Supporting Information

A Stable Planar-chiral *N*-Heterocyclic Carbene with a 1,1´-Ferrocenediyl Backbone

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Contents

1. X-Ray Crystallography

Table S1. Crystallographic data

	3	**4**	**5**	[**A'-Np**H]BF_4	(R_pR_p-**10**)=C(O^-)(R_pR_p-**10**$^+$) (S_pS_p-**10**)=C(O^-)(S_pS_p-**10**$^+$)	**A'-Np**H−$CHCl_2$	**A-Np**H−CH_2CN	**A-Np**H−$CHCl_2$	(*E*)-[Fe{η^5-C_5H_4[NNp(CHO)]}-{η^5-C_5H_4(NHNp)}]
Chemical formula	$C_{24}H_{42}FeSi_2$	$C_{18}H_{24}Br_2Fe$	$C_{18}H_{24}FeN_6$	$C_{29}H_{47}BF_4FeN_2$	$C_{59}H_{92}Fe_2N_4O$	$C_{30}H_{48}Cl_2FeN_2$	$C_{23}H_{33}FeN_3$	$C_{22}H_{32}Cl_2FeN_2$	$C_{21}H_{32}FeN_2O$
Formula mass	442.61	456.04	380.28	566.35	985.06	563.45	407.37	451.25	384.33
Crystal system	tetragonal	monoclinic	triclinic	triclinic	monoclinic	monoclinic	monoclinic	monoclinic	triclinic
Space group	*P* -4 2_1 *c*	*P* $2_1/n$	*P* -1	*P* -1	*P* $2_1/n$	*P* $2_1/c$	*P* $2_1/c$	*P* $2_1/c$	*P* -1
a/Å	16.9122(6)	10.8421(6)	6.9683(10)	10.4182(8)	11.2320(3)	21.5012(12)	16.1859(9)	10.2598(5)	9.9201(11)
b/Å	16.9122(6)	8.8940(6)	10.7377(17)	11.9766(12)	21.6146(8)	8.0519(2)	6.2591(4)	23.3257(15)	10.7066(11)
c/Å	17.8911(6)	19.0588(10)	13.687(2)	13.5263(11)	22.6191(6)	18.5315(9)	21.5457(12)	10.0167(5)	11.0762(13)
α/°	90	90	100.971(12)	83.236(7)	90	90	90	90	85.767(9
β/°	90	97.876(4)	105.110(12)	82.779(6)	96.622(2)	110.721(4)	97.799(4)	113.568(4)	72.107(8)
γ/°	90	90	105.110(12)	82.822(7)	90	90	90	90	64.675(8)
Unit cell volume/Å^3	5117.3(3)	1820.50(19)	964.6(3)	1652.3(2)	5454.7(3)	3000.7(2)	2162.6(2)	2197.2(2)	1009.6(2)
Temperature/K	143(2)	143(2)	223(2)	163(2)	173(2)	100(2)	173(2)	173(2)	100(2)
Crystal size/mm	0.48×0.28×0.20	0.51×0.31×0.17	0.23×0.17×0.03	0.12×0.11×0.04	0.15×0.14×0.08	0.40×0.15×0.03	0.60×0.27×0.17	0.29×0.18×0.03	0.07×0.03×0.02
Z	8	4	2	2	4	4	4	4	2
μ/mm^{-1}	0.690	5.210	0.794	0.497	0.574	0.701	0.709	0.939	0.757
No. of reflections measured	30646	8806	8120	12061	28548	15039	13417	10163	7806
Independent reflections [R_{int}]	4414 [0.0351]	3126 [0.0559]	3344 [0.1201]	5785 [0.0555]	9882 [0.0365]	5445 [0.0391]	3821 [0.0877]	3968 [0.0251]	3731 [0.0840]
Final R_1 (wR_2) [$I > 2\sigma(I)$]	0.0302 (0.0708)	0.0248 (0.0635)	0.0599 (0.1138)	0.0506 (0.1309)	0.0387 (0.0883)	0.0346 (0.0808)	0.0439 (0.1215)	0.0279 (0.0671)	0.0741 (0.1987)
Final R_1 (wR_2) [all data]	0.0350 (0.0733)	0.0291 (0.0648)	0.0990 (0.1273)	0.0699 (0.1433)	0.0590 (0.0976)	0.0448 (0.0880)	0.0506 (0.1254)	0.0349 (0.0713)	0.0862 (0.2122)
Absorption correction T_{min}/T_{max}	Integration 0.821/0.885	Integration 0.198/0.466	Integration 0.863/0.981	Integration 0.95/0.981	Integration 0.920/0.954	Integration 0.72/0.964	Integration 0.636/0.907	Integration 0.865/0.965	Integration 0.947/0.987
Goodness of fit on F^2	1.007	1.049	0.828	1.062	1.015	0.992	1.093	1.053	1.054
CCDC number	1063561	1063562	1063566	1063567	1063565	1063568	1063563	1063569	1063564

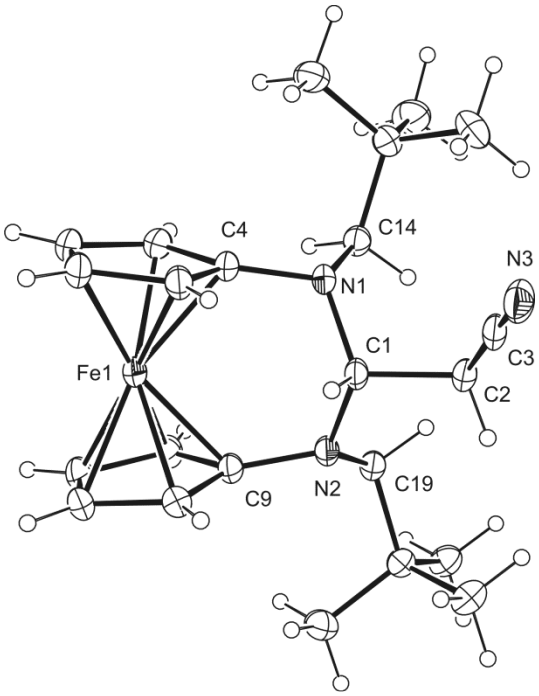

Figure S1. Molecular structure of **A-Np**H−CH_2CN in the crystal (ellipsoids drawn at the 30% probability level). Selected bond lengths [Å] and bond angles [deg]: C1−C2 1.553(3), C1−N1 1.484(3), C1−N2 1.488(3), C2−C3 1.469(4), C3−N3 1.150(4), C4−N1 1.435(3), C9−N2 1.433(3); N1−C1−N2 118.3(2), C2−C3−N3 176.5(3), C1−N1−C4 112.5(2), C1−N2−C9 113.6(2).

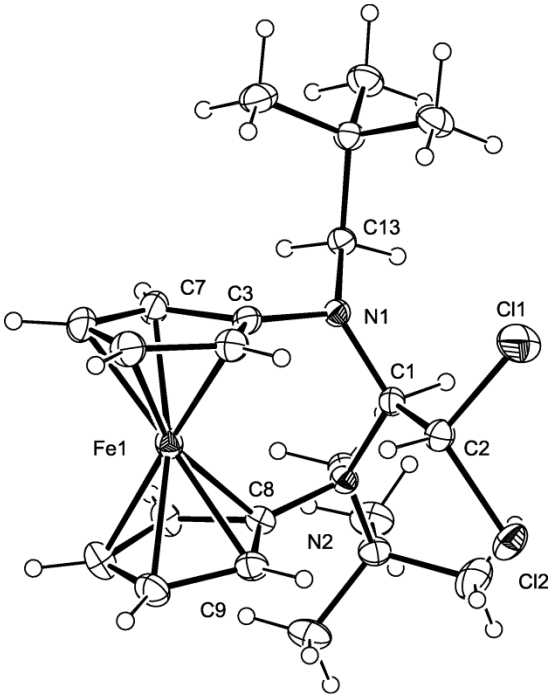

Figure S2. Molecular structure of **A-Np**H−$CHCl_2$ in the crystal (ellipsoids drawn at the 30% probability level). Selected bond lengths [Å] and bond angles [deg]: C1−C2 1.539(3), C1−N1 1.471(2), C1−N2 1.466(2), C2−Cl1 1.769(2), C2−Cl2 1.778(2), C3−N1 1.415(3), C8−N2 1.421(2); N1−C1−N2 118.1(1), Cl1−C2−Cl2 107.8(1), C1−N1−C3 118.1(1), C1−N2−C8 118.0(1).

