Electronic Supplementary Material (ESI) for Chemical Communications

Supporting information for:

A C_{3v}-symmetrical tribenzotriquinacene-based threefold *N*-heterocyclic carbene. Coordination to rhodium(I) and stereoelectronic properties

Candela Segarra, Jens Linke, Elena Mas-Marzá, Dietmar Kuck and Eduardo Peris

General methods. All operations were carried out by using standard Schlenk techniques under nitrogen atmosphere unless otherwise stated. Solvents were purified on MBraun SPS or purchased from Aldrich and degassed prior to use by purging with nitrogen and kept over molecular sieves. All other reagents were used as received from commercial suppliers. Column chromatrography was performed using the solvent systems indicated on silica gel (63-200 μm). NMR spectra were recorded on a Varian Mercury 300 and a Varian NMR System 500 MHz spectrometers, and referenced (^{1}H, ^{13}C) as follows: $CDCl_3$ (δ 7.26, 77.16), CD_2Cl_2 (δ 5.32, 53.84), CD_3CN (δ 1.94, 1.32), C_6D_6 (δ 7.16, 128.06). Electrospray mass spectra (ESIMS) were recorded on a Micromass Quatro LC instrument; nitrogen was employed as drying and nebulizing gas. Accurate mass measurements were performed by use of a Q-TOF premier mass spectrometer with electrospray source (Waters, Manchester, UK) operating at a resolution of ca. 16 000 (fwhm). Elemental analyses were carried out on a EuroEA3000 Eurovector Analyzer. $[Rh(COD)Cl]_2$[1], $[RhCl(BimNtBu_2)(COD)]$[2] (BimN*t*Bu = 1,3-di(*tert*-butyl)-benzimidazolylidene), 1,3-bis(2,6-diisopropylphenyl) imidazolium chloride (IPr·HCl)[3], and hexabromotribenzotriquinacene[4] were synthesized as previously reported.

1. Synthesis and characterization of compounds

1.1. Synthesis of 2,3,6,7,8b,10,11-Hexakis(tert-butylamine)-4b,8b,12b,12d-tetramethyl-4b,8b,12b,12d-tetrahydrodibenzo[2,3:4,5]pentaleno[1,6-*ab*]indene (5). A mixture of $[Pd(OAc)_2]$ (4.8 mg, 0.022 mmol), 1,3-bis(2,6-diisopropylphenyl) imidazolium chloride (IPr·HCl, 18 mg, 0.043 mmol), NaO*t*Bu (6 mg, 0.065 mmol) and toluene (10 mL) was stirred for 30 min at room temperature. After this time, the solution was added *via* oven dried cannula into a Schlenk containing hexabromotribenzotriquinacene (250 mg, 0.31 mmol) and NaO*t*Bu (214 mg, 2.22 mol) in toluene (10 mL). T*ert*-butylamine (0.233 mL, 2.22 mmol) was added and the resulting mixture was refluxed for 12 h. The cooled reaction mixture was filtered over Celite and concentrated under reduced pressure, yielding the desired product as a dark brown solid. Yield: 232 mg (99%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 6.81 (s, 6H, CH_{arom}), 2.36 (s, 3H, C$H_{3\ central}$), 1.52 (s, 9H, CH_3), 1.26 (s, 54H, C(CH_3)$_3$). ^{13}C NMR (125 MHz, $CDCl_3$): δ 141.5 ($C_{q\ arom}$), 138.0 ($C_{q\ arom}$), 114.7 (*C*H$_{arom}$), 71.1 (*C*CH$_{3\ central}$), 61.7 (*C*CH$_3$), 51.9 (*C*(CH$_3$)$_3$), 30.3 (C(*C*H$_3$)$_3$), 26.3 (*C*H$_3$), 16.6 (*C*H$_{3\ central}$). Electrospray MS

(20 V, *m/z*): 763.5 $[M + H]^+$. HRMS (+)-ESI-TOF-MS of $[M + H]^+$, monoisotopic peak 763.6363, calcd 763.6366, ε_r = 1.5 ppm Satisfactory elemental analysis could not be obtained due to the light sensitive nature of the compound.

1.2. Synthesis of compound 6

A mixture of compound **5** (232 mg, 0.3 mmol), HBF_4 (0.138 mL, 1.0 mmol, 54% in Et_2O) and triethylorthoformate (40 mL) was refluxed for 4 h under aerobic conditions and cooled to room temperature. Addition of Et_2O afforded a precipitate, which was collected by filtration and washed with methanol. Precipitation from CH_3CN/Et_2O gave compound **6** as a light beige solid. Slow evaporation of a concentrated solution of compound **6** in CH_3CN gave crystals suitable for X-ray crystallography. Yield: 322 mg (95 %). ^{1}H NMR (500 MHz, CD_3CN): δ 8.49 (s, 3H, NC*H*N) 8.21 (s, 6H, CH_{arom}), 1.99 (s, 9H, CH_3), 1.84 (s, 54H, C(CH_3)$_3$), 1.58 (s, 3H, C$H_{3\ central}$). ^{13}C NMR (125 MHz, CD_3CN): δ 148.9 ($C_{q\ arom}$), 139.4 ($C_{q\ arom}$), 133.3 (N*C*HN), 111.7 (*C*H$_{arom}$), 72.3 (*C*CH$_{3\ central}$), 64.2 (*C*CH$_3$), 62.4 (*C*(CH$_3$)$_3$), 28.8 (C(*C*H$_3$)$_3$), 26.8 (*C*H$_3$), 16.8 (*C*H$_{3\ central}$). Electrospray MS (20 V, *m/z*): 265.4 $[M]^{3+}$. HRMS (+)-ESI-TOF-MS of $[M + H]^+$, monoisotopic peak 265.2014, calcd 265.2018, ε_r = 1.5 ppm.

