Electronic Supplementary Information

A stable tetrazagallole and its radical anion dimer

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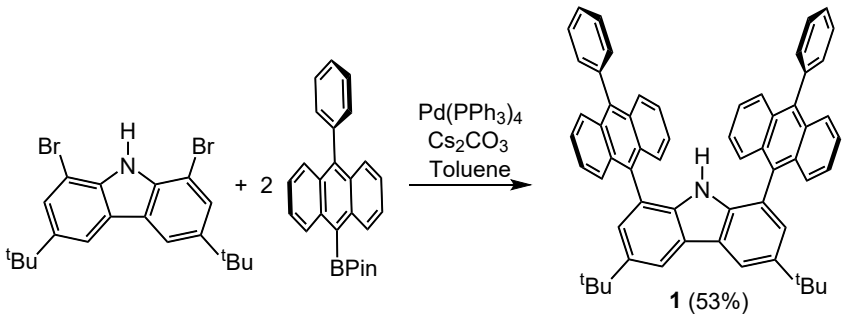
Content

Experimental section

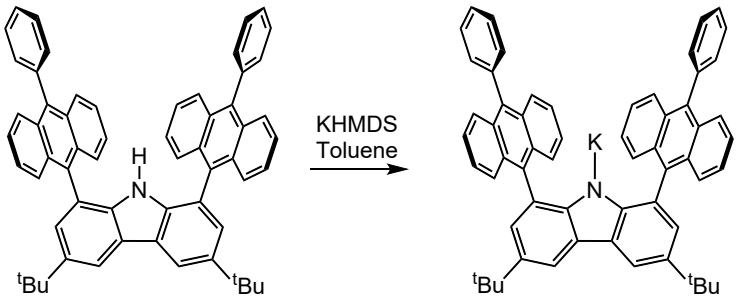
General considerations: All experiments were carried out under dry oxygen-free nitrogen using standard Schlenk techniques or in a N_2 filled-glove box. Solvents were dried by standard methods and stored in activated 4 Å molecule sieve in the glovebox. The NMR spectra were recorded on Bruker spectrometers (AV400) referenced to residual solvent signals as internal standards. The solutions of samples in the deuterated solvent were sealed off in a NMR tube under vacuum for measurements. UV/Vis spectra were recorded on the Lambda 750 spectrometer at room temperature. Element analyses were performed on an Elementar Vario EL III instrument. Cyclic voltammetry measurement was performed on a CHI660E electrochemical workstation with platinum as the working electrode and $Ag/AgNO_3$ (0.1 M in CH_3CN) as the reference electrode under a nitrogen atmosphere, THF was used as the solvent and *n*-Bu_4NPF_6 (10^{-1} M) was used as electrolyte. Magnetic measurements were performed using a Quantum Design SQUID VMS magnetometer. EPR spectra were obtained using JEOL JES-X320 X-band variable-temperature apparatus. For the single crystal X-ray structure analyses the crystals were each mounted on a glass capillary in perfluorinated oil and measured in a cold N_2 flow. The data for all compounds were collected on a Bruker D8 CMOS detector at 120 K. The structures were solved by direct methods and all refined on F^2 with the SHELX-2018/3 software package. The positions of the H atoms were calculated and considered isotropically according to a riding model. SQUEEZE was used to remove the highly disordered solvent molecules in the crystal structures of **1** (0.5 *n*-hexane), **4** (1 *n*-hexane and 1.5 toluene) and $\{[K(18\text{-c-}6)]^+[\mathbf{4}]^{\bullet-}\}_2$ (4.5 THF). Commercially available reagents were purchased from Energy Chemical and used as received. 1,8-dibromo-3,6-di-tert-butyl-carbazole,[1] GaI[2] and 1-azido-4-(tert-butyl)benzene[3] were synthesized according to the reported procedure.

Synthesis of the ligand LH (1)



To a dried 350 ml ACE tube containing 1,8-dibromo-3,6-di-tert-butyl-carbazole (4.37 g, 10.00 mmol), 4,4,5,5-tetramethyl-2-(10-phenylanthracen-9-yl)-1,3,2-dioxaborolane (8.37 g, 22.00 mmol), cesium carbonate Cs_2CO_3 (19.55 g, 60.00 mmol) and $Pd(PPh_3)_4$ (1.73 g, 1.50 mmol) were added dry toluene (120 mL) in a glovebox. The reaction mixture was heated to 100 °C under stirring for 48 h. The orange turbid mixture was cooled to room temperature and then poured into 800 mL of water. The mixture was transferred into a separation funnel, the organic phase was separated. The aqueous phase was extracted with 3 x 50 ml of dichloromethane. The combined organic phases were washed once with 50 ml of brine and dried over Na_2SO_4. After drying, all the volatiles were removed and the residue purified by column chromatography on silica gel eluting with dichloromethane. The obtained solid was washed with diethyl ether (50 mL) to afford analytically pure product. Crystals suitable for X-ray diffraction analysis were obtained from the CH_2Cl_2 solution layered with *n*-hexane at room temperature. The molecular structure of **1** is depicted in Fig. S1. Yield: 4.14 g, 5.28 mmol, 53%. ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K, ppm): δ 1.59 (s, 18H, C(C$\underline{H}_3$)$_3$), 7.06 (s, 1H, N$\underline{H}$), 7.18-7.25 (m, 8H, Ar-$\underline{H}$), 7.40-7.45 (m, 4H, Ar-$\underline{H}$), 7.55-7.66 (m, 16H, Ar-$\underline{H}$), 8.48 (d, 2H, Ar-$\underline{H}$); ^{13}C NMR ($CDCl_3$, 100 MHz, 298 K, ppm): δ 32.3 (C($\underline{C}$H$_3$)$_3$), 35.1 ($\underline{C}$(CH$_3$)$_3$), 116.0, 120.9, 123.6, 125.1, 125.5, 126.7, 127.1, 127.5, 127.6, 128.4, 128.5, 130.0, 130.1, 131.3, 131.4, 133.3, 137.6, 138.0, 139.0, 143.0. Elemental analysis for $C_{60}H_{49}N$ (%): Cacld: C 91.91, H 6.30, N 1.79; Found: C 91.64, H 6.24, N 1.65.

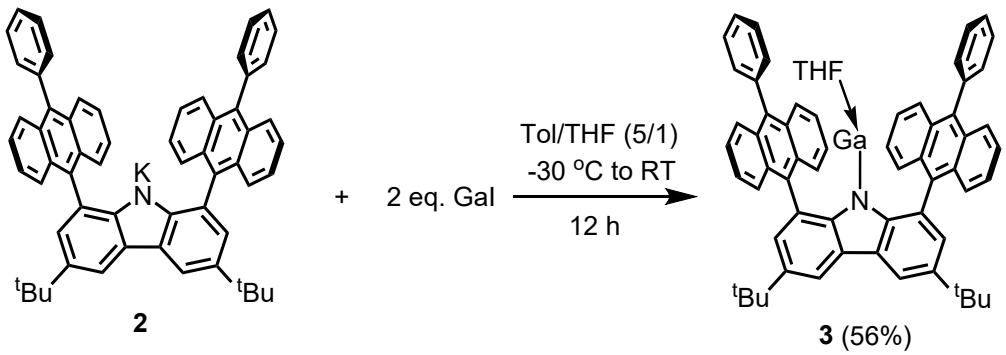
Synthesis of the potassium salt LK (2)



2 (92%)

In a N_2-filled glovebox, the ligand **1** (2.35 g, 3.00 mmol, 1 eq.) and KHMDS (658 mg, 3.30 mmol, 1.1 eq.) were dissolved in 30 mL of toluene at –30 °C. The reaction mixture was stirred vigorously at ambient temperature for 12 h, and a large amount of red solid was produced. The reaction mixture was placed in a –30 °C refrigerator for 1 h and then filtered. The dark red solid was washed with 10 mL of *n*-hexane and dried under vacuo for 1 h to give the potassium salt LK (**2**), which was directly used for subsequent reactions. Yield: 2.27 g, 2.76 mmol, 92%. Crystals of $LK(THF)_2$ suitable for single-crystal X-ray diffraction analysis were grown from THF/*n*-hexane solution at room temperature. The molecular structure is depicted in Fig. S2. ^{1}H NMR (THF-d_8, 400 MHz, 298 K, ppm): δ 1.45 (s, 18H, C($C\underline{H}_3$)$_3$), 7.07-7.14 (m, 12H, Ar-<u>*H*</u>), 7.36-7.38 (m, 2H, Ar-<u>*H*</u>), 7.43-7.46 (m, 8H, Ar-<u>*H*</u>), 7.51-7.56 (m, 2H, Ar-<u>*H*</u>), 7.84-7.87 (m, 4H, Ar-<u>*H*</u>), 7.33 (d, 2H, Ar-<u>*H*</u>). The ^{13}C NMR data was not obtained due to low solubility, see Figure S14 for details.