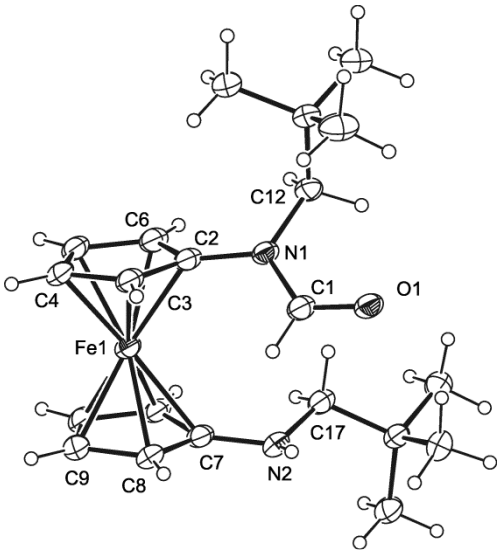

Figure S3. Molecular structure of (*E*)-[Fe{η^5-C_5H_4[NNp(CHO)]}{η^5-C_5H_4(NHNp)}]in the crystal (ellipsoids drawn at the 30% probability level). Selected bond lengths [Å] and bond angles [deg]: C1−N1 1.349(4), C1−O1 1.230(6), C2−N1 1.415(7), C7−N2 1.381(6); C1−N1−C2 119.9(4), C7−N2−C17 120.0(4).

2. Electrochemistry

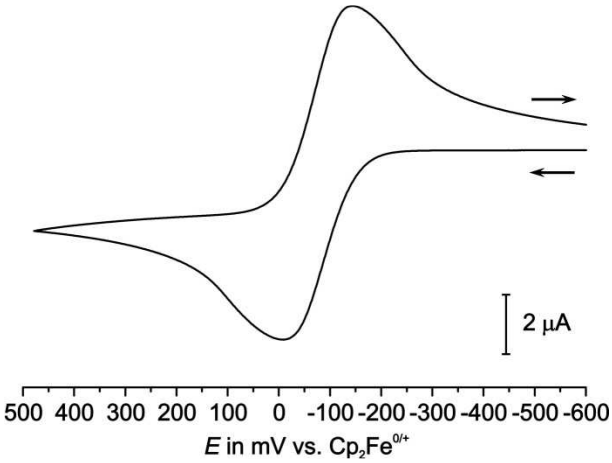

Figure S4. CV of 1,1'-di-*tert*-butylferrocene (**1**) in 0.1 M THF/NBu_4PF_6 at v = 100 mV s^{-1}.

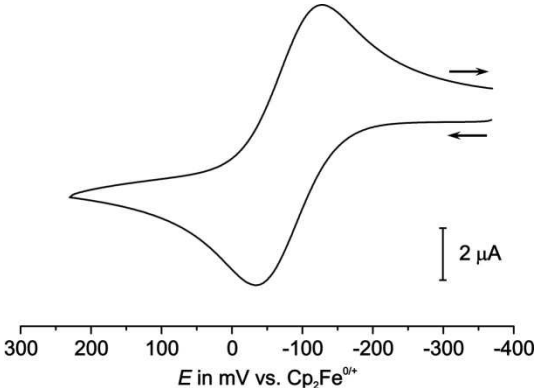

Figure S5. CV of *rac*-fc'$(NH{=}CHtBu)_2$ (**8**) in 0.1 M THF/NBu_4PF_6 at v = 100 mV s^{-1}.

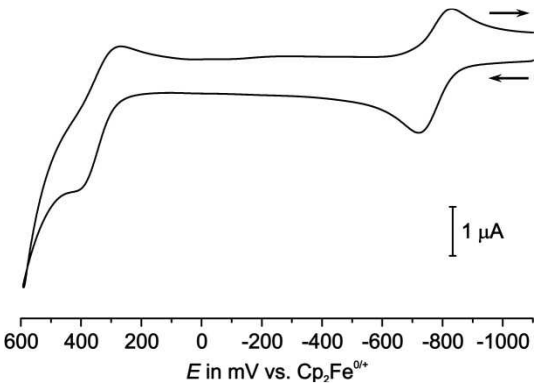

Figure S6. CV of *rac*-fc'$(NHNp)_2$ (**9**) in 0.1 M THF/NBu_4PF_6 at v = 100 mV s^{-1}.

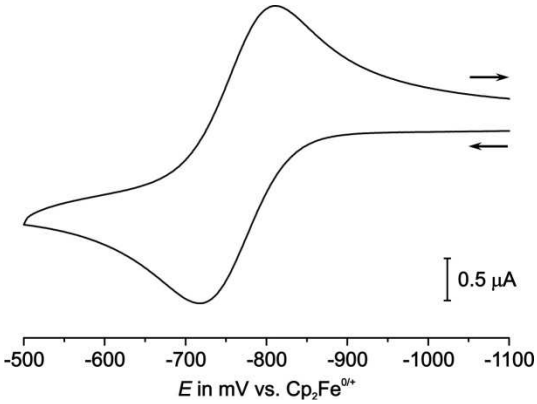

Figure S7. CV of the first anodic wave of *rac*-fc'$(NHNp)_2$ (**9**) in 0.1 M THF/NBu_4PF_6 at v = 100 mV s^{-1}.

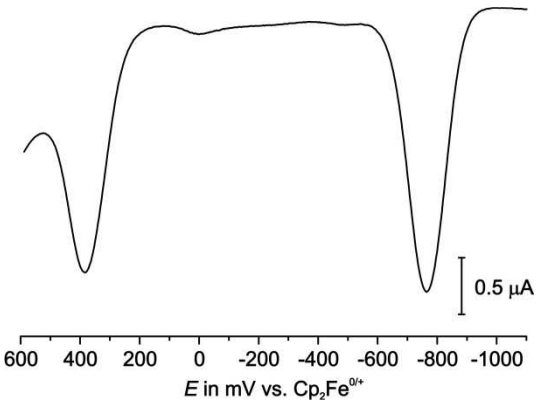

Figure S8. Square wave voltammogram of *rac*-fc'$(NHNp)_2$ (**9**) in 0.1 M THF/NBu_4PF_6.

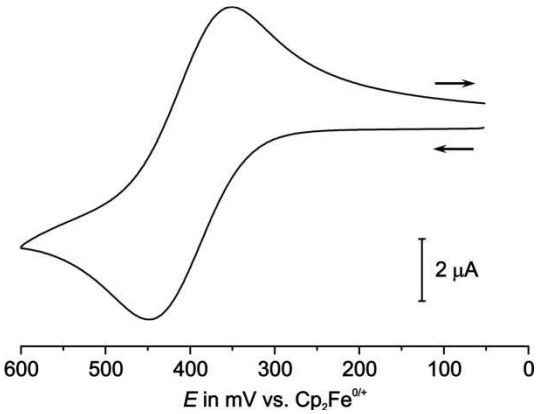

Figure S9. CV of [**A'-Np**H]BF_4 in 0.1 M THF/NBu_4PF_6 at v = 100 mV s^{-1}.

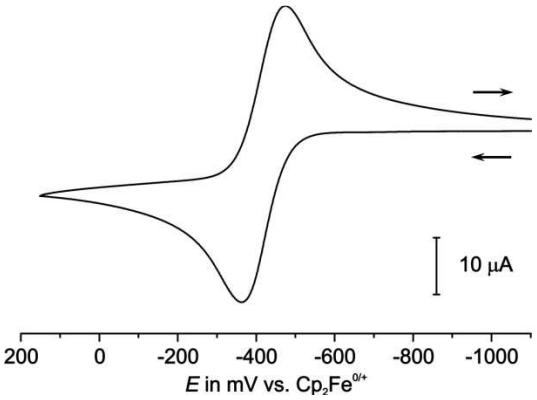

Figure S10. CV of **A-Np**(H_2O) in 0.1 M THF/NBu_4PF_6 at v = 100 mV s^{-1}.

3. EPR Spectroscopy

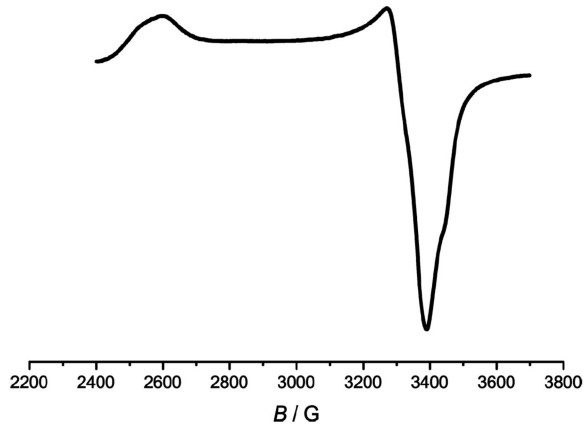

Figure S11. EPR spectrum of the chemically oxidized ($[FeCp_2]PF_6$) hydrolysis products of **A-Np**.