1.3. Synthesis of compound 3

Under inert atmosphere, a Wilmad® (LPV) NMR tube with a Teflon-lined cap was charged with **6** (20 mg, 0.019 mmol), NaO*t*Bu (1.8 mg, 0.019 mmol) and dried C_6D_6 (0.6 mL). To this suspension, NaHMDS (1M in THF, 0.074 mL, 0.074 mmol, 3.9 equiv.) was added and the reaction mixture was stirred at room temperature for 2h. Formation of carbene **2** was identified by NMR and HRMS techniques. ^{1}H NMR (300 MHz, C_6D_6): δ 7.65 (s, 6H, CH_{arom}), 1.79 (s, 3H, C$H_{3\ central}$), 1.77 (s, 54H, C(CH_3)$_3$), 1.74 (s, 9H, CH_3). ^{13}C NMR (125 MHz, C_6D_6): δ 225.8 ($C_{carbene}$) 142.8 ($C_{q\ arom}$), 136.4 ($C_{q\ arom}$), 107.4 (*C*H$_{arom}$), 72.6 (*C*CH$_{3\ central}$), 61.8 (*C*CH$_3$), 57.3 (*C*(CH$_3$)$_3$), 30.8 (C(*C*H$_3$)$_3$), 27.3 (*C*H$_3$), 17.0 (*C*H$_{3\ central}$). HRMS (+)-ESI-TOF-MS of $[M + H]^+$, monoisotopic peak 793.5903, calcd 793.5897, ε_r = 0.8 ppm.

1.4. Synthesis of compound 7

A Schlenk tube containing a suspension of compound **6** (200 mg, 0.19 mmol) in THF (10 mL) was placed in an ice bath kept at 0 °C. KHMDS was then added dropwise (0.5 M in toluene, 1.48 mL, 0.74 mmol, 3.9 equiv.) and the slurry was stirred at 0 ºC for 30 min. The resulting cloudy dark brown solution was filtered through cannula into another Schlenck charged with a solution of $[Rh(COD)Cl]_2$ (154 mg, 0.313 mmol) in THF (10

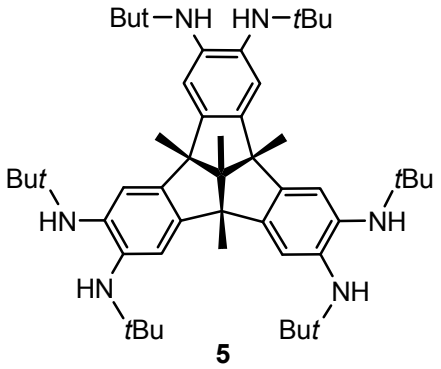
mL). The reaction mixture was stirred at ambient temperature for 12h. THF was then removed under reduced pressure. The crude soid was purified by column chromatrography. Elution with CH_2Cl_2 separated a yellow band containing $[Rh(COD)Cl]_2$. Further elution with CH_2Cl_2/Acetone (9:1) separated a light yellow band that contained compound **7**. Compound **7** was obtained as a pale yellow solid by precipitation from CH_2Cl_2/hexane. Yield: 94 mg (32 %). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.61 (s, 3H, CH_{arom}), 7.58 (s, 3H, CH_{arom}), 4.98 (br., 6H, COD), 3.00 (br., 3H, COD), 2.71 (br., 3H, COD), 2.44 (br., 12H, COD), 2.37 (s, 27 H, C(CH_3)$_3$), 2.36 (s, 27 H, C(CH_3)$_3$), 1.97 (s, 9H, CH_3), 1.83 (s, 3H, C$H_{3\ central}$), 1.78 (br., 12H, COD). ^{13}C NMR (125 MHz, CD_2Cl_2): δ 195.8 (d, $^1J_{Rh\text{-}C}$ = 49.0 Hz, Rh-$C_{carbene}$), 195.6 (d, $^1J_{Rh\text{-}C}$ = 49.0 Hz, Rh-$C_{carbene}$), 142.8 ($C_{q\ arom}$), 136.5 ($C_{q\ arom}$), 108.6 (CH$_{arom}$), 93.3 (d, $^1J_{Rh\text{-}C}$ = 15.8 Hz, Rh-CH$_{COD}$), 72.6 (CCH$_{3\ central}$), 68.0 (d, $^1J_{Rh\text{-}C}$ = 15.8 Hz, Rh-CH$_{COD}$), 62.0 (CCH$_3$), 60.5 (C(CH$_3$)$_3$), 32.5 (C(CH$_3$)$_3$), 29.6 (CH$_2$-COD), 29.0 (CH$_2$-COD). 27.3 (CH$_3$), 16.7 (CH$_{3\ central}$). Electrospray MS (20 V, *m*/*z*): 516.6 $[M - 3\ Cl + 3\ CH_3CN]^{3+}$.

2. Electrochemical measurements

The measurements were carried out using a GPES equipped PGSTAT-30 potentiostat from Autolab at room temperature. A three-electrode configuration was used, where two Pt microelectrodes were connected to the working electrode and counter electrode and a Ag wire was used as the pseudo-reference electrode. The redox potential of ferrocene (445 mV) was used to calibrate the potential scale. Measurements performed on 10 mM analyte in CH_2Cl_2 with 0.1 mM $[NBu_4]PF_6$, at a 100 mV s^{-1} scan rate.