Synthesis of the Ga(I) compound LGa(THF) (3)

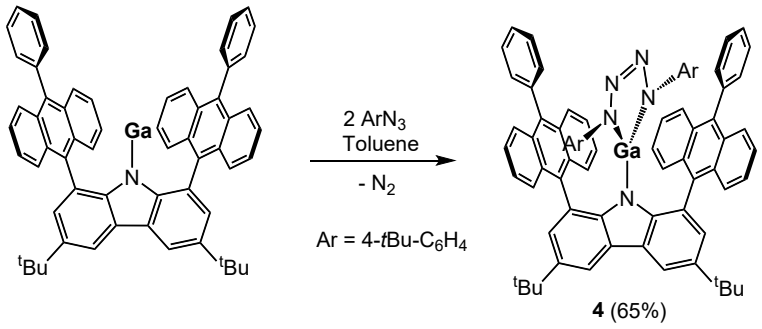


2 **3** (56%)

In a N_2-filled glovebox, **2** (1.64 g, 2.00 mmol, 1 eq.) and GaI (787 mg, 4.00 mmol, 2

eq.) were dissolved in 40 mL of cooled toluene (–30 °C). After the dark red reaction mixture was stirred for 1 h at room temperature, 8 mL of THF was added. The resulting reaction mixture was stirred vigorously at ambient temperature for another 12 h. The mixture was filtered and the obtained solid was washed with toluene (3 × 5 mL) to afford the product **3** containing KI, which can be used for further reaction directly. The pure product could be obtained by dissolving in THF, filtered and remove the volatiles under vacuo. The crystals suitable for X-ray diffraction analysis were grown from THF/n-hexane solution at –30 °C. Yield (without THF based on **2**): 0.95 g, 1.12 mmol, 56%. ^{1}H NMR (C_6D_6, 400 MHz, 298 K, ppm): δ 1.59 (s, 18H, C(C$\underline{H}_3$)$_3$), 6.85-7.02 (m, 12H, Ar-$\underline{H}$), 7.11-7.26 (m, 6H, Ar-$\underline{H}$), 7.58 (s, 2H, Ar-$\underline{H}$), 7.61 (s, 2H, Ar-$\underline{H}$), 7.67 (s, 2H, Ar-$\underline{H}$), 7.89 (s, 2H, Ar-$\underline{H}$), 7.92 (s, 2H, Ar-$\underline{H}$), 8.78 (s, 2H, Ar-$\underline{H}$). The ^{13}C NMR data was not obtained due to the low solubility of **3**, the recorded spectrum is shown in Fig. S16. Elemental analysis for $C_{60}H_{48}NGa$ (%): Cacld: C 84.51, H 5.67, N 1.64; Found: C 84.19, H 5.94, N 1.49.

Synthesis of the 6π aromatic tetrazagallole 4

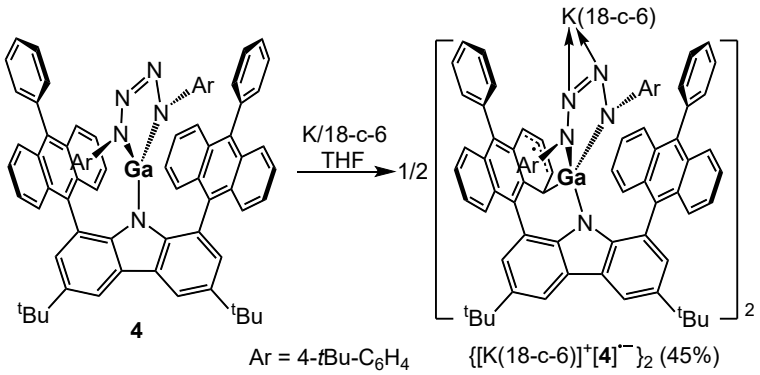


4 (65%)

In a N_2-filled glovebox, to a suspension of **3** (0.43 g, 0.50 mmol) in toluene (20 mL) was added 1-azido-4-(tert-butyl)benzene (0.175 g, 1.00 mmol) at –30 °C. The mixture turned clear gradually under stirring. After stirring for 12 h at room temperature, all the volatile was removed under vacuo, and the residue was washed with *n*-hexane (2 × 10 mL) to afford the product **4** as a yellow solid. Yield: 0.33 g, 0.28 mmol, 56%. Orange crystals suitable for X-ray diffraction analysis were obtained from toluene/*n*-hexane solution at room temperature. ^{1}H NMR (C_6D_6, 400 MHz, 298K, ppm): δ 1.16 (s, 18H, C(C$\underline{H}_3$)$_3$), 1.51 (s, 18H, C(C$\underline{H}_3$)$_3$), 6.24 (br, 3H, Ar-$\underline{H}$), 6.37 (br, 4H, Ar-$\underline{H}$),

6.47-6.51 (m, 4H, Ar-*H*), 6.55-6.60 (m, 4H, Ar-*H*), 7.07-7.19 (m, 7H, Ar-*H*), 7.37-7.43 (m, 6H, Ar-*H*), 7.69-7.71 (m, 6H, Ar-*H*), 8.07 (d, 2H, Ar-*H*), 8.85 (d, 2H, Ar-*H*). ^{13}C NMR (C_6D_6, 100 MHz, 298 K, ppm): δ 31.4 (C(*C*H$_3$)$_3$), 31.9 (C(*C*H$_3$)$_3$), 33.6 (*C*(CH$_3$)$_3$), 34.8 (*C*(CH$_3$)$_3$), 116.1, 116.5, 123.0, 124.1, 124.8, 125.2, 127.2, 127.3, 127.4, 127.8, 128.7, 130.1, 130.7, 131.3, 131.8, 138.5, 141.0, 142.1, 142.8, 144.1, 144.3. Elemental analysis for $C_{80}H_{74}GaN_5$ (%): Cacld: C 81.76, H 6.35, N 5.96; Found: C 81.44, H 6.37, N 5.84.

One-electron reduction of 4 to the radical anion salt



In a N_2-filled glovebox, **4** (0.12 g, 0.10 mmol) and elemental potassium (3.9 mg, 0.10 mmol) were placed in a 50 mL Schlenk flask, and THF (15 mL) was added at room temperature. The mixture was stirred and the yellow solution gradually became orange. After stirring for 12 h, the solution was filtered. The filtrate was concentrated to ca. 5 mL and 18-c-6 (26.1 mg, 0.10 mmol) was added. The mixture was left at room temperature and orange crystals of the radical anion salt $\{[K(18\text{-c-}6)]^+[\mathbf{4}]^{\bullet-}\}_2$ were formed after 24 h, which were suitable for single crystal X-ray diffraction analysis. Yield: 67 mg, 0.045 mmol, 45%. Elemental analysis for $C_{92}H_{98}GaKN_5O_6$ (%): Cacld: C 74.73, H 6.68, N 4.74; Found: C 74.35, H 6.37, N 4.84.

Table S1. Crystal data and refinement of 1-3

	1•CH_2Cl_2	**2**	**3**•C_4H_8O
formula	$C_{61}H_{51}Cl_2N$	$C_{68}H_{64}KNO_2$	$C_{68}H_{64}GaNO_2$
formula weight	868.92	966.30	996.92
crystal system	Monoclinic	Triclinic	Monoclinic
space group	*P*2(1)	*P*-1	*P*2(1)
a/Å	9.1578(9)	14.3228(12)	9.1948(7)
b/Å	21.5786(17)	14.5543(11)	21.6490(15)
c/Å	13.1159(12)	14.8790(11)	13.2822(9)
α/deg		66.692(2)	
β/deg	91.515(3)	66.937(2)	90.634(3)
γ/deg		74.731(2)	
V/Å^3	2591.0(4)	2599.2(4)	2643.8(3)
Z	2	2	2
ρ_{calcd}/g·cm^{-3}	1.114	1.235	1.252
μ/mm^{-1}	0.163	0.151	0.696
F(000)	916	1028	1052
crystal size/mm^3	0.38 x 0.26 x 0.15	0.24 x 0.20 x 0.18	0.10 x 0.06 x 0.04
θ range/deg	2.747–24.998	1.821–25.346	2.895–52.988
index ranges	-10 ≤ h ≤ 10	–17 ≤ *h* ≤ 17	–10 ≤ *h* ≤ 10
	–25 ≤ *k* ≤ 25	–18 ≤ *k* ≤ 17	–25 ≤ *k* ≤ 23
	–15 ≤ *l* ≤ 15	–17 ≤ *l* ≤ 17	–15 ≤ *l* ≤ 15
collected data	34677	60726	21678
unique data	9042 (R_{int} = 0.1055)	9502 (R_{int} = 0.0954)	8707 (R_{int} = 0.0804)
completeness to *θ*	99.7%	99.8%	99.9 %
data/restraints/parameters	9042 / 49 / 588	9502 / 0 / 655	8707 / 626 / 695
GOF on F^2	1.070	1.104	1.073
final *R* indices [*I*>2□(*I*)]	R_1 = 0.0546	R_1 = 0.0453	R_1 = 0.0986
	wR_2 = 0.1232	wR_2 = 0.1194	wR_2 = 0.2755
R indices (all data)	R_1 = 0.1010	R_1 = 0.0739	R_1 = 0.1220
	wR_2 = 0.1563	wR_2 = 0.1329	wR_2 = 0.2898
Largest diff peak/hole (e·Å^{-3})	0.236/–0.269	0.413/–0.420	0.980/–1.462

Table S2. Crystal data and refinement of 4 and $[K(18\text{-c-}6)]^+[4]^{\bullet-}$

