-3.12795900	2.21304900
C	5.04558500	4.68250800	0.66518200
C	3.55886700	6.23173500	-0.59087400
C	4.94641200	4.58957200	-1.84386600
C	-4.96273600	4.70977400	0.98597700
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C	-4.06259400	-0.34269700	0.64648400
C	-2.61424400	-0.94864100	-1.19036100
C	-4.70399700	-1.58361000	0.58877200
C	-4.29043400	-2.47540100	-0.40237800
C	-5.82285000	-1.90556600	1.58408600
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C	-2.90489600	-3.20837500	-2.38627200
C	-6.37147000	-3.32131100	1.39542600
C	-6.97372600	-0.90744800	1.38142900
C	-5.28247200	-1.78350400	3.01706800
C	-1.80719300	-2.69953600	-3.32120700
C	-2.42479600	-4.50045500	-1.70725700
C	-4.15083200	-3.50647400	-3.23511200
C	1.08949600	-1.31668000	3.11533600
C	2.39138900	-0.89588800	3.73028200
H	4.43910000	2.12852400	-0.46530900
H	1.32694500	5.11664600	-0.52291600
H	-1.31692100	5.12915200	-0.42681900
H	-4.44822000	2.16588500	-0.21316900
H	1.60216200	-0.77874500	-1.78696900
H	4.66809000	-3.51731300	-0.52768200
H	4.49226100	0.43503900	1.12562200
H	1.69528000	-3.51553100	-4.22102700
H	2.96620300	-2.27571100	-4.05110100
H	1.32220500	-1.96829300	-3.44903900
H	0.77216700	-4.69095200	-2.17254900
H	0.54271800	-3.17974400	-1.25166800
H	1.55603900	-4.46371800	-0.58356900
H	3.07184000	-5.19087000	-3.20824600
H	3.75751300	-5.04892700	-1.58405300
H	4.44014300	-4.08753200	-2.92285000
H	6.36405400	-3.41598100	2.85792200
H	5.21825300	-4.01683400	1.63815500
H	4.67288200	-2.84711000	2.85853100
H	7.96330600	-2.66414100	1.01643400
H	7.39379300	-1.57021200	-0.27222500
H	6.84109700	-3.25947200	-0.22494800
H	7.24112500	-1.10271300	2.77650300
H	5.58852800	-0.46233400	2.85682900
H	6.69365600	0.06986300	1.56024400
H	5.74499600	5.34448200	-1.92113500
H	4.30852500	4.67261500	-2.73724200
H	5.42076400	3.59737500	-1.86138700
H	5.84372400	5.44063300	0.62487800
H	5.52652700	3.69461500	0.71685900
H	4.47949500	4.82971000	1.59775300
H	4.38197100	6.96036400	-0.64167000
H	2.97335600	6.45691900	0.31379000
H	2.91706300	6.39835200	-1.46961400
H	-4.35458100	7.00167100	-0.32148100
H	-2.94801600	6.44048200	-1.24531500
H	-2.89560500	6.47058900	0.53893500
H	-5.75458000	5.47531900	1.00341700
H	-4.34196800	4.83783700	1.88600200
H	-5.44934200	3.72545700	1.05074300
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H	-5.49552700	3.66682500	-1.52944300
H	-4.42561800	4.74486700	-2.45351700
H	-4.35469100	0.38876000	1.40286300

