Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Electronic Supplementary Materials

Search for Blues Brothers: X-ray Crystallographic/Spectroscopic Characterization of Tetraarylbenzidine Cation Radical as a Product of Aging of Solid Magic Blue

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S1. NMR Spectroscopy of aged MB^0

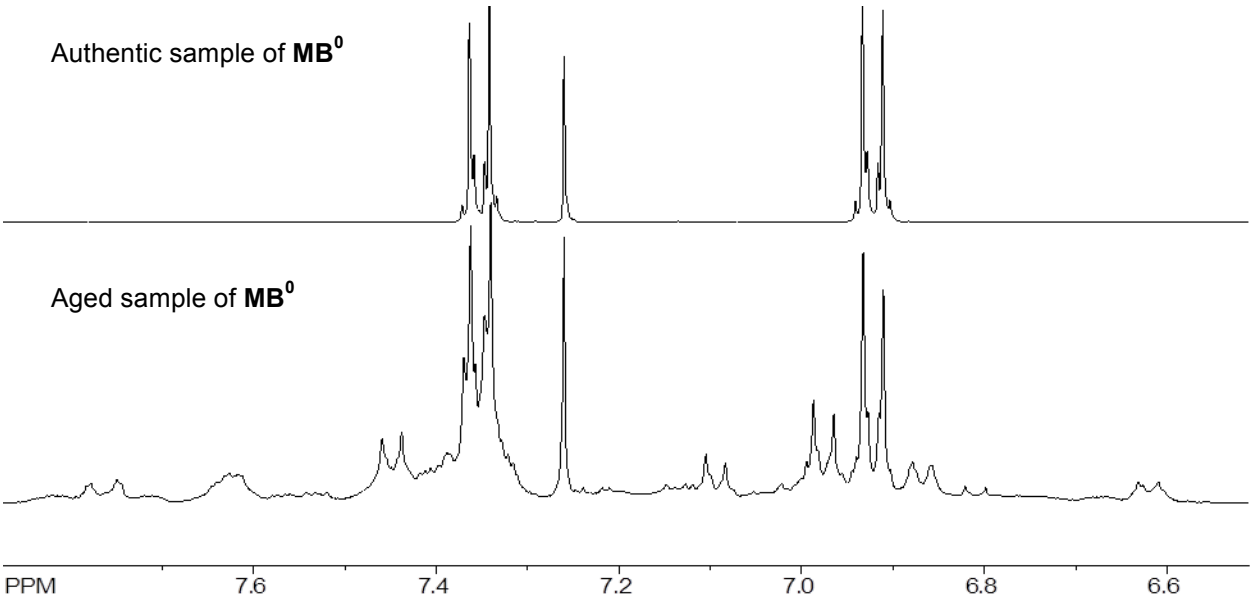


Fig. S1: Comparison of the ^{1}H NMR spectra of aged sample of $MB^{+\bullet}$ reduced by Zn dust or ferrocene (bottom) and the authentic sample of neutral MB^0 (top).

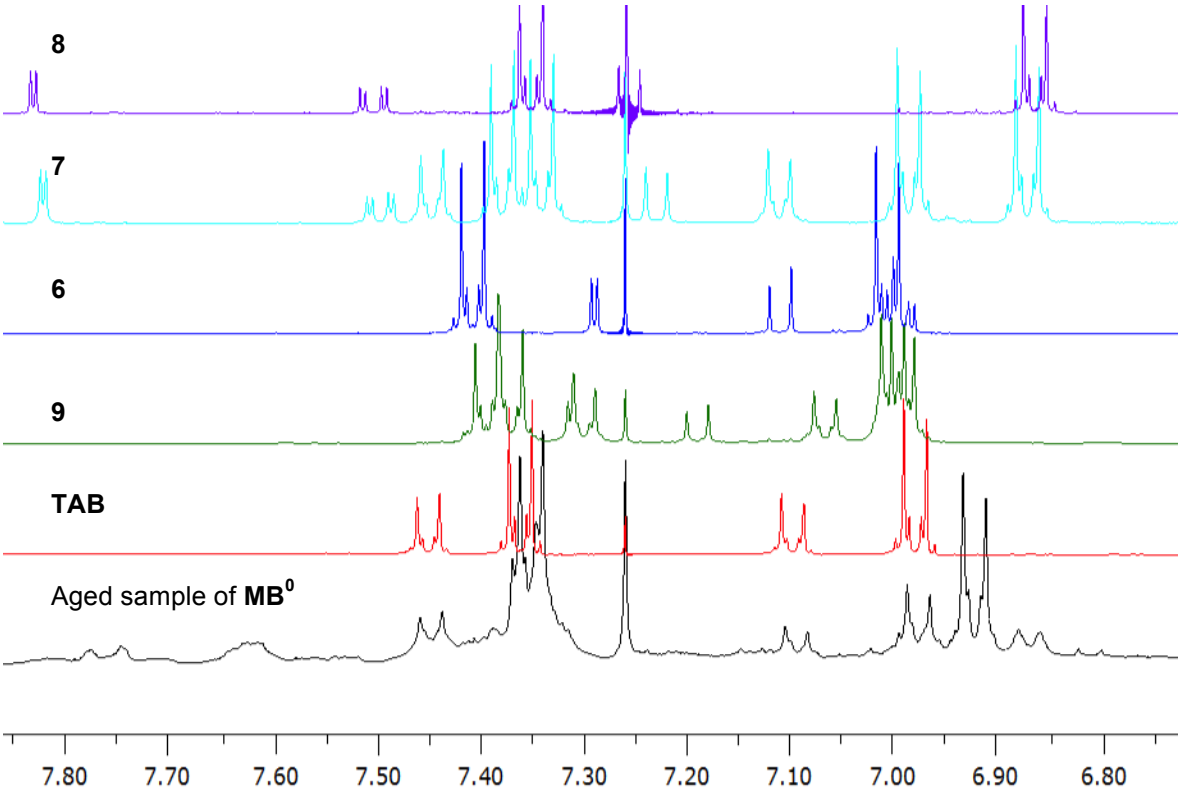


Fig. S2. Comparison of the ^{1}H NMR spectra of the aged sample of $MB^{+\bullet}$, reduced to MB^0 by using ferrocene (identical to that in Fig. S1 in the ESI), and NMR spectra of authentic **TAB** and **6**-**9**.

S2. MALDI Spectroscopy of aged sample of MB^0

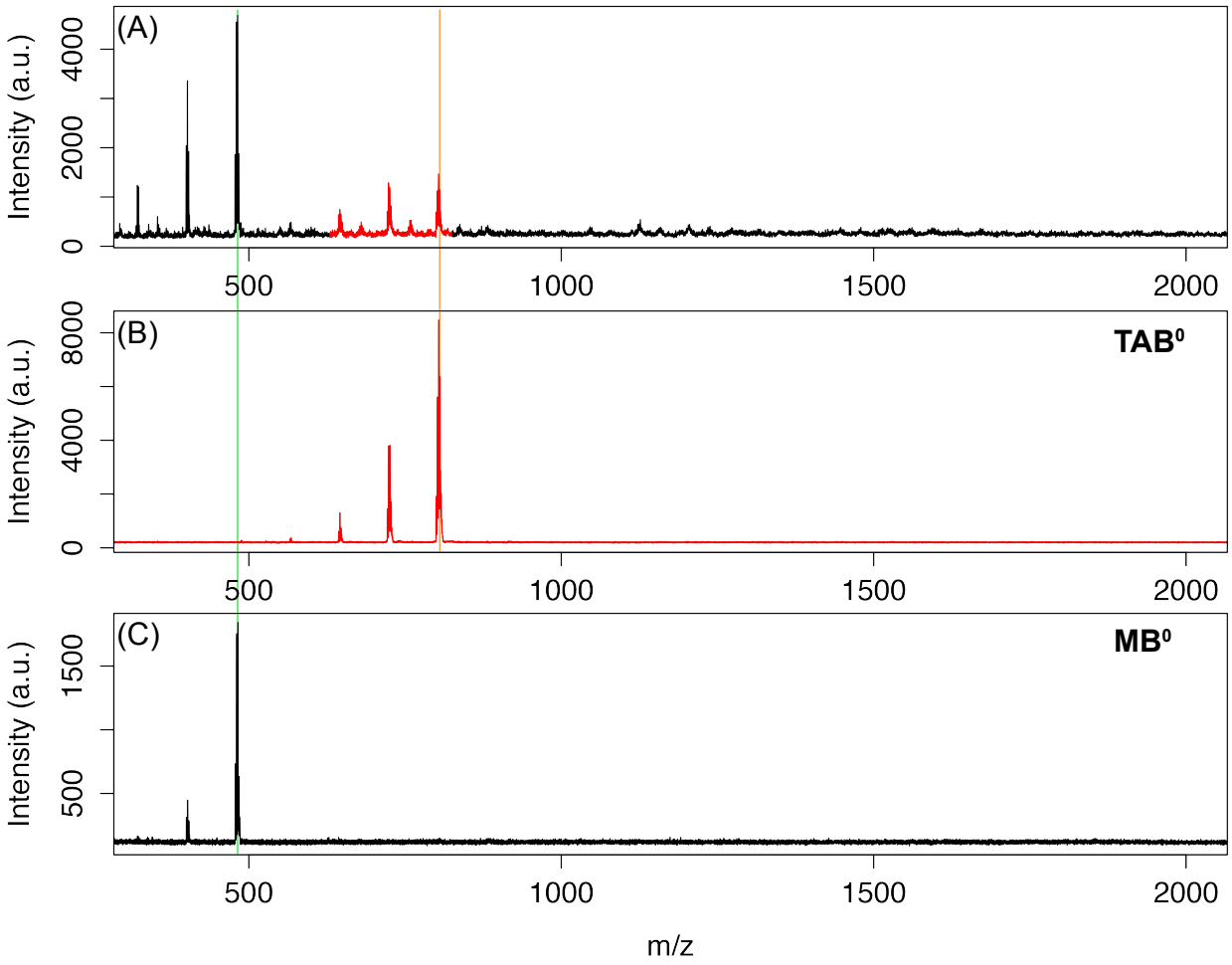


Fig. S3. MALDI-TOF mass spectra of the aged sample of $\mathbf{MB^{+\bullet}}$, reduced to $\mathbf{MB^0}$ using ferrocene in dichloromethane [The NMR spectrum of the same sample is shown above in Fig. S1 of the ESI] (A), and authentic samples of $\mathbf{TAB^0}$ (B) and $\mathbf{MB^0}$ (C).

S3. Cyclic Voltammetry of TAB and 4-9

The CV cell was of an air-tight design with high vacuum Teflon valves and Viton O-ring seals to allow an inert atmosphere to be maintained without contamination by grease. The working electrode consisted of an adjustable platinum disk embedded in a glass seal to allow periodic polishing (with a fine emery cloth) without changing the surface area (~1 mm^2) significantly. The reference SCE electrode (saturated calomel electrode) and its salt bridge were separated from the catholyte by a sintered glass frit. The counter electrode consisted of a platinum gauze that was separated from the working electrode by ~3 mm. The CV measurements were carried out in a solution of 0.1 M supporting electrolyte (tetra-*n*-butylammonium hexafluorophosphate) and the substrate in dry CH_2Cl_2 under an argon atmosphere at 22 ºC. All the cyclic voltammograms were recorded at a sweep rate of 50 mV sec^{-1} and were IR compensated (Fig. S4). The oxidation potentials (E_{ox}, calculated by taking the average of anodic and cathodic peaks) were referenced to the added (equimolar) ferrocene.

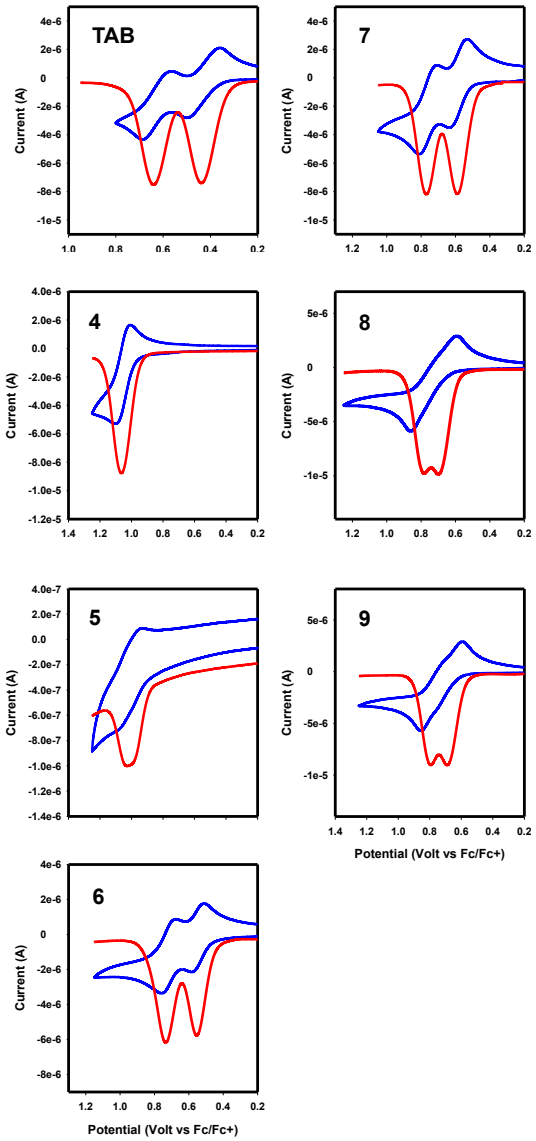
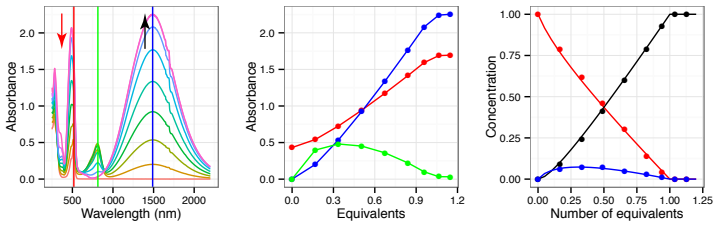


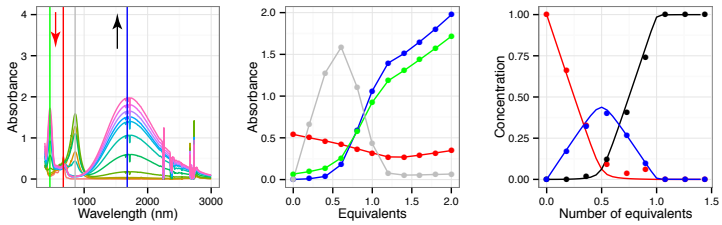
Fig. S4. Cyclic and square-wave voltammograms of **TAB** and **4**-**9** (Chart 1 of the Manuscript). Poor CV quality of **5** was due to its poor solubility in CH_2Cl_2.

S4. Redox Titrations of TAB and 6-9

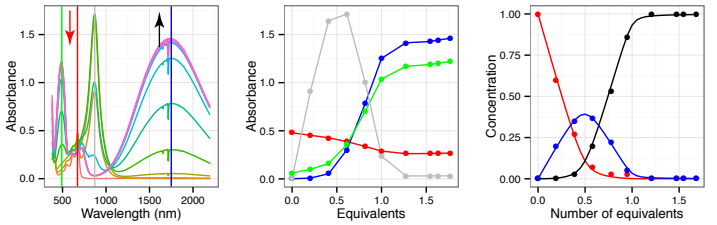
A: TAB^{0} (0.99 mM) + **THEO$^{+\bullet}$** $SbCl_6^-$ (59 uM) → **TAB$^{+\bullet}$** $SbCl_6^-$ + **THEO^{0}**



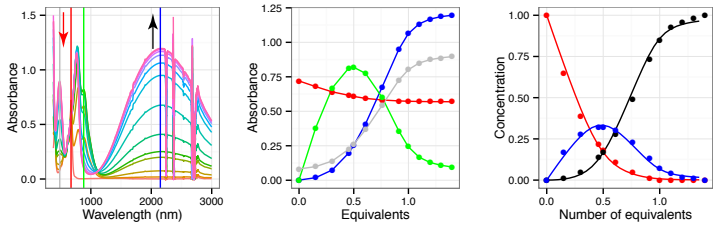
B: 6 (1.18 mM) + **NAP$^{+\bullet}$** $SbCl_6^-$ (58 uM) → **6$^{+\bullet}$** $SbCl_6^-$ + **NAP^{0}**



C: 7 (1.05 mM) + **NAP$^{+\bullet}$** $SbCl_6^-$ (52 uM) → **7$^{+\bullet}$** $SbCl_6^-$ + **NAP^{0}**



D: 8 (1.01 mM) + **NAP$^{+\bullet}$** $SbCl_6^-$ (77 uM) → **8$^{+\bullet}$** $SbCl_6^-$ + **NAP^{0}**



E: 9 (1.00 mM) + **NAP$^{+\bullet}$** $SbCl_6^-$ (57 uM) → **9$^{+\bullet}$** $SbCl_6^-$ + **NAP^{0}**

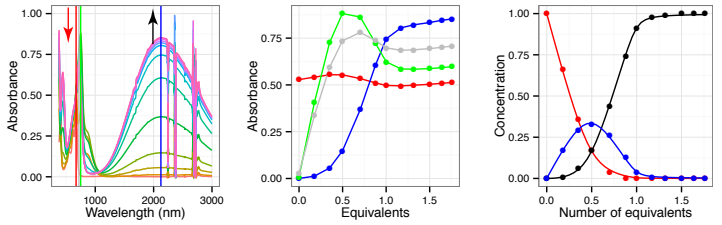


Fig. S5. Spectral changes attendant upon the reduction of **TAB** and **6**-**9** (**A**-**E**, as denoted) by **THEO$^{+\bullet}$** $SbCl_6^-$ and **NAP$^{+\bullet}$** $SbCl_6^-$ in CH_2Cl_2 at 22 ºC as well as the corresponding molar fraction plots against the number of added equivalents of neutral electron donor (i.e. **TAB** and **6**-**9**). See also Table S4.

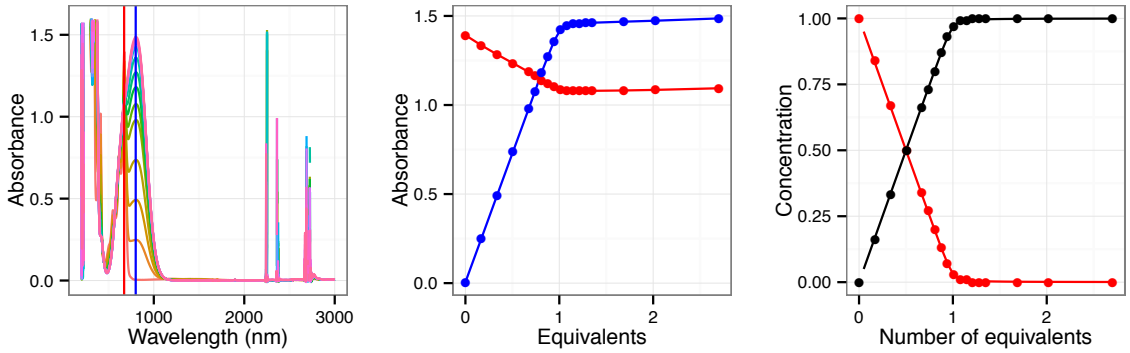


Fig. S6. Spectral changes attendant upon the reduction of 3.03 mM **BC** by 0.15 mM **NAP**$^{+\bullet}$ $SbCl_6^-$ in CH_2Cl_2 at 22 ºC as well as the corresponding molar fraction plot against the number of added equivalents of neutral **BC**.

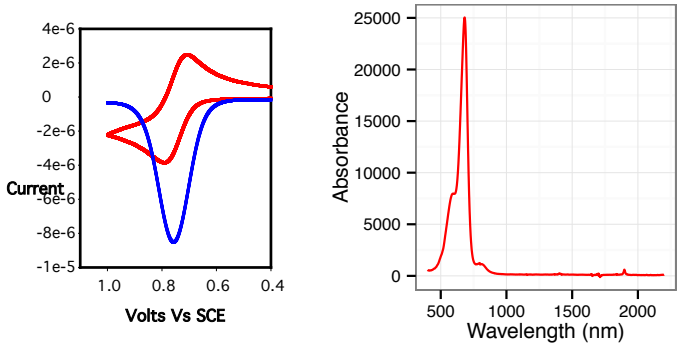


Fig. S7. (Left) Cyclic and square-wave voltammograms of 5 mM **10** in CH_2Cl_2 (22 ºC) containing 0.2 M tetra-*n*-butylammonium hexafluorophosphate at v = 200 mV s^{-1}. (Right) The molar absorptivity spectrum of **10** cation radical in CH_2Cl_2 (22 ºC).

S5. Crystal data and structure refinement

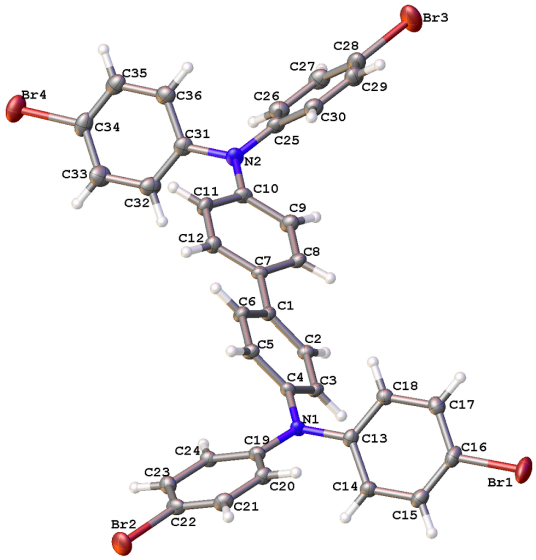


Fig. S8. ORTEP diagram of **TAB**.

Table S1. Crystal data and structure refinement for **TAB**

Identification code	raj25b
Empirical formula	$C_{36}H_{24}Br_4N_2$
Formula weight	803.95
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	15.3203(2)
b/Å	15.5925(2)
c/Å	19.8315(3)
α/°	87.2838(12)
β/°	81.2554(13)
γ/°	82.7604(12)
Volume/Å^3	4643.06(12)
Z	6
ϱ_{calc}g/cm^3	1.725
μ/mm^{-1}	6.559
F(000)	2363.0
Crystal size/mm^3	0.4519 × 0.2202 × 0.0592
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	5.72 to 148.1
Index ranges	-19 ≤ h ≤ 19, -19 ≤ k ≤ 19, -24 ≤ l ≤ 21
Reflections collected	88456
Independent reflections	18598 [R_{int} = 0.0359, R_{sigma} = 0.0223]
Data/restraints/parameters	18598/0/1135
Goodness-of-fit on F^2	1.014
Final R indexes [I>=2σ (I)]	R_1 = 0.0369, wR_2 = 0.0957
Final R indexes [all data]	R_1 = 0.0425, wR_2 = 0.1009
Largest diff. peak/hole / e Å^{-3}	2.42/-1.52

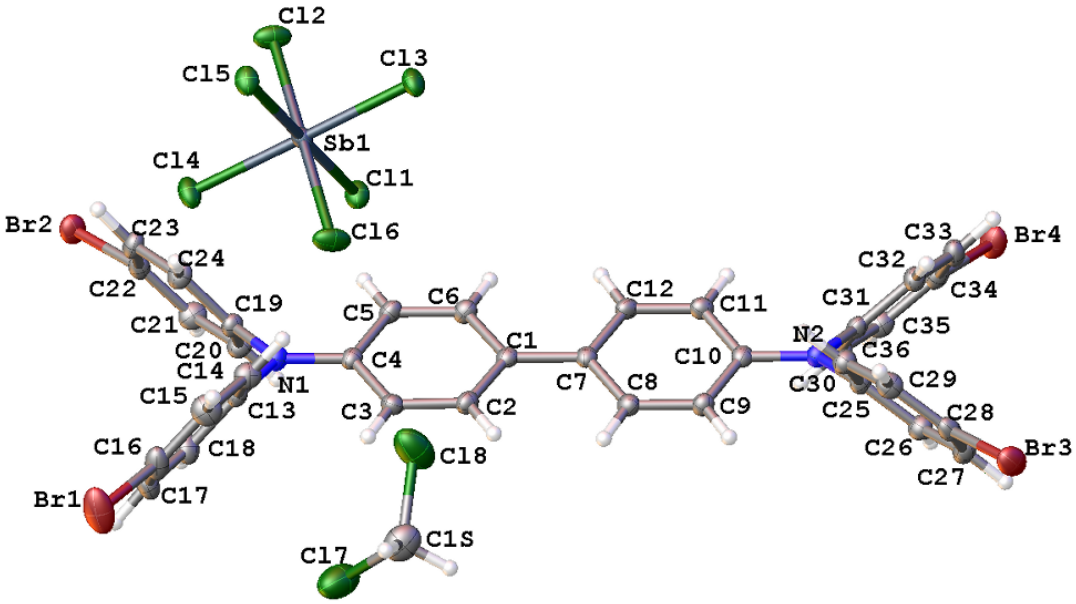


Fig. S9. ORTEP diagram of **TAB**$^{+\bullet}$.

Table S2. Crystal data and structure refinement for **TAB**$^{+\bullet}$

Identification code	raj25f
Empirical formula	C37H26N2Cl8Br4Sb
Formula weight	1223.59
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	P21/n
a/Å	15.37545(18)
b/Å	14.15367(14)
c/Å	19.4760(2)
α/°	90.00
β/°	91.4952(10)
γ/°	90.00
Volume/Å3	4236.90(8)
Z	4
ϱcalcg/cm3	1.918
μ/mm-1	14.474
F(000)	2356.0
Crystal size/mm3	0.2391 × 0.105 × 0.0323
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.24 to 148.2
Index ranges	-18 ≤ h ≤ 19, -17 ≤ k ≤ 17, -19 ≤ l ≤ 23
Reflections collected	41012
Independent reflections	8456 [Rint = 0.0366, Rsigma = 0.0238]
Data/restraints/parameters	8456/0/469
Goodness-of-fit on F2	1.023
Final R indexes [I>=2σ (I)]	R1 = 0.0266, wR2 = 0.0628
Final R indexes [all data]	R1 = 0.0310, wR2 = 0.0659
Largest diff. peak/hole / e Å-3	1.36/-1.10

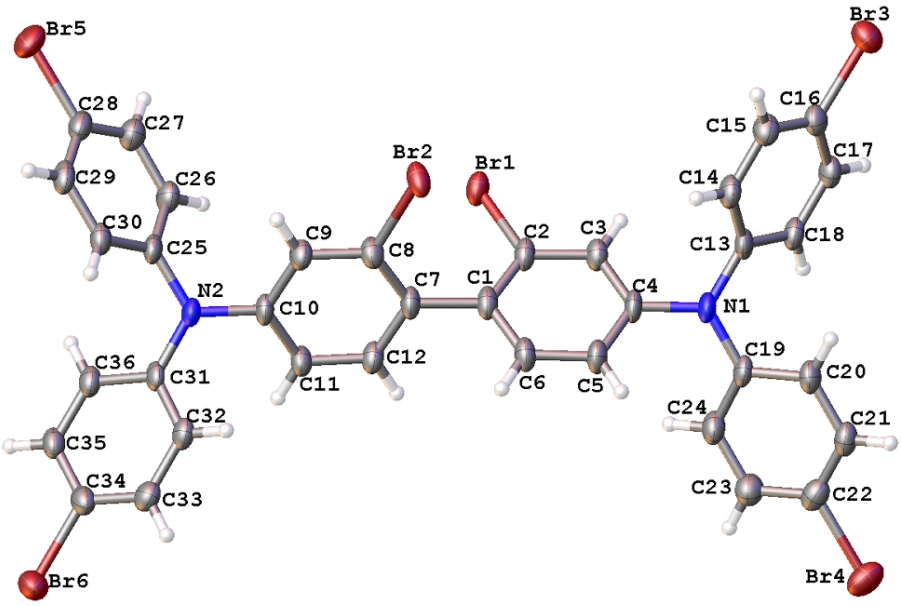


Fig. S10. ORTEP diagram of **9**.

Table S3. Crystal data and structure refinement for **9**

Identification code	raj25j
Empirical formula	C36H22N2Br6
Formula weight	962.02
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	10.1188(2)
b/Å	13.8839(3)
c/Å	16.4081(5)
α/°	107.983(2)
β/°	106.750(2)
γ/°	96.924(2)
Volume/Å3	2043.19(9)
Z	2
ϱcalcg/cm3	1.564
μ/mm-1	7.282
F(000)	924.0
Crystal size/mm3	0.3829 × 0.1448 × 0.0709
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.04 to 147.4
Index ranges	-12 ≤ h ≤ 12, -14 ≤ k ≤ 17, -20 ≤ l ≤ 20
Reflections collected	38897
Independent reflections	8166 [Rint = 0.0378, Rsigma = 0.0219]
Data/restraints/parameters	8166/0/397
Goodness-of-fit on F2	1.052
Final R indexes [I>=2σ (I)]	R1 = 0.0334, wR2 = 0.0931
Final R indexes [all data]	R1 = 0.0371, wR2 = 0.0955
Largest diff. peak/hole / e Å-3	1.42/-1.10

S6. Computational Details

Electronic structure calculations were performed with the Gaussian 09 package, revision D01.[1] For the density functional theory (DFT) calculations we used calibrated (see Ref.[2] for details) B1LYP functional[3] that contains 40% contribution (denoted as B1LYP-40) of the exact exchange with 6-31G(d) basis set by Pople and co-workers[4] (see refs [5,6] and references therein for the detailed discussion concerning self-interaction error). Solvent effects were included using the implicit integral equation formalism polarizable continuum model (IEF-PCM, also referred as PCM)[7-11] with the dichloromethane solvent parameters (ε = 8.93). In all DFT calculations, ultrafine Lebedev's grid was used with 99 radial shells per atom and 590 angular points in each shell. The wave function stability tests[12,13] was performed to ensure absence of solutions with lower energy. The values of $<S^2>$ operator after spin annihilation were confirmed to be close to the expectation value of 0.75, thus indicating that spin contamination was not an issue for the performed calculations. Energies of vertical electronic excitations were computed using the time-dependent density functional theory (TD-DFT) method.[13-17] Tight cutoffs on forces and atomic displacement were used to determine the convergence in geometry optimization procedure. Hessians were calculated for the optimized structures to confirm absence of imaginary frequencies.

Table S4. Wavelengths and oscillator strengths corresponding to the lowest-energy transition in the cation radicals of compounds in Chart 1 of the Manuscript, obtained from the TD-DFT calculations [B1LYP-40/6-31G(d)+PCM(CH_2Cl_2)] ($\lambda_{D0\rightarrow D1}$ and f_{osc}) as well as the lowest-energy transition of cation radicals (λ_{max}(CR) and ε_{max}(CR)) and dications (λ_{max}(DC) and ε_{max}(DC)) of these compounds obtained by spectroscopic redox titration

Compound	$\lambda_{D0\rightarrow D1}$, nm	f_{osc}	λ_{max}(CR), nm	ε_{max}(CR), M^{-1} cm^{-1}	λ_{max}(DC), nm	ε_{max}(DC), M^{-1} cm^{-1}
MB	604	0.30	728	28200	-	-
1	686	0.35	757[18]	-	-	-
2	721	0.24	805[18]	-	-	-
3	823	0.14	880[18]	-	-	-
4	1291	0.03	820[18]	-	-	-
5	1526	0.27	854, 2500	-	-	-
TAB	1353	1.00	1490	38100	807	112600
6	1420	0.73	1735	24000	860	66500
7	1304	0.56	1750	24500	869	87700
8	1339	0.21	2150	15000	883	25590
9	1428	0.30	2128	15000	752	41750

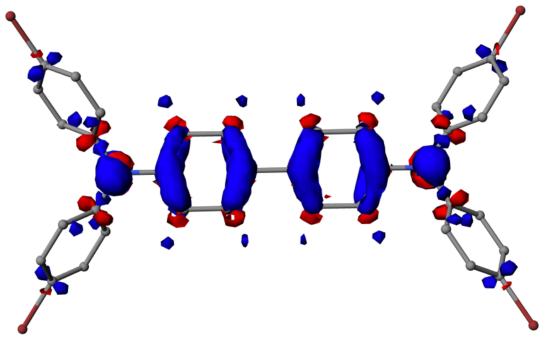


Fig. S11. Difference between the spatial electron density distributions in the **TAB** and **TAB**$^{+\bullet}$, with the geometries corresponding to **TAB**$^{+\bullet}$ [B1LYP-40/6-31G(d)+PCM(CH_2Cl_2)].

