Supporting Information

Fluorescent Benzene-centered Mono-, Bis- and Tris-Triazapentadiene-Boron Complexes

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Theoretical Calculations

To investigate the electronic structures and the electronic transitions of the mono-, bis- and tris triazapentadiene boron compounds, complete DFT-geometry optimizations followed by TD-DFT calculations for 20 states of compound **14a-c** and **14e** were performed in the gas phase using the B3LYP[1] functional and the def2-TZVP basis set[2] as implemented in Gaussian09[3].

Calculations for Compound 14a:

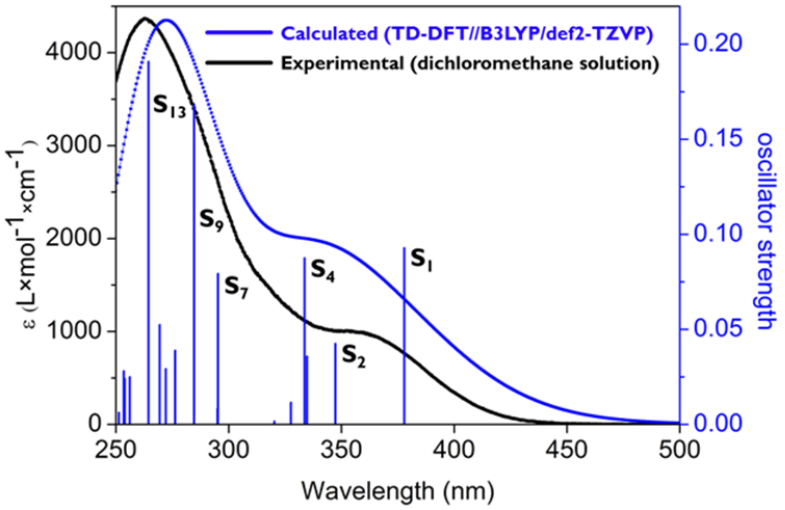


Figure S 1. The experimental (black, y1-axis) and calculated (blue) UV/VIS spectrum of **14a** with the associated oscillator strength (y2-axis) of the different excited states S_1, S_2, S_4, S_7, S_9, S_{13}. The calculated extinction coefficient was normalized to ε = 4 400 L·mol^{-1}·cm^{-1} (factor 4.8).

To gain better insight into the transitions relevant (based on the oscillator strength) for the different absorption bands in the UV spectrum, the transitions to S_1, S_2, S_4 contributing to the longest wavelength absorption and S_7, S_9 and S_{13} which contribute the most to the shorter wavelength absorption band, were studied in more detail (Table S 1).

Table S 1. Selected TD-DFT calculation data/results of compound **14a**.[a]

Excited state	Transition energy / eV	Main CI coefficient[b]	Oscillator strength *f*
S_1	3.2813 (378 nm)	98 % (HOMO → LUMO)	0.0928
S_2	3.5698 (347 nm)	96 % (HOMO−1 → LUMO)	0.0425
S_4	3.7158 (334 nm)	43 % (HOMO−3 → LUMO) 29% (HOMO−2 → LUMO) 24 % (HOMO−4 → LUMO)	0.0875
S_7	4.1987 (295 nm)	90 % (HOMO−6 → LUMO)	0.0793
S_9	4.3551 (285 nm)	46 % (HOMO−7 → LUMO) 41 % (HOMO−8 → LUMO)	0.1683
S_{13}	4.6879 (264 nm)	51 % (HOMO−9 → LUMO) 34 % (HOMO−10 → LUMO)	0.1908

[a] TD-DFT calculations on the B3LYP/def2-TZVP level of theory. [b] Transitions which are significantly involved in the CI wave function. Only transitions contributing more than 10 % to the CI wave function are listed. Additionally, all transitions quoted in the table sum up to a CI wave function contribution of more than 90 %. This value is obtained by multiplying the CI coefficient by itself followed by multiplication by two.

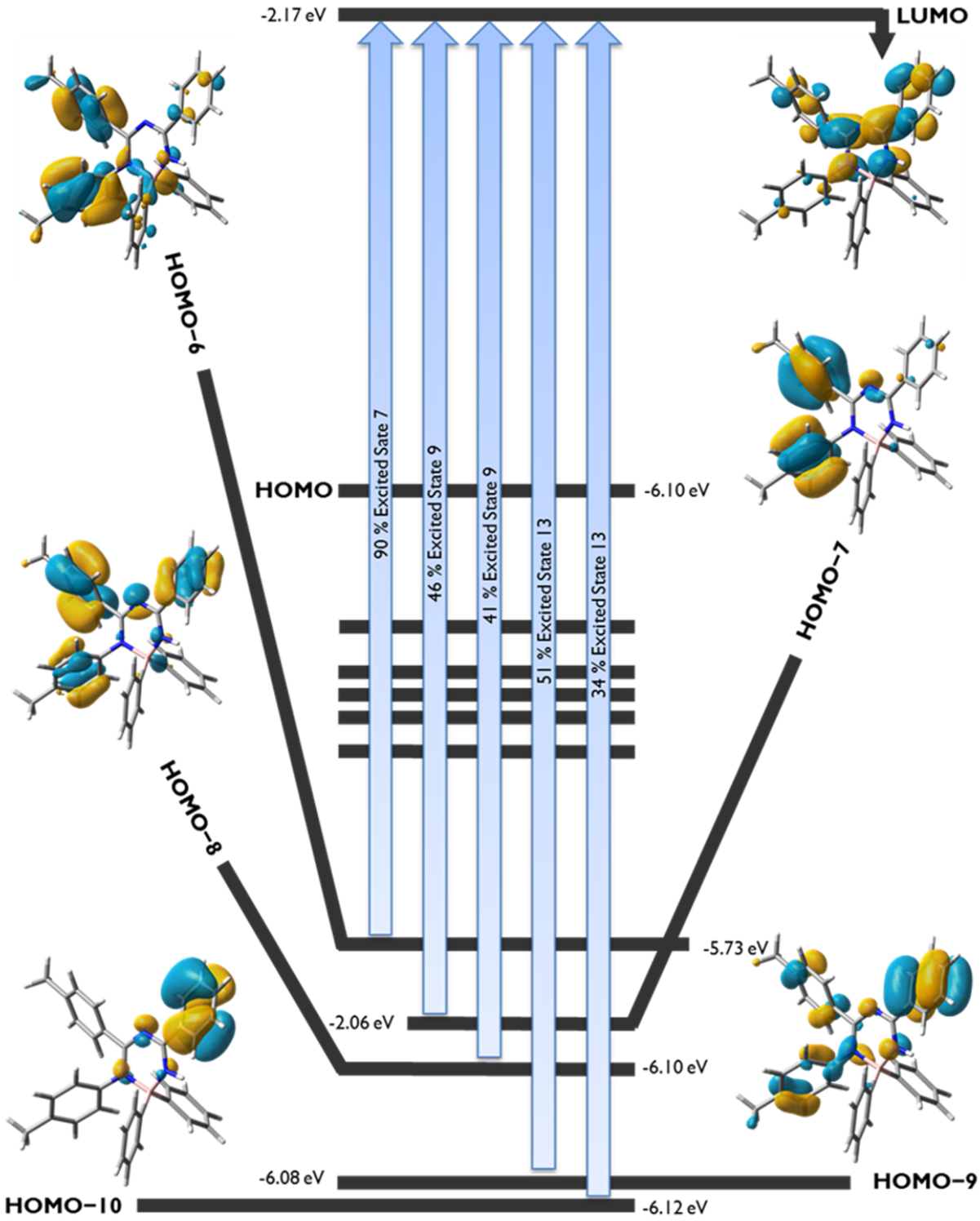


Figure S 2. KOHN-SHAM orbital pictures and energies with main transitions of **14a** which contribute the most to the longest wavelength absorption at around 350 nm. (TD//B3LYP/def2-TZVP).

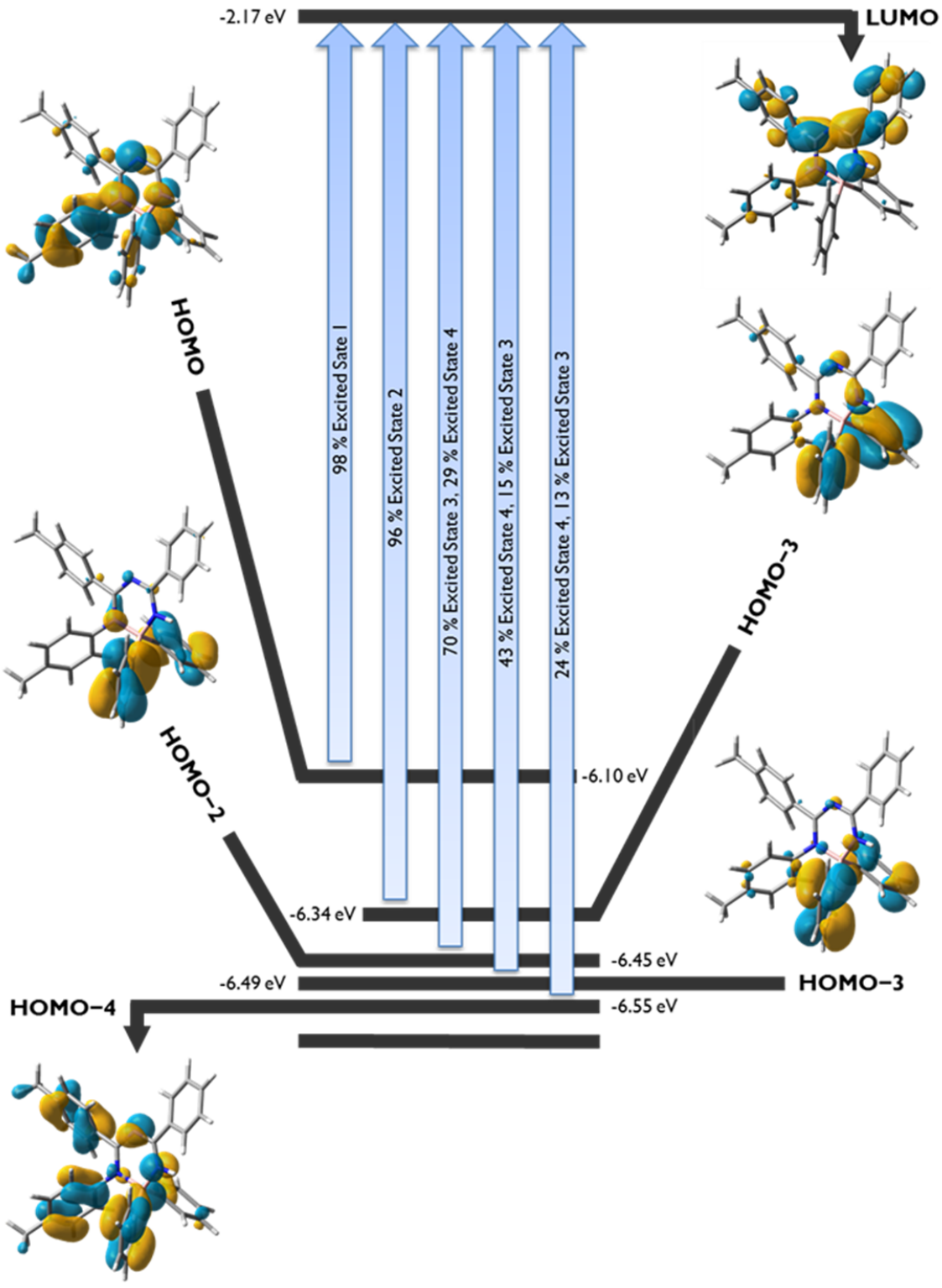


Figure S 3. KOHN-SHAM orbital pictures and energies with main transitions of **14a** which contribute the most to the shortest wavelength absorption at around 260 nm. (TD//B3LYP/def2-TZVP).

Calculations for Compound 14b:

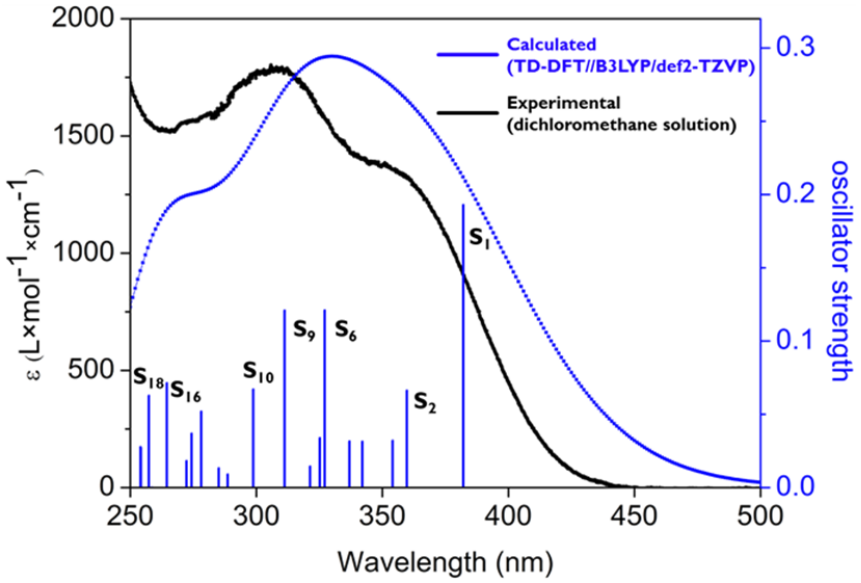


Figure S 4. The experimental (black, y1-axis) and calculated (blue) UV/VIS spectrum of **14b** with the associated oscillator strength (y2-axis) of the different excited states S_1, S_2, S_6, S_9, S_{10}, S_{16} and S_{18}. The calculated extinction coefficient was normalized to ε = 1 750 $L \cdot mol^{-1} \cdot cm^{-1}$ (factor 9.7).

The experimental spectrum shows a band at $\lambda_{abs,\ max}$ = 308 nm and a shoulder at λ_{abs} = 350 nm. The calculated spectrum is slightly shifted to longer wavelength compared to the experimental spectrum ($\lambda_{abs,\ max}$ = 331 nm). The shoulder at λ_{abs} = 350 nm is also barely visible in the calculated spectrum. The relevant transitions to S_1, S_2, S_6, S_9, S_{10}, S_{16} and S_{18}, which contribute the most to the calculated absorption bands are listed in Table S 2 and shown in Figure S % in m ore detail.Table S 2Table S 2. **Selected TD-DFT calculation data/results of compound** 14b**.**[a]

Excited state	Transition energy / eV	Main CI coefficient [b]	Oscillator strength *f*
S_1	3.2448 (382 nm)	98 % (HOMO → LUMO)	0.1929
S_2	3.4467 (360 nm)	97 % (HOMO−1 → LUMO)	0.0662
S_6	3.7904 (327 nm)	58 % (HOMO−6 → LUMO) 12 % (HOMO−5 → LUMO)	0.1210
S_9	3.9842 (311 nm)	66 % (HOMO−8 → LUMO)	0.1209

		12 % (HOMO−6 → LUMO)	
S_{10}	4.1495 (299 nm)	27 % (HOMO−10 → LUMO) 21 % (HOMO−9 → LUMO) 19 % (HOMO−13 → LUMO) 11 % (HOMO−11 → LUMO)	0.0670
S_{16}[c]	4.6871 (265 nm)	85 % (HOMO−1 → LUMO+1)	0.0713
S_{18}[c]	4.8172 (257 nm)	41 % (HOMO → LUMO+3) 23 % (HOMO → LUMO+2)	0.0627

[a] TD-DFT calculations on the B3LYP/def2-TZVP level of theory. [b] Transitions which are significantly involved at the CI wave function. Only transitions contributing more than 10% to the CI wave function are listed. Additionally, all transitions quoted in the table sum up to a CI wave function contribution of more than 90%. This value is obtained by multiplying the CI coefficient by itself followed by multiplication by two. [c] The calculated transitions of this excited state only sum up to a CI wave function contribution of 85%, thus characterizing the CI wave function insufficiently.

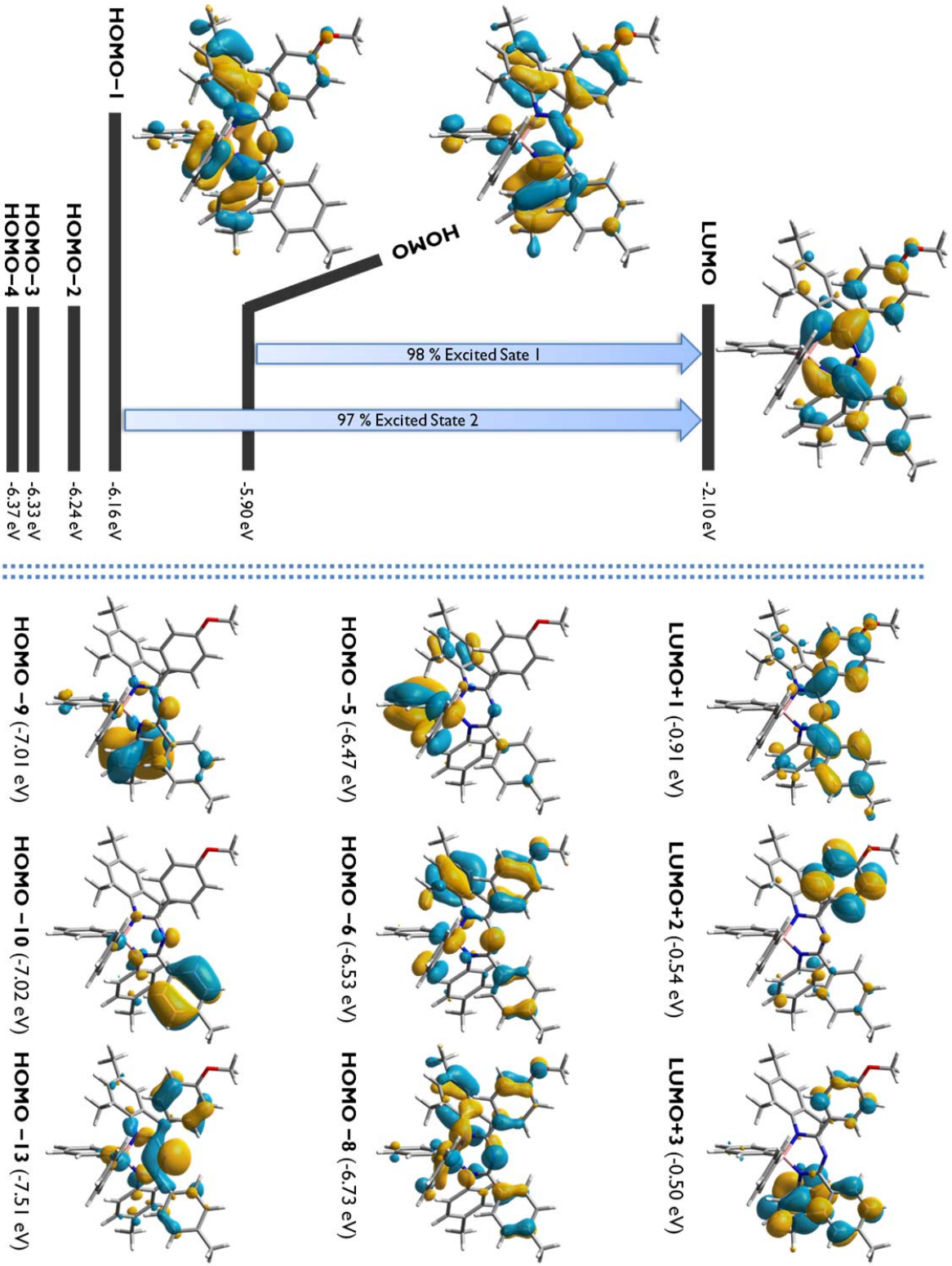


Figure S 5. Selected KOHN-SHAM orbital pictures and energies with main transitions of **14b** (TD//B3LYP/def2-TZVP).

Calculations for Compound 14c:

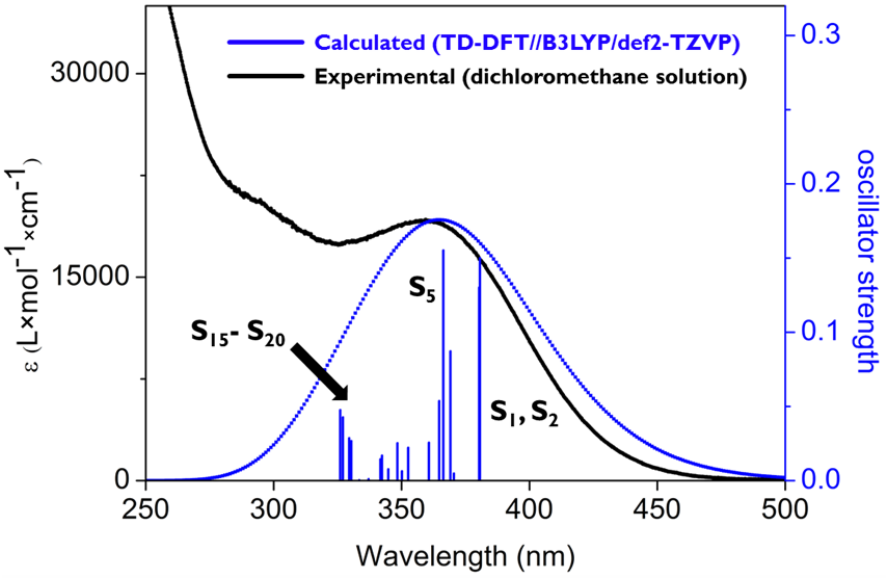


Figure S 6. The experimental (black, y1-axis) and calculated (blue) UV/VIS spectrum of **14c** with the associated oscillator strength (y2-axis) of the different excited states S_1, S_2, S_5, S_{15}-S_{20}. The calculated extinction coefficient was normalized to ε = 19 100 $L \cdot mol^{-1} \cdot cm^{-1}$ (factor 1.5).

The experimental spectrum shows the longest wavelength absorption band at $\lambda_{abs,\,max}$ = 359 nm, while the corresponding calculated band is only different by 6 nm at $\lambda_{abs,\,max}$ = 365 nm. This is described most accurately by the excited states S_1, S_2, S_5. A second band at λ_{abs} = 294 nm is described by S_{15} to S_{20} which are mostly transitions with high energies from low-lying HOMO−ℕ to higher LUMO+ℕ. See Table S 3 and Figure S 7, Figure S 8 for more details.

Table S 3. Selected TD-DFT calculation data/results of compound **14c**.[a]

Excited state	Transition energy / eV	Main CI coefficient [b]	Oscillator strength *f*
S_1	3.2570 (381 nm)	34 % (HOMO → LUMO+1) 32 % (HOMO → LUMO) 29% (HOMO−1 → LUMO)	0.1500
S_2	3.2599 (380 nm)	43 % (HOMO → LUMO) 40 % (HOMO−1 → LUMO) 11 % (HOMO−1 → LUMO+1)	0.1302
S_5	3.3843 (366 nm)	49 % (HOMO−3 → LUMO) 29 % (HOMO−4 → LUMO)	0.1552

[a] TD-DFT calculations on the B3LYP/def2-TZVP level of theory. [b] Transitions which are significantly involved at the CI wave function. Only transitions contributing more than 10% to the CI wave function are listed. Additionally, all transitions quoted in the table sum up to a CI wave function contribution of more than 90%. This value is obtained by multiplying the CI coefficient by itself followed by multiplication by two.