3. Spectra

3.1. ^{1}H and ^{13}C NMR spectra of 5



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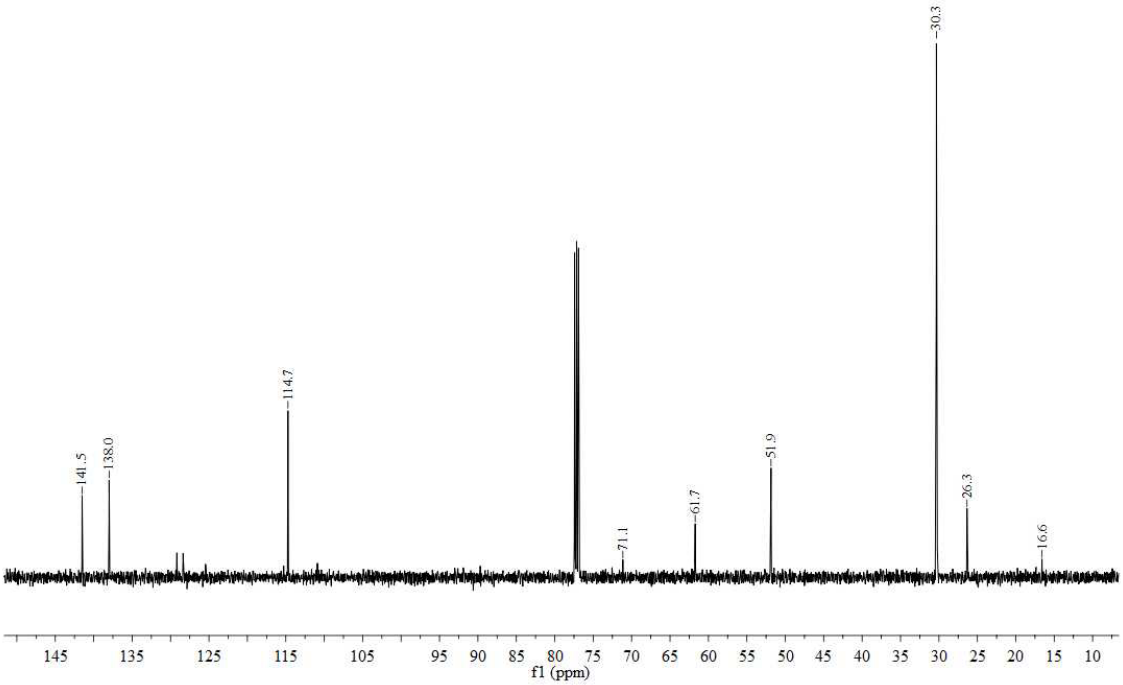
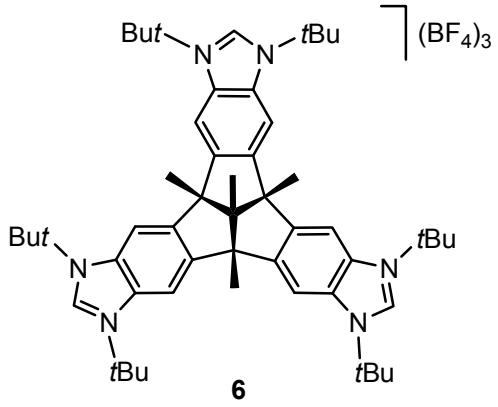


3.2. ^{1}H and ^{13}C NMR spectra of 6



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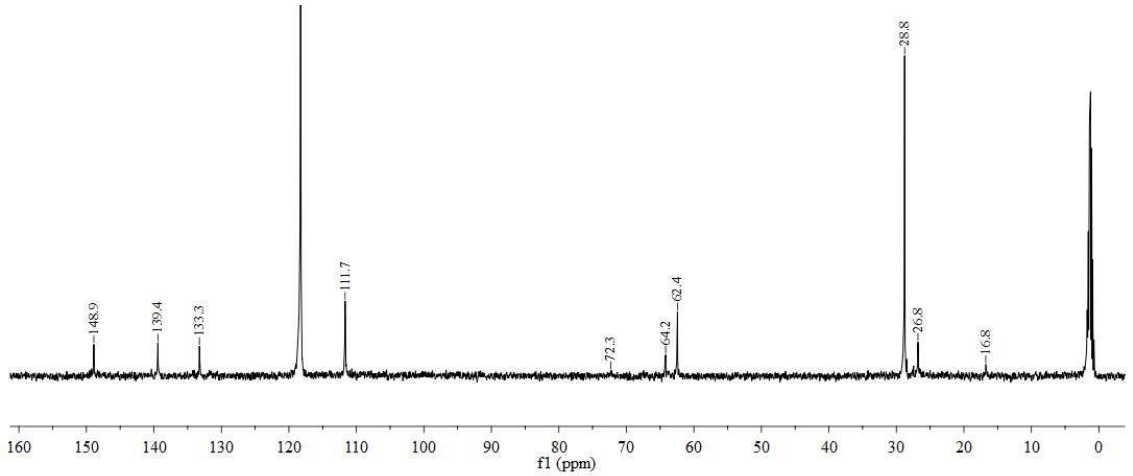
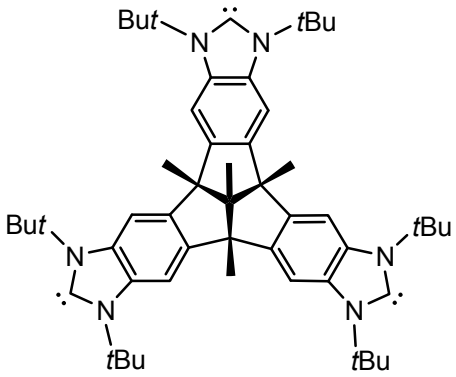


