Electronic supplementary information

for

Ruthenium tris(σ-B-H) borate complexes: synthesis, structure, and reactivity

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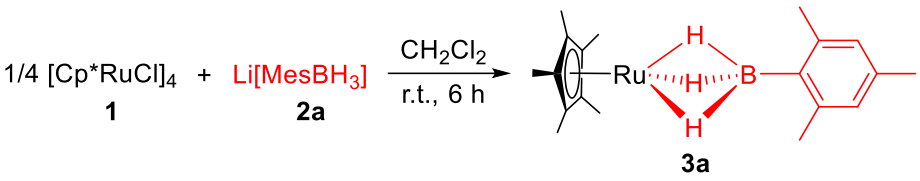
Contents

General information

X-ray diffraction: Single-crystal X-ray diffraction data were collected on a Bruker Smart APEX II CCD single-crystal diffractometer or a Bruker D8 Venture diffractometer equipped with a Photon 100 CMOS detector using Mo_{Ka} radiation (λ = 0.71073 Å). All of the data were corrected for absorption effects using the multi-scan technique. Final unit cell parameters were based on all observed reflections from integration of all frame data. The structures were solved with the ShelXT structure solution program using Intrinsic Phasing and refined with the ShelXL refinement package using Least Squares minimization that implanted in Olex2. For all compounds, all non-H atoms were refined anisotropically unless otherwise stated, and hydrogen atoms were introduced at their geometric positions and refined as riding atoms unless otherwise stated. *Exceptions and special features:* For compounds **3a** and **3c** the C_5Me_5 group, for compound **3b** the Tipp group were found disordered over two positions. Several restraints (SADI, SIMU, ISOR, EADP and EXYZ) were used in order to improve refinement stability. CCDC 2194525-2194527, 2150382, 2150385 and 2150386 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures/.

NMR spectra and crystallographic data of compound 3a



Scheme S1

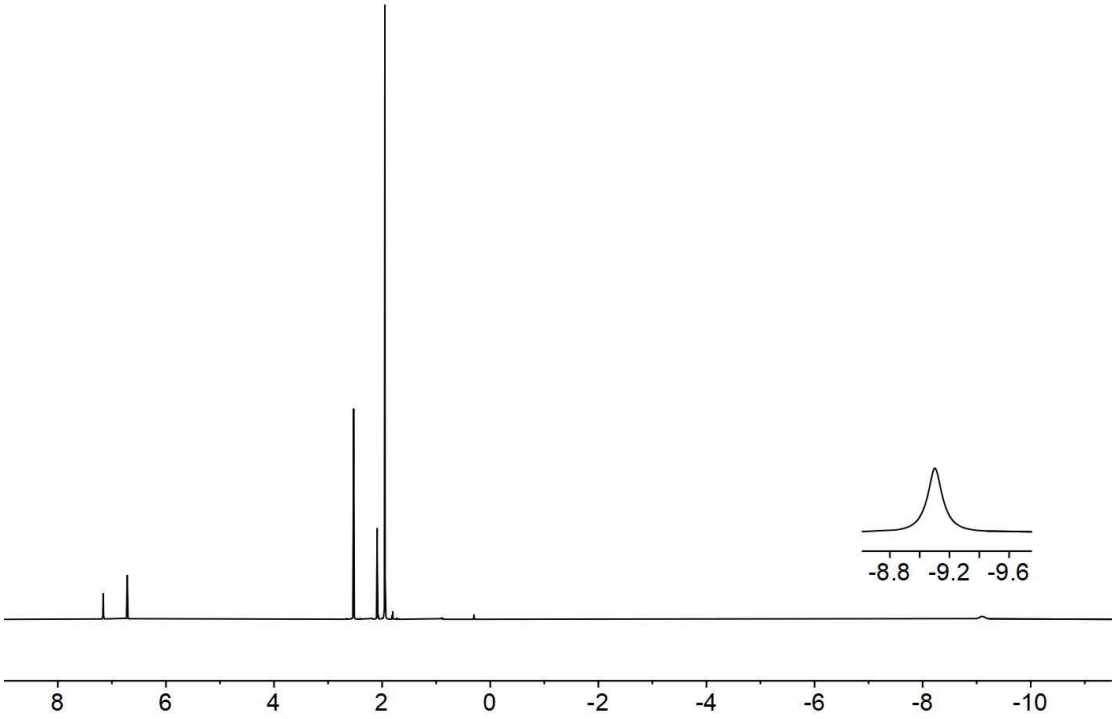


Figure S1. ^{1}H NMR (400 MHz, 298 K, C_6D_6) spectrum of compound **3a**.

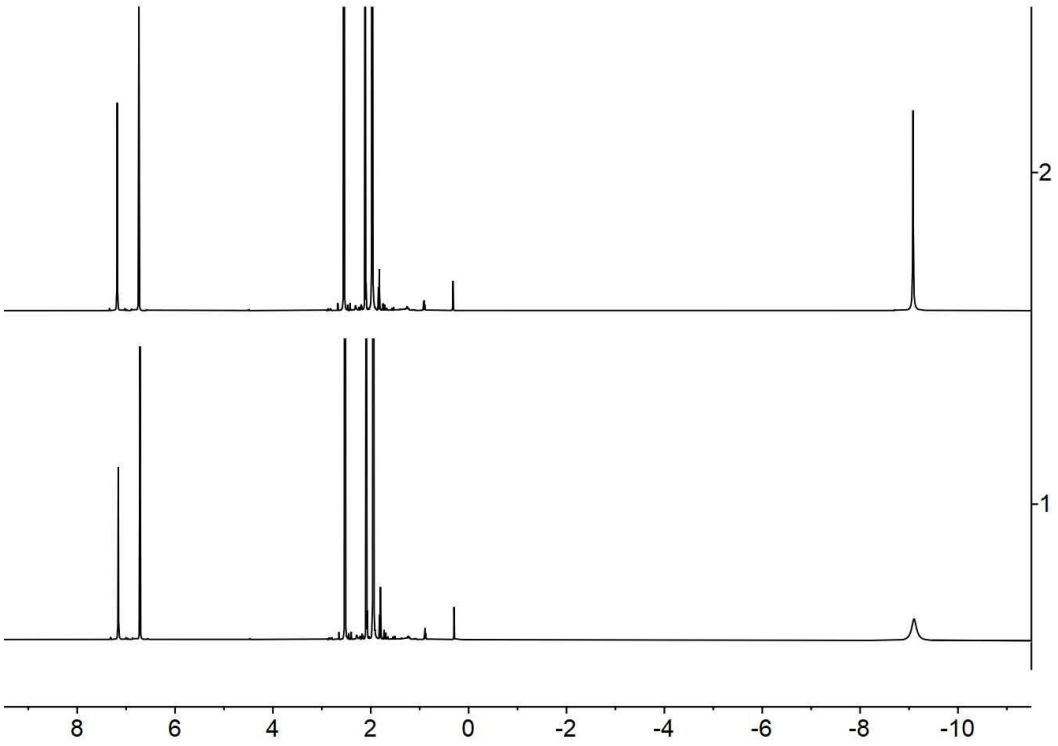


Figure S2. (1) ^{1}H NMR (400 MHz, 298 K, C_6D_6) and (2) $^{1}H\{^{11}B\}$ NMR (400 MHz, 298 K, C_6D_6) spectra of compound **3a**.

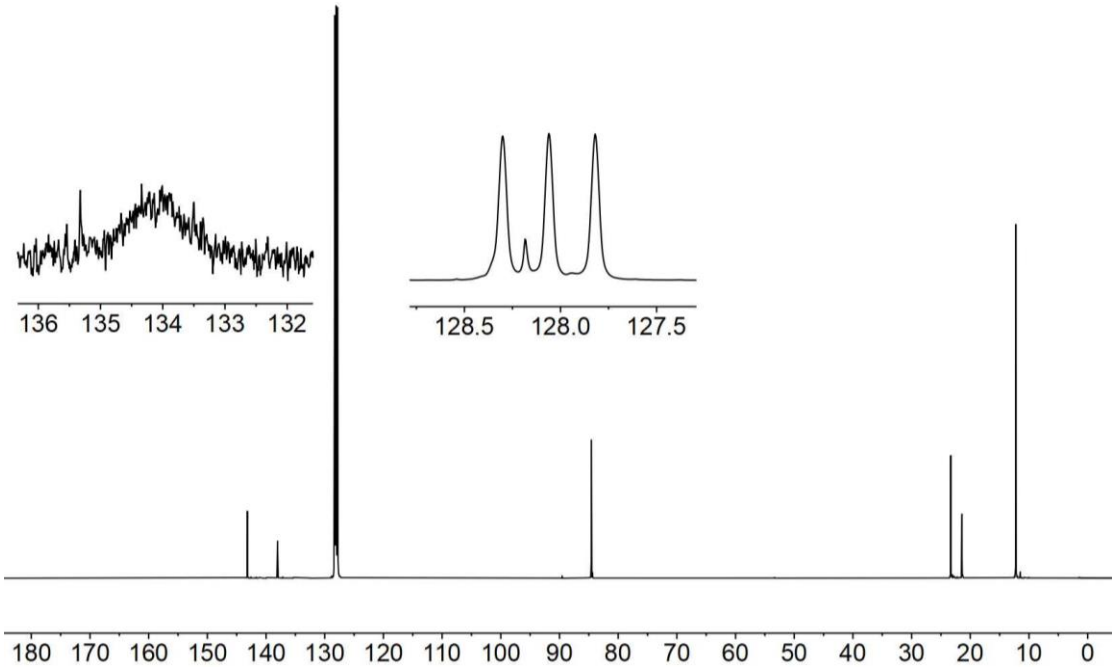


Figure S3. $^{13}C\{^{1}H\}$ NMR (101 MHz, 298 K, C_6D_6) spectrum of compound **3a**.

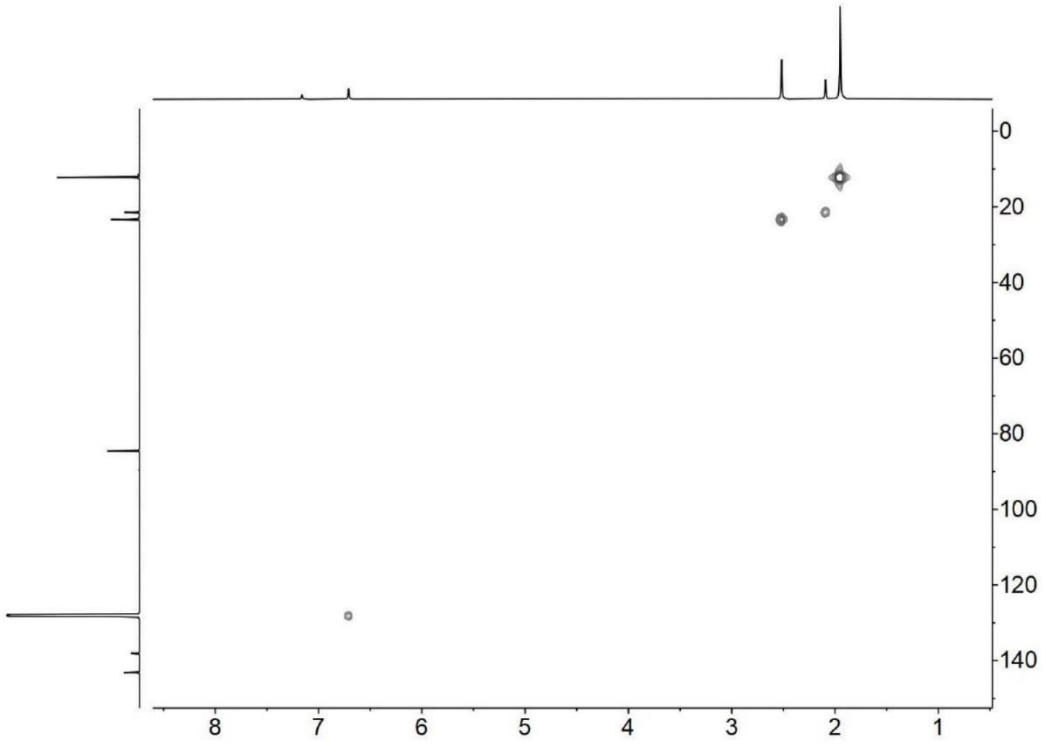


Figure S4. ^{1}H-^{13}C GHSQC (400 MHz/101 MHz, 298 K, C_6D_6) spectrum of compound **3a**.

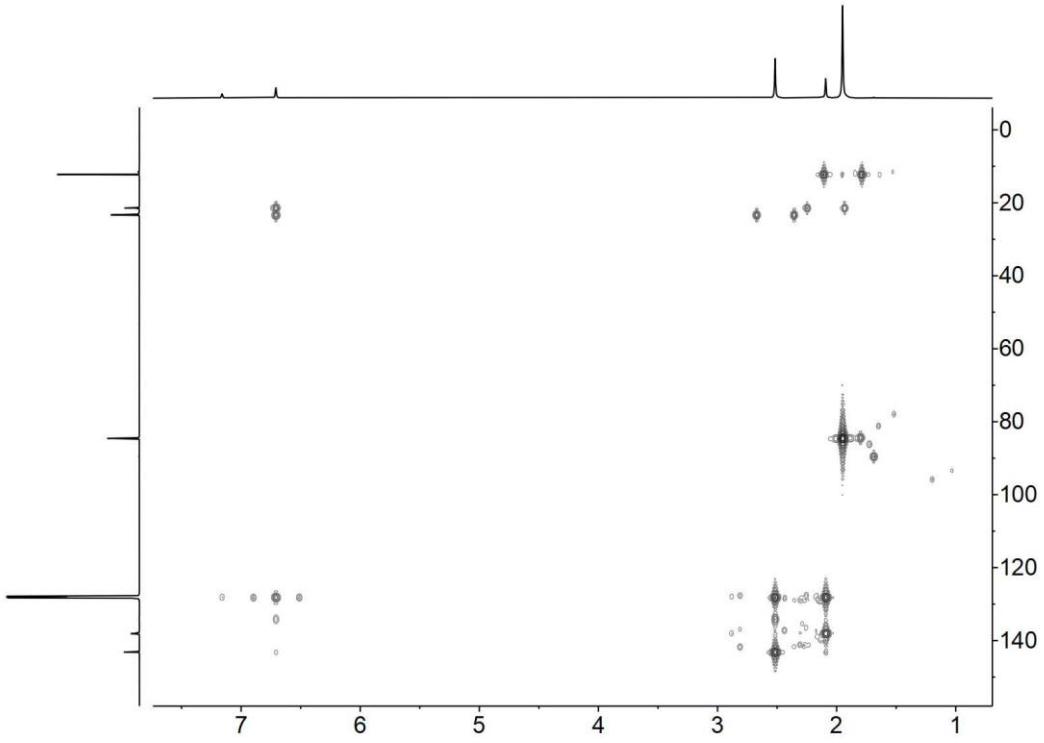


Figure S5. ^{1}H-^{13}C GHMBC (400 MHz/101 MHz, 298 K, C_6D_6) spectrum of compound **3a**.