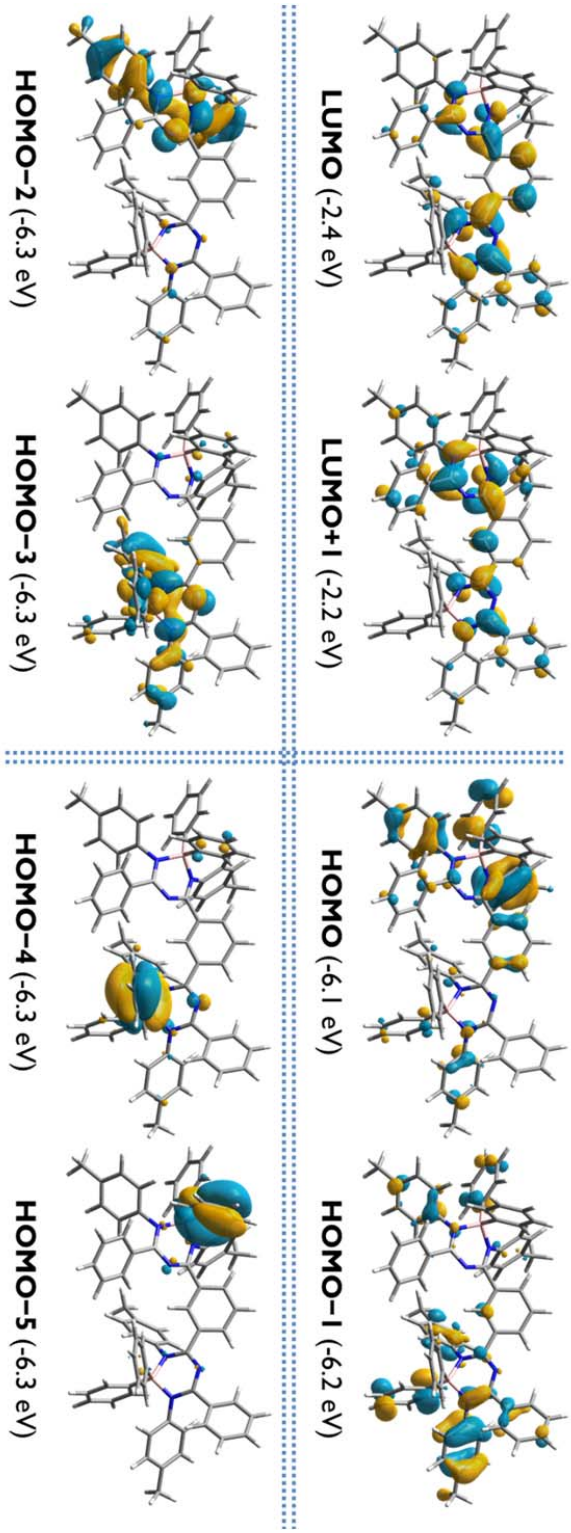


Figure S 7. Selected KOHN-SHAM molecular orbital pictures of **14c**. The degree of similarity of the energy levels can be particularly observed within the pairs HOMO/HOMO-1, HOMO-2/HOMO-3 and HOMO-4/HOMO-5.

The shapes of the LUMO and LUMO+1 molecular orbitals are quite similar and only differ in the differently pronounced electron delocalization in the left (LUMO+1) and right (LUMO) part of the molecule. Notably all energies of the relevant molecular orbitals are quite similar resulting in a greater amount of excited states which contribute to the CI wave function of this molecule compared to **14a**, **b**.

Since the shape of the respective molecular orbitals involved in the relevant transitions are similar, it is sufficient to only have a closer look at the HOMO→LUMO, HOMO−2→LUMO and the HOMO−4→LUMO transition to adequately describe the CI wave function.

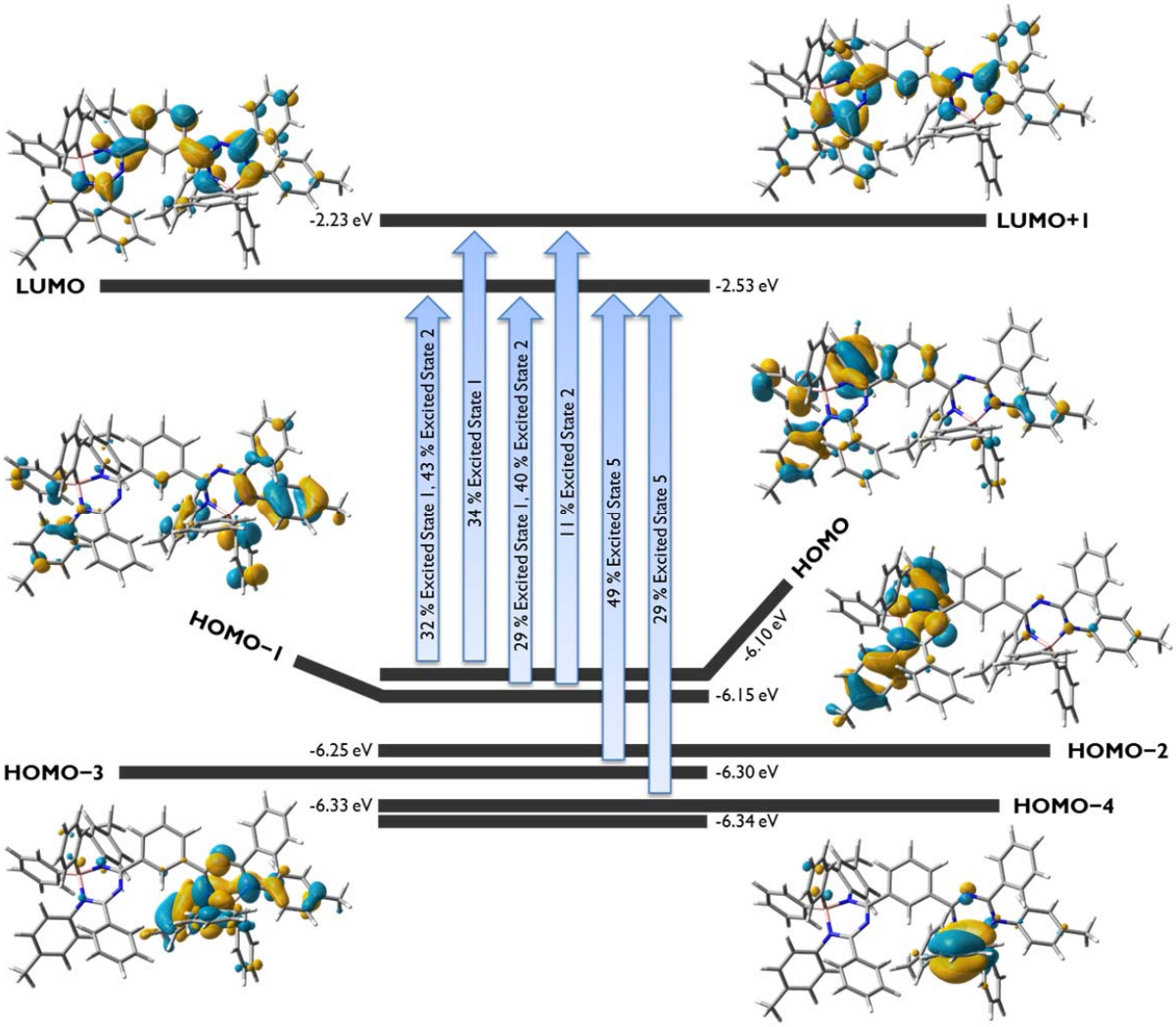


Figure S 8. Relevant transitions which are contributing more than 10% to the excited states S_1 (95%), S_2 (94%), S_5 (78%) and the respective KOHN-SHAM molecular orbital pictures of **14c**.

Calculations for Compound 14e:

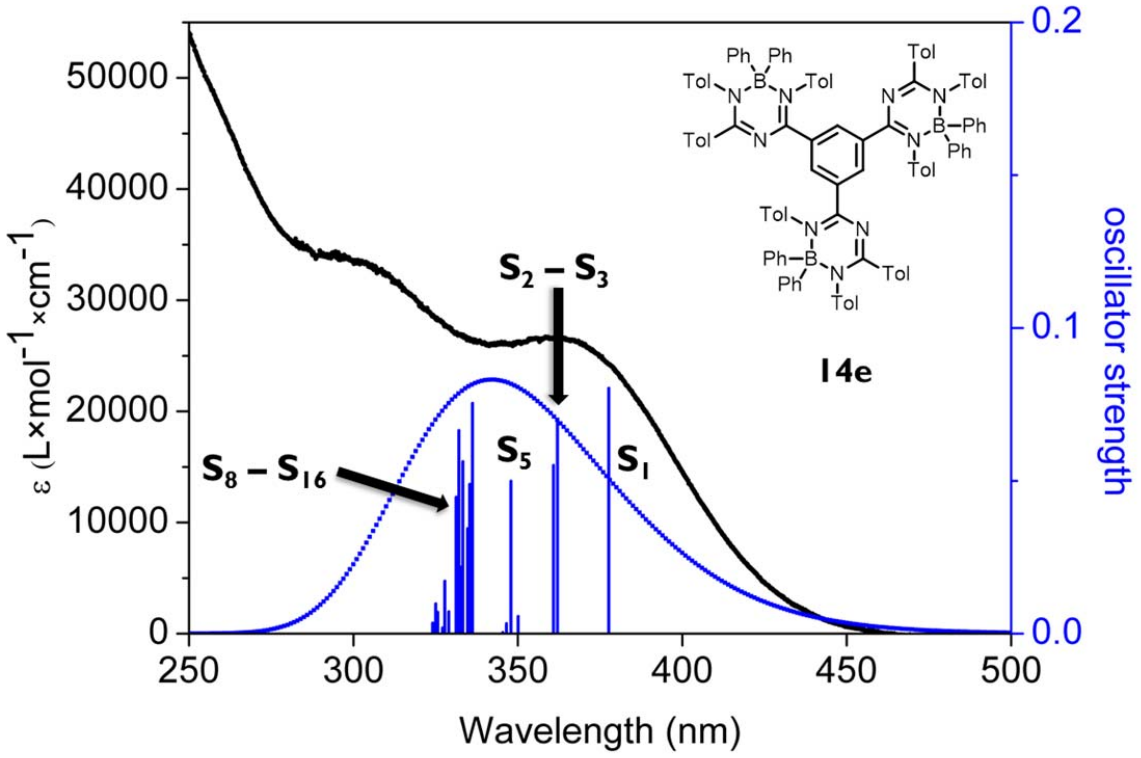


Figure S 9. The experimental (black, y1-axis) and calculated (blue) UV/VIS spectrum of **14e** with the associated oscillator strength (y2-axis) of the different excited states S_1-S_3, S_4-S_6 and S_7-S_{10}.

The highest oscillator strength are $f = 0.1406$ for S_1 at $\lambda_{abs} = 405$ nm, $f = 0.1166$ for S_2 at $\lambda_{abs} = 403$ nm and $f = 0.1028$ for S_3 at $\lambda_{abs} = 401$ nm (Table S 4).

Table S 4. Selected TD-DFT calculation data/results of compound **14e**.[a]

Excited state	Transition energy / eV	Main CI coefficient [b]	Oscillator strength *f*
S_1	3.2829 (378 nm)	93 % (HOMO → LUMO)	0.0803
S_2	3.4247 (362 nm)	62 % (HOMO−2 → LUMO+1) 15 % (HOMO−2 → LUMO) 12 % (HOMO−2 → LUMO+2)	0.0698
S_3	3.4359 (361 nm)	51 % (HOMO−1 → LUMO+1) 19 % (HOMO−1 → LUMO+2) 18 % (HOMO−1 → LUMO)	0.0551
S_5	3.5639 (348 nm)	76 % (HOMO−3 → LUMO)	0.0499
S_8[c]	3.6874 (336 nm)	60 % (HOMO−7 → LUMO) 14 % (HOMO−6 → LUMO)	0.0754
S_9[c]	3.6970 (335 nm)	15 % (HOMO → LUMO+2) 13 % (HOMO−4 → LUMO) 11 % (HOMO−7 → LUMO) 10 % (HOMO−5 → LUMO+1)	0.0489
S_{10}[c]	3.7037 (335 nm)	38 % (HOMO−4 → LUMO+1) 11 % (HOMO → LUMO+2)	0.0344
S_{11}[c]	3.7200 (333 nm)	32 % (HOMO−9 → LUMO) 12 % (HOMO → LUMO+2) 10 % (HOMO−5 → LUMO+1)	0.0563
S_{12}	3.7271 (333 nm)	24 % (HOMO−6 → LUMO+1) 13 % (HOMO−6 → LUMO) 13 % (HOMO−6 → LUMO+2)	0.0218
S_{13}	3.7335 (332 nm)	39 % (HOMO−8 → LUMO+1) 12 % (HOMO−5 → LUMO+1) 11 % (HOMO−8 → LUMO) 11 % (HOMO−8 → LUMO+2)	0.0665
S_{14}	3.7427 (331 nm)	45 % (HOMO → LUMO+2) 17 % (HOMO−9 → LUMO)	0.0447

[a] TD-DFT calculations on the B3LYP/def2-TZVP level of theory. [b] Transitions which are significantly involved at the CI wave function. Only transitions contributing more than 10% to the CI wave function are listed. Additionally, all transitions quoted in the table sum up to a CI wave function contribution of more than 90%. This value is obtained by multiplying the CI coefficient by itself followed by multiplication by two. [c] The calculated transitions of this excited state only sum up to a CI wave function contribution of 80% to 88%, thus characterizing the CI wave function insufficiently.

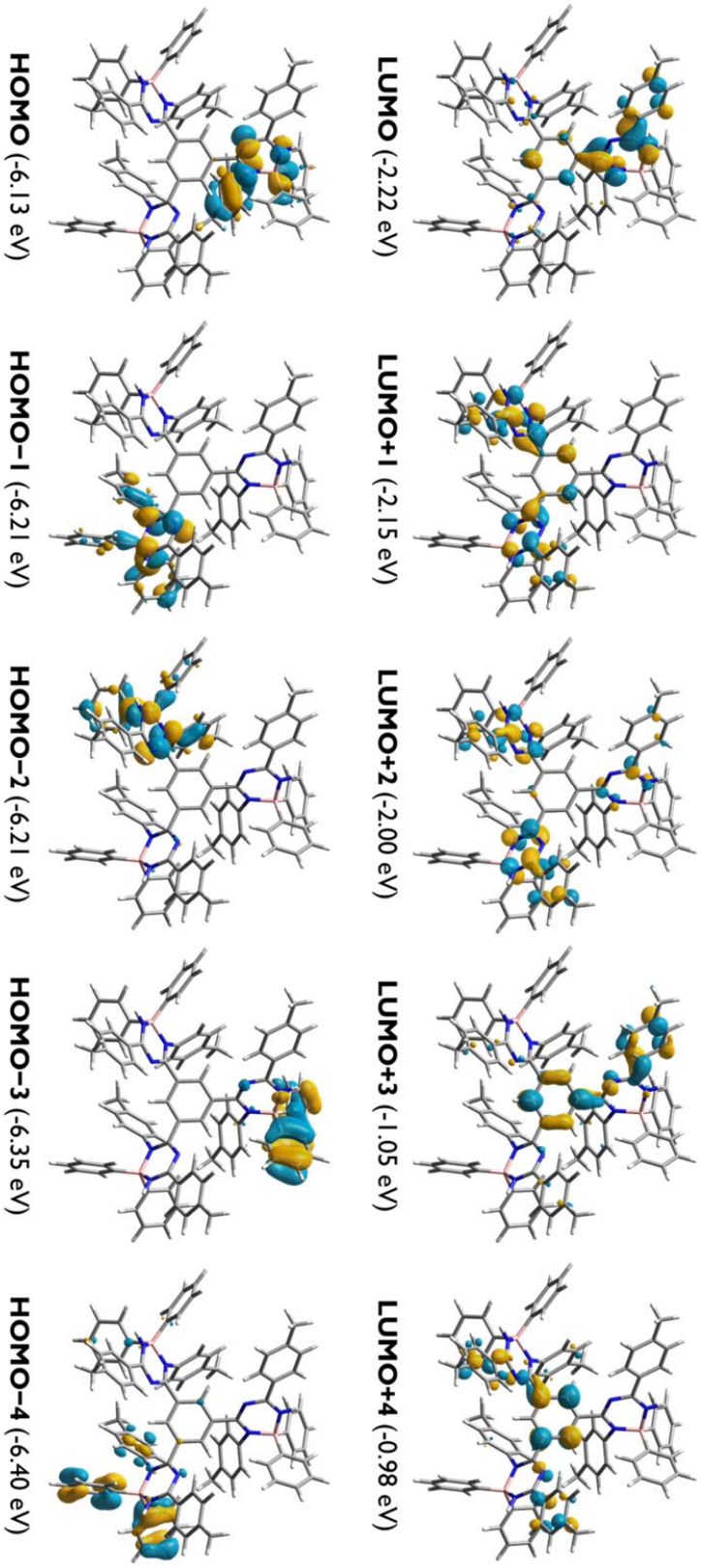


Figure S 10. Selected KOHN-SHAM molecular orbital pictures of **14e**.

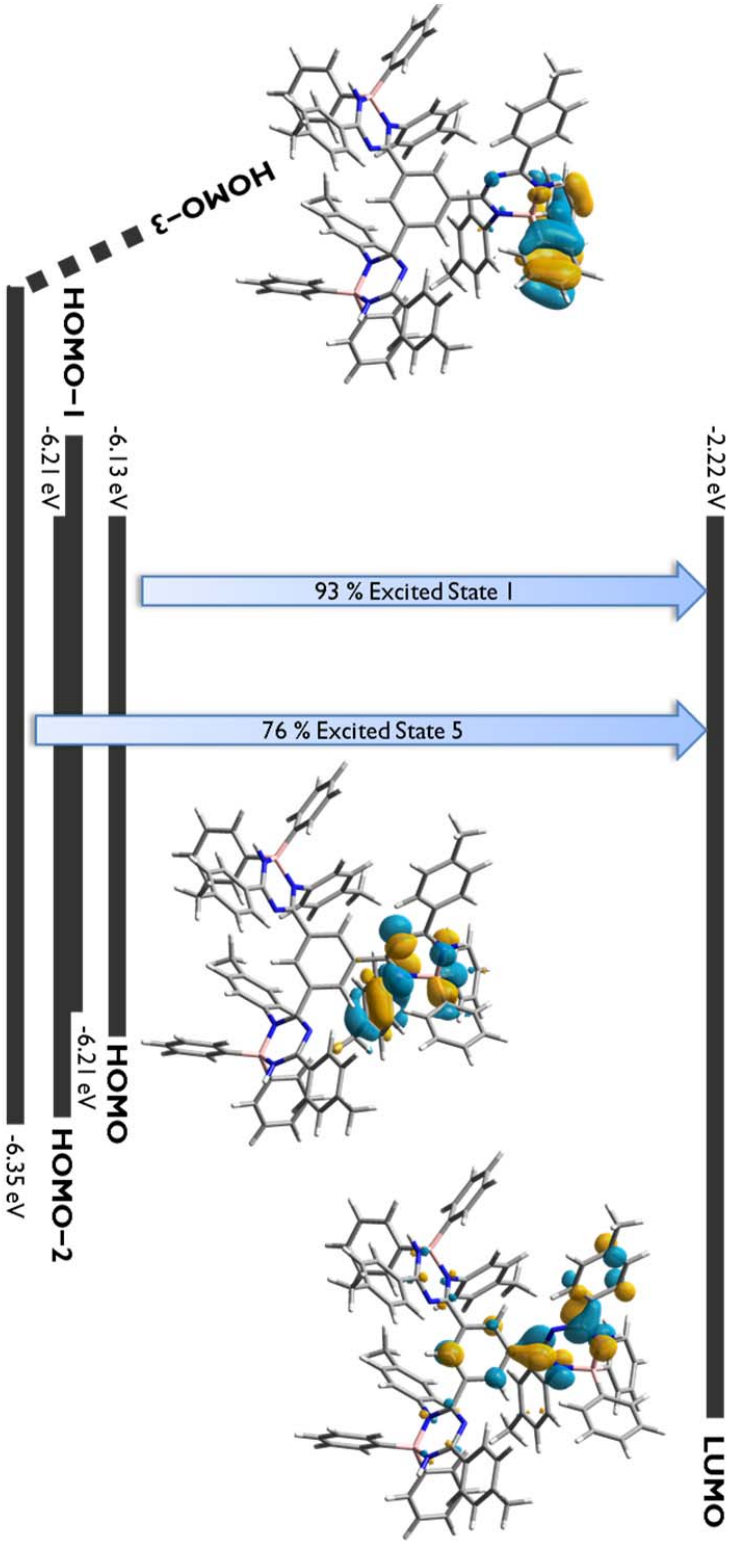


Figure S 11. Transitions contributing to the excited states S_1 (93%) S_5 (76%) and the relevant KOHN-SHAM molecular orbitals.

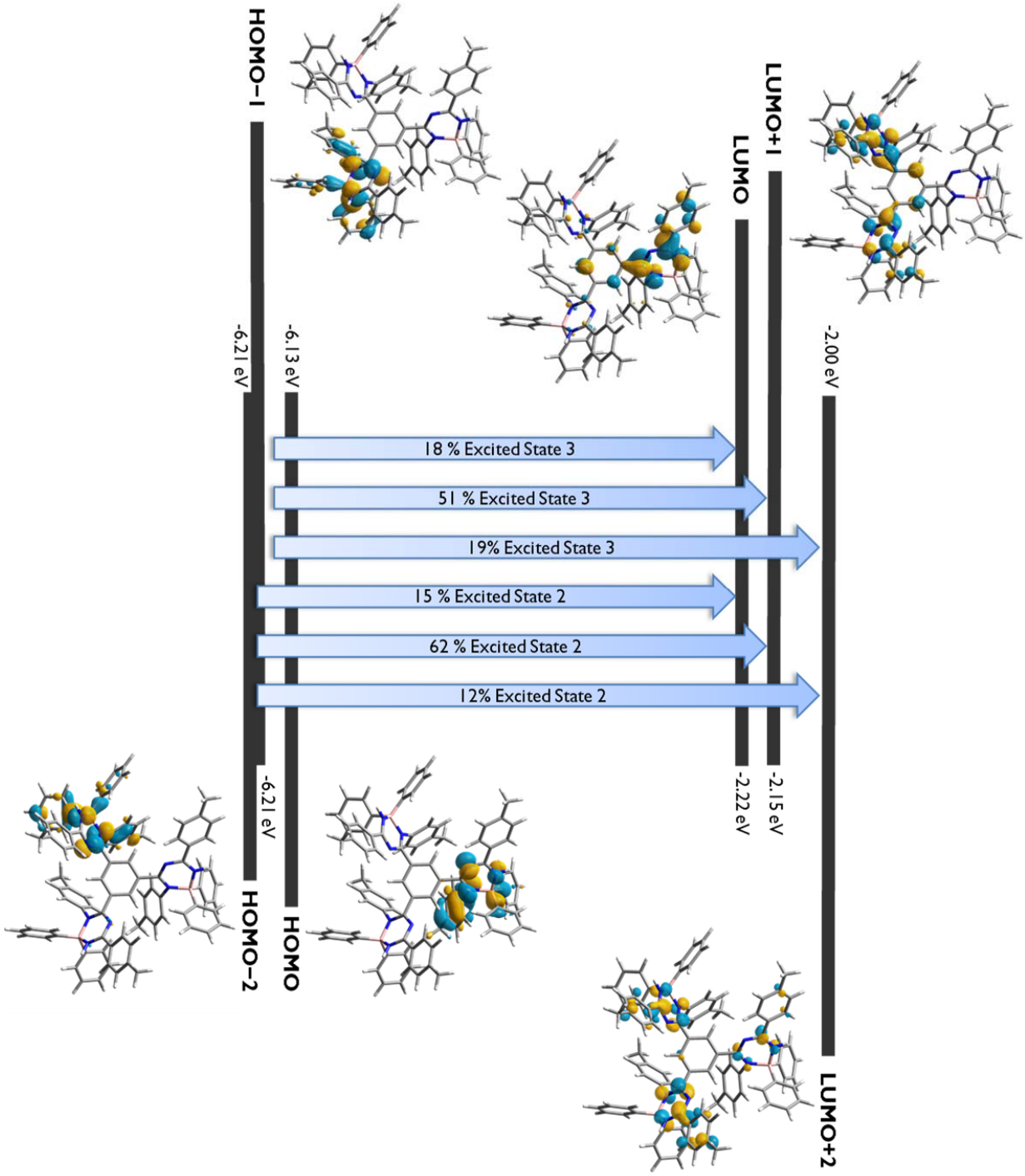


Figure S 12. Transitions contributing to the excited states S_2 (89%), S_3 (88%) and the relevant KOHN-SHAM molecular orbitals.