Table S5. Comparison of the bond lengths (in Å) of **TAB^{0}** (N) and **TAB$^{+\bullet}$** (CR), obtained by X-ray crystallography and by DFT calculations

		X-ray			DFT		
Atom1	Atom2	N	CR	Δ	N	CR	Δ
C1	**C2**	1.391	1.410	0.019	1.399	1.417	0.018
C2	**C3**	1.385	1.374	-0.011	1.385	1.369	-0.016
C1	**C6**	1.394	1.424	0.030	1.399	1.417	0.018
C3	**C4**	1.385	1.416	0.031	1.396	1.415	0.019
C4	**C5**	1.384	1.418	0.034	1.396	1.415	0.019
C5	**C6**	1.392	1.365	-0.027	1.385	1.369	-0.016
N1	**C4**	1.428	1.367	-0.061	1.417	1.374	-0.043
N1	**C13**	1.416	1.442	0.026	1.413	1.427	0.014
N1	**C19**	1.408	1.443	0.035	1.413	1.427	0.014
C13	**C14**	1.402	1.392	-0.010	1.397	1.394	-0.003
C13	**C18**	1.392	1.382	-0.010	1.397	1.394	-0.003
C14	**C15**	1.386	1.389	0.003	1.387	1.386	-0.001
C15	**C16**	1.377	1.376	-0.001	1.387	1.388	0.001
C16	**C17**	1.391	1.378	-0.013	1.387	1.388	0.001
C17	**C18**	1.386	1.387	0.001	1.387	1.386	-0.001
Br1	**C16**	1.903	1.907	0.004	1.906	1.899	-0.007
C19	**C20**	1.402	1.390	-0.012	1.397	1.394	-0.003
C19	**C24**	1.394	1.384	-0.010	1.397	1.394	-0.003
C20	**C21**	1.383	1.387	0.004	1.387	1.386	-0.001
C21	**C22**	1.383	1.385	0.002	1.387	1.388	0.001
C22	**C23**	1.385	1.387	0.002	1.387	1.388	0.001
C23	**C24**	1.390	1.386	-0.004	1.387	1.386	-0.001
Br2	**C22**	1.904	1.894	-0.010	1.906	1.899	-0.007
C1	**C7**	1.484	1.448	-0.036	1.479	1.441	-0.038
C7	**C12**	1.396	1.421	0.025	1.399	1.417	0.018
C7	**C8**	1.397	1.422	0.025	1.399	1.417	0.018
C8	**C9**	1.389	1.365	-0.024	1.385	1.369	-0.016
C9	**C10**	1.390	1.412	0.022	1.396	1.415	0.019
C10	**C11**	1.393	1.417	0.024	1.396	1.415	0.019
C11	**C12**	1.389	1.370	-0.019	1.385	1.369	-0.016
N2	**C10**	1.423	1.372	-0.051	1.417	1.374	-0.043
N2	**C25**	1.418	1.434	0.016	1.413	1.427	0.014
N2	**C31**	1.414	1.434	0.020	1.413	1.427	0.014
C25	**C26**	1.400	1.391	-0.009	1.397	1.394	-0.003
C25	**C30**	1.391	1.392	0.001	1.397	1.394	-0.003
C26	**C27**	1.385	1.383	-0.002	1.387	1.386	-0.001

		X-ray			DFT		
Atom1	Atom2	N	CR	Δ	N	CR	Δ
C27	**C28**	1.382	1.383	0.001	1.387	1.388	0.001
C28	**C29**	1.388	1.384	-0.004	1.387	1.388	0.001
C29	**C30**	1.389	1.394	0.005	1.387	1.386	-0.001
Br3	**C28**	1.904	1.900	-0.004	1.906	1.899	-0.007
C31	**C32**	1.396	1.392	-0.004	1.397	1.394	-0.003
C31	**C36**	1.397	1.393	-0.004	1.397	1.394	-0.003
C32	**C33**	1.387	1.386	-0.001	1.387	1.386	-0.001
C33	**C34**	1.390	1.384	-0.006	1.387	1.388	0.001
C34	**C35**	1.378	1.376	-0.002	1.387	1.388	0.001
C35	**C36**	1.386	1.384	-0.002	1.387	1.386	-0.001
Br4	**C34**	1.902	1.898	-0.004	1.906	1.899	-0.007

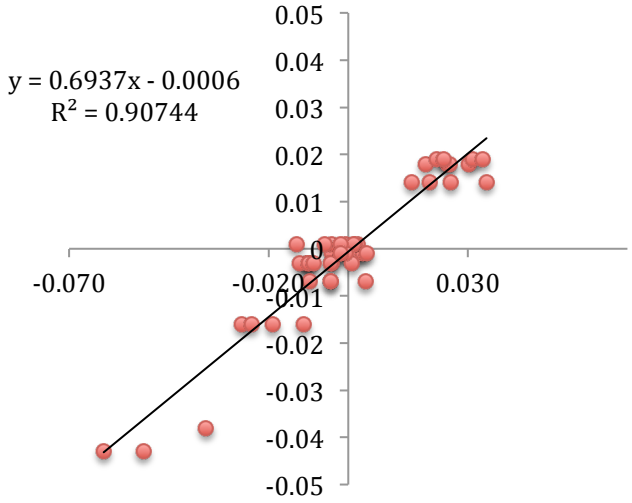


Fig. S12. Comparison of the oxidation-induced bond length changes (in Å) in **TAB** obtained by means of X-ray crystallography (abscissa) and DFT calculations (ordinate).

S7. General Experimental Methods and Materials.

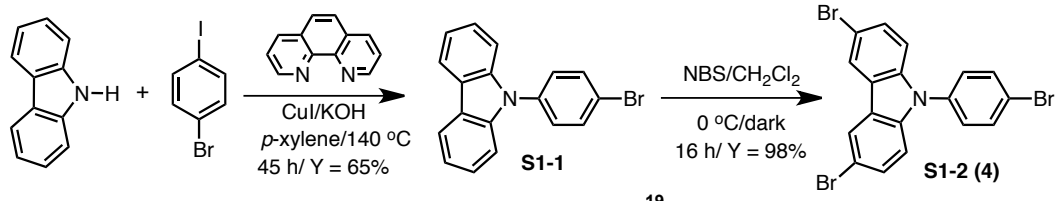
All reactions were performed under an argon atmosphere unless otherwise noted. All commercial reagents were used without further purification unless otherwise noted. Dichloromethane (Aldrich) was repeatedly stirred with fresh aliquots of concentrated sulfuric acid (~10 % by volume) until the acid layer remained colorless. After separation, CH_2Cl_2 layer was washed successively with water, 5% aqueous sodium bicarbonate, water, and saturated aqueous sodium chloride and dried over anhydrous calcium chloride. The CH_2Cl_2 was distilled twice from P_2O_5 under an argon atmosphere and stored in a Schlenk flask equipped with a Teflon valve fitted with Viton O-rings. Acetonitrile was stirred with molecular sieves overnight, filtered, and again stirred with $CaCl_2$ overnight. After that it was filtered and distilled twice from P_2O_5 under an argon atmosphere and stored in a Schlenk flask equipped with a Teflon valve fitted with Viton O-rings. The hexanes and toluene were distilled over P_2O_5 under an argon atmosphere and then refluxed over calcium hydride (~12 h). After distillation from CaH_2, the solvents were stored in Schlenk flasks under an argon atmosphere. Tetrahydrofuran (THF) was dried initially by distilling over lithium aluminum hydride under an argon atmosphere and stored in a Schlenk flask equipped with a Teflon valve fitted with Viton O-rings. NMR spectra were recorded on Varian 400 MHz NMR spectrometers.

S8. Synthesis of compounds in Chart 1.

Synthetic schemes for the preparation of compounds in Chart 1 (in the manuscript) are presented below in individual schemes S1-S8 together with the detailed experimental procedures for the each step of synthesis and their characterization data (i.e. numerical spectroscopic data) as well as $^{1}H/^{13}C$ NMR spectra are given below. Note that identity of each molecule was further confirmed by MALDI mass spectrometry.

S8.1. Synthesis of 3, 6-dibromo-9-(4′-bromophenyl)-9*H*-carbazole (S1-2 or 4).

Scheme S1.

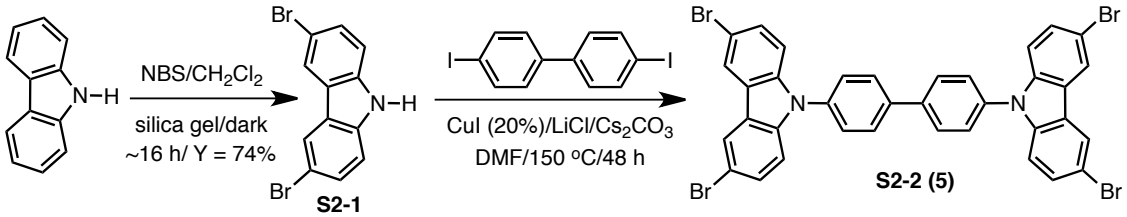


Preparation of 9-**(4-bromophenyl)-9*H*-carbazole (S1-1).**[19] A mixture of carbazole (1.0 g, 5.98 mmol), 4-bromoiodobenzene (1.86 g, 6.58 mmol), CuI (1.13 g, 5.98 mmol), 1,10-phenanthroline (1.05 g, 5.86 mmol) and KOH (1.50 g, 26.8 mmol) in *p*-xylene (50 mL) was stirred at ~140 °C for 45 hours. The reaction mixture was cooled to room temperature and the resulting suspension was filtered and residue was washed with *p*-xylene (3x 10mL). To the resulting filtrate CH_2Cl_2 (160 mL) was added and it was washed with water and dried over anhydrous $MgSO_4$. After removal of the solvent in vacuo, the crude product was purified on a silica gel chromatography with hexanes as eluent to afford compound **S1-1** as a solid. Yield: 1.26 g (65%). m.p. 146-147 ºC (lit.[19] m.p. 149-150 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.3 (t, 2H, *J* = 7.24 Hz), 7.41 (m, 6H), 7.73 (d, 2H, *J* = 7.70 Hz), 8.14 (d, 2H, *J* = 7.70 Hz); ^{13}C NMR (400 MHz, $CDCl_3$) δ 109.71, 120.37, 120.56, 121.03, 123.62, 126.25, 128.88, 133.27, 136.95, 140.73.

Preparation of 3,6-dibromo-9-(4-bromophenyl)-9*H*-carbazole (S1-2 or 4).[20] Compound **S1-1** (1.0 g, 3.10 mmol) was dissolved in dichloromethane (17 mL) in a Schlenk flask wrapped with aluminum foil. NBS (1.36 g, 7.69 mmol) was added as solid at 0 °C in the dark and the reaction mixture was stirred overnight (~16 h). It was quenched with water and extracted with dichloromethane (3 x 40 mL). The combined organic extracts were dried over anhydrous $MgSO_4$ and filtered. The organic layer was evaporated under reduced pressure. The residue was purified by silica gel chromatography with hexanes as the eluent to afford **S1-2** (**4**) as a crystalline solid. Yield: 1.46 g (98%). m.p. 208-210 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 (d, 2H, *J* = 8.75 Hz), 7.38 (d, 2H, *J* = 8.76 Hz), 7.50 (dd, 2H, *J* = 8.75 Hz, 1.9 Hz), 7.74 (d, 2H, *J* = 8.76 Hz), 8.18 (d, 2H, *J* = 1.9 Hz); ^{13}C NMR (400 MHz, $CDCl_3$) δ 111.46, 113.54, 121.90, 123.51, 124.21, 128.72, 129.74, 133.57, 136.00, 139.77.

S8.2. Synthesis of 4,4'-*bis*(3,6-dibromo-9H-carbazol-9-yl)-1,1'-biphenyl (S2-2 or 5)

Scheme S2.

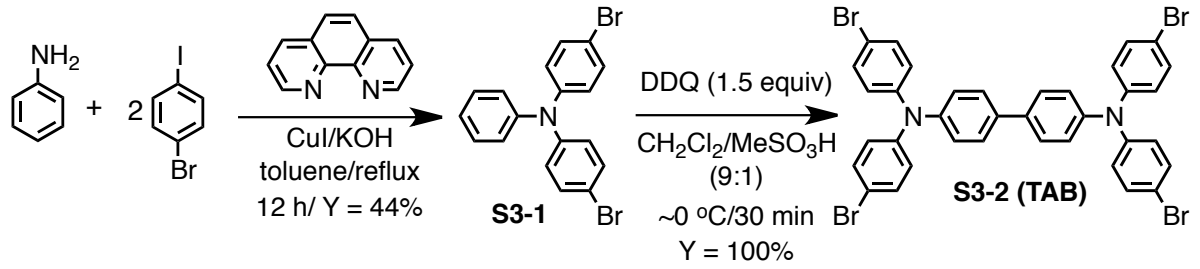


Preparation of 3,6-dibromo-9H-carbazole (S2-1).[21] Carbazole (0.5 g, 3.0 mmol) was dissolved in CH_2Cl_2 (100 mL) and SiO_2 (10 g, dried beforehand at 120 °C) and NBS (1.07 g, 6.0 mmol) was added slowly. The reaction mixture was stirred overnight (~16 h) at 22 °C in the absence of light under argon atmosphere. The mixture was filtered and the silica gel was washed with CH_2Cl_2 (3 x 30 mL). The combined organic layers were washed with brine (3 x 20 mL), dried over anhydrous $MgSO_4$, filtered, and evaporated to give **S2-1** as a greenish solid, which was further purified by crystallization from a mixture of ethanol and water (70:30). Yield: 0.724 g (74%). m.p. 203-205 ºC (lit.[22] m.p. 204-206 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, 2H, *J* = 8.4 Hz), 7.52 (dd, 2H, *J* = 8.59 Hz, 2.0 Hz), 8.09 (br s, 1H), 8.12 (d, 2H, *J* = 2.0 Hz); ^{13}C NMR (400 MHz, $CDCl_3$) δ 112.43, 112.82, 123.45, 124.28, 129.50, 138.52.

Preparation of 4,4'-*bis*(3,6-dibromo-9H-carbazol-9-yl)-1,1'-biphenyl (S2-2 or 5).[23] Compound **S2-1** (0.59 g, 1.83 mmol), Cs_2CO_3 (0.59 g, 1.83 mmol), 4,4′-diiodobiphenyl (0.41 g, 1.01 mmol), CuI (0.035 g, 0.183 mmol), LiCl (0.077 g, 1.83 mmol) and DMF (6 mL) were added in a sealed tube with screw cap and stirred in a ~150 °C oil bath. After 48 hour, the reaction mixture was cooled to room temperature and was diluted with saturated aqueous ammonium chloride. The product was extracted with ethyl acetate and then with chloroform. The combined organic extracts were dried over anhydrous $MgSO_4$, filtered and the solvent was evaporated under reduced pressure. The compound **S2-2 (or 5)** is partially soluble in most common organic solvents and therefore the accurate yield was determined. m.p. > 400 ºC ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm = 7.36 (d, 2H, *J* = 8.70 Hz), 7.55 (dd, 2H, *J* = 8.89 Hz, 1.88 Hz), 7.65 (d, 2H, *J* = 8.33 Hz), 7.91 (d, 2H, *J* = 8.28 Hz), 8.23 (d, 2H, *J* = 1.88 Hz). ^{13}C NMR was not taken due to poor solubility in $CDCl_3$.

S8.3. Synthesis of *tetrakis*-(4-bromophenyl)benzidine (S3-2 or TAB).

Scheme S3.



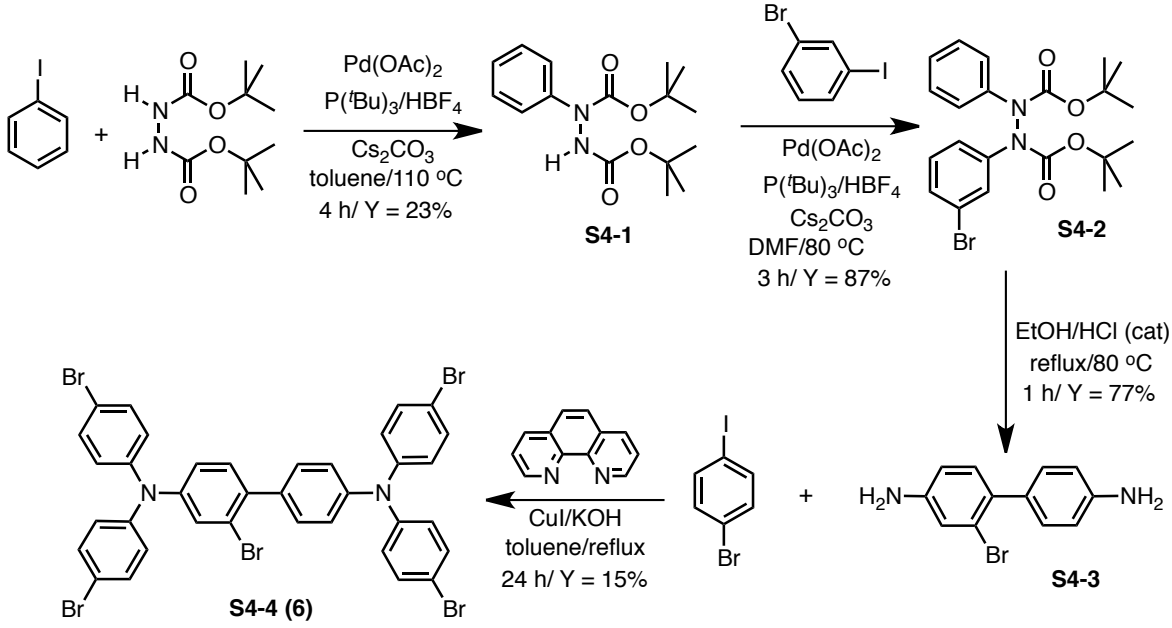
Preparation of 4-bromo-*N*-(4-bromophenyl)-*N*-phenylaniline (S3-1).[24] In a dry Schlenk flask a mixture of aniline (1.1 g, 12 mmol), 1-bromo-4-iodobenzene (8.5 g, 30 mmol), CuI (0.07 g, 0.36 mmol), 1,10-phenanthroline (0.065 g, 0.36 mmol), potassium hydroxide (5.2 g, 92 mmol) and toluene (60 mL) was stirred under an argon atmosphere at reflux for overnight (~16 h). The resulting mixture was then cooled to room temperature and poured into distilled water. The products were extracted with dichloromethane (4 × 50 mL), and the organic layers were dried over anhydrous $MgSO_4$. The solvent was evaporated under reduced pressure, and the resulting crude product was purified by silica gel column chromatography using hexanes as an eluent to obtain **S1-1** as a colorless viscous liquid. Yield: 2.14 g (44%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.94 (d, 4H, *J* = 8.9 Hz), 7.06 (m, 3H), 7.27 (m, 2H), 7.34 (d, 4H, *J* = 8.9 Hz); ^{13}C NMR (400 MHz, $CDCl_3$) δ 115.60, 123.88, 124.74, 125.55, 129.70, 132.48, 146.66, 147.04.

Preparation of S3-2 (TAB).[25,26] In a dry Schlenk flask compound **S1-1** (0.32 g, 0.79 mmol) was dissolved in dry dichloromethane (27 mL), cooled to 0°C and after 5 minutes methanesulfonic acid (3 mL) was added under an argon atmosphere. DDQ (2,3-dichloro-5,6-dicyanobenzoquinone) (0.27 g, 1.2 mmol) was added as solid, and the resulting mixture was stirred for 30 minutes. The reaction was quenched with saturated aqueous $NaHCO_3$ solution (50 mL) and extracted with dichloromethane (3 x 25 mL). The organic extracts were washed with water, and dried over anhydrous $MgSO_4$. Solvent was removed under reduced pressure and the resulting crude solid was crystallized from acetonitrile to afford **TAB** as a colorless crystalline solid in nearly quantitative yield. m.p. 226-227 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97

(d, 4H, *J* = 8.93 Hz), 7.09 (d, 2H, *J* = 8.64 Hz), 7.36 (d, 4H, *J* = 8.93 Hz), 7.45 (d, 2H, *J* = 8.7 Hz); ^{13}C NMR (400 MHz, $CDCl_3$) δ 115.88, 124.68, 125.78, 127.85, 132.60, 135.63, 146.16, 146.53.

S8.4. Synthesis of 2-bromo-*N*^{4},*N*^{4},*N*$^{4'}$,*N*$^{4'}$-*tetrakis*(4-bromophenyl)-[1,1'-biphenyl]-4,4'-diamine (S4-4 or 6)

Scheme S4.



Preparation of di-*tert*-butyl-1-phenylhydrazine-1,2-dicarboxylate (S4-1).[27] A sealed tube were charged with iodobenzene (1.83 g , 8.97 mmol), di-*tert*-butylhydrazine-1,2-dicarboxylate (2.5 g, 10.76 mmol), $Pd(OAc)_2$ (0.1 g, 0.45 mmol), P(t-Bu)$_3$·HBF_4 (0.26 g, 0.89 mmol), Cs_2CO_3 (4.09 g, 12.55 mmol) and dry toluene (20 mL) at room temperature. The reaction mixture was degassed, tube was filled with with argon, sealed with a screw cap and heated at 110 °C for 4h. The reaction mixture was then cooled to room temperature and filtered through a short pad of silica gel using ethyl acetate as the eluent. The organic solution was concentrated and purified by flash column chromatography on silica gel (hexanes:ethyl acetate = 10:1) to afford hydrazide **S4-1** as a pale yellow solid. Yield = 0.75 g (23%). m.p. 78-80 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.49 (s, 18H), 6.81/6.60 (rotamers, 2 x br s, 1H, NHBoc), 7.13 – 7.17 (m, 1H), 7.33 – 7.29 (m, 2H), 7.40 (m, 2H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 28.26, 28.31, 81.6, 82.3, 123.8, 125.6, 128.5, 142.3, 153.7, 155.5.

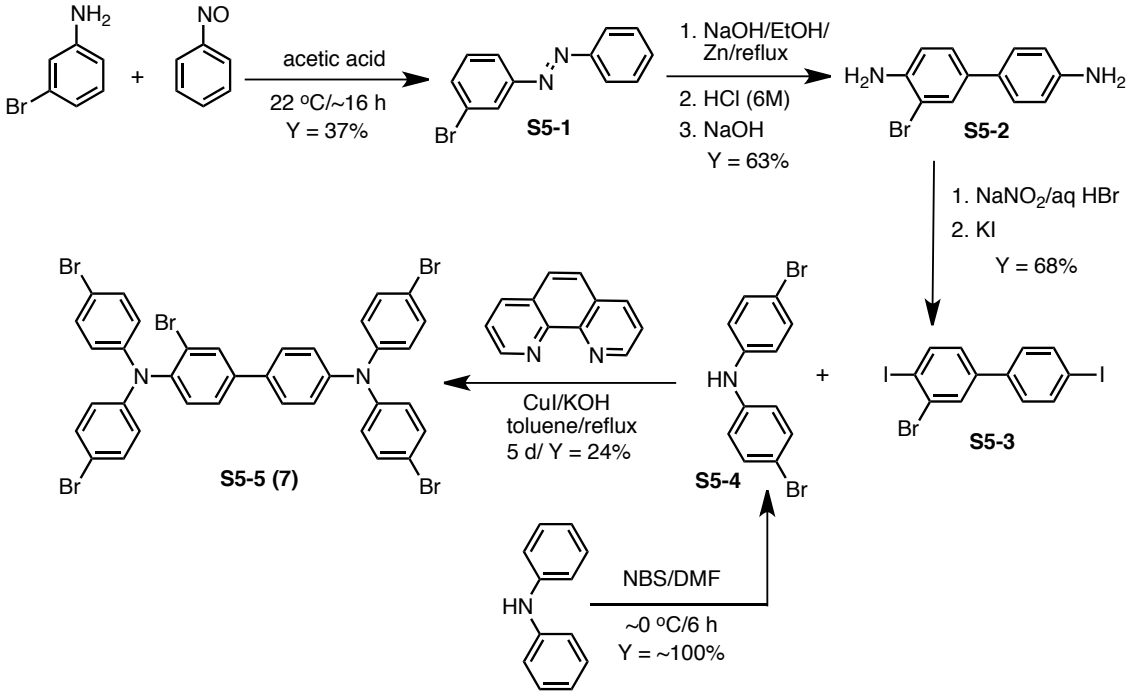
Preparation of di-*tert*-butyl-1-(3-bromophenyl)-2-phenylhydrazine-1,2-dicarboxylate (S4-2).[28] A sealed tube was charged with 1-bromo-3-iodobenzene (0.41 g, 1.46 mmol), **S4-1** (0.41 g, 1.32 mmol), CuI (0.28 g, 1.46 mmol), 1,10-phenanthroline (0.26 g, 1.46 mmol), Cs_2CO_3 (0.47 g, 1.46 mmol) and DMF (3.0 mL) at room temperature. The reaction mixture was degassed, tube was filled with argon, sealed with screw cap and heated at 80 °C for 3 h. The reaction mixture was then cooled to room temperature and filtered through a short pad of silica gel using ethyl acetate as the eluent. The organic solution was concentrated and purified by flash column chromatography on silica gel using hexanes as the eluent to afford compound **S4-2**. Yield: 0.54 g, 87%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14-7.18 (t, 2H, *J* = 7.9 Hz), 7.26-7.40 (m, 6H), 7.66 (bs, 1H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 28.26, 28.29, 83.3, 83.5, 121.1 (bs), 122.7, 122.9 (bs), 126.4, 129.0, 129.3, 130.5, 135.0, 141.5, 143.1, 153.4, 153.6.

Preparation of 2-bromo-[1,1'-biphenyl]-4,4'-diamine (S4-3).[28] A Schlenk flask was charged with **S4-2** (0.47 g, 1.01 mmol), 10 mL of ethanol and 0.5 mL of conc. HCl at room temperature. The reaction mixture was heated to reflux for 1 h. The resulting mixture was then cooled to 0 °C, neutralized with aqueous $NaHCO_3$, extracted with dichloromethane and dried over anhydrous $MgSO_4$, filtered and the solvent was evaporated under reduced pressure. The crude product was purified by silica gel chromatography to afford **S4-3** which was rather unstable and was used in the next step without further purification. Yield: ~77%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.71 (bs, 4H), 6.63 (dd, 1H, *J* = 8.23 Hz, 2.4 Hz), 6.70 (d, 2H, *J* = 8.63 Hz), 6.97 (d, 1H, *J* = 2.38 Hz), 7.08 (d, 1H, *J* = 8.23 Hz), 7.18 (d, 2H, *J* = 8.63 Hz); ^{13}C NMR (400 MHz, $CDCl_3$) δ 114.35, 114.56, 119.07, 123.33, 130.65, 131.57, 131.86, 132.70, 145.51, 146.33.

2-bromo-*N*^{4},*N*^{4},*N*$^{4'}$,*N*$^{4'}$-*tetrakis*(4-bromophenyl)-[1,1'-biphenyl]-4,4'-diamine (S4-4 or 6).[24] In a dry Schlenk flask, a mixture of **S4-3** (0.28 g, 1.06 mmol), 1-bromo-4-iodobenzene (1.23 g, 4.36 mmol), CuI (0.08 g, 0.42 mmol), 1,10-phenanthroline (0.076 g, 0.42 mmol), potassium hydroxide (0.45 g, 8.15 mmol) and toluene (20 mL) was stirred and refluxed under argon atmosphere for 24h. The mixture was then cooled to room temperature and poured into distilled water. The products were extracted with dichloromethane (4 x 50 mL) and the organic layers were dried over anhydrous $MgSO_4$, filtered and evaporated under reduced pressure. The resulting crude product was purified by silica gel column chromatography using hexanes as the eluent. The brown solid was further purified by multiple treatment with charcoal (20 mg) in dichloromethane (100 mL). The resulting solid was crystallized from a mixture of acetonitrile and dichloromethane to afford **S4-4** (or **6**) as pale yellow solid. Yield: 0.14 g, (15%). m.p. 244-246 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.99 (m, 9H), 7.06 (d, 2H, *J* = 8.68 Hz), 7.19 (d, 1H, *J* = 8.40 Hz), 7.30 (m, 3H), 7.38 (m, 8H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 116.03, 116.64, 122.54, 123.12, 123.17, 126.04, 126.16, 127.73, 130.68, 131.86, 132.61, 132.79, 135.40, 136.53, 145.97, 146.30, 146.44, 147.09.

S8.5. Synthesis of 3-bromo-*N*^{4},*N*^{4},*N*$^{4'}$,*N*$^{4'}$-*tetrakis*(4-bromophenyl)-[1,1'-biphenyl]-4,4'-diamine (S5-5 or 7).

Scheme 5.



Preparation of (*E*)-1-(3-bromophenyl)-2-phenyldiazene (S5-1)[29] To a solution of nitrosobenzene (5.25 g, 49.01 mmol) in glacial acetic acid (40 mL), 2-bromoaniline (10.11 g, 58.81 mmol) was added resulting immediately into a green solution. The mixture was stirred overnight (~16 h) at 22 ^{o}C after which time it turned deep red. The reaction mixture was poured into 700 mL of water. Aqueous NaOH (50 g in 300 mL water) was added slowly until the solution was almost neutralized (tested by pH paper). **[Caution: Addition of alkali to this reaction mixture is highly exothermic!]** The resulting solution was extracted with diethyl ether (3 x 100 mL) and the combined ether extracts were washed with aqueous Na_2CO_3 solution (2 x 100 mL). The ethereal solution was then treated with a mixture of diethyl ether and HCl (30 mL HCl in 50 mL diethyl ether). The precipitated 2-bromoaniline hydrochloride was filtered off, and the filtrate evaporated to about 100 mL. The red solution containing bromoazobenzene **S5-1** was subjected to column chromatography on basic alumina using diethyl ether as the eluent. The resulting red oil from chromatographic separation solidified upon treating with ethanol-solid carbon dioxide (dry ice). The red solid mass was allowed to warm to 0 °C and was filtered. Yield: 4.84 g (37%). m.p. 35-36 ºC (lit.[22] m.p. 36 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (td, 1H, *J* = 7.61 Hz, 1.67 Hz, 0.65 Hz), 7.40 (td, 1H, 7.7 Hz, 1.67 Hz, 0.70 Hz), 7.53 (m, 3H), 7.68 (dd, 1H, *J* = 7.96 Hz, 1.75 Hz), 7.76 (dd, 1H, *J* = 7.88 Hz, 1.33 Hz), 7.98 (m, 2H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 117.95, 123.58, 125.89, 128.14, 129.33, 131.75, 132.04, 133.89, 149.76, 152.76.

Preparation of 3-bromo-[1,1'-biphenyl]-4,4'-diamine (S5-2).[29] To a solution of bromoazobenzene **S5-1** (3.26 g) in ethanol (40 mL) zinc dust (1.70 g, 26.20 mmol) was added and the mixture was stirred. An aqueous ethanolic solution of NaOH (2 g NaOH dissolved in 5.0 mL water + 35 mL ethanol) was added to the above reaction mixture and it was refluxed until the red color disappeared (~2 h). It was then cooled to ambient temperature and filtered into an excess of concentrated hydrochloric acid. The solid Zn-residue was washed with warm ethanol and the washings were added to the main filtrate. The resulting precipitate of 3-bromobenzidine hydrochloride was filtered and the precipitate was added to an aqueous NaOH solution (20 g NaOH in 300 mL H_2O) and stirred for 20 min, and then extracted with dichloromethane (3 x 30 mL) and dried over anhydrous $MgSO_4$. The solvent was removed under reduced pressure and crude product was crystallized from dilute aqueous HCl solution to afford pure **S5-2**. Yield: 2.08 g (63%). m.p. 79-81 ºC (lit.[22] m.p. 81 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.69 (bs, 2H), 4.06 (bs, 2H), 6.72 (d, 2H, *J* = 8.71 Hz), 6.79 (d, 1H, *J* = 8.31 Hz), 7.31 (m, 3H), 7.60 (d, 1H, *J* = 2.17 Hz); ^{13}C NMR (400 MHz, $CDCl_3$) δ 109.94, 115.55, 116.11, 126.46, 127.41, 130.30, 130.39, 133.11, 142.57, 145.54.

Preparation of 3-bromo-4,4'-diiodo-1,1'-biphenyl (S5-3).[30] To a stirred solution of **S5-2** (0.5 g, 1.90 mmol) in 48% HBr (3.0 mL) and water (10.0 mL) at 0 °C was added slowly an aqueous solution of $NaNO_2$ (0.393 g, 5.70 mmol in 5 mL H_2O). The resulting mixture was stirred vigorously for 1h at ~0 °C. A cold aqueous solution of KI (6.30 g, 38 mmol in 10.0 mL H_2O) was added in above reaction mixture dropwise and it was allowed to stir and warm to room temperature stir during the course of overnight (~16 h). The reaction mixture was then diluted with dichloromethane (100 mL) and washed with 10% aqueous NaOH solution (100 mL) and $Na_2S_2O_3$ solution (100 mL) and dried over anhydrous $MgSO_4$, filtered, and the solvent was removed under reduced pressure. The resulting crude product was purified through flash column chromatography using hexanes as the eluent to afford pure **S5-3**. Yield: 0.63 g (68%). m.p. 81-83 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 (dd, 1H, *J* = 8.23 Hz, 2.14 Hz), 7.26 (d, 2H, *J* = 8.04 Hz), 7.77 (d, 2H, *J* = 8.60 Hz), 7.80 (d, 1H, *J* = 2.14 Hz), 7.90 (d, 1H, *J* = 8.23 Hz); ^{13}C NMR (400 MHz, $CDCl_3$) δ 94.37, 100.29, 126.99, 128.78, 130.55, 131.03, 138.28, 138.32, 140.78, 141.85.