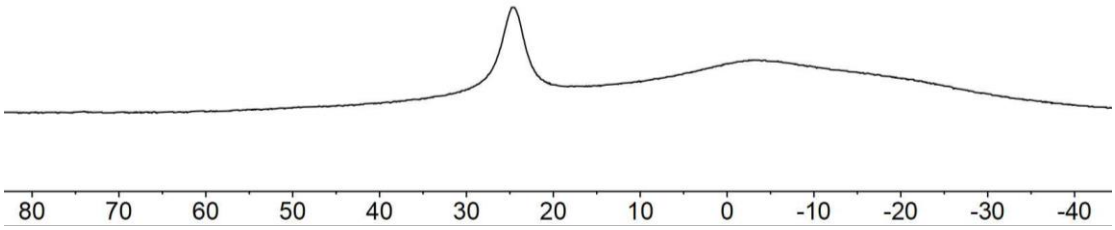


Figure S6. ^{11}B NMR (128 MHz, 298 K, C_6D_6) spectrum of compound **3a**.

X-ray crystal structure analysis of compound 3a: formula $C_{19}H_{29}BRu$, M = 369.30, yellow crystal, 0.35 x 0.15 x 0.1 mm, a = 17.5721(3), b = 7.85900(10), c = 27.1629(4) Å, α = 90, β = 97.2870(10), γ = 90°, V = 3720.88(10) Å^3, ρ_{calc} = 1.318 g·cm^{-3}, μ = 0.835 mm^{-1}, empirical absorption correction (0.6805 ≤ T ≤ 0.7456), Z = 8, monoclinic, space group $P2_1/n$ (No. 14), λ = 0.71073 Å, T = 173 K, ω and φ scans, 17923 reflections collected (±h, ±k, ±l), 8180 independent (R_{int} = 0.0250) and 6766 observed reflections [I>2σ(I)], 236 refined parameters, R = 0.0260, wR^2 = 0.0637, max. (min.) residual electron density 0.41 (-0.41) e.Å^{-3}.

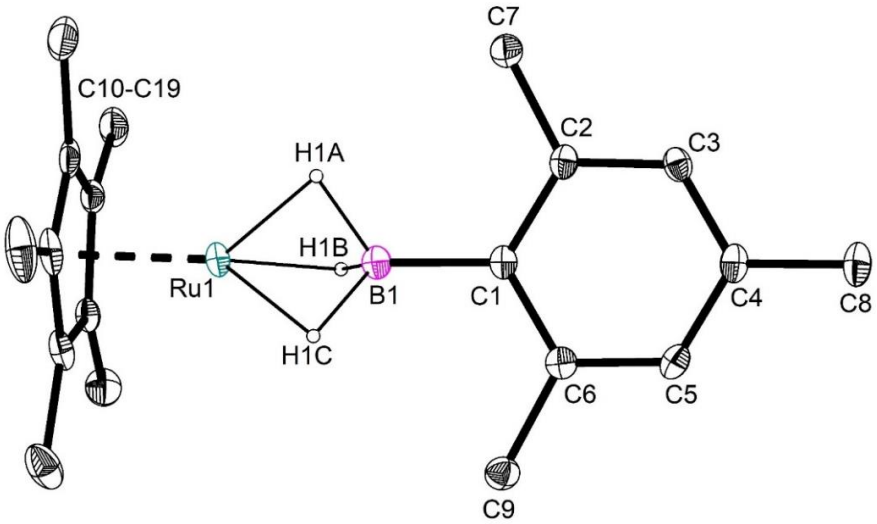
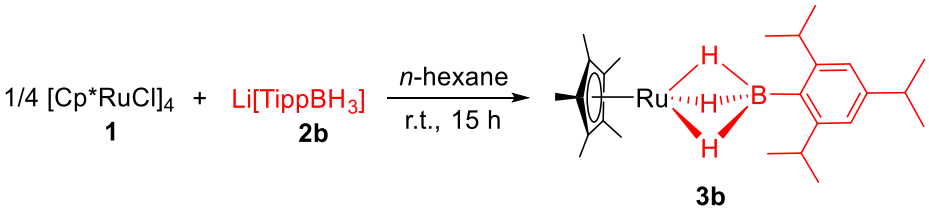


Figure S7. Molecular structure of compound **3a** (thermal ellipsoids are shown at the 30% probability level).

NMR spectra and crystallographic data of compound 3b



Scheme S2

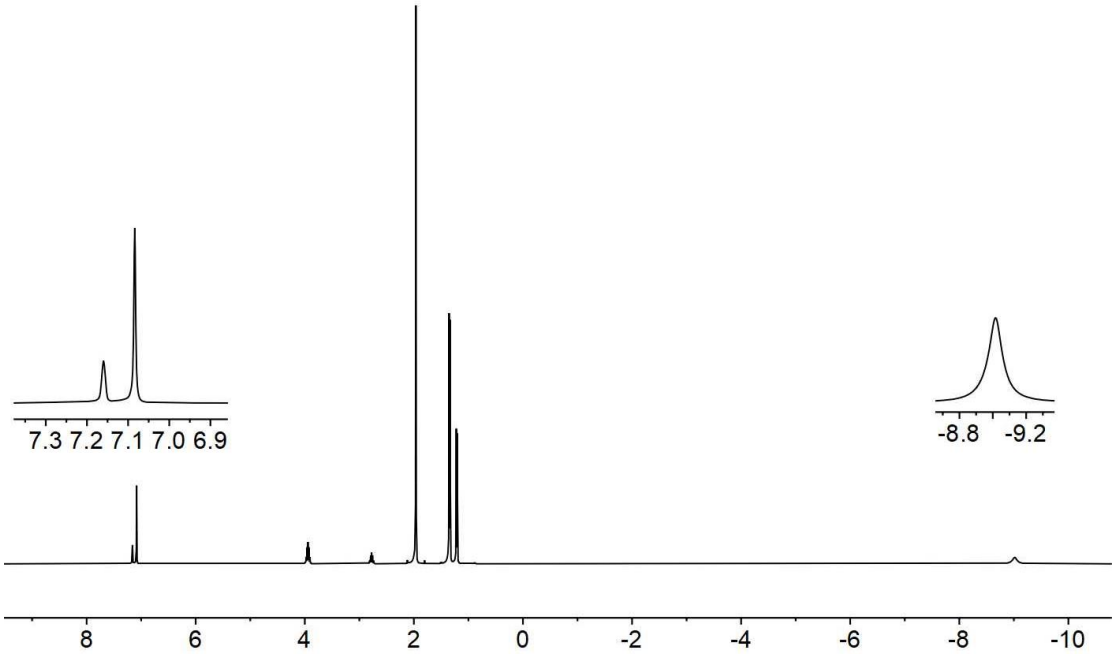


Figure S8. ^{1}H NMR (400 MHz, 298 K, C_6D_6) spectrum of compound **3b**.

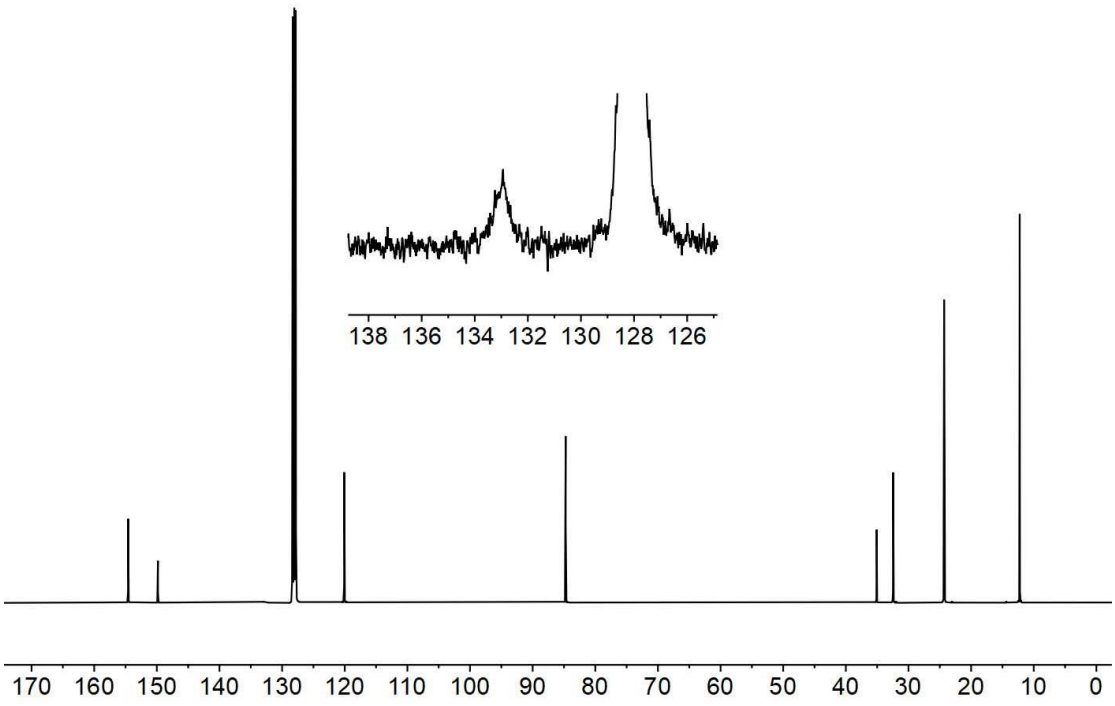


Figure S9. $^{13}C\{^{1}H\}$ NMR (101 MHz, 298 K, C_6D_6) spectrum of compound **3b**.

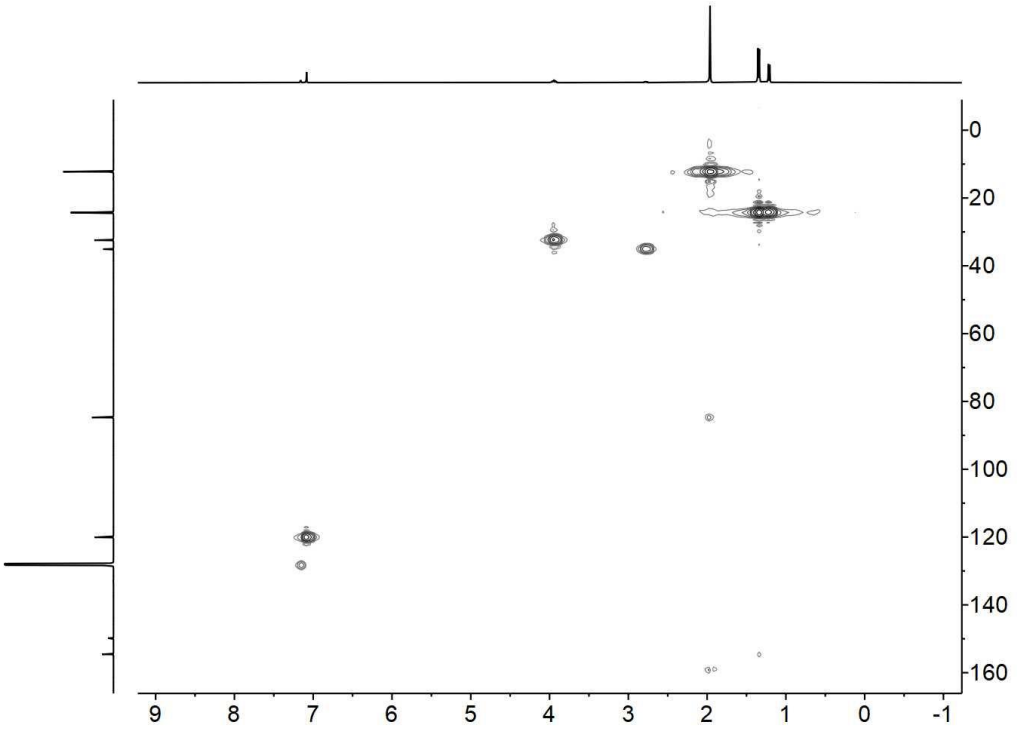


Figure S10. ^{1}H-^{13}C GHSQC (400 MHz/101 MHz, 298 K, C_6D_6) spectrum of compound **3b**.

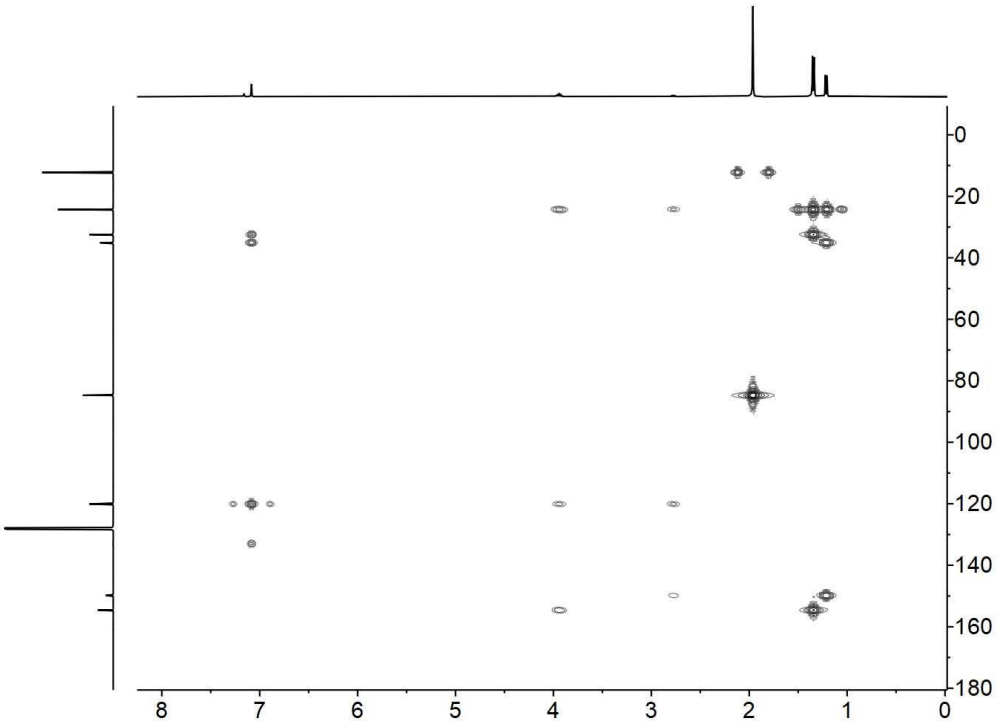


Figure S11. ^{1}H-^{13}C GHMBC (400 MHz/101 MHz, 298 K, C_6D_6) spectrum of compound **3b**.

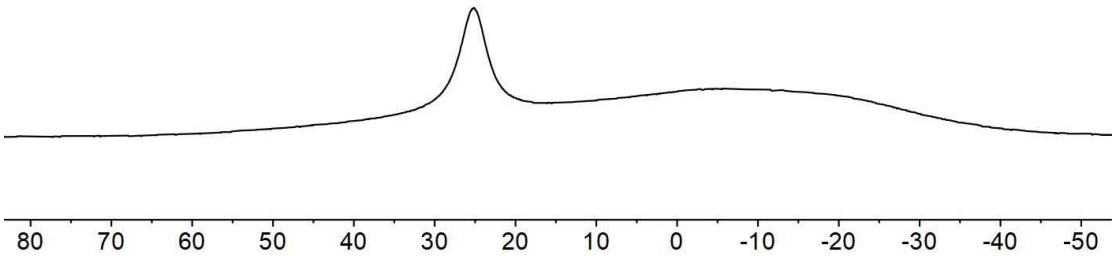


Figure S12. ^{11}B NMR (128 MHz, 298 K, C_6D_6) spectrum of compound **3b**.