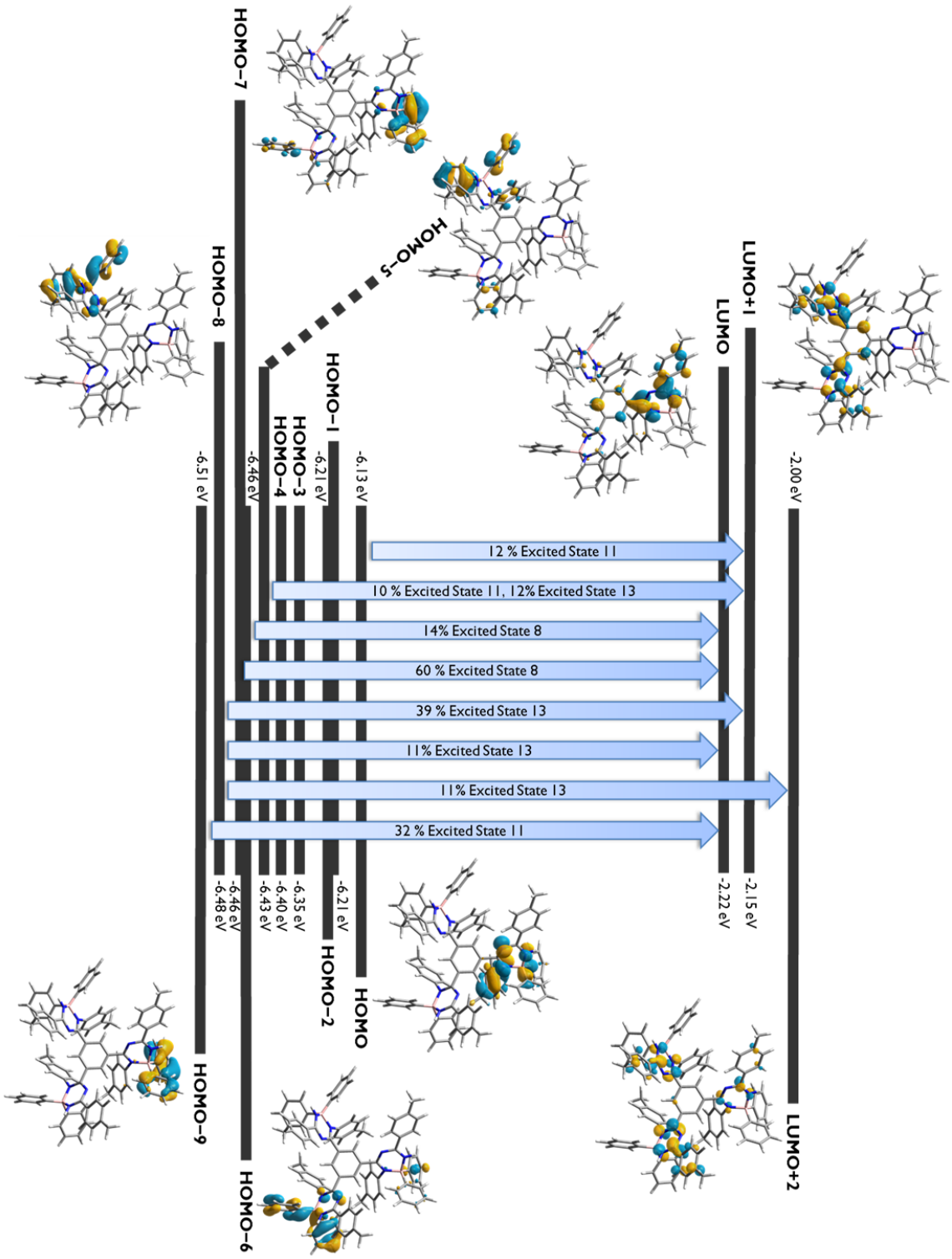


Figure S 13. Transitions from the band accumulation S8-S16 contributing to the excited states with the highest oscillator strengths S_8 (74%), S_{11} (54%), S_{13} (73%) and the relevant KOHN-SHAM molecular orbitals.

Calculated optimized geometrical data (Cartesian Coordinates) and TD-DFT-Results (B3LYP/def2-TZVP)

14a E_{tot} = -1503.4273497 au (NIMAG = 0)

Symbol	X	Y	Z
B	-0.626516	-1.259825	0.222161
N	0.414872	-0.050361	0.006767
C	0.008929	1.219891	-0.013701
N	-1.269499	1.600025	-0.116939
C	-2.226261	0.680251	-0.278588
N	-1.997273	-0.605131	-0.172822
C	-0.318855	-2.475783	-0.815854
C	0.388575	-3.63048	-0.456909
C	0.657498	-4.645725	-1.36884
C	0.219295	-4.538864	-2.683801
C	-0.483666	-3.405321	-3.07334
C	-0.741512	-2.396296	-2.150483
C	1.786994	-0.385345	-0.250809
C	2.529408	-1.123263	0.665219
C	3.846692	-1.464677	0.383202
C	4.455595	-1.093748	-0.814175
C	3.693421	-0.366419	-1.730169
C	2.378296	-0.022375	-1.459559
C	5.874793	-1.487536	-1.127869
C	0.962695	2.362466	0.084235
C	2.0212	2.374545	0.995276
C	2.833393	3.491318	1.119285
C	2.636537	4.622596	0.325422
C	1.574283	4.606742	-0.579482
C	0.740767	3.503942	-0.688713
C	3.553441	5.811284	0.429973
C	-3.590755	1.181011	-0.589226
C	-3.931416	2.493686	-0.251593
C	-5.2038	2.979787	-0.516584
C	-6.14883	2.168997	-1.135938
C	-5.814508	0.866208	-1.489379
C	-4.545961	0.374462	-1.215288
H	-2.794817	-1.217981	-0.256929
C	-0.744944	-1.688379	1.792456
C	-0.334456	-0.853425	2.840257
C	-0.547041	-1.179395	4.176733
C	-1.195464	-2.361914	4.511028
C	-1.626216	-3.207909	3.495086
C	-1.400699	-2.872521	2.164356
H	0.737361	-3.744019	0.562084
H	1.209343	-5.522845	-1.051567
H	0.423676	-5.329109	-3.396004
H	-0.829422	-3.305433	-4.095723
H	-1.284091	-1.518585	-2.486126
H	2.081271	-1.423942	1.601769
H	4.410021	-2.033331	1.113984
H	4.131748	-0.071704	-2.676856
H	1.801452	0.528336	-2.190801
H	5.904883	-2.292281	-1.867879
H	6.39525	-1.839807	-0.236868
H	6.439464	-0.648802	-1.540208
H	2.20517	1.515273	1.62385
H	3.636381	3.482835	1.847117
H	1.389553	5.475662	-1.200539
H	-0.096706	3.519108	-1.372099
H	3.052705	6.729695	0.121344
H	3.916529	5.945855	1.44993
H	4.429762	5.684593	-0.212755
H	-3.185101	3.115224	0.221642
H	-5.458303	3.995087	-0.239934
H	-7.139644	2.55099	-1.347124
H	-6.539869	0.233673	-1.984823
H	-4.299489	-0.633875	-1.524249
H	0.163795	0.082673	2.61541
H	-0.210277	-0.506379	4.956693
H	-1.363981	-2.620782	5.549211
H	-2.134981	-4.133125	3.739631
H	-1.740376	-3.556463	1.394593

14a TD-DFT Output

```
Excited State   1:      Singlet-A      3.2813 eV  377.85 nm  f=0.0928  <S**2>=0.000
    130 -> 131        0.69860
 This state for optimization and/or second-order correction.
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-A      3.5698 eV  347.32 nm  f=0.0425  <S**2>=0.000
    129 -> 131        0.69241

 Excited State   3:      Singlet-A      3.7040 eV  334.73 nm  f=0.0358  <S**2>=0.000
    126 -> 131       -0.25505
    127 -> 131        0.27822
    128 -> 131        0.59028

 Excited State   4:      Singlet-A      3.7158 eV  333.67 nm  f=0.0875  <S**2>=0.000
    126 -> 131       -0.34906
    127 -> 131        0.46424
    128 -> 131       -0.37874

 Excited State   5:      Singlet-A      3.7849 eV  327.58 nm  f=0.0115  <S**2>=0.000
    125 -> 131       -0.13797
    126 -> 131        0.51307
    127 -> 131        0.44589
    129 -> 131        0.10819

 Excited State   6:      Singlet-A      3.8712 eV  320.27 nm  f=0.0016  <S**2>=0.000
    125 -> 131        0.68470
    126 -> 131        0.16403

 Excited State   7:      Singlet-A      4.1987 eV  295.29 nm  f=0.0793  <S**2>=0.000
    122 -> 131        0.12748
    123 -> 131       -0.10501
    124 -> 131        0.67185

 Excited State   8:      Singlet-A      4.2023 eV  295.04 nm  f=0.0082  <S**2>=0.000
    119 -> 131        0.33850
    120 -> 131        0.11077
    122 -> 131       -0.31577
    123 -> 131        0.46385
    124 -> 131        0.18205

 Excited State   9:      Singlet-A      4.3551 eV  284.69 nm  f=0.1683  <S**2>=0.000
    119 -> 131       -0.17964
    120 -> 131       -0.10499
    122 -> 131        0.45237
```

123 -> 131 0.47886

Excited State 10: Singlet-A 4.4881 eV 276.25 nm f=0.0388 <S**2>=0.000
119 -> 131 0.45501
120 -> 131 0.24800
121 -> 131 0.19587
122 -> 131 0.37472
123 -> 131 -0.12611

Excited State 11: Singlet-A 4.5556 eV 272.16 nm f=0.0292 <S**2>=0.000
130 -> 132 0.67857

Excited State 12: Singlet-A 4.6023 eV 269.40 nm f=0.0524 <S**2>=0.000
119 -> 131 -0.31667
120 -> 131 0.43086
121 -> 131 0.38567
121 -> 133 -0.11132

Excited State 13: Singlet-A 4.6879 eV 264.48 nm f=0.1908 <S**2>=0.000
120 -> 131 -0.41435
121 -> 131 0.50393
130 -> 133 -0.16274

Excited State 14: Singlet-A 4.8405 eV 256.14 nm f=0.0249 <S**2>=0.000
120 -> 131 -0.12436
121 -> 131 0.10248
130 -> 133 0.60099
130 -> 134 0.18957
130 -> 135 -0.17651

Excited State 15: Singlet-A 4.8821 eV 253.96 nm f=0.0239 <S**2>=0.000
129 -> 132 0.66577
130 -> 135 -0.12053

Excited State 16: Singlet-A 4.8912 eV 253.48 nm f=0.0281 <S**2>=0.000
130 -> 133 -0.22581
130 -> 134 0.63687

Excited State 17: Singlet-A 4.9336 eV 251.31 nm f=0.0062 <S**2>=0.000
129 -> 132 0.17875
130 -> 133 0.11990
130 -> 134 0.13146
130 -> 135 0.59545

Excited State 18: Singlet-A 5.0048 eV 247.73 nm f=0.0159 <S**2>=0.000
128 -> 132 0.68829

Excited State 19: Singlet-A 5.0295 eV 246.51 nm f=0.0179 <S**2>=0.000
126 -> 132 -0.39739
127 -> 132 0.53627

Excited State 20: Singlet-A 5.0931 eV 243.43 nm f=0.0047 <S**2>=0.000
125 -> 132 -0.12296
126 -> 132 0.48645
127 -> 132 0.44794
130 -> 135 -0.10561

14b E_{tot}=-1967.0893804 au (NIMAG = 0)

Symbol	X	Y	Z
B	0.415773	-0.958492	0.848299
N	-1.010939	-0.425934	0.297836
C	-1.138658	0.899092	0.204914
N	-0.086896	1.729933	0.287110
C	1.145766	1.279710	0.056757
N	1.442913	-0.025937	0.013214
C	-2.012628	-1.304289	-0.264837
C	-2.736147	-2.196425	0.546650
C	-3.655946	-3.050409	-0.055023
H	-4.213408	-3.732581	0.577445
C	-3.884439	-3.058017	-1.427508
C	-3.154286	-2.169186	-2.204740
H	-3.303257	-2.158252	-3.278913
C	-2.217673	-1.295005	-1.655398
C	-2.600169	-2.230890	2.044688
H	-1.564732	-2.303010	2.365935
H	-3.141688	-3.084865	2.450701
H	-3.010791	-1.330799	2.510031
C	-4.863320	-4.020482	-2.045968
H	-5.764303	-4.118140	-1.437416
H	-4.425825	-5.018737	-2.138620
H	-5.161560	-3.697852	-3.044085
C	-1.457055	-0.385105	-2.584841
H	-1.518462	-0.756927	-3.607477
H	-0.404036	-0.312537	-2.315488
H	-1.864545	0.628864	-2.578950
C	-2.443132	1.584605	0.007036
C	-3.650249	1.109828	0.540050
H	-3.671254	0.189082	1.100427
C	-4.827811	1.812692	0.386405
H	-5.752727	1.448597	0.813386
C	-4.843865	3.017506	-0.322737
C	-3.653123	3.512497	-0.855272
H	-3.630441	4.445413	-1.398970
C	-2.474080	2.802929	-0.674299
H	-1.550149	3.203359	-1.064056
O	-6.049387	3.628924	-0.430801
C	-6.130999	4.864989	-1.124633
H	-5.515602	5.631890	-0.646073
H	-7.175910	5.162541	-1.081147
H	-5.828695	4.756229	-2.170006
C	2.184342	2.333627	-0.095443
C	1.883839	3.535108	-0.736020
H	0.901517	3.671224	-1.165455
C	2.827856	4.548813	-0.823218
H	2.575096	5.468571	-1.337752
C	4.090881	4.409015	-0.249235
C	4.377652	3.213463	0.415215
H	5.344252	3.084403	0.888668
C	3.448121	2.189568	0.485378
H	3.694608	1.280314	1.015037
C	5.115316	5.508665	-0.329236
H	5.418203	5.838275	0.667682
H	4.728494	6.374966	-0.865953
H	6.018299	5.170089	-0.843557
C	2.559435	-0.478795	-0.754424
C	2.728762	-0.032455	-2.065637
H	2.012195	0.658040	-2.490759
C	3.801123	-0.465497	-2.833937
H	3.903885	-0.100193	-3.849176
C	4.734702	-1.367878	-2.328897
C	4.545360	-1.827375	-1.024165
H	5.243743	-2.541778	-0.603351
C	3.479651	-1.397754	-0.249140
H	3.360677	-1.786121	0.749994
C	5.906175	-1.833367	-3.152128
H	6.845140	-1.422777	-2.770246
H	5.808809	-1.522361	-4.192606
H	5.999131	-2.921364	-3.132303
C	0.610295	-0.552378	2.428309
C	1.818235	-0.843677	3.083852
H	2.600383	-1.373206	2.554688
C	2.060420	-0.492877	4.406628
H	3.008721	-0.746554	4.866082
C	1.088607	0.180168	5.138263
H	1.269405	0.459098	6.169137
C	-0.116182	0.490044	4.523210
H	-0.885110	1.021013	5.072212
C	-0.341657	0.127890	3.197704
H	-1.294249	0.394650	2.760828
C	0.611949	-2.536870	0.520907
C	0.650364	-3.022635	-0.795731
H	0.571486	-2.331708	-1.625293
C	0.798149	-4.372177	-1.087831
H	0.822471	-4.700280	-2.120306
C	0.915667	-5.300027	-0.058540
H	1.032130	-6.354067	-0.280072
C	0.879543	-4.855702	1.255955
H	0.967143	-5.563707	2.071800

C	0.730071	-3.498863	1.532459	H	0.706492	-3.186585	2.568513

14a TD-DFT Output

Excited State 1: Singlet-A 3.2448 eV 382.10 nm f=0.1929 <S**2>=0.000
170 -> 171 0.70095
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.4467 eV 359.71 nm f=0.0662 <S**2>=0.000
169 -> 171 0.69784

Excited State 3: Singlet-A 3.5018 eV 354.06 nm f=0.0320 <S**2>=0.000
168 -> 171 0.69867

Excited State 4: Singlet-A 3.6246 eV 342.06 nm f=0.0314 <S**2>=0.000
165 -> 171 -0.13879
166 -> 171 -0.14117
167 -> 171 0.65559

Excited State 5: Singlet-A 3.6796 eV 336.95 nm f=0.0316 <S**2>=0.000
162 -> 171 0.14300
165 -> 171 0.12582
166 -> 171 0.64059
167 -> 171 0.20125

Excited State 6: Singlet-A 3.7904 eV 327.10 nm f=0.1210 <S**2>=0.000
162 -> 171 -0.20290
163 -> 171 0.15123
164 -> 171 0.54062
165 -> 171 -0.24738
166 -> 171 0.16448
167 -> 171 -0.13875

Excited State 7: Singlet-A 3.8127 eV 325.18 nm f=0.0338 <S**2>=0.000
163 -> 171 0.33490
164 -> 171 0.14912
165 -> 171 0.58239

Excited State 8: Singlet-A 3.8586 eV 321.32 nm f=0.0144 <S**2>=0.000
163 -> 171 0.56359
164 -> 171 -0.32896
165 -> 171 -0.23375

Excited State 9: Singlet-A 3.9842 eV 311.19 nm f=0.1209 <S**2>=0.000

159 -> 171 0.12471
161 -> 171 -0.13061
162 -> 171 0.57234
163 -> 171 0.16854
164 -> 171 0.24451
166 -> 171 -0.14305

Excited State 10: Singlet-A 4.1495 eV 298.79 nm f=0.0670 <S**2>=0.000
157 -> 171 0.30878
158 -> 171 -0.15892
159 -> 171 -0.23407
160 -> 171 0.36663
161 -> 171 0.32652
162 -> 171 0.22670

Excited State 11: Singlet-A 4.2954 eV 288.65 nm f=0.0090 <S**2>=0.000
160 -> 171 0.47909
161 -> 171 -0.47897
162 -> 171 -0.10796

Excited State 12: Singlet-A 4.3491 eV 285.08 nm f=0.0132 <S**2>=0.000
157 -> 171 -0.20759
158 -> 171 0.15989
159 -> 171 0.41931
160 -> 171 0.30648
161 -> 171 0.26601
170 -> 172 -0.18898

Excited State 13: Singlet-A 4.4575 eV 278.14 nm f=0.0519 <S**2>=0.000
158 -> 171 0.17844
161 -> 171 0.15057
170 -> 172 0.63755

Excited State 14: Singlet-A 4.5199 eV 274.31 nm f=0.0369 <S**2>=0.000
157 -> 171 0.35506
158 -> 171 -0.34363
159 -> 171 0.41326
161 -> 171 -0.11034
170 -> 172 0.10402
170 -> 174 -0.14598

Excited State 15: Singlet-A 4.5530 eV 272.31 nm f=0.0182 <S**2>=0.000
157 -> 171 0.38211
158 -> 171 0.45806
166 -> 173 -0.10822
170 -> 172 -0.12757
170 -> 173 -0.21282

Excited State 16: Singlet-A 4.6871 eV 264.52 nm f=0.0713 <S**2>=0.000
169 -> 172 0.65382

Excited State 17: Singlet-A 4.7937 eV 258.64 nm f=0.0001 <S**2>=0.000
168 -> 172 0.66133
169 -> 172 0.13948
170 -> 174 0.11408

Excited State 18: Singlet-A 4.8172 eV 257.38 nm f=0.0627 <S**2>=0.000
159 -> 171 0.15384
168 -> 172 -0.20113
169 -> 172 0.10001
169 -> 174 -0.11354
170 -> 173 0.34204
170 -> 174 0.45383
170 -> 175 -0.13326

Excited State 19: Singlet-A 4.8767 eV 254.24 nm f=0.0271 <S**2>=0.000
157 -> 171 0.15114
158 -> 171 0.11797
170 -> 173 0.35990
170 -> 174 -0.10274
170 -> 175 0.48352

Excited State 20: Singlet-A 4.8800 eV 254.07 nm f=0.0277 <S**2>=0.000
158 -> 171 -0.19916
169 -> 173 -0.15260
170 -> 173 -0.32610
170 -> 174 0.36667
170 -> 175 0.34841

14c E_{tot} = -3236.7325782 au (NIMAG = 0)

Symbol	X	Y	Z
C	-1.199183	0.987844	1.147844
C	-1.158664	1.982901	2.125445
C	0.061819	2.461849	2.580156
C	1.247968	1.989441	2.037956
C	1.224671	0.994625	1.057336
C	-0.00377	0.475821	0.648411
C	-2.499094	0.383129	0.723711
C	2.483123	0.396663	0.519805
H	0.088484	3.209893	3.361844
H	2.190315	2.381624	2.391163
H	-2.077708	2.36532	2.546258
H	-0.022515	-0.339566	-0.059078
N	3.54717	1.128782	0.216786
N	2.435634	-0.929439	0.388866
C	3.509593	-1.640082	0.037488
N	4.722795	-1.123721	-0.102319
C	5.883176	-1.977017	-0.082721
C	6.141762	-2.750987	1.047089
C	6.788599	-2.006362	-1.138432
C	7.918519	-2.812677	-1.066071
C	7.270204	-3.553822	1.107129
C	8.183447	-3.600032	0.052859
H	6.612357	-1.405664	-2.017976
H	5.459824	-2.712759	1.886029
H	7.448008	-4.147694	1.996317
H	8.606348	-2.827091	-1.903747
C	3.22284	-3.087674	-0.185669
C	2.341289	-3.743035	0.677413
C	2.022032	-5.078789	0.476004
C	2.552104	-5.767273	-0.609797
C	3.404501	-5.112448	-1.492455
C	3.746375	-3.784476	-1.277727
H	4.413998	-3.2877	-1.966719
H	1.350465	-5.578142	1.162621
H	1.908658	-3.193128	1.501173
H	2.299051	-6.807844	-0.77105
H	3.808071	-5.637303	-2.349011
N	-3.543081	1.127239	0.373809
N	-2.505478	-0.949058	0.768242
C	-3.588531	-1.647213	0.409057
N	-4.765269	-1.099509	0.153668
B	-5.033077	0.487614	0.319549
C	-3.357374	-3.122975	0.352156
C	-4.189056	-4.028354	1.013636
C	-3.902086	-5.386791	0.996824
C	-2.794553	-5.859757	0.302454
C	-1.957872	-4.963131	-0.353404
C	-2.227121	-3.602133	-0.312256
H	-5.056529	-3.6738	1.551299
H	-2.580488	-6.921033	0.279268
H	-4.548639	-6.076228	1.524737
H	-1.557859	-2.900521	-0.790446
H	-1.085554	-5.319674	-0.885877
C	-5.843988	-1.89042	-0.381465
C	-7.013946	-2.079389	0.346198
C	-8.055733	-2.824326	-0.192477
C	-7.966003	-3.387118	-1.464989
C	-6.789813	-3.177736	-2.185939
C	-5.743935	-2.436145	-1.657702
H	-7.106308	-1.651116	1.3343
H	-8.956121	-2.969704	0.393225
H	-4.846323	-2.273848	-2.23902
H	-6.690488	-3.59527	-3.181178
C	-5.813458	0.976368	-1.023052
C	-5.754115	0.758008	1.763993
C	-6.671844	1.793228	1.999733
C	-7.219251	2.031611	3.257123
C	-6.860982	1.236854	4.33908
C	-5.946599	0.208197	4.145242
C	-5.410183	-0.019469	2.882147
H	-7.928206	2.840611	3.389872
H	-6.963899	2.442053	1.184456
H	-5.648318	-0.417627	4.978233
H	-7.285852	1.41747	5.318889
H	-4.700235	-0.830967	2.773683
C	-5.115258	1.132062	-2.2292
C	-7.203083	1.139821	-1.095221
C	-7.852063	1.468609	-2.282062
C	-5.747264	1.460964	-3.422346
C	-7.125486	1.639566	-3.452999
H	-7.625725	1.898211	-4.378365
H	-5.164401	1.575745	-4.328855
H	-7.806978	0.986461	-0.211227