	4	$[K(18\text{-c-}6)]^+[\mathbf{4}]^{\bullet-}$
formula	$C_{80}H_{74}GaN_5$	$C_{92}H_{98}GaKN_5O_6$
formula weight	1175.16	1478.57
crystal system	Monoclinic	Monoclinic
space group	*P*2(1)/*c*	*P*2(1)/*n*
a/Å	13.7438(9)	17.3847(5)
b/Å	46.807(3)	17.2277(5)
c/Å	22.5165(13)	33.7309(11)
α/deg		
β/deg	102.572(3)	94.097(2)
γ/deg		
V/Å^3	14137.7(15)	10076.5(5)
Z	8	4
ρ_{calcd}/g·cm^{-3}	1.104	0.975
μ/mm^{-1}	0.563	0.721
F(000)	4960	3132
crystal size/mm^3	0.12 x 0.08 x 0.04	0.16 x 0.12 x 0.10
θ range/deg	2.981–54.035	2.285–54.271
index ranges	-16 ≤ h ≤ 16	–20 ≤ *h* ≤ 20
	–52 ≤ *k* ≤ 56	–16 ≤ *k* ≤ 20
	–27 ≤ *l* ≤ 23	–40 ≤ *l* ≤ 40
collected data	179327	120448
unique data	25914 (R_{int} = 0.0717)	17796 (R_{int} = 0.1125)
completeness to *θ*	99.8%	99.9%
data/restraints/parameters	25914 / 154 / 1587	17796 / 252 / 974
GOF on F^2	1.034	1.039
final *R* indices [*I*>2□(*I*)]	R_1 = 0.0489	R_1 = 0.0782
	wR_2 = 0.1274	wR_2 = 0.1984
R indices (all data)	R_1 = 0.0774	R_1 = 0.1473
	wR_2 = 0.1421	wR_2 = 0.2441
Largest diff peak/hole (e·Å^{-3})	0.332/–0.501	1.335/–0.998

Selected crystal structures and NMR spectra

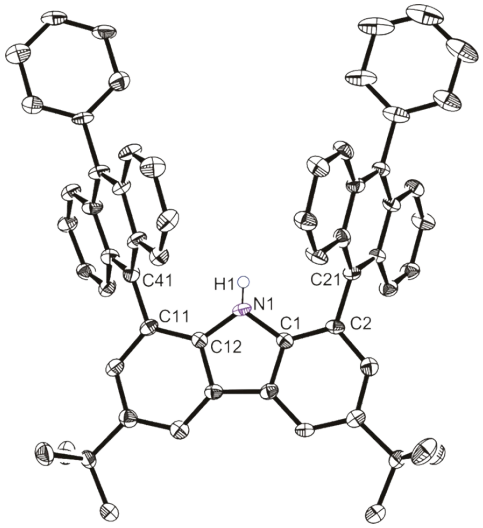


Fig. S1. Thermal ellipsoid drawing of the molecular structure of **1** at 50% probability. Hydrogen atoms (except H1) and solvent molecules were omitted for clarity. Selected bond lengths (Å): C1–N1 1.402(6), C1–C2 1.391(7), C2–C21 1.493(7), C11–C12 1.387(7), C11–C41 1.510(7), C12–N1 1.392(7).

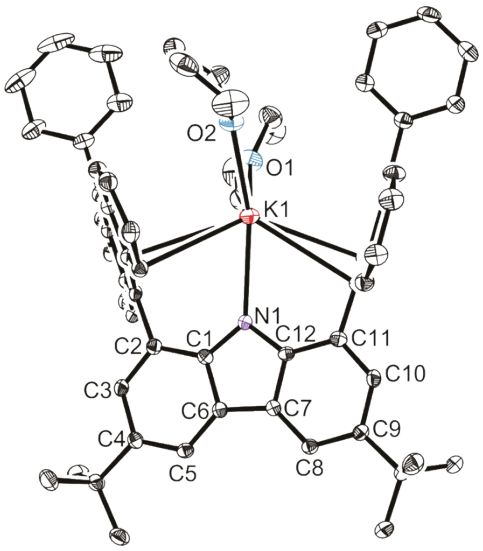


Fig. S2. Thermal ellipsoid drawing of the molecular structure of **2** at 50% probability. Hydrogen atoms were omitted for clarity. Selected bond lengths (Å) and angles (°): C1–N1 1.384(2), C1–C2 1.417(2), C1–C6 1.424(2), C11–C12 1.417(2), C12–N1 1.379(2), K1–O1 2.7111(14), K1–O2 2.7156(16), K1–N1 2.7638(15); O2-K1-O1 83.75(4), O2-K1-N1 114.85(5), O1-K1-N1 158.20(5).

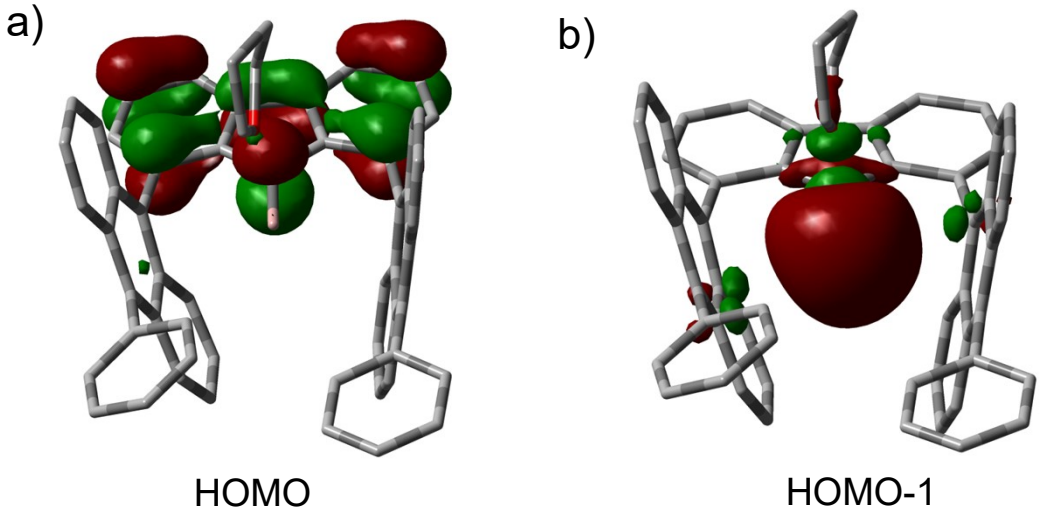


Fig. S3. Selected molecular orbitals of **3'**. Isovalue = 0.04.

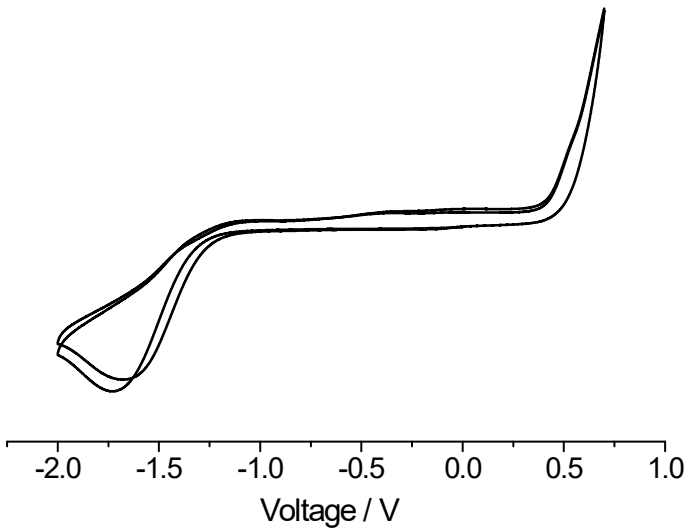


Fig. S4. Cyclic voltammogram of **4** measured in THF solution at room temperature, containing 0.1 M nBu$_4$PF$_6$, measured at 100 mV/s.

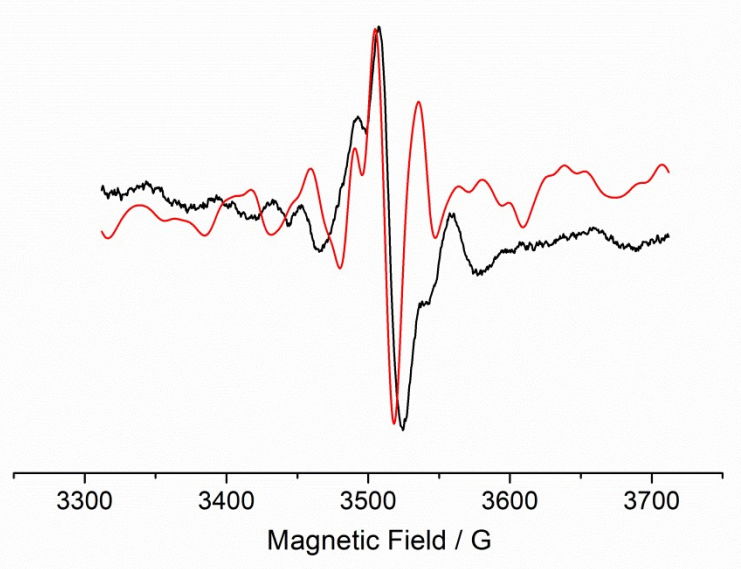


Fig. S5. Experimental (black line) and simulated (red line) EPR spectra of $\{[K(18\text{-}c\text{-}6)]^{+}[\mathbf{4}]^{\bullet-}\}_2$ measured in solid state at room temperature. The weak signal is most probably attributed to unidentified Ga-centered monoradical impurity according to simulation, since the coupling constants to the Ga nucleus are comparable to those of the Ga-based radical anion $[(t\mathrm{Bu}_2\mathrm{MeSi})_3\mathrm{Ga}]^{\bullet-}$.[4] Parameters for simulation: g = [2.001 2.001 2.008]; A(^{14}N)= [30 30 150] MHz; A(^{69}Ga) = [130 130 380] MHz; A(^{71}Ga) = [200 200 450] MHz.