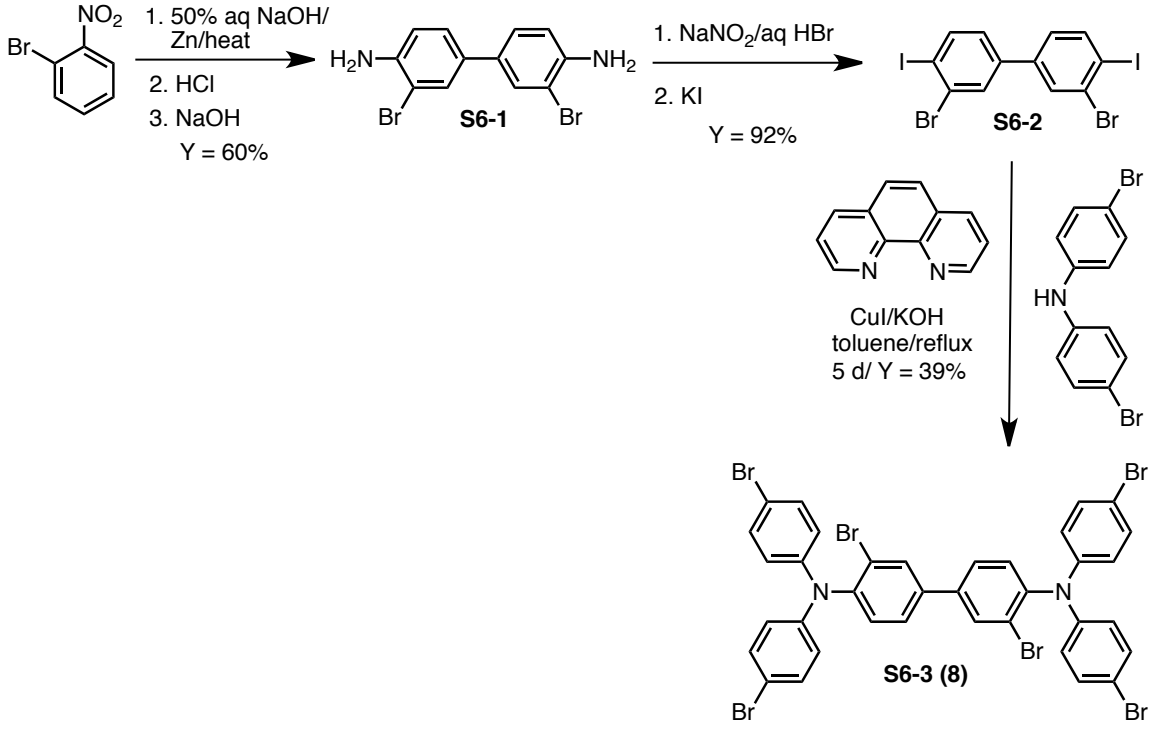
Preparation of *bis*(4-bromophenyl)amine (S5-4).[31] A solution of *N*-bromosuccinimide (5.27 g, 29.6 mmol) in DMF (25 mL) was added dropwise during the course of 30 min to a stirred solution of diphenylamine (2.5 g, 14.8 mmol) in DMF (25 mL) at ~0 °C. The resulting mixture was stirred at ~0 °C for 6 h. Water was added and the precipitate was filtered, washed with water and dried in vacuo to afford **S5-4** as a colorless solid. Yield: 4.83 g (~100%). m.p. 104-106 ºC (lit.[32,33] m.p. 105-107 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.65 (bs, 1H), 6.91 (d, 4H, *J* = 8.75 Hz), 7.36 (d, 4H, *J* = 8.75 Hz); ^{13}C NMR (400 MHz, $CDCl_3$) δ 113.56, 119.65, 132.55, 141.86.

Preparation of 3-bromo-$N^4,N^4,N^{4'},N^{4'}$-*tetrakis*(4-bromophenyl)-[1,1'-biphenyl]-4,4'-diamine (S5-5 or 7).[24] In a dry Schlenk flask, a mixture of **S5-3** (0.40 g, 0.82 mmol), *bis*(4-bromophenyl)amine (**S5-4**,

0.56 g, 1.73 mmol), CuI (0.033 g, 0.173 mmol), 1,10-phenanthroline (0.031 g, 0.173 mmol), potassium hydroxide (0.77 g, 13.84 mmol) and toluene (30 mL) was refluxed under an argon atmosphere for 5 d. After which time it was cooled to room temperature and poured into distilled water, and extracted with dichloromethane (4 x 20 mL). The organic layers were dried over anhydrous $MgSO_4$, filtered, and the solvent evaporated under reduced pressure. The resulting crude product was purified by silica gel column chromatography using hexanes as the eluent to afford **S5-5 (or 7)**. Yield: 0.18 g (24%). m.p. 213-215 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.87 (d, 4H, *J* = 8.95 Hz), 6.98 (d, 4H, *J* = 8.95 Hz), 7.11 (d, 2H, *J* = 8.74 Hz) 7.23 (d, 1H, *J* = 8.25 Hz), 7.34 (d, 4H, *J* = 8.95 Hz), 7.38 (d, 4H, *J* = 8.95 Hz), 7.44 (d, 2H, *J* = 8.75 Hz), 7.49 (dd, 1H, *J* = 8.28 Hz, 2.17 Hz), 7.82 (d, 1H, *J* = 2.09 Hz); ^{13}C NMR (400 MHz, $CDCl_3$) δ 115.18, 116.27, 123.72, 123.81, 124.23, 126.03, 127.37, 128.14, 131.46, 132.39, 132.69, 132.78, 133.64, 140.38, 143.35, 145.75, 146.31, 147.05.

S8.6. Synthesis 3,3'-dibromo-*N*^{4},*N*^{4},*N*$^{4'}$,*N*$^{4'}$-*tetrakis*(4-bromophenyl)-[1,1'-biphenyl]-4,4'-diamine (S6-3 or 8).

Scheme S6.



Preparation of 3,3'-dibromo-[1,1'-biphenyl]-4,4'-diamine (S6-1).[34] A mixture of *o*-nitrobromobenzene (5.5 g) and 50% aqueous sodium hydroxide (1.5 mL) was stirred at 60 °C, and zinc dust was added intermittently in small portions such that the temperature did not exceed beyond 70-80 °C. After 3.5 g of zinc had been added, the resulting sludge was diluted with water (12.5 mL) and 20% aqueous sodium hydroxide (7.5 mL). Another portion of zinc (5 g) was added at once and the resulting mixture was stirred at 70-80 °C until it was nearly colorless. The resulting mixture was cooled to room temperature and poured slowly into 25% sulfuric acid (50 mL) cooled to ~10 °C and then filtered. The blackish-ash colored solid was triturated with diethyl ether (2 x 100 mL). Combined ether extracts were dried over anhydrous $MgSO_4$, filtered, and evaporated under reduced pressure. The crude solid was dissolved in 50 mL ether and slowly poured into a stirred concentrated HCl (20 mL) cooled in an ice bath. 0 °C). After stirring for 1 hour, the precipitated salt was filtered and washed with ether. The hydrochloride salt was suspended in excess 10% aqueous sodium hydroxide and heated on a steam bath for 1h. The

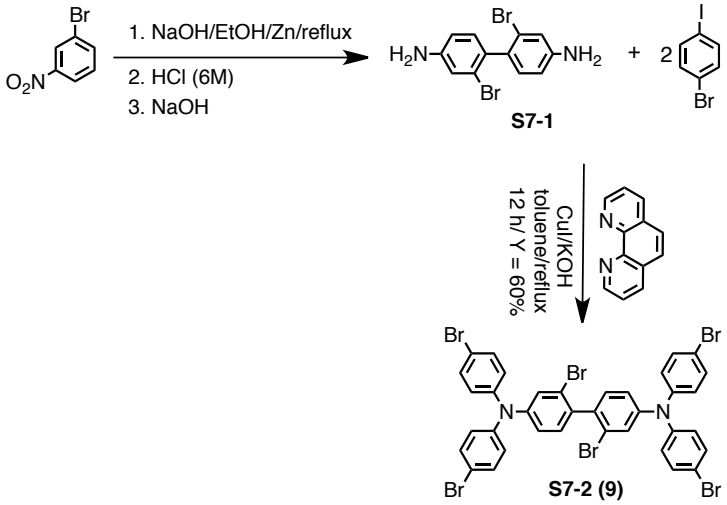
free base was extracted from the cooled mixture with ether and the ether extracts were dried over anhydrous $MgSO_4$ and evaporated. The crude product was crystallized from a mixture of ethanol and water to afford pure **S6-1**. Yield: 2.79 g (60%). m.p. 128-129 ºC (lit.[34] m.p. 127-129 ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.09 (bs, 4H), 6.79 (d, 2H, *J* = 8.28 Hz), 7.25 (dd, 2H, *J* = 8.28 Hz, 2.10 Hz), 7.56 (d, 2H, *J* = 2.10 Hz); ^{13}C NMR (400 MHz, $CDCl_3$) δ 109.90, 116.13, 126.54, 130.44, 131.71, 143.04.

Preparation of 3,3'-dibromo-4,4'-diiodo-1,1'-biphenyl (S6-2).[31] Using a slightly modified literature procedure, a stirred solution of **S6-1** (0.5 g, 1.46 mmol) in a mixture of 48% HBr (3.0 mL) and water (10.0 mL) at ~0 °C was added dropwise an aqueous solution of $NaNO_2$ (0.302 g, 4.38 mmol in 5 mL H_2O). After addition of $NaNO_2$, the reaction mixture was stirred vigorously for 1h at ~-5 °C. A cold aqueous solution of KI (4.84 g, 29.2 mmol in 10 mL H_2O) was added to the above reaction mixture slowly, and it was stirred overnight (~16 h) and was allowed to warm to room temperature. The reaction mixture was diluted with dichloromethane (100 mL) and washed with aqueous 10% NaOH solution (100 mL) and aqueous $Na_2S_2O_3$ solution (100 mL). Combined organic extracts were dried over anhydrous $MgSO_4$, filtered, and evaporated under reduced pressure. The crude product was purified by silica get column chromatography using hexanes as the eluent to afford pure **S6-2**. Yield: 0.76 g (92%). m.p. 179-181 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15 (dd, 2H, *J* = 8.27 Hz, 2.18 Hz), 7.78 (d, 2H, *J* = 2.18 Hz), 7.91 (d, 2H, *J* = 8.27 Hz); ^{13}C NMR (400 MHz, $CDCl_3$) δ 101.14, 126.98, 130.73, 131.02, 140.53, 140.93.

Preparation of 3,3'-dibromo-*N*^{4},*N*^{4},*N*$^{4'}$,*N*$^{4'}$-*tetrakis*(4-bromophenyl)-[1,1'-biphenyl]-4,4'-diamine (S6-3 or 8).[24] In a dry Schlenk flask, a mixture of compound **S6-2** (0.40 g, 0.71 mmol), *bis*(4-bromophenyl)amine **10** (0.48 g, 1.48 mmol), CuI (0.28 g, 0.148 mmol), 1,10-phenanthroline (0.26 g, 0.148 mmol), potassium hydroxide (0.66 g, 11.90 mmol) and toluene (30 mL) was refluxed under an argon atmosphere for 5 d. The mixture was then cooled to room temperature and poured into distilled water and extracted with dichloromethane (4 x 50 mL). The organic layer was dried over anhydrous $MgSO_4$, filtered, evaporated. The crude product was purified by silica gel column chromatography using hexanes as the eluent to afford pure **S6-3** (**8**). Yield: 0.27 g (39%). m.p. 228-230 ºC ^{1}H NMR (400 MHz, CD_2Cl_2) δ 6.87 (d, 8H, *J* = 8.95 Hz), 7.27 (d, 2H, *J* = 8.25 Hz), 7.35 (d, 8H, *J* = 8.95 Hz), 7.55 (dd, 2H, *J* = 8.25 Hz, 2.20 Hz), 7.87 (d, 2H, *J* = 2.20 Hz); ^{13}C NMR (400 MHz, CD_2Cl_2) δ 115.52, 124.13, 124.24, 128.16, 132.00, 132.71, 133.50, 139.06, 144.68, 146.12.

S8.7. Synthesis of 2,2'-dibromo-*N*^{4},*N*^{4},*N*$^{4'}$,*N*$^{4'}$-*tetrakis*(4-bromophenyl)-[1,1'-biphenyl]-4,4'-diamine (S7-2 or 9).

Scheme S7.

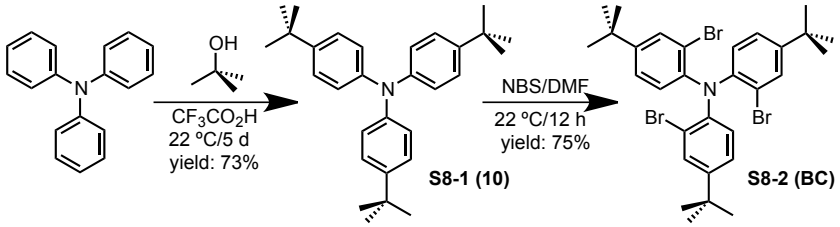


Preparation of 2,2'-dibromo-[1,1'-biphenyl]-4,4'-diamine (S7-1).[35] To a stirred solution of 3-bromonitrobenzene (5.5 g, 27.2 mmol) in ethanol (60 mL) were added in portions a solution of sodium hydroxide (2.5 g in 15 mL water) and zinc powder (10 g). The mixture was brought to 70 °C and after 15 minutes, more zinc (6 g) was added. After an additional 15 min, the mixture became pale yellow. It was then brought to a boil and filtered under an argon atmosphere. The zinc residue was washed with ethanol (2 x 10 mL). The combined filtrate was mixed with water (50 mL), and the mixture was cooled in an ice bath, which resulted in a pale yellow precipitate. The filtered precipitate was added to hydrochloric acid (6 M, 50 mL) and stirred at 60 °C for 15 minutes, then cooled rapidly. The solid benzidine hydrochloride was collected, washed with 6M hydrochloric acid and diethyl ether, and suspended in warm water containing excess sodium hydroxide. This mixture was extracted with diethyl ether (3 x 50 mL) and the extracts were dried over anhydrous $MgSO_4$, filtered, and evaporated. The crude benzidine **S7-1** was crystallized from ethanol-water mixture. Yield: 0.85 g (18%). m.p. 150-152 ºC (lit. [35] m.p. 151-153ºC). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.74 (br s. 4 H for NH_2), 6.64 (dd, 2H, *J* = 8.18 Hz, 2.36 Hz), 6.97 (d, 2H, *J* = 2.33 Hz), 7.00 (d, 2H, *J* = 8.18 Hz); ^{13}C NMR (400 MHz, $CDCl_3$) δ 113.95, 118.44, 124.95, 132.17, 132.24, 146.99.

Preparation of 2,2'-dibromo-*N*^{4},*N*^{4},*N*$^{4'}$,*N*$^{4'}$-*tetrakis*(4-bromophenyl)-[1,1'-biphenyl]-4,4'-diamine (S7-2 or 9).[24] In a dry Schlenk flask, a mixture of **S7-1** (0.4 g, 1.17 mmol), 1-bromo-4-iodobenzene (1.35 g, 4.8 mmol), CuI (0.013 g, 0.07 mmol), 1,10-phenanthroline (0.012 g, 0.07 mmol), potassium hydroxide (0.502 g, 8.96 mmol), and toluene (35 mL) was refluxed under an argon atmosphere for 24 h. The mixture was then cooled to room temperature and poured into distilled water. The crude product was extracted with dichloromethane (4 x 50 mL) and the combined organic layers were dried over anhydrous $MgSO_4$, filtered, and evaporated. The crude product was purified by silica gel column chromatography using hexanes as the eluent to afford **S7-2** (or **9**) as a brown-colored solid. The colored impurities were removed by repeated treatments (3 times) with charcoal (20 mg) in refluxing dichloromethane (25 mL) followed by crystallization from a mixture of acetonitrile and chloroform to afford shiny crystals of **S7-2** (or **9**). Yield: 0.67 g (60%). m.p. 278-280 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.00 (m, 10H), 7.11 (d, 2H, *J* = 8.32 Hz), 7.29 (d, 2H, *J* = 2.37 Hz), 7.40 (d, 8H, *J* = 8.80 Hz); ^{13}C NMR (400 MHz, $CDCl_3$) δ 116.89, 121.56, 124.53, 126.38, 126.45, 131.95, 132.87, 135.93, 145.91, 147.67.

S8.8. Synthesis of *tris*(2-bromo-4-(*tert*-butyl)phenyl)amine (S8-2 or BC)

Scheme S8.



Preparation of *tris*(4-(*tert*-butyl)phenyl)amine (S8-1 or 10).[36] A mixture of triphenylamine (1.23 g, 5 mmol), 2-methylpropane-2-ol (5 ml), and trifluoroacetic acid (20 mL) was stirred at 22 °C for 5 days. After which time the resulting precipitate thus formed was filtered, dried and recrystallized from a mixture of dichloromethane and hexanes to afford pure **S8-1** (**or 10**). Yield: 1.5 g (73%), m.p. 286-288 ºC (lit.[37] m.p. 276-278 ºC). ^{1}H NMR ($CDCl_3$) δ 1.30 (s, 27H), 7.01 (d, *J* = 8.3Hz, 6H), 7.23 (d, *J* = 8.3Hz, 6H); ^{13}C NMR ($CDCl_3$) δ 31.37, 34.14, 123.42, 125.93, 145.09, 145.44.

Preparation of *tris*(2-bromo-4-(*tert*-butyl)phenyl)amine (S8-2 or BC). A solution of 4-(*tert*-butyl)phenyl)amine (0.35 g, 0.85 mmol) in dichloromethane (15 mL) was added a solution of NBS (0.53 g, 2.96 mmol) in DMF (5 mL) dropwise under an argon atmosphere, and stirred overnight (~16 h) at 22 °C. The reaction mixture was quenched with water and extracted with dichloromethane (3 x 25 mL). Combined organic extracts were dried over anhydrous $MgSO_4$, filtered, and evaporated. The crude product was filtered through a short pad of silica gel using dichloromethane as the elutant followed by recrystallization from a mixture of dichloromethane and hexanes to afford pure **S8-2** (or **BC**). Yield: 0.42 g

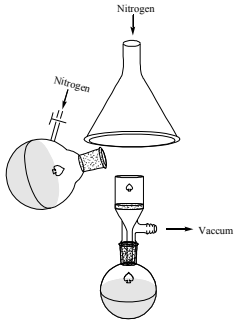
(75%), m.p. 238-240 ºC. $^{1}H^{1}$ NMR ($CDCl_3$) δ 1.30 (s, 27H), 6.74 (d, *J* = 8.36Hz, 3H), 7.19 (d, *J* = 8.36Hz, 2.23Hz, 3), 7.56 (d, *J* = 2.23Hz, 3H); ^{13}C NMR ($CDCl_3$) δ 31.48, 34.60, 121.23, 125.07, 126.70, 131.60, 143.51, 148.87.

S8.9. General procedures for preparative isolation cation-radical hexachloroantimonate salts.

Preparation of $MB^{+\bullet}SbCl_6^-$ using $NO^+SbCl_6^-$. A 50-mL flask fitted with a Schlenk adaptor was charged with nitrosonium hexachloroantimonate (44 mg, 0.12 mmol) was added a cold solution (~0 ^{o}C) of MB^{o} (58 mg, 0.12 mmol) in anhydrous dichloromethane (5 mL) under an argon atmosphere at -10 ^{o}C. The solution immediately took on a blue coloration and was stirred (while slowly bubbling argon through the solution to entrain gaseous NO) for 10 min to yield a blue solution of $\mathbf{MB^{+\bullet}}SbCl_6^-$. To this solution was then added dry ether (15 mL) to precipitate the dissolved $\mathbf{MB^{+\bullet}}SbCl_6^-$ salt. The microcrystalline precipitate was filtered using a medium-grade sintered-glass funnel under a blanket of dry nitrogen and washed with dry diethyl ether (2 x 5 mL) using a basic apparatus set-up shown below. The resulting salt was dried *in vacuo* at room temperature to afford $\mathbf{MB^{+\bullet}}SbCl_6^-$ in essentially quantitative yield (0.89 g, 91%).

Preparation of $MB^{+\bullet}SbCl_6^-$ using $SbCl_5$. A solution of $\mathbf{MB^0}$ (0.96 g, 2 mmol) in anhydrous dichloromethane (20 mL) in a flask equipped with a dropping funnel and argon inlet and outlet adapters. The dropping funnel was charged with a solution of $SbCl_5$ in dichloromethane (2 mL, 1 M) and the flask was cooled in a dry ice-acetone bath (approximately –78 ^{o}C). The $SbCl_5$ solution was slowly added (3-5 min) under a flow of argon. The reaction mixture immediately turned blue and a large amount of dark-blue material precipitated. The resultant mixture was warmed to ~0 ^{o}C during 5-10 min, and anhydrous diethyl ether (30 mL) was added to precipitate the dissolved $\mathbf{MB^{+\bullet}}SbCl_6^-$ salt. The dark-blue microcrystalline precipitate was suction filtered using a medium-grade sintered-glass funnel under a blanket of dry argon and washed with dry diethyl ether (2 x 20 mL) using a basic apparatus set-up shown below. The resulting salt was dried *in vacuo* at room temperature to afford $\mathbf{MB^{+\bullet}}SbCl_6^-$ in 88% yield (1.43 g, 88%).

A basic apparatus for filtration of cation-radical salts under argon atmosphere. A large inverted funnel, connected to a argon outlet, positioned above the sintered glass funnel is generally sufficient for maintaining an inert atmosphere during filtration of the cation radical salt (see sketch of the apparatus below).



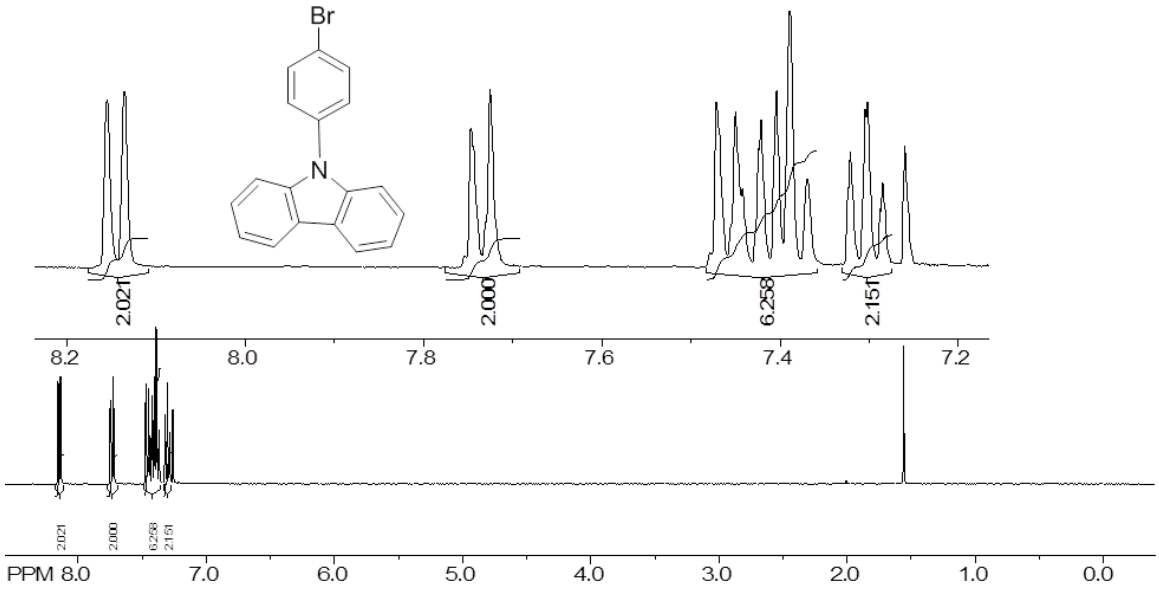
Similar procedures were used for preparative isolation of $BC^{+\bullet}SbCl_6^-$.

S8.10. Preparation of the $TAB^{+\bullet}SbCl_6^-$ salt.

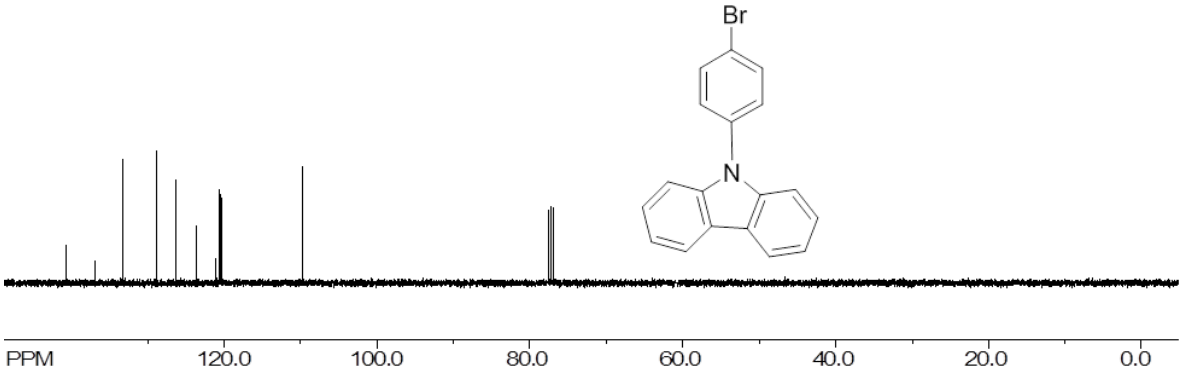
A 25 mL schlenk tube equipped with a magnetic stir bar was charged with a solution of the tetrakis (4-bromophenyl) benzidine **TAB** (30 mg, 0.037 mmol) in anhydrous dichloromethane (5 mL) under argon atmosphere. Then triethyloxonium hexachloroantimonate $\mathbf{Et_3O^+SbCl_6^-}$ (32 mg, 0.074 mmol) was added under an argon atmosphere at ~0 °C and stirred for 30 minutes. The mixture immediately took on a yellowish-orange coloration which intensified with time. The dark colored mixture was layered with dry toluene (10 mL) and kept it in refrigerator for overnight which gives an orange colored crystal of $\mathbf{TAB^{+\bullet}SbCl_6^-}$.

S9. NMR Spectroscopy

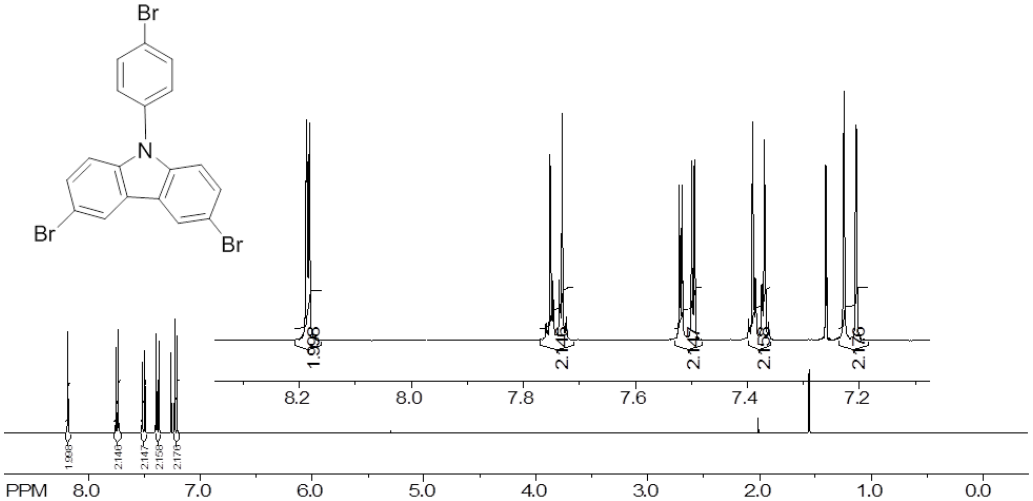
^{1}H NMR spectrum of S1-1 in $CDCl_3$



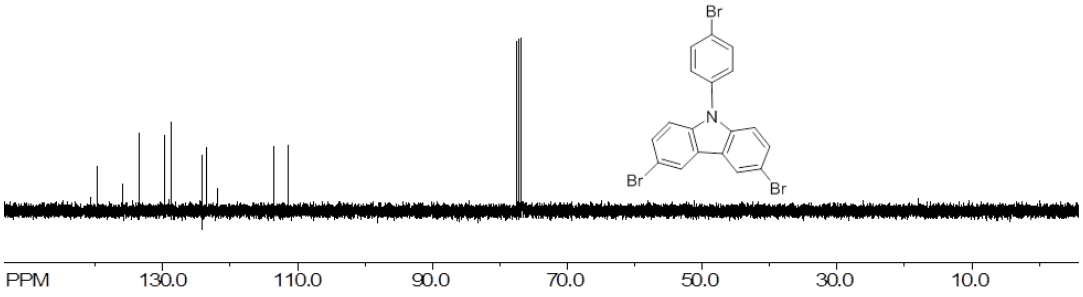
^{13}C NMR spectrum of S1-1 in $CDCl_3$



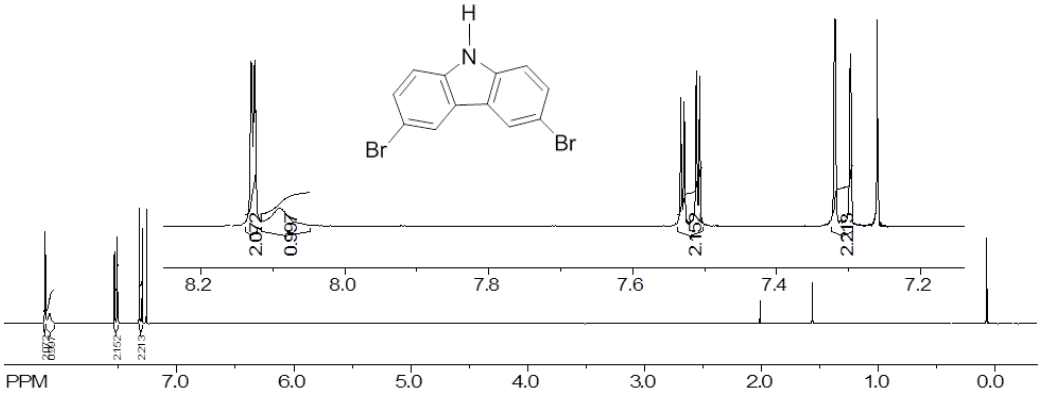
^{1}H NMR spectrum of S1-2 (4) in $CDCl_3$



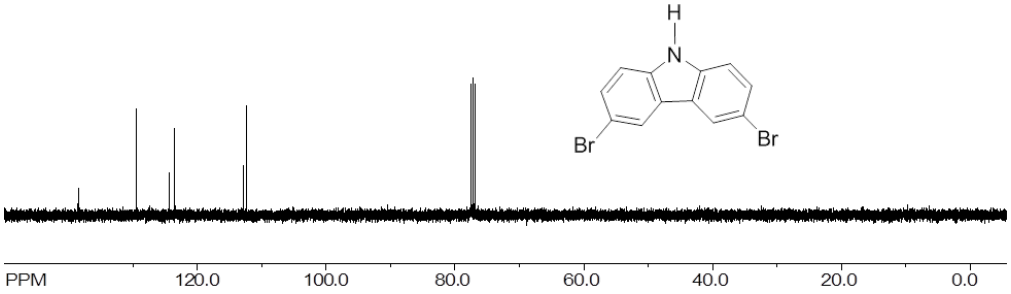
^{13}C NMR spectrum of S1-2 (4) in $CDCl_3$