4. Plots of NMR Spectra

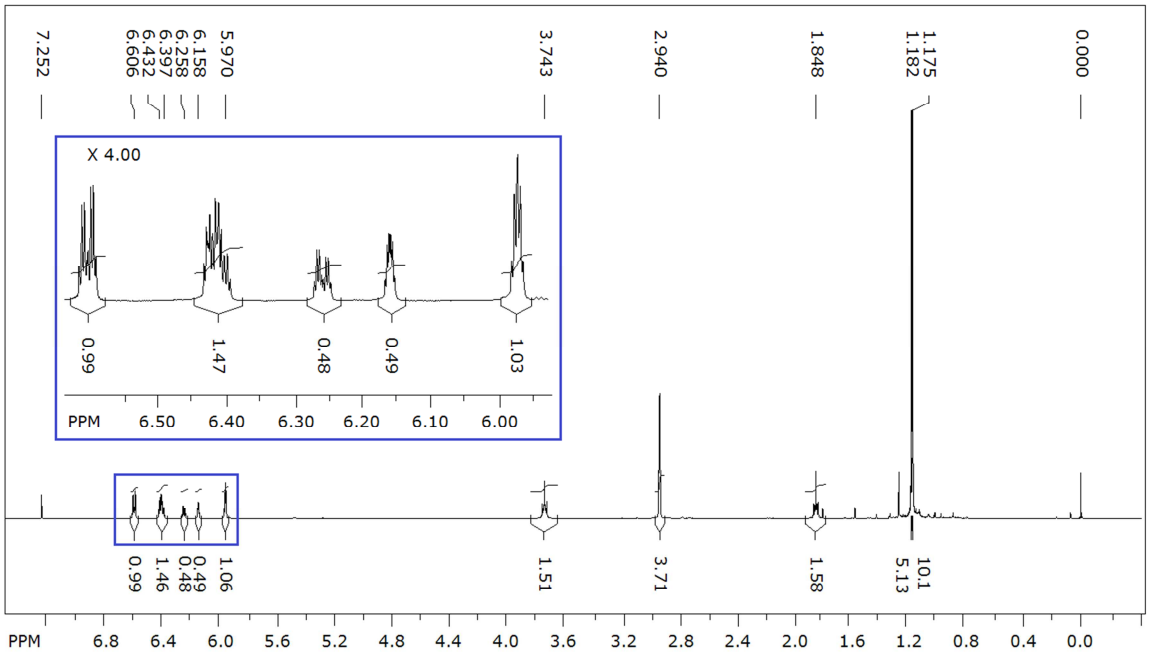

Figure S12. ^{1}H NMR spectrum of *tert*-butylcyclopentadiene ($CDCl_3$, 399.9 MHz).

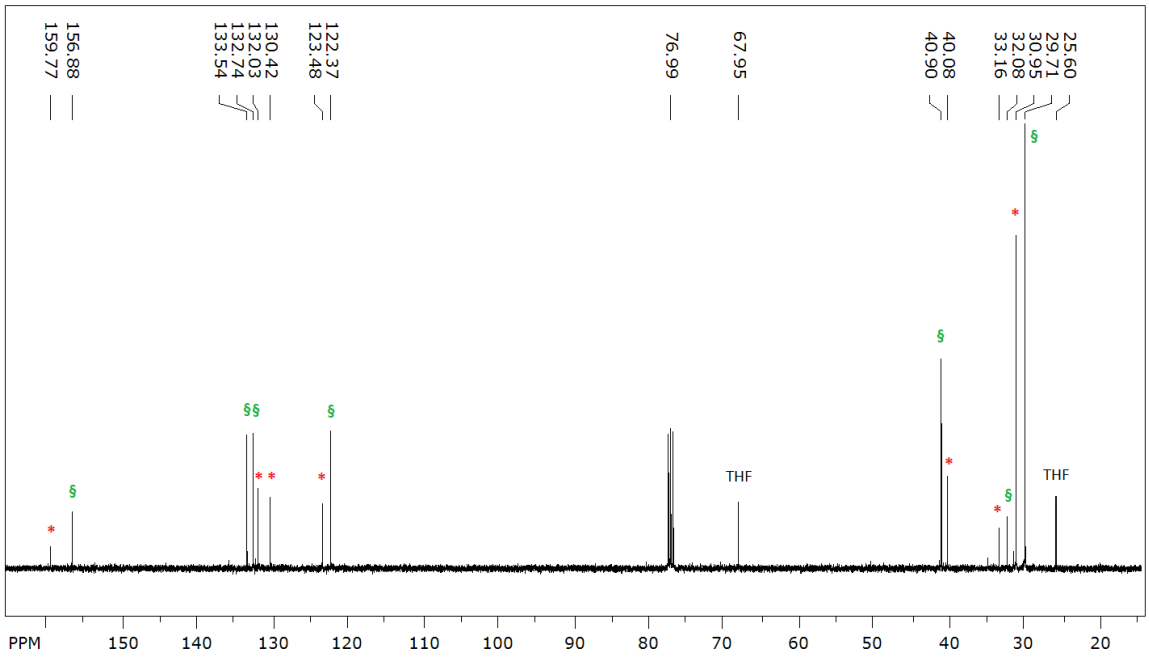

Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum of *tert*-butylcyclopentadiene ($CDCl_3$, 100.5 MHz). Signals marked with (§) and (*) belong to 2- and 1-*tert*-butylcyclopentadiene respectively.

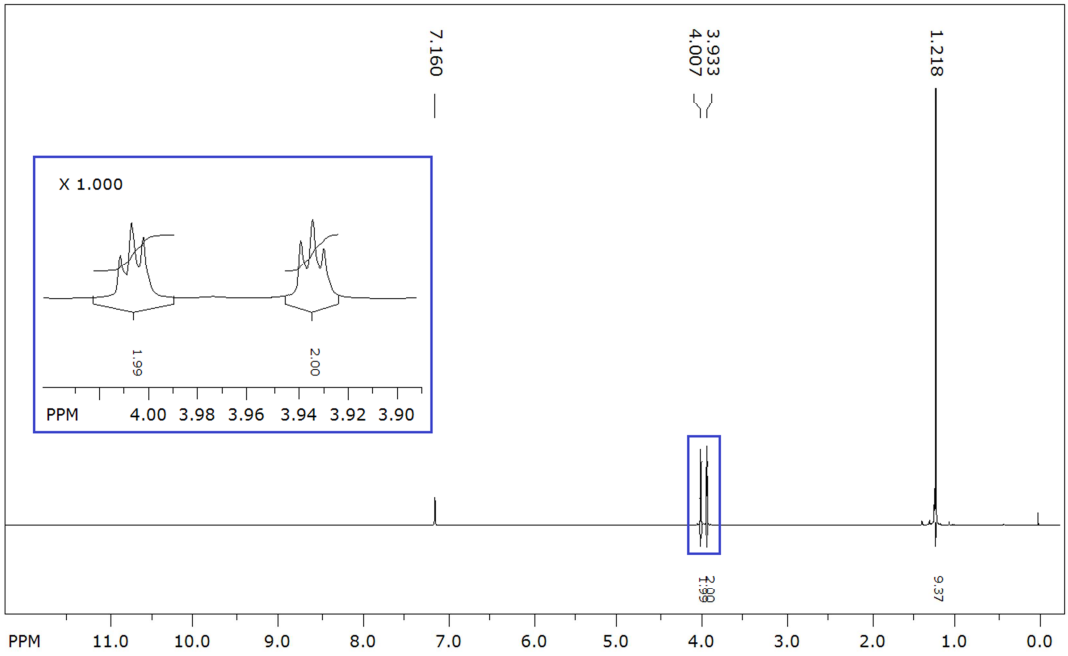

Figure S14. ^{1}H NMR spectrum of 1,1'-di-*tert*-butylferrocene (**1**) (C_6D_6, 399.9 MHz).

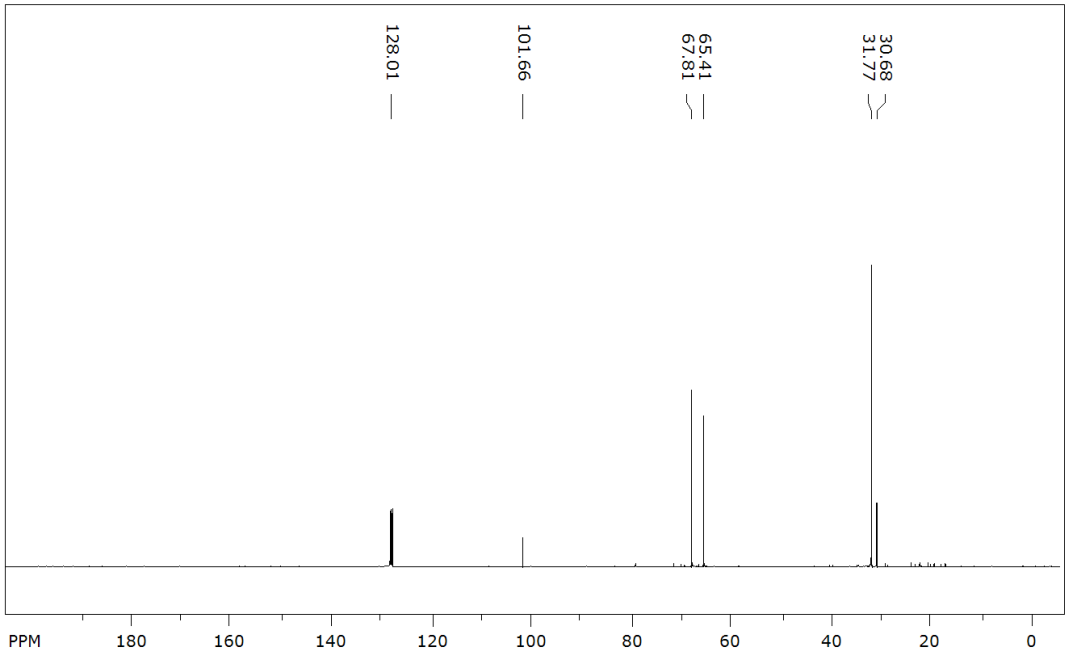

Figure S15. ^{13}C{^{1}H} NMR spectrum of 1,1'-di-*tert*-butylferrocene (**1**) (C_6D_6, 100.5 MHz).