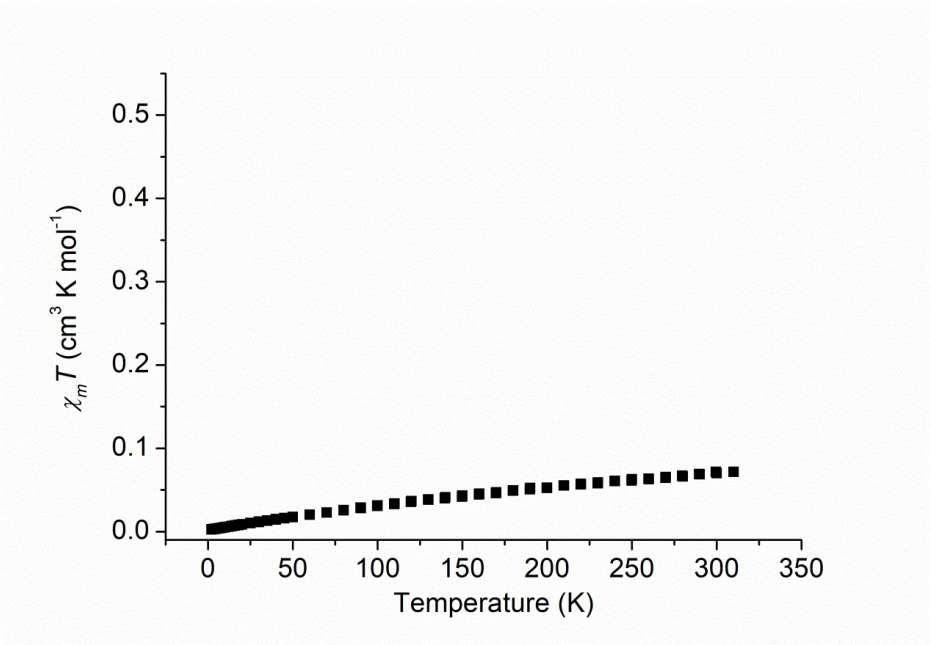


Fig. S6. The $\chi_m T$-T plots of $\{[K(18\text{-}c\text{-}6)]^{+}[\mathbf{4}]^{\bullet-}\}_2$ measured in solid state.

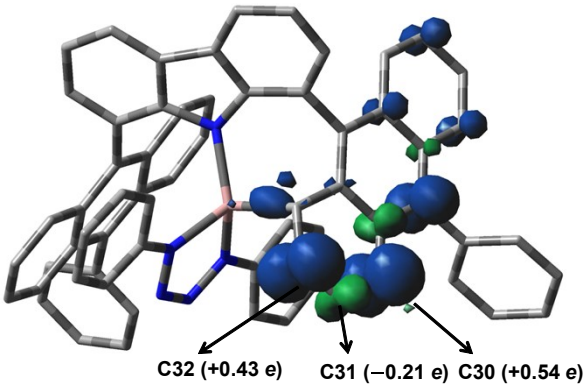


Fig. S7. Spin density map of [**4'**]$^{\bullet-}$. Isovalue = 0.04.

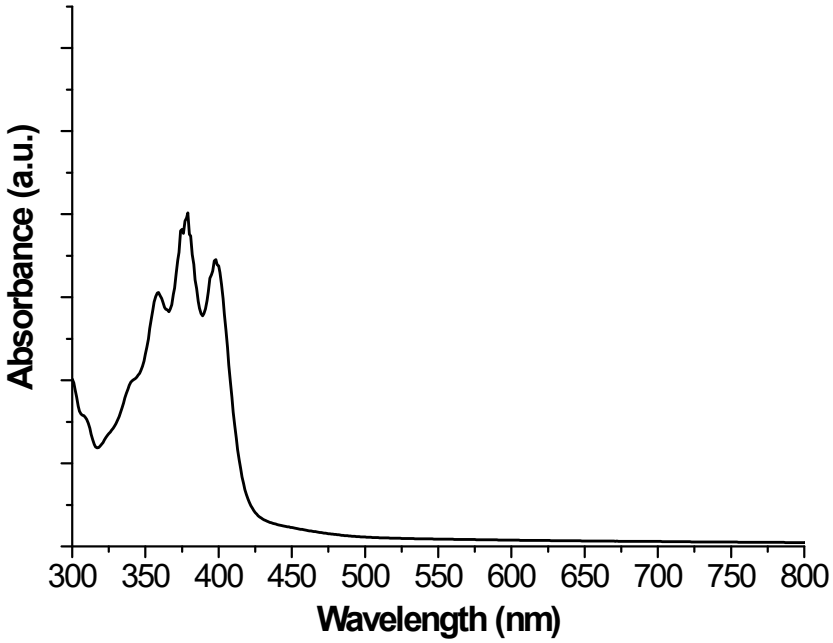


Fig. S8. UV-Vis spectrum of **3** in THF at room temperature.

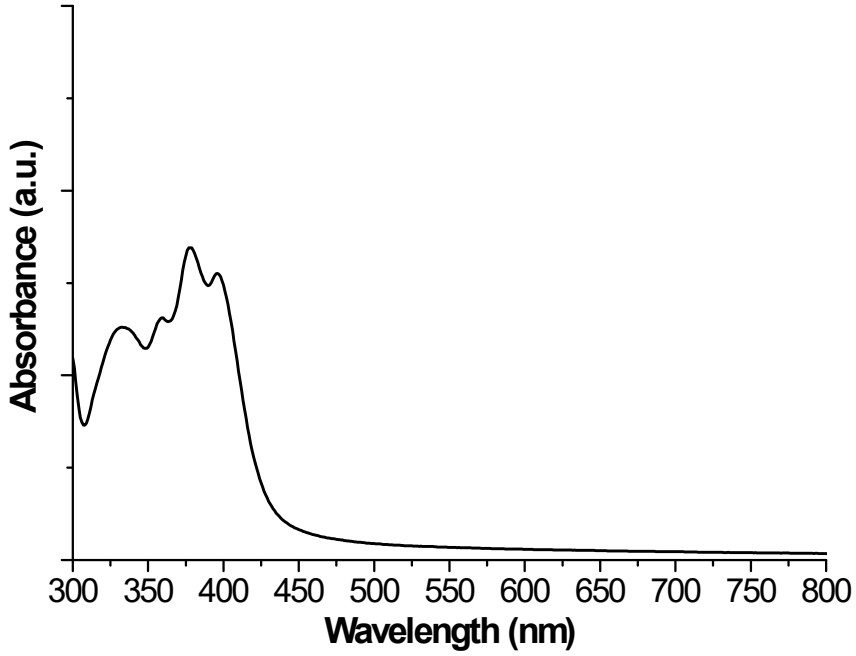


Fig. S9. UV-Vis spectrum of **4** in THF at room temperature.

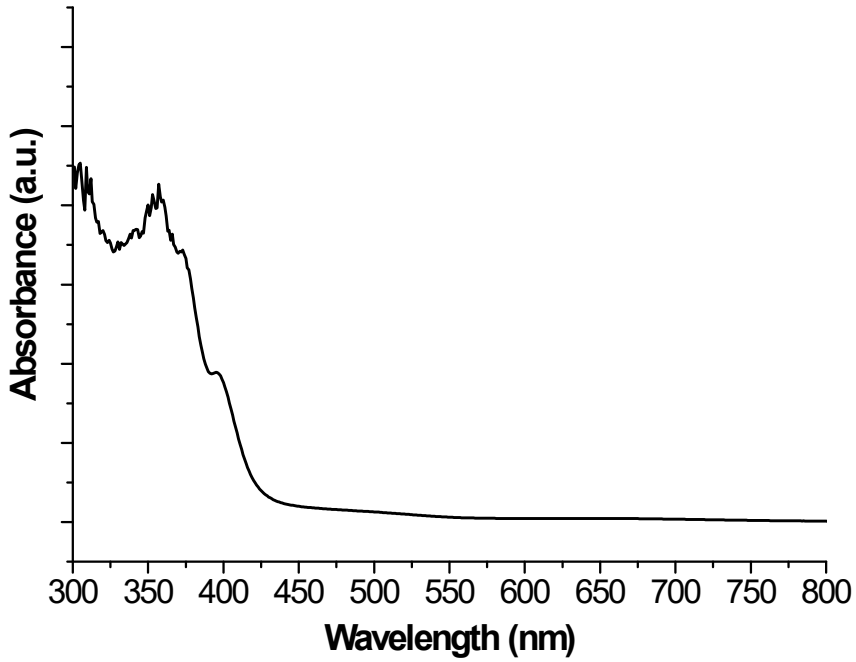


Fig. S10. UV-Vis spectrum of $\{[K(18\text{-}c\text{-}6)]^{+}[4]^{\bullet-}\}_2$ in THF at room temperature.