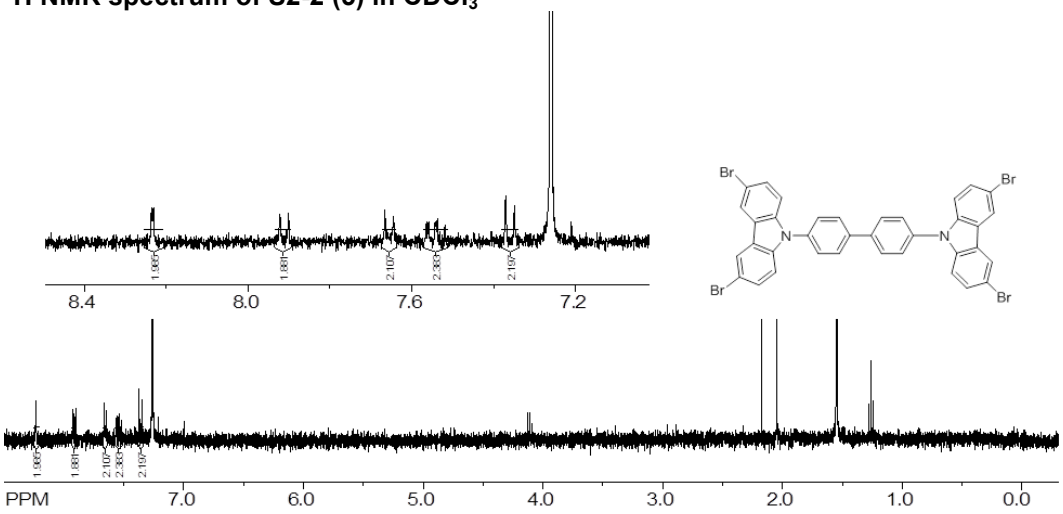
^{1}H NMR spectrum of S2-1in $CDCl_3$



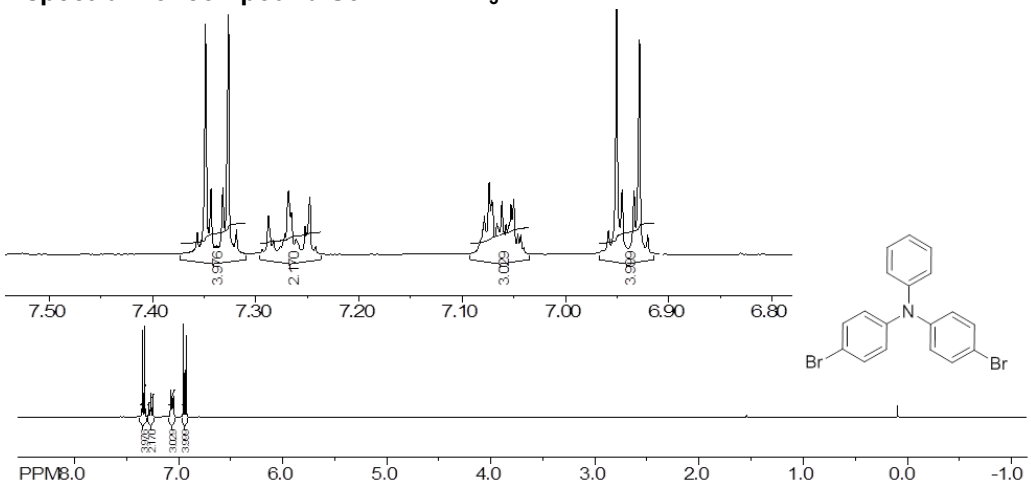
^{13}C NMR spectrum of S2-1 in $CDCl_3$



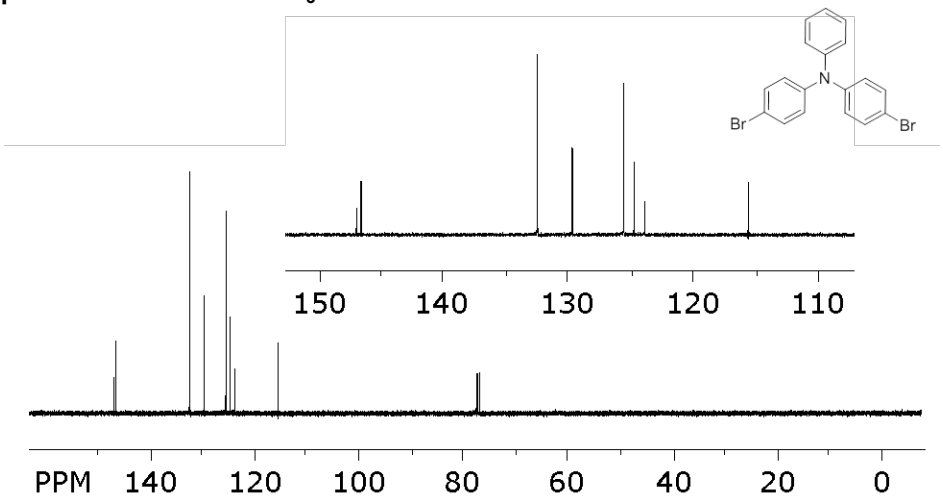
^{1}H NMR spectrum of S2-2 (5) in $CDCl_3$



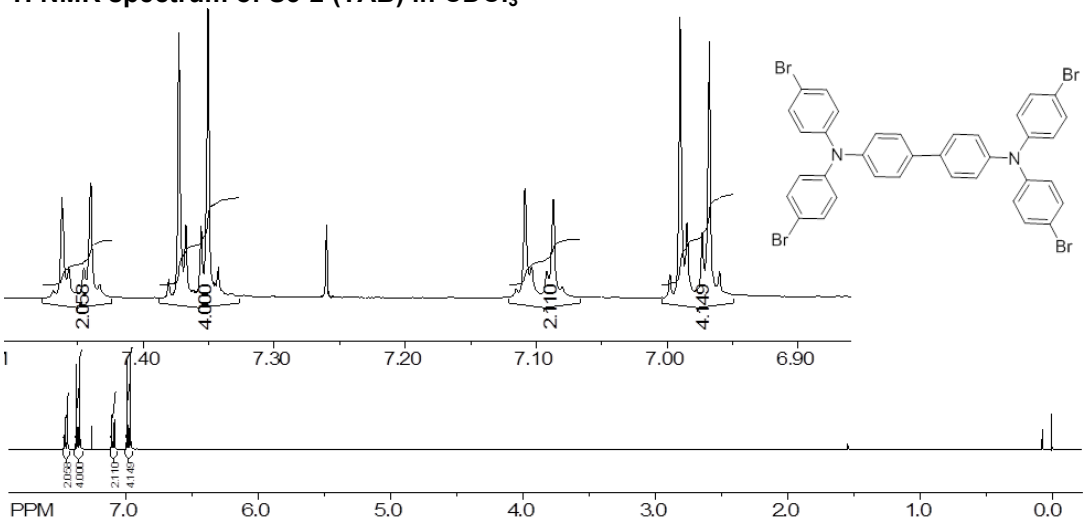
^{1}H NMR spectrum of compound S3-1 in $CDCl_3$



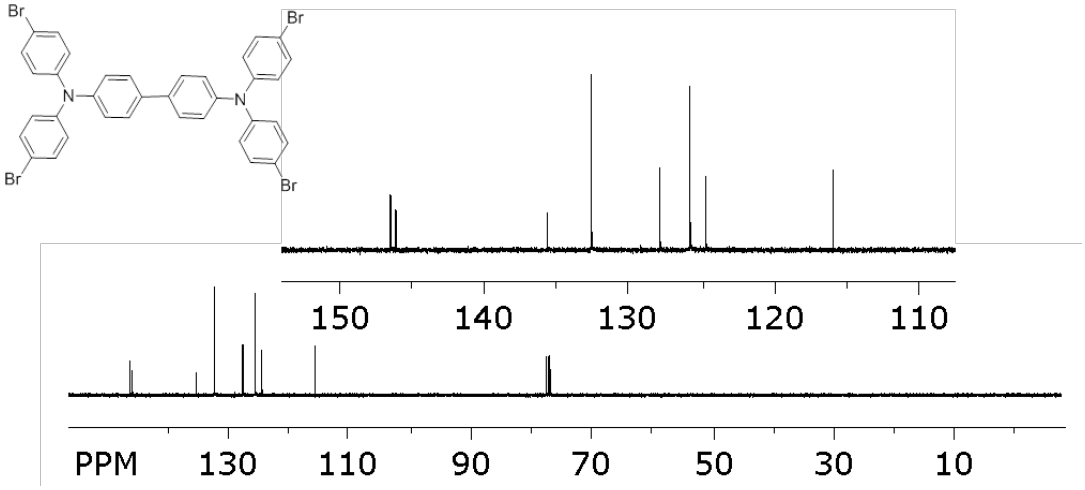
^{13}C NMR spectrum of S3-1 in $CDCl_3$



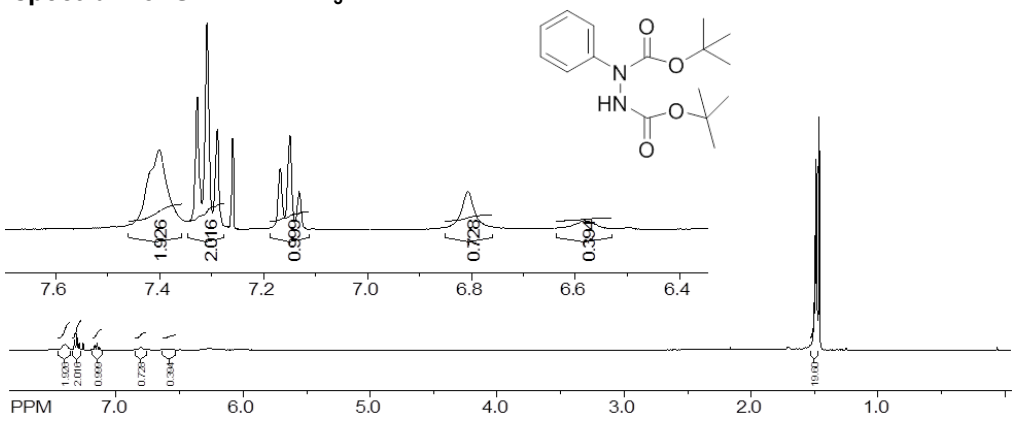
^{1}H NMR spectrum of S3-2 (TAB) in $CDCl_3$



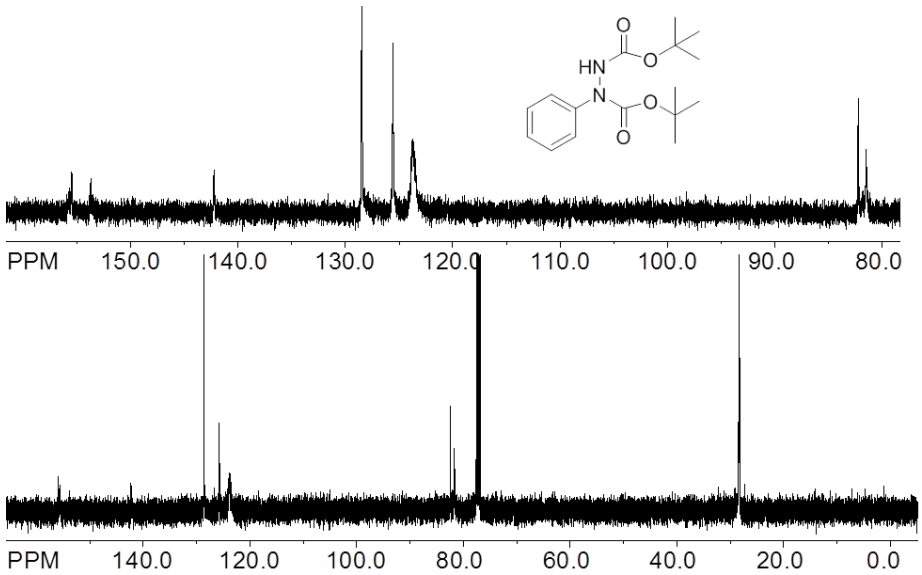
^{13}C NMR spectrum of S3-2 (TAB) in $CDCl_3$



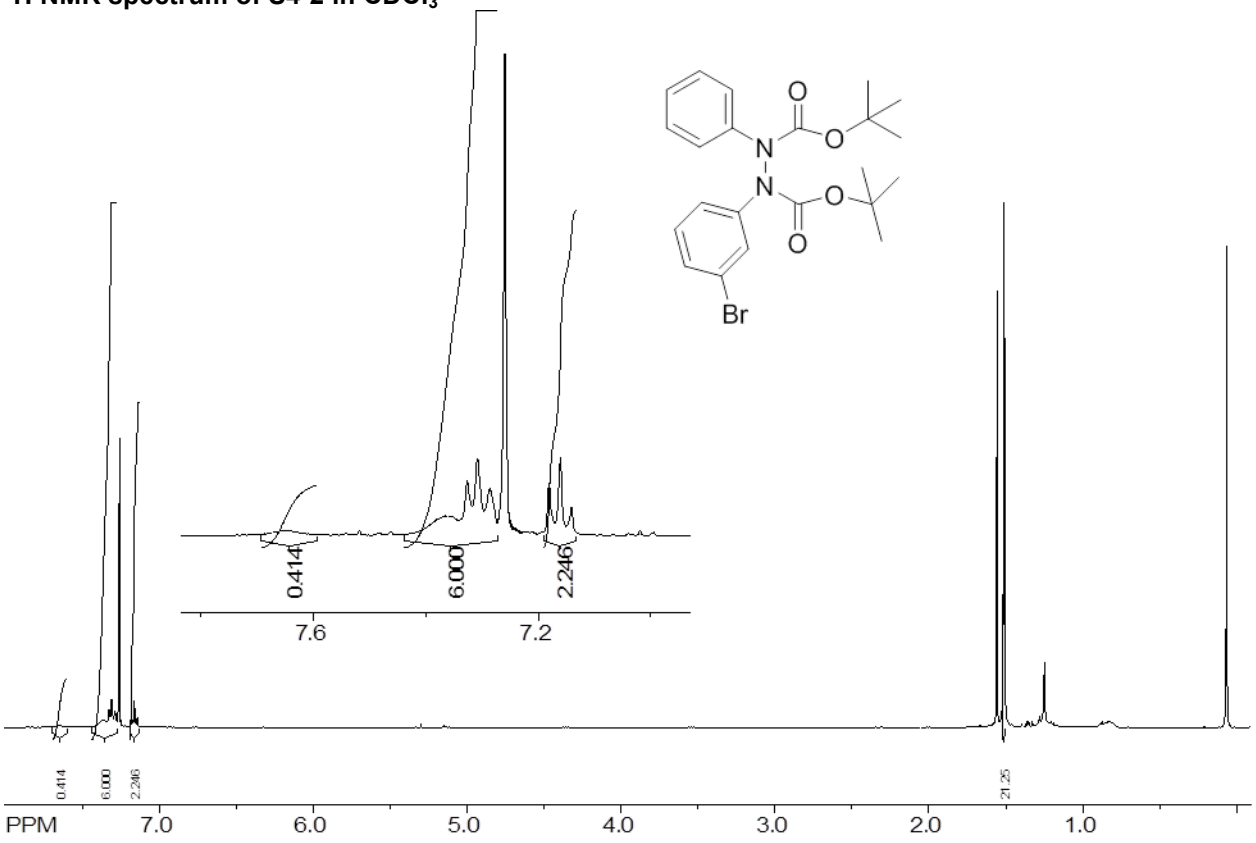
^{1}H NMR spectrum of S4-1 in $CDCl_3$



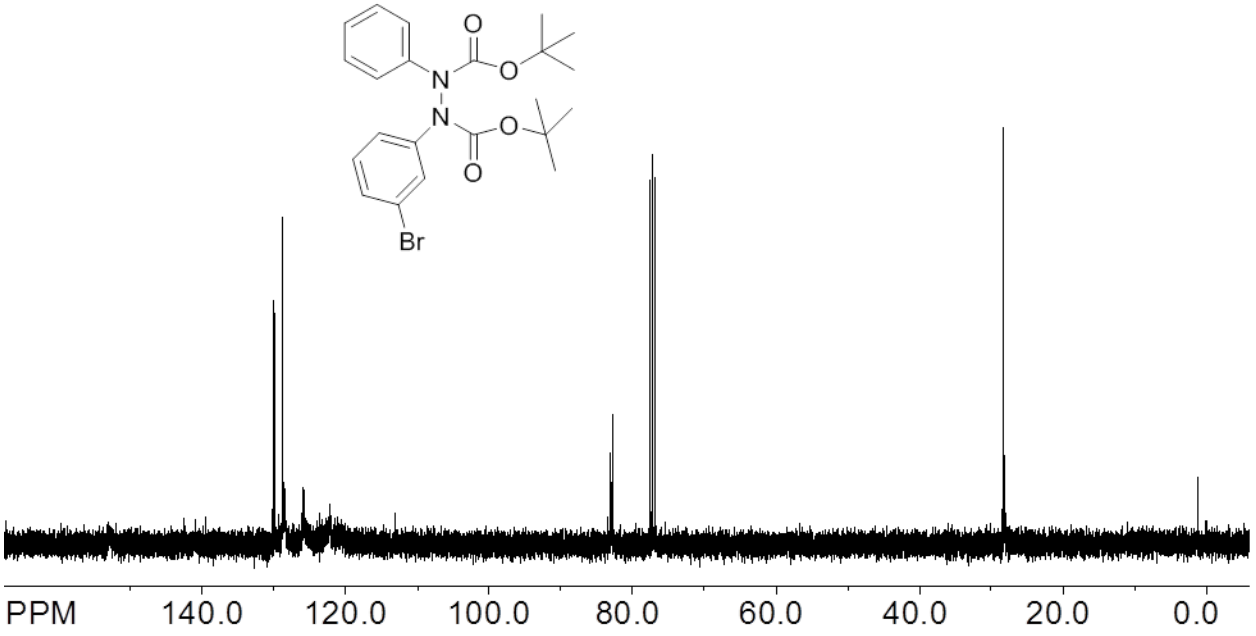
^{13}C NMR spectrum of S4-1 in $CDCl_3$



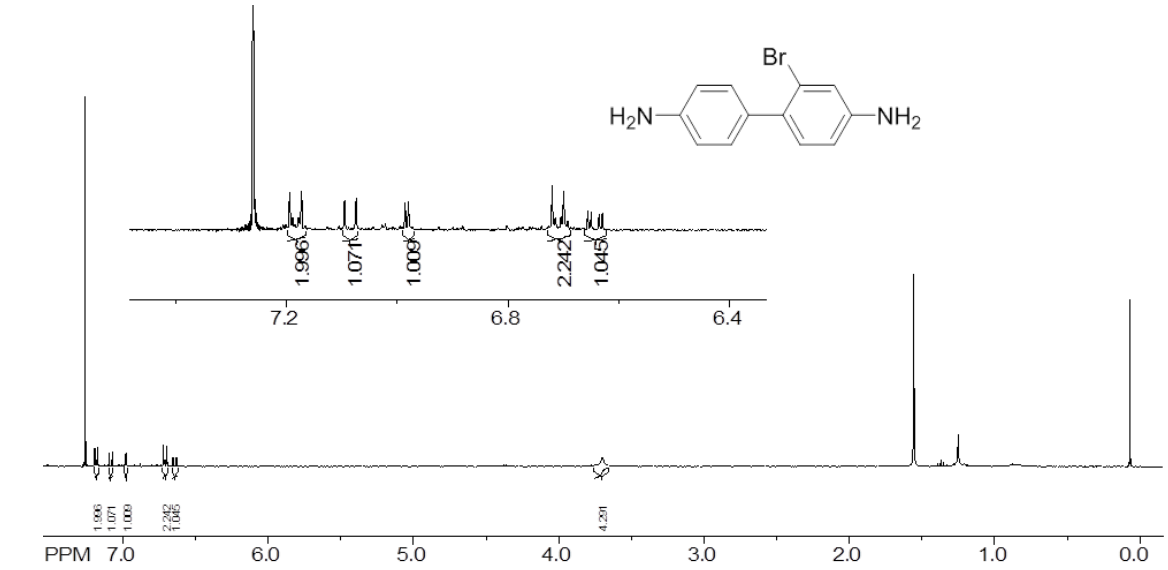
^{1}H NMR spectrum of S4-2 in $CDCl_3$



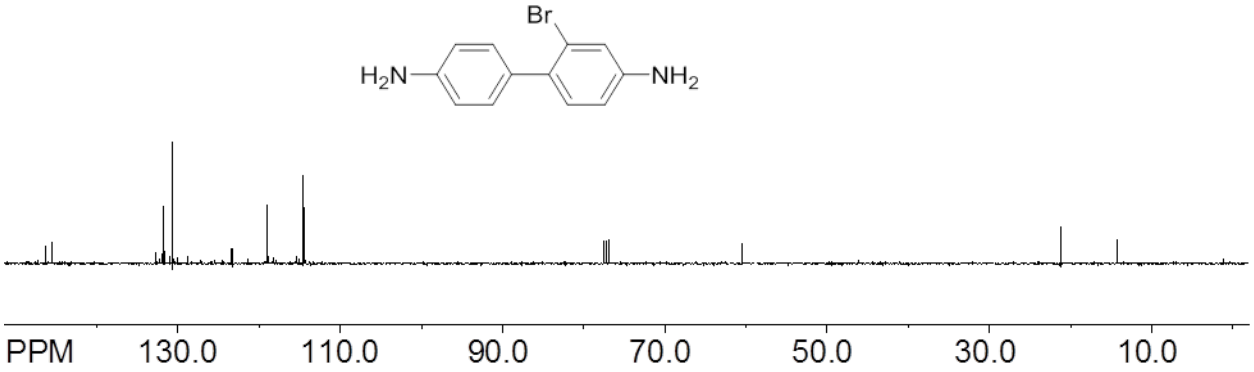
^{13}C NMR spectrum of S4-2 in $CDCl_3$



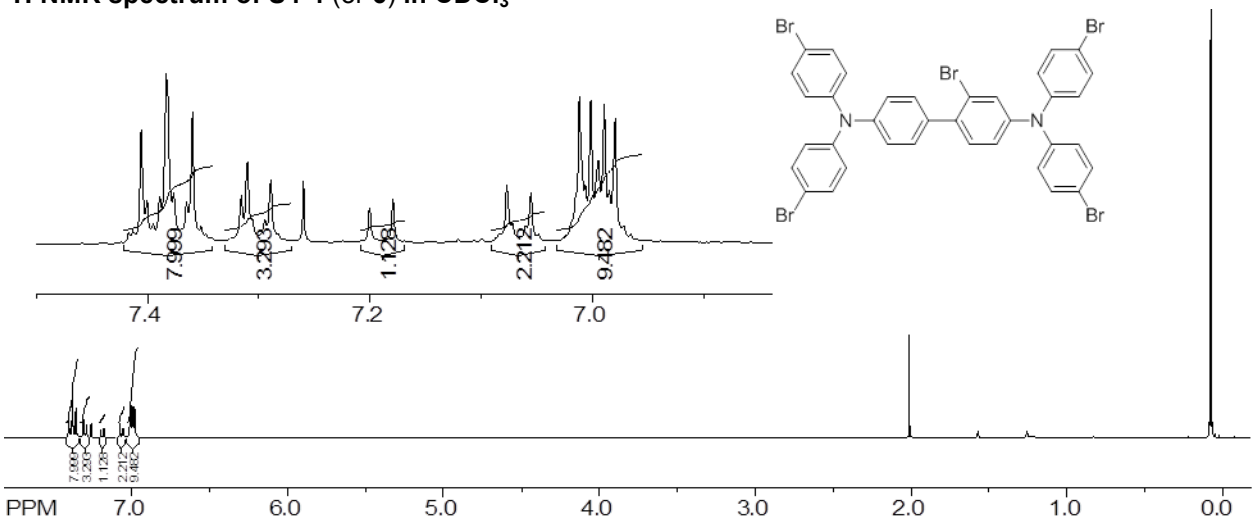
^{1}H NMR spectrum of S4-3 in $CDCl_3$



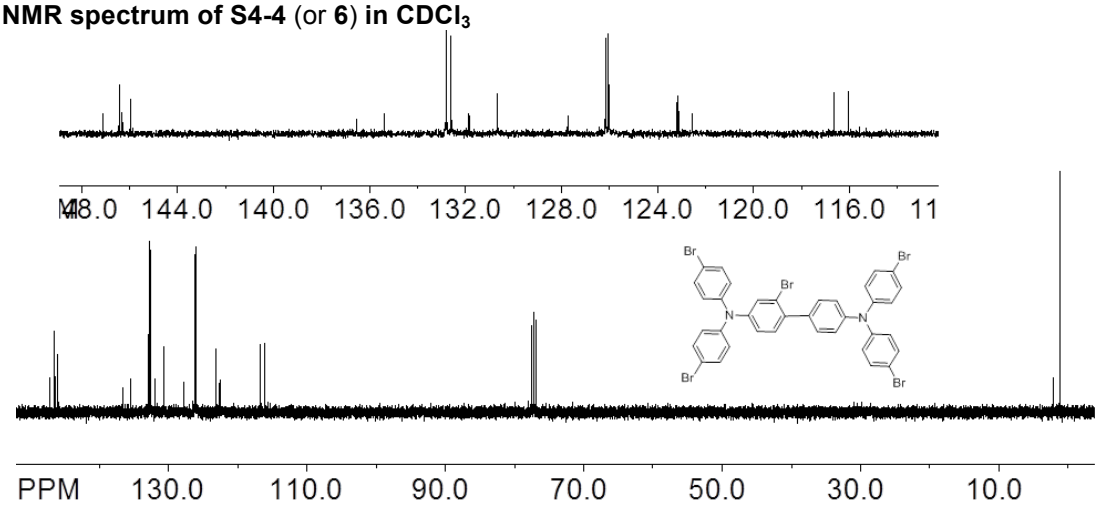
^{13}C NMR spectrum of S4-3 in $CDCl_3$



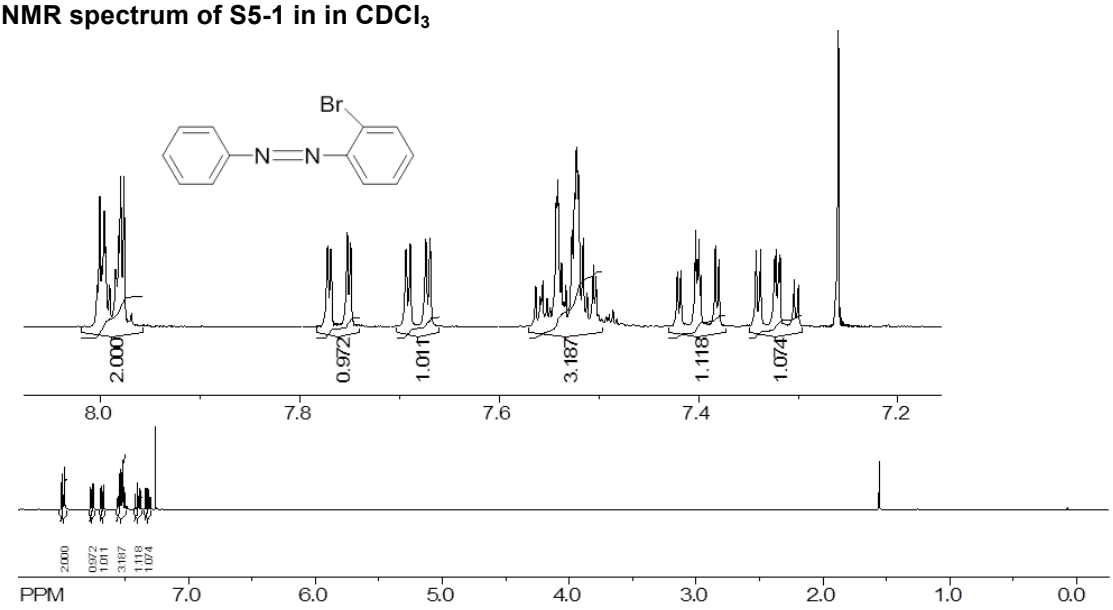
^{1}H NMR spectrum of S4-4 (or **6**) **in $CDCl_3$**



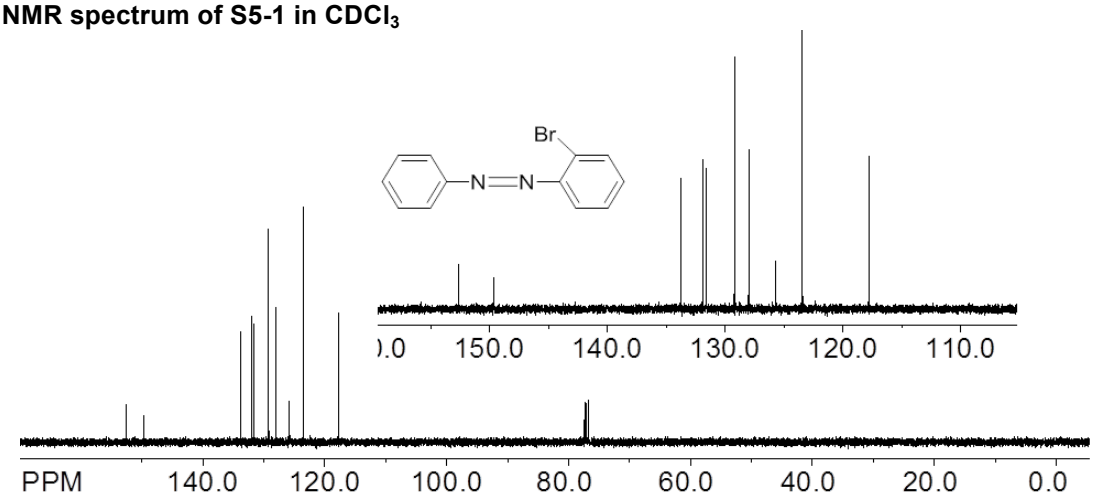
^{13}C NMR spectrum of S4-4 (or **6**) **in $CDCl_3$**



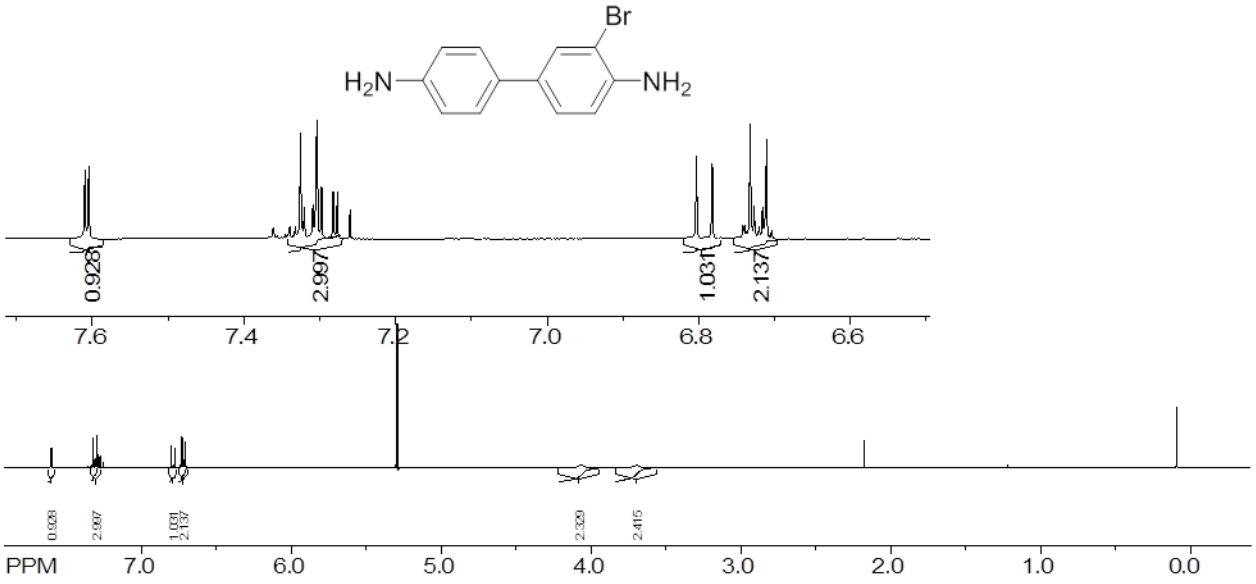
^{1}H NMR spectrum of S5-1 in in $CDCl_3$



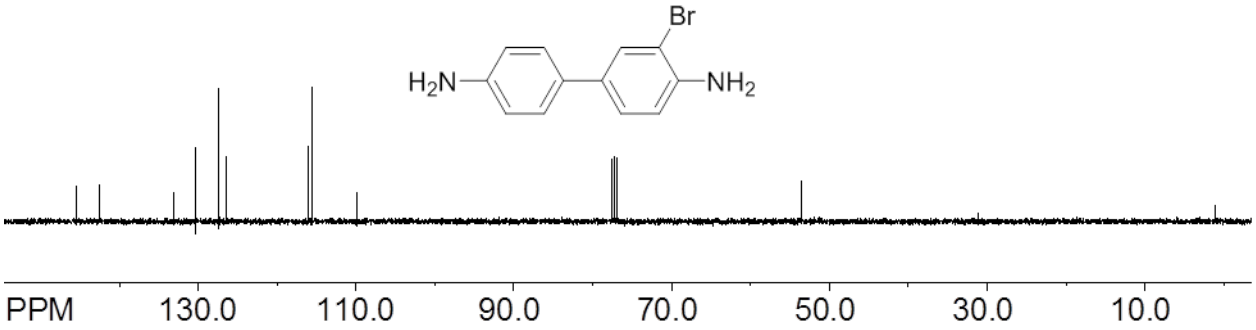
^{13}C NMR spectrum of S5-1 in $CDCl_3$



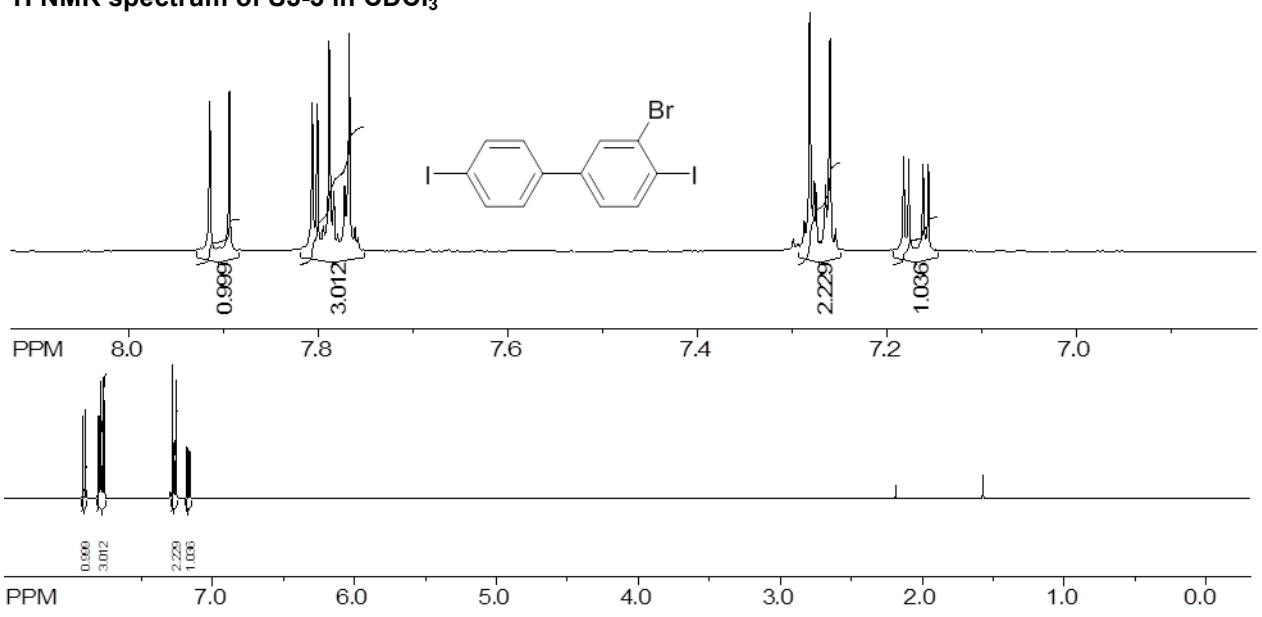
^{1}H NMR spectrum of S5-2 in in $CDCl_3$