H	-8.929581	1.58435	-2.290386
H	-4.042465	0.984208	-2.245148
C	3.418413	2.543278	-0.015182
C	2.596509	2.993159	-1.046197
C	2.48458	4.348405	-1.317193
C	3.195951	5.295705	-0.580614
C	4.0227	4.831294	0.441413
C	4.141546	3.475912	0.722456
H	4.792408	3.145728	1.518333
H	4.587728	5.540988	1.03481
H	1.840671	4.672988	-2.126349
H	2.053382	2.274318	-1.645246
C	-3.352903	2.520153	0.064467
C	-4.02239	3.518295	0.763128
C	-3.838815	4.854919	0.426326
C	-2.988494	5.237022	-0.60782
C	-2.319488	4.225411	-1.300204
C	-2.499178	2.891339	-0.974908
H	-4.67502	3.256726	1.581418
H	-4.36986	5.614241	0.988512
H	-1.978281	2.1268	-1.535848
H	-1.654159	4.484298	-2.115916
C	-2.788881	6.68468	-0.970052
H	-3.431326	7.334272	-0.375459
H	-3.014056	6.864096	-2.024026
H	-1.754052	6.995128	-0.803389
C	3.102256	6.763465	-0.903208
H	2.110148	7.028261	-1.272104
H	3.822274	7.041038	-1.678726
H	3.313842	7.377929	-0.027161
C	9.426239	-4.44583	0.13889
H	9.227034	-5.398537	0.632622
H	10.206063	-3.938973	0.714804
H	9.833877	-4.655158	-0.850736
C	-9.110941	-4.165489	-2.057208
H	-9.753717	-4.580913	-1.280163
H	-8.753904	-4.98816	-2.678936
H	-9.73324	-3.526138	-2.690262
B	4.988421	0.467635	-0.083634
C	6.003206	0.752664	1.162497
C	5.432095	0.979551	-1.56798
C	5.514446	0.783739	2.477691
C	6.348687	0.931889	3.580446
C	7.722276	1.049773	3.401059
C	8.241116	1.005989	2.112935
C	7.393055	0.857035	1.0192
H	7.832194	0.806061	0.031567
H	4.448451	0.687454	2.653116
H	5.927418	0.952216	4.578858
H	8.379194	1.167557	4.254238
H	9.310845	1.082967	1.957134
C	4.854263	0.406971	-2.711392
C	5.129534	0.864475	-3.99532
C	6.29205	2.063083	-1.788983
C	6.577472	2.532807	-3.068082
C	6.001064	1.932079	-4.18014
H	4.662384	0.390301	-4.850764
H	6.222309	2.293916	-5.17686
H	4.165903	-0.424286	-2.600971
H	6.743687	2.566897	-0.944421
H	7.248812	3.3742	-3.19428

14c TD-DFT Output

Excited State 1: Singlet-A 3.2570 eV 380.66 nm f=0.1500 <S**2>=0.000
277 -> 280 0.10952
278 -> 280 0.38113
279 -> 280 -0.40247
279 -> 281 0.41485
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.2599 eV 380.33 nm f=0.1302 <S**2>=0.000
278 -> 280 0.44978
278 -> 281 0.24030
279 -> 280 0.46231

Excited State 3: Singlet-A 3.3469 eV 370.45 nm f=0.0049 <S**2>=0.000
275 -> 280 0.46679
275 -> 281 0.23532
276 -> 280 0.36595
276 -> 281 0.19634
277 -> 280 -0.19675

Excited State 4: Singlet-A 3.3592 eV 369.09 nm f=0.0872 <S**2>=0.000
274 -> 280 -0.10323
275 -> 280 0.16448
275 -> 281 0.11661
277 -> 280 0.50229
277 -> 281 -0.35538
278 -> 281 0.20249

Excited State 5: Singlet-A 3.3843 eV 366.35 nm f=0.1552 <S**2>=0.000
274 -> 281 0.18663
275 -> 280 -0.38073
275 -> 281 -0.13072
276 -> 280 0.49668
276 -> 281 0.15049
277 -> 281 -0.14814

Excited State 6: Singlet-A 3.3997 eV 364.70 nm f=0.0537 <S**2>=0.000
274 -> 280 0.50555
274 -> 281 -0.41702
275 -> 281 -0.13702
276 -> 281 0.13327

Excited State 7: Singlet-A 3.4372 eV 360.71 nm f=0.0256 <S**2>=0.000
277 -> 281 -0.17737
278 -> 280 -0.30764

279 -> 280 0.21999
279 -> 281 0.52498

Excited State 8: Singlet-A 3.5162 eV 352.61 nm f=0.0222 <S**2>=0.000
272 -> 280 -0.10506
273 -> 280 0.16576
276 -> 281 0.27767
277 -> 281 0.12190
278 -> 280 -0.10441
278 -> 281 0.50930
279 -> 280 -0.21364

Excited State 9: Singlet-A 3.5408 eV 350.16 nm f=0.0064 <S**2>=0.000
272 -> 280 0.61177
272 -> 281 0.26648
273 -> 281 -0.12469
278 -> 281 0.11742

Excited State 10: Singlet-A 3.5589 eV 348.38 nm f=0.0253 <S**2>=0.000
272 -> 281 -0.10983
273 -> 280 0.49135
273 -> 281 -0.42564
278 -> 281 -0.16345

Excited State 11: Singlet-A 3.5955 eV 344.83 nm f=0.0077 <S**2>=0.000
270 -> 280 0.23330
270 -> 281 0.10183
276 -> 280 0.11419
277 -> 280 0.36653
277 -> 281 0.46914
278 -> 280 -0.12799
279 -> 281 0.11001

Excited State 12: Singlet-A 3.6216 eV 342.35 nm f=0.0169 <S**2>=0.000
270 -> 280 0.54102
270 -> 281 0.22030
271 -> 281 0.14790
276 -> 280 -0.11419
276 -> 281 0.13409
277 -> 281 -0.22311
278 -> 281 -0.11399

Excited State 13: Singlet-A 3.6283 eV 341.72 nm f=0.0145 <S**2>=0.000
270 -> 280 -0.18271
270 -> 281 -0.16410
276 -> 280 -0.21161
276 -> 281 0.51712

277 -> 280 0.14928
278 -> 280 0.10545
278 -> 281 -0.23708

Excited State 14: Singlet-A 3.6349 eV 341.09 nm f=0.0252 <S**2>=0.000
269 -> 280 0.10922
270 -> 281 0.11609
271 -> 280 0.50856
271 -> 281 -0.42727

Excited State 15: Singlet-A 3.6778 eV 337.11 nm f=0.0011 <S**2>=0.000
274 -> 281 -0.10879
275 -> 280 -0.30427
275 -> 281 0.60937

Excited State 16: Singlet-A 3.7186 eV 333.42 nm f=0.0004 <S**2>=0.000
274 -> 280 0.46440
274 -> 281 0.49494
275 -> 280 0.10387

Excited State 17: Singlet-A 3.7527 eV 330.38 nm f=0.0267 <S**2>=0.000
268 -> 280 0.60703
268 -> 281 0.26017
269 -> 280 0.12315
269 -> 281 0.12949

Excited State 18: Singlet-A 3.7623 eV 329.54 nm f=0.0287 <S**2>=0.000
268 -> 281 0.13894
269 -> 280 0.51679
269 -> 281 -0.40876

Excited State 19: Singlet-A 3.7908 eV 327.06 nm f=0.0427 <S**2>=0.000
254 -> 280 0.14420
263 -> 280 -0.12422
266 -> 280 0.31549
266 -> 281 0.14131
267 -> 280 -0.19322
267 -> 281 -0.21240
269 -> 281 0.12882
273 -> 280 -0.25256
273 -> 281 -0.29476

Excited State 20: Singlet-A 3.8030 eV 326.01 nm f=0.0476 <S**2>=0.000
255 -> 280 0.11235
255 -> 281 -0.14373
264 -> 281 -0.10458
265 -> 280 0.11664

265 -> 281	-0.12166
266 -> 280	-0.21560
266 -> 281	0.17795
267 -> 280	-0.35313
267 -> 281	0.36183
272 -> 281	0.12067
273 -> 281	-0.10591

14e: E_{tot} = -4045.60335017au (NIMAG = 0)

Symbol	X	Y	Z
6	0.272222	4.780795	1.359475
6	0.801557	2.774233	0.334189
7	1.810209	3.279416	-0.373459
5	2.418495	4.736806	-0.048060
7	1.280079	5.403432	0.800931
6	0.389469	1.340623	0.225183
6	1.320692	0.306135	0.231680
6	0.903902	-1.024047	0.233340
6	-0.456540	-1.314078	0.248190
6	-1.400955	-0.287441	0.239280
6	-0.971565	1.035010	0.238625
6	1.945032	-2.092844	0.356575
6	-2.846621	-0.654551	0.366300
7	2.000454	-3.132149	-0.465445
5	3.125127	-4.285686	-0.302306
7	3.713717	-3.987291	1.121079
6	3.637786	-2.835179	1.745876
7	2.785985	-1.874108	1.374493
6	4.348427	-4.077191	-1.363455
6	2.447639	-5.763445	-0.295271
6	2.301223	-6.539756	-1.453542
6	1.690131	-7.788545	-1.431930
6	1.201414	-8.307912	-0.237797
6	1.327938	-7.562237	0.927822
6	1.940259	-6.312547	0.890288
6	5.187049	-5.136875	-1.740529
6	6.314883	-4.944425	-2.533044
6	6.647348	-3.670877	-2.977899
6	5.844904	-2.596594	-2.610805
6	4.723010	-2.803370	-1.815606
6	4.063668	-1.619636	3.878120
6	4.827955	-1.365324	5.003889
6	6.035649	-2.033458	5.227071
6	6.452278	-2.964623	4.276416
6	5.687695	-3.230996	3.148803
6	6.856736	-1.748248	6.455283
6	4.477691	-2.567341	2.936565
6	1.112496	-3.219777	-1.598960
6	1.315036	-2.419100	-2.717153
6	0.475699	-2.530123	-3.819897
6	-0.577291	-3.441508	-3.842195
6	-0.769200	-4.237993	-2.710735
6	0.061497	-4.135135	-1.605026
6	-1.481750	-3.569512	-5.039812
1	4.324665	-4.681346	1.526171
7	-3.071157	-1.515441	1.366701
6	-4.325599	-1.775271	1.746711
7	-5.365702	-1.237971	1.151970
5	-5.345009	-0.547465	-0.255960
7	-3.782082	-0.162117	-0.435384
6	-5.810255	-1.681816	-1.334207
6	-6.274352	0.785902	-0.204641
6	-6.467656	1.479021	0.998138
6	-7.235749	2.637764	1.072353
6	-7.838484	3.145505	-0.072038
6	-7.662532	2.482851	-1.282225
6	-6.894853	1.325064	-1.340365
6	-4.913026	-2.626230	-1.853381
6	-5.327290	-3.678101	-2.663535
6	-6.672958	-3.828833	-2.978076
6	-7.591346	-2.920420	-2.466164
6	-7.161880	-1.870324	-1.660145
6	-4.506659	-2.672922	2.911181
6	-3.469602	-2.833696	3.833596
6	-3.628362	-3.659994	4.934601
6	-4.816506	-4.361952	5.149111
6	-5.841175	-4.214926	4.212463
6	-5.693090	-3.383763	3.112560
6	-0.702901	5.520164	2.197880
6	2.609726	5.592833	-1.420048
6	1.515387	6.235553	-2.016295
6	1.632705	6.961580	-3.197606
6	2.865952	7.064350	-3.829532
6	3.969666	6.432885	-3.267526
6	3.837393	5.713507	-2.084416
6	3.731082	4.648137	0.916309
6	4.013738	3.528329	1.710223
6	5.071768	3.507160	2.614274
6	5.882575	4.625585	2.764401
6	5.620971	5.758585	2.002065
6	4.565838	5.762126	1.095842
6	-0.857453	6.905668	2.108696
6	-1.774806	7.570011	2.909452
6	-2.564966	6.878014	3.827728
6	-2.407056	5.492632	3.912103
6	-1.500754	4.820983	3.108298
6	-3.575702	7.593962	4.681783
6	-4.993088	-5.236583	6.360431
6	-3.422739	0.666398	-1.560484
6	-3.697330	2.032813	-1.548496

6	-3.372471	2.820853	-2.642238	1	-8.124924	2.868932	-2.183110
6	-2.774876	2.275500	-3.780771	1	-6.770726	0.832401	-2.296910
6	-2.508241	0.908424	-3.778642	1	-3.859295	-2.552775	-1.611826
6	-2.827184	0.109558	-2.686305	1	-4.600062	-4.385844	-3.044207
6	-2.427388	3.143475	-4.961655	1	-7.001130	-4.645673	-3.609249
6	2.322844	2.589974	-1.524807	1	-8.645145	-3.027152	-2.696021
6	1.487240	2.313724	-2.602334	1	-7.902913	-1.179147	-1.276825
6	1.990220	1.696723	-3.740558	1	-2.543470	-2.301566	3.669364
6	3.335348	1.346818	-3.842415	1	-2.812678	-3.766315	5.640262
6	4.163707	1.639733	-2.757129	1	-6.763688	-4.769204	4.338548
6	3.672504	2.255177	-1.615108	1	-6.496312	-3.327633	2.388208
6	3.883289	0.679060	-5.076202	1	0.537869	6.165129	-1.550796
1	1.384150	6.383661	1.017873	1	0.762044	7.446289	-3.624126
1	-6.267937	-1.424784	1.564286	1	2.966076	7.629262	-4.748405
7	0.064233	3.466762	1.206647	1	4.937173	6.502092	-3.750918
1	2.377936	0.520093	0.268640	1	4.715474	5.235263	-1.668426
1	-0.799133	-2.335797	0.302636	1	3.394438	2.642484	1.628270
1	-1.681274	1.845687	0.282030	1	5.260124	2.616636	3.202398
1	2.667195	-6.157006	-2.398349	1	6.707895	4.614901	3.465869
1	1.594651	-8.358078	-2.348978	1	6.243684	6.639247	2.108563
1	0.727780	-9.281920	-0.216852	1	4.393017	6.656428	0.507634
1	0.948902	-7.951497	1.865573	1	-0.284918	7.481728	1.392059
1	2.012760	-5.746115	1.812731	1	-1.881448	8.644097	2.815221
1	4.956667	-6.141864	-1.408300	1	-3.006023	4.930667	4.619442
1	6.933734	-5.791960	-2.804083	1	-1.390440	3.748361	3.175546
1	7.522012	-3.516376	-3.597917	1	-4.586681	7.454011	4.288392
1	6.097637	-1.594696	-2.937758	1	-3.572123	7.212614	5.704408
1	4.134184	-1.939103	-1.531624	1	-3.381146	8.666012	4.716790
1	3.135392	-1.092990	3.709002	1	-5.402137	-4.662583	7.197282
1	4.483728	-0.632015	5.724259	1	-4.042541	-5.658261	6.689339
1	7.394206	-3.482095	4.412915	1	-5.682073	-6.058536	6.162316
1	6.065248	-3.933497	2.416014	1	-4.161717	2.478330	-0.680773
1	7.089708	-0.683983	6.535665	1	-3.592995	3.881606	-2.608987
1	7.796829	-2.299525	6.443988	1	-2.047103	0.451547	-4.646225
1	6.315022	-2.027691	7.362632	1	-2.606147	-0.947739	-2.712136
1	2.127650	-1.707121	-2.731112	1	-3.289295	3.728293	-5.290446
1	0.653382	-1.896113	-4.680425	1	-1.633422	3.852428	-4.712376
1	-1.578414	-4.958866	-2.693638	1	-2.085744	2.545628	-5.806890
1	-0.102951	-4.767295	-0.744155	1	0.442816	2.592589	-2.555982
1	-2.505959	-3.272768	-4.799504	1	1.322115	1.499091	-4.570478
1	-1.138247	-2.944502	-5.864364	1	5.217136	1.388483	-2.805891
1	-1.521616	-4.601444	-5.396087	1	4.337104	2.477414	-0.792450
1	-5.998737	1.112165	1.905093	1	4.158800	-0.360246	-4.877309
1	-7.362338	3.143271	2.022689	1	4.781171	1.186695	-5.435109
1	-8.438821	4.045846	-0.022167	1	3.152187	0.679671	-5.885043

14e TD-DFT Output

Excitation energies and oscillator strengths:

```
Excited State   1:      Singlet-A      3.2829 eV  377.67 nm  f=0.0803  <S**2>=0.000
   348 -> 349        0.68092
   348 -> 351       -0.15425
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) =  -4045.48270684
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State   2:      Singlet-A      3.4247 eV  362.03 nm  f=0.0698  <S**2>=0.000
   346 -> 349        0.27601
   346 -> 350        0.55754
   346 -> 351        0.24292
   347 -> 349       -0.13184
   347 -> 351       -0.13016

Excited State   3:      Singlet-A      3.4359 eV  360.85 nm  f=0.0551  <S**2>=0.000
   346 -> 349       -0.12545
   346 -> 351       -0.12479
   347 -> 349       -0.29729
   347 -> 350        0.50599
   347 -> 351       -0.30906

Excited State   4:      Singlet-A      3.5414 eV  350.10 nm  f=0.0057  <S**2>=0.000
   348 -> 350        0.68019

Excited State   5:      Singlet-A      3.5639 eV  347.89 nm  f=0.0499  <S**2>=0.000
   345 -> 349        0.61820
   345 -> 351       -0.14530
   346 -> 349       -0.13601
   347 -> 349        0.16361
   347 -> 350        0.10695

Excited State   6:      Singlet-A      3.5779 eV  346.53 nm  f=0.0033  <S**2>=0.000
   345 -> 349        0.18661
   346 -> 349        0.57834
   346 -> 350       -0.27900
   347 -> 349       -0.12675

Excited State   7:      Singlet-A      3.5896 eV  345.39 nm  f=0.0004  <S**2>=0.000
   345 -> 349       -0.16507
   346 -> 349        0.17316
   347 -> 349        0.54749
   347 -> 350        0.34107
```

Excited State 8: Singlet-A 3.6874 eV 336.23 nm f=0.0754 <S**2>=0.000
339 -> 349 -0.11966
341 -> 349 0.54682
341 -> 351 -0.13819
342 -> 349 -0.26854
344 -> 349 -0.12237
348 -> 351 -0.12189

Excited State 9: Singlet-A 3.6970 eV 335.37 nm f=0.0489 <S**2>=0.000
331 -> 350 -0.11674
337 -> 350 -0.10422
338 -> 349 0.10550
340 -> 349 -0.11060
340 -> 350 -0.15347
341 -> 349 0.23395
342 -> 350 -0.12616
343 -> 349 -0.12385
343 -> 350 -0.21886
344 -> 349 0.25628
344 -> 350 -0.13384
344 -> 351 0.21179
348 -> 351 0.27427

Excited State 10: Singlet-A 3.7037 eV 334.76 nm f=0.0344 <S**2>=0.000
338 -> 350 0.11922
340 -> 350 -0.13687
342 -> 349 -0.12021
342 -> 350 0.14878
342 -> 351 -0.10406
343 -> 349 -0.12099
343 -> 350 -0.13124
343 -> 351 -0.10616
344 -> 349 -0.11457
344 -> 350 0.43705
344 -> 351 -0.14682
348 -> 351 0.23516

Excited State 11: Singlet-A 3.7200 eV 333.29 nm f=0.0563 <S**2>=0.000
333 -> 349 -0.20345
336 -> 349 -0.19234
339 -> 349 0.39998
341 -> 349 0.12175
343 -> 350 0.22258
344 -> 349 -0.21419
348 -> 351 0.24497

Excited State 12: Singlet-A 3.7271 eV 332.66 nm f=0.0218 <S**2>=0.000

339 -> 349 0.17822
340 -> 350 0.11944
341 -> 350 0.13961
341 -> 351 -0.12450
342 -> 349 -0.25533
342 -> 350 0.34549
342 -> 351 -0.25098
343 -> 350 -0.19329
344 -> 349 0.15919
344 -> 350 -0.17678
344 -> 351 0.14675
347 -> 350 -0.11004

Excited State 13: Singlet-A 3.7335 eV 332.09 nm f=0.0665 <S**2>=0.000
340 -> 349 0.23842
340 -> 350 0.43950
340 -> 351 0.23007
342 -> 350 -0.15527
343 -> 349 -0.16268
343 -> 350 -0.24107
343 -> 351 -0.15266
344 -> 350 0.13244
348 -> 351 0.11049

Excited State 14: Singlet-A 3.7427 eV 331.27 nm f=0.0447 <S**2>=0.000
339 -> 349 -0.29297
342 -> 350 0.10600
343 -> 349 0.20585
343 -> 350 0.14396
344 -> 350 -0.17687
348 -> 351 0.47312

Excited State 15: Singlet-A 3.7685 eV 329.00 nm f=0.0072 <S**2>=0.000
332 -> 349 -0.10500
338 -> 349 -0.16098
340 -> 350 -0.10413
343 -> 350 -0.22260
344 -> 349 -0.24319
345 -> 350 0.21136
346 -> 351 0.15367
347 -> 349 -0.12040
347 -> 350 0.18797
347 -> 351 0.35887

Excited State 16: Singlet-A 3.7824 eV 327.79 nm f=0.0172 <S**2>=0.000
333 -> 349 0.26926
336 -> 349 0.24864

337 -> 349 0.20868
338 -> 349 0.17079
339 -> 349 0.36524
344 -> 349 0.10836
347 -> 351 0.21198

Excited State 17: Singlet-A 3.7901 eV 327.12 nm f=0.0019 <S**2>=0.000
333 -> 349 -0.12586
334 -> 349 0.13488
337 -> 349 -0.17007
338 -> 349 0.10119
339 -> 349 -0.14590
340 -> 350 0.10543
342 -> 350 0.10984
343 -> 349 -0.18712
343 -> 350 0.13487
344 -> 349 0.12047
345 -> 350 -0.14078
346 -> 350 0.11632
347 -> 350 0.17663
347 -> 351 0.42145

Excited State 18: Singlet-A 3.8072 eV 325.66 nm f=0.0070 <S**2>=0.000
334 -> 350 0.10118
337 -> 349 -0.13389
337 -> 351 -0.10254
338 -> 349 -0.14820
338 -> 350 0.39614
338 -> 351 -0.14846
342 -> 350 -0.10586
346 -> 350 0.10985
346 -> 351 -0.29292

Excited State 19: Singlet-A 3.8148 eV 325.01 nm f=0.0098 <S**2>=0.000
331 -> 350 0.13210
334 -> 350 -0.12872
337 -> 349 0.17695
337 -> 350 0.40567
337 -> 351 0.13550
338 -> 349 -0.19268
338 -> 351 -0.19395
339 -> 350 -0.10946
340 -> 349 -0.11732
340 -> 350 -0.14223
343 -> 350 -0.11094
345 -> 350 -0.14175
346 -> 351 -0.11848

Excited State 20: Singlet-A 3.8258 eV 324.07 nm f=0.0035 <S**2>=0.000

338 -> 350	0.23467
338 -> 351	-0.10533
344 -> 349	0.12674
345 -> 350	-0.20406
346 -> 350	-0.19576
346 -> 351	0.51036
347 -> 350	0.10064