3.3. ^{1}H and ^{13}C NMR spectra of 3



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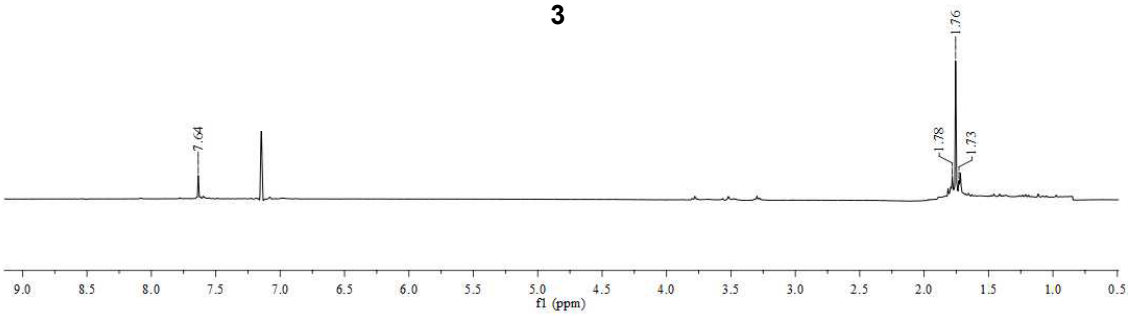
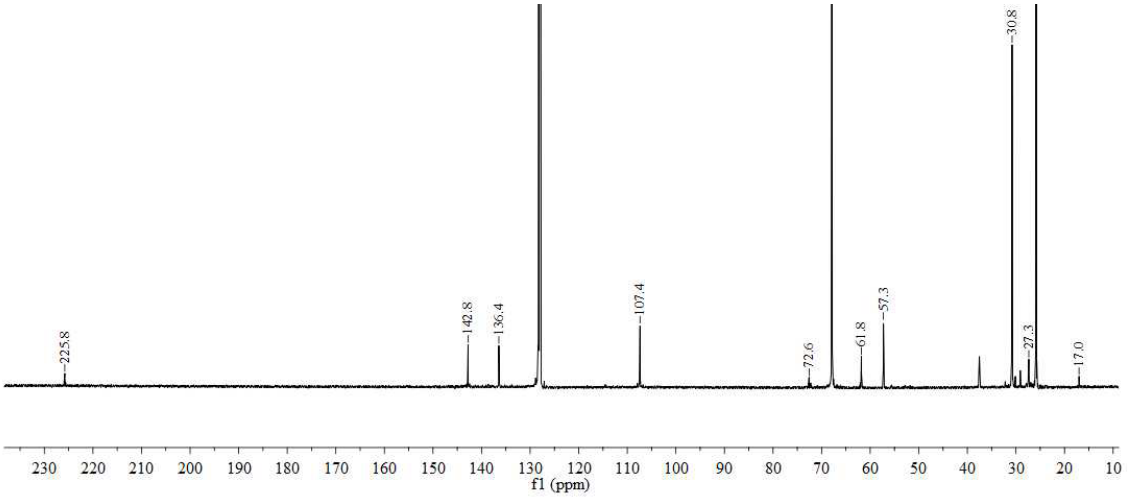
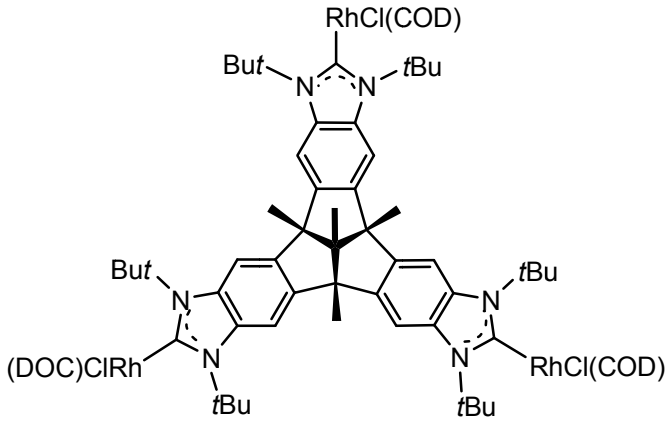