X-ray crystal structure analysis of compound 3b: formula $C_{25}H_{41}BRu$, M = 453.46 g/mol, yellow crystal, 0.25 x 0.2 x 0.1mm, a = 9.2828(4), b = 14.0011(6), c = 9.3396(4) Å, α = 90, β = 97.9350(10), γ = 90°, V = 1202.24(9) Å^3, ρ_{calc} = 1.253 g·cm^{-3}, μ = 0.659 mm^{-1}, empirical absorption correction (0.6624≤ T ≤ 0.7456), Z = 2, monoclinic, space group $P2_1$ (No. 4), λ = 0.71073 Å, T = 170 K, ω and φ scans, 5807 reflections collected

(±*h*, ±*k*, ±*l*), 3533 independent (R_{int} = 0.0635) and 3185 observed reflections [$I>2\sigma(I)$], 407 refined parameters, R = 0.0328, wR^2 = 0.0867, max. (min.) residual electron density 0.31（-0.66) e.Å^{-3}.

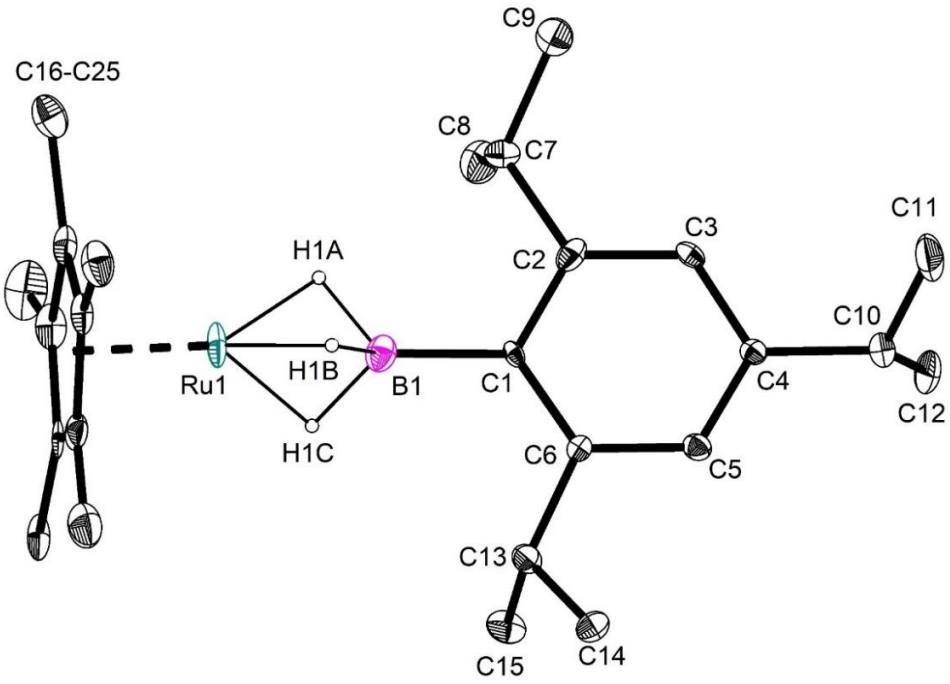
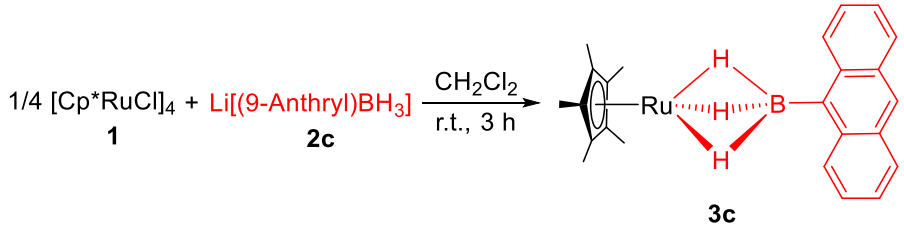


Figure S13. Molecular structure of compound **3b** (thermal ellipsoids are shown at the 30% probability level).

NMR spectra and crystallographic data of compound 3c



Scheme S3

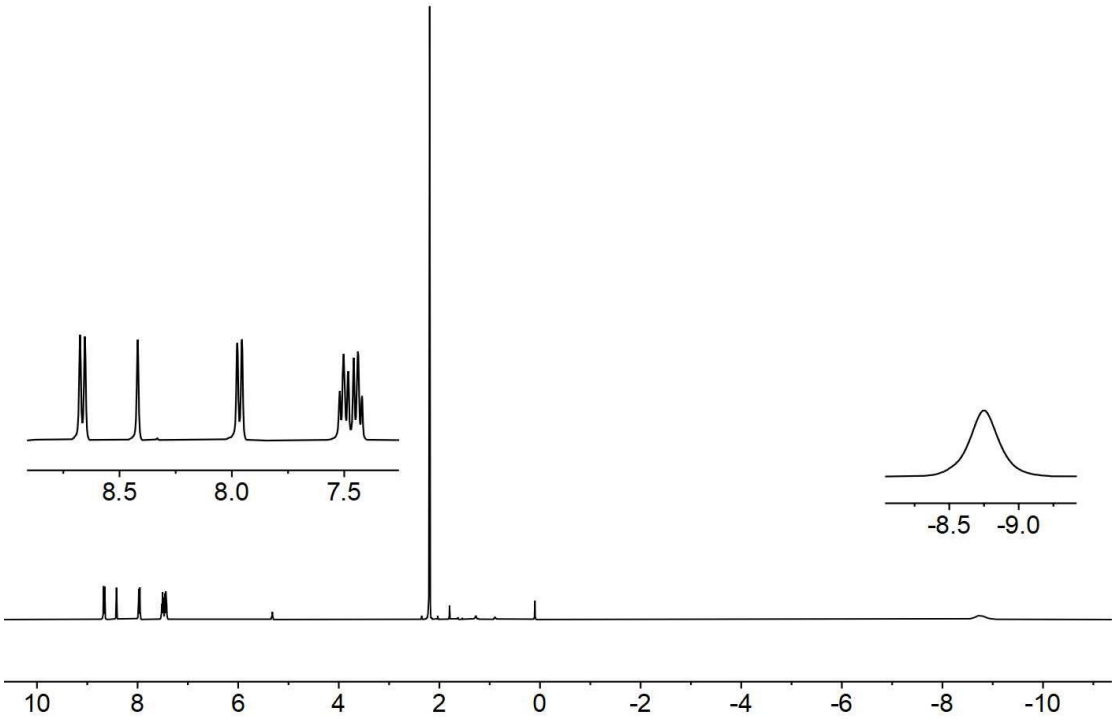


Figure S14. ^{1}H NMR (400 MHz, 298 K, CD_2Cl_2) spectrum of compound **3c**.

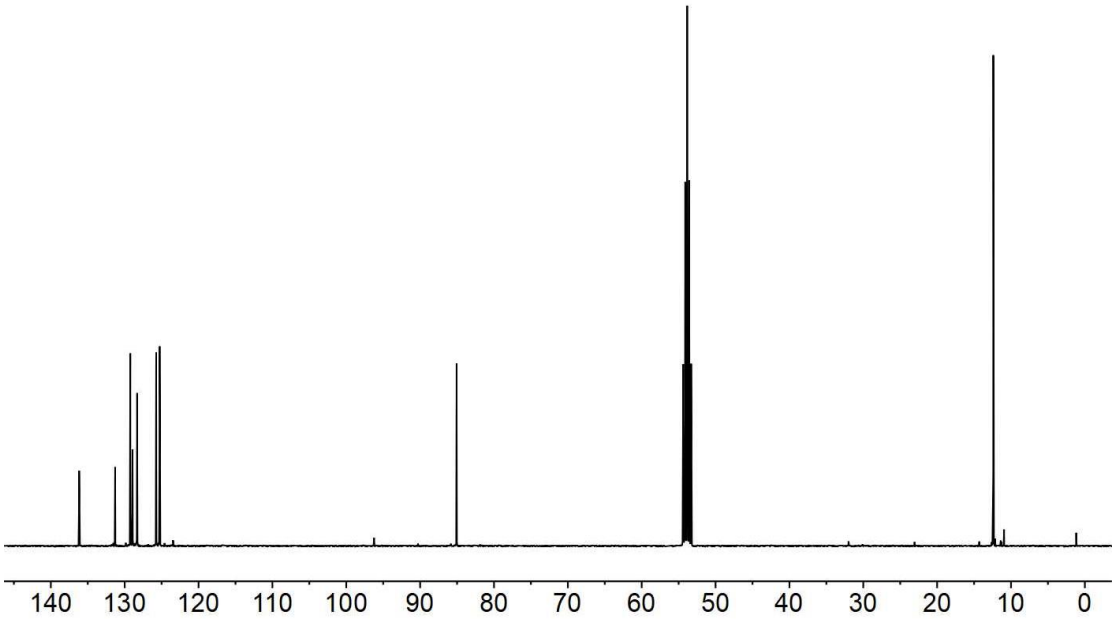


Figure S15. $^{13}C\{^{1}H\}$ NMR (101 MHz, 298 K, CD_2Cl_2) spectrum of compound **3c**.

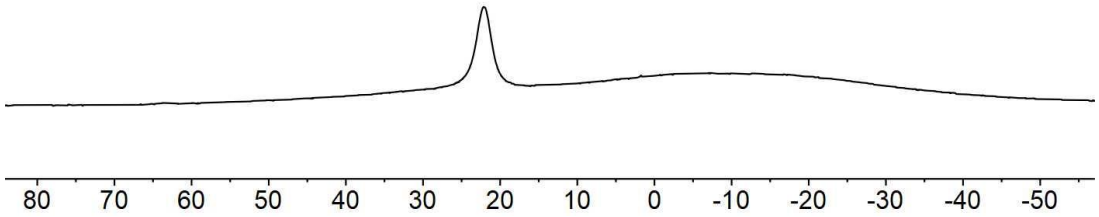


Figure S16. ^{11}B NMR (128 MHz, 298 K, CD_2Cl_2) spectrum of compound **3c**.

X-ray crystal structure analysis of compound 3c: formula $C_{24}H_{27}BRu$, M = 427.33 g/mol, yellow crystal, 0.27 x 0.15 x 0.1 mm, a = 11.932(3), b = 13.828(4), c = 14.862(4) Å, α = 114.054(7), β = 99.367(7), γ = 104.778(8)°, V = 2064.0(10) Å^3, ρ_{calc} = 1.375 g·cm^{-3}, μ = 0.763 mm^{-1}, empirical absorption correction (0.6700 ≤ T ≤ 0.7457), Z = 4, triclinic, space group $P\bar{1}$ (No. 2), λ = 0.71073 Å, T = 150 K, ω and φ scans, 53949 reflections collected ($\pm h$, $\pm k$, $\pm l$), 10113 independent (R_{int} = 0.0657) and 7500 observed reflections [$I>2\sigma(I)$], 599 refined parameters, R = 0.0363, wR^2 = 0.0897, max. (min.) residual electron density 0.48 (-0.65) e.Å^{-3}.

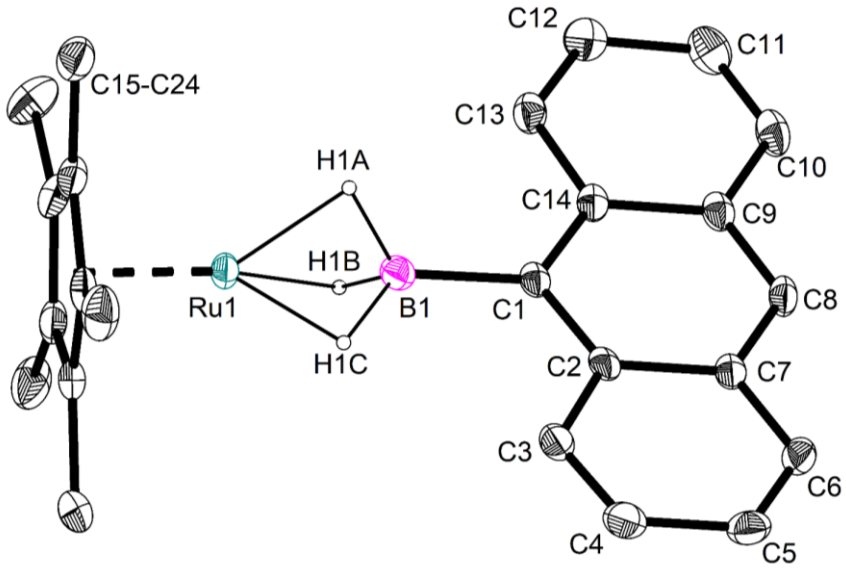


Figure S17. Molecular structure of compound **3c** (thermal ellipsoids are shown at the 30% probability level).

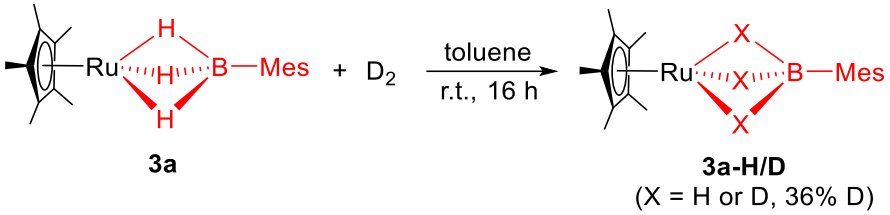
Thermal stability tests of ruthenium tris(σ-B-H) borates 3a-c

Table S1. Thermal stability data of ruthenium tris(σ-B-H) borates **3a-c** in solution

	Ar	50 °C	110 °C	130 °C	150 °C
3a	Mes	●	●	◇	■
3b	Tipp	●	●	●	◇
3c	9-Anthryl	◇	■	–	–

All reactions were carried out for 10 h in toluene-d_8 under a nitrogen atmosphere. ● = Stable, ◇ = Partly decomposed, ■ = Completely decomposed.

Reaction of 3a with D_2



Scheme S4

In a Schlenk tube (10 mL), compound **3a** (73.9 mg, 0.20 mmol) was dissolved in toluene (5 mL). The tube was evacuated under -78 °C, and then refilled with D_2 atmosphere (0.8 bar). After stirring for 16 h at room temperature, the solvent was removed under vacuum to give a yellow solid. The ^{1}H NMR spectroscopy studies revealed a 36% decrease in the intensity of the hydride signal, which indicated that D-D/B-H oxidative addition and H/D exchange were occurred. Deuterium incorporation was also confirmed by the ^{2}H NMR spectroscopy in toluene.