Def2-TZVP basis set details as obtained from EMSL Basis Set Exchange Library[2] (https://bse.pnl.gov/bse/portal)

```
 !  Def2-TZVP  EMSL  Basis Set Exchange Library   8/8/12 8:15 AM
 ! Elements                      References
 ! --------                     ----------
 ! H He Li Be B C N O F Ne Na Mg Al Si P S Cl Ar K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge
 As Se Br Kr Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe Cs Ba La Hf Ta W Re Os
 Ir Pt Au Hg Tl Pb Bi Po At Rn: F. Weigend and R. Ahlrichs, Balanced basis sets of split valence,
 triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of
 accuracy Phys. Chem. Chem. Phys. 2005, 7, 3297-3305.
 !
 ****
 H     0
 S   3   1.00
      34.0613410           0.60251978E-02
       5.1235746           0.45021094E-01
       1.1646626           0.20189726
 S   1   1.00
       0.32723041          1.0000000
 S   1   1.00
       0.10307241          1.0000000
 P   1   1.00
       0.8000000           1.0000000
 ****
 B     0
 S   6   1.00
    8564.8660687           0.22837198155E-03
    1284.1516263           0.17682576447E-02
     292.27871604          0.91407080516E-02
      82.775469176         0.36342638989E-01
      27.017939269           0.11063458441
       9.8149619660          0.23367344321
 S   2   1.00
       3.9318559059          0.41818777978
       1.6595599712          0.22325473798
 S   1   1.00
       0.35762965239         1.0000000
 S   1   1.00
       0.14246277496         1.0000000
 S   1   1.00
       0.60560594768E-01           1.0000000
 P   4   1.00
      22.453875803           0.50265575179E-02
       5.1045058330          0.32801738965E-01
       1.4986081344            0.13151230768
       0.50927831315           0.33197167769
 P   1   1.00
       0.18147077798         1.0000000
 P   1   1.00
       0.64621893904E-01     1.0000000
 D   1   1.00
       0.66100000            1.0000000
 D   1   1.00
       0.19900000            1.0000000
 F   1   1.00
       0.49000000            1.0000000
 ****
 C     0
 S   6   1.00
    13575.3496820          0.22245814352E-03
     2035.2333680          0.17232738252E-02
      463.22562359         0.89255715314E-02
      131.20019598         0.35727984502E-01
       42.853015891          0.11076259931
       15.584185766          0.24295627626
 S   2   1.00
        6.2067138508         0.41440263448
        2.5764896527         0.23744968655
 S   1   1.00
        0.57696339419         1.0000000
 S   1   1.00
        0.22972831358         1.0000000
 S   1   1.00
        0.95164440028E-01           1.0000000
 P   4   1.00
       34.697232244           0.53333657805E-02
        7.9582622826          0.35864109092E-01
        2.3780826883          0.14215873329
        0.81433208183         0.34270471845
 P   1   1.00
        0.28887547253         1.0000000
 P   1   1.00
        0.10056823671         1.0000000
```

```
D   1   1.00
     1.09700000          1.0000000
D   1   1.00
     0.31800000          1.0000000
F   1   1.00
     0.76100000          1.0000000
****
N     0
S   6   1.00
  19730.8006470         0.21887984991E-03
   2957.8958745         0.16960708803E-02
    673.22133595        0.87954603538E-02
    190.68249494        0.35359382605E-01
     62.295441898         0.11095789217
     22.654161182         0.24982972552
S   2   1.00
      8.9791477428        0.40623896148
      3.6863002370        0.24338217176
S   1   1.00
     0.84660076805         1.0000000
! Elements                   References
! --------                   ----------
! Y-Cd(ecp-28), Hf-Hg(ecp-46): D. Andrae,U. Haeussermann, M.Dolg, H.Stoll, H.Preuss,
Theor.Chim.Acta, 1990, 77, 123?141.
! In-Sb(ecp-28), Tl-Bi(ecp-46): B. Metz, H. Stoll, M. Dolg, J. Chem. Phys., 2000, 113,
2563?2569.
! Te-Xe(ecp-28), Po-Rn(ecp-46): K. A. Peterson, D. Figgen, E. Goll, H. Stoll, M. Dolg, J. Chem.
Phys., 2003, 119, 11113?11123.
! Rb(ecp-28), Cs(ecp-46): T.Leininger, A.Nicklass, W.Kuechle, H.Stoll, M.Dolg, A.Bergner,
Chem. Phys. Lett., 1996, 255, 274?280.
! Sr(ecp-28), Ba(ecp-46): M. Kaupp, P. V. Schleyer, H. Stoll and H. Preuss, J. Chem. Phys.,
1991, 94, 1360?1366.!
S   1   1.00
     0.33647133771         1.0000000
S   1   1.00
     0.13647653675         1.0000000
P   4   1.00
    49.200380510        0.55552416751E-02
    11.346790537        0.38052379723E-01
     3.4273972411         0.14953671029
     1.1785525134         0.34949305230
P   1   1.00
     0.41642204972         1.0000000
P   1   1.00
     0.14260826011         1.0000000
D   1   1.00
     1.65400000          1.0000000
D   1   1.00
     0.46900000          1.0000000
F   1   1.00
     1.09300000          1.0000000
****
```

X-Ray Crystal Structure Analysis

General Procedures. For **14a-c**, and **14e**: Data sets were collected with a Nonius KappaCCD diffractometer or a Rigaku CCD diffractometer with rotating anode generator. Programs used: data collection, COLLECT (R. W. W. Hooft, Bruker AXS, 2008, Delft, The Netherlands) and CrystalClear (Rigaku Corp., 2000); data reduction Denzo-SMN (Z. Otwinowski, W. Minor, Methods Enzymol. 1997, 276, 307-326); absorption correction, Denzo (Z. Otwinowski, D. Borek, W. Majewski, W. Minor, Acta Crystallogr. 2003, A59, 228-234); structure solution SHELXS-97 (G. M. Sheldrick, Acta Crystallogr. 1990, A46, 467-473); structure refinement SHELXL-97 (G. M. Sheldrick, Acta Crystallogr. 2008, A64, 112-122) and graphics, XP (BrukerAXS, 2000). R-values are given for observed reflections, and wR2 values are given for all reflections.

Exceptions and special features: The hydrogen at N1 atom in compound **14a** was refined freely. For compound **14e** a badly disordered acetonitril molecule was found in the asymmetrical unit and could not be satisfactorily refined. The program SQUEEZE (A. L. Spek J. Appl. Cryst., 2003, 36, 7-13) was therefore used to remove mathematically the effect of the solvent. The quoted formula and derived parameters are not included the squeezed solvent molecule.

X-Ray data for 14a

formula $C_{34}H_{30}BN_3$, M = 491.42, yellow crystal, 0.30 x 0.15 x 0.15 mm, a = 14.9147(6), b = 10.5759(4), c = 16.7471(8) Å, β = 90.479(2)°, V = 2640.7(2) Å^3, ρ_{calc} = 1.236 gcm^{-3}, μ = 0.551 mm^{-1}, empirical absorption correction ($0.852 \leq T \leq 0.921$), Z = 4, monoclinic, space group $P2_1/n$ (No. 14), λ = 1.54178 Å, T = 223(2) K, ω and φ scans, 11940 reflections collected ($\pm h$, $\pm k$, $\pm l$), [(sinθ)/λ] = 0.60 Å^{-1}, 3995 independent (R_{int} = 0.039) and 3482 observed reflections [$I>2\sigma(I)$], 348 refined parameters, R = 0.050, wR^2 = 0.134, max. (min.) residual electron density 0.22 (-0.25) e.Å^{-3}, the hydrogen at N1 atom was refined freely; others were calculated and refined as riding atoms.

CCDC 1011607 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (internat.) +44(1223)336-033, E-mail: deposit@ccdc.cam.ac.uk].

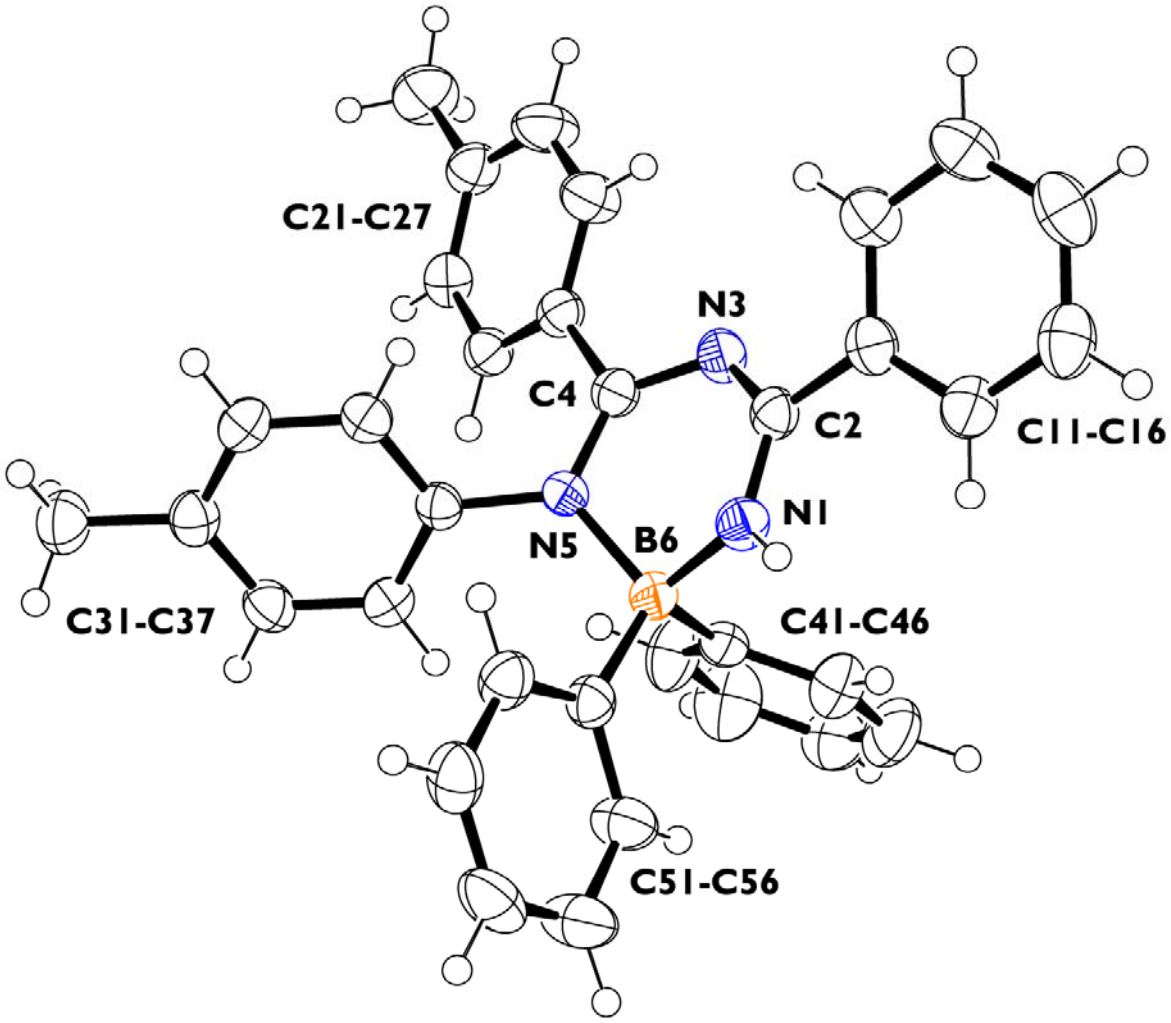


Figure S 14. Oak Ridge Thermal Ellipsoid Plot (ORTEP) of **14a**. Thermal ellipsoids shown at a 50% probability level.

X-Ray data for 14b

formula $C_{44}H_{42}BN_3O$, M = 639.62, yellow crystal, 0.35 x 0.30 x 0.02 mm, a = 41.2640(6), b = 10.5501(2), c = 16.9777(3) Å, β = 100.091(1)°, V = 7276.7(2) Å^3, ρ_{calc} = 1.168 gcm^{-3}, μ = 0.069 mm^{-1}, empirical absorption correction ($0.976 \leq T \leq 0.998$), Z = 8, monoclinic, space group $C2/c$ (No. 15), λ = 0.71073 Å, T = 223(2) K, ω and φ scans, 26763 reflections collected ($\pm h$, $\pm k$, $\pm l$), [(sinθ)/λ] = 0.62 Å^{-1}, 7286 independent (R_{int} = 0.053) and 4708 observed reflections [$I>2\sigma(I)$], 448 refined parameters, R = 0.076, wR^2 = 0.182, max. (min.) residual electron density 0.24 (-0.19) e.Å^{-3}, hydrogen atoms were calculated and refined as riding atoms.

CCDC 1011608 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (internat.) +44(1223)336-033, E-mail: deposit@ccdc.cam.ac.uk].

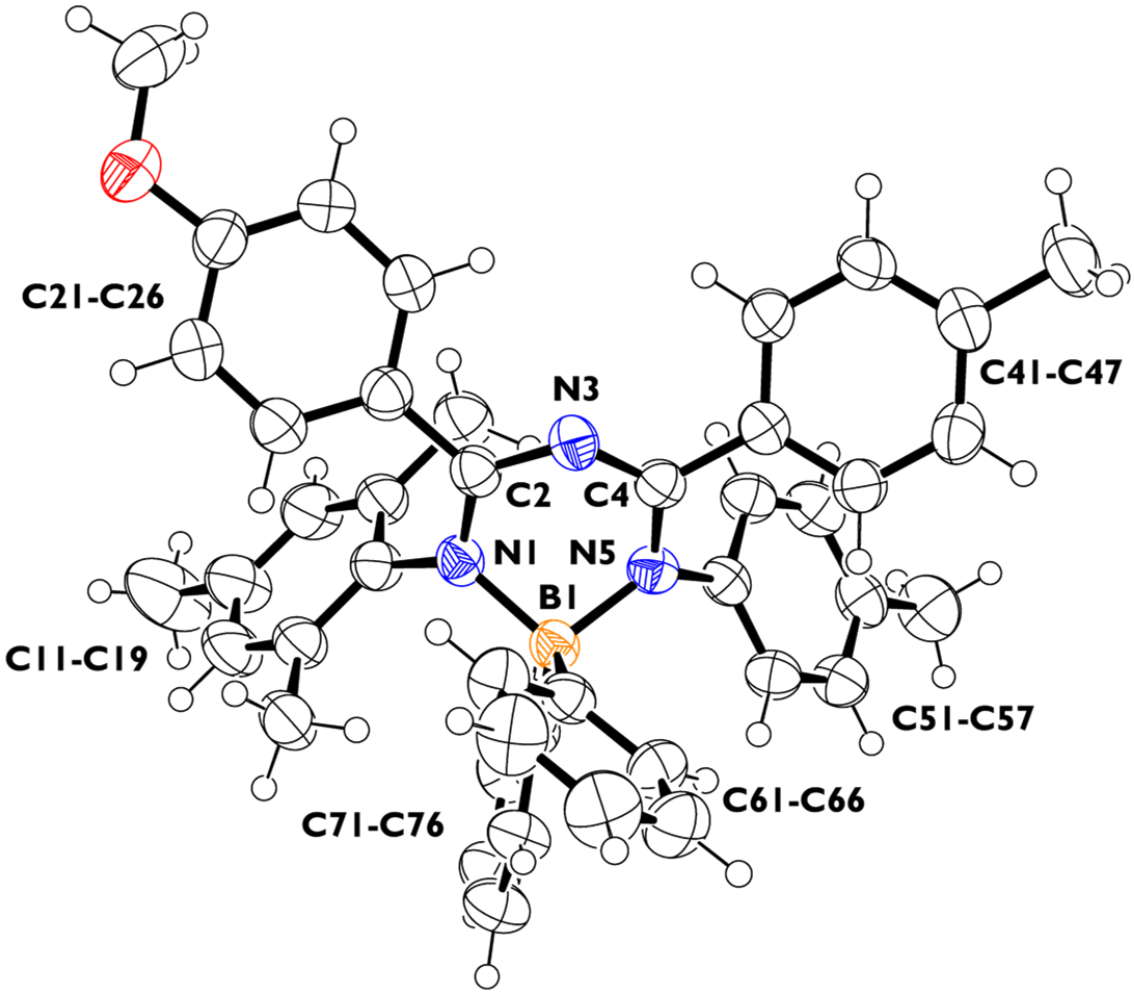


Figure S 15. Oak Ridge Thermal Ellipsoid Plot (ORTEP) of **14b**. Thermal ellipsoids shown at a 50% probability level.

X-Ray data for 14c

formula $C_{74}H_{62}B_2N_6 \cdot C_2H_3N$, M = 1097.97, yellow crystal, 0.60 x 0.40 x 0.03 mm, a = 19.1756(3), b = 10.4129(2), c = 30.5970(5) Å, β = 96.906(1)°, V = 6065.1(2) Å^3, ρ_{calc} = 1.202 gcm^{-3}, μ = 0.070 mm^{-1}, empirical absorption correction ($0.959 \leq T \leq 0.997$), Z = 4, monoclinic, space group $P2_1/c$ (No. 14), λ = 0.71073 Å, T = 223(2) K, ω and φ scans, 80106 reflections collected ($\pm h$, $\pm k$, $\pm l$), [(sinθ)/λ] = 0.67 Å^{-1}, 14872 independent (R_{int} = 0.083) and 10287 observed reflections [$I>2\sigma(I)$], 771 refined parameters, R = 0.062, wR^2 = 0.153, max. (min.) residual electron density 0.23 (-0.20) e.Å^{-3}, hydrogen atoms were calculated and refined as riding atoms.

CCDC 1011609 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (internat.) +44(1223)336-033, E-mail: deposit@ccdc.cam.ac.uk].

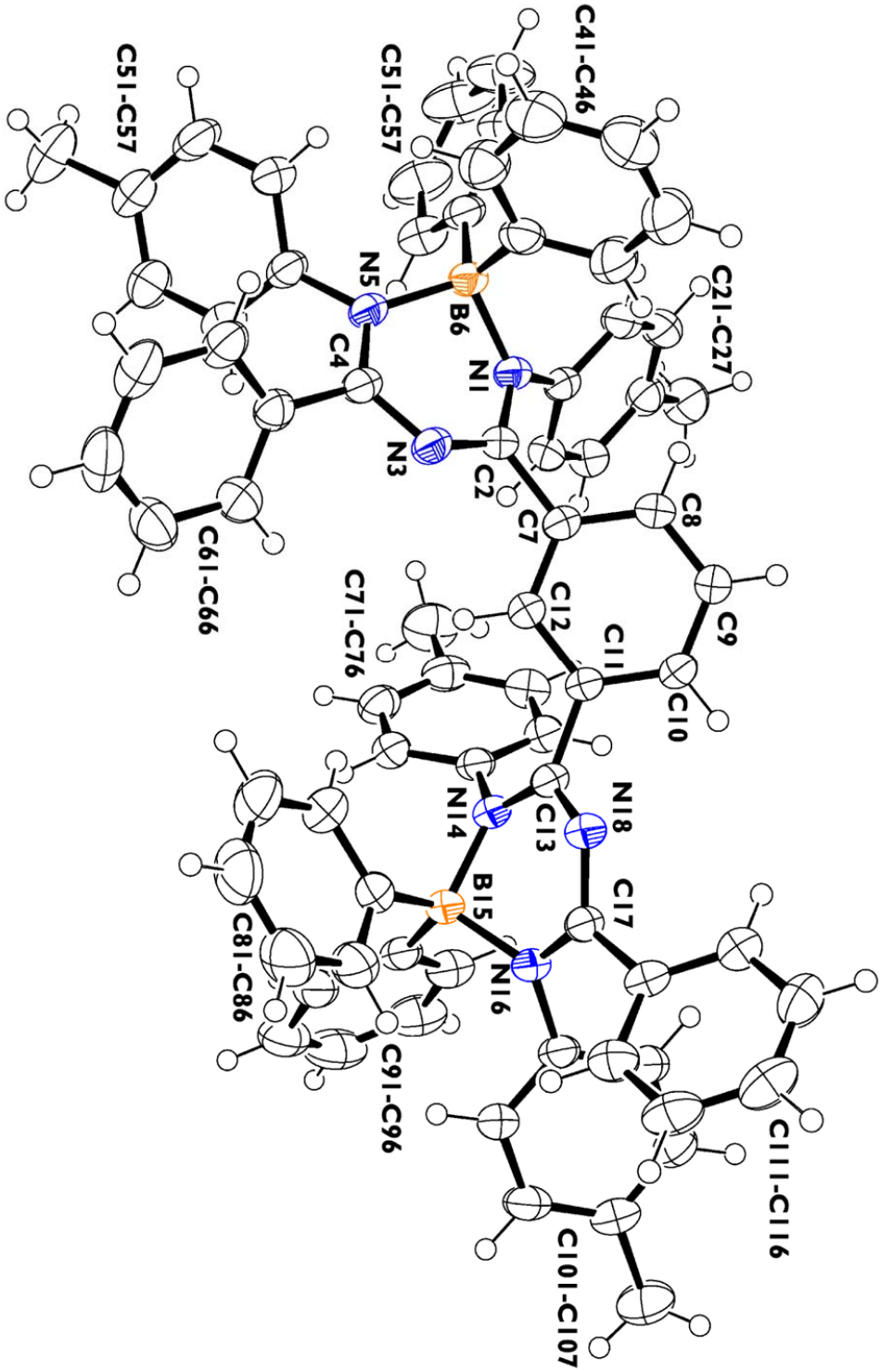


Figure S 16. Oak Ridge Thermal Ellipsoid Plot (ORTEP) of **14c**. Thermal ellipsoids shown at a 50% probability level.

X-Ray data for 14e

formula $C_{111}H_{96}B_3N_9$, M = 1588.40, yellow crystal, 0.10 x 0.06 x 0.02 mm, a = 14.8875(9), b = 20.1518(13), c = 32.0673(8) Å, V = 9620.5(9) Å^3, ρ_{calc} = 1.097 gcm^{-3}, μ = 0.487 mm^{-1}, empirical absorption correction ($0.952 \leq T \leq 0.990$), Z = 4, orthorhombic, space group $P2_12_12_1$ (No. 19), λ = 1.54178 Å, T = 223(2) K, ω and φ scans, 46596 reflections collected ($\pm h$, $\pm k$, $\pm l$), [$(\sin\theta)/\lambda$] = 0.60 Å^{-1}, 15310 independent (R_{int} = 0.173) and 6941 observed reflections [$I>2\sigma(I)$], 1117 refined parameters, R = 0.083, wR^2 = 0.184, max. (min.) residual electron density 0.16 (-0.19) e.Å^{-3}, hydrogen atoms were calculated and refined as riding atoms.

CCDC 1011610 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (internat.) +44(1223)336-033, E-mail: deposit@ccdc.cam.ac.uk].

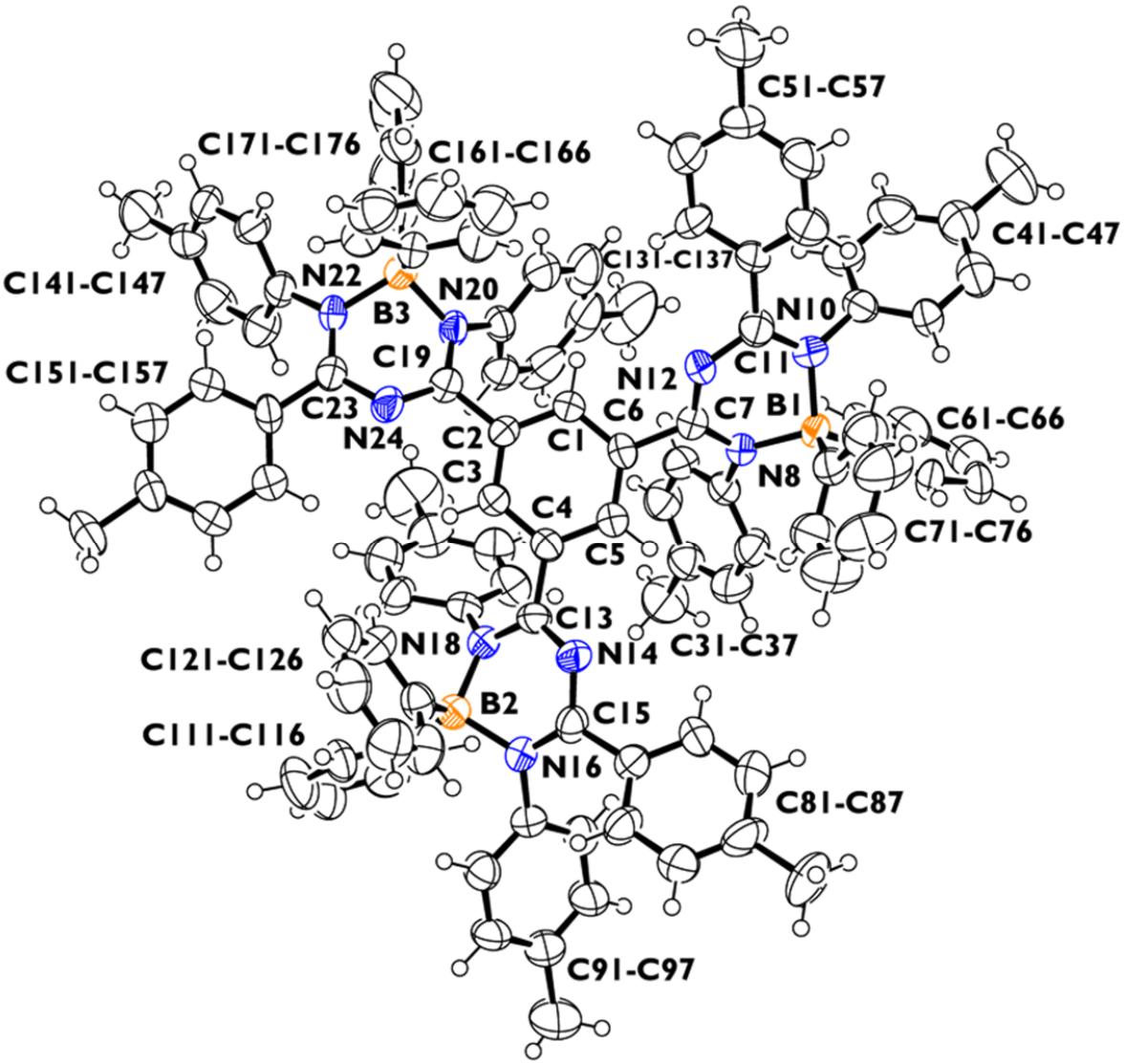
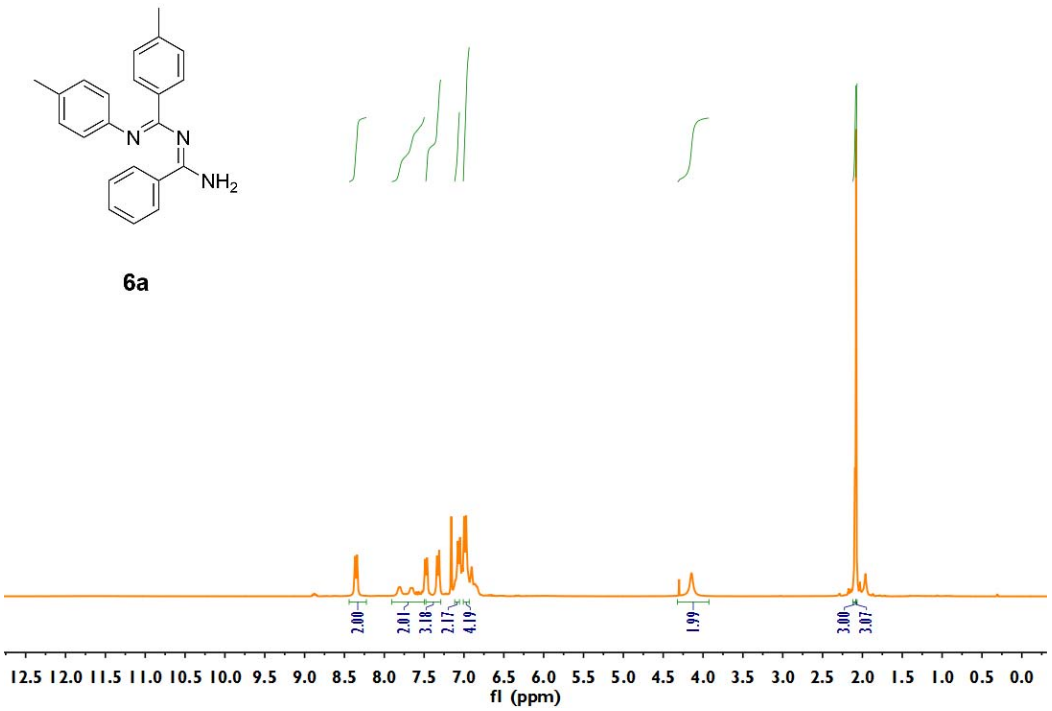


Figure S 17. Oak Ridge Thermal Ellipsoid Plot (ORTEP) of **14e**. Thermal ellipsoids shown at a 50% probability level.