3.4. ^{1}H and ^{13}C NMR spectra of 7



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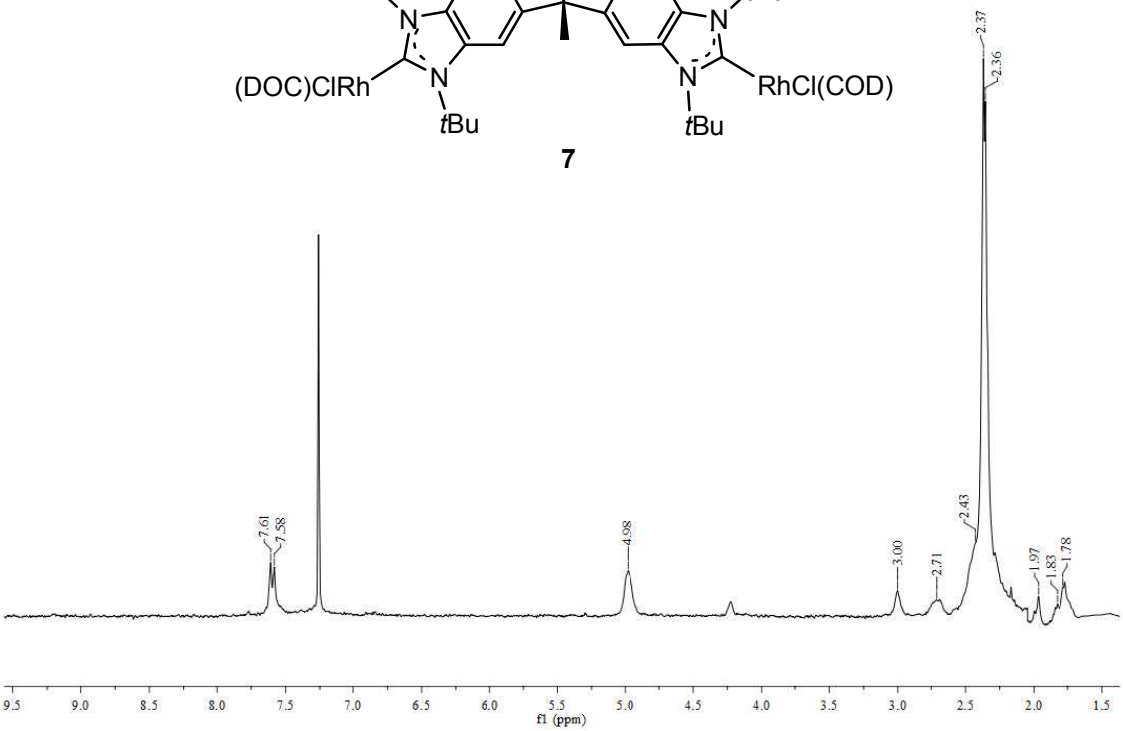
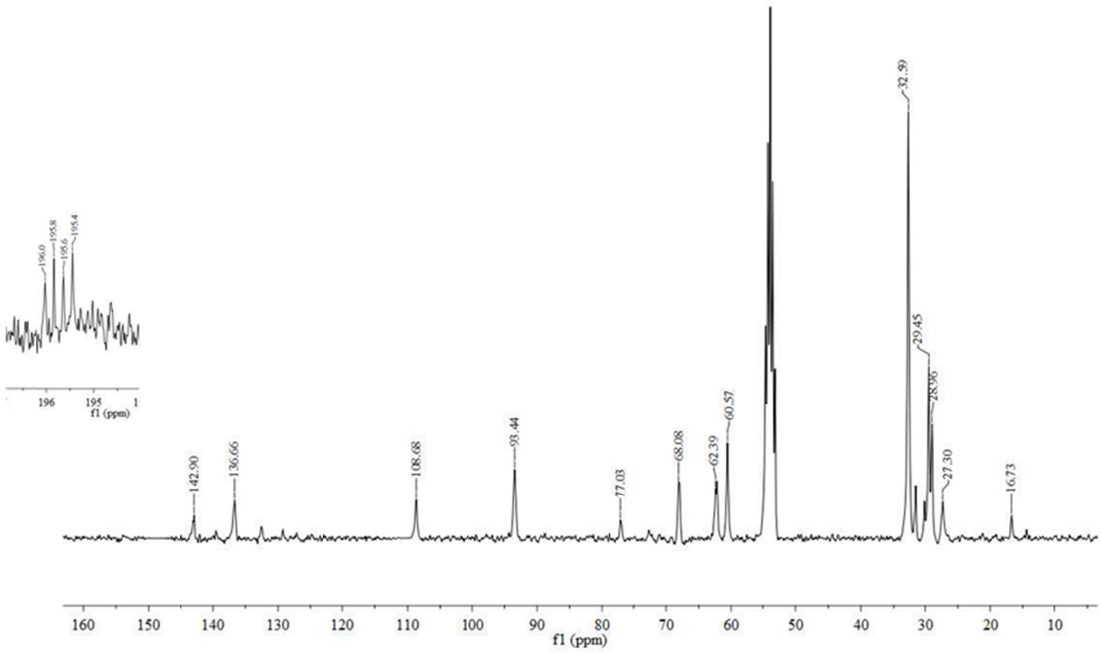
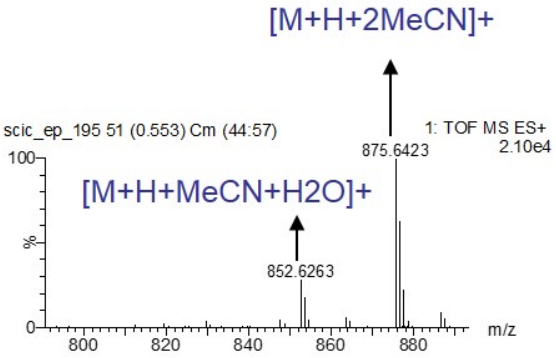
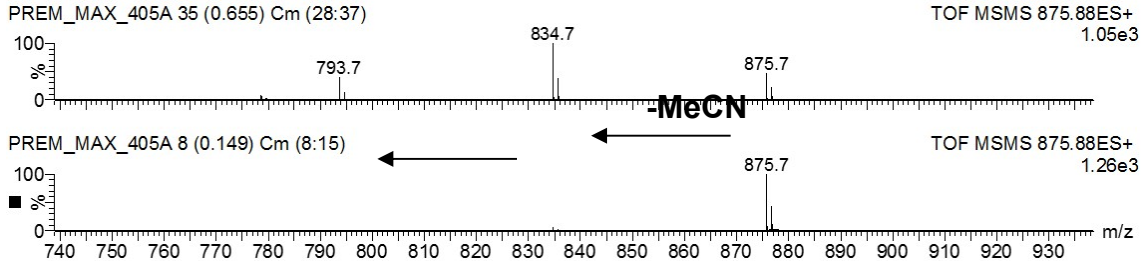
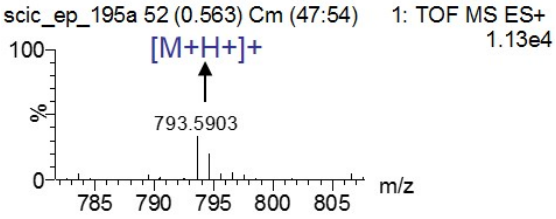




3.5. High Resolution Mass Spectra of 3







4. X-Ray Crystallography

X-Ray Diffraction studies for complex 6. Crystals suitable for X-ray study of **6** were obtained by slow evaporation of a concentrated solution of the compound in CH_3CN. Diffraction data was collected on a Agilent SuperNova diffractometer equipped with an Atlas CCD detector using Mo-Kα radiation (λ = 0.71073 Å). Single crystals were mounted on a MicroMount® polymer tip (MiteGen) in a random orientation. Absorption corrections based on the multiscan method were applied.[5] The structures were solved by direct methods in SHELXS-97 and refined by the full-matrix method based on F^2 with the program SHELXL-97 using the OLEX software package.[6, 7]

Key details of the crystal and structure refinement data are summarized in Supplementary Table S1. Further crystallographic details may be found in the respective CIF which was deposited at the Cambridge Crystallographic Data Centre, Cambridge, UK. The reference number for **1** was assigned as 950746.