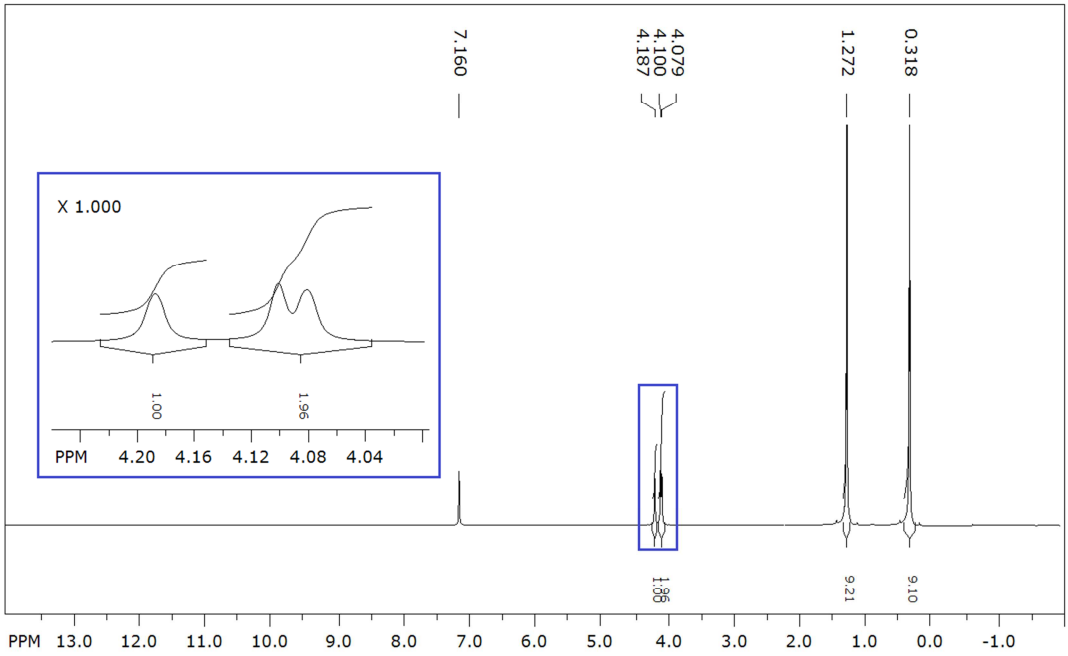

Figure S16. ^{1}H NMR spectrum of *rac*-fc'$(SiMe_3)_2$ (**3**) (C_6D_6, 399.9 MHz).

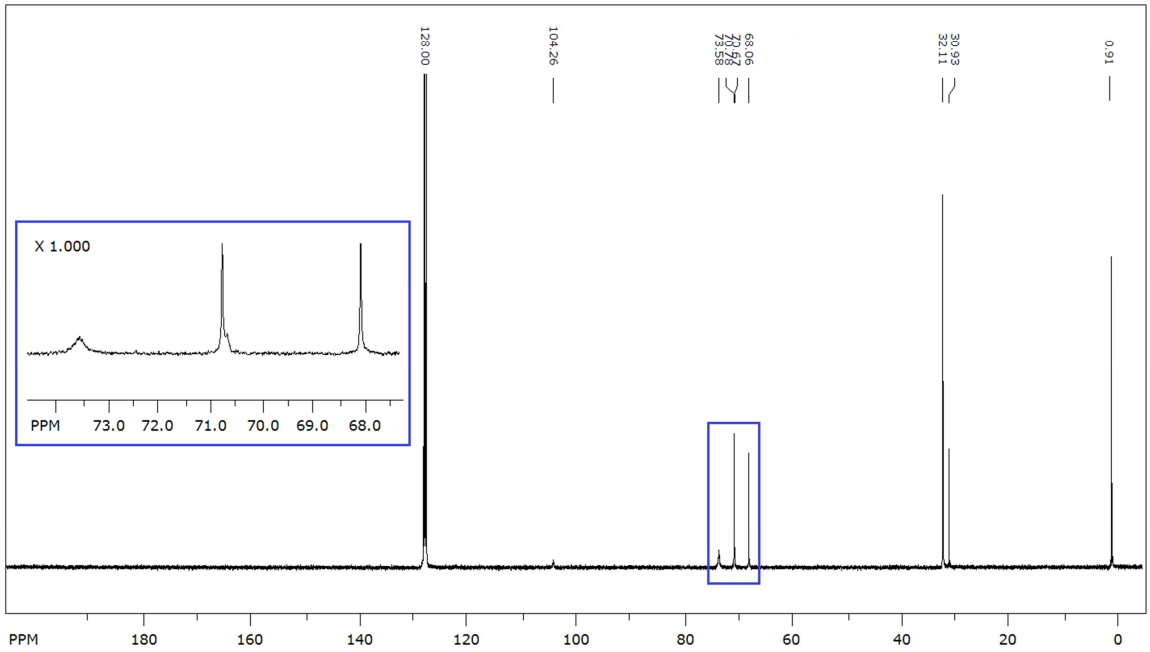

Figure S17. $^{13}C\{^{1}H\}$ NMR spectrum of *rac*-fc'$(SiMe_3)_2$ (**3**) (C_6D_6, 100.5 MHz).

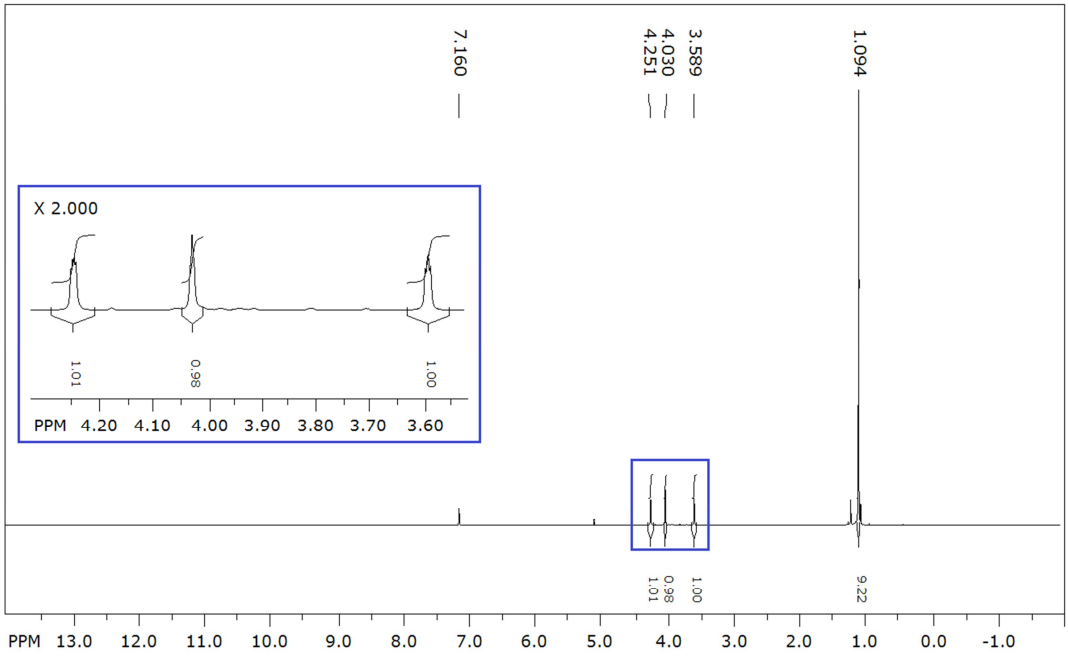

Figure S18. ^{1}H NMR spectrum of *rac*-fc'Br$_2$ (**4**) (C_6D_6, 399.9 MHz).