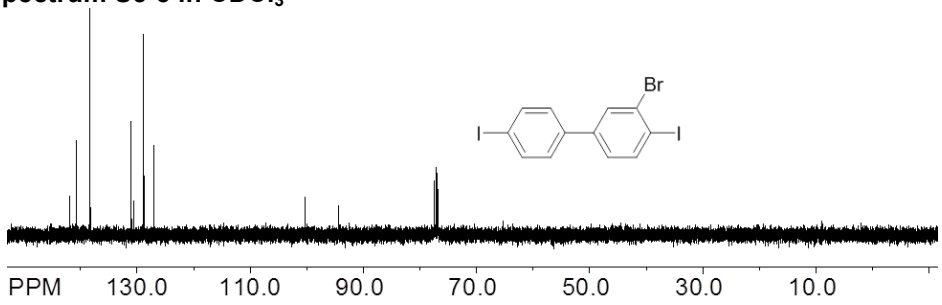
^{13}C NMR spectrum of S5-2 in $CDCl_3$



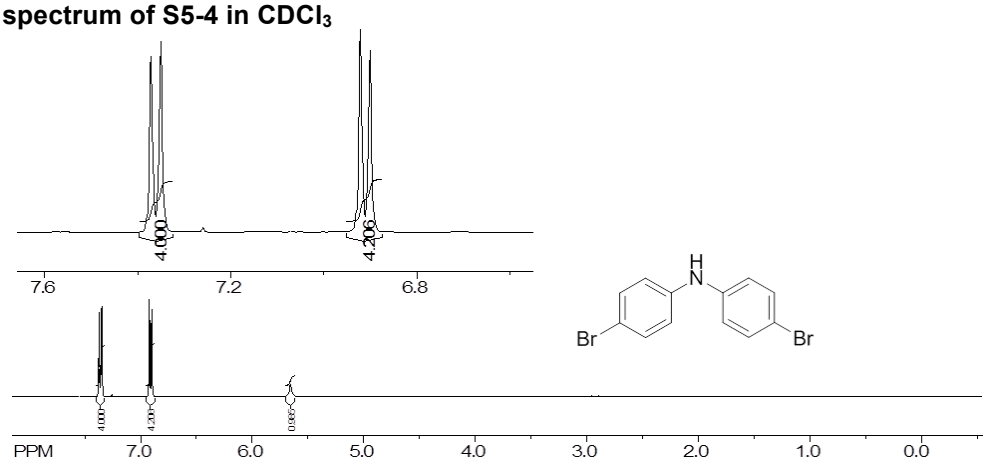
^{1}H NMR spectrum of S5-3 in $CDCl_3$



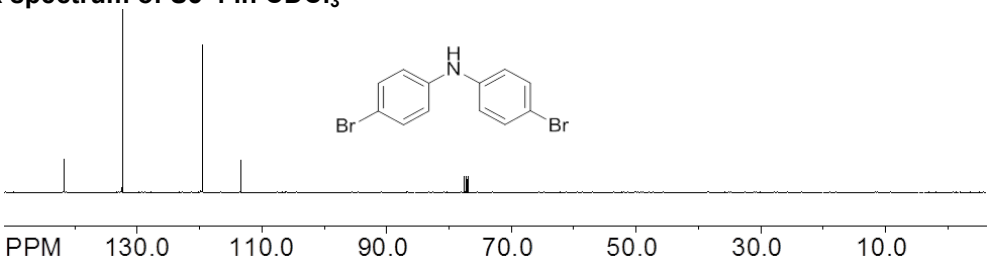
^{13}C NMR spectrum S5-3 in $CDCl_3$



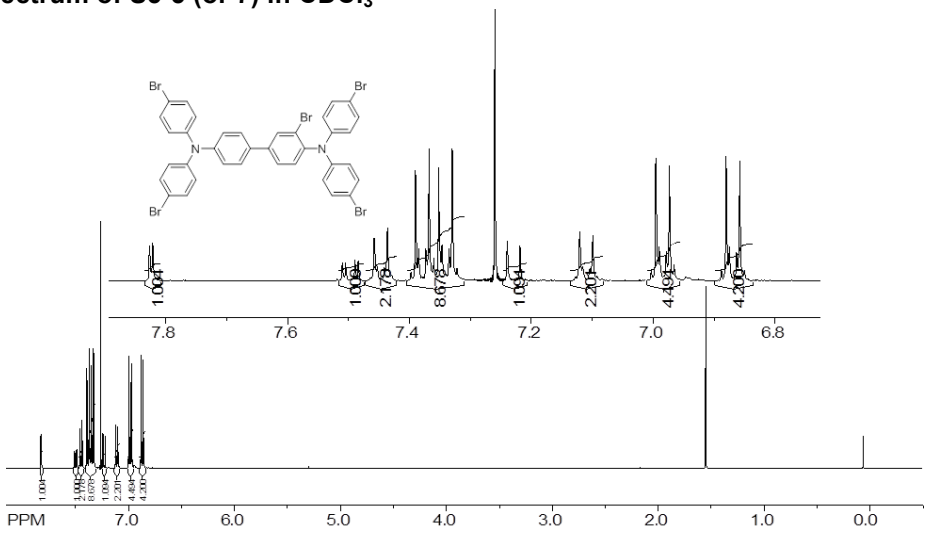
^{1}H NMR spectrum of S5-4 in $CDCl_3$



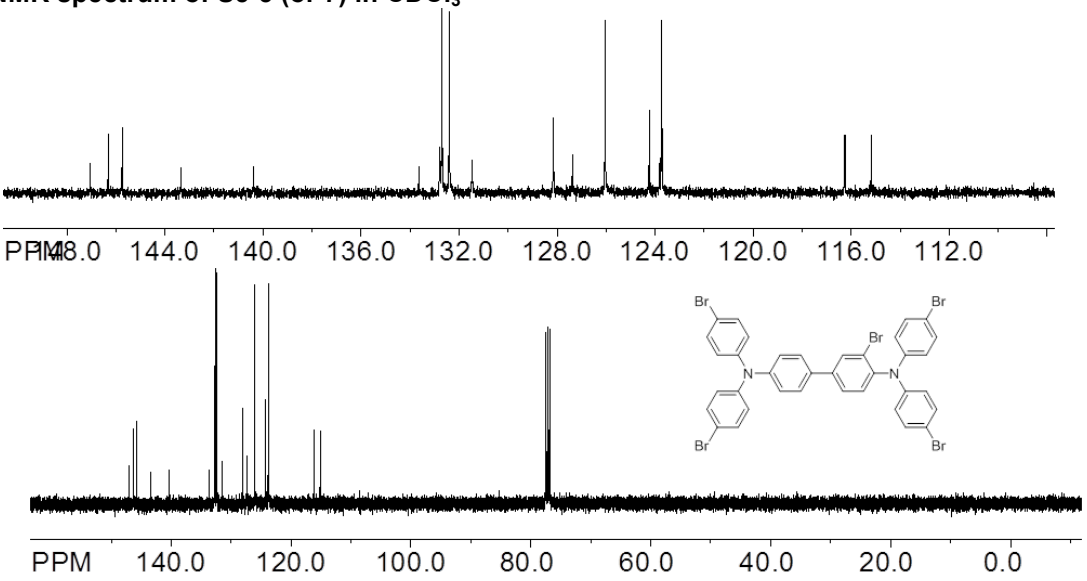
^{13}C NMR spectrum of S5-4 in $CDCl_3$



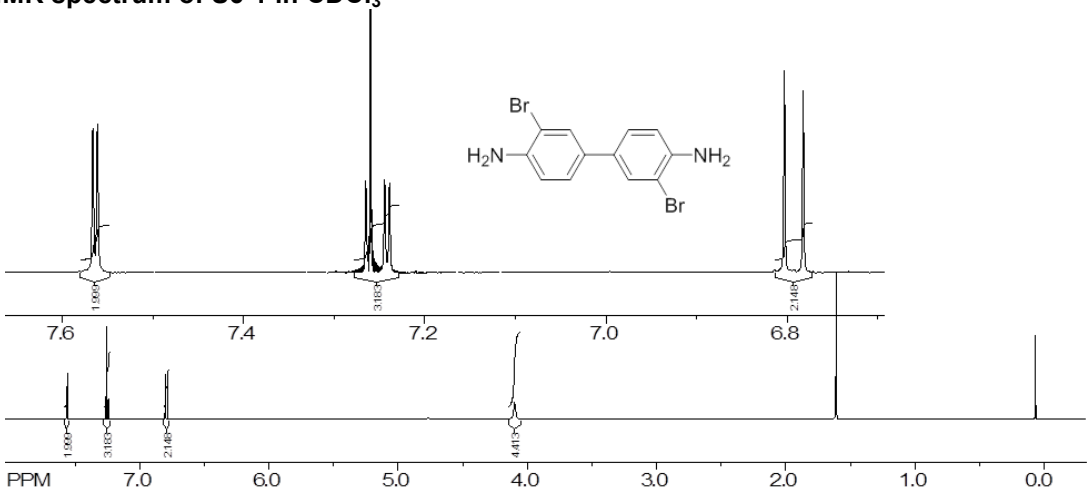
^{1}H NMR spectrum of S5-5 (or 7) in $CDCl_3$



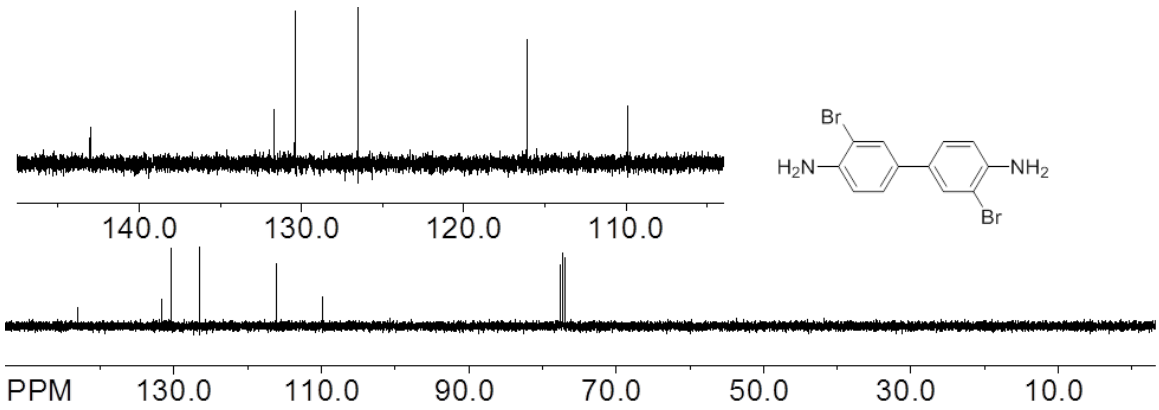
^{13}C NMR spectrum of S5-5 (or 7) in $CDCl_3$



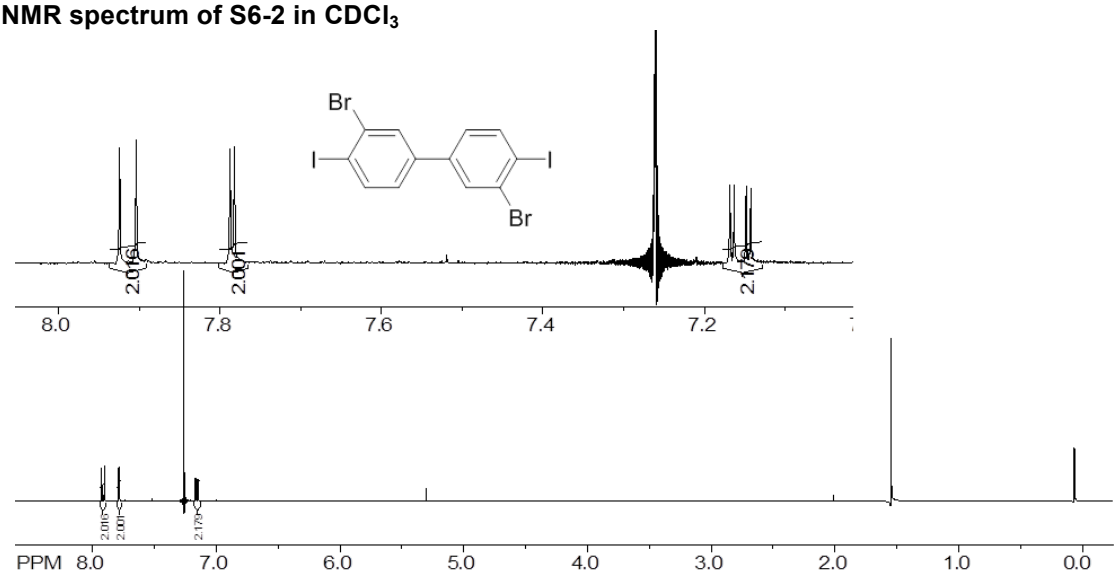
^{1}H NMR spectrum of S6-1 in $CDCl_3$



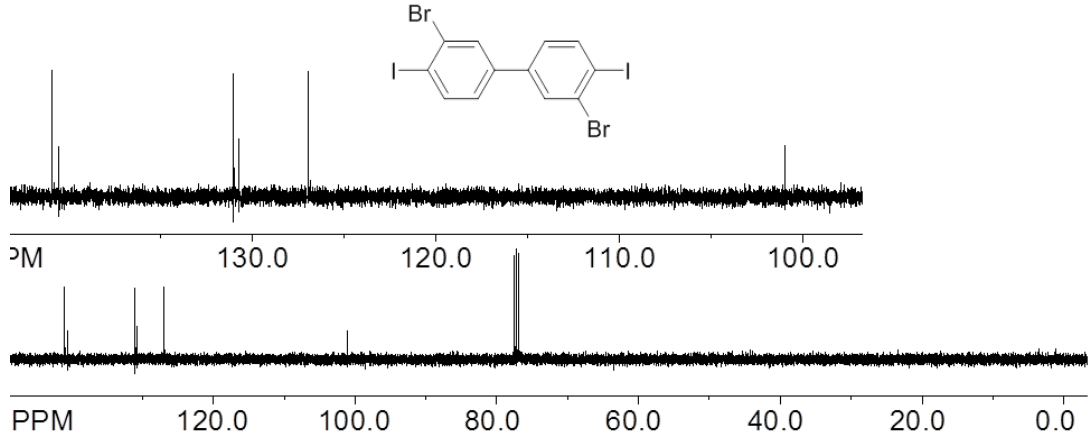
^{13}C NMR spectrum of S6-1 in $CDCl_3$



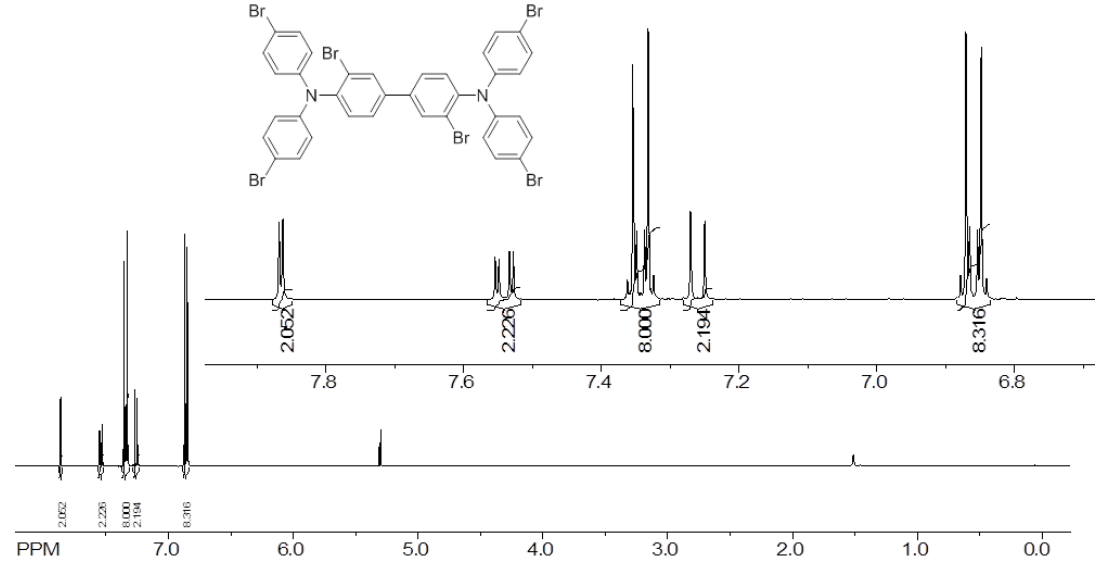
^{1}H NMR spectrum of S6-2 in $CDCl_3$



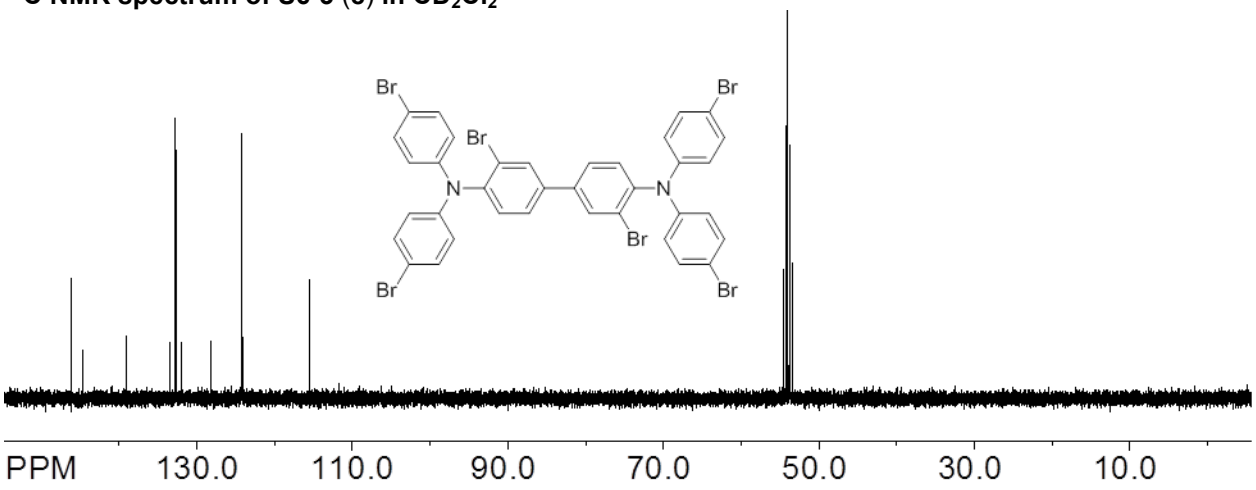
^{13}C NMR spectrum of S6-2 in $CDCl_3$



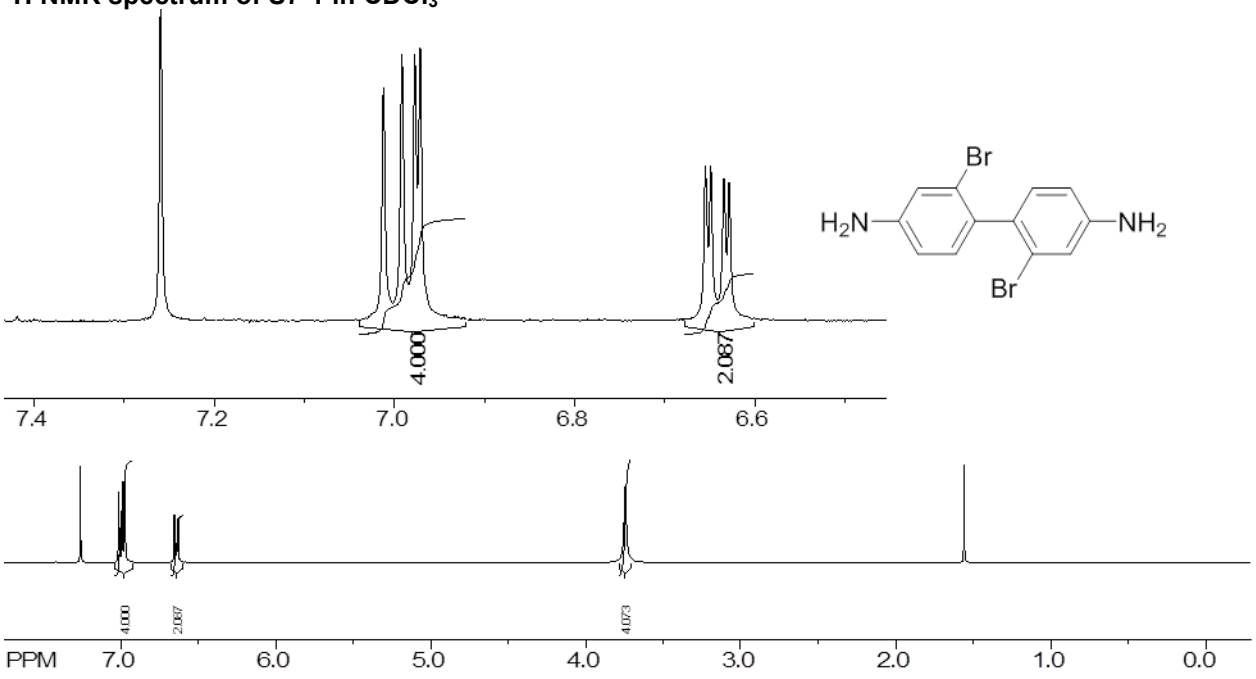
^{1}H NMR spectrum of S6-3 (8) in CD_2Cl_2



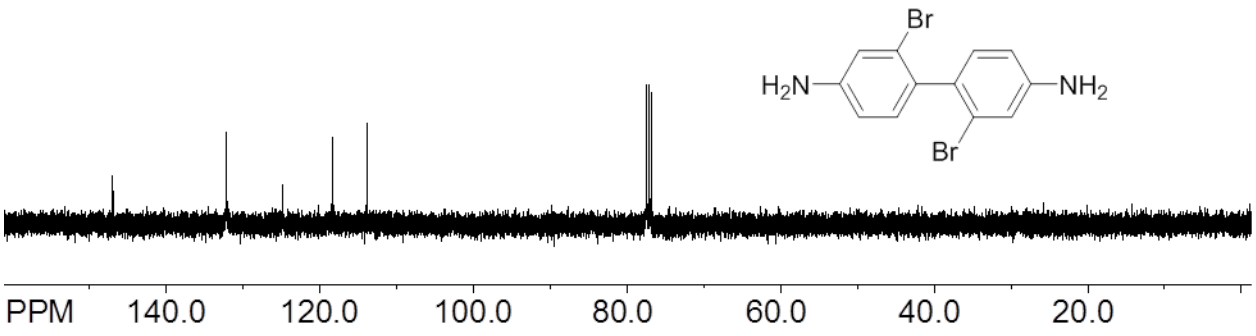
^{13}C NMR spectrum of S6-3 (8) in CD_2Cl_2



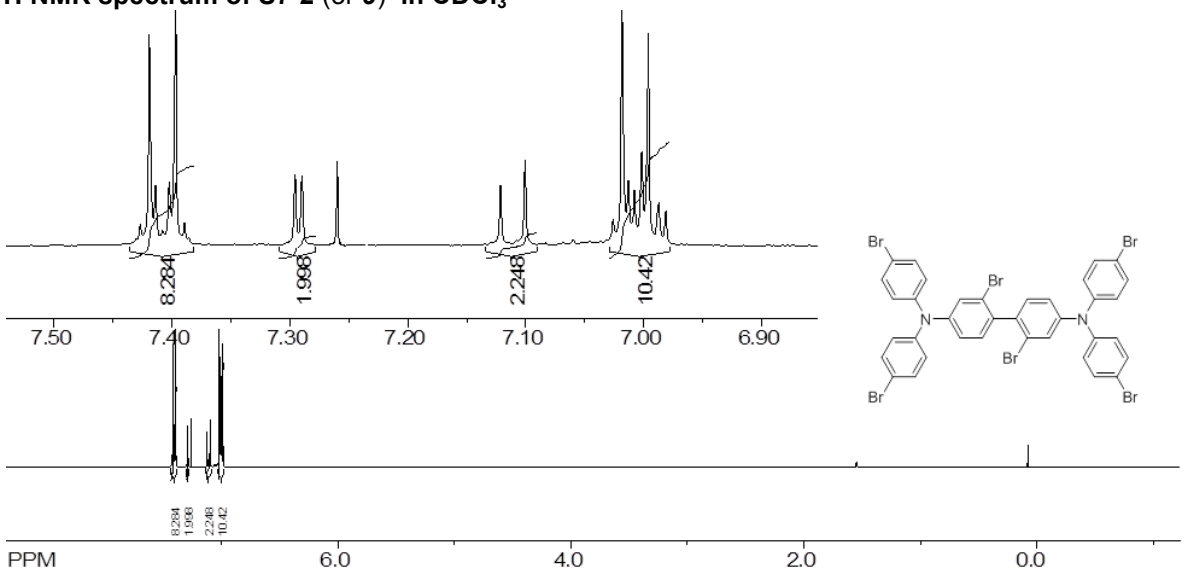
^{1}H NMR spectrum of S7-1 in $CDCl_3$



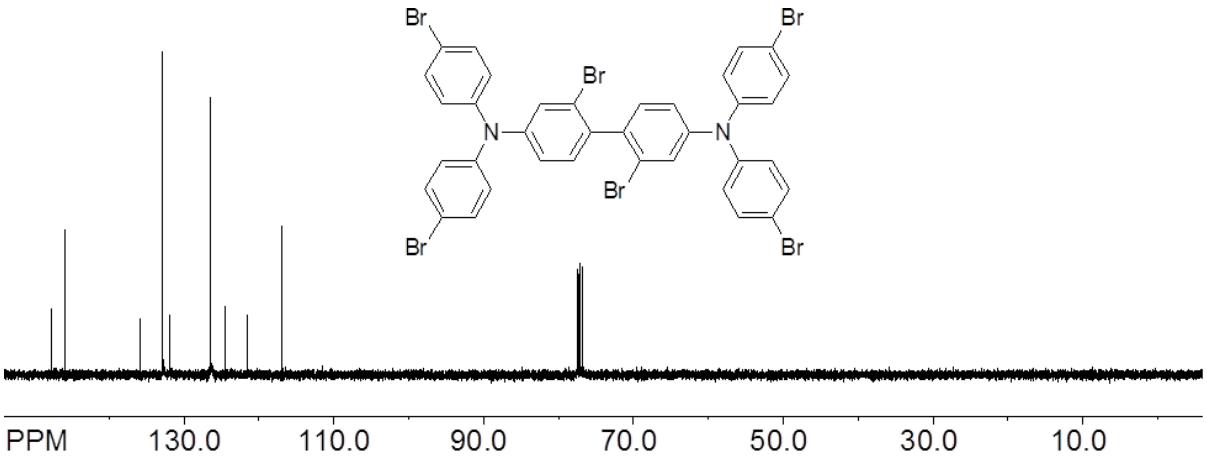
^{13}C NMR spectrum of S7-1 in $CDCl_3$



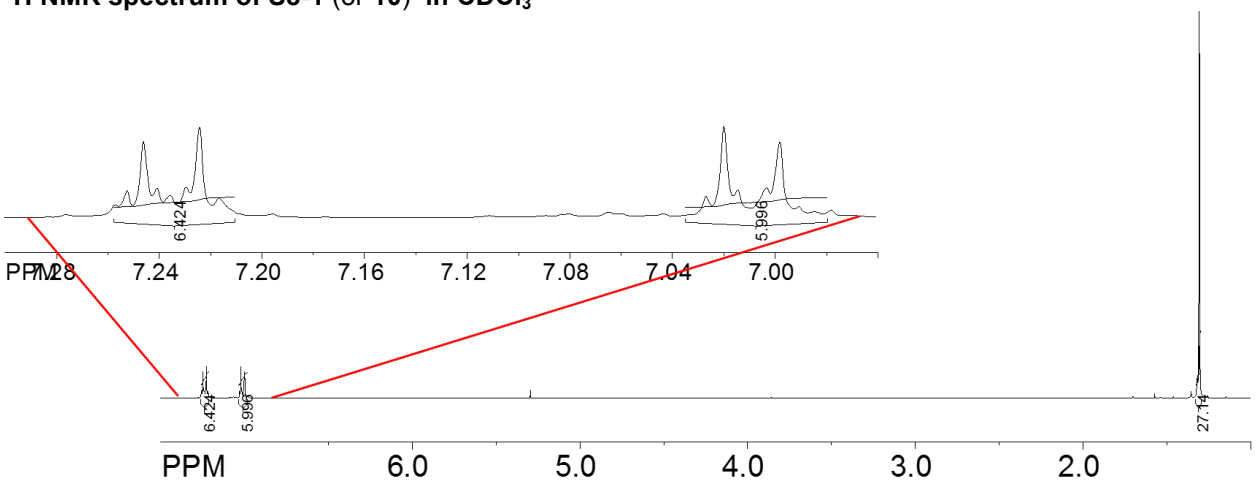
^{1}H NMR spectrum of S7-2 (or **9**) **in $CDCl_3$**



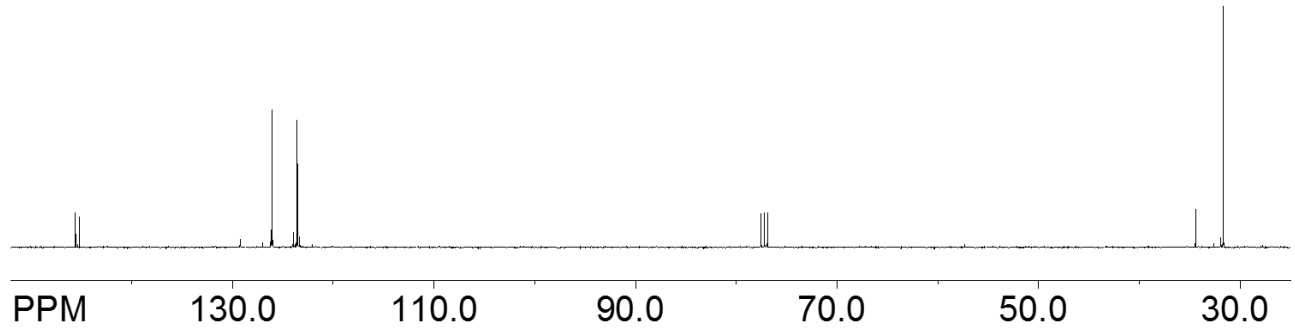
^{13}C NMR spectrum of S7-2 (or **9**) **in $CDCl_3$**



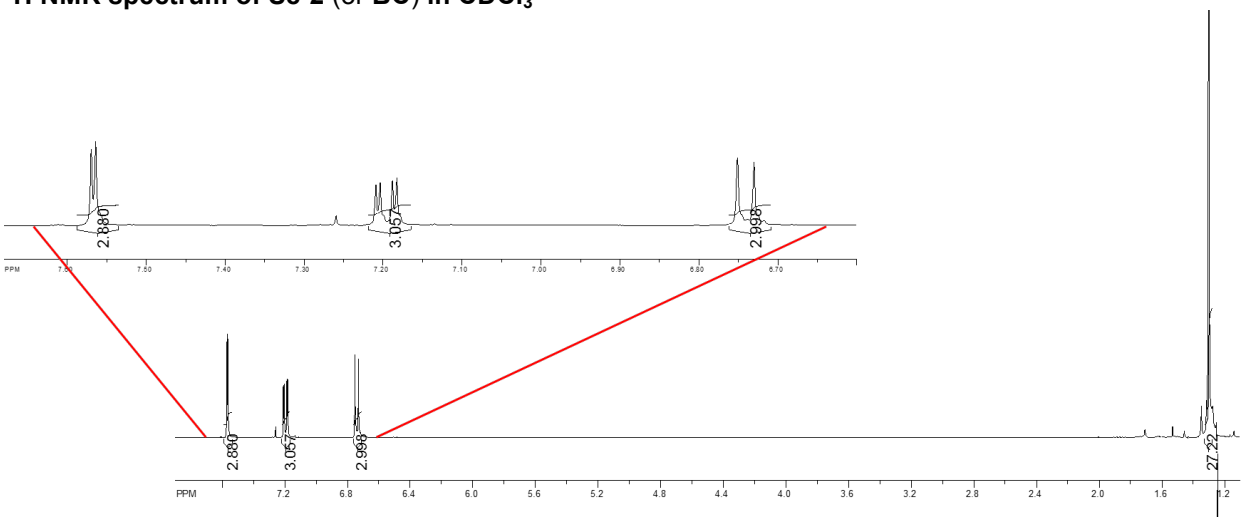
^{1}H NMR spectrum of S8-1 (or **10**) **in $CDCl_3$**