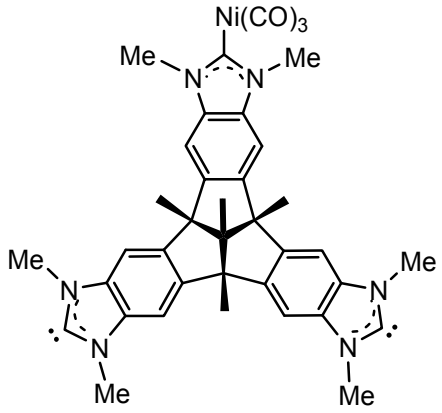
Supplementary Table S1. Summary of crystal data, data collection, and structure refinement details.

	6
Empirical formula	$C_{53}H_{72}B_3F_{12}N_6$
Formula weight	1053.60
Temperature/K	200.00(14)
Crystal system	hexagonal
Space group	$P6_3cm$
a/Å	15.7431(5)
b/Å	15.7431(5)
c/Å	12.5624(5)
α/°	90.00
β/°	90.00
γ/°	120.00
Volume/$Å^3$	2696.41(16)
Z	2
$\rho_{calc}mg/mm^3$	1.298
m/mm^{-1}	0.886
F(000)	1110.0
Crystal size/mm^3	0.14 × 0.11 × 0.1
2Θ range for data collection	6.48 to 144.94°
Index ranges	$-18 \le h \le 14$, $-15 \le k \le 18$, $-15 \le l \le 15$
Reflections collected	16021
Independent reflections	1899[R(int) = 0.0284]
Data/restraints/parameters	1899/1/128
Goodness-of-fit on F^2	1.026
Final R indexes [I>=2σ (I)]	$R_1 = 0.0696$, $wR_2 = 0.1947$
Final R indexes [all data]	$R_1 = 0.0754$, $wR_2 = 0.2093$
Largest diff. peak/hole / e $Å^{-3}$	0.68/-0.27
Flack parameter	0.0(5)

5. Computational details

The DFT calculations presented in this work were carried out as reported in the literature for ditopic NHC complexes.[8] The calculated atomic coordinates are collected in Supplementary Tables S2, S3 and S4.

Supplementary Table S2



A

mono-Ni(CO)$_3$ complex

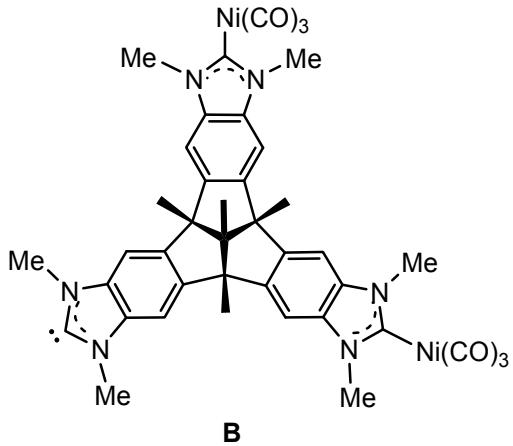
Ni1	3.4831	5.8310	0.2515
C2	4.4075	4.8785	-0.9645
C3	2.2466	6.7383	-0.6906
C4	4.5337	6.9711	1.1630
C5	2.6939	4.5808	1.5717
O6	4.9749	4.2993	-1.7688
O7	1.5209	7.3269	-1.3482
O8	5.1939	7.6972	1.7463
N9	1.4385	4.5772	2.1013
N10	3.3049	3.4934	2.1211
C11	1.2436	3.4964	2.9470
C12	0.4177	5.5656	1.8418
C13	2.4511	2.7965	2.9606
C14	4.6753	3.0999	1.8889
C15	0.1545	3.0802	3.6974

H16	0.8892	6.4439	1.4121
H17	-0.0657	5.8453	2.7794
H18	-0.3340	5.1814	1.1483
C19	2.6204	1.6528	3.7259
H20	5.1837	3.9130	1.3788
H21	5.1709	2.9109	2.8432
H22	4.7232	2.1991	1.2724
H23	-0.7772	3.6312	3.6868
C24	0.3181	1.9270	4.4583
H25	3.5631	1.1207	3.7372
C26	1.5261	1.2277	4.4723
C27	-0.7251	1.2922	5.3572
C28	1.4792	0.0155	5.3819
C29	0.0173	0.0449	6.0026
C30	-1.2675	2.3317	6.3472
C31	-1.8621	0.6838	4.5592
C32	2.6342	0.0710	6.3908
C33	1.5301	-1.2806	4.5963
C34	0.0379	0.1095	7.5249
C35	-0.7276	-1.2513	5.4655
H36	-2.0105	1.8984	7.0184
H37	-1.7577	3.1422	5.8032
H38	-0.4690	2.7783	6.9421
C39	-1.8595	-0.7101	4.6140
C40	-2.8361	1.3820	3.8502
H41	2.6144	0.9908	6.9778
H42	2.6169	-0.7835	7.0691