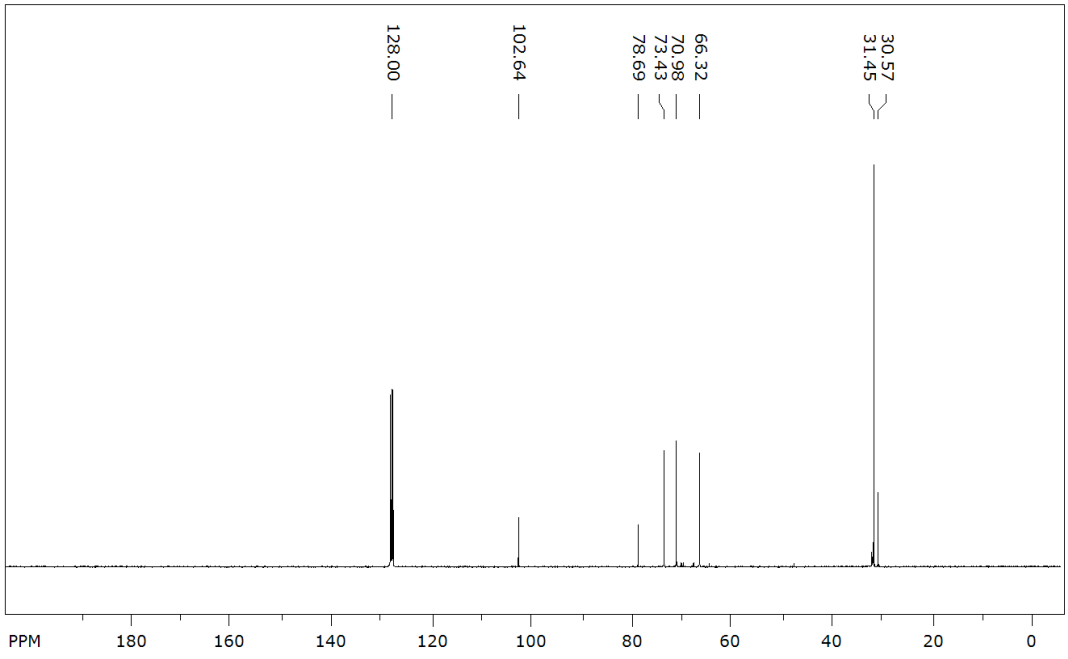

Figure S19. ^{13}C{^{1}H} NMR spectrum of *rac*-fc'Br$_2$ (**4**) (C_6D_6, 100.5 MHz).

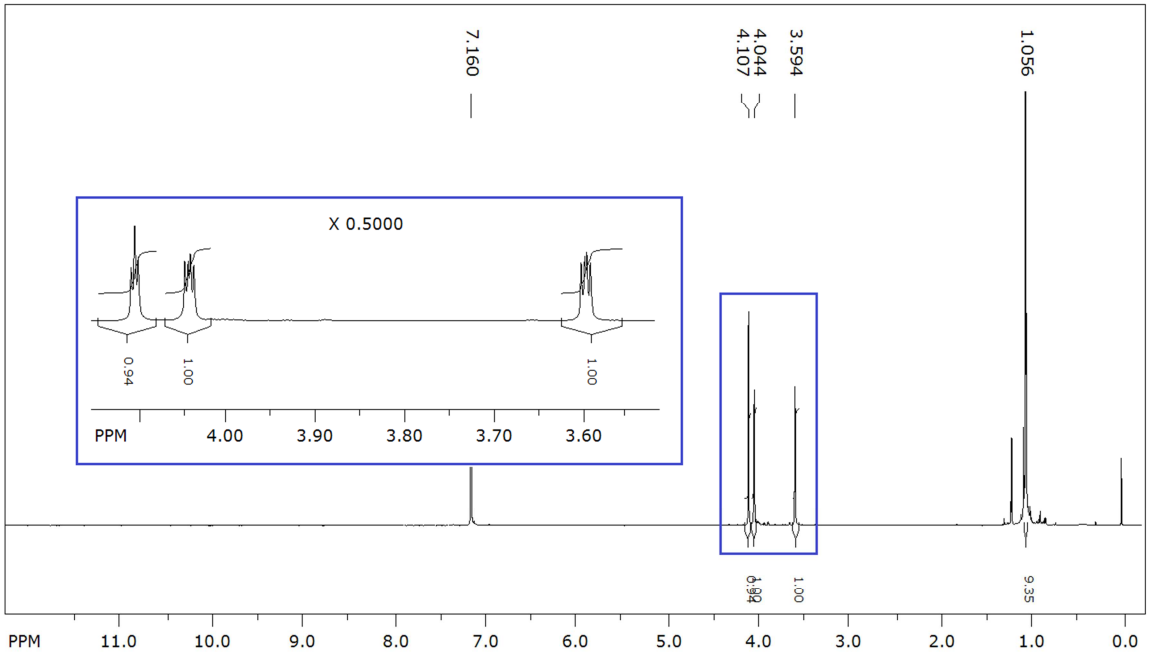

Figure S20. ^{1}H NMR spectrum of *rac*-fc'$(N_3)_2$ (**5**) (C_6D_6, 399.9 MHz).

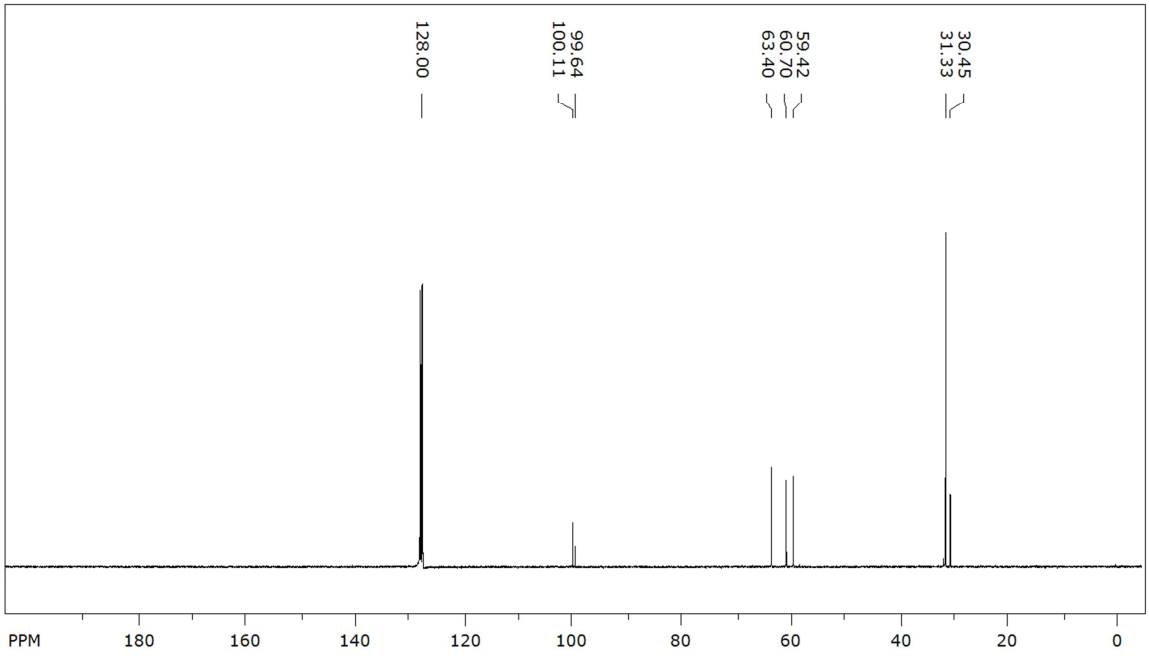

Figure S21. ^{13}C{^{1}H} NMR spectrum of *rac*-fc'$(N_3)_2$ (**5**) (C_6D_6, 100.5 MHz).

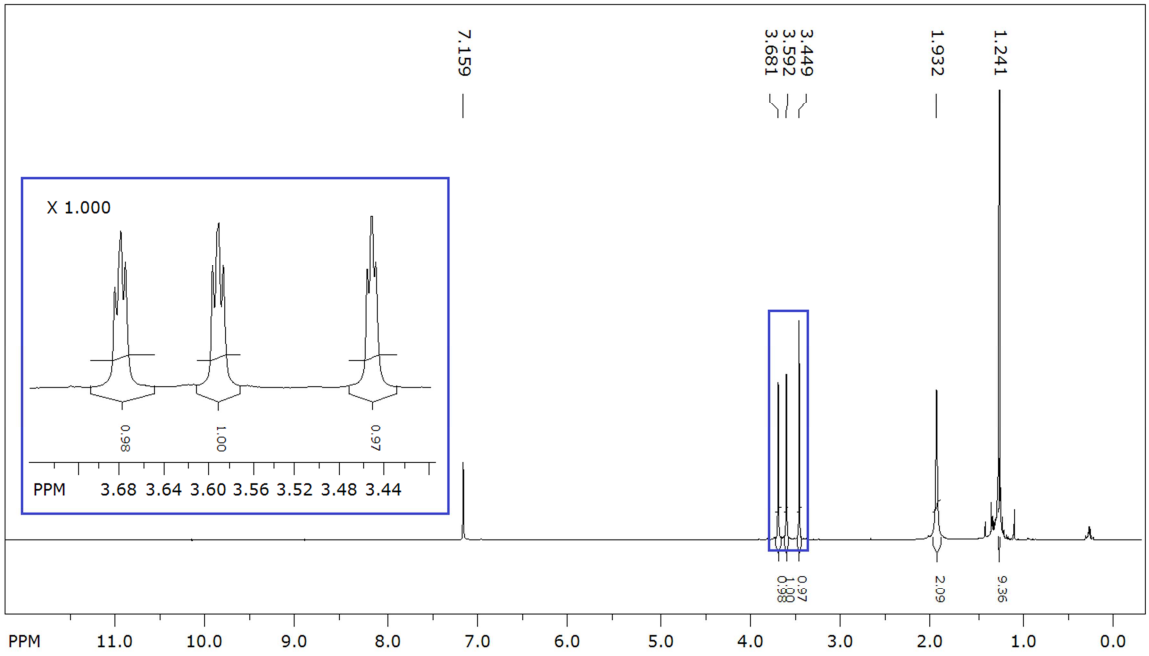

Figure S22. ^{1}H NMR spectrum of *rac*-fc'$(NH_2)_2$ (**6**) (C_6D_6, 399.9 MHz).