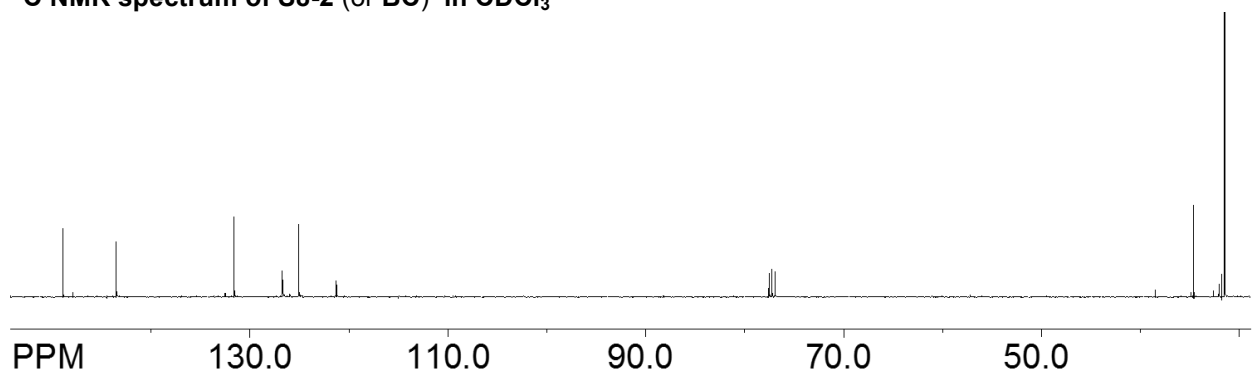
^{13}C NMR spectrum of S8-1 (or **10**) **in $CDCl_3$**



^{1}H NMR spectrum of S8-2 (or **BC**) **in $CDCl_3$**



^{13}C NMR spectrum of S8-2 (or **BC**) **in $CDCl_3$**



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S11. Archive entries from the calculation files

The archive entries, formerly intended for the Browse Quantum Chemistry Database System, are organized as a simple list of data fields separated by backslash symbols, which is wrapped in 70-char text lines. The script 'Parse.Archive.pl', written in Perl, converts archive entry into human readable format. To use this script,