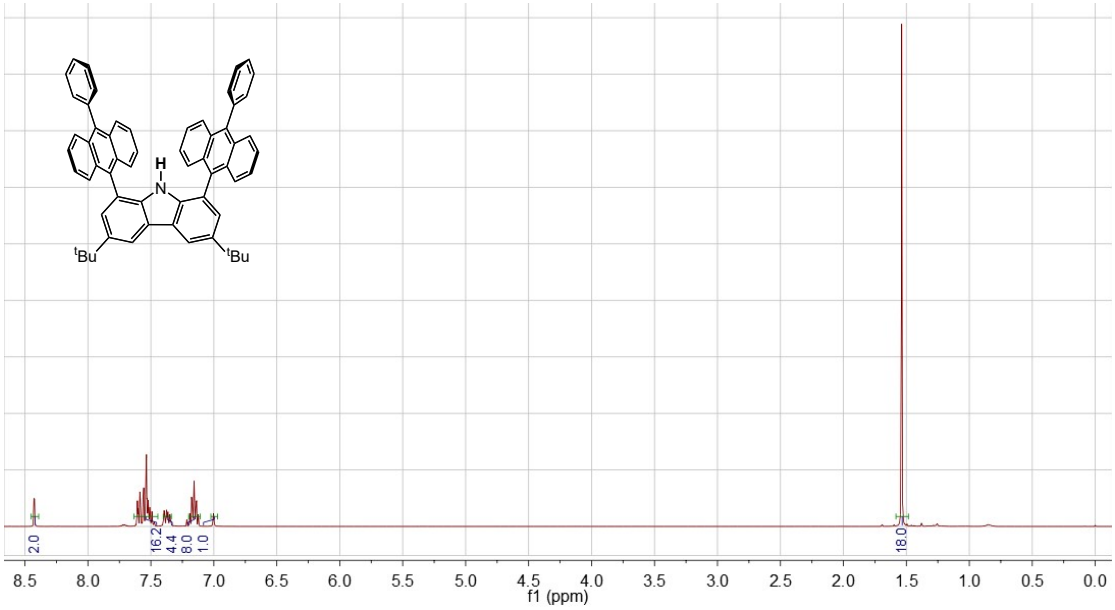


Fig. S11. ^{1}H NMR ($CDCl_3$) of **1**.

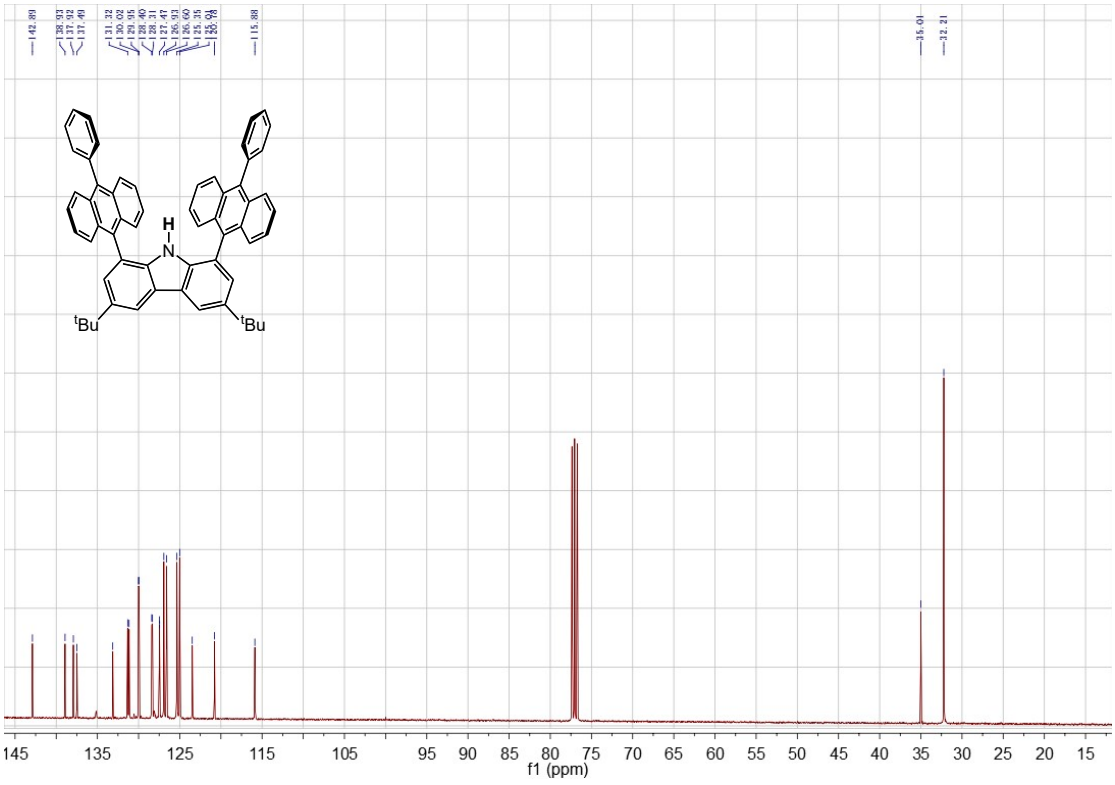


Fig. S12. ^{13}C NMR ($CDCl_3$) of **1**.

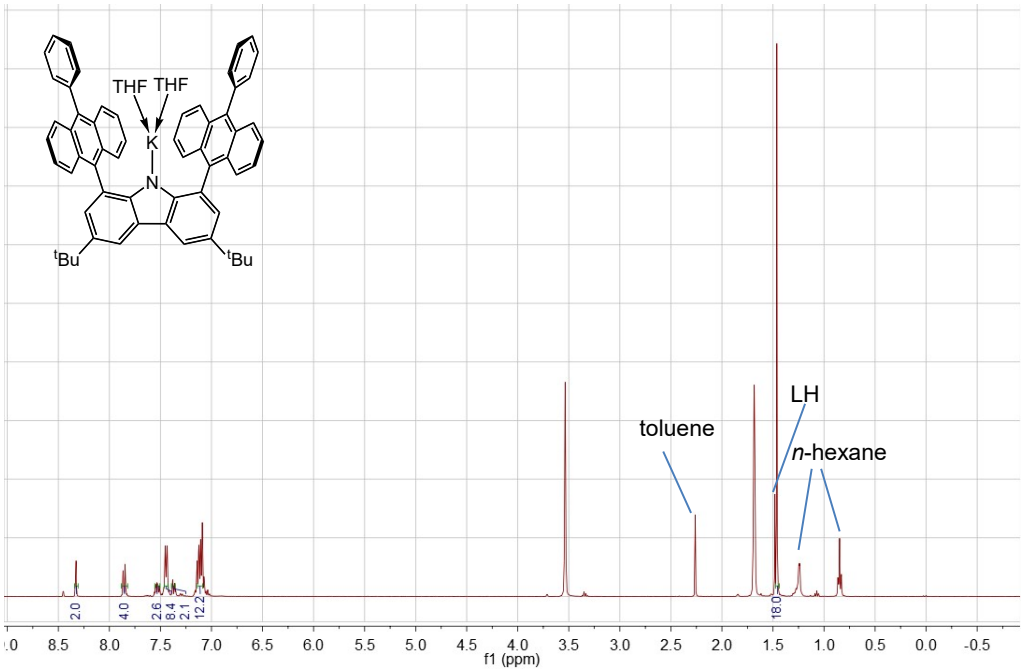


Fig. S13. ^{1}H NMR (THF-d_8) of **2**.

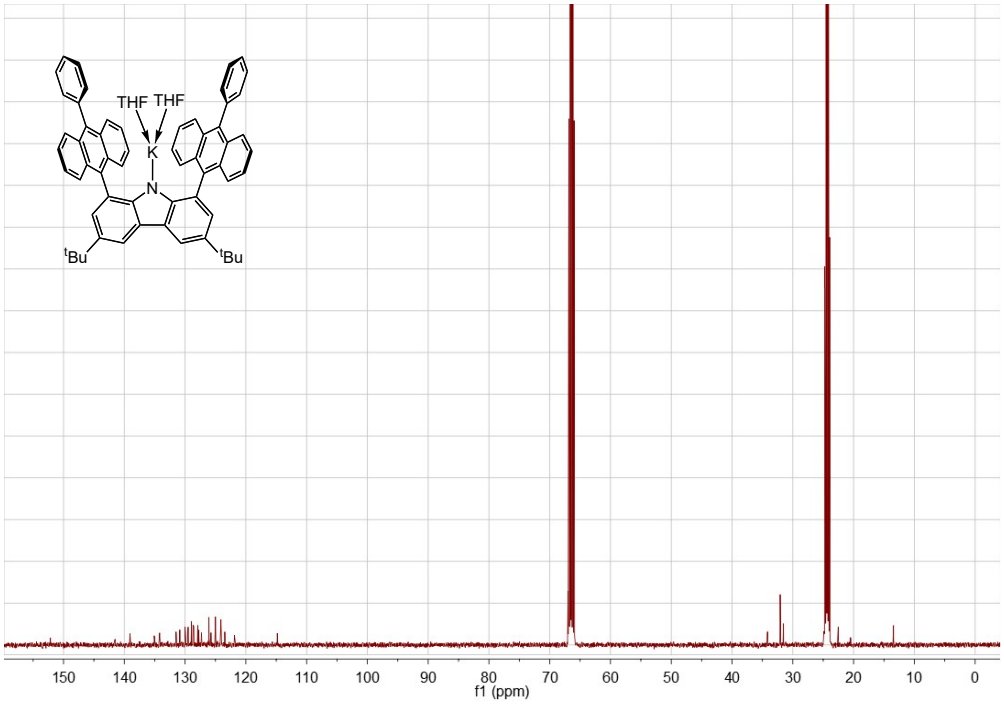


Fig. S14. ^{13}C NMR (THF-d_8) of **2**.