H43	3.5900	0.0446	5.8628
C44	0.3187	-1.9712	4.6370
C45	2.6318	-1.7843	3.9096
H46	-0.9711	0.1272	7.9380
H47	0.5511	1.0031	7.8816
H48	0.5495	-0.7524	7.9544
C49	-1.2843	-2.1932	6.5419
C50	-2.8298	-1.4642	3.9597
C51	-3.7958	0.6300	3.1903
H52	-2.8563	2.4644	3.8173
C53	0.1578	-3.1936	3.9902
C54	2.4675	-2.9964	3.2571
H55	3.5812	-1.2636	3.8878
H56	-2.0312	-1.6979	7.1645
H57	-0.4930	-2.5880	7.1813
H58	-1.7734	-3.0474	6.0688
C59	-3.7920	-0.7691	3.2436
H60	-2.8440	-2.5460	4.0091
N61	-4.8913	0.9689	2.4108
C62	1.2510	-3.6885	3.2961
H63	-0.7745	-3.7434	4.0286
N64	3.3190	-3.7847	2.4980
N65	-4.8855	-1.1720	2.4921
C66	-5.5774	-0.1218	1.9684
C67	-5.2747	2.3229	2.0914
N68	1.4574	-4.8436	2.5573
C69	2.7211	-4.9259	2.0551

C70	4.6894	-3.4465	2.1983
C71	-5.2613	-2.5485	2.2769
H72	-4.4791	2.8329	1.5419
H73	-5.5003	2.8881	2.9995
H74	-6.1650	2.2729	1.4693
C75	0.4536	-5.8559	2.3337
H76	5.0990	-4.2490	1.5899
H77	4.7452	-2.5075	1.6414
H78	5.2768	-3.3531	3.1155
H79	-6.1516	-2.5510	1.6528
H80	-5.4840	-3.0439	3.2255
H81	-4.4625	-3.0944	1.7683
H82	0.9043	-6.6344	1.7230
H83	0.1191	-6.2881	3.2804
H84	-0.4088	-5.4384	1.8076

Supplementary Table S3



B

bis-Ni(CO)$_3$ complex

Ni1	3.4909	5.8319	0.2485
C2	4.4409	4.8849	-0.9527

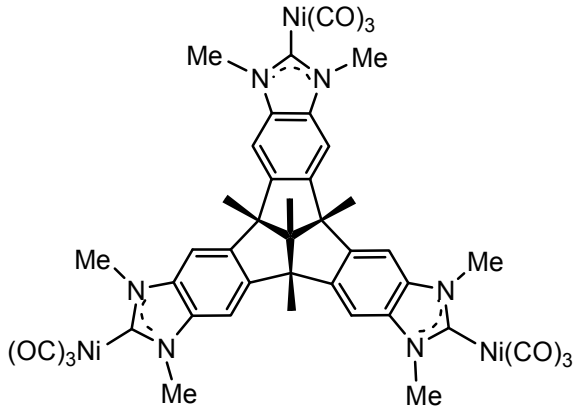
C3	2.2536	6.7188	-0.7127
C4	4.5182	6.9905	1.1635
C5	2.7016	4.5808	1.5660
O6	5.0244	4.3092	-1.7476
O7	1.5277	7.2944	-1.3812
O8	5.1636	7.7282	1.7486
N9	1.4411	4.5681	2.0840
N10	3.3173	3.5013	2.1266
C11	1.2482	3.4898	2.9326
C12	0.4144	5.5468	1.8103
C13	2.4620	2.8007	2.9608
C14	4.6939	3.1204	1.9094
C15	0.1564	3.0685	3.6762
H16	0.8832	6.4282	1.3841
H17	-0.0821	5.8243	2.7416
H18	-0.3255	5.1543	1.1089
C19	2.6339	1.6624	3.7334
H20	5.1995	3.9376	1.4029
H21	5.1815	2.9383	2.8690
H22	4.7571	2.2193	1.2947
H23	-0.7790	3.6129	3.6561
C24	0.3228	1.9207	4.4446
H25	3.5824	1.1411	3.7578
C26	1.5361	1.2313	4.4716
C27	-0.7205	1.2867	5.3436
C28	1.4898	0.0220	5.3853
C29	0.0270	0.0505	6.0043

C30	-1.2733	2.3318	6.3222
C31	-1.8529	0.6636	4.5504
C32	2.6439	0.0771	6.3950
C33	1.5426	-1.2758	4.6025
C34	0.0459	0.1333	7.5257
C35	-0.7119	-1.2550	5.4816
H36	-2.0163	1.9001	6.9945
H37	-1.7668	3.1335	5.7685
H38	-0.4801	2.7895	6.9156
C39	-1.8493	-0.7291	4.6277
C40	-2.8278	1.3491	3.8303
H41	2.6225	0.9968	6.9818
H42	2.6265	-0.7771	7.0736
H43	3.6006	0.0519	5.8684
C44	0.3346	-1.9731	4.6523
C45	2.6421	-1.7735	3.9099
H46	-0.9636	0.1517	7.9373
H47	0.5541	1.0339	7.8717
H48	0.5609	-0.7205	7.9670
C49	-1.2549	-2.1936	6.5676
C50	-2.8208	-1.4949	3.9886
C51	-3.7877	0.5856	3.1841
H52	-2.8492	2.4307	3.7797
C53	0.1755	-3.1965	4.0092
C54	2.4780	-2.9885	3.2624
H55	3.5854	-1.2436	3.8754
H56	-2.0012	-1.6986	7.1907

H57	-0.4574	-2.5781	7.2055
H58	-1.7416	-3.0545	6.1040
C59	-3.7844	-0.8127	3.2621
H60	-2.8368	-2.5756	4.0582
N61	-4.8840	0.9110	2.4005
C62	1.2687	-3.6843	3.3100
H63	-0.7550	-3.7482	4.0496
N64	3.3374	-3.7681	2.5047
N65	-4.8789	-1.2284	2.5200
C66	-5.5712	-0.1872	1.9788
C67	-5.2679	2.2594	2.0577
N68	1.4662	-4.8421	2.5763
C69	2.7268	-4.9028	2.0606
C70	4.7086	-3.3978	2.2414
C71	-5.2563	-2.6084	2.3295
H72	-4.4731	2.7593	1.4981
H73	-5.4924	2.8404	2.9559
H74	-6.1589	2.1982	1.4377
C75	0.4464	-5.8516	2.4081
Ni76	3.4409	-6.3261	0.8820
H77	5.2453	-4.2791	1.9047
H78	4.7658	-2.6232	1.4731
H79	5.1701	-3.0311	3.1598
H80	-6.1482	-2.6208	1.7079
H81	-5.4771	-3.0871	3.2870
H82	-4.4595	-3.1635	1.8277
H83	0.9063	-6.7330	1.9705