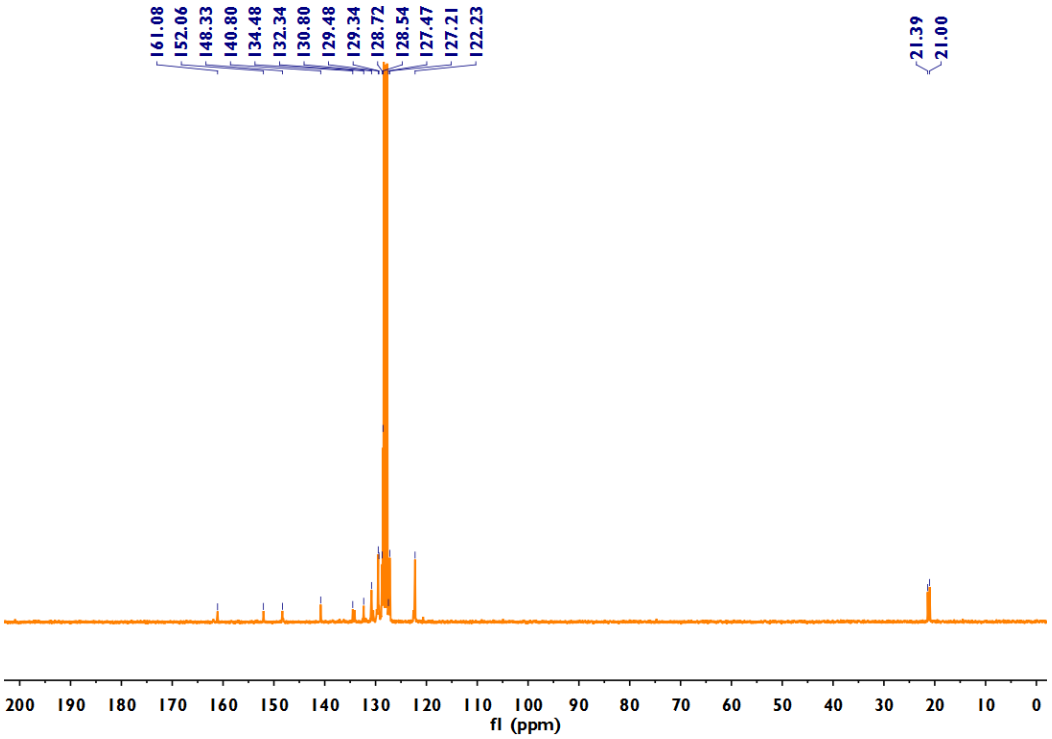
NMR Spectra

6a: ^{1}H NMR

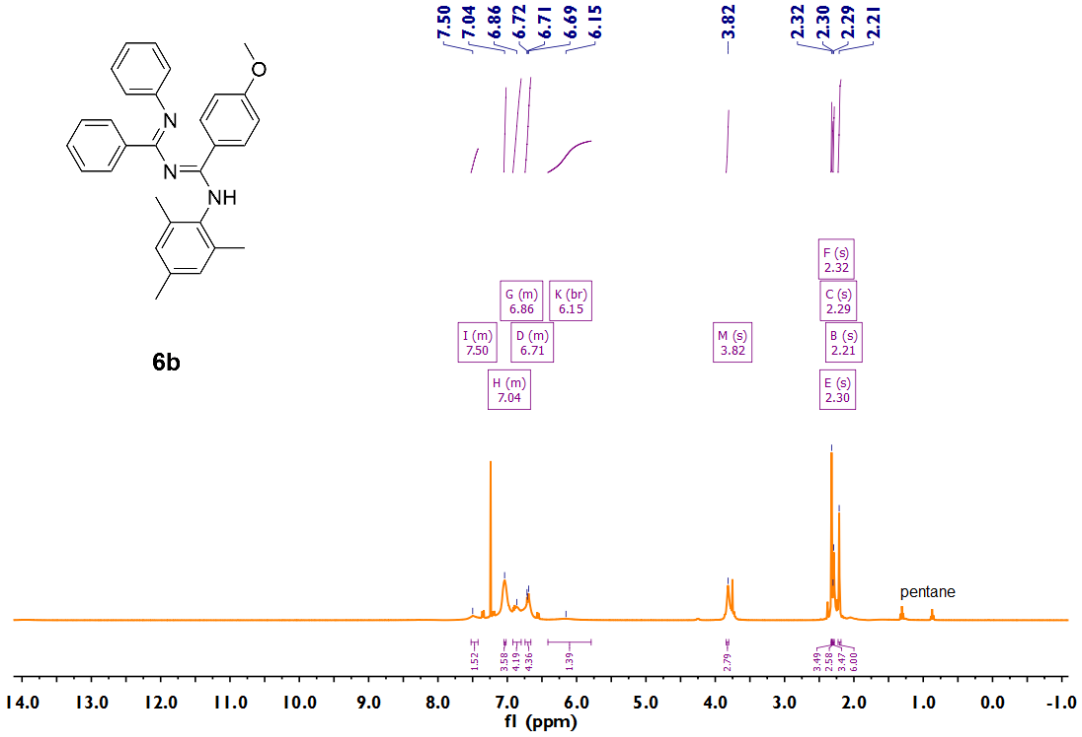


6a

6a: ^{13}C NMR

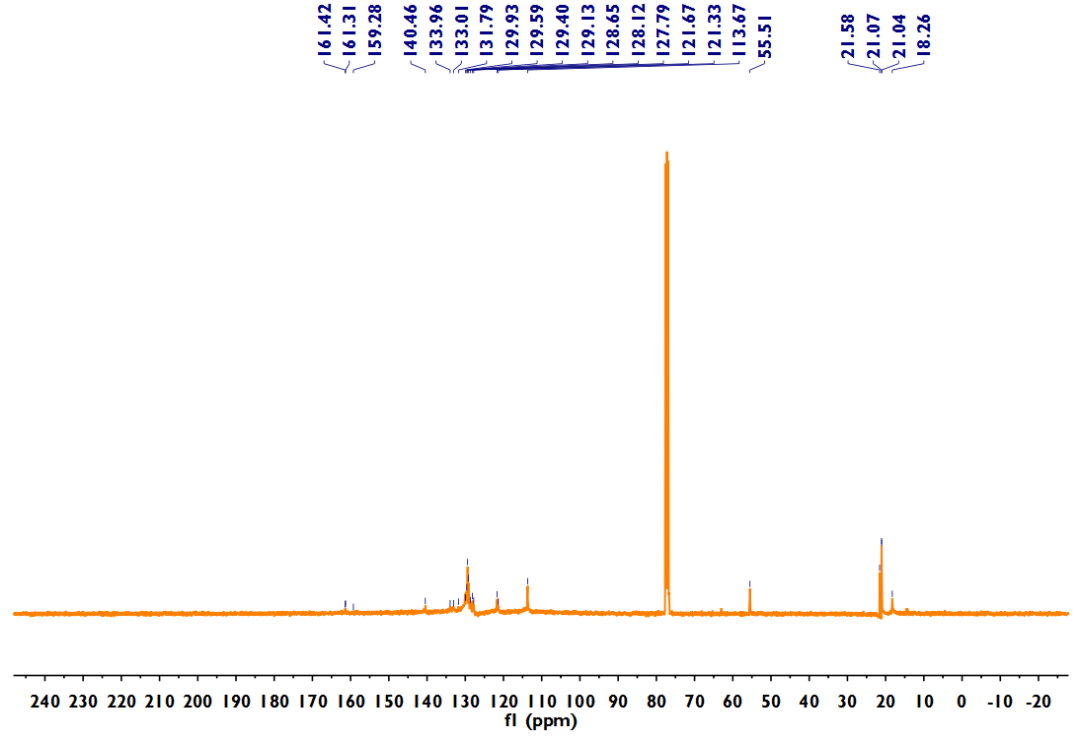


6b: ^{1}H NMR

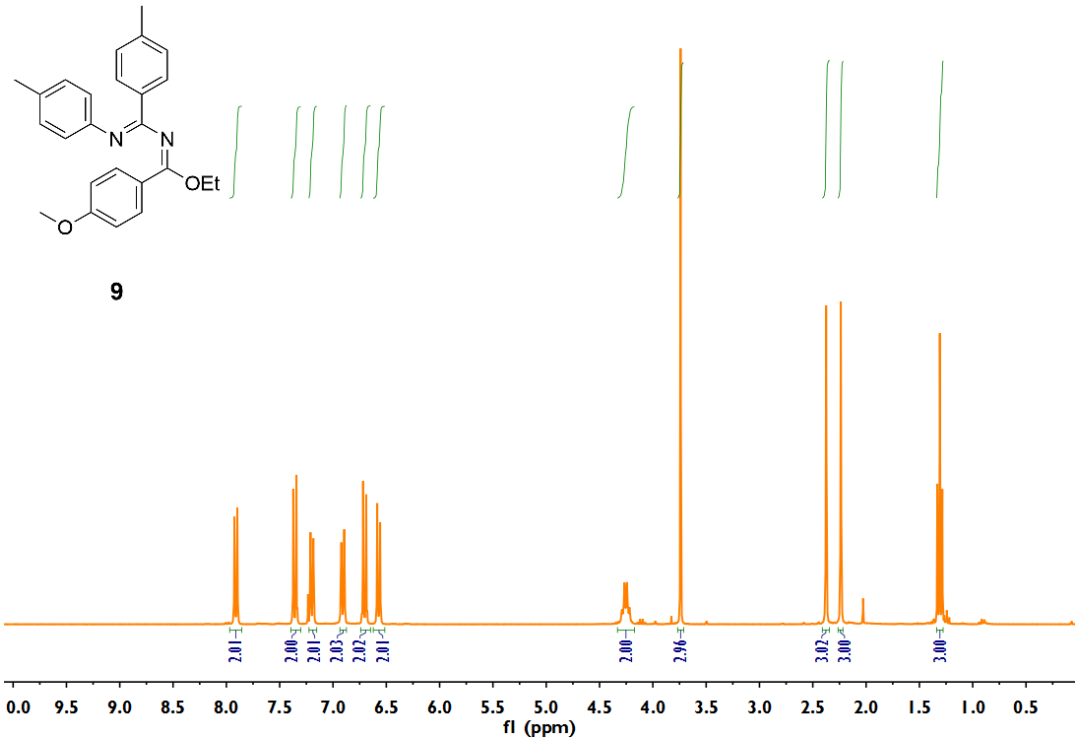


6b

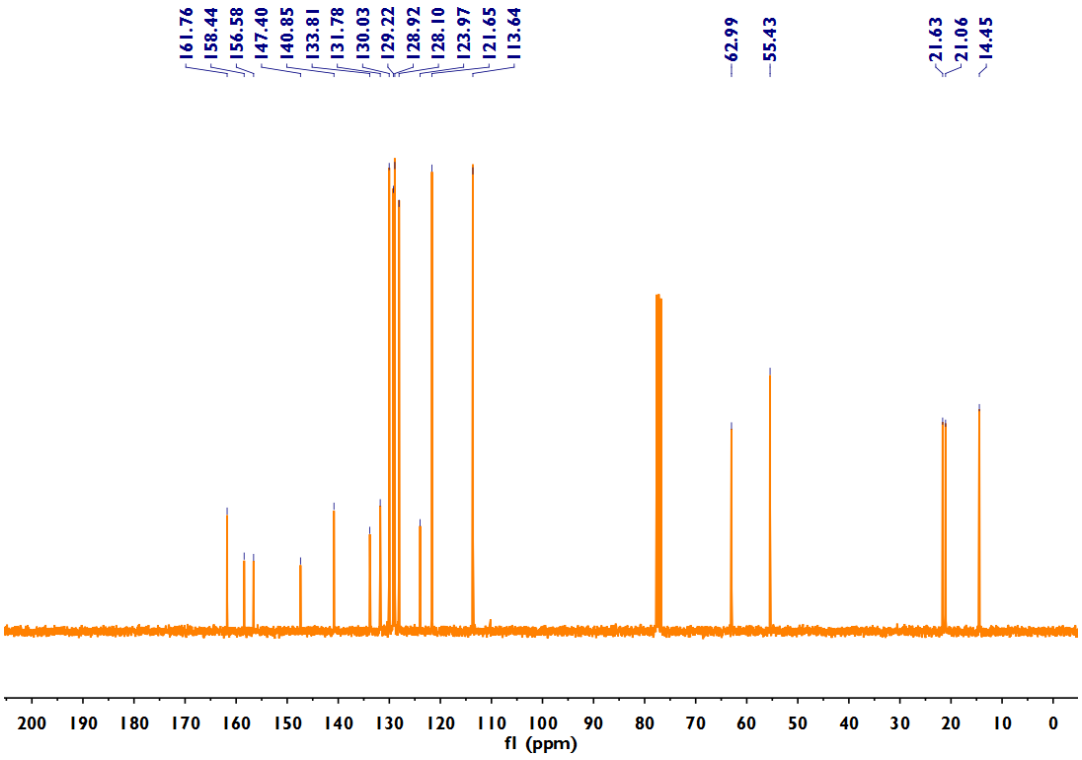
6b: ^{13}C NMR



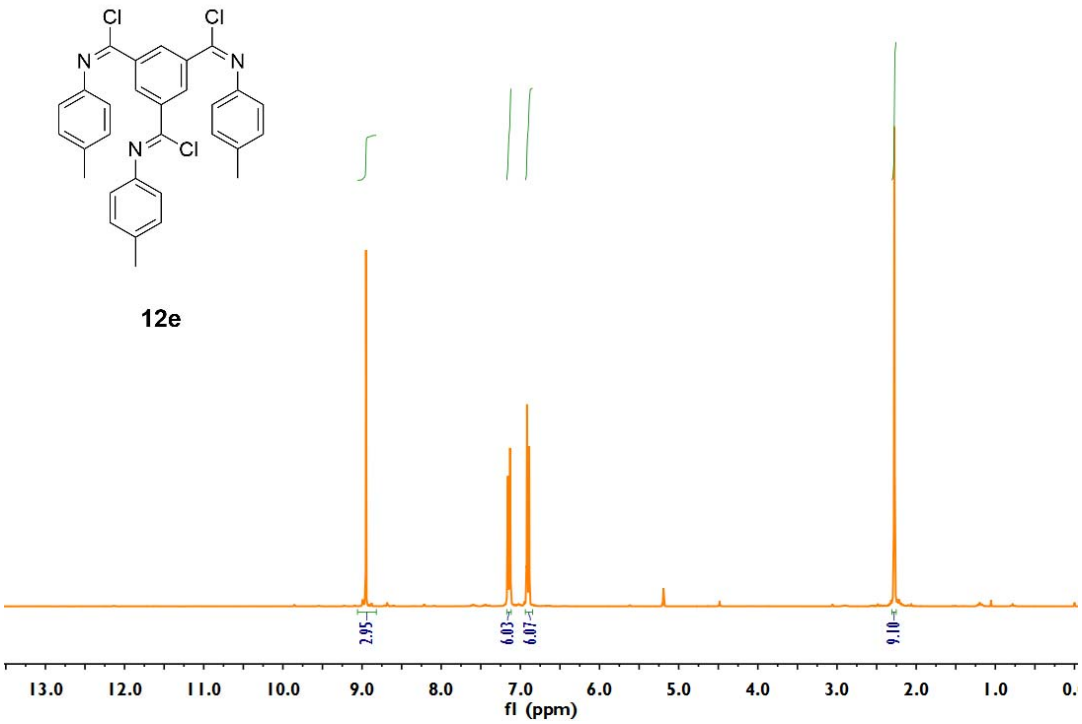
9: ^{1}H NMR



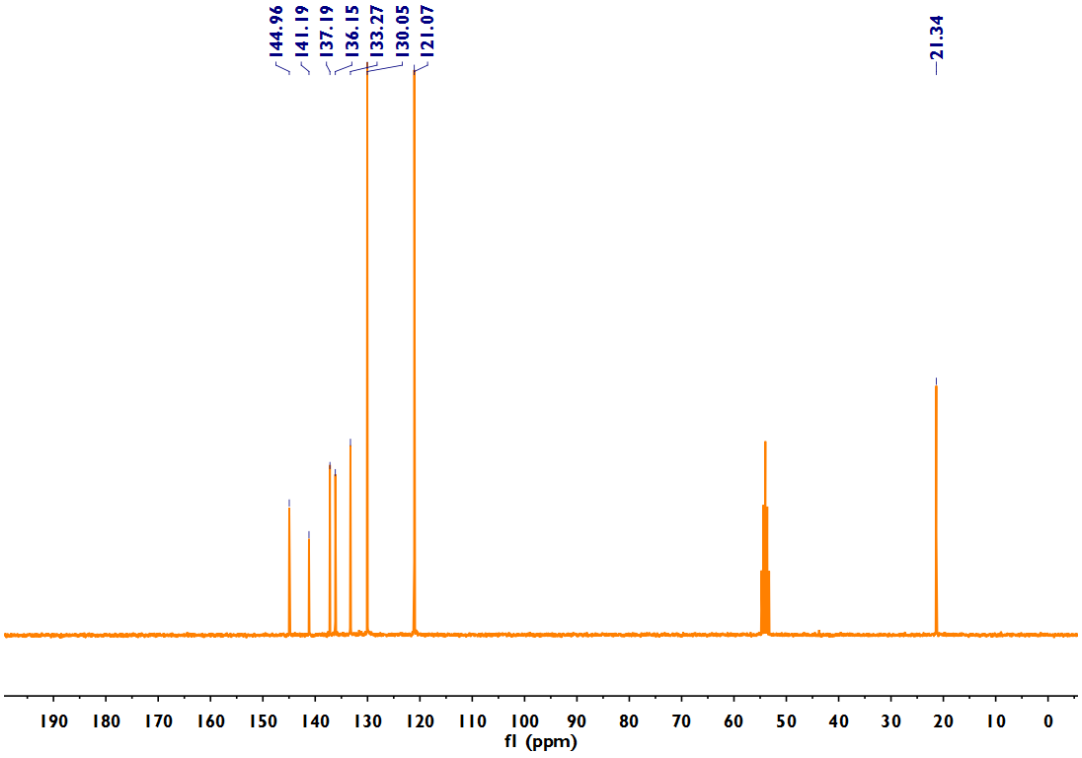
9: ^{13}C NMR



12e: ^{1}H NMR



12e: ^{13}C NMR



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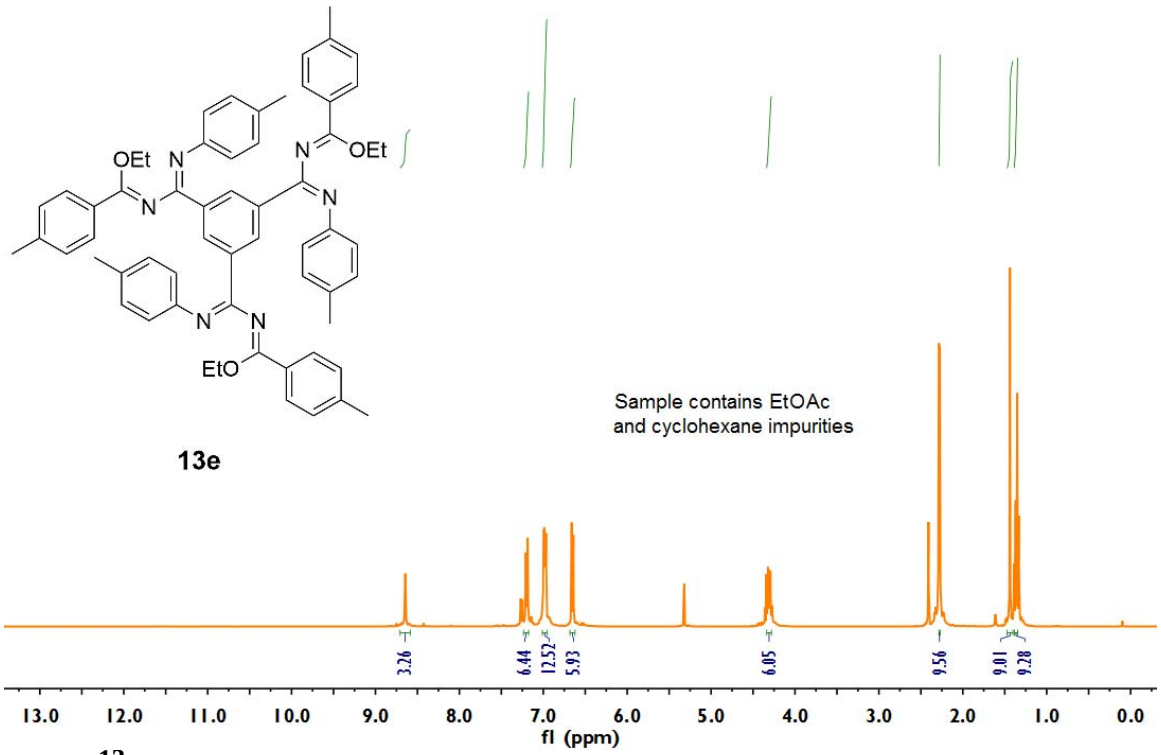