H	-4.78598000	-3.44278300	-0.48232700
H	-1.81395300	-0.66768300	-1.87490300
H	-6.07490200	-2.01985800	3.74512400
H	-4.92369300	-0.76703800	3.23562400
H	-4.44186300	-2.47259100	3.18663900
H	-7.79250600	-1.11494400	2.08912900
H	-7.37807900	-0.97481000	0.35938100
H	-6.64620000	0.13028900	1.54608100
H	-7.16420000	-3.51436000	2.13426600
H	-5.59006800	-4.08295400	1.54107700
H	-6.81073300	-3.46285700	0.39577900
H	-3.91098700	-4.24195900	-4.01978600
H	-4.52158800	-2.59226000	-3.72411200
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H	-2.12823800	-5.24671100	-2.46194400
H	-3.21446000	-4.94949600	-1.08657400
H	-1.56093900	-4.30497400	-1.05641200
H	-1.56963100	-3.46641900	-4.07441300
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H	-2.11977100	-1.79049600	-3.85777900
H	-0.07010700	0.16663200	4.13175200
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H	-2.32035500	-2.70003300	1.74312600
H	-0.23011500	-3.85321800	1.16001400
H	2.01322500	-2.91431700	1.92250800
H	2.77405000	-1.68523200	4.39994700
H	2.29133000	0.02903700	4.31636700
H	3.15759000	-0.73752300	2.95675600

5.4.24 [(^{dtbp}Cbz)Li(Tol)] – 3rd excited state

0 1

Li	-0.02934000	-0.80418200	1.09967300
N	-0.01442000	0.83177500	-0.17753800
C	-1.37403900	-2.33699500	2.09517400
C	-0.20329700	-2.97384400	1.73241600
C	-1.35173200	-1.15356100	2.89103800
C	1.07890000	-2.45465900	2.15636000
C	-0.08254300	-0.74477400	3.45525500
C	-1.09280400	1.66051600	-0.23857100
C	1.06449600	1.65436000	-0.28646900
C	2.44394700	1.33704800	-0.32910100
C	0.68234400	3.06122000	-0.36979800
C	3.32468500	2.41018200	-0.41494500
C	2.99932700	-0.03924100	-0.33035400
C	2.96895200	3.80303200	-0.46123400
C	1.63400500	4.11259200	-0.44824000
C	4.08678700	4.83963600	-0.53704000
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C	-1.65625500	4.12199900	-0.35926400
C	-2.99186200	3.81981400	-0.30366600
C	-3.35264700	2.42804200	-0.25348900
C	-4.10597400	4.86297500	-0.31177000
C	-2.47351600	1.35078600	-0.22553300
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C	2.48829900	-1.02243300	-1.17664600
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C	2.53353900	-3.34637500	-2.21515300
C	4.75149000	-1.56685300	0.39853600
C	5.95945700	-1.92783300	1.26824100
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C	7.13810900	-2.32389500	0.36598600
C	5.58395900	-3.10887600	2.17751100
C	4.99493800	4.69402700	0.69491700
C	3.53340700	6.26486100	-0.56600000
C	4.90942400	4.60922800	-1.81508900
C	-4.95108500	4.70851400	0.96316500
C	-3.54658700	6.28550900	-0.35398900
C	-4.99396900	4.65048200	-1.54858400
C	-4.07039200	-0.34396400	0.64679300
C	-2.63596700	-0.95662700	-1.19658100

C	-4.72050400	-1.58216700	0.59018100
C	-4.31253600	-2.47764900	-0.39881200
C	-5.83794300	-1.89738700	1.58925300
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C	-6.98306400	-0.89157700	1.39227400
C	-5.29160700	-1.78081400	3.02049300
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C	-4.16338800	-3.54644700	-3.21733900
C	1.09438600	-1.38032000	3.11107900
C	2.40292200	-0.97679400	3.72335300
H	4.38597300	2.15955700	-0.47448200
H	1.28035300	5.14273800	-0.49755100
H	-1.30004700	5.15064000	-0.42051100
H	-4.41645600	2.18032100	-0.26216100
H	1.60519400	-0.78685300	-1.77259100
H	4.72136600	-3.48853700	-0.55519900
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H	1.72611100	-3.51017900	-4.22828000
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H	3.78979300	-5.03557200	-1.58577700
H	4.46987100	-4.08126000	-2.93090600
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H	6.70125100	0.11524700	1.55502300
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H	4.42687000	4.85672700	1.62365600
H	4.36264800	6.98669300	-0.61315400
H	2.94656800	6.49219700	0.33727900
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H	-1.55516000	-4.29014500	-1.04126800
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H	2.30990500	-0.06821300	4.33569400
H	3.16044700	-0.79791900	2.94535900

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