H84	0.0227	-6.1138	3.3795
H85	-0.3498	-5.4945	1.7507
C86	4.9068	-5.8306	-0.0386
C87	3.8196	-7.7414	1.9255
C88	2.1967	-6.7091	-0.3617
O89	5.8203	-5.5827	-0.6782
O90	4.0668	-8.6347	2.5919
O91	1.4369	-6.9494	-1.1794

Supplementary Table S3



C

tris-Ni(CO)$_3$ complex

Ni1	-0.4840	7.0362	-1.6315
C2	-0.4168	5.4852	-0.4026
C3	-2.0486	7.1925	-2.5095
C4	-0.1829	8.5111	-0.6466
C5	0.7638	6.8041	-2.9092
N6	0.7099	4.9020	0.0974
N7	-1.4432	4.7427	0.1010
O8	-2.9993	7.3425	-3.1248
O9	0.0000	9.4456	-0.0172
O10	1.5263	6.6666	-3.7476

C11	0.4112	3.7993	0.8796
C12	2.0597	5.3646	-0.1304
C13	-0.9812	3.6950	0.8807
C14	-2.8476	4.9947	-0.1254
C15	1.2076	2.9109	1.5857
H16	2.0111	6.3427	-0.6004
H17	2.5862	5.4511	0.8221
H18	2.6021	4.6764	-0.7829
C19	-1.6335	2.6958	1.5867
H20	-2.9607	6.0094	-0.4936
H21	-3.2591	4.2957	-0.8572
H22	-3.3921	4.8963	0.8152
C23	0.5556	1.9011	2.2865
H24	2.2858	3.0084	1.5897
C25	-0.8360	1.7957	2.2867
H26	-2.7139	2.6279	1.5914
C27	1.2140	0.8294	3.1332
C28	-1.3253	0.6367	3.1332
C29	0.0000	0.0000	3.7348
C30	1.9732	-0.1739	2.2867
C31	2.1560	1.4731	4.1595
C32	-1.9242	-0.4694	2.2865
C33	-2.3537	1.1306	4.1595
C34	0.1112	-1.4661	3.1332
C35	0.0000	0.0000	5.2587
C36	1.3686	-1.4317	2.2865
C37	3.1514	0.0668	1.5867

H38	2.6345	0.7243	4.7926
H39	1.6324	2.1911	4.7925
H40	2.9513	2.0164	3.6445
C41	-3.1247	-0.4097	1.5857
C42	-1.1371	-1.6219	2.2867
H43	-2.7138	0.3182	4.7925
H44	-1.9446	1.9194	4.7926
H45	-3.2219	1.5477	3.6445
C46	0.1977	-2.6037	4.1595
H47	0.9144	-0.4388	5.6590
H48	-0.8372	-0.5725	5.6590
H49	-0.0771	1.0113	5.6590
C50	1.9171	-2.5013	1.5857
C51	3.6906	-0.9977	0.8807
H52	3.6328	1.0364	1.5914
C53	-3.4959	-1.5436	0.8796
H54	-3.7482	0.4754	1.5897
C55	-1.5179	-2.7626	1.5867
H56	1.0813	-2.5093	4.7925
H57	0.2707	-3.5641	3.6445
H58	-0.6900	-2.6437	4.7926
C59	3.0847	-2.2558	0.8796
H60	1.4624	-3.4837	1.5897
N61	4.8289	-1.1215	0.1010
C62	-2.7094	-2.6973	0.8807
N63	-4.6002	-1.8362	0.0974
H64	-0.9189	-3.6643	1.5914

N65	3.8903	-3.0658	0.0974
C66	4.9587	-2.3816	-0.4026
C67	5.7493	-0.0313	-0.1254
N68	-3.3857	-3.6212	0.1010
C69	-4.5419	-3.1036	-0.4026
C70	-5.6757	-0.8985	-0.1304
C71	3.6160	-4.4661	-0.1304
Ni72	6.3355	-3.0989	-1.6315
H73	6.6847	-0.4407	-0.4936
H74	5.9364	0.4895	0.8152
H75	5.3498	0.6746	-0.8572
C76	-2.9017	-4.9634	-0.1254
Ni77	-5.8515	-3.9372	-1.6315
H78	-6.4985	-1.4297	-0.6004
H79	-6.0139	-0.4859	0.8221
H80	-5.3509	-0.0847	-0.7829
H81	2.7488	-4.5917	-0.7829
H82	3.4277	-4.9653	0.8221
H83	4.4874	-4.9130	-0.6004
C84	7.2532	-1.8221	-2.5095
C85	7.4623	-4.0972	-0.6466
C86	5.5106	-4.0636	-2.9092
H87	-3.7240	-5.5687	-0.4936
H88	-2.5442	-5.3858	0.8152
H89	-2.0907	-4.9703	-0.8572
C90	-6.2744	-2.7405	-2.9092
C91	-5.2046	-5.3704	-2.5095

C92	-7.2794	-4.4139	-0.6466
O93	7.8584	-1.0738	-3.1248
O94	8.1801	-4.7228	-0.0172
O95	5.0103	-4.6551	-3.7476
O96	-6.5366	-2.0115	-3.7476
O97	-4.8591	-6.2687	-3.1248
O98	-8.1801	-4.7228	-0.0172

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