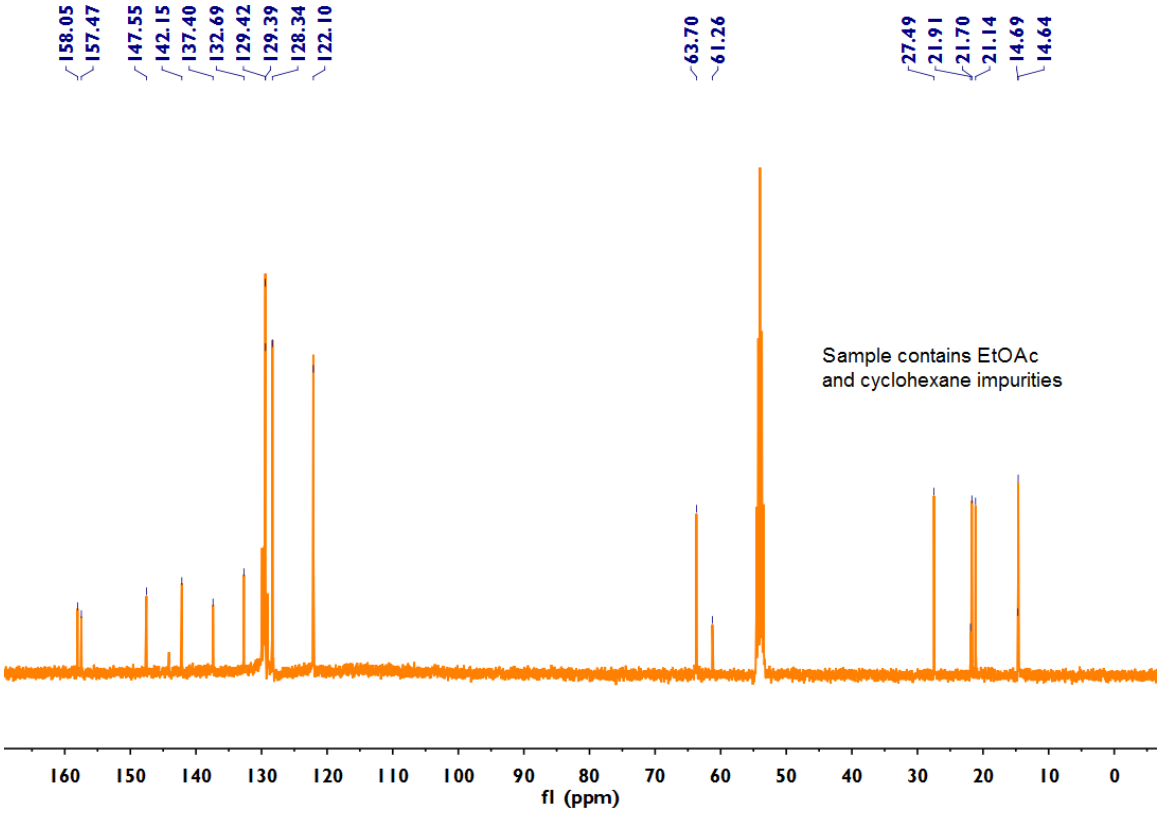
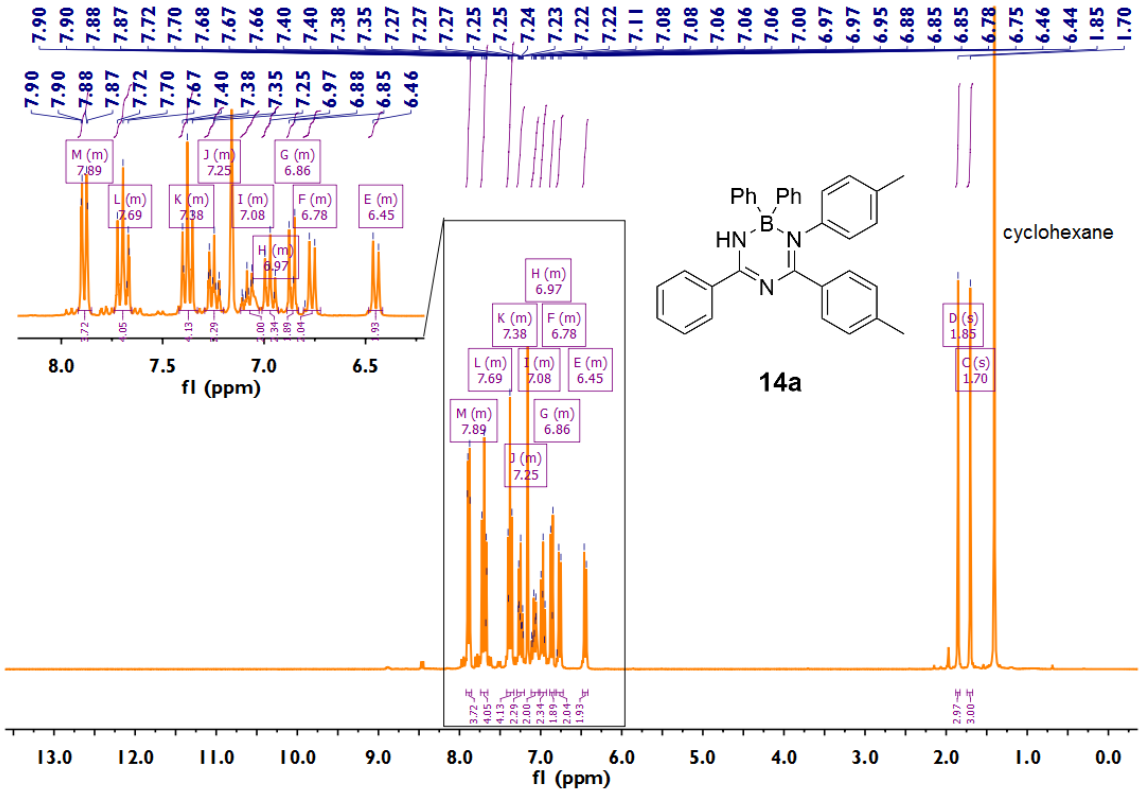


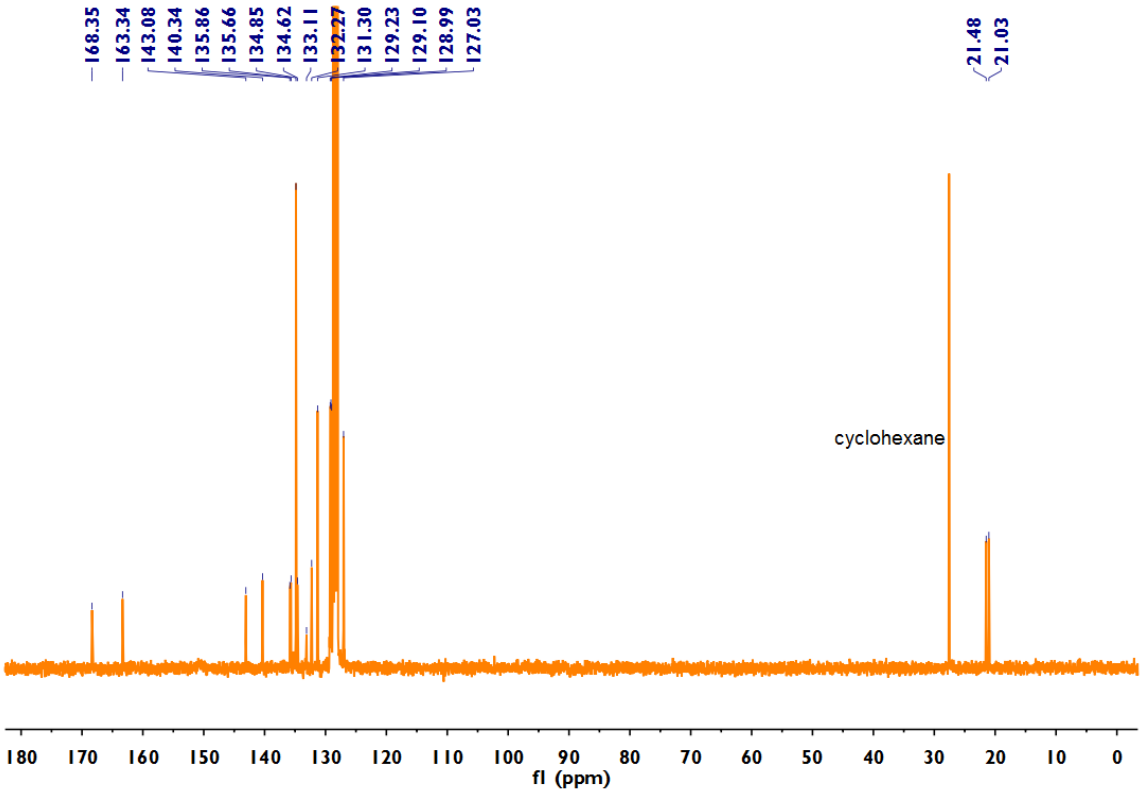
13e: ^{13}C NMR



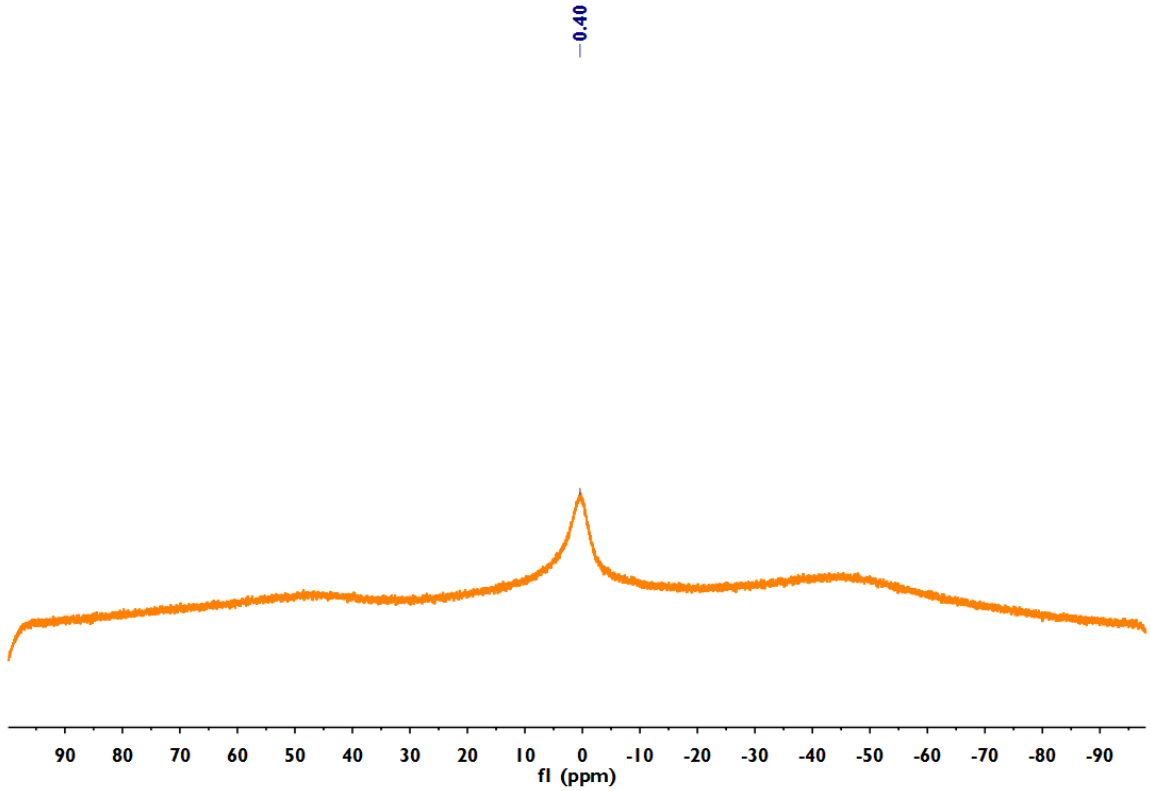
14a: ^{1}H NMR



14a: ^{13}C NMR



14a: ^{11}B NMR



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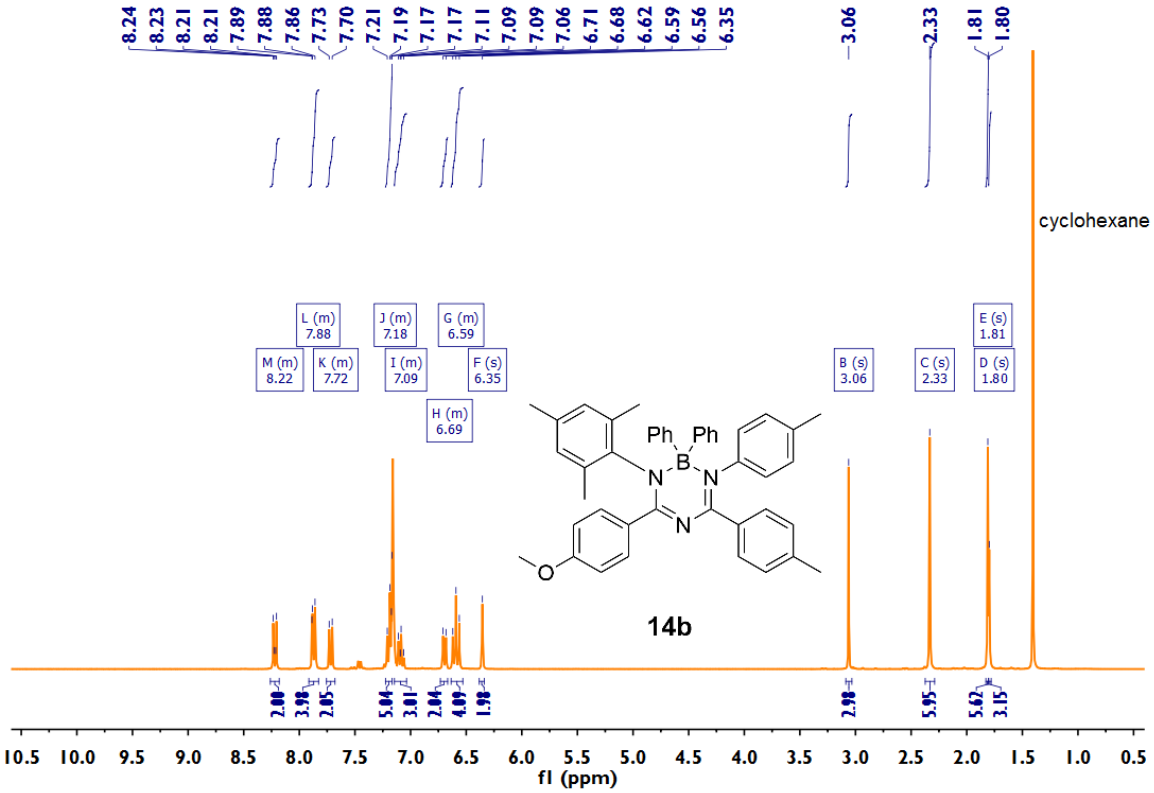
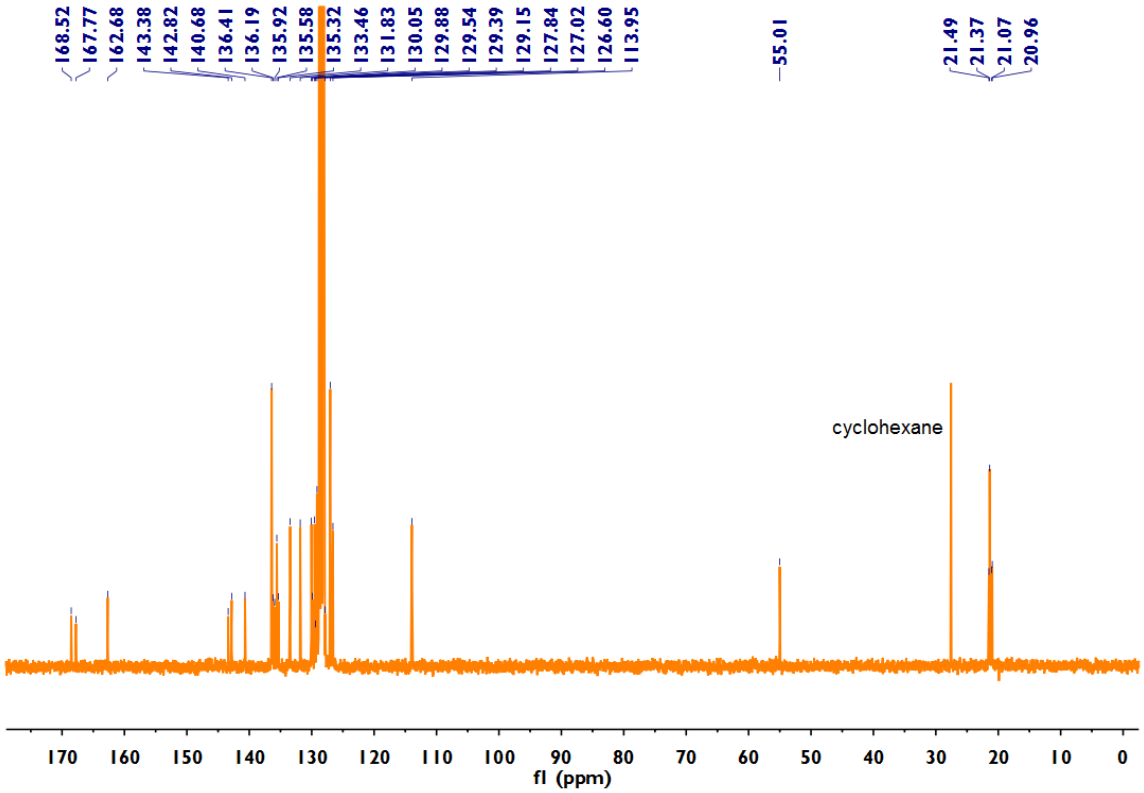
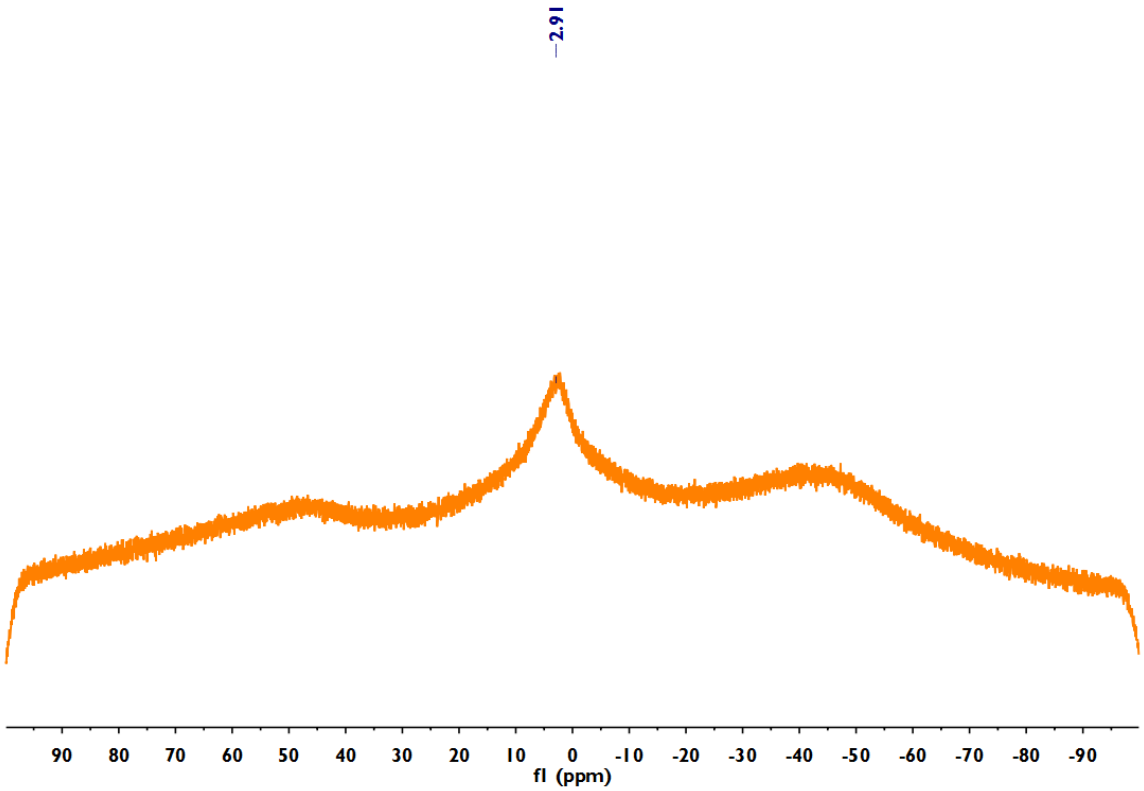


14b: ^{13}C NMR



14b: ^{11}B NMR



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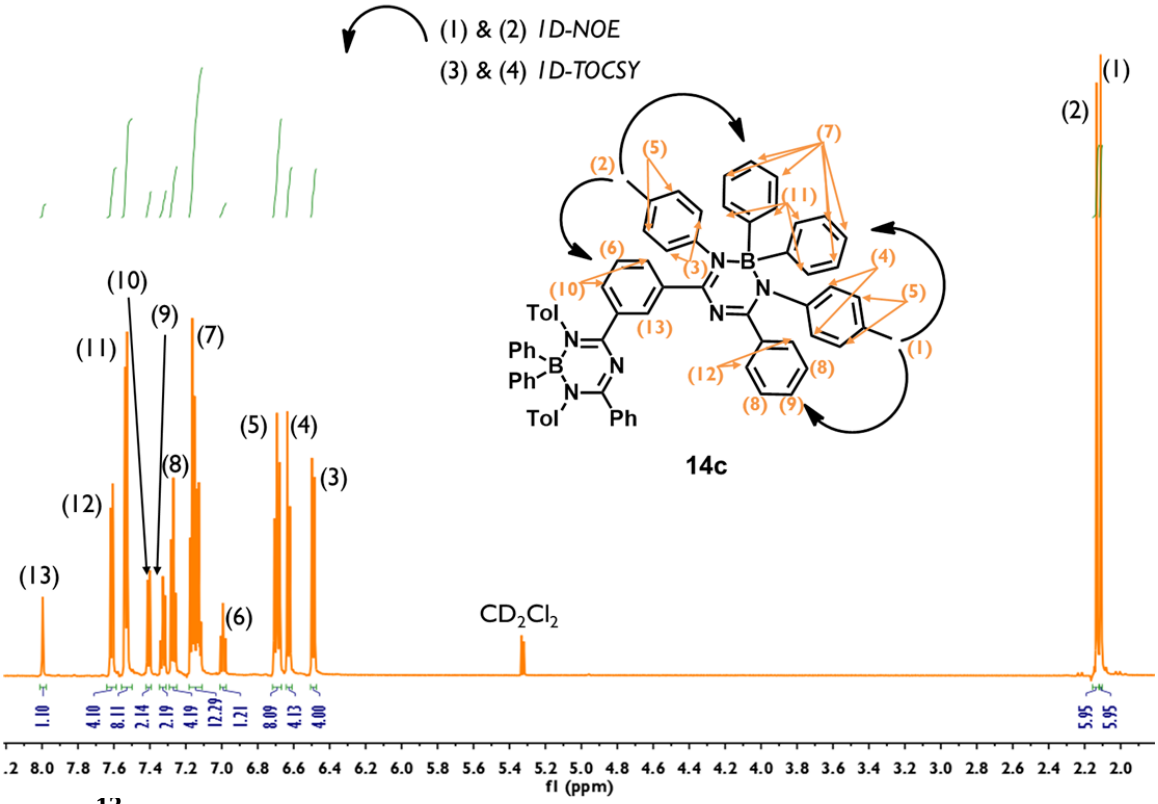