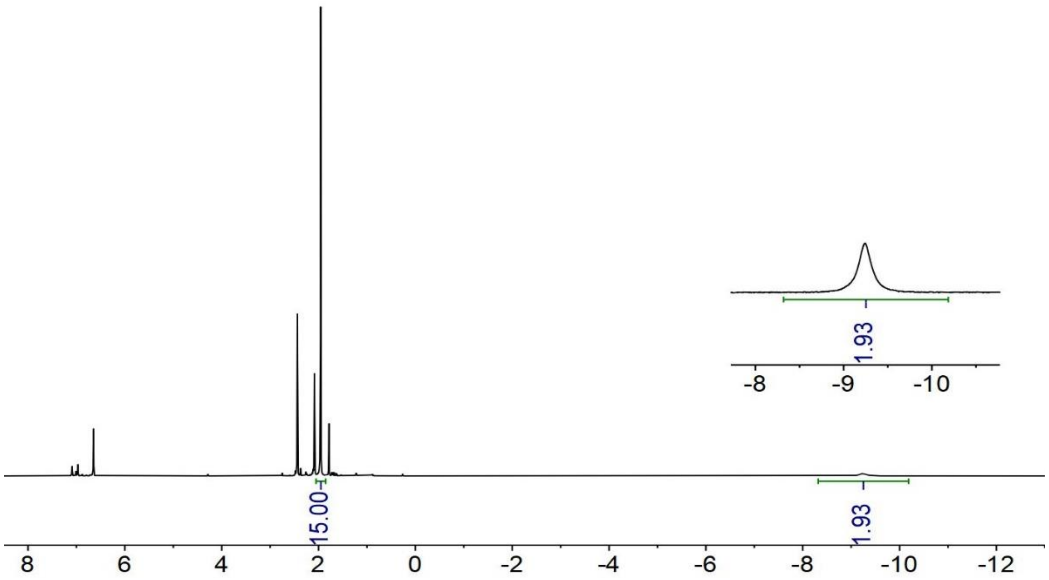


Figure S18. ^{1}H NMR (400 MHz, 298 K, toluene-d_8) spectrum of compound **3a-H/D**.

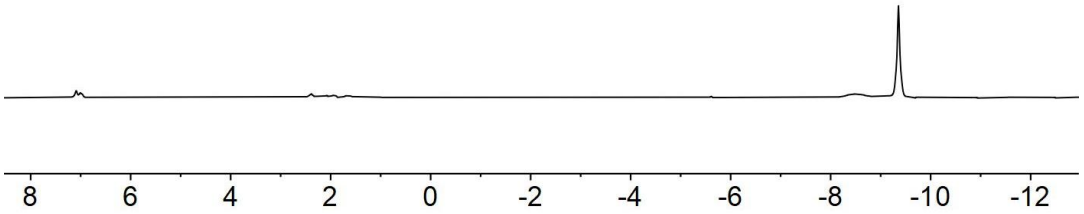
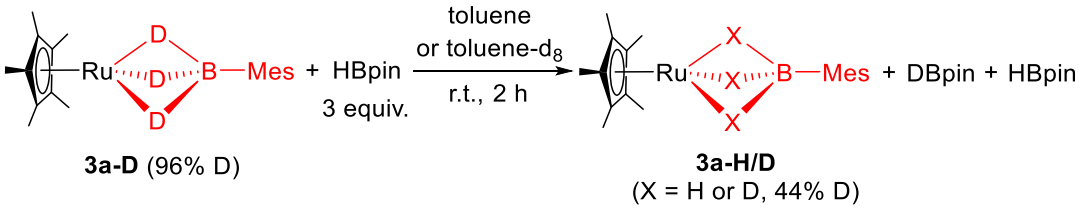


Figure S19. ^{2}H NMR (77 MHz, 298 K, toluene) spectrum of compound **3a-H/D**.

Reaction of 3a-D with HBpin



3a-D (96% D)

3a-H/D
(X = H or D, 44% D)

Scheme S5

Following the same procedure of synthesis of compound **3a**, reaction of [Cp*RuCl]$_4$ and Li[MesBD$_3$] gave **3a-D** as a yellow crystalline solid, which was 96% deuterium as determined by ^{1}H NMR. In an NMR tube, compound **3a-D** (11.2 mg, 0.03 mmol) and HBpin (11.5 mg, 0.09 mmol) were dissolved in toluene-d$_8$ (0.6 mL). After 2 h at room temperature, NMR experiments were conducted. ^{1}H NMR spectroscopy studies revealed there was only 44% deuterium according to the integration of the hydride signal, indicating that B-H/B-D oxidative addition and H/D exchange were occurred. Additionally, the concomitant formation of DBpin via the H/D exchange process was judged by ^{11}B NMR, which was also confirmed by

^{2}H NMR spectroscopy of the same reaction in toluene.

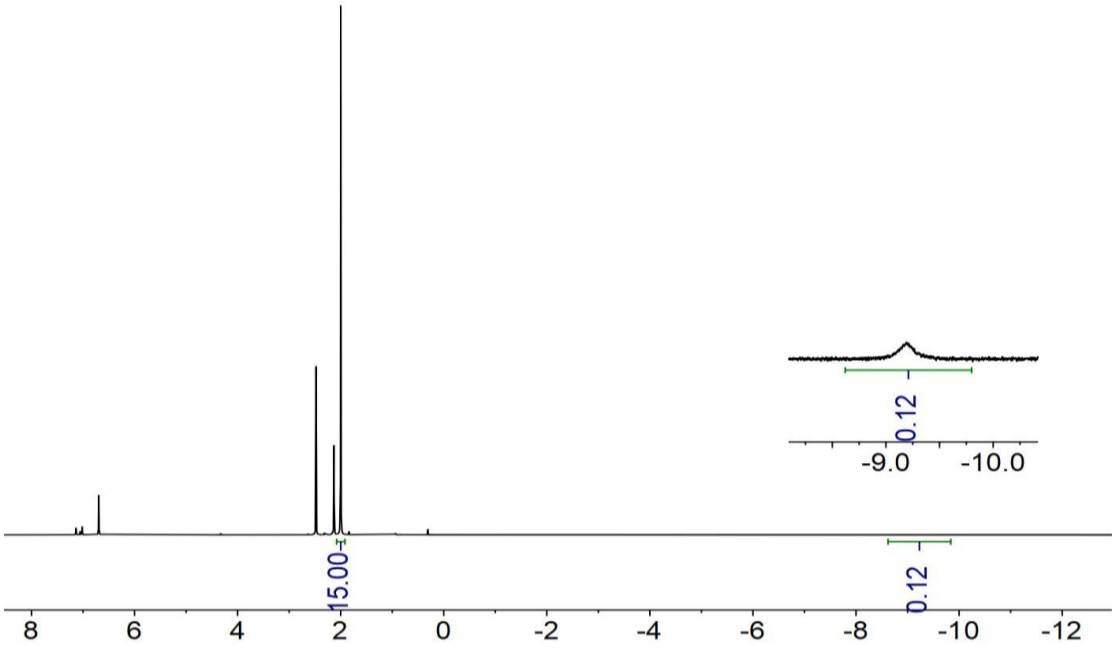


Figure S20. ^{1}H NMR (400 MHz, 298 K, toluene-d_8) spectrum of compound **3a-D**.

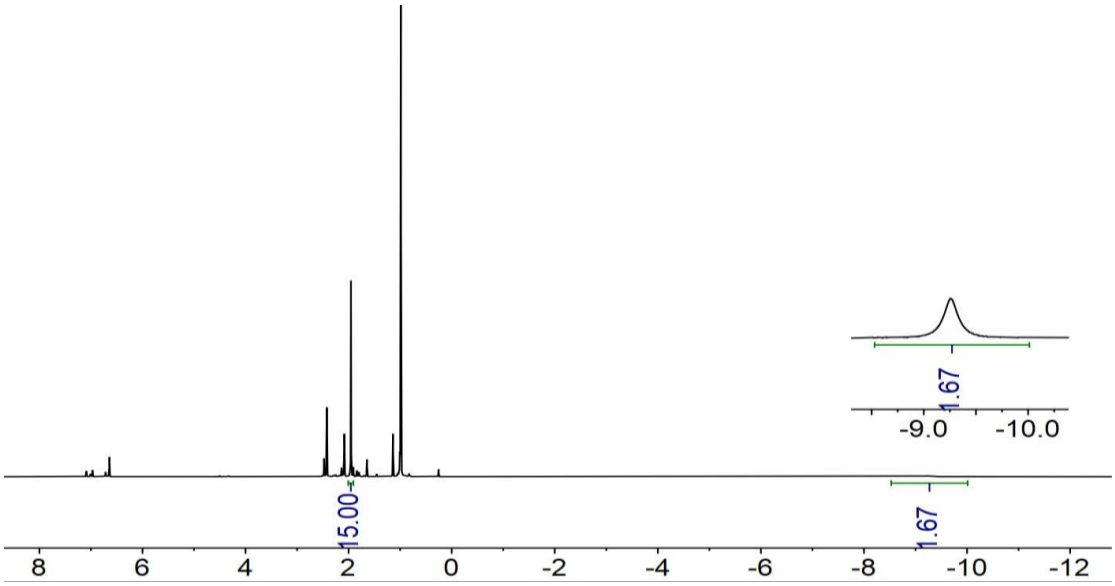


Figure S21. ^{1}H NMR (400 MHz, 298 K, toluene-d_8) spectrum of the reaction between compound **3a-D** and HBpin.

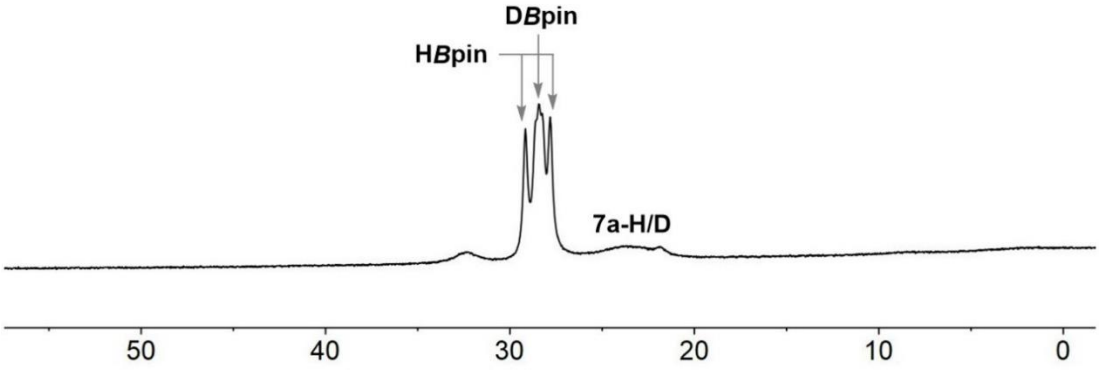


Figure S22. ^{11}B NMR (128 MHz, 298 K, toluene-d_8) spectrum of the reaction between compound **3a-D** and HBpin.

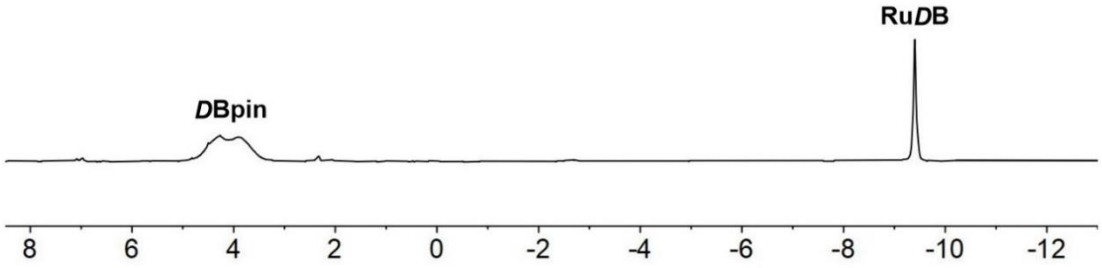
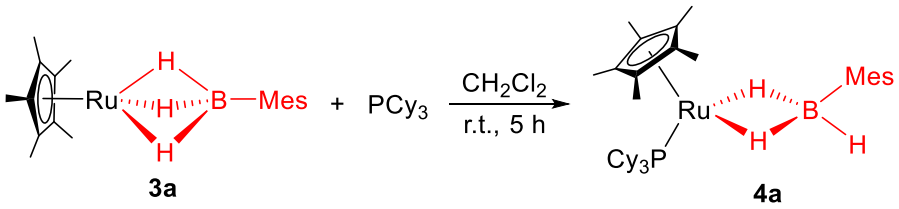


Figure S23. ^{2}H NMR (77 MHz, 298 K, toluene) spectrum of the reaction between compound **3a-D** and HBpin.

NMR spectra and crystallographic data of compound 4a



Scheme S6

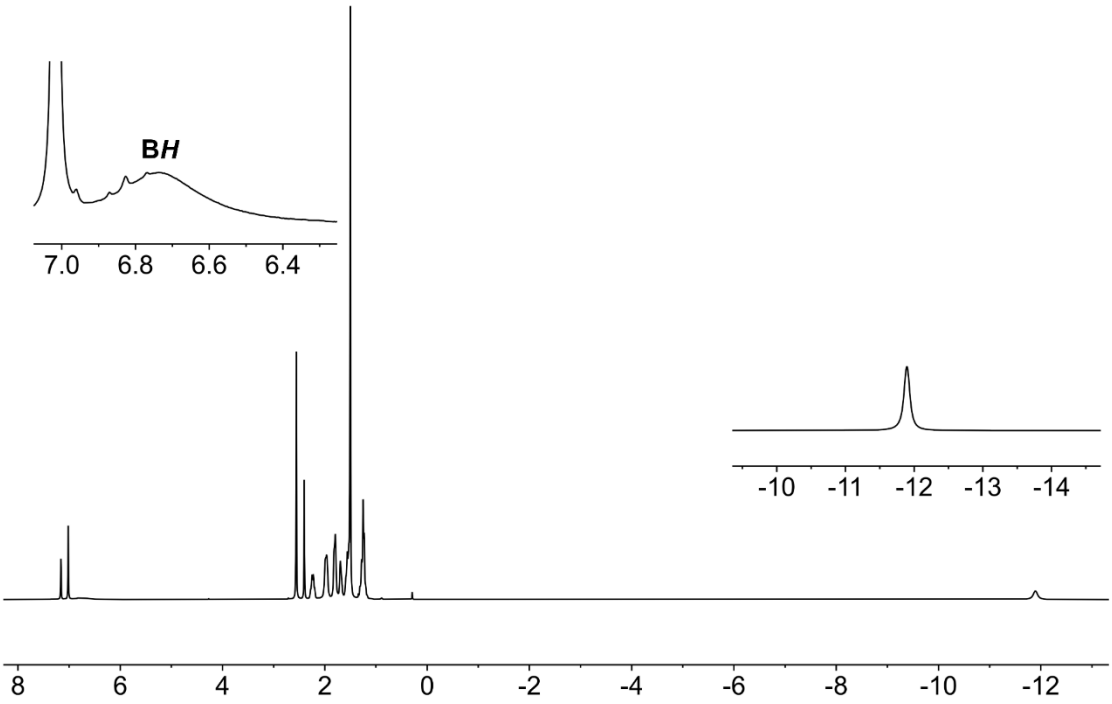


Figure S24. ^{1}H NMR (400 MHz, 298 K, C_6D_6) spectrum of **4a**.