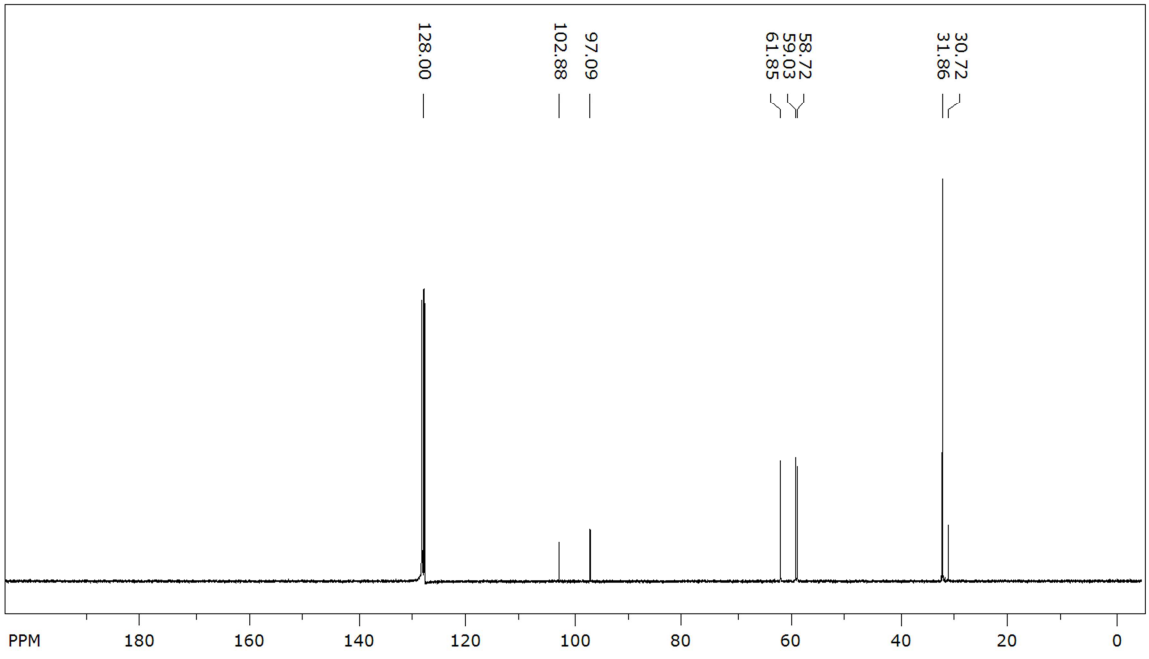

Figure S23. ^{13}C{^{1}H} NMR spectrum of *rac*-fc'$(NH_2)_2$ (**6**) (C_6D_6, 100.5 MHz).

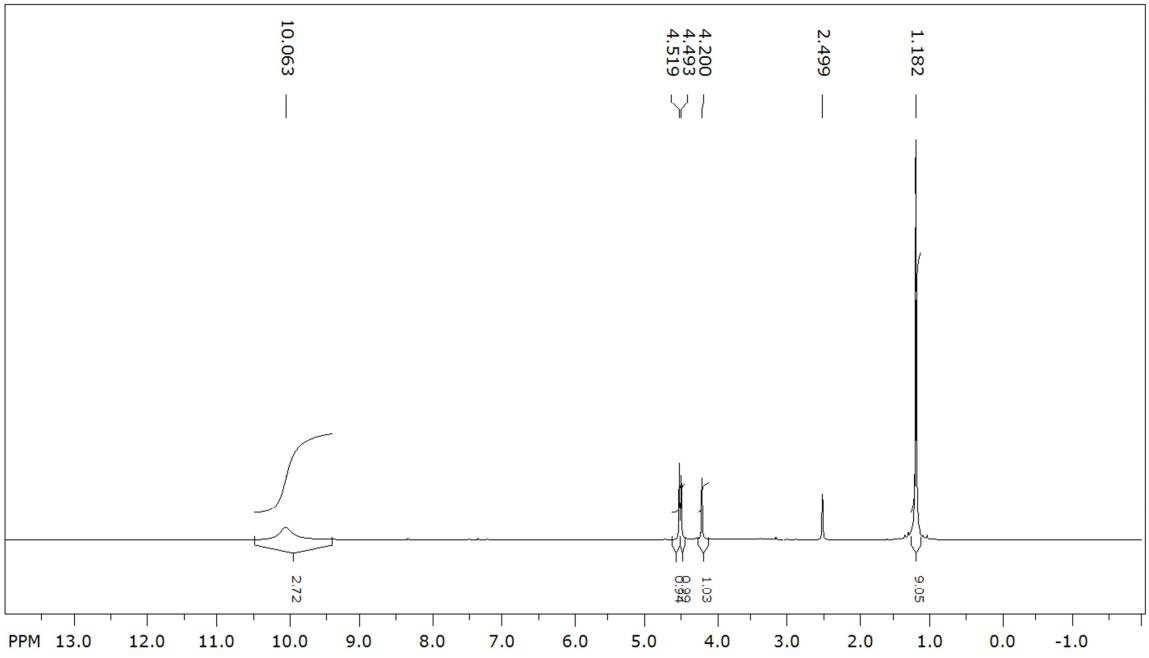

Figure S24. ^{1}H NMR spectrum of [**6**H$_2$]Cl$_2$ (DMSO-d_6, 399.9 MHz).

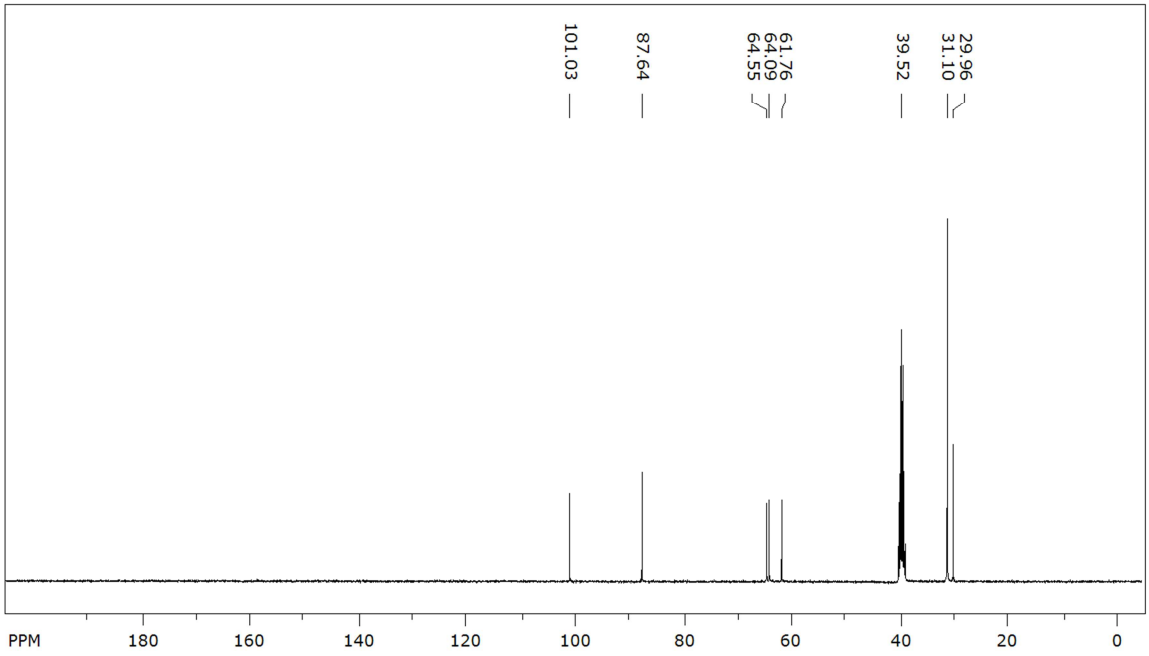

Figure S25. ^{13}C{^{1}H} NMR spectrum of [**6**H$_2$]Cl$_2$ (DMSO-d_6, 100.5 MHz).