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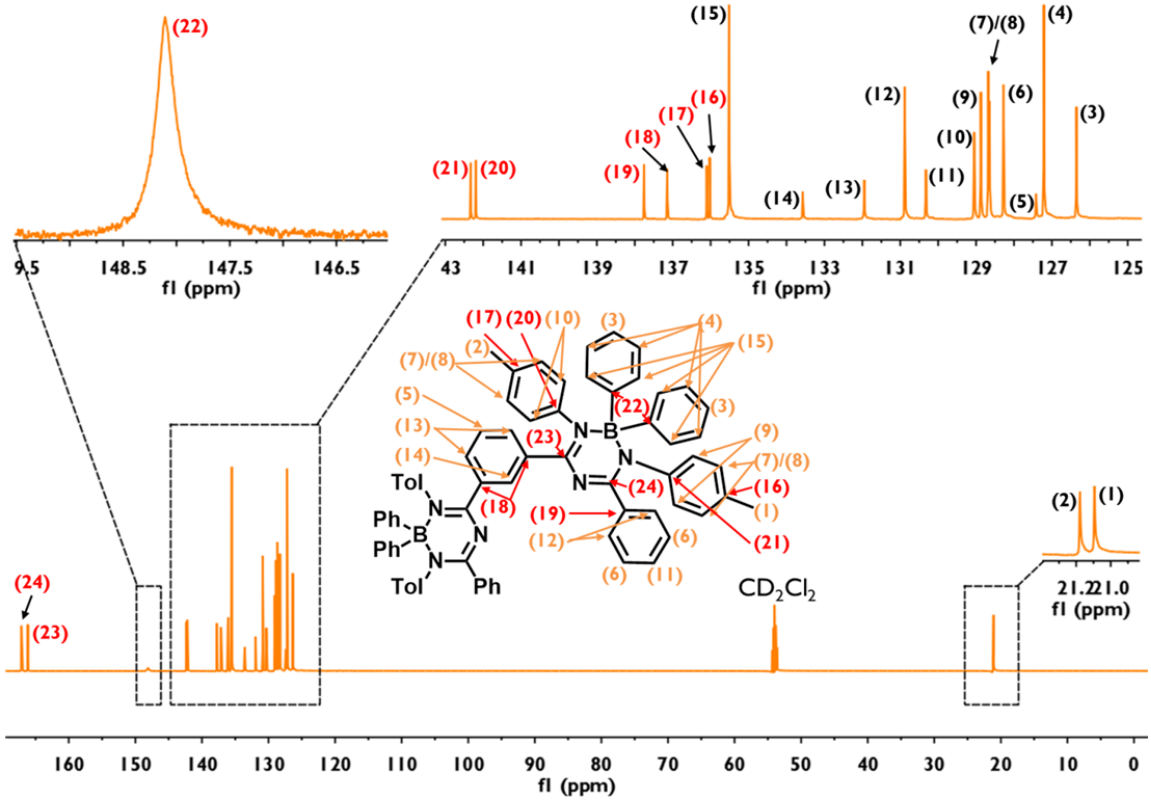

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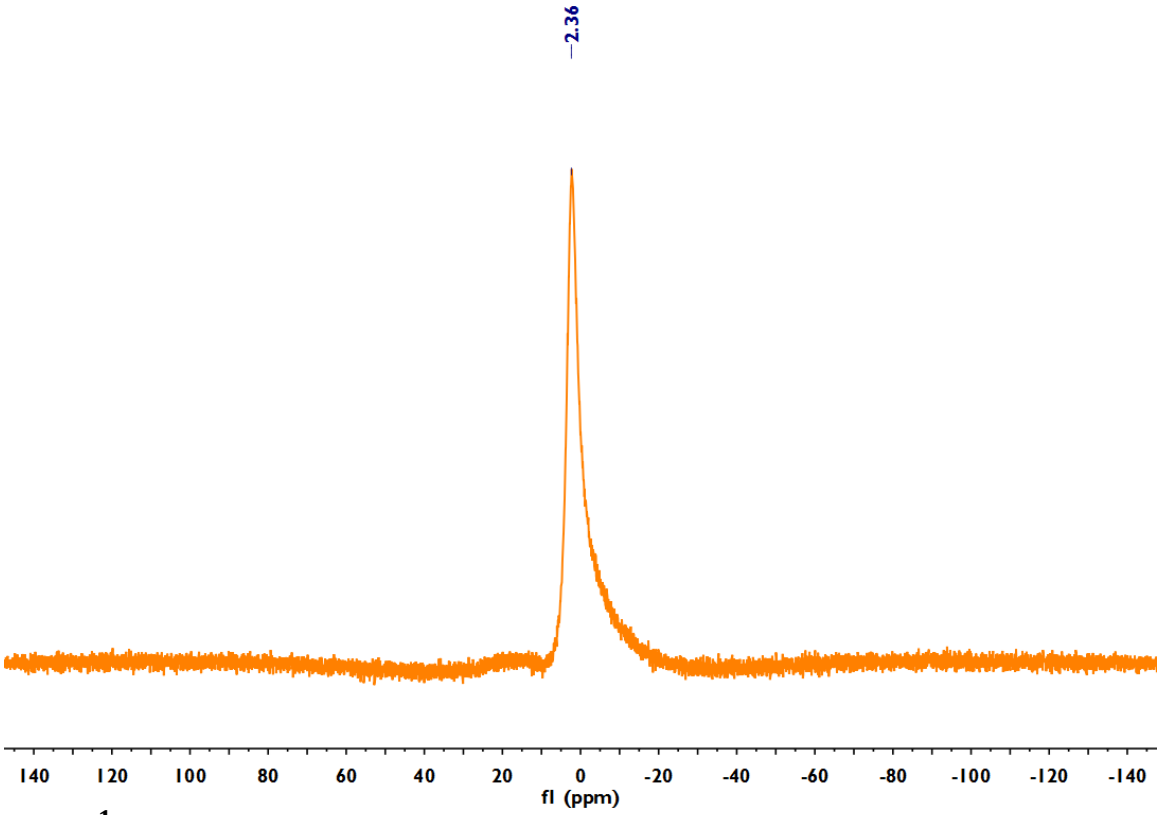
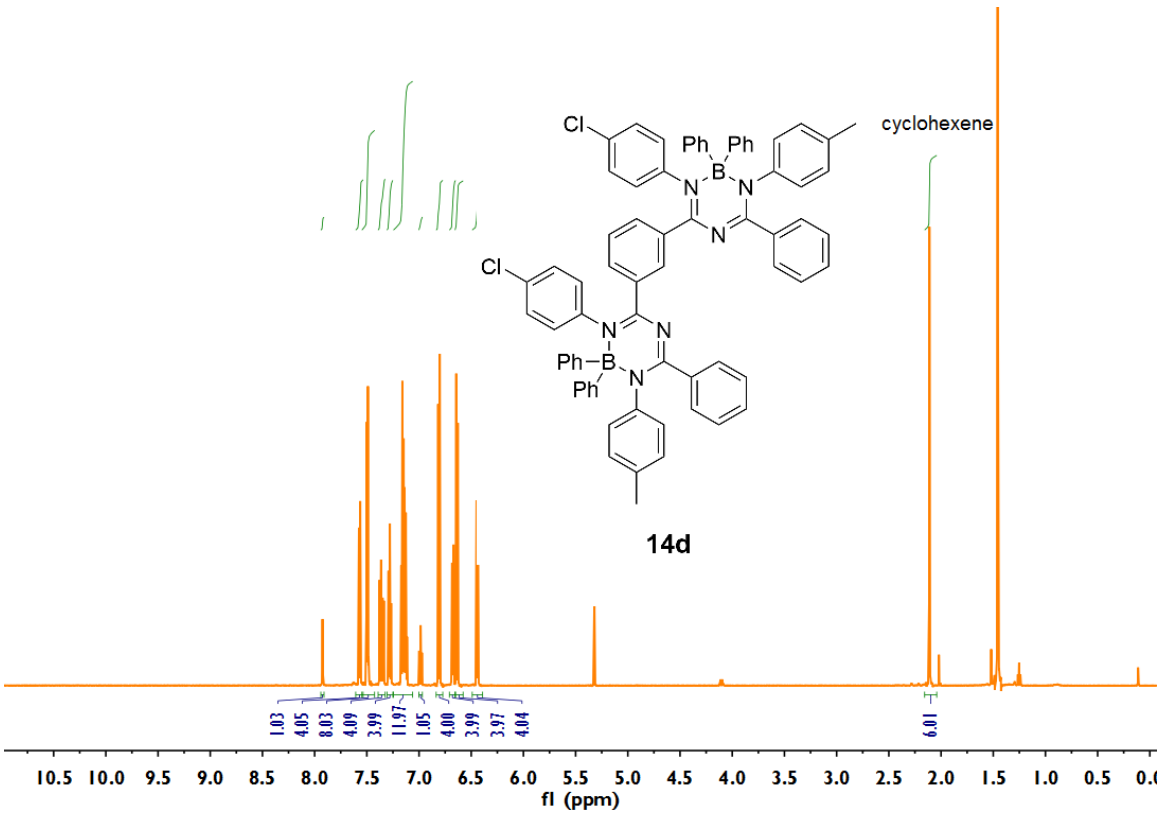


14d: ^{1}H NMR



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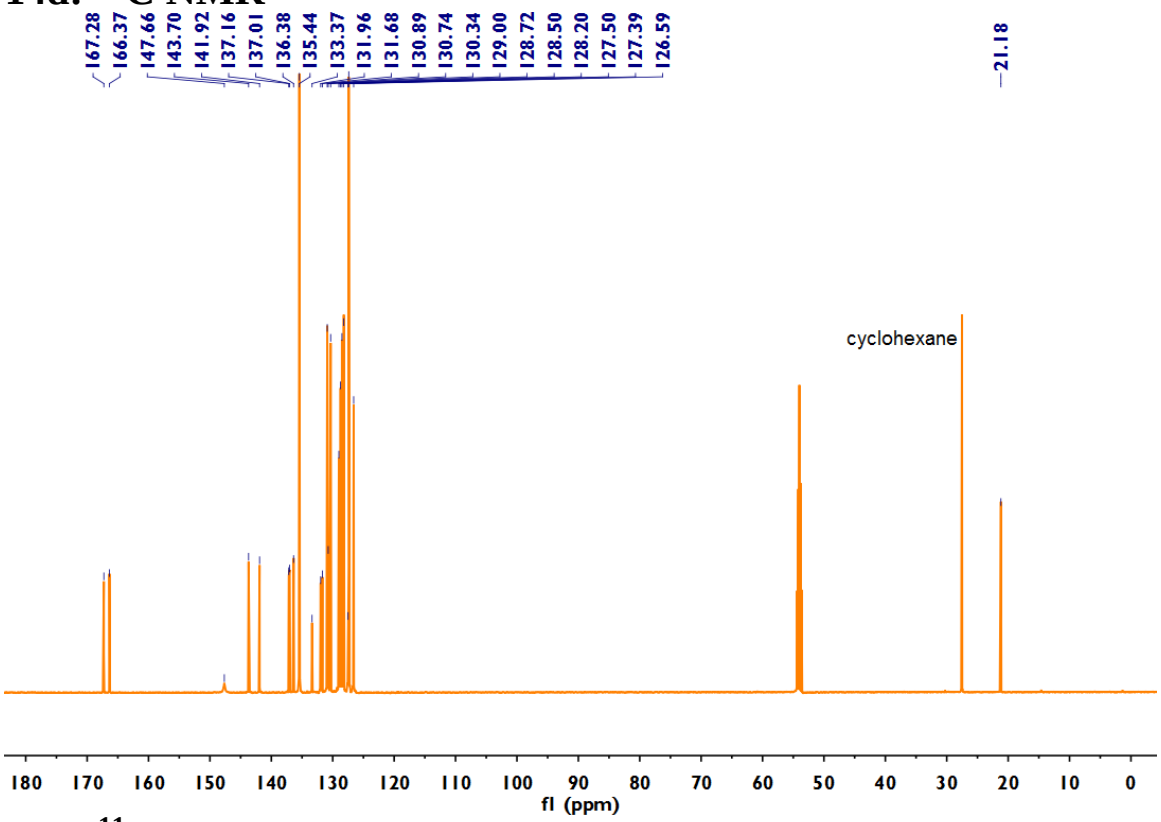

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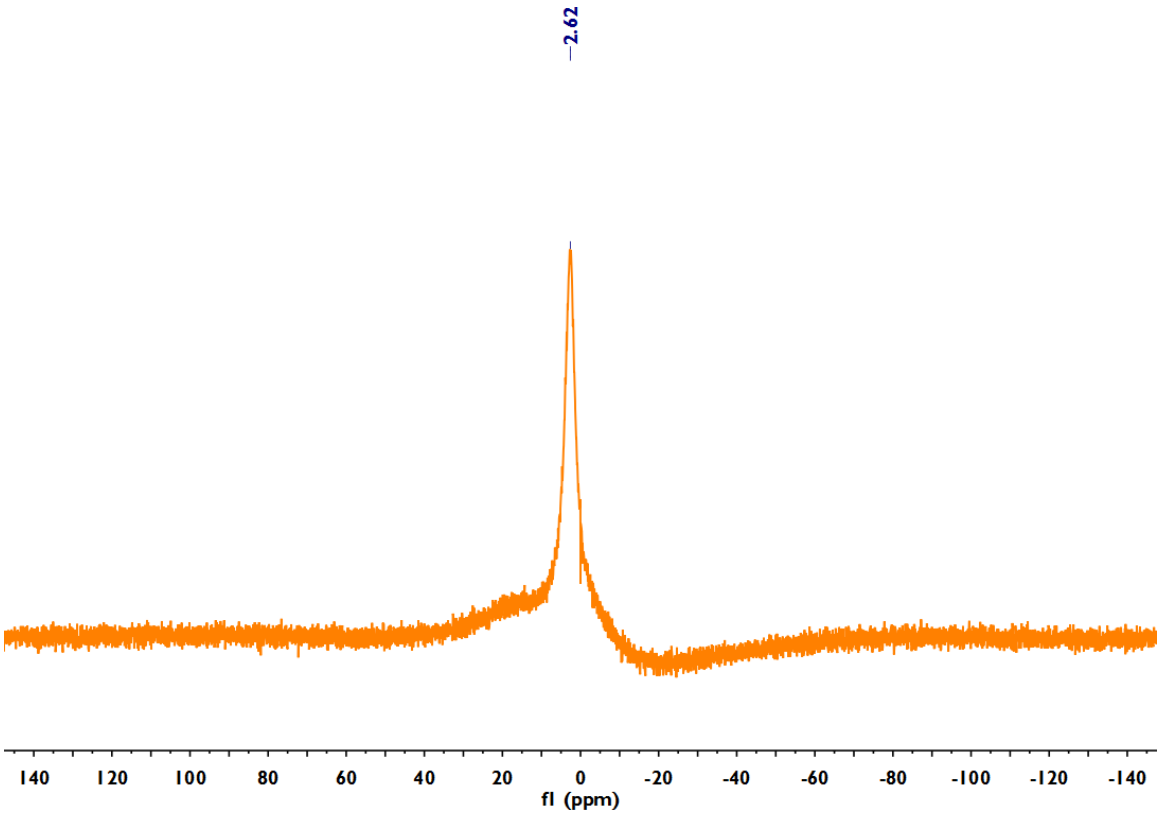
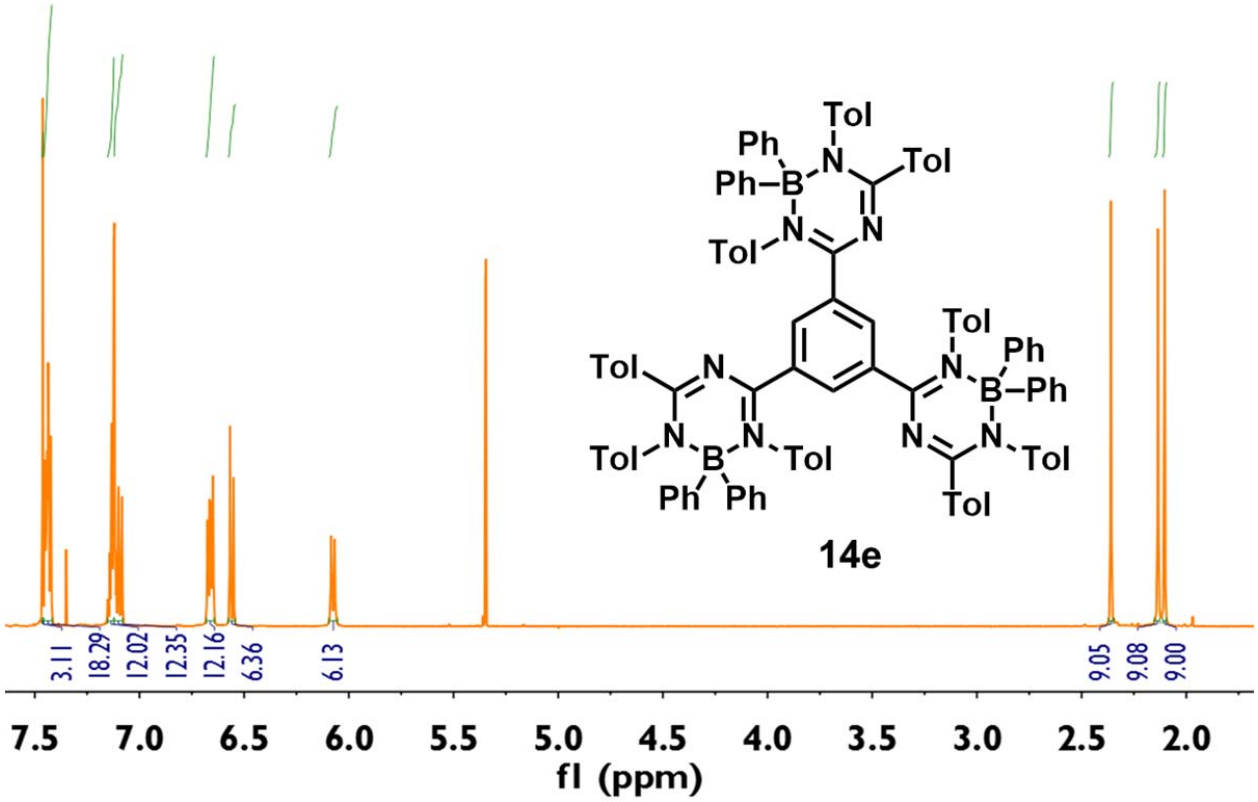
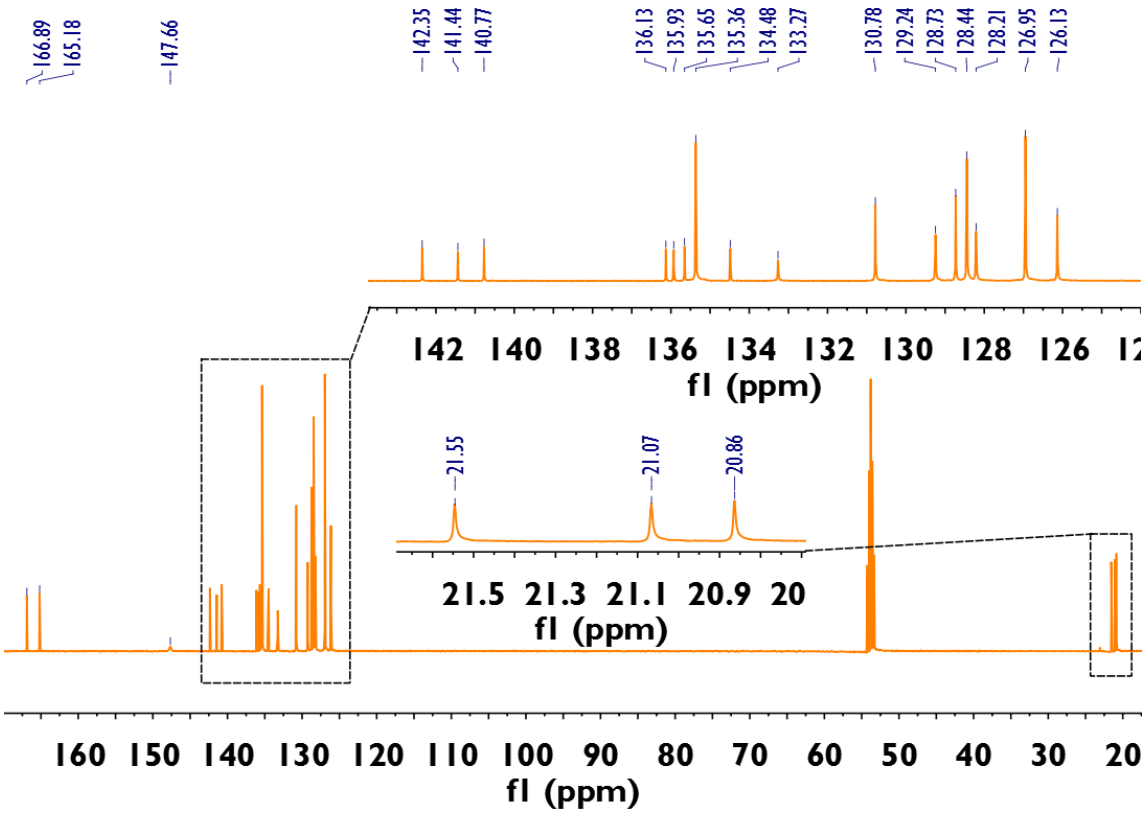


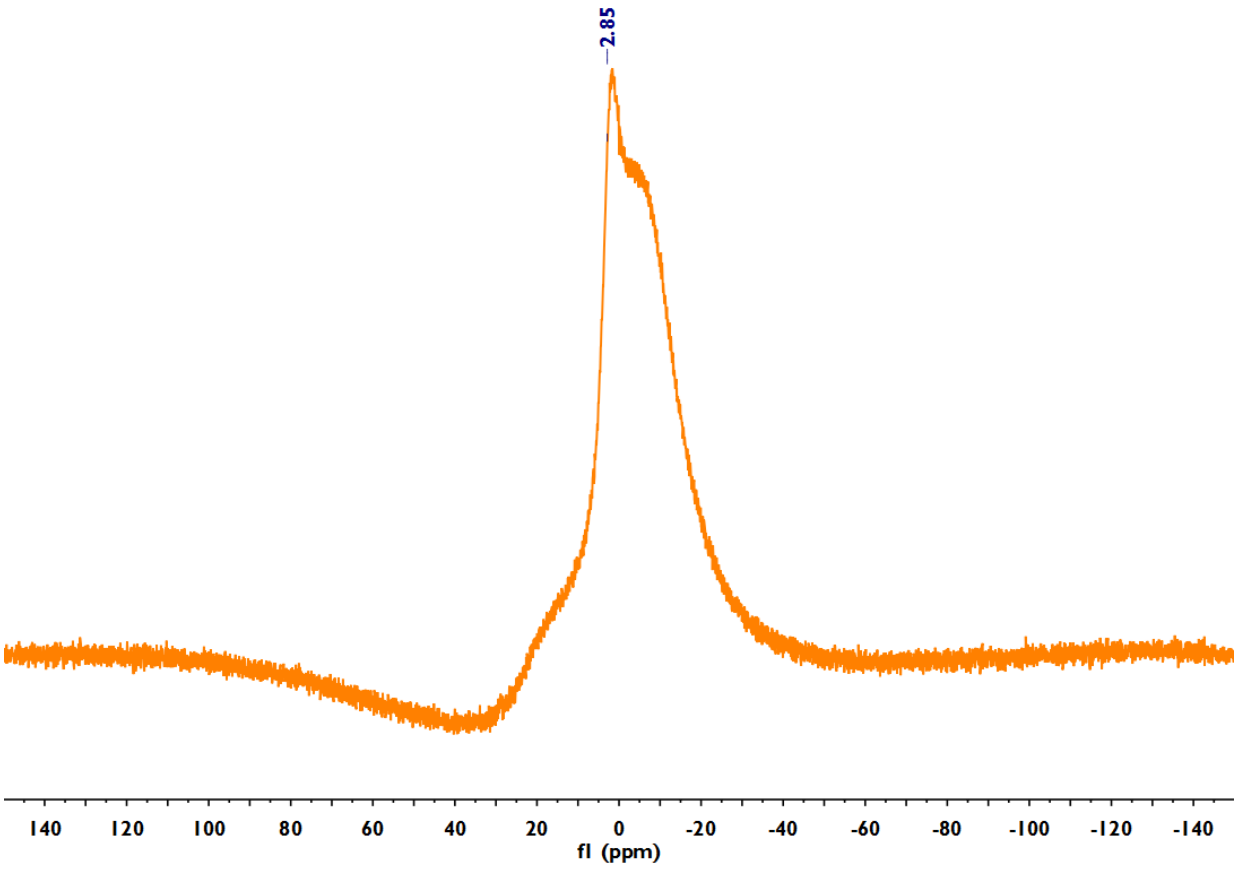
14e: ^{1}H NMR



14e: ^{13}C NMR



14e: ^{11}B NMR



References

[1] Becke, A. D. *J. Chem. Phys.*, 1**993,** *98,* 5648-5652. C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785-789.

[2] Feller, D*., J. Comp. Chem.* **1996**, *17*, 1571-1586; Schuchardt, K.L., Didier, B.T., Elsethagen, T., Sun, L., Gurumoorthi, V., Chase, J., Li, J., and Windus, T.L.J. *Chem. Inf. Model.* **2007**, *47*, 1045-1052, doi:10.1021/ci600510j.

[3] Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, M. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.