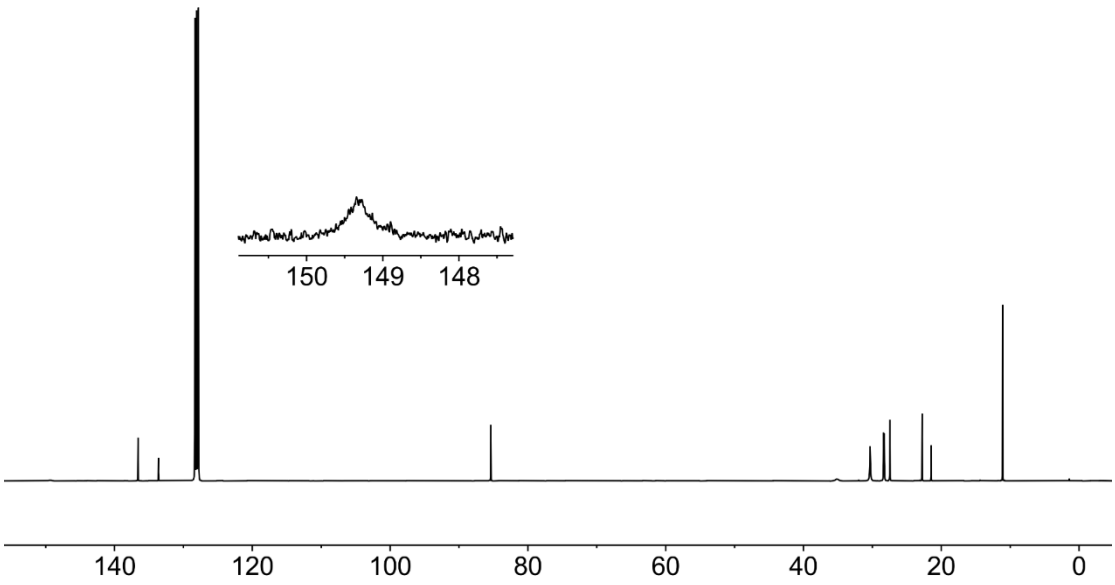


Figure S25. ^{13}C{^{1}H} NMR (101 MHz, 298 K, C_6D_6) spectrum of **4a**.

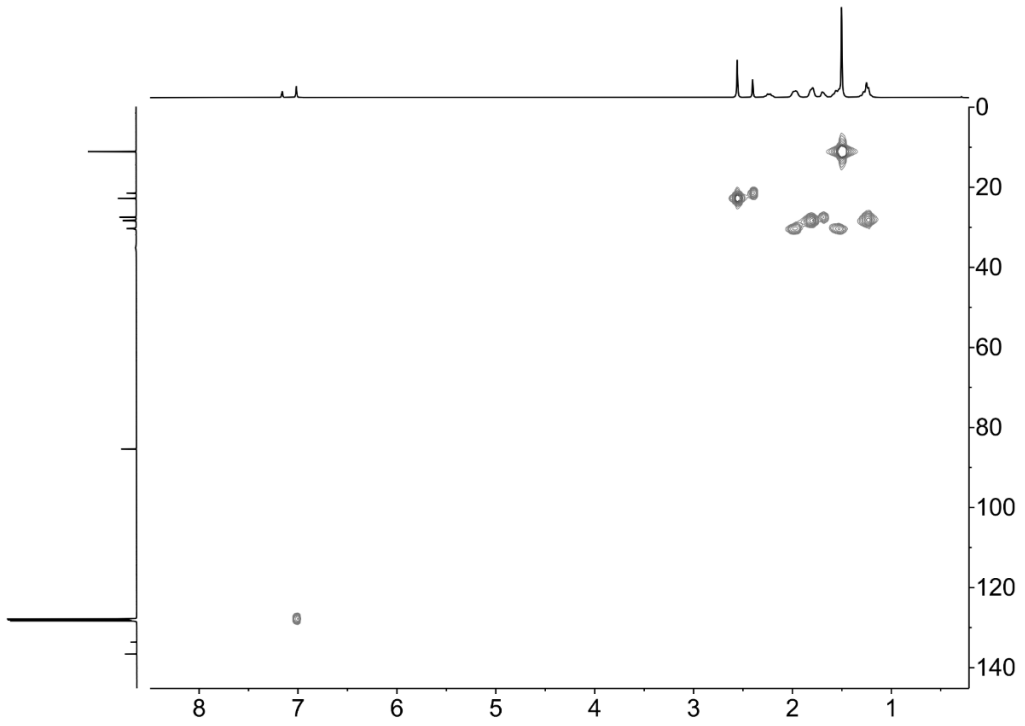


Figure S26. ^{1}H-^{13}C GHSQC (400 MHz/101 MHz, 298 K, C_6D_6) spectrum of **4a**.

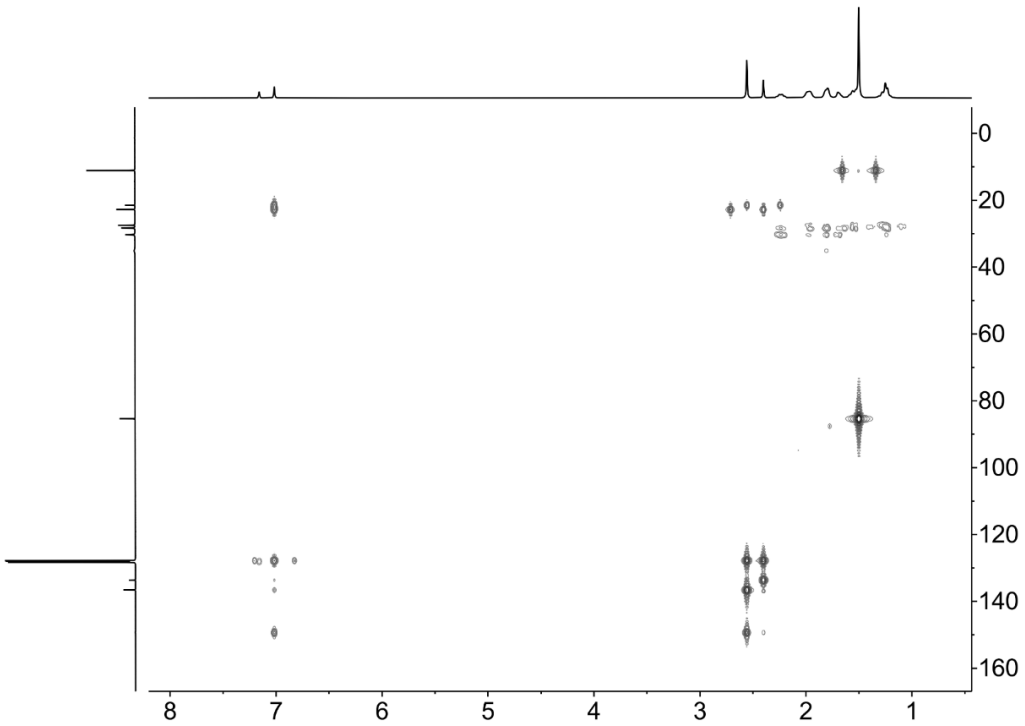


Figure S27. ^{1}H-^{13}C GHMBC (400 MHz/101 MHz, 298 K, C_6D_6) spectrum of **4a**.

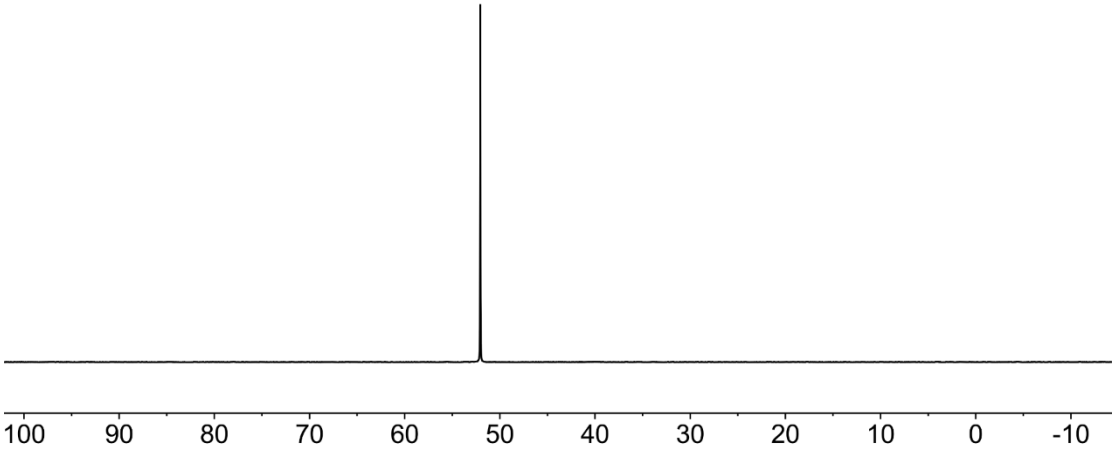


Figure S28. $^{31}P\{^{1}H\}$ NMR (162 MHz, 298 K, C_6D_6) spectrum of **4a**.

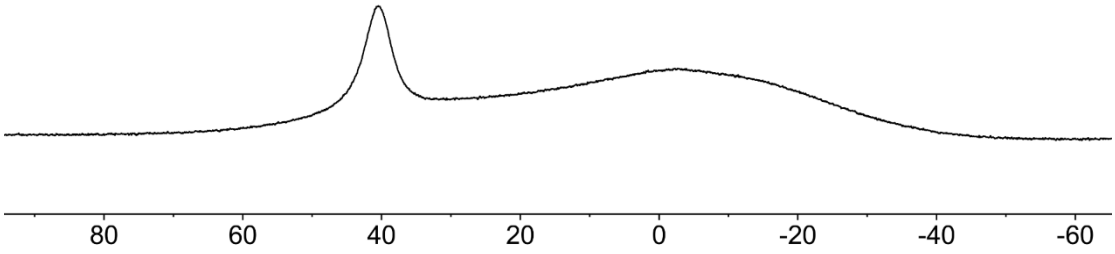


Figure S29. ^{11}B NMR (128 MHz, 298 K, C_6D_6) spectrum of **4a**.

X-ray crystal structure analysis of compound 4a: formula $C_{37}H_{62}BPRu$, M = 649.71, red crystal，0.38 x 0.26 x 0.18 mm，a = 10.0172(2), b = 12.1842(2), c = 16.9434(3) Å, α = 65.7160(10), β = 81.0310(10), γ = 64.7590(10)°, V = 1704.54(6) Å^3, ρ_{calc} = 1.266 g·cm^{-3}, μ = 0.530 mm^{-1}, empirical absorption correction (0.6758≤ T ≤ 0.7456), Z = 2, triclinic, space group $P\bar{1}$ (No. 2), λ = 0.71073 Å, T = 173 K, ω and φ scans, 8260 reflections collected (±h, ±k, ±l), 5799 independent (R_{int} = 0.0145) and 5378 observed reflections [I>2σ(I)], 381 refined parameters, R = 0.0243, wR^2 = 0.0610, max. (min.) residual electron density 0.59 (-0.55) e.Å^{-3}.

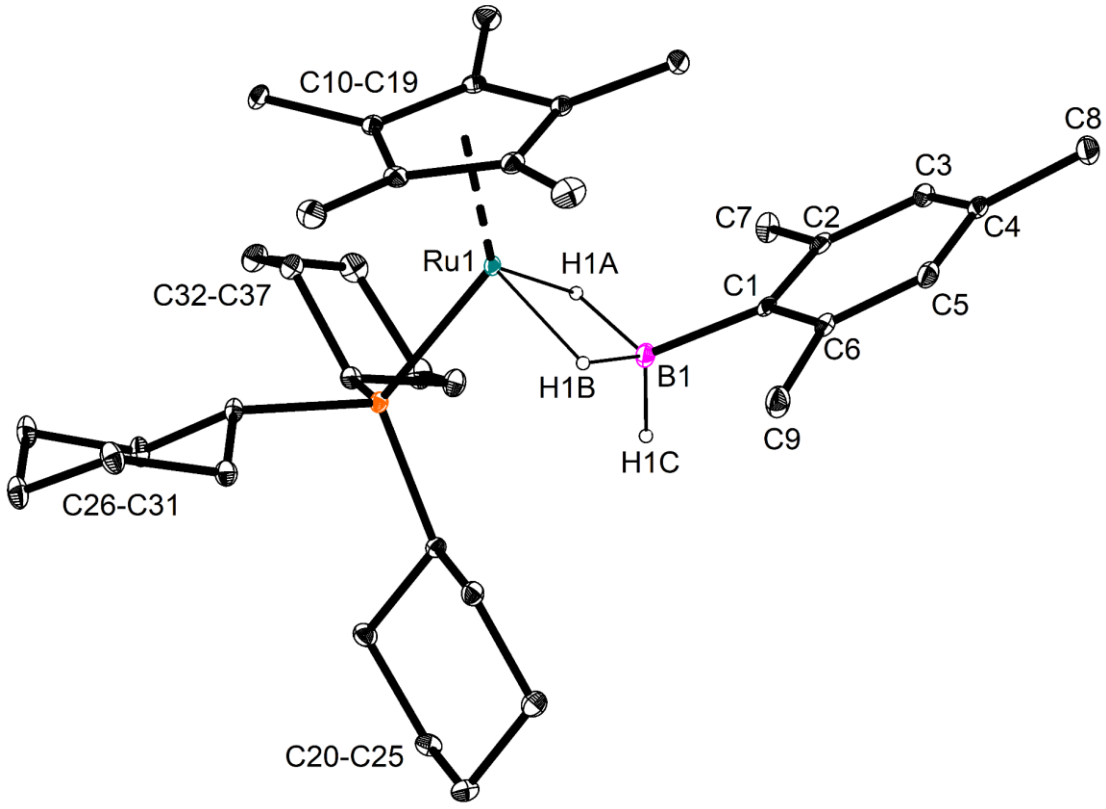
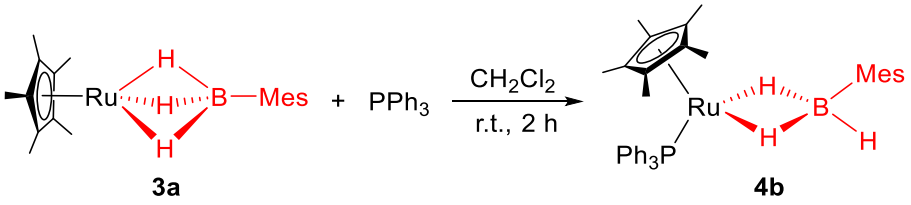


Figure S30. Molecular structure of **4a** (thermal ellipsoids are shown at the 30% probability level).