1. Check if Perl interpreter is installed on the system. To do this, run the command 'perl –v' in console. If console returns a message like 'command not found', please obtain and install a Perl interpreter (www.perl.org/get.html; Perl is Open Source software licensed under GNU GPL).
2. Save the script code, listed below, as a file named 'Parse.Archive.pl'.
3. Select an archive entry of interest and save it as another file (e.g. 'A.txt').
4. Run the command 'perl Parse.Archive.pl A.txt > A-parsed.txt' in console. The parsed archive entry will be stored in the file 'A-parsed.txt' in this example. In some cases, absolute path to the Perl interpreter might need to be provided.

```
# --- Parse.Archive.pl ---

# Merge all strings in one line
my $s='';
while (<>) {chomp;$s .= $_}
$_ = $s;

#     Some     PDF     viewers     (like     Mac     OS's     Preview)     might     substitute
# 'end of line' symbols by the white space symbols,
# To remove these extra white spaces, please uncomment the following lines:
# my $str_length = 70;
# my $index = $str_length;
# while (length($_) > $index) {
#     substr $_,$index,1,'';
#     $index += $str_length;
# }

# Replace all backslashes by new-line symbols
s:\\:\n:g;

# Print the resulting output
print;

# --- END ---
```

```
MB
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079387708\C,-9.5011427469,0.5428860739,-4.871548501\H,-9.0858538483,1.1346975762,-5.6723950921\C,-8.917796385,0.5678315904,-3.6136332479\H,-8.0473200212,1.182613732,-3.4430402729\N,1.0891252081,-0.3054101106,-0.5054902372\C,-0.3236708274,-0.286668678,-0.6167359586\C,-1.1243603214,-0.0799246151,0.5080506144\H,-0.6628904143,0.0510552502,1.4754823118\C,-2.5046825756,-0.054876719,0.393050362\H,-3.0990780991,0.081958336,1.2848923573\C,-3.1385220811,-0.2499659603,-0.8389257046\C,-2.3245745833,-0.4640575463,-1.9566203564\H,-2.7750350547,-0.5873306101,-2.93093085\C,-0.9431303046,-0.4749679183,-1.8535852868\H,-0.3390962422,-0.6198492866,-2.7368782678\C,1.7472389875,0.6731756123,0.27255725\C,1.3306594778,2.0066061275,0.2364303717\H,0.5064464486,2.2931463428,-0.3986574554\C,1.9657038163,2.9684892194,1.0076093136\H,1.6361784733,3.9952158177,0.9712528023\C,3.0369679061,2.6023925262,1.808867772\Br,3.919900875,3.9232465289,2.8609019083\C,3.4731199634,1.286612655,1.8542816896\H,4.3016680968,1.0069063345,2.4862012906\C,2.8225436684,0.325722974,1.0948246436\H,3.1513342221,-0.7011691782,1.1426660962\C,1.8339589314,-1.3038793845,-1.1724260211\C,3.0308715603,-0.987006126,-1.8205022329\H,3.3885565938,0.0313253052,-1.8185882405\C,3.7659611745,-1.9674558343,-2.4699271732\H,4.6883780021,-1.7115486015,-2.9676392755\C,3.2951237166,-3.2718848952,-2.49014362\Br,4.2959065617,-4.6195971784,-3.3919059723\C,2.1047949323,-3.6075161077,-1.8623683213\H,1.7480707838,-4.6256563378,-1.8756657276\C,1.3832943606,-2.6263335911,-1.1990341522\H,0.4644480329,-2.8890490476,-0.6975379578\\Version=EM64L-G09RevD.01\HF=-11781.5869503\RMSD=6.954e-09\RMSF=1.883e-07\Dipole=-0.0042999,-0.0032716,-0.0040352\Quadrupole=-14.7030353,13.3748535,1.3281818,1.045689,-1.3824329,-8.5452543\PG=C01 [X(C36H24Br4N2)]\\@

1
1\1\GINC-HPC-CN121\FOpt\RBLYP\6-31G(d)\C18H11Br4N1\TALIPOVM\27-Feb-2015\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Title\\0,1\N,-0.0007738506,-0.0434827104,0.0631200765\C,1.4170899781,-0.0654709023,0.0340817933\C,2.167569594,0.9234183251,0.6714968442\H,1.6675591559,1.7143714978,1.2099751867\C,3.5535123243,0.8979554945,0.6166430712\H,4.1304749437,1.6647555151,1.1095230601\C,4.1880233449,-0.1099372194,-0.0954120433\Br,6.0903984,-0.1377455904,-0.1853234875\C,3.4595598067,-1.0981382702,-0.7405900175\H,3.9628017977,-1.883029194,-1.283190556\C,2.0744148503,-1.0781925389,-0.6641836433\C,-0.7188649104,0.1

44841841,1.2571704313\C,-0.1825046911,-0.2585362988,2.485219481\H,0.79
06765107,-0.7220525756,2.5229815524\C,-0.892738213,-0.079017619,3.6613
324722\H,-0.4660158705,-0.3951074417,4.6006366317\C,-2.1572318127,0.48
99373884,3.6205578027\Br,-3.1380424795,0.729068189,5.237429485\C,-2.71
32883807,0.8837254846,2.4143147709\H,-3.6959664131,1.3283238318,2.3844
555123\C,-1.9939012833,0.7178630663,1.2397012428\H,-2.4295725325,1.041
735133,0.3074392502\C,-0.6835496191,-0.1224867012,-1.1768187202\C,-1.4
755034,-1.2215207397,-1.5198347468\Br,-1.6126307014,-2.6923636713,-0.3
35741977\C,-2.1469777078,-1.2821614624,-2.7321385519\H,-2.7538876914,-
2.1383332704,-2.9754991683\C,-2.0038751456,-0.2340307814,-3.6276437045
\Br,-2.9115659416,-0.3129945306,-5.2945962503\C,-1.2069945936,0.862163
5082,-3.3321072696\H,-1.1016918851,1.6699249907,-4.0385672611\C,-0.560
1457218,0.9095114681,-2.107165847\H,0.0537772373,1.761546276,-1.855850
8819\H,1.4966349011,-1.8587204921,-1.1360445382\\Version=EM64L-G09RevD
.01\HF=-11033.5093124\RMSD=6.795e-09\RMSF=7.792e-07\Dipole=0.1802492,0
.4788767,-0.8346802\Quadrupole=-5.7183536,8.5651722,-2.8468187,-0.3404
671,6.0647903,-1.7112942\PG=C01 [X(C18H11Br4N1)]\\@

2
1\1\GINC-HPC-CN122\FOpt\RBLYP\6-31G(d)\C18H10Br5N1\TALIPOVM\27-Feb-201
5\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent
=Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\
\Title\\0,1\N,0.0323991243,-0.2656902543,0.0604466603\C,1.4338418959,-
0.0774505948,0.0164543716\C,2.078327765,0.7980493143,0.8906904469\H,1.
5080418426,1.3647887015,1.610175425\C,3.4571882928,0.9533526554,0.8438
055131\H,3.946209902,1.6329343968,1.5242564258\C,4.1939724526,0.244228
2917,-0.0905295455\Br,6.0850222186,0.4651176929,-0.1654547405\C,3.5702
847908,-0.6274510062,-0.9724885657\H,4.14992272,-1.1844200213,-1.69204
0624\C,2.1964091319,-0.7927582072,-0.9108832502\C,-0.6913432967,0.0426
819894,1.2393263019\C,-0.499589217,-0.6659245332,2.4308210756\Br,0.712
1025522,-2.1163456822,2.5034355206\C,-1.2055911923,-0.3498961527,3.581
4809697\H,-1.0389233553,-0.9085953175,4.4874118445\C,-2.1407762539,0.6
721082573,3.5392928773\Br,-3.1220007556,1.0958299647,5.1103243117\C,-2
.3733884215,1.3803257785,2.3709970251\H,-3.1022705989,2.1746144302,2.3
458623589\C,-1.6407441571,1.0652274427,1.2372914035\H,-1.8045128213,1.
6236220991,0.3281195656\C,-0.6877736182,-0.3362467338,-1.1588147481\C,
-1.6102460274,-1.3570871356,-1.406086583\Br,-1.8825825562,-2.731550889
7,-0.1320056967\C,-2.334369313,-1.4063534982,-2.589211058\H,-3.0438246

149,-2.1995754419,-2.7568295768\C,-2.113808603,-0.4365139858,-3.553156
0342\Br,-3.0922393183,-0.507612605,-5.1800695918\C,-1.189148139,0.5779
177021,-3.3516099639\H,-1.0252509066,1.3292102598,-4.1075314841\C,-0.4
921894546,0.6223799594,-2.1556076437\H,0.2204433092,1.4146091902,-1.98
18979702\H,1.7132366229,-1.4877260669,-1.580575021\\Version=EM64L-G09R
evD.01\HF=-13604.570837\RMSD=6.389e-09\RMSF=9.546e-07\Dipole=-0.572824
1,0.8950503,-0.541744\Quadrupole=-7.8601909,6.4727544,1.3874365,-2.242
9277,-0.2289601,0.1769917\PG=C01 [X(C18H10Br5N1)]\\@

3
1\1\GINC-HPC-CN123\FOpt\RBLYP\6-31G(d)\C18H9Br6N1\TALIPOVM\27-Feb-2015
\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=
Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\
Title\\0,1\N,0.0170584323,-0.3285767362,0.0468010921\C,1.4164369632,-0
.1032054793,0.014905915\C,1.9718471787,1.0384133702,0.5922735051\H,1.3
185695578,1.7568152948,1.064083409\C,3.3387882895,1.2695822576,0.57008
80481\H,3.7486052237,2.1591734679,1.021159915\C,4.1658509064,0.3506060
644,-0.0561678727\Br,6.0406666153,0.6558379029,-0.1136146771\C,3.65035
08068,-0.798146387,-0.6362234206\H,4.2998631607,-1.5195483952,-1.10351
72858\C,2.2836632792,-1.0233635154,-0.5833289995\C,-0.6861960224,-0.03
28171186,1.2418244794\C,-0.4751820755,-0.7765764384,2.4075048264\Br,0.
6992488412,-2.2586779659,2.3894063231\C,-1.1436222658,-0.4786575637,3.
5846772238\H,-0.9647271685,-1.0636380357,4.4715037644\C,-2.0609310632,
0.5607468314,3.5927483865\Br,-2.990274156,0.9629967649,5.2007809784\C,
-2.3154657957,1.3001960738,2.4485326475\H,-3.032568886,2.1053902454,2.
4633549954\C,-1.619970232,1.0021625303,1.2866458575\H,-1.8005361865,1.
5831884294,0.3948263031\C,-0.697320854,-0.3073575932,-1.1777504935\C,-
1.6883908413,-1.2553589619,-1.4528035929\Br,-2.0383966766,-2.648736360
7,-0.2229528275\C,-2.4051247496,-1.226684086,-2.6388755938\H,-3.165503
4672,-1.9656213794,-2.8297900483\C,-2.1086245935,-0.2534746969,-3.5805
975354\Br,-3.0788335663,-0.2199817646,-5.2142046364\C,-1.1136638143,0.
6840749576,-3.3529005548\H,-0.8882851803,1.43600494,-4.0922142333\C,-0
.4234918695,0.6536042233,-2.1507162186\H,0.3423010207,1.3898471863,-1.
9581459074\Br,1.6106491889,-2.6423980618,-1.2919237724\\Version=EM64L-
G09RevD.01\HF=-16175.6332131\RMSD=8.293e-09\RMSF=1.038e-06\Dipole=-0.0
509784,1.4357324,-0.1620333\Quadrupole=-3.0693404,6.0030299,-2.9336896
,-0.2889807,0.0416814,-0.9929343\PG=C01 [X(C18H9Br6N1)]\\@

4

1\1\GINC-HPC-CN21\FOpt\RBLYP\6-31G(d)\C18H10Br3N1\TALIPOVM\07-Jan-2015
\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=
Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\
Title\\0,1\N,-0.1478215742,0.0233887988,0.2753260128\C,1.2160799905,0.
2265675141,0.1061336777\C,2.1784946463,0.5929441262,1.0430294916\H,1.9
254010553,0.7565265563,2.0789681568\C,3.4844618801,0.7472265071,0.6082
781469\H,4.2542105513,1.0292854076,1.3092128188\C,3.8117646035,0.54163
75562,-0.7349701287\Br,5.6276470276,0.7636585985,-1.2789360969\C,2.865
056148,0.1875010682,-1.6765304875\H,3.1408518382,0.0405095949,-2.70925
59152\C,1.5475926368,0.0306844936,-1.2499331649\C,-0.8569612572,0.1294
146787,1.4985215959\C,-0.5149820183,-0.6849046721,2.5752554488\H,0.280
7630381,-1.4071797375,2.4715972615\C,-1.2008210812,-0.5767476873,3.777
0993192\H,-0.9363905614,-1.2047363418,4.6130992763\C,-2.2400407174,0.3
360547684,3.8836732857\Br,-3.1920815143,0.4780022473,5.5249074787\C,-2
.5988088544,1.1473469247,2.8170705777\H,-3.4054187128,1.8563957306,2.9
162216862\C,-1.8960795151,1.048012552,1.6242563211\H,-2.1499377577,1.6
894861097,0.7937795491\C,-0.6985349602,-0.3017206371,-0.9580411803\C,-
2.0154277932,-0.6147761554,-1.283708389\H,-2.7952739636,-0.6234227903,
-0.5382005421\C,-2.3043107419,-0.9213696691,-2.6031360713\H,-3.3150053
072,-1.1671407726,-2.8886026478\C,-1.2932029433,-0.9165170295,-3.56819
88906\Br,-1.7477479225,-1.3423691196,-5.3723102458\C,0.0189507403,-0.6
173846584,-3.2568000404\H,0.7834682862,-0.6263213385,-4.0181663386\C,0
.3208047536,-0.3084526236,-1.9317499659\\Version=EM64L-G09RevD.01\HF=-
8461.2802922\RMSD=8.435e-09\RMSF=1.397e-06\Dipole=-0.7026628,0.1055621
,1.2126379\Quadrupole=-0.6351577,3.6915399,-3.0563822,-3.3356188,2.811
1071,-2.6833656\PG=C01 [X(C18H10Br3N1)]\\@

5

1\1\GINC-HPC-CN119\FOpt\RBLYP\6-31G(d)\C36H20Br4N2\TALIPOVM\26-Feb-201
5\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent
=Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\
\Title\\0,1\N,-8.8250626182,-0.1712990662,-1.2897630234\C,-7.410894183
5,-0.1902305407,-1.1785874986\C,-6.7664388695,0.6704241221,-0.29389687
35\H,-7.3452607729,1.3699670911,0.2907124024\C,-5.3849339879,0.6422383
512,-0.1816490441\H,-4.9000486393,1.3316819002,0.4937126506\C,-4.61382
78047,-0.2286636387,-0.9579007297\C,-5.2771827493,-1.0795565064,-1.847
5453282\H,-4.7113066493,-1.7832395093,-2.4400510089\C,-6.6594192081,-1

.0698506392,-1.9533699972\H,-7.1582340552,-1.7545944888,-2.6230428707\
C,-9.7248406215,-0.4067260604,-0.258328645\C,-9.4786193693,-0.72931248
67,1.0736667264\H,-8.4738912853,-0.8220207588,1.4554445896\C,-10.56641
5458,-0.9327833167,1.9063587565\H,-10.4096229015,-1.1826416853,2.94387
09206\C,-11.868215224,-0.8186167976,1.4101479755\Br,-13.3308334883,-1.
105657754,2.6025747132\C,-12.1269093265,-0.5089493616,0.0890928622\H,-
13.1407605074,-0.4336895284,-0.2723815743\C,-11.0392789616,-0.30243734
33,-0.7576021655\C,-9.5462310687,0.0843402658,-2.4488371509\C,-10.9247
947989,0.0137051734,-2.161626911\C,-11.8610772712,0.2454108066,-3.1677
088259\H,-12.9205910798,0.1959317672,-2.9695511055\C,-11.3912048038,0.
5458605141,-4.4314309509\Br,-12.6415161538,0.8667110551,-5.8375377936\
C,-10.0253549416,0.6267614159,-4.7175377611\H,-9.7019104644,0.87059153
42,-5.7172272992\C,-9.0866597212,0.3980552071,-3.7252613563\H,-8.03256
25698,0.4654382999,-3.9447733383\N,1.0736023281,-0.3064567055,-0.50712
51341\C,-0.3405800404,-0.2876171196,-0.6193463586\C,-1.1300347286,-0.0
997887072,0.5120682492\H,-0.6627801634,0.0079997205,1.4796615451\C,-2.
5113051077,-0.073220288,0.3968946143\H,-3.1091212624,0.0515197634,1.28
7676332\C,-3.1374168947,-0.2493910609,-0.841046448\C,-2.3291876992,-0.
4455703711,-1.9652619614\H,-2.7823061539,-0.556291215,-2.9393641526\C,
-0.946781081,-0.4565865867,-1.8613625605\H,-0.3360141665,-0.5788831893
,-2.7435255798\C,1.8637810164,0.7247285707,-0.016351844\C,1.4883136441
,1.9849504714,0.4416052156\H,0.4541865806,2.2913673234,0.4656888665\C,
2.4851620611,2.8466183477,0.8680027687\H,2.2274142541,3.8295782201,1.2
296837951\C,3.825415454,2.4512630142,0.8306813531\Br,5.1583935403,3.67
6960904,1.4342529405\C,4.2127792292,1.2080191439,0.3698435599\H,5.2546
838792,0.9287278196,0.3441290152\C,3.2174950037,0.3331204128,-0.062205
8076\C,1.9039929289,-1.3593660067,-0.8682244664\C,3.2431694318,-1.0036
767577,-0.6071494563\C,4.2708904929,-1.9055465983,-0.8774197301\H,5.30
2484195,-1.6539660481,-0.6858269518\C,3.9288636872,-3.1391004009,-1.39
64561964\Br,5.3078326996,-4.4010903246,-1.7827430289\C,2.6015622407,-3
.4988561289,-1.6470337133\H,2.3785918956,-4.4754404112,-2.0470557207\C
,1.5727942227,-2.610206186,-1.3825830824\H,0.5479480667,-2.8893576278,
-1.571356407\\Version=EM64L-G09RevD.01\HF=-11779.2503508\RMSD=2.735e-0
9\RMSF=1.595e-07\Dipole=-0.0037983,0.0016351,-0.0021718\Quadrupole=-50
.7991257,23.0523436,27.746782,0.6886328,-6.1920737,3.7020354\PG=C01 [X
(C36H20Br4N2)]\\@

6

1\1\GINC-HPC-CN121\FOpt\RBLYP\6-31G(d)\C36H23Br5N2\TALIPOVM\26-Feb-201
5\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent
=Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\
\Title\\0,1\N,-8.8409270259,-0.1783610992,-1.2831355573\C,-7.435115393
9,-0.2057525128,-1.1143931527\C,-6.7908777581,0.775435576,-0.356705107
\H,-7.3688752638,1.5708150255,0.0893321256\C,-5.4175512865,0.741431712
7,-0.1821146285\H,-4.9434085804,1.5159414561,0.4013888636\C,-4.6383362
037,-0.2589745745,-0.770353676\C,-5.2895617121,-1.2251401808,-1.540839
0287\H,-4.7144080615,-2.0178832698,-1.9977957244\C,-6.6663383746,-1.21
0821578,-1.7028554896\H,-7.1476819995,-1.9836414849,-2.2830665955\C,-9
.6792708438,0.1095341194,-0.1820765626\C,-9.4101007499,-0.4332734848,1
.0769861106\H,-8.5599165041,-1.0848520367,1.2090668313\C,-10.224666882
8,-0.1441869733,2.1615614674\H,-10.0080376842,-0.5689796531,3.12936578
21\C,-11.3275398988,0.6783318009,1.9861327579\Br,-12.4562087047,1.0681
492504,3.4710687009\C,-11.6190924553,1.2210716954,0.7435610583\H,-12.4
740083163,1.8667355134,0.6160121147\C,-10.790375273,0.9432591879,-0.33
32141833\H,-11.0072738696,1.3783422898,-1.2968715603\C,-9.4050890004,-
0.446126632,-2.5513638925\C,-10.5417186344,-1.2500959408,-2.6694951214
\H,-10.9899943302,-1.6781958599,-1.7858827752\C,-11.1015097678,-1.5069
516341,-3.9121788468\H,-11.9788811206,-2.1296971398,-3.9922268023\C,-1
0.5125285051,-0.973213281,-5.0487296858\Br,-11.2708519653,-1.334335821
1,-6.7590578621\C,-9.378431948,-0.1800626838,-4.9562060137\H,-8.930173
1977,0.2382463887,-5.8439685067\C,-8.8340970705,0.0883044216,-3.709218
0341\H,-7.9605558198,0.7177293602,-3.6341158625\N,1.0898154695,-0.2955
276569,-0.5262094303\C,-0.3202860689,-0.295343227,-0.5739183049\C,-1.0
669044687,-0.2489488526,0.6039384015\H,-0.5682857672,-0.2371735946,1.5
592028612\C,-2.4511051178,-0.233252934,0.5526576857\Br,-3.359158213,-0
.2287862948,2.2339565843\C,-3.1603347346,-0.2773281793,-0.6511959054\C
,-2.3834964321,-0.3464020502,-1.8149023345\H,-2.8898801407,-0.36542473
03,-2.7689577305\C,-1.0006897653,-0.3471394502,-1.7919207626\H,-0.4472
0897,-0.376362401,-2.7177284452\C,1.7714774498,0.5196297856,0.40923142
74\C,1.3715073727,1.8404265764,0.624319018\H,0.5393431819,2.2462851853
,0.0694277093\C,2.034861564,2.6387733706,1.5441415328\H,1.719277958,3.
6580041107,1.7036154158\C,3.1172104862,2.1210927579,2.2402705879\Br,4.
0394498885,3.2187056681,3.4944808124\C,3.5371324779,0.8152820244,2.035
1039336\H,4.3752007382,0.4175692446,2.5858856292\C,2.8578202563,0.0158
670302,1.1277012647\H,3.1729776906,-1.0054921854,0.9774821014\C,1.8290
743568,-1.1185696407,-1.4094833189\C,2.9653836046,-0.623435742,-2.0529

271824\H,3.2761774151,0.396249798,-1.8833738606\C,3.6995901482,-1.4290
67124,-2.91056425\H,4.5758414982,-1.0379421164,-3.4036351615\C,3.28602
13598,-2.73268313,-3.1416851912\Br,4.2837476231,-3.8385492092,-4.32918
65163\C,2.1558183493,-3.2420281227,-2.5195714117\H,1.8454931853,-4.259
7698519,-2.6978766032\C,1.4364821517,-2.4373364097,-1.6484597922\H,0.5
66059655,-2.8367946062,-1.150559907\\Version=EM64L-G09RevD.01\HF=-1435
2.6471063\RMSD=7.590e-09\RMSF=1.985e-07\Dipole=0.4788407,-0.0057941,-0
.676238\Quadrupole=-14.9976988,16.450378,-1.4526792,0.8385689,2.692381
,-10.4943945\PG=C01 [X(C36H23Br5N2)]\\@

7
1\1\GINC-HPC-CN55\FOpt\RBLYP\6-31G(d)\C36H23Br5N2\TALIPOVM\05-Aug-2015
\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=
Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\
Title\\0,1\N,-8.8162017097,-0.1579435948,-1.3125594234\C,-7.4077479633
,-0.1800243578,-1.1881869956\C,-6.7744500961,0.4782573825,-0.131237386
\H,-7.3645227123,1.0242842202,0.5892063474\C,-5.3954351511,0.446507898
2,-0.0087095739\H,-4.9329212051,0.9859833445,0.8052520973\C,-4.5967532
274,-0.2242118448,-0.9403977127\C,-5.2405882767,-0.8721773815,-1.99938
42369\C,-6.6200822913,-0.8606136818,-2.119865727\H,-7.0918298851,-1.39
01147791,-2.9337875434\C,-9.6312789109,-0.3032958927,-0.1659009185\C,-
9.3191470192,-1.2510648308,0.8118604378\H,-8.4531584473,-1.8832889405,
0.6882555041\C,-10.1118616161,-1.3901002872,1.9413336956\H,-9.86274885
09,-2.1254720062,2.6904510134\C,-11.2354535206,-0.5901835568,2.0882536
834\Br,-12.3342968592,-0.7864641312,3.6321866489\C,-11.5695126392,0.35
08121164,1.1256893083\H,-12.4406811373,0.9748504024,1.2505302536\C,-10
.7625151648,0.4978793978,0.007333859\H,-11.0123195066,1.2406099841,-0.
7349419361\C,-9.4126557501,0.0111687643,-2.5837476468\C,-10.520288756,
-0.754540734,-2.9558544341\H,-10.9192777468,-1.4880433174,-2.271874938
6\C,-11.1138493303,-0.5838649765,-4.1976986438\H,-11.968587917,-1.1805
726178,-4.475764275\C,-10.5873025355,0.3450230656,-5.0828840985\Br,-11
.3917602607,0.5736369431,-6.7947221216\C,-9.4826809717,1.1097118624,-4
.7380091081\H,-9.0836820486,1.8361264559,-5.4287451792\C,-8.9048345175
,0.9474754668,-3.4877190296\H,-8.0548550253,1.5526313846,-3.2115513471
\N,1.1091682273,-0.288024016,-0.4490323241\C,-0.3062142953,-0.27679705
78,-0.5539867593\C,-1.1389218997,-0.3293537338,0.5655608109\Br,-0.3758
636256,-0.4963931063,2.2952486216\C,-2.5182256855,-0.3064515768,0.4463
666368\C,-3.12335982,-0.2470874604,-0.8121575643\C,-2.294021064,-0.216

8943439,-1.9381655378\H,-2.7288400802,-0.1503798005,-2.9242016298\C,-0
.915775791,-0.2276090132,-1.8072710865\H,-0.2870083483,-0.1839345746,-
2.6844935306\C,1.7897700969,0.8329298154,0.0547963828\C,1.2012742597,2
.1009373078,0.0137771729\H,0.2251425906,2.2294752462,-0.4270250506\C,1
.8603226269,3.2067796674,0.5305357569\H,1.3928328408,4.1784498065,0.49
01249777\C,3.1221512211,3.0574011349,1.0828770545\Br,4.0354060276,4.57
77604771,1.782329071\C,3.7257547486,1.8095549814,1.1330396012\H,4.7037
771281,1.6932387975,1.5738438418\C,3.059335357,0.7036490945,0.63012029
11\H,3.5268956687,-0.2662146033,0.6937554152\C,1.7944771492,-1.4296906
128,-0.9344085932\C,2.8554450676,-1.3074303428,-1.8331403867\H,3.17490
41805,-0.3283710768,-2.1571008453\C,3.5020515157,-2.4358647672,-2.3157
720072\H,4.3206666927,-2.3365070659,-3.011397181\C,3.0717241694,-3.691
7281547,-1.9121491782\Br,3.9477115326,-5.2435350483,-2.5858297069\C,2.
0155619508,-3.834765956,-1.0247693206\H,1.6949972308,-4.8152965075,-0.
7091330468\C,1.3868516893,-2.7012124986,-0.5303356771\H,0.5839523129,-
2.7983251007,0.1847787832\H,-4.6598276781,-1.4278581965,-2.721305704\H
,-3.1224849475,-0.3734634724,1.3370701395\\Version=EM64L-G09RevD.01\HF
=-14352.6489104\RMSD=9.297e-09\RMSF=2.704e-07\Dipole=-0.7869787,-0.222
6023,-0.8374613\Quadrupole=-7.2966343,5.4063442,1.89029,-1.7017777,-1.
2600326,-5.9459652\PG=C01 [X(C36H23Br5N2)]\\@

8
1\1\GINC-HPC-CN109\FOpt\RBLYP\6-31G(d)\C36H22Br6N2\TALIPOVM\05-Aug-201
5\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent
=Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\
\Title\\0,1\N,-8.8388052707,-0.252409146,-1.3465874065\C,-7.4263648232
,-0.2779421346,-1.2235580934\C,-6.7554914399,0.7938272097,-0.634933355
5\H,-7.3340416195,1.6399758801,-0.2947513777\C,-5.3779900344,0.7931722
921,-0.4977213649\H,-4.8915122596,1.6522964255,-0.060630408\C,-4.61394
76453,-0.2833041332,-0.9574778148\C,-5.2788298204,-1.3639736901,-1.541
3361355\C,-6.6586263568,-1.360439739,-1.6591007173\Br,-7.5157321844,-2
.8929273408,-2.3759936045\C,-9.6024025307,-0.2590450563,-0.1525158656\
C,-9.337249039,-1.2156083644,0.8276736824\H,-8.5838353414,-1.967128151
2,0.6453711133\C,-10.0440631548,-1.2178629365,2.0213859955\H,-9.833839
1122,-1.9594694208,2.7761073481\C,-11.0357903466,-0.2696980536,2.22379
51636\Br,-12.0189469586,-0.2745073823,3.8553214381\C,-11.3248373622,0.
6813739931,1.255686729\H,-12.0942207436,1.4180927414,1.4264043401\C,-1
0.6001111614,0.69056706,0.0728513781\H,-10.809297055,1.4386440649,-0.6

768928294\C,-9.4371611298,-0.1329932334,-2.6130822853\C,-10.7353055142
,-0.6044486905,-2.8389531616\H,-11.2877749443,-1.0685674385,-2.0372009
86\C,-11.3220819581,-0.4923399857,-4.0891624326\H,-12.3237580065,-0.86
06710365,-4.2481497964\C,-10.6090478246,0.0767134537,-5.1342484545\Br,
-11.4127184328,0.2232090719,-6.8565664797\C,-9.3174833347,0.5375100583
,-4.9367210197\H,-8.7654254384,0.982346571,-5.7501117336\C,-8.73791302
78,0.4387660842,-3.6801483575\H,-7.7375231252,0.8143186735,-3.53173969
3\N,1.0885324488,-0.2953688291,-0.4669020832\C,-0.3256842293,-0.286037
1314,-0.5726722328\C,-1.144927335,0.2538952182,0.4213889211\Br,-0.3682
506861,0.9388003749,2.0103167957\C,-2.5241223006,0.264017968,0.2973432
486\C,-3.1391539147,-0.2902527871,-0.8274747095\C,-2.3264553935,-0.853
056782,-1.8156695847\H,-2.7714835154,-1.2706286799,-2.7063171674\C,-0.
9479192823,-0.8444202778,-1.6889759893\H,-0.3290259578,-1.2641399994,-
2.4682213264\C,1.8140239673,0.9044029024,-0.5670848385\C,1.2735955426,
2.0101997575,-1.2303625785\H,0.3006193656,1.941848982,-1.691292341\C,1
.9773464478,3.2029865802,-1.3112962992\H,1.5470870251,4.047124642,-1.8
276046536\C,3.2361124992,3.2966163888,-0.7401580471\Br,4.2107284213,4.
9305489885,-0.8605695228\C,3.7926661189,2.2113984496,-0.0791896345\H,4
.7686146673,2.2899652985,0.3742976474\C,3.0814111709,1.025928382,0.014
0630194\H,3.5119532279,0.1940201157,0.5488303943\C,1.7297630643,-1.554
0066861,-0.3485549012\C,2.7811022195,-1.9120388088,-1.1937956407\H,3.1
272050931,-1.2179873684,-1.9448264236\C,3.3843899069,-3.1557798263,-1.
0770184411\H,4.1959184859,-3.4290390495,-1.7332185288\C,2.9199757601,-
4.0508383129,-0.1238370881\Br,3.7362632841,-5.7652501569,0.0278232132\
C,1.8725284152,-3.7162056541,0.7213477276\H,1.5253761807,-4.4153366708
,1.465971816\C,1.287530948,-2.462983761,0.6127638496\H,0.4920930591,-2
.1787812939,1.2851555283\H,-4.7267271145,-2.2299486462,-1.8703964088\H
,-3.1197605949,0.6702290275,1.0992724645\\Version=EM64L-G09RevD.01\HF=
-16923.7100884\RMSD=8.070e-09\RMSF=3.052e-07\Dipole=-0.0083198,-0.0085
192,0.0018159\Quadrupole=-13.7848084,7.9120073,5.8728011,-10.7847213,-
12.4866675,-1.3554751\PG=C01 [X(C36H22Br6N2)]\\@

9
1\1\GINC-HPC-CN124\FOpt\RBLYP\6-31G(d)\C36H22Br6N2\TALIPOVM\27-Feb-201
5\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent
=Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\
\Title\\0,1\N,-8.839332106,-0.1454387432,-1.2944184349\C,-7.4385949544
,-0.2211908797,-1.153291934\C,-6.7259828276,0.7914358381,-0.5051280366

\H,-7.247682096,1.6515767001,-0.1152355801\C,-5.3533632928,0.6983647888,-0.3694884757\H,-4.8191049634,1.4937722567,0.1289292541\C,-4.6236753993,-0.3800150777,-0.8804951645\C,-5.3576026996,-1.3741473105,-1.5267773084\Br,-4.483285715,-2.9165884807,-2.2307276756\C,-6.7355183389,-1.3152445108,-1.6587524914\H,-7.2612300064,-2.1195597938,-2.1463125529\C,-9.6349362561,0.3553351846,-0.2353592079\C,-9.3851019136,-0.0260047217,1.0845740653\H,-8.5814885483,-0.7129716527,1.3022207947\C,-10.1615400214,0.4692460129,2.1218008313\H,-9.9617674967,0.1692609642,3.1386494759\C,-11.2065702319,1.3356068497,1.8370276094\Br,-12.2835241009,2.0074934762,3.2573679273\C,-11.4784608844,1.719105708,0.5320840102\H,-12.2888372321,2.3988183444,0.3195692651\C,-10.6866569848,1.2353813158,-0.4987891561\H,-10.8862329973,1.5438185903,-1.513778533\C,-9.4623649658,-0.5955249593,-2.4841255007\C,-10.6118438665,-1.38585112,-2.4258277155\H,-11.022024581,-1.6660503799,-1.4675199233\C,-11.2330182231,-1.8163937203,-3.5890029949\H,-12.1207242515,-2.4270506612,-3.5349414216\C,-10.6917209351,-1.4704369923,-4.8181453025\Br,-11.5340470414,-2.0699151426,-6.417852682\C,-9.5454233788,-0.6934195671,-4.8987183355\H,-9.1353304287,-0.4220953634,-5.8589543611\C,-8.9399014035,-0.25028281,-3.7323564712\H,-8.0571793323,0.3681514754,-3.7920476807\N,1.0904009757,-0.2921550294,-0.5223932909\C,-0.3166142781,-0.3294243666,-0.6055736419\C,-1.0884746497,-0.4870810158,0.5459941054\H,-0.6130759335,-0.598820448,1.5064963575\C,-2.4708265051,-0.5095139355,0.4555717347\Br,-3.4434666368,-0.7498925809,2.0789629729\C,-3.1439241674,-0.3995229738,-0.7607778247\C,-2.3471334699,-0.2577672533,-1.901586685\H,-2.8322065316,-0.159385595,-2.8615532961\C,-0.9669344053,-0.2125482272,-1.8370968024\H,-0.39053614,-0.0799477222,-2.7394411971\C,1.7239988754,0.368513919,0.5583979592\C,1.2886528677,1.629321871,0.9719652444\H,0.4661591873,2.1069470108,0.4614808742\C,1.9045397182,2.2764497509,2.0328140613\H,1.5621196029,3.2504424618,2.3457732005\C,2.974941553,1.6686749492,2.6724064326\Br,3.8323346449,2.5600788171,4.1209428709\C,3.4297038743,0.4213151597,2.2713661259\H,4.258169655,-0.047709557,2.7788205981\C,2.7973195589,-0.2290257539,1.2219219109\H,3.139195847,-1.2064660562,0.9172166718\C,1.8784231823,-0.9357918158,-1.5071900308\C,3.0135458852,-0.3076297261,-2.0238449805\H,3.2849479986,0.6782703786,-1.6781690475\C,3.7968031851,-0.9379127822,-2.979299842\H,4.6718903412,-0.4451128177,-3.3733039938\C,3.4338604332,-2.1965946206,-3.435231391\Br,4.4993815355,-3.0601539607,-4.7570926103\C,2.3058329798,-2.8350083699,-2.9414977641\H,2.0348995925,-3.8175814983,-3.2951052059\C,1.5371539233,-2.20754701,-1.972301485\H,0.66

79947748,-2.7092968206,-1.5749683244\\Version=EM64L-G09RevD.01\HF=-169
23.7087315\RMSD=4.827e-09\RMSF=2.458e-07\Dipole=0.0376995,0.7551559,-0
.3874958\Quadrupole=-5.088289,10.14156,-5.053271,-5.1341874,1.3295688,
-13.2224058\PG=C01 [X(C36H22Br6N2)]\\@

MC, tris(2-bromo-4-(tert-butyl)phenyl)amine
1\1\GINC-HPC-CN119\FOpt\RBLYP\6-31G(d)\C30H36Br3N1\TALIPOVM\27-Mar-201
5\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent
=Dichloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\
\Title\\0,1\N,0.0166035312,-0.6088477398,0.0448941486\C,1.420513168,-0
.4069297177,0.0316320179\C,1.9983617139,0.7171073717,0.6237021514\H,1.
3547867431,1.4426716665,1.0991167392\C,3.3684413235,0.9140981105,0.610
6126181\H,3.7628925161,1.8013658631,1.0836336678\C,4.2339426181,0.0073
265486,-0.0097352773\C,5.745215754,0.2625556107,-0.0199632625\C,3.6577
389046,-1.1173901059,-0.5970567529\H,4.2688822751,-1.8639358629,-1.074
8963067\C,2.2855625865,-1.3241749504,-0.5623427398\Br,1.5963300065,-2.
9293719458,-1.3049817036\C,-0.6928871556,-0.3053234015,1.2350486982\C,
-0.5257442208,-1.0625120576,2.3983565101\Br,0.6085737677,-2.584739442,
2.3795398408\C,-1.2002308701,-0.7541493659,3.5656627521\H,-1.028797239
8,-1.3734435948,4.432005629\C,-2.1038769456,0.311669205,3.6260228573\C
,-2.8386628266,0.609891354,4.9378587771\C,-2.2921778403,1.0489932723,2
.4584440271\H,-2.9785874343,1.8800918922,2.4416718749\C,-1.5956481827,
0.7519540019,1.2937485459\H,-1.7528381882,1.351017985,0.4087808938\C,-
0.6820522536,-0.5412063145,-1.1877028794\C,-1.6927233742,-1.4533561602
,-1.5052413764\Br,-2.0989846637,-2.867355913,-0.3056510823\C,-2.387734
619,-1.3771615613,-2.6983953587\H,-3.1581570146,-2.1081515808,-2.88683
98465\C,-2.0901032266,-0.4010294775,-3.6547849314\C,-2.8767458161,-0.3
631823817,-4.9698858643\C,-1.0645288917,0.4920752525,-3.3498307661\H,-
0.7872465651,1.2650553071,-4.0482435691\C,-0.3835953803,0.4278279149,-
2.1406360614\H,0.3975723629,1.1429129011,-1.9280108742\C,-3.7807059903
,1.8134217931,4.8100892301\C,-1.8107766801,0.9180615033,6.0424589609\C
,-3.6759468326,-0.6159753056,5.3478033938\H,-4.4173604183,-0.854215753
5,4.5845157628\H,-4.2030199675,-0.4154004259,6.2817333663\H,-3.0560251
347,-1.4989352897,5.5001617455\H,-3.2419925397,2.7239586333,4.54627572
44\H,-4.2772190225,1.9889433555,5.7644025025\H,-4.5553412317,1.6448402
851,4.0616114408\H,-1.2075586536,1.7884143338,5.7818711877\H,-1.134952
6728,0.0807197044,6.2133883152\H,-2.3218758683,1.1293948722,6.98286515
48\C,6.51829997,-0.8471638616,-0.7430125594\C,6.2598158511,0.342620902

6,1.4293220733\C,6.0314350457,1.5950069393,-0.7374861953\H,6.074724585
2,-0.5915236971,1.960543871\H,5.7795364508,1.1462129452,1.9865742008\H
,7.334671673,0.5295081513,1.436465303\H,6.382556601,-1.8162731281,-0.2
621480948\H,7.5837320109,-0.6179331265,-0.7260270731\H,6.2175726017,-0
.9377029437,-1.7871938301\C,-2.4146851884,0.7774950958,-5.8850852158\C
,-4.3732172531,-0.1618538777,-4.6671787786\C,-2.6830820511,-1.69311116
19,-5.7220080044\H,-4.5414154027,0.7775347399,-4.1394272735\H,-4.77566
85752,-0.9676753793,-4.0541362263\H,-4.9441090928,-0.1352563476,-5.596
4725047\H,-1.6309108061,-1.8590574048,-5.9553575756\H,-3.2403592977,-1
.67884402,-6.6598326624\H,-3.035547166,-2.5439239654,-5.1397678209\H,-
2.550279697,1.7530264751,-5.4172786959\H,-3.0021730229,0.767429638,-6.
8031430657\H,-1.3657775884,0.6743260503,-6.1640576294\H,5.6842053571,1
.5635454597,-1.7707830927\H,7.1041093453,1.7939514062,-0.7466020624\H,
5.5423760994,2.4345607206,-0.2444569686\\Version=EM64L-G09RevD.01\HF=-
8933.888762\RMSD=9.612e-09\RMSF=4.436e-07\Dipole=-0.0208964,2.1036988,
-0.1872739\Quadrupole=6.3803515,-12.6858584,6.3055069,0.4099598,0.0725
399,1.8173194\PG=C01 [X(C30H36Br3N1)]\\@

Tris(4-(tert-butyl)phenyl)amine
1\1\GINC-HPC-CN124\FOpt\RBLYP\6-31G(d)\C30H39N1\TALIPOVM\05-Aug-2015\0
\\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=Di
chloromethane) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Ti
tle\\0,1\N,0.0107567965,0.0335724355,-0.0250885033\C,1.4259608278,0.04
80087317,-0.0202020759\C,2.1316161366,0.9401720762,0.7916678159\H,1.59
01098319,1.632322439,1.4194404609\C,3.5166278419,0.9422405407,0.798113
8325\H,4.0203267752,1.6490084178,1.4424359785\C,4.2658149197,0.0782463
466,-0.0091720179\C,5.7975348823,0.1252552517,0.0257721314\C,3.5463646
954,-0.7987610439,-0.8211602654\H,4.0639110101,-1.4945556087,-1.462863
8485\C,2.1566874078,-0.8249323918,-0.8237960063\C,-0.7020194007,0.1493
563273,1.1919928526\C,-0.2868300171,-0.5401791026,2.3345860897\C,-0.98
48542294,-0.4165895919,3.5242743725\H,-0.6272342714,-0.9676880218,4.38
26113028\C,-2.1329153611,0.3769233187,3.6345777942\C,-2.8772983655,0.4
733271181,4.9710783924\C,-2.5396612179,1.0504430993,2.4827591646\H,-3.
4132768662,1.6830688712,2.5022927099\C,-1.8380354054,0.9506605883,1.28
69450751\H,-2.1778992927,1.4988124332,0.4206405502\C,-0.6923659951,-0.
0894193301,-1.2476087086\C,-1.8087419556,-0.9236018709,-1.3513728416\C
,-2.4961159085,-1.0345002634,-2.5485055509\H,-3.3539789907,-1.69118986
37,-2.5827221158\C,-2.1018757131,-0.3423535877,-3.6997495308\C,-2.8889

883831,-0.5067445887,-5.0047947962\C,-0.980365422,0.4787382556,-3.5817
843406\H,-0.6283147619,1.0441904664,-4.4303680826\C,-0.2920724415,0.61
4020937,-2.381686544\H,0.5644863968,1.2696670794,-2.327700348\C,-4.103
1458585,1.3914579239,4.8882147606\C,-1.9305392023,1.0342421666,6.04865
51042\C,-3.3556328374,-0.9276073374,5.3963486534\H,-4.038154984,-1.346
9108863,4.656160511\H,-3.8821714415,-0.8744841116,6.3507732826\H,-2.52
33976571,-1.620888957,5.5147225259\H,-3.8279502516,2.411828211,4.61965
30152\H,-4.5984356436,1.4280705464,5.8587833628\H,-4.8307043099,1.0316
563972,4.160072807\H,-1.5825113123,2.0322088193,5.7794273155\H,-1.0549
332285,0.400768678,6.1874782411\H,-2.4466090829,1.1028736929,7.0078113
943\C,6.4319087939,-0.8983748202,-0.9241414189\C,6.2895640458,-0.17717
1032,1.4535812304\C,6.2793955598,1.5277873342,-0.3900293078\H,5.971548
1585,-1.1705524485,1.7722805745\H,5.9066272815,0.544072158,2.174960959
8\H,7.3795594535,-0.1413035047,1.4942677569\H,6.1532970647,-1.91998657
89,-0.6639089285\H,7.5182427623,-0.8275933166,-0.8647782634\H,6.146029
6386,-0.7206671471,-1.961294037\C,-2.3040845842,0.3348445579,-6.145905
6301\C,-4.3486637255,-0.0671999293,-4.785037896\C,-2.8644049608,-1.984
5497931,-5.4380621287\H,-4.3986373387,0.980603502,-4.4864601851\H,-4.8
376675908,-0.6590666885,-4.0118628084\H,-4.9222726454,-0.1845742579,-5
.7060169758\H,-1.8419524321,-2.3216843873,-5.6124881027\H,-3.427283173
3,-2.1172622211,-6.3635704517\H,-3.3071898252,-2.6349406178,-4.6842764
82\H,-2.3202882279,1.4000668958,-5.9134138303\H,-2.8950785534,0.185600
584,-7.0498431004\H,-1.2761361619,0.0510073248,-6.3733876499\H,5.95511
07319,1.7657049717,-1.4038107088\H,7.3692622068,1.5774150581,-0.362685
8933\H,5.8952989404,2.3013484183,0.2742813169\H,-2.1367819935,-1.48469
03074,-0.4888149595\H,0.5866702467,-1.1735355458,2.2870031109\H,1.6366
386151,-1.5282628199,-1.4573001115\\Version=EM64L-G09RevD.01\HF=-1220.
6967916\RMSD=4.641e-09\RMSF=2.487e-07\Dipole=-0.0040013,-0.0075319,0.0
15959\Quadrupole=3.013266,-6.0173197,3.0040538,0.2279432,0.1473069,0.8
948516\PG=C01 [X(C30H39N1)]\\@

MB Cation Radical

1\1\GINC-HPC-CN8\Stability\UBLYP\6-31G(d)\C18H12Br3N1(1+,2)\TALIPOVM\0
4-Jun-2014\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(np
a) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=2
00) int(grid=ultrafine)\\Title\\1,2\N,0,0.0097087448,-0.0043564374,-0.
000447635\C,0,1.4144624996,0.0238734621,-0.0017888503\C,0,2.0972217721

,0.8891608479,0.8665337016\H,0,1.5474577487,1.5542853719,1.513059653\C
,0,3.4774182714,0.9215945526,0.8586152984\H,0,4.0068605379,1.598748908
4,1.5090226165\C,0,4.1777925643,0.0856372002,-0.0078145579\Br,0,6.0632
48853,0.1298861896,-0.0136258973\C,0,3.511611703,-0.7818745272,-0.8702
478597\H,0,4.0680975534,-1.4348719877,-1.5228178631\C,0,2.131247663,-0