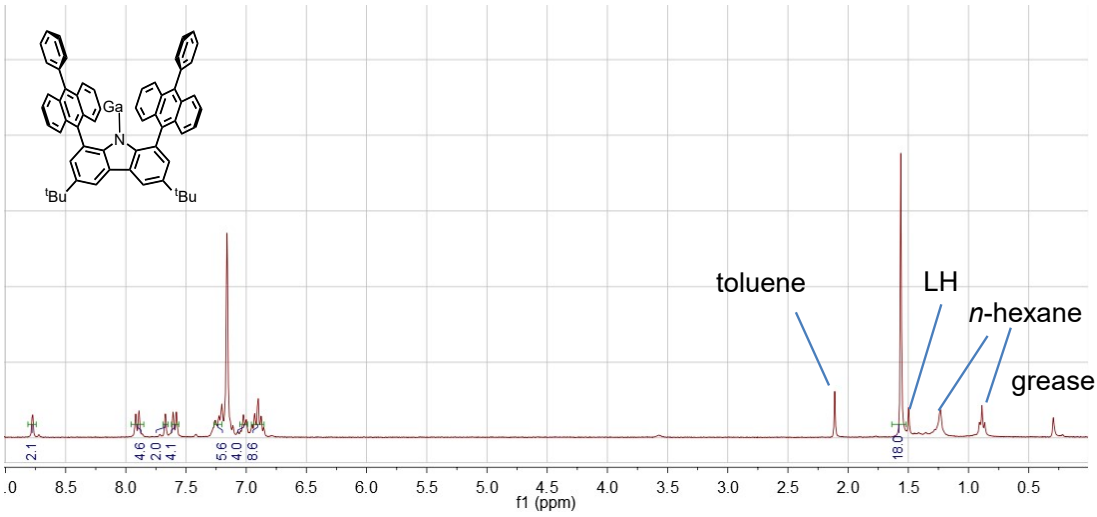


Fig. S15. ^{1}H NMR (C_6D_6) of **3**.

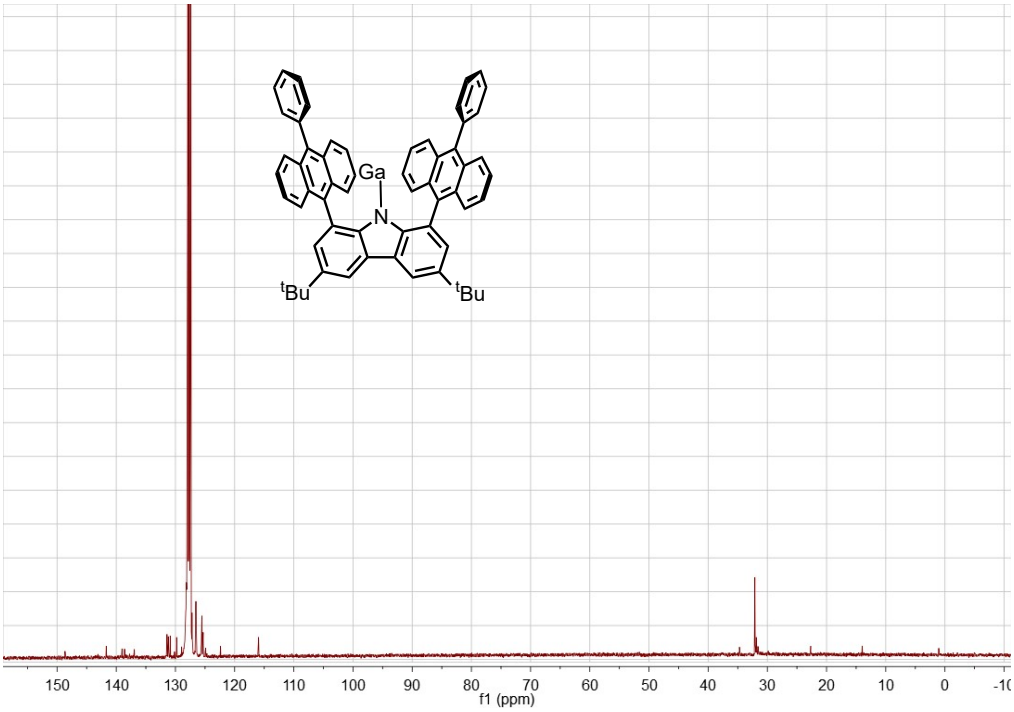


Fig. S16. ^{13}C NMR (C_6D_6) of **3**.

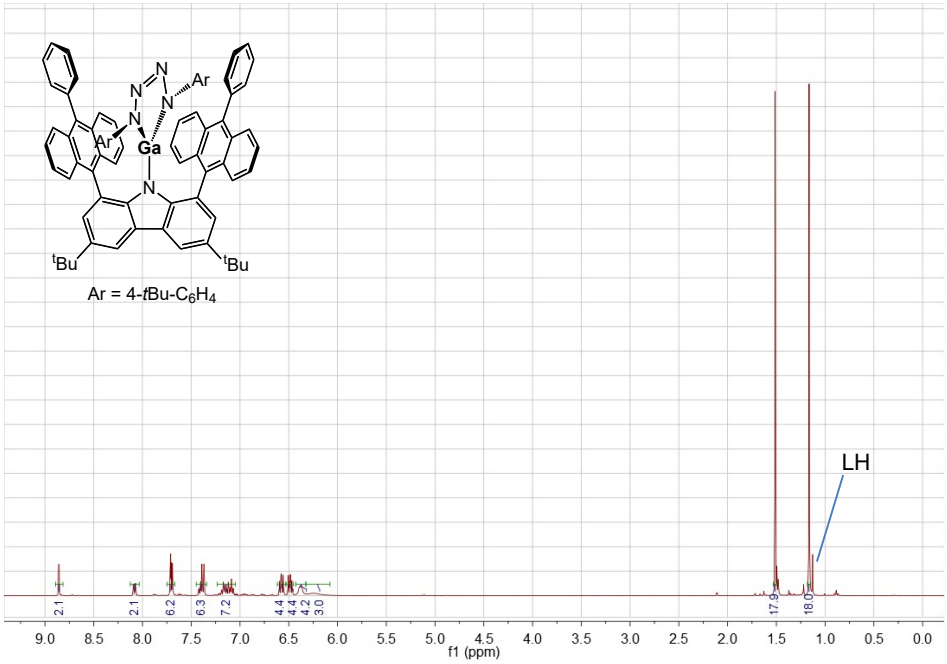


Fig. S17. ^{1}H NMR (C_6D_6) of **4**.

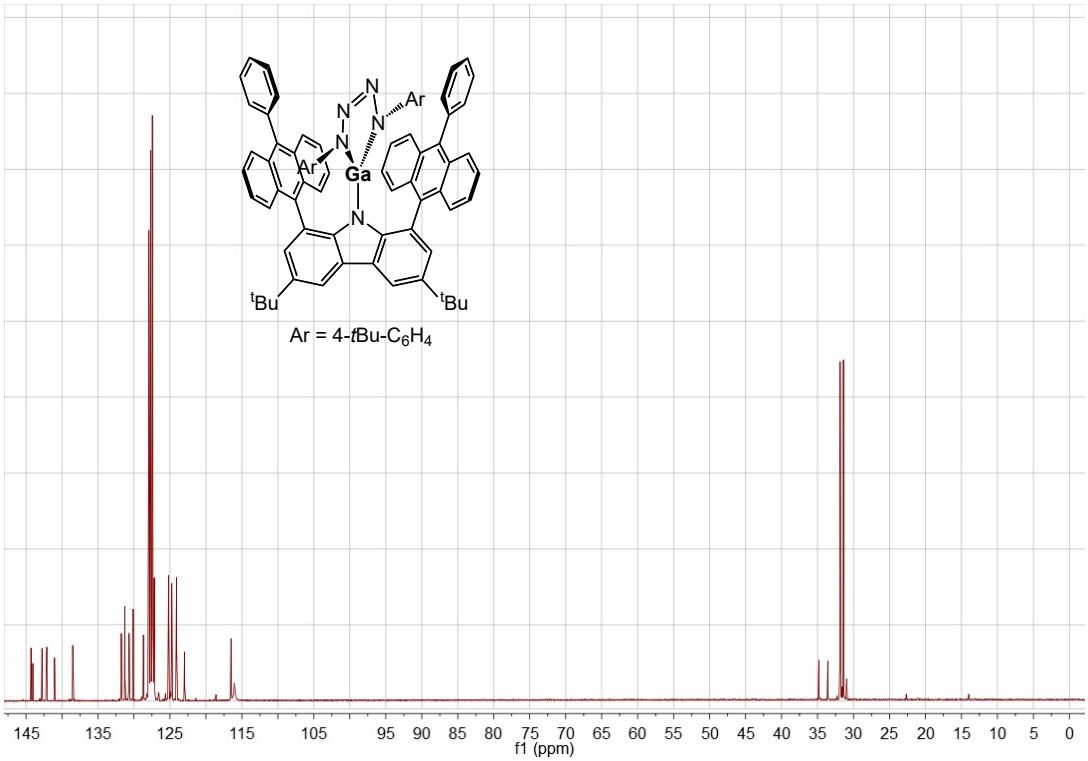


Fig. S18. ^{13}C NMR (C_6D_6) of **4**.