NMR spectra and crystallographic data of compound 4b



Scheme S7

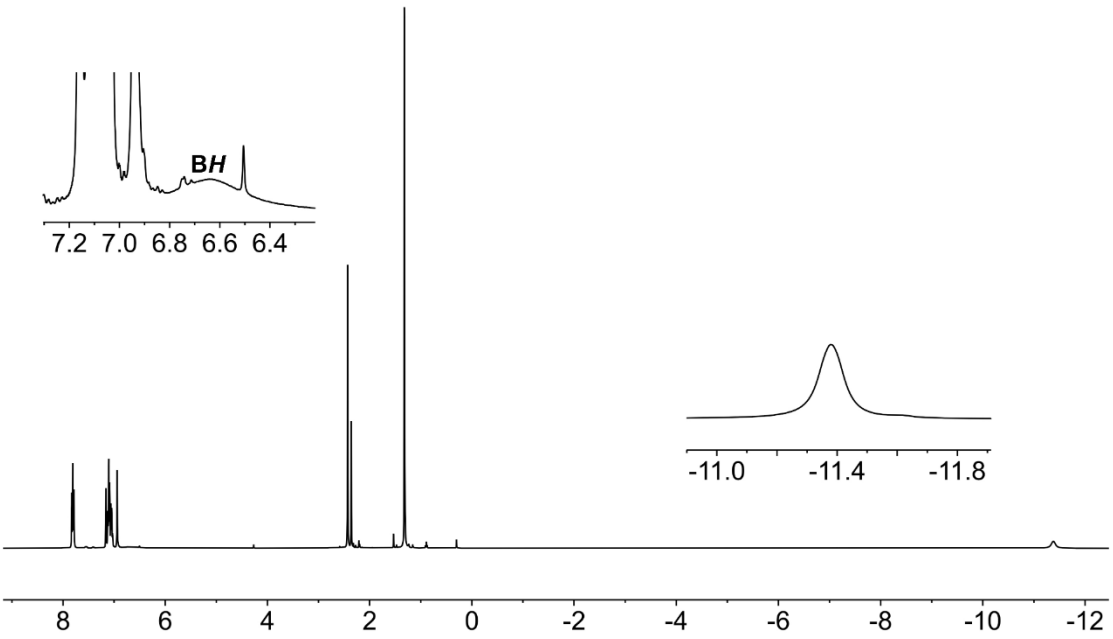


Figure S31. ^{1}H NMR (400 MHz, 298 K, C_6D_6) spectrum of **4b**.

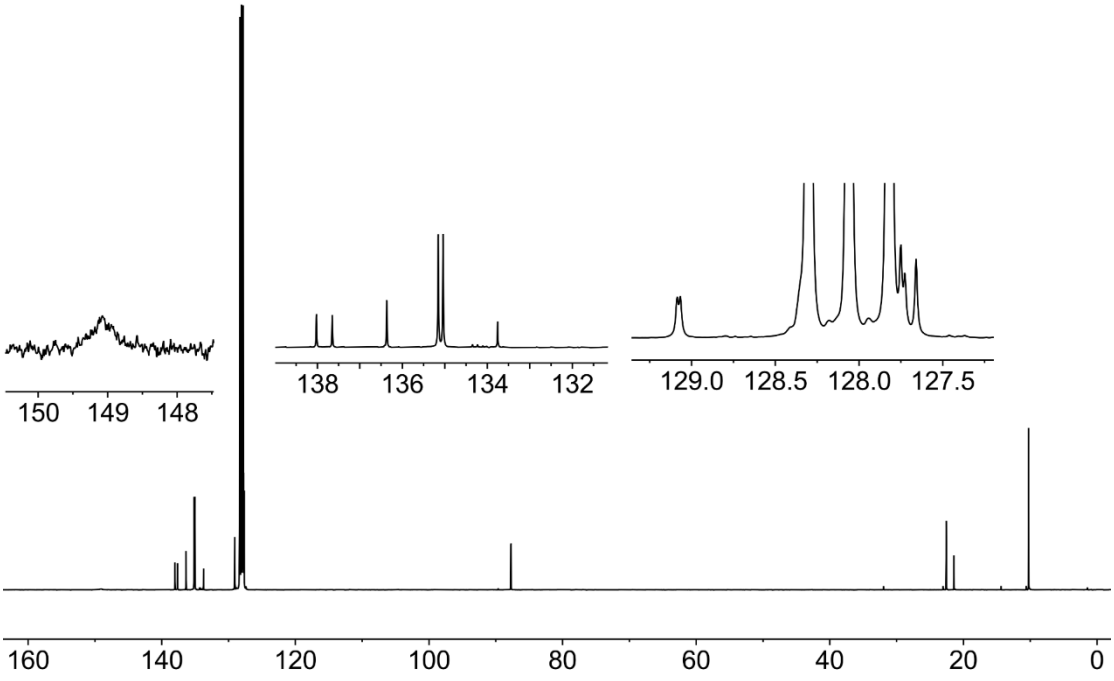


Figure S32. ^{13}C{^{1}H} NMR (101 MHz, 298 K, C_6D_6) spectrum of **4b**.

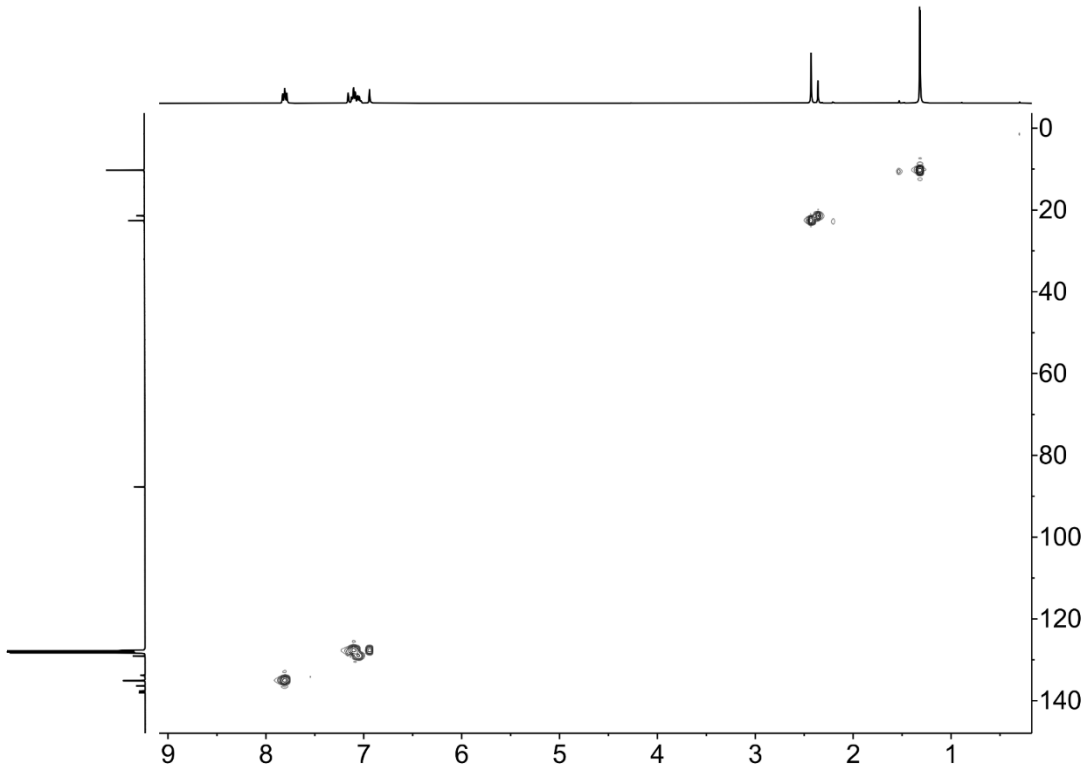


Figure S33. ^{1}H-^{13}C GHSQC (400 MHz/101 MHz, 298 K, C_6D_6) spectrum of **4b**.

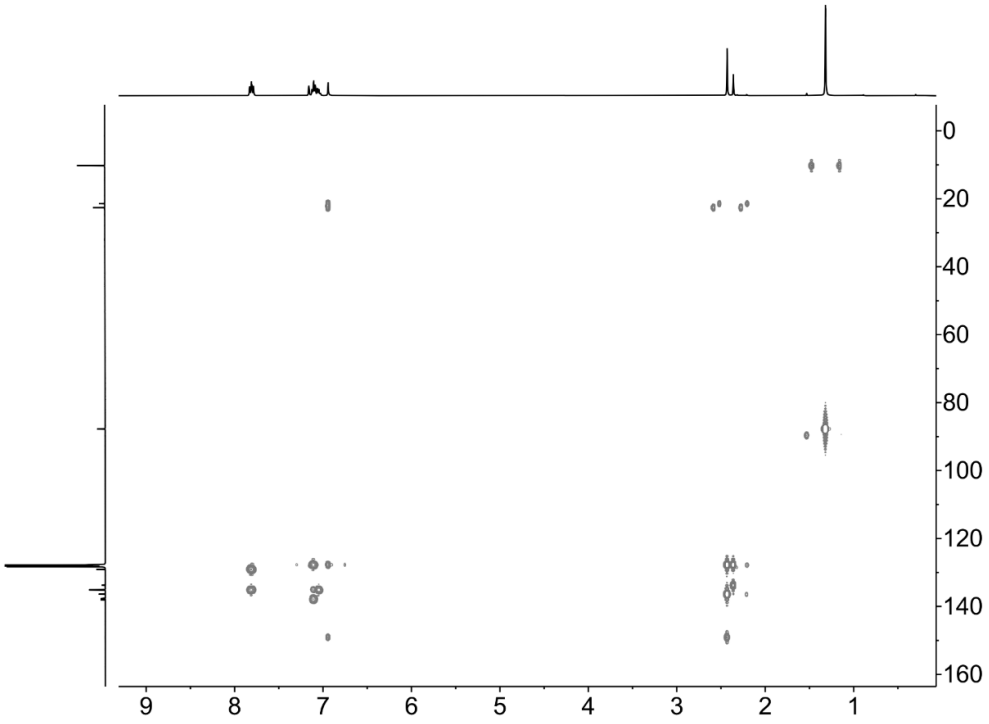


Figure S34. ^{1}H-^{13}C GHMBC (400 MHz/101 MHz, 298 K, C_6D_6) spectrum of **4b**.

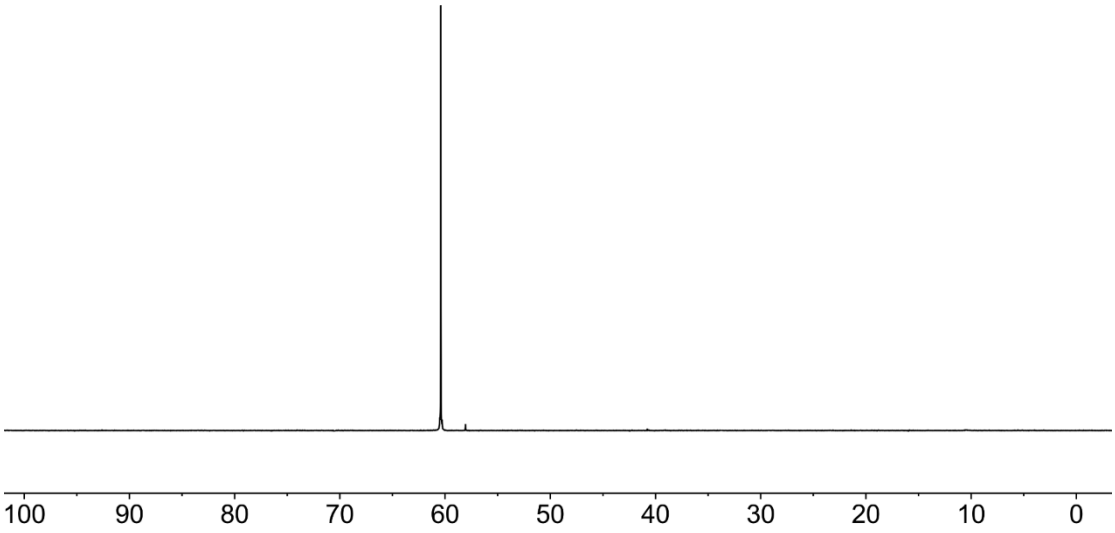


Figure S35. $^{31}P\{^{1}H\}$ NMR (162 MHz, 298 K, C_6D_6) spectrum of **4b**.

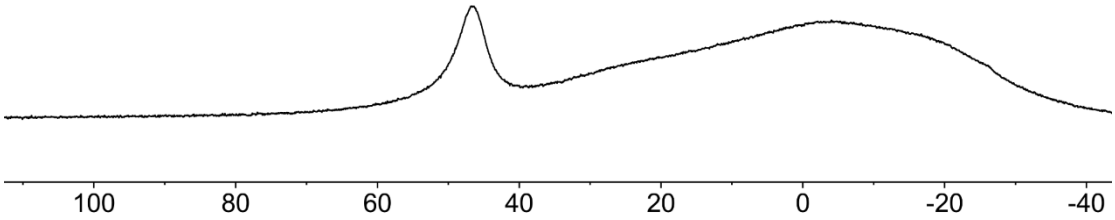


Figure S36. ^{11}B NMR (128 MHz, 298 K, C_6D_6) spectrum of **4b**.

X-ray crystal structure analysis of compound 4b: formula $C_{37}H_{44}BPRu$, M = 631.57, yellow crystal，0.27 x 0.24 x 0.2 mm，a = 9.61760(10), b = 10.06670, c = 17.7082(2) Å, α = 85.50, β = 88.45, γ = 69.31°, V = 1598.95(3) Å^3, ρ_{calc} = 1.312 g·cm^{-3}, μ = 0.564 mm^{-1}, empirical absorption correction ($0.6672 \leq T \leq 0.7465$), Z = 2, triclinic, space group $P\bar{1}$ (No. 2), λ = 0.71073 Å, T = 173 K, ω and φ scans, 15972 reflections collected ($\pm h$, $\pm k$, $\pm l$), 9529 independent (R_{int} = 0.0143) and 8868 observed reflections [$I>2\sigma(I)$], 381 refined parameters, R = 0.0238, wR^2 = 0.0609, max. (min.) residual electron density 0.68 (-0.86) e.Å^{-3}.

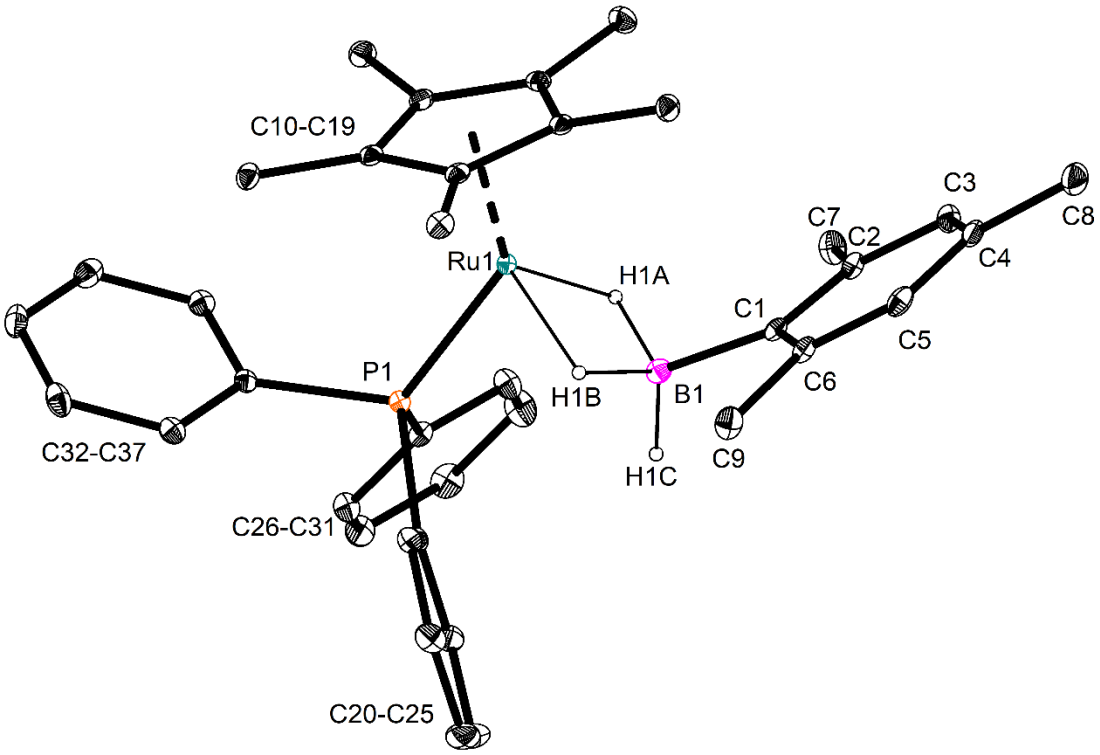
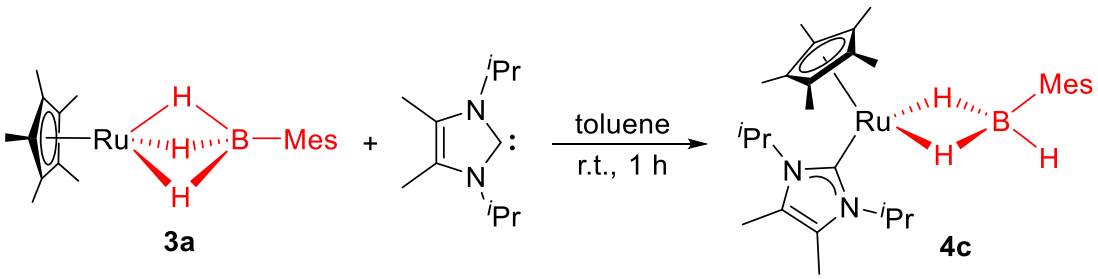


Figure S37. Molecular structure of **4b** (thermal ellipsoids are shown at the 30% probability level).