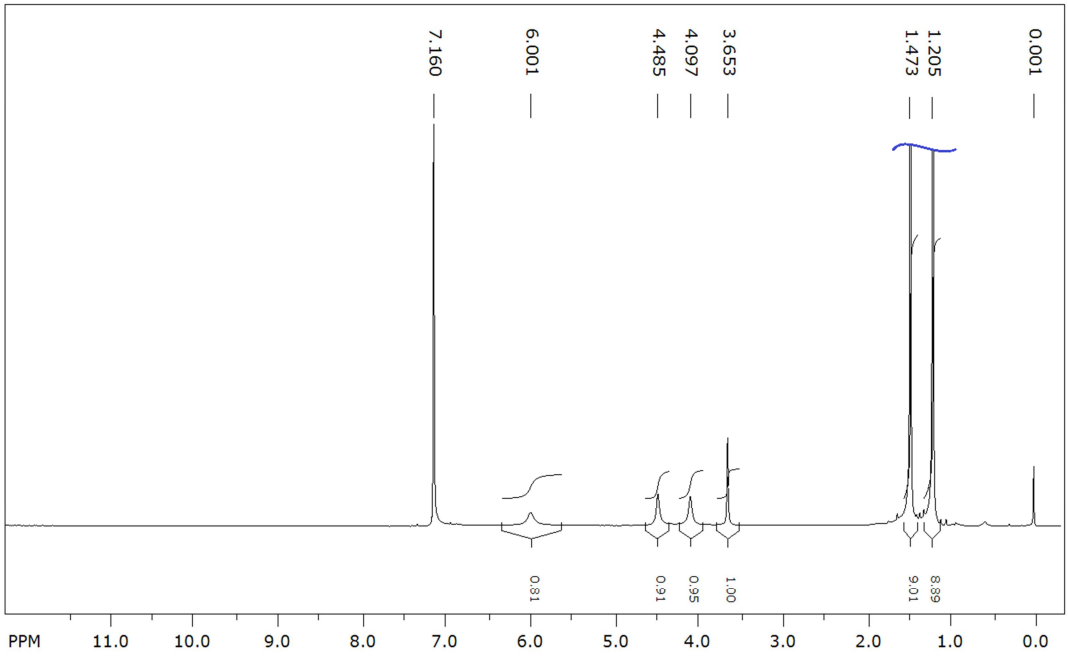

Figure S26. ^{1}H NMR spectrum of *rac*-fc'(NHBoc)$_2$ (**7**) (C_6D_6, 399.9 MHz).

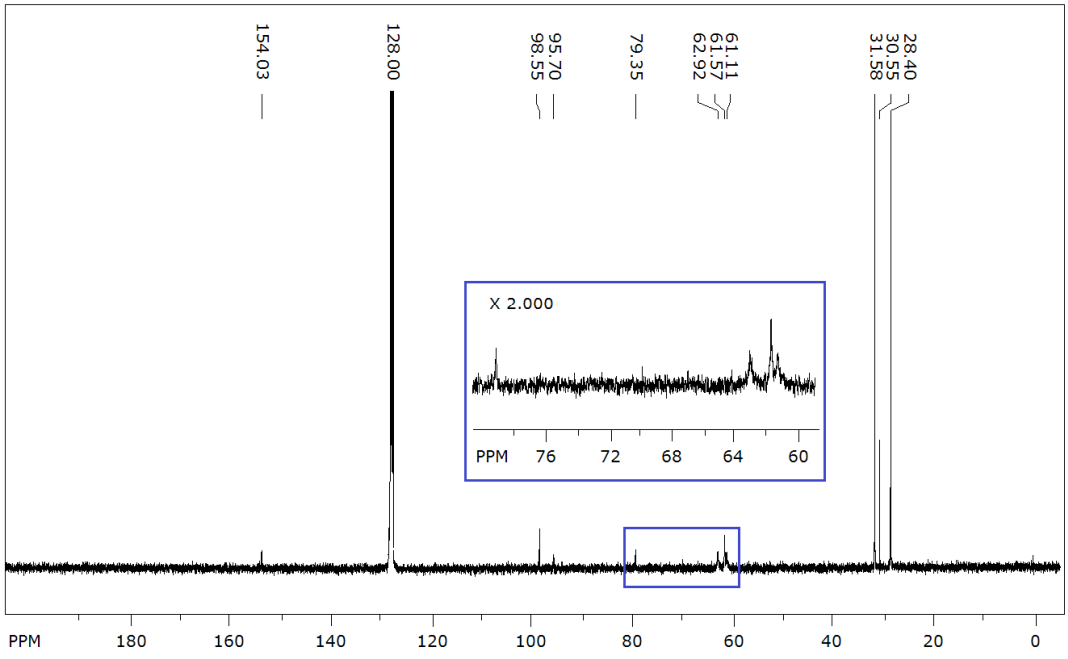

Figure S27. ^{13}C{^{1}H} NMR spectrum of *rac*-fc'(NHBoc)$_2$ (**7**) (C_6D_6, 100.5 MHz).

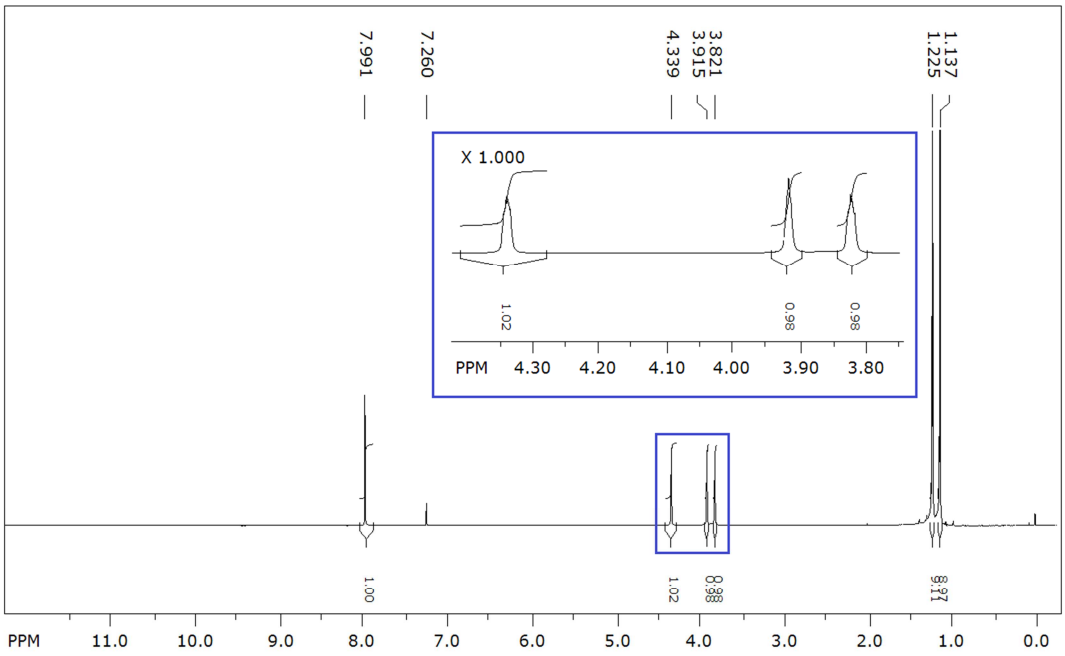

Figure S28. ^{1}H NMR spectrum of *rac*-fc'(N=CH*t*Bu)$_2$ (**8**) ($CDCl_3$, 399.9 MHz).