Theoretical calculations

All the calculations were performed with Gaussian 09 program suite.[5] All the geometry optimizations were performed with the WB97XD functional and 6-31G*basis set.[6,7] Frequency calculations were carried out to confirm that all optimized geometries correspond to energy minima. In addition, the natural bond orbital (NBO) analysis[8] was obtained at the same level.

Coordinates of the studied molecules

3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	31	0	-0.253106	0.121943	0.017994
2	7	0	-2.250215	0.222866	-0.481887
3	6	0	-5.031790	3.195622	0.257105
4	6	0	3.110053	2.719957	0.193029
5	6	0	0.939113	2.768313	1.450932
6	6	0	0.628305	-3.447167	0.000238
7	6	0	-5.417469	1.936340	-0.179917
8	1	0	-6.468489	1.706276	-0.334330
9	6	0	-1.675096	-3.869326	0.753669
10	1	0	-2.740766	-3.716727	0.624530
11	6	0	-4.435187	0.972643	-0.422846
12	6	0	-3.077892	-0.791293	-0.898819
13	6	0	1.977569	-1.255209	-2.733998

14	1	0	3.044265	-1.356638	-2.564722
15	6	0	-0.782357	-3.263076	-0.187354
16	6	0	-1.211688	2.844764	0.252832
17	6	0	-5.056341	-2.564567	-1.704412
18	6	0	-3.705335	-2.951449	-1.709288
19	1	0	-3.435643	-3.953410	-2.033439
20	6	0	3.904520	-3.624561	-1.090089
21	1	0	3.557819	-4.317222	-1.851940
22	6	0	0.918480	3.037803	-0.972660
23	6	0	1.626946	2.543231	2.687482
24	1	0	2.710482	2.504577	2.679115
25	6	0	-0.514668	3.007581	-0.963548
26	6	0	-4.438910	-0.395398	-0.888452
27	6	0	-0.498064	2.760000	1.463267
28	6	0	-3.072154	1.289134	-0.209746
29	6	0	-1.172588	2.581828	2.714275
30	1	0	-2.257733	2.585836	2.715974
31	6	0	1.629081	2.878304	0.231249
32	6	0	1.539476	-2.780904	-0.836438
33	6	0	-3.672991	3.513914	0.431434
34	1	0	-3.390491	4.518144	0.736597
35	6	0	-1.254406	-2.451881	-1.237927
36	6	0	-2.676357	2.577150	0.197587
37	6	0	-5.429422	-1.293391	-1.292367
38	1	0	-6.476214	-1.000729	-1.289120
39	6	0	2.987339	-2.768879	-0.477663
40	6	0	1.511799	-0.395705	-3.681752
41	1	0	2.208132	0.194224	-4.269788
42	6	0	-0.475972	2.413184	3.872402
43	1	0	-1.005039	2.297154	4.814079

44	6	0	-1.210975	-4.638051	1.778769
45	1	0	-1.909540	-5.096700	2.472739
46	6	0	-2.697700	-2.085555	-1.303928
47	6	0	1.588056	3.151790	-2.232819
48	1	0	2.671239	3.191873	-2.245738
49	6	0	0.947489	2.384644	3.857861
50	1	0	1.490517	2.225342	4.784824
51	6	0	-0.778149	-0.976389	-3.169302
52	1	0	-1.843605	-0.874557	-3.341987
53	6	0	1.077153	-2.009109	-1.913813
54	6	0	0.888562	3.227572	-3.398910
55	1	0	1.416667	3.320644	-4.343513
56	6	0	-0.335905	-1.856061	-2.127562
57	6	0	0.113104	-0.262339	-3.910240
58	1	0	-0.241469	0.421278	-4.674746
59	6	0	-0.532323	3.178042	-3.389690
60	1	0	-1.078409	3.231081	-4.327012
61	6	0	5.346301	3.547162	0.612972
62	1	0	6.000983	4.332451	0.979603
63	6	0	0.186404	-4.850375	1.943458
64	1	0	0.543819	-5.476036	2.755993
65	6	0	5.690412	-2.701765	0.244113
66	1	0	6.739472	-2.675575	0.524120
67	6	0	4.780946	-1.844645	0.859732
68	1	0	5.118518	-1.138198	1.612246
69	6	0	3.965653	3.719481	0.661507
70	1	0	3.542762	4.635119	1.066022
71	6	0	1.073435	-4.269849	1.086981
72	1	0	2.138995	-4.425930	1.216650
73	6	0	3.436730	-1.876847	0.502625

74	1	0	2.729366	-1.194821	0.970445
75	6	0	5.249858	-3.591226	-0.732086
76	1	0	5.953885	-4.261834	-1.216038
77	6	0	-1.209807	3.071488	-2.213524
78	1	0	-2.293198	3.035448	-2.204951
79	6	0	5.885507	2.374339	0.091200
80	1	0	6.962703	2.240898	0.051453
81	6	0	3.659562	1.546061	-0.332844
82	1	0	2.993823	0.773358	-0.709471
83	6	0	5.038987	1.375027	-0.383141
84	1	0	5.449047	0.454087	-0.787226
85	8	0	-1.075341	-0.724081	1.925373
86	6	0	-0.084245	-1.183138	2.860914
87	1	0	0.567764	-0.334791	3.094061
88	1	0	0.508764	-1.962866	2.376588
89	6	0	-2.395991	-0.822569	2.474872
90	1	0	-2.877932	-1.719950	2.071274
91	1	0	-2.958635	0.055901	2.153954
92	6	0	-2.180527	-0.911804	3.979203
93	1	0	-3.010519	-1.406753	4.490007
94	1	0	-2.060695	0.091711	4.398745
95	6	0	-0.864171	-1.690870	4.071733
96	1	0	-1.050566	-2.764811	3.971367
97	1	0	-0.328248	-1.520059	5.008892
98	1	0	-5.783225	3.955334	0.449366
99	1	0	-5.812252	-3.272638	-2.030023

4

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	31	0	0.769452	-0.001208	-0.011758
2	7	0	2.393535	-0.004245	-0.873636
3	7	0	0.417568	0.000181	1.805814
4	7	0	-0.919128	0.002233	2.039105
5	7	0	-1.665395	0.002933	1.024157
6	7	0	-1.050005	0.001471	-0.201064
7	6	0	3.161006	-1.120968	-1.165266
8	6	0	2.770502	-2.457310	-1.053524
9	6	0	3.716665	-3.415713	-1.398789
10	1	0	3.447005	-4.465592	-1.328712
11	6	0	4.997591	-3.052415	-1.842953
12	6	0	5.362870	-1.718483	-1.965410
13	1	0	6.352921	-1.447499	-2.320586
14	6	0	4.433515	-0.733336	-1.626495
15	6	0	4.435895	0.717682	-1.626957
16	6	0	5.368463	1.699566	-1.966509
17	1	0	6.357617	1.425119	-2.321524
18	6	0	5.007547	3.034766	-1.844900
19	6	0	3.727821	3.402534	-1.400959
20	1	0	3.461585	4.453332	-1.331567
21	6	0	2.778543	2.447445	-1.055055
22	6	0	3.164673	1.109767	-1.165956
23	6	0	1.373865	-2.766567	-0.629009
24	6	0	1.070206	-2.988023	0.729539
25	6	0	2.088812	-2.990861	1.733439
26	1	0	3.115094	-2.810836	1.431741
27	6	0	1.782232	-3.197109	3.043464

28	1	0	2.565546	-3.166724	3.794180
29	6	0	0.434125	-3.397474	3.443731
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31	6	0	-0.564166	-3.421519	2.517421
32	1	0	-1.590196	-3.585337	2.825587
33	6	0	-0.286175	-3.247172	1.124449
34	6	0	-1.291609	-3.355623	0.147352
35	6	0	-0.976765	-3.207194	-1.216815
36	6	0	-1.967066	-3.357069	-2.239429
37	1	0	-2.992941	-3.546447	-1.946048
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39	1	0	-2.405701	-3.374749	-4.317225
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42	6	0	0.660107	-2.761611	-3.002852
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46	6	0	-3.177521	-4.989607	0.347336
47	1	0	-2.532148	-5.737291	-0.105687
48	6	0	-4.478020	-5.318507	0.716259
49	1	0	-4.846134	-6.327249	0.553302
50	6	0	-5.302879	-4.357245	1.294565
51	1	0	-6.318365	-4.612843	1.582787
52	6	0	-4.818774	-3.069017	1.503875
53	1	0	-5.455733	-2.314819	1.957162
54	6	0	-3.518187	-2.737862	1.135423
55	1	0	-3.131937	-1.736799	1.301342
56	6	0	1.382896	2.761527	-0.630811
57	6	0	1.079971	2.985424	0.727500