NMR spectra and crystallographic data of compound 4c



Scheme S8

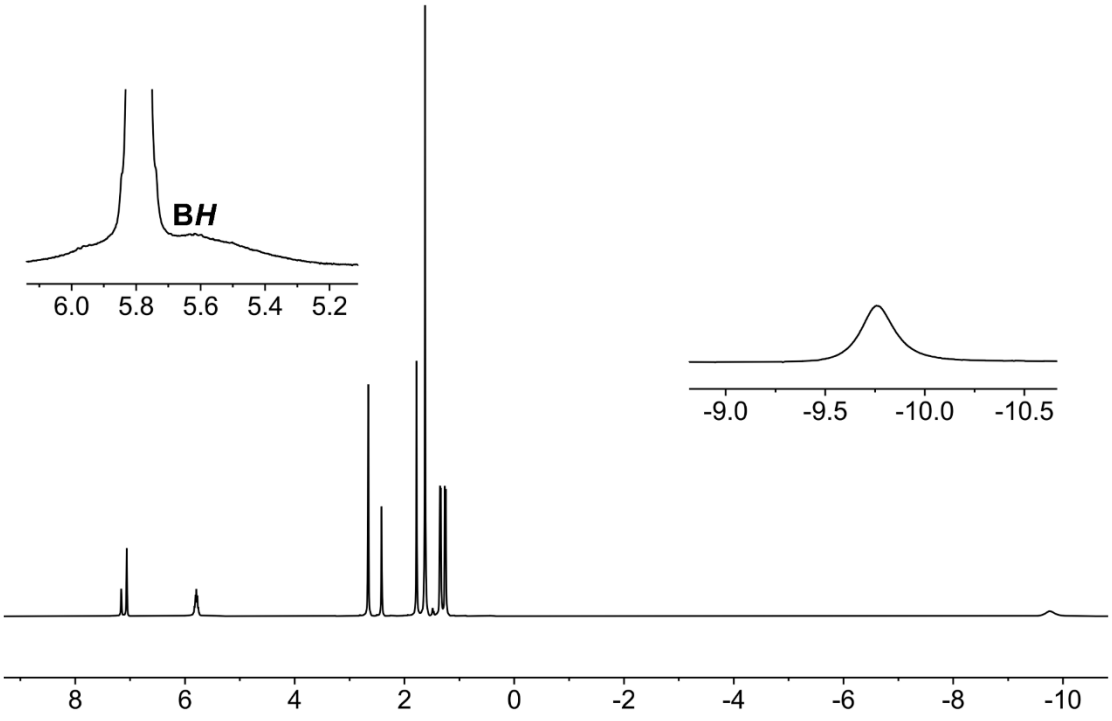


Figure S38. ^{1}H NMR (400 MHz, 298 K, C_6D_6) spectrum of **4c**.

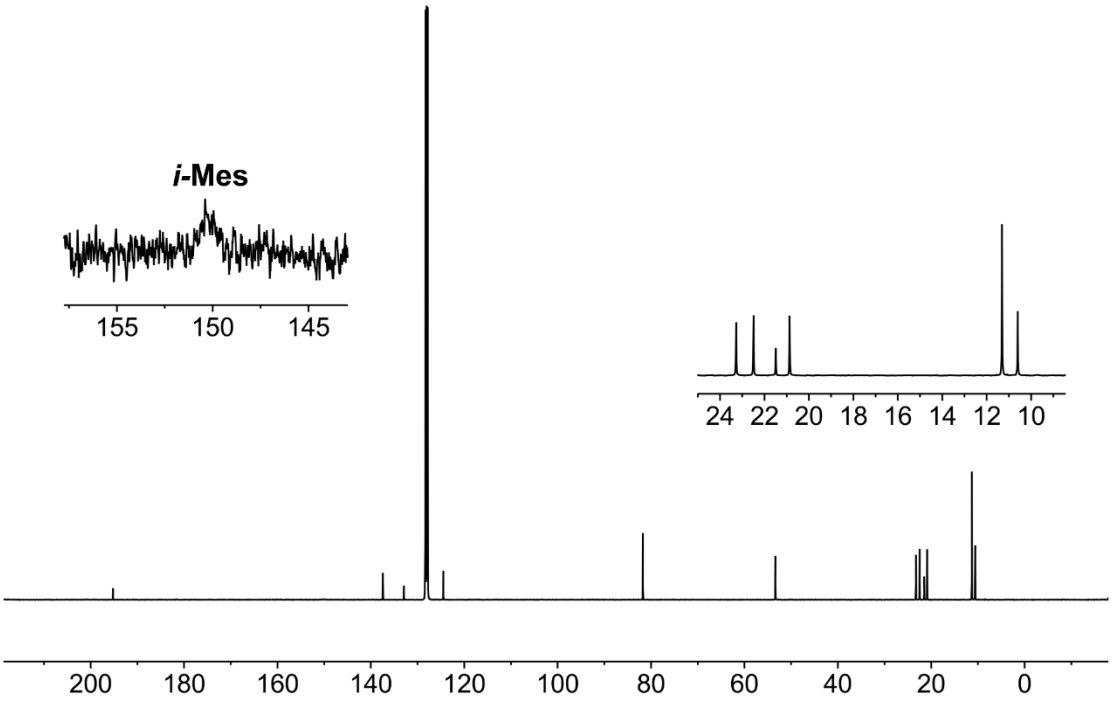


Figure S39. ^{13}C{^{1}H} NMR (101 MHz, 298 K, C_6D_6) spectrum of **4c**.

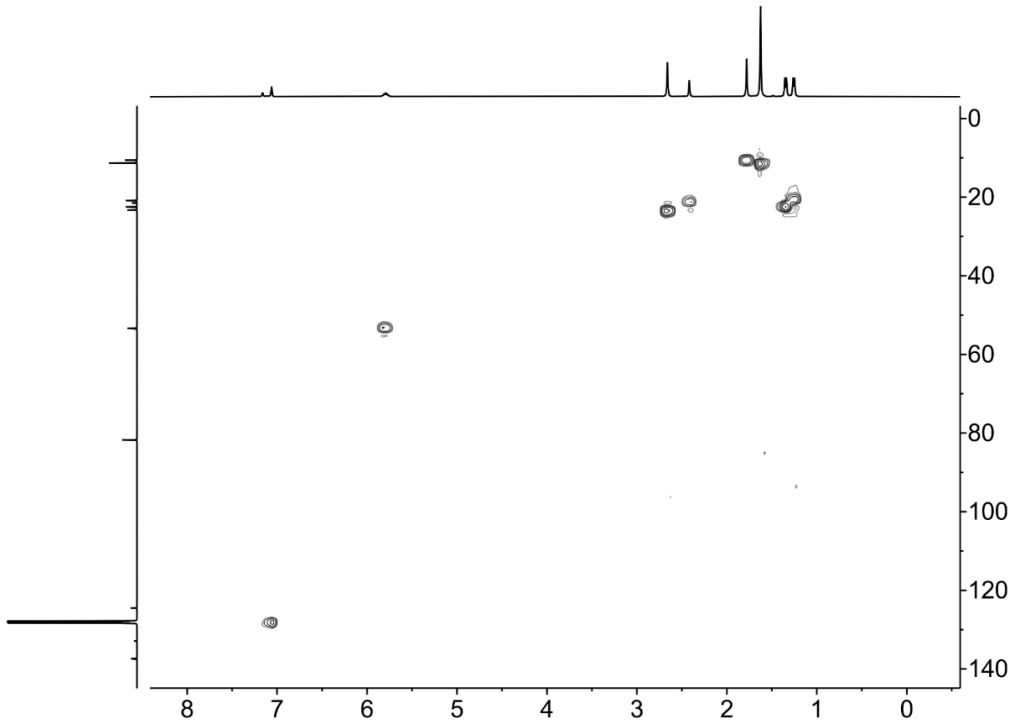


Figure S40. ^{1}H-^{13}C GHSQC (400 MHz/101 MHz, 298 K, C_6D_6) spectrum of **4c**.

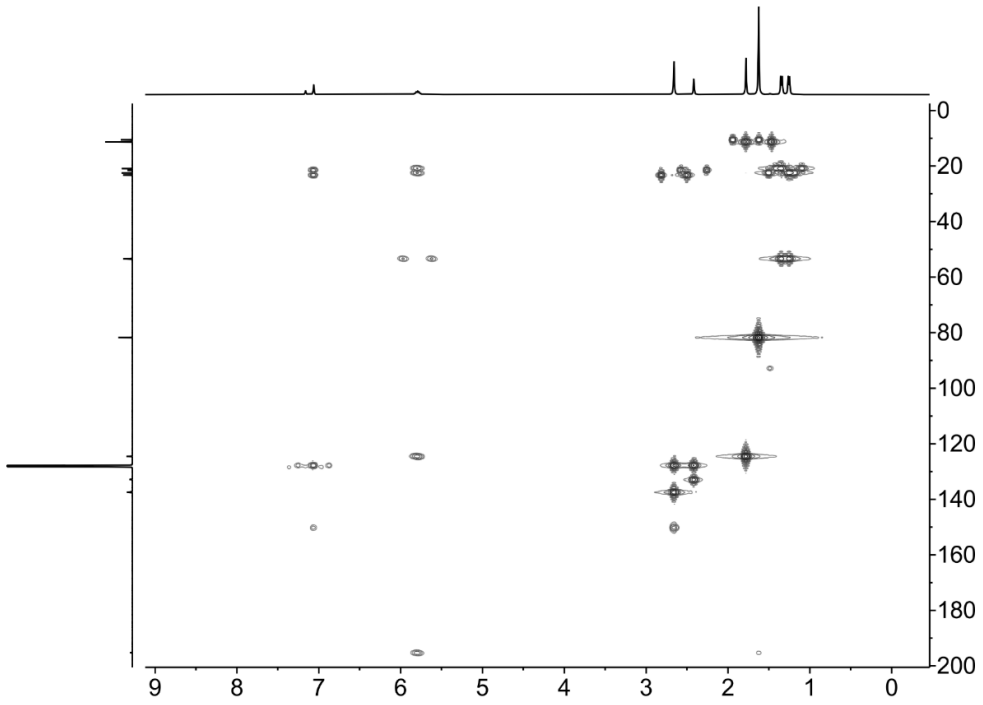


Figure S41. ^{1}H-^{13}C GHMBC (400 MHz/101 MHz, 298 K, C_6D_6) spectrum of **4c**.

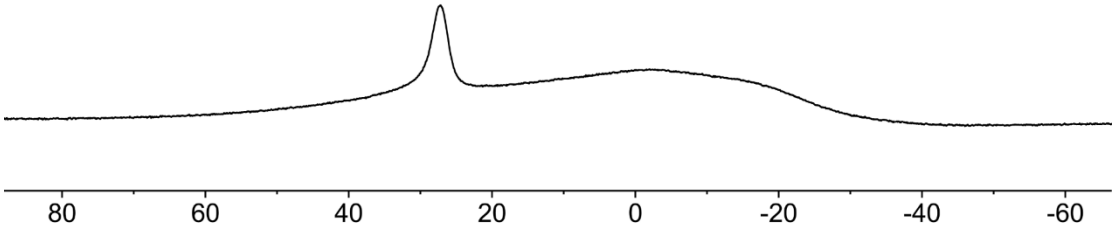


Figure S42. ^{11}B NMR (128 MHz, 298 K, C_6D_6) spectrum of **4c**.

X-ray crystal structure analysis of compound 4c: formula $C_{30}H_{49}BN_2Ru$, M = 549.59, yellow crystal, 0.42 x 0.25 x 0.12 mm，a = 10.782(4), b = 12.152(4), c = 12.316(4) Å, α = 112.688(8), β = 97.811(8), γ = 90.370(9)°, V = 1471.9(9) Å^3, ρ_{calc} = 1.240 g·cm^{-3}, μ = 0.552 mm^{-1}, empirical absorption correction (0.6855≤ T ≤ 0.7465), Z = 2, triclinic, space group $P\bar{1}$ (No. 2), λ = 0.71073 Å, T = 120 K, ω and φ scans, 44116 reflections collected (±h, ±k, ±l), 8964 independent (R_{int} = 0.0425) and 8100 observed reflections [I>2σ(I)], 503 refined parameters, R = 0.0249, wR^2 = 0.0606, max. (min.) residual electron density 0.47 (-0.72) e.Å^{-3}.