.8113122067,-0.8721607684\H,0,1.6088865065,-1.5006068411,-1.5161539462
\C,0,-0.6924723882,0.0999679041,1.2119835681\C,0,-0.2075485371,-0.5467
001652,2.3589499\H,0,0.683134565,-1.152087836,2.3047926597\C,0,-0.8991
943091,-0.4435515243,3.5492908702\H,0,-0.5424473716,-0.9538142458,4.42
92551721\C,0,-2.0688710954,0.3111179812,3.5993081205\Br,0,-3.006868118
7,0.4561153437,5.2289094836\C,0,-2.5584115202,0.9605133882,2.468493460
8\H,0,-3.4563096342,1.5541060645,2.5271293082\C,0,-1.8748866927,0.8528
724045,1.2737513339\H,0,-2.2310412705,1.3765827943,0.4010631672\C,0,-0
.6918458444,-0.1333214701,-1.2102981865\C,0,-1.8512265428,-0.922061570
9,-1.2663457236\H,0,-2.1877316945,-1.4549418298,-0.3914189822\C,0,-2.5
362873077,-1.0523749848,-2.457825465\H,0,-3.4159402288,-1.6731391203,-
2.511574173\C,0,-2.0717955534,-0.3898614838,-3.5916751728\Br,0,-3.0120
678396,-0.564968971,-5.2169096776\C,0,-0.925290353,0.3999965027,-3.547
5924284\H,0,-0.5883066372,0.9199185653,-4.4296623713\C,0,-0.2319056115
,0.5261359022,-2.3605733217\H,0,0.6397695679,1.1590618189,-2.311745433
9\\Version=EM64L-G09RevD.01\HF=-8462.2554141\S2=0.801744\S2-1=0.\S2A=0
.752641\RMSD=4.529e-09\Dipole=-0.0106403,-0.0098607,-0.0075292\Quadrup
ole=3.9564258,-7.8688168,3.912391,0.2201757,-0.0183929,1.1660148\PG=C0
1 [X(C18H12Br3N1)]\\@

TAB Cation Radical
1\1\GINC-HPC-CN12\Stability\UBLYP\6-31G(d)\C36H24Br4N2(1+,2)\TALIPOVM\
07-Jan-2015\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(n
bo) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=
200) int(grid=ultrafine)\\Title\\1,2\N,0,-8.7975634224,-0.1789951434,-
1.2869055209\C,0,-7.4285181887,-0.2003063963,-1.178248679\C,0,-6.76774
83695,0.5210045801,-0.1554636941\H,0,-7.3411338585,1.1270894105,0.5263
536948\C,0,-5.4033404127,0.4949268499,-0.0520622908\H,0,-4.9430067219,
1.1001257993,0.7122304172\C,0,-4.5948971654,-0.2428352641,-0.952189641
\C,0,-5.2722609899,-0.9586875953,-1.9704236394\H,0,-4.7144545401,-1.57
86417051,-2.6535941038\C,0,-6.6359966227,-0.9441554476,-2.0846829873\H
,0,-7.1118959997,-1.534728432,-2.8500517631\C,0,-9.6242074225,0.137844
5732,-0.1680351332\C,0,-9.4676353253,-0.5471702673,1.0360894656\H,0,-8

.7177979844,-1.3185460369,1.1258926325\C,0,-10.2834512851,-0.2481008081,2.1169465861\H,0,-10.1672941942,-0.7796392356,3.0480547703\C,0,-11.2601802563,0.7285363145,1.9810221238\Br,0,-12.3832351449,1.1362712153,3.4570296493\C,0,-11.4335218569,1.4105446619,0.7840328343\H,0,-12.1942959989,2.1693685597,0.6927400445\C,0,-10.6116882335,1.1134661051,-0.2919853804\H,0,-10.7330876583,1.6434333771,-1.2243721282\C,0,-9.4491534801,-0.4673791889,-2.5224823747\C,0,-10.4878483421,-1.3961040622,-2.5562770563\H,0,-10.7799381981,-1.9126274182,-1.6548017114\C,0,-11.1427517576,-1.6630612355,-3.748435964\H,0,-11.9430140003,-2.3853096345,-3.7780644287\C,0,-10.7517055375,-0.9984691122,-4.9031411496\Br,0,-11.6469320887,-1.3633243902,-6.5375414725\C,0,-9.7214491406,-0.0687344741,-4.8830757383\H,0,-9.4353239112,0.450308296,-5.7840471156\C,0,-9.0734512037,0.2007966167,-3.6870312603\H,0,-8.2845725766,0.9369801771,-3.6574160043\N,0,1.0452756947,-0.3076726825,-0.5106745049\C,0,-0.3239328063,-0.2954975821,-0.6171315874\C,0,-1.1364750615,0.0899994864,0.4757672736\H,0,-0.679599611,0.3403345276,1.4189833183\C,0,-2.5001259383,0.1044524862,0.3611920844\H,0,-3.078124742,0.3583569923,1.2351360835\C,0,-3.15820008,-0.263096739,-0.8387603599\C,0,-2.3302831737,-0.6500282423,-1.92179489\H,0,-2.7708140748,-0.8932368507,-2.8753192775\C,0,-0.9653575581,-0.6664918976,-1.8229393854\H,0,-0.3729869428,-0.928679843,-2.6839430536\C,0,1.718818192,0.4798729643,0.4699397229\C,0,1.4601759094,1.8460250233,0.5710292936\H,0,0.7463181723,2.3114649246,-0.0915614639\C,0,2.1292136182,2.6118576027,1.5139115482\H,0,1.9343129003,3.6696495051,1.5913287017\C,0,3.0629504309,2.0057015898,2.3427793418\Br,0,3.9863123842,3.0534040154,3.6295603338\C,0,3.3372518368,0.6480386412,2.2452507872\H,0,4.0630554394,0.1890690762,2.8975175175\C,0,2.661339517,-0.1154526484,1.3062049387\H,0,2.8610701666,-1.1732177261,1.2271316118\C,0,1.8508078697,-1.1079558108,-1.374139503\C,0,2.9312074301,-0.5337577842,-2.0417478648\H,0,3.1419740523,0.5181455478,-1.924138362\C,0,3.7327189395,-1.3109219862,-2.8633675068\H,0,4.565800434,-0.8677712785,-3.3853701998\C,0,3.4461728694,-2.661161575,-3.0137869901\Br,0,4.5417608553,-3.7269311767,-4.1406771157\C,0,2.3762053777,-3.2466968353,-2.3515923602\H,0,2.1716502675,-4.2992679783,-2.4662985239\C,0,1.5810772704,-2.4674313856,-1.5248578336\H,0,0.758802249,-2.9176730493,-0.9898647562\\Version=EM64L-G09RevD.01\HF=-11781.4041041\S2=0.774777\S2-1=0.\S2A=0.750401\RMSD=1.611e-09\Dipole=-0.0027809,-0.0168931,0.0039737\Quadrupole=74.8697035,-36.2148223,-38.6548812,2.9670235,17.284988,-3.1289354\PG=C01 [X(C36H24Br4N2)]\\@

1 Cation Radical

1\1\GINC-HPC-CN116\Stability\UBLYP\6-31G(d)\C18H11Br4N1(1+,2)\TALIPOVM
\27-Feb-2015\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(
nbo) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc
=200) int(grid=ultrafine)\\Title\\1,2\N,0,0.0124103599,-0.0289898284,0
.0602298815\C,0,1.4115364712,-0.0239510615,0.027520718\C,0,2.142738925
7,0.8324345841,0.8684548691\H,0,1.630861894,1.5175004872,1.5250941767\
C,0,3.5214716894,0.8335414048,0.8136984492\H,0,4.0876337744,1.50247586
67,1.441300039\C,0,4.1744684503,-0.0187680711,-0.0748330646\Br,0,6.056
627427,-0.0151606607,-0.1461192402\C,0,3.4599570366,-0.8692217676,-0.9
17801491\H,0,3.9800797556,-1.530316755,-1.5917523842\C,0,2.0818485773,
-0.8677030888,-0.8738874591\C,0,-0.6972847724,0.1529052566,1.242260126
\C,0,-0.1798496978,-0.3224642945,2.463235609\H,0,0.7521510115,-0.86362
14937,2.4839514539\C,0,-0.8960587753,-0.148213201,3.6270648832\H,0,-0.
5126803696,-0.5269956895,4.5605805009\C,0,-2.1313890302,0.4985697566,3
.5847964536\Br,0,-3.1041037063,0.7405503896,5.1763897024\C,0,-2.661007
5142,0.9646376955,2.3803838911\H,0,-3.6130647407,1.469900445,2.3658178
904\C,0,-1.9530802761,0.7876296451,1.2125384106\H,0,-2.347035255,1.167
8301906,0.2839448111\C,0,-0.6860321281,-0.1686958766,-1.1719659991\C,0
,-1.6161786537,-1.1932869632,-1.3915668538\Br,0,-1.9387318647,-2.53134
35454,-0.100899187\C,0,-2.2801110295,-1.2775075552,-2.6043939166\H,0,-
2.9864474773,-2.072292112,-2.7765774198\C,0,-2.0124984841,-0.342331882
7,-3.595856234\Br,0,-2.9292891348,-0.4619679059,-5.2415775486\C,0,-1.0
804309247,0.6698047403,-3.4024279759\H,0,-0.8814970399,1.3893538081,-4
.1795714859\C,0,-0.4174350094,0.7466230174,-2.1923007039\H,0,0.2979182
607,1.535086453,-2.0174241958\H,0,1.5212722501,-1.5401919878,-1.502936
7062\\Version=EM64L-G09RevD.01\HF=-11033.3095455\S2=0.799597\S2-1=0.\S
2A=0.752327\RMSD=3.931e-09\Dipole=0.7377384,0.9617989,0.3341703\Quadru
pole=3.1257612,-8.8529066,5.7271454,-0.9415046,0.0975285,1.2880656\PG=
C01 [X(C18H11Br4N1)]\\@

2 Cation Radical

1\1\GINC-HPC-CN118\Stability\UBLYP\6-31G(d)\C18H10Br5N1(1+,2)\TALIPOVM
\27-Feb-2015\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(
nbo) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc
=200) int(grid=ultrafine)\\Title\\1,2\N,0,0.059160922,-0.1093020788,0.
0469278998\C,0,1.4266812962,-0.0166250247,0.0134414003\C,0,2.124321269

,0.7256073863,0.9986763511\H,0,1.5788105201,1.2532505932,1.7637691666\
C,0,3.4917676384,0.8180045598,0.9461573539\H,0,4.0250336293,1.40112446
,1.6790908246\C,0,4.1931721028,0.1659950026,-0.0768906013\Br,0,6.06024
00377,0.289946799,-0.1349008845\C,0,3.5210174478,-0.5752616734,-1.0559
042847\H,0,4.077380565,-1.0854365988,-1.8251803791\C,0,2.1517762476,-0
.6643336601,-1.0180748338\C,0,-0.680755881,0.1238999254,1.2380843856\C
,0,-0.4388744223,-0.580420217,2.427650619\Br,0,0.8173450592,-1.9828880
572,2.5195607583\C,0,-1.1867454793,-0.3065929649,3.559672111\H,0,-1.00
67080003,-0.8587477488,4.4667212923\C,0,-2.1799679706,0.6630959433,3.5
071185664\Br,0,-3.1859868151,1.0315877578,5.0601725201\C,0,-2.44940488
78,1.3551487579,2.3329862861\H,0,-3.2231497184,2.10469023,2.3020753325
\C,0,-1.7022442799,1.0767053866,1.2047129961\H,0,-1.8906937923,1.61812
21869,0.2909597695\C,0,-0.6679219582,-0.2816355599,-1.1666584767\C,0,-
1.5682469297,-1.3381591229,-1.3482689029\Br,0,-1.7712830131,-2.6884707
732,-0.0485370255\C,0,-2.2867215929,-1.4404878665,-2.5276351806\H,0,-2
.9709827042,-2.260027804,-2.6709317149\C,0,-2.1019454018,-0.4909284735
,-3.5249904209\Br,0,-3.0942546345,-0.6358482686,-5.1243065105\C,0,-1.1
999688006,0.5537387636,-3.3698356641\H,0,-1.0656844996,1.2851156358,-4
.1498484888\C,0,-0.4842003759,0.65066167,-2.1907503527\H,0,0.204512134
9,1.4685176108,-2.0435252593\H,0,1.6313522876,-1.2642467768,-1.7461386
529\\Version=EM64L-G09RevD.01\HF=-13604.3650606\S2=0.793807\S2-1=0.\S2
A=0.751658\RMSD=1.901e-09\Dipole=1.3677863,1.5413947,-0.8558761\Quadru
pole=7.2866676,-9.1534437,1.8667761,-0.7625947,-0.5279036,1.7831215\PG
=C01 [X(C18H10Br5N1)]\\@

3 Cation Radical
1\1\GINC-HPC-CN119\Stability\UBLYP\6-31G(d)\C18H9Br6N1(1+,2)\TALIPOVM\
27-Feb-2015\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(n
bo) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=
200) int(grid=ultrafine)\\Title\\1,2\N,0,0.011564937,-0.1412758293,0.0
24698473\C,0,1.4100721289,-0.0249210136,0.0035751571\C,0,2.0113189125,
1.0176860838,0.7246208349\H,0,1.3881173103,1.7166846833,1.2599231363\C
,0,3.3789260598,1.1892056997,0.7074382967\H,0,3.8324471485,2.008326835
,1.2408498215\C,0,4.1627616301,0.3020688632,-0.0255114077\Br,0,6.02979
34045,0.5280234822,-0.067224274\C,0,3.5939868157,-0.7621132693,-0.7205
599573\H,0,4.2172092238,-1.4666003198,-1.2454254525\C,0,2.2240254361,-
0.9319498949,-0.7038684804\C,0,-0.6833920507,0.0444095736,1.229577075\
C,0,-0.3516596255,-0.6660548973,2.4005499818\Br,0,0.9098496797,-2.0626

13296,2.3747026878\C,0,-1.04501722,-0.4299174881,3.5706760004\H,0,-0.8
046761841,-0.9873455039,4.4604638\C,0,-2.0774904565,0.504542209,3.5810
311952\Br,0,-3.0036140942,0.8252432063,5.1864900207\C,0,-2.442536295,1
.1926538801,2.4268813495\H,0,-3.2430889582,1.9136855428,2.4493805737\C
,0,-1.7508157341,0.9543183218,1.2586736854\H,0,-1.9983886525,1.5037884
845,0.3640288145\C,0,-0.6989662286,-0.2273440174,-1.1820422506\C,0,-1.
7657221655,-1.1317431315,-1.3573758721\Br,0,-2.1672379918,-2.43558933,
-0.0604796992\C,0,-2.4586458297,-1.1591793966,-2.550950441\H,0,-3.2618
3307,-1.8630665211,-2.6912053874\C,0,-2.0872453464,-0.2986021551,-3.58
09010627\Br,0,-3.0484781451,-0.3390580754,-5.197021083\C,0,-1.01317233
91,0.5765327081,-3.4408926173\H,0,-0.7360096093,1.236168402,-4.2466962
962\C,0,-0.3217491478,0.6026044613,-2.2487978399\H,0,0.4914307617,1.29
83950563,-2.1138229423\Br,0,1.5050256955,-2.4811433536,-1.4953958399\\
Version=EM64L-G09RevD.01\HF=-16175.4184626\S2=0.792901\S2-1=0.\S2A=0.7
51793\RMSD=4.163e-09\Dipole=-0.0722546,2.055044,-0.2422459\Quadrupole=
4.4641838,-8.8036655,4.3394817,0.4357642,-0.024532,1.4967178\PG=C01 [X
(C18H9Br6N1)]\\@

4 Cation Radical
1\1\GINC-HPC-CN10\Stability\UBLYP\6-31G(d)\C18H10Br3N1(1+,2)\TALIPOVM\
07-Jan-2015\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(n
bo) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=
200) int(grid=ultrafine)\\Title\\1,2\N,0,-0.1392697746,0.0217333371,0.
261874543\C,0,1.2258782093,0.199996653,0.1095946497\C,0,2.1743080081,0
.5680414826,1.0635657353\H,0,1.9087122389,0.7505704192,2.0920179126\C,
0,3.487368551,0.7064963007,0.6414881825\H,0,4.2524177941,0.9850117427,
1.3474414621\C,0,3.8217995814,0.4963221696,-0.696381828\Br,0,5.6132855
524,0.6947571589,-1.2355432171\C,0,2.8640163239,0.1537827495,-1.663478
7446\H,0,3.1541854294,0.0169408381,-2.6927567891\C,0,1.5615128875,0.01
09492948,-1.2499820351\C,0,-0.8478876976,0.1276204743,1.4843383745\C,0
,-0.4195088298,-0.6027395175,2.592902381\H,0,0.4246167843,-1.270121379
6,2.5156230719\C,0,-1.1157524316,-0.5006797057,3.7851260086\H,0,-0.803
5685111,-1.0715990743,4.6445616443\C,0,-2.2262157204,0.3325478671,3.85
83944778\Br,0,-3.1733941145,0.4721761854,5.4884533206\C,0,-2.654147882
8,1.0649513601,2.7569592429\H,0,-3.5095134707,1.7166166954,2.832847561
8\C,0,-1.9639513108,0.9608332,1.5614135192\H,0,-2.2675739069,1.5484377
266,0.7091061645\C,0,-0.7036407703,-0.2775024535,-0.9673850501\C,0,-2.
0295437236,-0.5830734525,-1.2731444662\H,0,-2.7988164247,-0.6066131767

,-0.51867115\C,0,-2.3322635481,-0.8719203642,-2.5946464667\H,0,-3.3458
025774,-1.108467951,-2.8740976315\C,0,-1.328618729,-0.8669636901,-3.56
34052298\Br,0,-1.7749235355,-1.2643134438,-5.3475489269\C,0,0.01126803
54,-0.5872861428,-3.2526847366\H,0,0.7653244168,-0.6092602151,-4.02305
78393\C,0,0.316399147,-0.2956450885,-1.9450341413\\Version=EM64L-G09Re
vD.01\HF=-8461.0705649\S2=0.797075\S2-1=0.\S2A=0.752007\RMSD=1.941e-09
\Dipole=-0.0614785,0.0129333,0.1174327\Quadrupole=7.4847643,-14.167199
5,6.6824351,0.2474078,0.4736128,1.9506668\PG=C01 [X(C18H10Br3N1)]\\@

5 Cation Radical
1\1\GINC-HPC-CN17\Stability\UBLYP\6-31G(d)\C36H20Br4N2(1+,2)\TALIPOVM\
27-Feb-2015\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(n
bo) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=
200) int(grid=ultrafine)\\Title\\1,2\N,0,-8.8139961036,-0.1758982829,-
1.2977513168\C,0,-7.4136507136,-0.1919499972,-1.1870635804\C,0,-6.7809
263481,0.5923766901,-0.2159627664\H,0,-7.3603646762,1.2519201226,0.410
8132444\C,0,-5.4052486523,0.5749568659,-0.1176246159\H,0,-4.92905642,1
.223688634,0.6006495104\C,0,-4.6220446093,-0.2274950915,-0.9631129334\
C,0,-5.2803507604,-1.0101979009,-1.9255413551\H,0,-4.7124848925,-1.671
5074488,-2.561033748\C,0,-6.6541745661,-0.9926093619,-2.0479163545\H,0
,-7.1426246096,-1.637845416,-2.7612048509\C,0,-9.709883593,-0.29241098
02,-0.2392918316\C,0,-9.449835019,-0.5140905868,1.1113876821\H,0,-8.44
68050063,-0.6098560867,1.4927345274\C,0,-10.5363613926,-0.627098623,1.
9657911054\H,0,-10.3760823397,-0.7912946294,3.0187674757\C,0,-11.83521
03621,-0.5429996024,1.4664679439\Br,0,-13.2880567762,-0.7059283357,2.6
563206084\C,0,-12.1002268771,-0.3587547816,0.1040778892\H,0,-13.116700
0651,-0.3259843083,-0.2535191385\C,0,-11.0252782548,-0.2357968852,-0.7
468430534\C,0,-9.5293376413,-0.0428914583,-2.4838645044\C,0,-10.909144
7711,-0.0745436115,-2.190899329\C,0,-11.8336323826,0.066380415,-3.2011
392911\H,0,-12.8944162609,0.0512156181,-3.0090090396\C,0,-11.352686226
1,0.2439053232,-4.5040945167\Br,0,-12.5938306491,0.4289635136,-5.91071
93019\C,0,-9.9898332368,0.3048081189,-4.7909512072\H,0,-9.6618478285,0
.4651278671,-5.8048289918\C,0,-9.0544717672,0.1729926364,-3.7756760237
\H,0,-8.0021390973,0.2511010208,-3.9928637655\N,0,1.0507250607,-0.3012
831901,-0.4985708988\C,0,-0.3571189747,-0.2840975506,-0.6137989801\C,0
,-1.1515973603,-0.0880996673,0.5152595102\H,0,-0.6892889785,0.02005470
83,1.4845492418\C,0,-2.5302411529,-0.0602363756,0.3967892779\H,0,-3.12
58965991,0.0660188031,1.2882268122\C,0,-3.1539147475,-0.2475878863,-0.

8431596471\C,0,-2.3417396119,-0.4544383058,-1.9652142891\H,0,-2.787302
239,-0.5672662816,-2.9419751814\C,0,-0.9619620737,-0.4626043015,-1.857
4497209\H,0,-0.3509990312,-0.585218793,-2.7387366477\C,0,1.8331405646,
0.692665488,0.082883819\C,0,1.4505417067,1.9111112031,0.6369834209\H,0
,0.4163155405,2.2141259629,0.6805821427\C,0,2.4421334351,2.7414122319,
1.1332981296\H,0,2.1776655351,3.6913155103,1.570405629\C,0,3.784186171
6,2.358070016,1.0682095699\Br,0,5.1086559778,3.5373212511,1.7703873207
\C,0,4.1785213438,1.1582444817,0.5079690943\H,0,5.2219467171,0.8883468
908,0.4588802405\C,0,3.1886904239,0.3162507656,0.005670165\C,0,1.89360
44286,-1.3139207731,-0.9482926818\C,0,3.2272036218,-0.9690717443,-0.65
19037663\C,0,4.2655002166,-1.8344393861,-0.9897122272\H,0,5.293203421,
-1.58892284,-0.7716504914\C,0,3.9393475999,-3.0252059031,-1.6099217242
\Br,0,5.3323690126,-4.2356064332,-2.0920167694\C,0,2.6170189588,-3.377
0972759,-1.8925599964\H,0,2.4048824619,-4.3208416667,-2.3697016328\C,0
,1.5776345397,-2.5235775225,-1.5606056714\H,0,0.5574059296,-2.80241485
34,-1.7722025193\\Version=EM64L-G09RevD.01\HF=-11779.0431166\S2=0.7945
16\S2-1=0.\S2A=0.751878\RMSD=1.519e-09\Dipole=-9.8308622,0.1253218,-0.
7987888\Quadrupole=172.2553734,-102.7765458,-69.4788276,5.8331971,39.0
006511,2.0212299\PG=C01 [X(C36H20Br4N2)]\\@

6 Cation Radical
1\1\GINC-HPC-CN116\Stability\UBLYP\6-31G(d)\C36H23Br5N2(1+,2)\TALIPOVM
\26-Feb-2015\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(
nbo) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc
=200) int(grid=ultrafine)\\Title\\1,2\N,0,-8.8030498147,-0.1790660885,
-1.2807824952\C,0,-7.4372725448,-0.2018498233,-1.1127297983\C,0,-6.803
8315512,0.6981917116,-0.2241816751\H,0,-7.3878969465,1.4510030318,0.27
95745069\C,0,-5.4448317369,0.6633363382,-0.0519433409\H,0,-4.986437275
8,1.3911739648,0.595222374\C,0,-4.6354971506,-0.2628380987,-0.74803646
1\C,0,-5.2792516146,-1.1417610612,-1.6482054588\H,0,-4.6977589215,-1.8
874255928,-2.1673250098\C,0,-6.6377643273,-1.1237825171,-1.8280590325\
H,0,-7.1035016891,-1.8479266387,-2.4761581506\C,0,-9.6605040965,0.2781
904888,-0.2452207427\C,0,-9.4696023645,-0.1629088129,1.0662414949\H,0,
-8.6789459231,-0.8607797793,1.2941556135\C,0,-10.3155522144,0.27479011
33,2.071311019\H,0,-10.1788392909,-0.0710698504,3.0832933556\C,0,-11.3
496941964,1.1485952313,1.7591091595\Br,0,-12.5083247485,1.7465155684,3
.132171607\C,0,-11.5529451118,1.5884933492,0.4558824847\H,0,-12.355901
2944,2.2714626651,0.2296314403\C,0,-10.7089506004,1.1495394394,-0.5491

394486\H,0,-10.8509195489,1.4956642964,-1.560964792\C,0,-9.3972495417,
-0.6155169572,-2.4956880752\C,0,-10.4974271572,-1.4745392127,-2.457266
0981\H,0,-10.8783036602,-1.8258545085,-1.5108460433\C,0,-11.0845693941
,-1.8943124577,-3.6381691934\H,0,-11.9259859519,-2.5681160826,-3.61594
37661\C,0,-10.5736317867,-1.4466145594,-4.8512960598\Br,0,-11.38037929
43,-2.018109669,-6.466282003\C,0,-9.4854091678,-0.5843635059,-4.900781
497\H,0,-9.1097939968,-0.232015347,-5.8480075025\C,0,-8.8959226246,-0.
1666104045,-3.7193276921\H,0,-8.0662197771,0.5228167141,-3.7454527701\
N,0,1.0537122581,-0.2965975798,-0.5224121041\C,0,-0.3312146941,-0.3069
069894,-0.5597188275\C,0,-1.0811655522,-0.1384923675,0.6168726191\H,0,
-0.5794045418,-0.0468389458,1.5648475199\C,0,-2.4578051831,-0.12964822
43,0.5801581401\Br,0,-3.3253557642,-0.0193324589,2.2737387613\C,0,-3.1
834748419,-0.2975842089,-0.6166579659\C,0,-2.4038490162,-0.5020294374,
-1.7739524082\H,0,-2.9075473936,-0.6087868596,-2.7225210245\C,0,-1.029
9961412,-0.49786437,-1.7643750074\H,0,-0.4905729051,-0.6155608912,-2.6
897133069\C,0,1.7585602427,0.3761455828,0.5161213427\C,0,1.4712716956,
1.7072254569,0.8176504442\H,0,0.7068719878,2.2321876753,0.2647707812\C
,0,2.1681978775,2.3635749729,1.821310812\H,0,1.9461404679,3.3934160899
,2.05237181\C,0,3.1652862693,1.6874179676,2.5098857529\Br,0,4.13074991
26,2.5870422534,3.8788263292\C,0,3.4716869858,0.3667091658,2.214249175
9\H,0,4.246595746,-0.1495762794,2.7585414114\C,0,2.7620606953,-0.28876
24943,1.219081461\H,0,2.9871815479,-1.3191436747,0.9892032947\C,0,1.81
86844713,-0.968086015,-1.5185519177\C,0,2.8487863334,-0.2952981895,-2.
1737503855\H,0,3.0492958114,0.7391995334,-1.9393798131\C,0,3.615938388
2,-0.9481751779,-3.1270701114\H,0,4.4115744645,-0.4260202977,-3.634631
6479\C,0,3.3405805686,-2.2743705044,-3.4289354073\Br,0,4.3850624463,-3
.1705631696,-4.7410343177\C,0,2.3179668891,-2.9584640277,-2.7872848052
\H,0,2.1205713481,-3.9925358307,-3.0219515592\C,0,1.5630246571,-2.3043
252474,-1.8248613781\H,0,0.777760284,-2.8349574021,-1.3077436177\\Vers
ion=EM64L-G09RevD.01\HF=-14352.4584426\S2=0.78582\S2-1=0.\S2A=0.751167
\RMSD=5.009e-09\Dipole=-4.3908464,-0.0618096,-1.266817\Quadrupole=125.
6250908,-63.6956504,-61.9294404,4.2599897,31.0531704,-2.0389486\PG=C01
[X(C36H23Br5N2)]\\@

7 Cation Radical
1\1\GINC-HPC-CN35\Stability\UBLYP\6-31G(d)\C36H23Br5N2(1+,2)\TALIPOVM\
05-Aug-2015\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(n
bo) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=

200) int(grid=ultrafine)\\Title\\1,2\N,0,-8.7859190432,-0.1546341487,-1.2930176832\C,0,-7.4116453786,-0.187222188,-1.1573732531\C,0,-6.7819089877,0.4384466517,-0.0585166713\H,0,-7.3717322678,0.9888843995,0.6563078833\C,0,-5.4158815978,0.4029703294,0.0644432421\H,0,-4.9602069709,0.9357531719,0.8837481847\C,0,-4.6042042652,-0.257367977,-0.8823597427\C,0,-5.2482940691,-0.8807327448,-1.9721309378\C,0,-6.6121533794,-0.8477521736,-2.1163568133\H,0,-7.0787662768,-1.3724454554,-2.9340036076\C,0,-9.6273753597,-0.0913226215,-0.1552320921\C,0,-9.3676747727,-0.9027781498,0.9535667383\H,0,-8.5385538133,-1.5929177187,0.9398370897\C,0,-10.1993511147,-0.8456022165,2.0579878415\H,0,-10.0119714768,-1.4784780537,2.9103709001\C,0,-11.286209475,0.0212400053,2.0499185228\Br,0,-12.4229879813,0.0990263255,3.5594855276\C,0,-11.5564345229,0.8291728113,0.9501501996\H,0,-12.3986289492,1.5021029264,0.9615421905\C,0,-10.7287457882,0.7701377959,-0.1561184977\H,0,-10.9206030073,1.4040337,-1.0075351394\C,0,-9.3870941457,-0.1850120927,-2.5762976744\C,0,-10.4937062287,-1.0083658709,-2.8039793046\H,0,-10.8725349679,-1.6392507892,-2.0152564808\C,0,-11.0847762399,-1.0349265023,-4.0541092688\H,0,-11.9288342196,-1.6791150107,-4.2407722865\C,0,-10.5742352854,-0.2320273731,-5.0689141859\Br,0,-11.3875084057,-0.2660397327,-6.7762421976\C,0,-9.4804528792,0.5977825791,-4.8505210555\H,0,-9.1062730771,1.227683125,-5.6413940678\C,0,-8.8847965878,0.6217452492,-3.6017154389\H,0,-8.0526953324,1.2825460491,-3.4146602939\N,0,1.072020644,-0.3842841086,-0.3482576979\C,0,-0.3269326527,-0.3572290339,-0.4539361024\C,0,-1.1728871509,-0.2372792442,0.6611702072\Br,0,-0.4655680435,-0.2154699622,2.4197317444\C,0,-2.5455673382,-0.1895577017,0.5190557801\C,0,-3.1493699027,-0.295703722,-0.7418453056\C,0,-2.3075142182,-0.4485389065,-1.8554994549\H,0,-2.7234417554,-0.4992610997,-2.8495507505\C,0,-0.9376760571,-0.4696436763,-1.7111502903\H,0,-0.3082524907,-0.5535406711,-2.583591247\C,0,1.7648229563,0.6816545183,0.2773683572\C,0,1.2809100916,1.9870931955,0.2019484593\H,0,0.3785390534,2.1985420378,-0.3513947944\C,0,1.9553114999,3.0250252767,0.8299506816\H,0,1.5752863297,4.0327349867,0.7679193312\C,0,3.1272499954,2.7572610689,1.5191560914\Br,0,4.0633856759,4.1790028452,2.3707524223\C,0,3.6292792884,1.4647206521,1.5962671317\H,0,4.5383231151,1.2639499551,2.1412559578\C,0,2.9426683852,0.4295365694,0.9839687689\H,0,3.3175574969,-0.5795598623,1.0606070795\C,0,1.7891709482,-1.3468193625,-1.1065562539\C,0,2.8615247142,-0.9742696766,-1.9176317778\H,0,3.1557406448,0.0620669127,-1.9809369898\C,0,3.5537299962,-1.9298371797,-2.6472452673\H,0,4.3817752498,-1.6377484139,-3.2738431151\C,0,3.1604347

544,-3.2583731002,-2.5770827686\Br,0,4.1019535938,-4.5690075204,-3.585
3581253\C,0,2.0922046807,-3.6463537745,-1.7809294752\H,0,1.8004467776,
-4.6833058966,-1.7248058573\C,0,1.4149833652,-2.6897955033,-1.04033483
01\H,0,0.5973753628,-2.9861698271,-0.4005283467\H,0,-4.6696320313,-1.4
40186541,-2.6894888728\H,0,-3.1493471116,-0.1252175344,1.4093236828\\V
ersion=EM64L-G09RevD.01\HF=-14352.4586894\S2=0.796361\S2-1=0.\S2A=0.75
2052\RMSD=6.375e-09\Dipole=-7.2624387,-0.0975202,-1.481826\Quadrupole=
148.1372831,-81.2267354,-66.9105477,3.6481436,33.4349545,-6.0083987\PG
=C01 [X(C36H23Br5N2)]\\@

8 Cation Radical
1\1\GINC-HPC-CN4\Stability\UBLYP\6-31G(d)\C36H22Br6N2(1+,2)\TALIPOVM\0
6-Aug-2015\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(nb
o) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=2
00) int(grid=ultrafine)\\Title\\1,2\N,0,-8.8281994578,-0.3557664458,-1
.291542406\C,0,-7.4239816882,-0.3814683467,-1.167545511\C,0,-6.7517586
912,0.6927046158,-0.5756597997\H,0,-7.3294978288,1.5393593674,-0.23717
60918\C,0,-5.3777344367,0.6968222694,-0.4353783473\H,0,-4.8996731671,1
.5610139431,0.0005773749\C,0,-4.6076693645,-0.374192011,-0.903528557\C
,0,-5.2705790302,-1.454135512,-1.493013769\C,0,-6.6496678117,-1.463927
7041,-1.6044890555\Br,0,-7.4770978189,-3.0148134636,-2.3137966462\C,0,
-9.5954303975,-0.0243623166,-0.1459093016\C,0,-9.3502574648,-0.6859898
844,1.0584142166\H,0,-8.5968631012,-1.4583879913,1.0986866326\C,0,-10.
0727486015,-0.3671791261,2.1981478308\H,0,-9.8793612189,-0.8832446832,
3.1255114757\C,0,-11.0591654856,0.6059012796,2.1272345407\Br,0,-12.063
7382126,1.0385428033,3.6854974037\C,0,-11.3253915794,1.2668571058,0.93
7104639\H,0,-12.0899883761,2.0266395239,0.893482236\C,0,-10.5864323764
,0.9569411799,-0.1955322694\H,0,-10.781149974,1.4806794675,-1.11884900
14\C,0,-9.4278943259,-0.4065171999,-2.5711832782\C,0,-10.6844184142,-0
.9957276133,-2.7348447447\H,0,-11.1961476409,-1.4157388426,-1.88262356
72\C,0,-11.2775789766,-1.0542876584,-3.9851106501\H,0,-12.247944433,-1
.5109297425,-4.1022262351\C,0,-10.6054672493,-0.5404571443,-5.08594803
97\Br,0,-11.4140898575,-0.6324634132,-6.8077958406\C,0,-9.3540958402,0
.0372748296,-4.9462680392\H,0,-8.8388519964,0.4401252932,-5.8042718382
\C,0,-8.7720270263,0.1113229944,-3.6882598704\H,0,-7.8051407636,0.5784
507395,-3.5796229933\N,0,1.0759113736,-0.3331237459,-0.4745893342\C,0,
-0.3358469967,-0.3403028164,-0.5352460082\C,0,-1.1432199092,0.27442034
45,0.4363720679\Br,0,-0.4081424777,1.0404879181,2.0006223485\C,0,-2.51

79370371,0.2526924825,0.309068202\C,0,-3.1396239753,-0.3752673907,-0.7
787281338\C,0,-2.3274774799,-1.0051004562,-1.7322906322\H,0,-2.7699626
192,-1.473722801,-2.5969237242\C,0,-0.9554745302,-0.9947599474,-1.6080
275785\H,0,-0.3394383571,-1.4544265671,-2.3652604082\C,0,1.7684467959,
0.8733926972,-0.3533957297\C,0,1.2383565561,2.0421410697,-0.9245832272
\H,0,0.320783285,2.0012612111,-1.4894076437\C,0,1.9151637932,3.2365053
719,-0.7978590604\H,0,1.5230274747,4.1329821191,-1.250176936\C,0,3.117
4503574,3.2736390067,-0.092693069\Br,0,4.0348684228,4.9094542103,0.084
8779008\C,0,3.6506897039,2.1228441165,0.4857408586\H,0,4.5710395133,2.
1716427941,1.044819834\C,0,2.9803091016,0.924761695,0.3571011279\H,0,3
.3641862472,0.0398125854,0.8384065765\C,0,1.7562023742,-1.5511315528,-
0.6117431757\C,0,2.9488304594,-1.6210964531,-1.3496538933\H,0,3.335162
8537,-0.7431035104,-1.8419758669\C,0,3.6020586195,-2.8295340488,-1.484
2618341\H,0,4.5078739551,-2.8938900342,-2.0651173904\C,0,3.0705477416,
-3.9680102782,-0.8820419943\Br,0,3.966375015,-5.6163185871,-1.06724759
06\C,0,1.8865482344,-3.9119445644,-0.1492475548\H,0,1.4952599452,-4.79
94051826,0.3211968333\C,0,1.2260521589,-2.7076580358,-0.0179377982\H,0
,0.3239711342,-2.6476483592,0.5698046754\H,0,-4.7185719178,-2.31900555
67,-1.8242250882\H,0,-3.1141772088,0.6937259525,1.0906927498\\Version=
EM64L-G09RevD.01\HF=-16923.512392\S2=0.798687\S2-1=0.\S2A=0.752307\RMS
D=5.149e-09\Dipole=8.925654,0.2991257,0.5107339\Quadrupole=7.7208343,8
.3421129,-16.0629471,-7.035331,-7.0268609,-3.4427337\PG=C01 [X(C36H22B
r6N2)]\\@

9 Cation Radical
1\1\GINC-HPC-CN120\Stability\UBLYP\6-31G(d)\C36H22Br6N2(1+,2)\TALIPOVM
\28-Feb-2015\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(
nbo) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc
=200) int(grid=ultrafine)\\Title\\1,2\N,0,-8.8007369443,-0.1709317355,
-1.2716000186\C,0,-7.4150979194,-0.2594969741,-1.1197197935\C,0,-6.709
9536061,0.66749093,-0.3400344956\H,0,-7.2339809696,1.4779580526,0.1402
713416\C,0,-5.3428091527,0.5605475582,-0.1962794029\H,0,-4.8240666424,
1.2969673766,0.3981419146\C,0,-4.5980565159,-0.4443711832,-0.829509501
2\C,0,-5.3217959818,-1.3575898138,-1.6038103233\Br,0,-4.4513329013,-2.
8256428578,-2.4528094511\C,0,-6.6945275731,-1.285962155,-1.7424847161\
H,0,-7.2087502523,-2.0350356636,-2.3204339196\C,0,-9.6101727067,0.3765
823661,-0.2400056738\C,0,-9.4585739074,-0.0458179831,1.0811377935\H,0,
-8.7193055751,-0.7937566939,1.325103586\C,0,-10.2545109735,0.485892135

9,2.0850606367\H,0,-10.1344569742,0.1555140911,3.1048810078\C,0,-11.21
83055005,1.4296066099,1.7604933613\Br,0,-12.3209168134,2.1526014141,3.
1328991693\C,0,-11.3921207147,1.8528582387,0.4508508249\H,0,-12.141701
8721,2.590036407,0.2095636327\C,0,-10.5813557397,1.3298837515,-0.54581
34614\H,0,-10.7034695685,1.6636344188,-1.5651551275\C,0,-9.4355404818,
-0.6434530663,-2.4519158365\C,0,-10.5484194917,-1.4792737004,-2.361883
1823\H,0,-10.9154525311,-1.78160982,-1.3927665788\C,0,-11.1877729378,-
1.9252959326,-3.5093729899\H,0,-12.0480028525,-2.571794915,-3.43479349
64\C,0,-10.7004247176,-1.5441397745,-4.750950152\Br,0,-11.5677183788,-
2.1622776303,-6.3280328613\C,0,-9.5915804536,-0.7174468103,-4.86101666
13\H,0,-9.2266916171,-0.418625865,-5.8311550643\C,0,-8.9673086503,-0.2
611000824,-3.7095866327\H,0,-8.1153183083,0.3972655527,-3.7886523459\N
,0,1.0814305827,-0.2911809185,-0.5256965984\C,0,-0.3133713908,-0.34308
05327,-0.5946981556\C,0,-1.0677879191,-0.4362308431,0.5837617212\H,0,-
0.5760030204,-0.5139534354,1.5388090458\C,0,-2.4441756591,-0.490718693
6,0.511963765\Br,0,-3.3807940104,-0.7017497007,2.1477781381\C,0,-3.126
7410599,-0.4512281703,-0.7171501625\C,0,-2.340685677,-0.3616445652,-1.
8797745022\H,0,-2.8370567116,-0.3026086596,-2.8350339507\C,0,-0.966989
8507,-0.3088810255,-1.8370295469\H,0,-0.3998698732,-0.1938116261,-2.74
65489524\C,0,1.714718336,0.3949216803,0.5283087913\C,0,1.1980164354,1.
6181470445,0.977776764\H,0,0.3341942051,2.0514574559,0.4990928125\C,0,
1.8241098252,2.2911279747,2.0089939186\H,0,1.4410941224,3.2401753677,2
.3476102172\C,0,2.9613729714,1.7417255676,2.5944601529\Br,0,3.81246228
29,2.6615145314,4.0056169113\C,0,3.4833555524,0.5271845429,2.157104747
2\H,0,4.3566149251,0.1075307159,2.6297019678\C,0,2.8641090197,-0.14522
90495,1.1216522932\H,0,3.2474539585,-1.0984148231,0.793780295\C,0,1.86
1022141,-0.9258439617,-1.5114705689\C,0,3.0224509329,-0.3033920737,-1.
9899682606\H,0,3.3052225169,0.6715273736,-1.6260012323\C,0,3.784173213
2,-0.924060486,-2.9605388034\H,0,4.6680336107,-0.4419805819,-3.3457579
918\C,0,3.3924228947,-2.1683856377,-3.4475822709\Br,0,4.4373495152,-3.
0144856896,-4.7720593285\C,0,2.245249614,-2.799808947,-2.9748484138\H,
0,1.9640086864,-3.7710059201,-3.348765905\C,0,1.4770123738,-2.17911117
28,-2.009016036\H,0,0.6028366817,-2.6744119873,-1.6172124438\\Version=
EM64L-G09RevD.01\HF=-16923.5139899\S2=0.799162\S2-1=0.\S2A=0.75237\RMS
D=6.384e-09\Dipole=7.7157403,0.8654373,0.2256081\Quadrupole=23.2815433
,-11.1828478,-12.0986955,-4.7077582,1.4058481,-0.822846\PG=C01 [X(C36H
22Br6N2)]\\@

MC, tris(2-bromo-4-(tert-butyl)phenyl)amine, Cation Radical
1\1\GINC-HPC-CN85\Stability\UBLYP\6-31G(d)\C30H36Br3N1(1+,2)\TALIPOVM\
27-Mar-2015\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(n
pa) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=
200) int(grid=ultrafine)\\Title\\1,2\N,0,0.0182808139,-0.3186067986,0.
0170389972\C,0,1.4175039247,-0.2363241242,0.0057776816\C,0,2.047509245
8,0.7711887332,0.7532928241\H,0,1.4390523306,1.4716288215,1.3040960433
\C,0,3.416878496,0.9017846536,0.7386652025\H,0,3.8618142715,1.70537097
18,1.3039817655\C,0,4.2285365899,0.0305609573,-0.006311921\C,0,5.74578
4311,0.2126808551,-0.0095591235\C,0,3.5956103238,-0.9936048203,-0.7182
938761\H,0,4.1752205322,-1.7153387594,-1.2668169746\C,0,2.2209760242,-
1.1367127231,-0.714173394\Br,0,1.4771979475,-2.6590193723,-1.546794159
4\C,0,-0.6813824349,-0.13184197,1.2194185494\C,0,-0.3854593646,-0.8608
400486,2.3866928318\Br,0,0.8474999656,-2.2912514113,2.3561052294\C,0,-
1.0880302982,-0.621075486,3.546518672\H,0,-0.8511066377,-1.2146605084,
4.4143468571\C,0,-2.1125121464,0.3377895396,3.6070822583\C,0,-2.851531
1503,0.564535536,4.9257863648\C,0,-2.4165904487,1.0344837238,2.4331524
429\H,0,-3.1930009016,1.7805406385,2.4258907792\C,0,-1.7235733948,0.80
11577502,1.2615891394\H,0,-1.9515021382,1.3711758419,0.3741091117\C,0,
-0.6858108835,-0.3721280644,-1.1950697611\C,0,-1.7714306233,-1.2450953
56,-1.4004515267\Br,0,-2.2200952333,-2.5597401792,-0.1209807678\C,0,-2
.4453005997,-1.2375824847,-2.6011370839\H,0,-3.2570586531,-1.934463784
2,-2.7312032218\C,0,-2.0771037739,-0.3813728293,-3.651895769\C,0,-2.86
75959474,-0.4148142453,-4.9595517435\C,0,-0.9779287649,0.4589701714,-3
.446716246\H,0,-0.6557859637,1.1354537827,-4.2200238953\C,0,-0.2907349
193,0.4603824236,-2.2490066552\H,0,0.5343132055,1.139498507,-2.0989065
413\C,0,-3.9258383503,1.6524341014,4.8075810977\C,0,-1.8384933868,0.99
39103905,6.0049477008\C,0,-3.5344302446,-0.7499038645,5.3531948669\H,0
,-4.2548424055,-1.0781318112,4.6038093404\H,0,-4.0673299898,-0.5971415
199,6.291837668\H,0,-2.8159789514,-1.553884482,5.5073554323\H,0,-3.500
5252657,2.6161750803,4.5269445184\H,0,-4.4161707542,1.7782567371,5.772
0394145\H,0,-4.6942926222,1.3888070778,4.0808291327\H,0,-1.3425534929,
1.9244890283,5.7284046265\H,0,-1.0718083739,0.2383059861,6.1710258178\
H,0,-2.3561913281,1.1542521576,6.9507610319\C,0,6.4594735296,-0.833893
6831,-0.8734266214\C,0,6.2691368847,0.094262372,1.4352884448\C,0,6.079
7220478,1.6117167686,-0.5645490849\H,0,6.0447648005,-0.8869404542,1.85
37518519\H,0,5.8359634163,0.8491394847,2.0901244521\H,0,7.351003371,0.
2279402285,1.4448317859\H,0,6.2913855463,-1.8473165245,-0.5086545019\H

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Tris(4-(tert-butyl)phenyl)amine Cation Radical

1\1\GINC-HPC-CN128\Stability\UBLYP\6-31G(d)\C30H39N1(1+,2)\TALIPOVM\05-Aug-2015\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(nbo) scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200) int(grid=ultrafine)\\Title\\1,2\N,0,0.01002419,0.0375290684,-0.027335456\C,0,1.4147002059,0.0526042626,-0.0212155493\C,0,2.1089733458,0.9001380449,0.8557292451\H,0,1.5644464613,1.5659661651,1.5065273199\C,0,3.4871408449,0.9087496748,0.8486687166\H,0,3.9949572589,1.5852056651,1.5187400593\C,0,4.2317170781,0.0807594394,-0.008438364\C,0,5.7598144831,0.1255171268,0.0281485523\C,0,3.5175618868,-0.7595341786,-0.8703334155\H,0,4.0403106951,-1.4254674647,-1.5363612007\C,0,2.1346057247,-0.7780038489,-0.8881998491\C,0,-0.6981312539,0.1472627879,1.1815529844\C,0,-0.2295411626,-0.4963531203,2.3369503821\C,0,-0.9361357765,-0.3834616337,3.5149870464\H,0,-0.5645419695,-0.9054801043,4.3832495334\C,0,-2.1177218348,0.3715686726,3.6040417045\C,0,-2.8595134197,0.4693020685,4.9376164559\C,0,-2.563009068,1.0079258325,2.4396844932\H,0,-3.454978254,1.6117110687,2.4574958674\C,0,-1.876235421,0.9003968847,1.2437930692\H,0,-2.2283899205,1.4241049128,0.3690070906\C,0,-0.6869286495,-0.0873729597,-1.240131396\C,0,-1.8566891076,-0.8600337857,-1.3071818933\C,0,-2.5279001603,-0.9798095114,-2.5047828137\H,0,-3.4125837634,-1.5970798062,-2.532224435\C,0,-2.0836653994,-0.3391585319,-3.6738928848\C,0,-2.8684063058,-0.5034251992,-4.9760016266\C,0,-0.9182976777,0.4307373448,-3

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)]\\@