58	6	0	2.098617	2.986199	1.731362
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61	1	0	2.576006	3.163021	3.791868
62	6	0	0.445314	3.400151	3.441222
63	1	0	0.214599	3.530789	4.493625
64	6	0	-0.552948	3.426191	2.514933
65	1	0	-1.578434	3.593659	2.822946
66	6	0	-0.275577	3.249268	1.122162
67	6	0	-1.280705	3.359756	0.144971
68	6	0	-0.966351	3.208926	-1.219046
69	6	0	-1.956194	3.360830	-2.241806
70	1	0	-2.981480	3.553658	-1.948617
71	6	0	-1.628885	3.259128	-3.559974
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73	6	0	-0.294358	2.961092	-3.946358
74	1	0	-0.047019	2.877581	-5.000674
75	6	0	0.669093	2.756394	-3.004645
76	1	0	1.684884	2.517260	-3.301057
77	6	0	0.374642	2.886378	-1.610131
78	6	0	-2.675434	3.705405	0.548233
79	6	0	-3.509036	2.749750	1.133750
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81	6	0	-4.808618	3.085136	1.501925
82	1	0	-5.447790	2.333301	1.956019
83	6	0	-5.288903	4.374578	1.291300
84	1	0	-6.303608	4.633499	1.579309
85	6	0	-4.461226	5.332779	0.711939
86	1	0	-4.826361	6.342435	0.547947
87	6	0	-3.161728	4.999646	0.343294

88	1	0	-2.514166	5.744938	-0.110544
89	6	0	1.250700	-0.000482	2.929177
90	6	0	0.749410	0.000928	4.230427
91	1	0	-0.322399	0.002547	4.382623
92	6	0	1.627445	0.000269	5.308646
93	1	0	1.224680	0.001389	6.317834
94	6	0	3.005697	-0.001771	5.110630
95	6	0	3.501244	-0.003166	3.807807
96	1	0	4.573189	-0.004764	3.631521
97	6	0	2.633975	-0.002535	2.726526
98	1	0	3.037598	-0.003636	1.717347
99	6	0	-1.881019	0.002333	-1.327005
100	6	0	-1.279129	0.000569	-2.584536
101	1	0	-0.196327	-0.001441	-2.679617
102	6	0	-2.056339	0.001353	-3.731329
103	1	0	-1.567193	-0.000048	-4.701045
104	6	0	-3.444901	0.003910	-3.647718
105	6	0	-4.044643	0.005690	-2.391894
106	1	0	-5.127330	0.007719	-2.304505
107	6	0	-3.275603	0.004920	-1.234506
108	1	0	-3.748409	0.006387	-0.261344
109	1	0	5.720461	3.810896	-2.104924
110	1	0	5.707970	-3.831036	-2.102471
111	1	0	3.683790	-0.002271	5.958480
112	1	0	-4.052482	0.004514	-4.547494

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[4]$^{\bullet-}$

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	

					Z
1	31	0	-0.241534	-1.000515	-0.747284
2	7	0	-0.340412	-2.145477	0.813507
3	7	0	-1.741877	-0.571509	-1.819170
4	7	0	-1.846857	0.768691	-2.069739
5	7	0	-1.013463	1.504541	-1.480907
6	7	0	-0.098469	0.883401	-0.669445
7	6	0	0.507801	-3.248123	0.893239
8	6	0	1.866728	-3.344183	0.529926
9	6	0	2.472133	-4.590564	0.689277
10	1	0	3.519994	-4.683172	0.415668
11	6	0	1.795951	-5.703740	1.202658
12	6	0	0.471433	-5.592023	1.595076
13	1	0	-0.059729	-6.440528	2.019282
14	6	0	-0.170032	-4.365133	1.435028
15	6	0	-1.492694	-3.901818	1.777162
16	6	0	-2.582331	-4.517421	2.390717
17	1	0	-2.535252	-5.565816	2.674598
18	6	0	-3.714892	-3.760628	2.646512
19	6	0	-3.740439	-2.400563	2.316389
20	1	0	-4.616366	-1.806719	2.563516
21	6	0	-2.669334	-1.758353	1.696703
22	6	0	-1.542776	-2.542007	1.392833
23	6	0	2.672857	-2.187001	0.051224
24	6	0	3.757696	-1.698407	0.851404
25	6	0	4.039617	-2.217562	2.140305
26	1	0	3.426107	-3.025898	2.522655
27	6	0	5.049337	-1.702507	2.918359
28	1	0	5.235579	-2.115865	3.906029

29	6	0	5.827128	-0.628588	2.443676
30	1	0	6.618517	-0.213025	3.061996
31	6	0	5.571067	-0.091875	1.205895
32	1	0	6.151141	0.755330	0.855965
33	6	0	4.537931	-0.602822	0.374125
34	6	0	4.229317	-0.012816	-0.885051
35	6	0	3.149773	-0.475266	-1.645778
36	6	0	2.805269	0.095943	-2.908365
37	1	0	3.410674	0.908769	-3.291763
38	6	0	1.734050	-0.386580	-3.676863
39	1	0	1.529168	0.067876	-4.642110
40	6	0	0.955500	-1.418993	-3.226488
41	1	0	0.118834	-1.784456	-3.815228
42	6	0	1.144200	-1.978558	-1.893678
43	1	0	0.895896	-3.039916	-1.808289
44	6	0	2.355996	-1.575669	-1.146815
45	6	0	5.011531	1.163856	-1.355996
46	6	0	6.332056	1.033673	-1.795129
47	1	0	6.791170	0.048498	-1.799846
48	6	0	7.055445	2.146575	-2.215786
49	1	0	8.081377	2.027661	-2.554780
50	6	0	6.464601	3.407357	-2.204192
51	1	0	7.028172	4.277432	-2.530997
52	6	0	5.147243	3.546014	-1.772929
53	1	0	4.675397	4.524681	-1.756953
54	6	0	4.425468	2.433894	-1.353029
55	1	0	3.397264	2.539702	-1.021618
56	6	0	-2.714499	-0.288473	1.467544
57	6	0	-1.859209	0.555417	2.200885
58	6	0	-0.932553	0.040064	3.165748

59	1	0	-0.893701	-1.029796	3.332379
60	6	0	-0.115697	0.867606	3.873471
61	1	0	0.581334	0.451885	4.595589
62	6	0	-0.140152	2.270285	3.645762
63	1	0	0.556700	2.914467	4.172999
64	6	0	-1.001982	2.801806	2.736852
65	1	0	-0.989652	3.867171	2.539382
66	6	0	-1.916907	1.975690	2.005967
67	6	0	-2.853015	2.520504	1.111000
68	6	0	-3.749938	1.682407	0.426169
69	6	0	-4.760790	2.208191	-0.441278
70	1	0	-4.841050	3.283539	-0.554760
71	6	0	-5.612159	1.387169	-1.116688
72	1	0	-6.369250	1.810091	-1.771617
73	6	0	-5.502565	-0.023152	-0.984730
74	1	0	-6.146110	-0.674490	-1.568101
75	6	0	-4.564998	-0.563035	-0.158674
76	1	0	-4.459574	-1.639536	-0.093612
77	6	0	-3.670718	0.262029	0.595334
78	6	0	-2.875461	3.987368	0.847561
79	6	0	-3.313241	4.897266	1.812978
80	1	0	-3.643713	4.524599	2.778857
81	6	0	-3.321598	6.264182	1.548452
82	1	0	-3.663808	6.959553	2.310416
83	6	0	-2.894200	6.737674	0.311101
84	1	0	-2.898348	7.804534	0.103909
85	6	0	-2.462137	5.836705	-0.659749
86	1	0	-2.126534	6.198120	-1.628009
87	6	0	-2.453808	4.470969	-0.395819
88	1	0	-2.116858	3.754128	-1.140688

89	6	0	-2.579043	-1.413768	-2.519931
90	6	0	-3.495704	-0.966207	-3.485004
91	1	0	-3.554825	0.095932	-3.688929
92	6	0	-4.323565	-1.871301	-4.134182
93	1	0	-5.030324	-1.501132	-4.873752
94	6	0	-4.267911	-3.235485	-3.850104
95	6	0	-3.355031	-3.682037	-2.897215
96	1	0	-3.294595	-4.740067	-2.655042
97	6	0	-2.512102	-2.791664	-2.246996
98	1	0	-1.829915	-3.160555	-1.483656
99	6	0	0.771207	1.720092	0.016555
100	6	0	0.804663	3.111765	-0.165663
101	1	0	0.140188	3.563587	-0.889502
102	6	0	1.676996	3.898755	0.578204
103	1	0	1.674260	4.975146	0.422061
104	6	0	2.546845	3.328876	1.504231
105	6	0	2.524240	1.946372	1.677703
106	1	0	3.199034	1.469918	2.383776
107	6	0	1.646261	1.154342	0.954605
108	1	0	1.624998	0.084791	1.141402
109	1	0	-4.577345	-4.210570	3.129854
110	1	0	2.321023	-6.649095	1.306325
111	1	0	3.236659	3.947578	2.070991
112	1	0	-4.924585	-3.935066	-4.359316

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