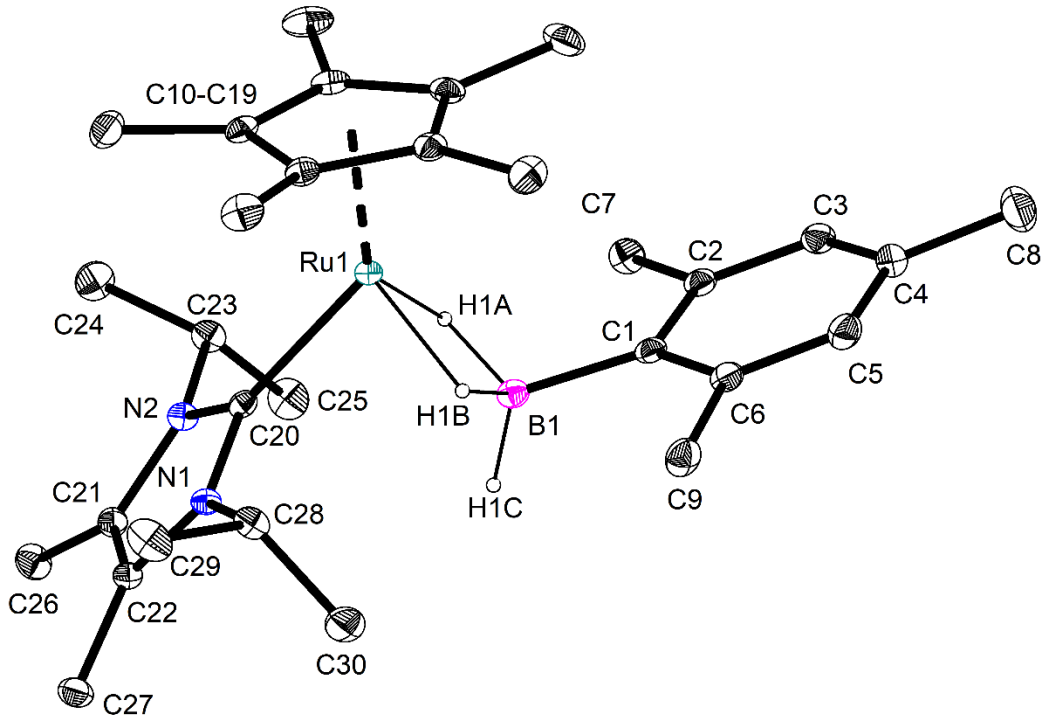


Figure S43. Molecular structure of **4c** (thermal ellipsoids are shown at the 30% probability level).

Computational details

Geometry optimizations of **3a-c** were performed at the BP86[1,2]/def2-TZVPP[3] level, in combination with RI[4] and the def2/J auxiliary basis set[5] planted in the ORCA4.2.1 suite of programs.[6,7] During the calculations, the D3 dispersion correction suggested by Grimme et al[8,9] was used to accelerate the calculation. All species were characterized as local minima by analytic frequency calculations. The natural population analysis (NPA) have been performed using the natural bond orbital (NBO) analysis. The topology of the electron density was conducted through the Multiwfn program package.[10] [(1) A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098-3100.

(2) J. P. Perdew, *Phys. Rev. B*, 1986. **33**, 8822-8824. (3) F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297-3305. (4) K. Eichkorn, O. Treutler, H. Öhm, M. Häser and R. Ahlrichs, *Chem. Phys. Lett.*, 1995, **242**, 652-660. (5) F. Weigend, *Phys. Chem. Chem. Phys.*, 2006, **8**, 1057-1065. (6) F. Neese, *WIREs. Comput. Mol. Sci.*, 2012, **2**, 73-78. (7) F. Neese, *WIREs. Comput. Mol. Sci.*, 2018, **8**, e1327; (8) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104; (9) S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456-1465. (10) T. Lu and F. W. Chen, *J. Comput. Chem.*, 2012, **33**, 580-592. (11) I. Mayer, I., *Chem. Phys. Lett.*, 1983, **97**, 270-274.]

Table S2 Calculated important geometrical parameters such as Ru-H, B-H and Ru-B bond lengths (in Å) and their corresponding average Mayer bond orders (MBO)[11] for the complexes **3a-c**. (Experimental values are given in parenthesis)

Molecules	bond	length	MBO	bond	length	MBO	bond	length	MBO
3a	Ru-H	1.767	0.441	Ru-B	1.945 (1.958)	0.625	B-1H	1.358	0.564
	Ru-H	1.758	0.475				B-2H	1.371	0.525
	Ru-H	1.753	0.464				B-3H	1.383	0.552
3b	Ru-H	1.764	0.395	Ru-B	1.944 (1.958)	0.621	B-1H	1.358	0.599
	Ru-H	1.752	0.46				B-2H	1.379	0.526
	Ru-H	1.745	0.439				B-3H	1.381	0.526
3c	Ru-H	1.759	0.461	Ru-B	1.946 (1.961)	0.668	B-1H	1.375	0.543
	Ru-H	1.771	0.399				B-2H	1.353	0.601
	Ru-H	1.754	0.435				B-3H	1.378	0.551

Table S3 Calculated Natural charges at boron (q_B) and metal center (q_{Ru}) for the complexes **3a-c**.

Molecules	q_B	q_{Ru}
3a	-0.023	-0.176
3b	-0.03	-0.182
3c	-0.04	-0.174

Table S4 Topological parameters at the bond critical points of the B-H and Ru-B bonds of **3a-c**. (All values are in a.u.)

Molecules	BCP	ρ(r)	$\nabla^2\rho(r)$	H(r)
3a	B-H	0.134	-0.212	-0.108
	B-H	0.129	-0.184	-0.095
	B-H	0.131	-0.200	-0.101
	Ru-B	0.130	0.034	-0.087
3b	B-H	0.134	-0.212	-0.108
	B-H	0.130	-0.188	-0.097
	B-H	0.129	-0.189	-0.096
	Ru-B	0.131	0.034	-0.088
3c	B-H	0.130	-0.192	-0.098
	B-H	0.134	-0.216	-0.111
	B-H	0.130	-0.197	-0.099
	Ru-B	0.130	0.036	-0.087

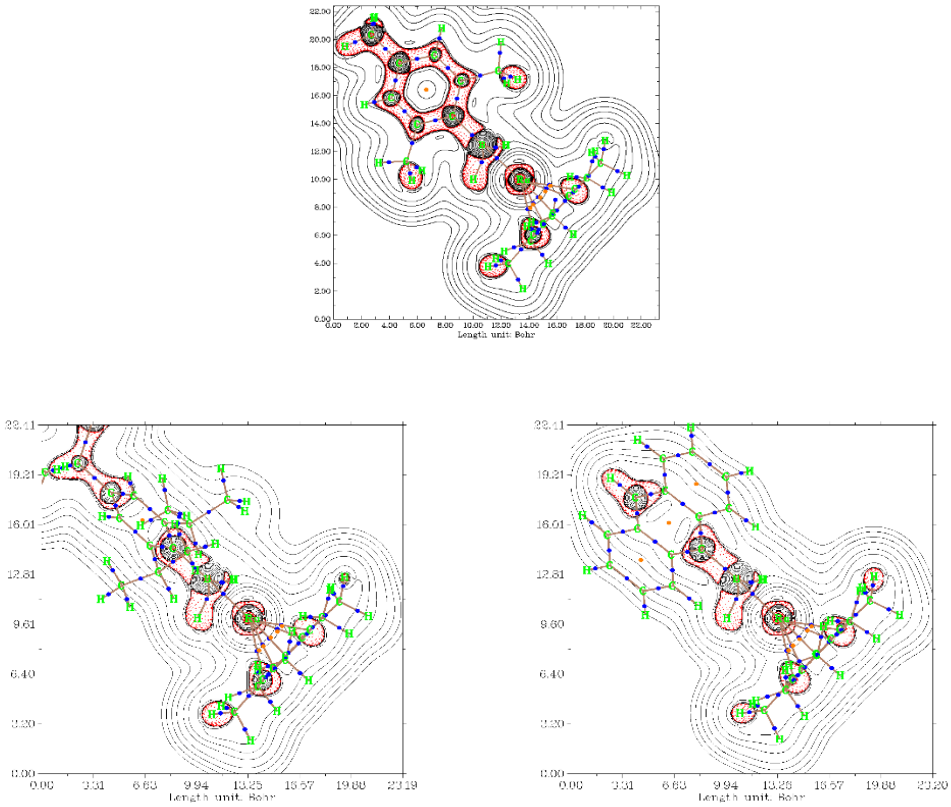


Fig. S44 Contour line diagrams of the $\nabla^2\rho(r)$ of **3a**(top), **3b** (left, bottom) and **3c** (right, bottom) in the plane of B-H-Ru. Dashed red lines indicate areas of charge concentration ($\nabla^2\rho(r) < 0$), while solid black lines show areas of charge depletion ($\nabla^2\rho(r) > 0$). Solid brown lines connecting the atomic nuclei are the bond paths. Blue and orange dots indicate BCPs and RCPs.

Cartesian coordinates for the calculated structure of **3a** (in Å).

C	-2.646502	8.776548	7.320186
C	-2.342181	6.799071	5.925728
C	-3.380382	7.241431	5.102660
H	-3.663069	6.637711	4.236024
C	-3.682552	9.185828	6.473686
H	-4.204789	10.120914	6.690354
C	-4.066854	8.434231	5.359418
C	-2.277709	9.642187	8.500035
H	-2.411456	9.105542	9.451230

H	-2.894829	10.548666	8.530783
H	-1.222371	9.947986	8.460238
C	-5.169555	8.902349	4.446162
H	-4.761397	9.289002	3.499784
H	-5.756118	9.706897	4.907838
H	-5.853602	8.081135	4.189646
C	-1.643822	5.501862	5.602641
H	-0.552259	5.626799	5.569862
H	-1.978900	5.107010	4.635517
H	-1.845260	4.739051	6.370220
C	-1.961248	7.565326	7.057378
B	-0.817304	7.065341	7.975668
Ru	0.632066	6.399230	9.088708
H	-0.668266	7.588823	9.219290
H	-0.792777	5.734194	8.302617
H	0.485315	7.185030	7.528082
C	1.457200	6.308740	11.092632
C	1.189535	4.973275	10.628197
C	2.748500	5.944627	9.184511
C	2.424484	6.917131	10.204055
C	0.874739	6.944176	12.314818
H	1.508449	6.749260	13.195007
H	-0.126744	6.551693	12.528064
H	0.790608	8.031846	12.197237
C	0.296307	3.971474	11.285084
H	0.860417	3.346528	11.997005
H	-0.164725	3.302444	10.547386
H	-0.513638	4.460649	11.839914
C	2.067045	3.469010	8.667855
H	2.339934	3.650952	7.621129
H	1.104035	2.943534	8.674283
H	2.821871	2.791219	9.099437
C	3.743400	6.132925	8.084439
H	3.783930	7.178933	7.757816
H	3.495136	5.518737	7.209947
H	4.753145	5.845855	8.420187
C	3.042434	8.269102	10.364247
H	3.945303	8.221310	10.995100
H	2.344196	8.974086	10.832776
H	3.335685	8.689339	9.394448
C	1.990174	4.746862	9.440398

Cartesian coordinates for the calculated structure of **3b** (in Å).

B	6.453515	13.992987	4.550730
H	7.065981	15.157124	4.213297
H	6.055192	13.588718	3.293663
H	7.588097	13.215074	4.673122
C	5.407979	13.939541	5.698087
C	4.915066	15.117180	6.322800
C	3.976329	15.011195	7.350847
H	3.595768	15.918258	7.820333
C	3.498820	13.771150	7.790497
C	3.985250	12.619531	7.170061
H	3.611457	11.650644	7.505431
C	4.922055	12.679706	6.132951
C	5.434480	16.486444	5.904784
H	5.624657	16.442290	4.821147
C	6.777197	16.777395	6.600273
H	6.642202	16.809914	7.691588
H	7.183916	17.746231	6.274963
H	7.520064	16.000984	6.373139
C	4.447634	17.635276	6.143896
H	3.463790	17.421542	5.705193
H	4.832422	18.559309	5.690946
H	4.304779	17.836541	7.214957
C	2.465847	13.677726	8.897804
H	2.270526	12.605819	9.065092
C	1.139389	14.337456	8.483401
H	0.378035	14.210760	9.267192
H	0.753818	13.898611	7.553656
H	1.273128	15.415748	8.314598
C	2.988596	14.270924	10.216408
H	3.924164	13.785898	10.524593
H	2.250512	14.141817	11.021629
H	3.186721	15.347140	10.111761
C	5.443688	11.391274	5.510253
H	5.797206	11.635457	4.497634
C	4.375506	10.298992	5.367483
H	4.045302	9.913744	6.343009
H	4.780445	9.446729	4.803957
H	3.490696	10.673615	4.836006
C	6.656766	10.873573	6.304248
H	7.456323	11.626631	6.339797
H	7.063916	9.961057	5.844892
H	6.368450	10.638245	7.338854
Ru	7.755771	13.968126	3.108223

C	8.058960	13.831563	0.963171
C	8.628683	15.061518	1.443996
C	9.665192	14.729657	2.403150
C	9.726338	13.294728	2.505546
C	8.731890	12.730664	1.620049
C	10.685260	12.515193	3.348148
H	10.251228	11.559185	3.664573
H	11.607366	12.296020	2.786700
H	10.966645	13.069907	4.251468
C	8.500363	11.276171	1.364193
H	7.458237	11.084723	1.079971
H	9.143346	10.906805	0.548508
H	8.714978	10.674296	2.256435
C	6.988507	13.705455	-0.072419
H	6.311993	14.569125	-0.056145
H	7.426487	13.640258	-1.081467
H	6.384580	12.804043	0.088490
C	8.270369	16.439530	0.988020
H	8.407038	17.173918	1.791854
H	8.902492	16.751437	0.140922
H	7.224224	16.492504	0.662421
C	10.555338	15.706473	3.101797
H	11.433062	15.955716	2.483668
H	10.026531	16.642388	3.321754
H	10.920959	15.302591	4.053239

Cartesian coordinates for the calculated structure of **3c** (in Å).

B	3.837121	9.923125	3.380534
C	3.992026	11.163302	4.302992
C	4.873010	11.168517	5.418963
C	5.622306	10.016783	5.812683
H	5.504478	9.096012	5.243890
C	6.470978	10.042505	6.893390
H	7.023649	9.143971	7.169321
C	6.634826	11.229264	7.659242
H	7.314200	11.234543	8.512056
C	5.932110	12.359668	7.324824
H	6.041862	13.275842	7.908056
C	5.035224	12.368876	6.213935
C	4.308912	13.517139	5.880868
H	4.438279	14.421428	6.480539
C	3.414600	13.533879	4.805296
C	2.666739	14.706051	4.481031
H	2.813146	15.598729	5.092036

C	1.783966	14.714458	3.430245
H	1.218522	15.615875	3.193137
C	1.603047	13.540549	2.648830
H	0.894441	13.551285	1.819695
C	2.311277	12.395425	2.927345
H	2.159504	11.504925	2.318948
C	3.246746	12.339123	4.006329
C	4.433782	7.318754	0.490136
C	3.148052	7.865325	0.111461
C	2.146564	7.313875	0.987003
C	2.808564	6.417785	1.915629
C	4.215395	6.429195	1.606935
C	5.735954	7.568978	-0.199866
H	5.768630	8.574934	-0.636828
H	5.899280	6.845181	-1.014925
H	6.579145	7.484648	0.497095
C	2.901450	8.799665	-1.029431
H	2.005212	9.408654	-0.859642
H	2.755203	8.239843	-1.966991
H	3.746842	9.483213	-1.176844
C	0.674070	7.560581	0.911306
H	0.207363	7.505407	1.902997
H	0.183409	6.812698	0.267465
H	0.455888	8.552684	0.497615
C	2.138002	5.579345	2.956117
H	2.802697	5.396740	3.809500
H	1.841448	4.601177	2.544855
H	1.233397	6.067519	3.338693
C	5.268204	5.617998	2.292256
H	6.235968	6.134443	2.286611
H	5.401282	4.648437	1.787041
H	5.001025	5.417074	3.336634
H	2.649175	9.232150	3.408243
H	4.698987	8.882724	3.458757
H	3.921902	10.149863	2.024173
Ru	3.588640	8.432934	2.154218