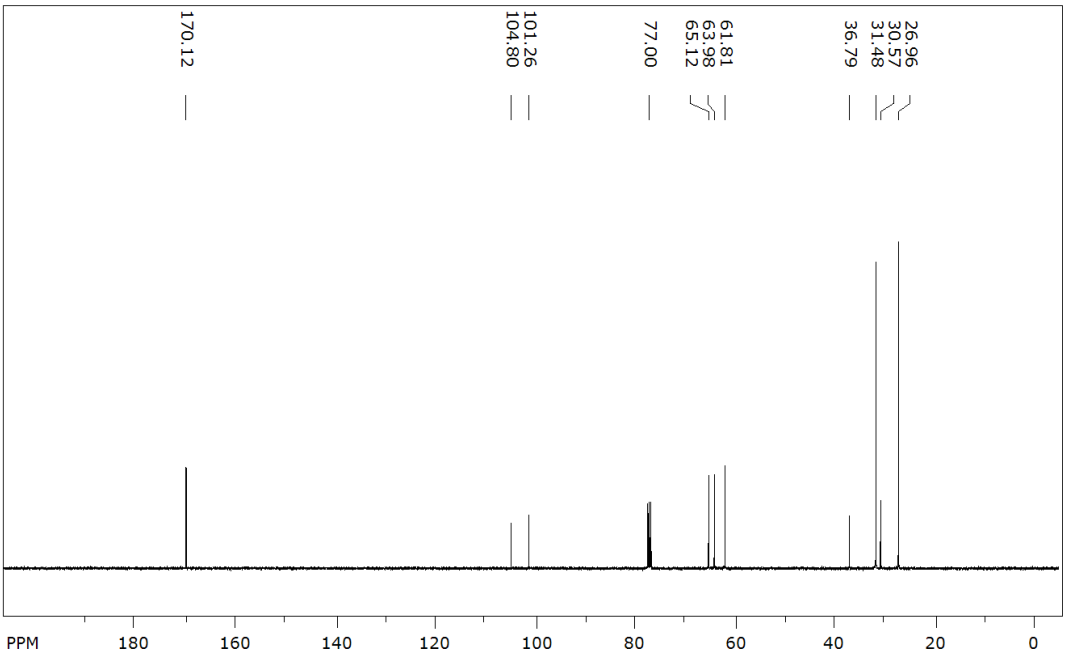

Figure S29. $^{13}C\{^{1}H\}$ NMR spectrum of *rac*-fc'(N=CH*t*Bu)$_2$ (**8**) ($CDCl_3$, 100.5 MHz).

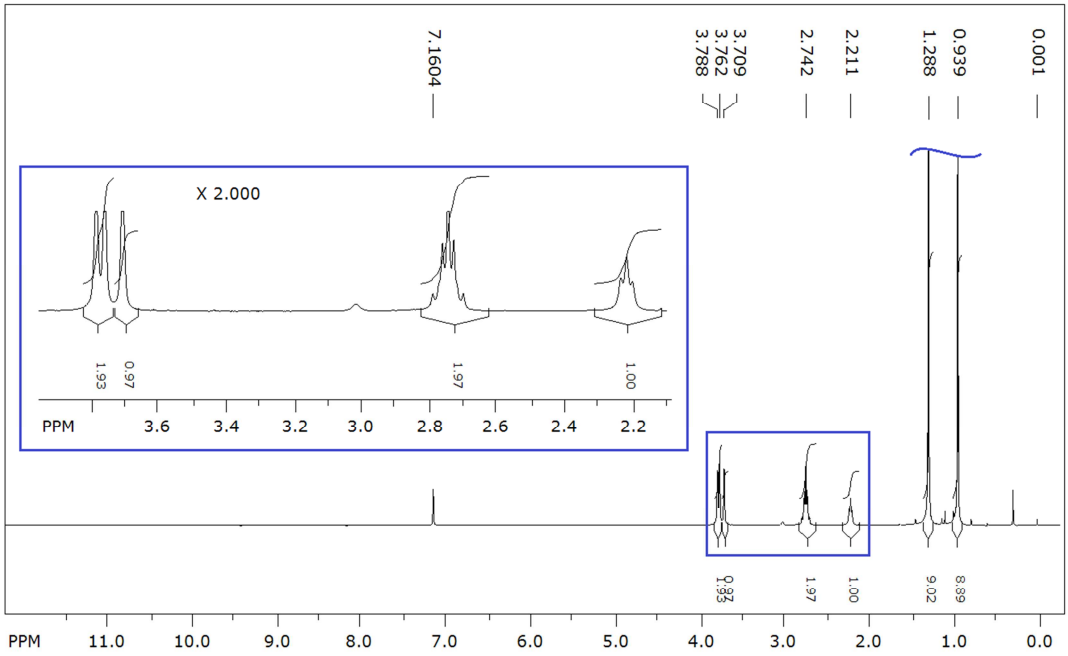

Figure S30. ^{1}H NMR spectrum of *rac*-fc'(NH-Np)$_2$ (**9**) (C_6D_6, 399.9 MHz).

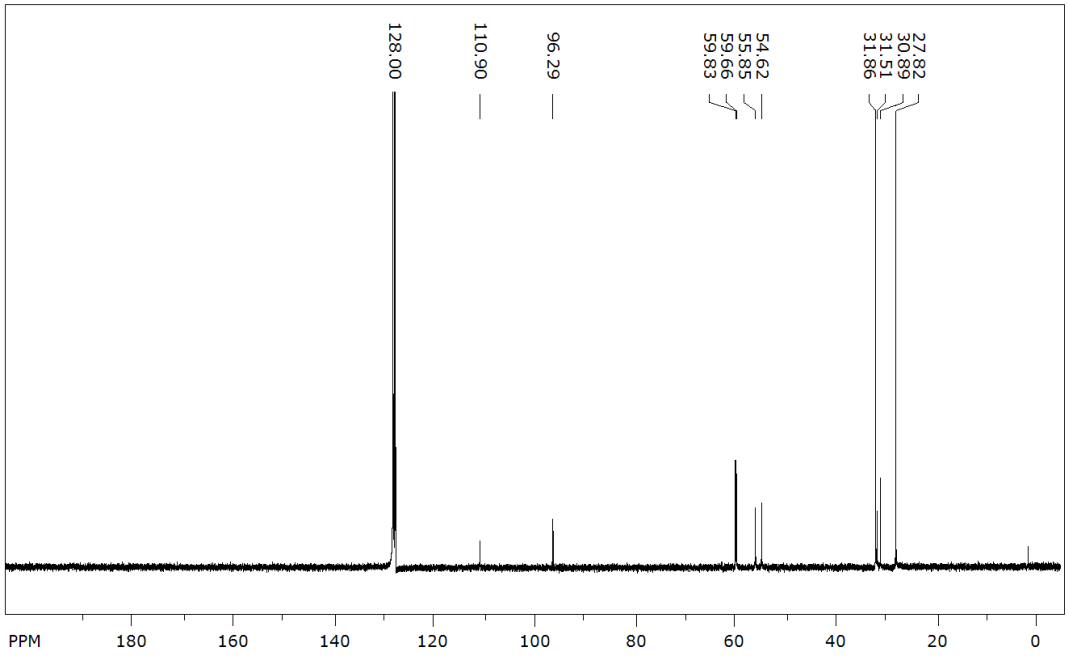

Figure S31. ^{13}C{^{1}H} NMR spectrum of *rac*-fc'(NH-Np)$_2$ (**9**) (C_6D_6, 100.5 MHz).

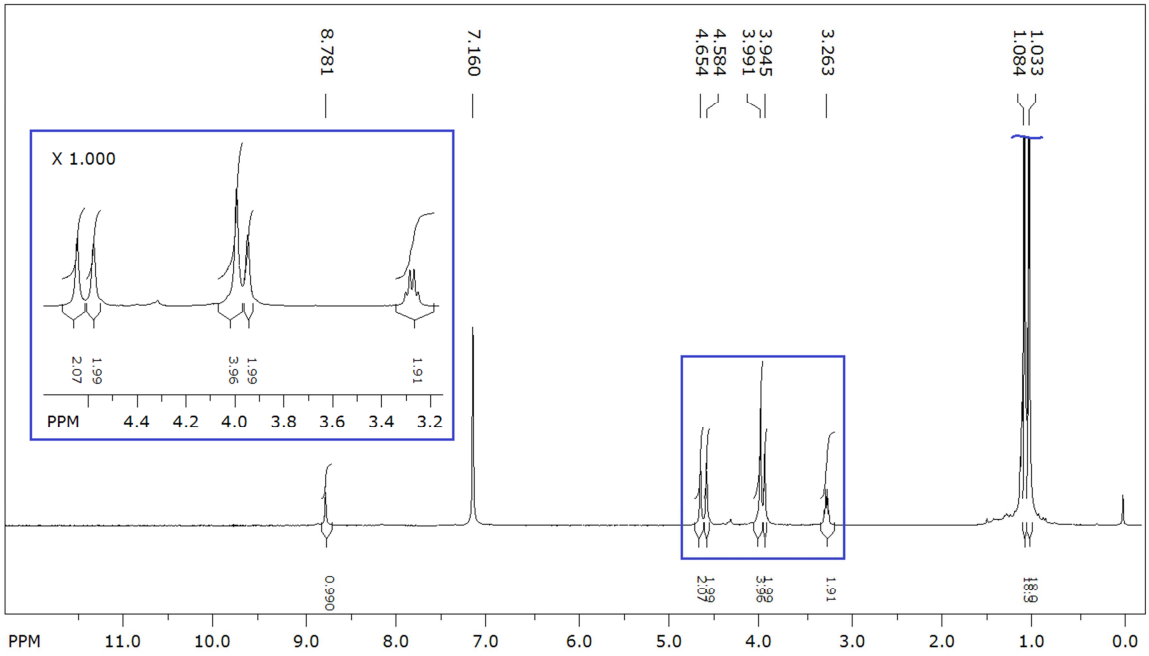

Figure S32. ^{1}H NMR spectrum of [**A'-Np**H]BF_4 (C_6D_6, 399.9 MHz).

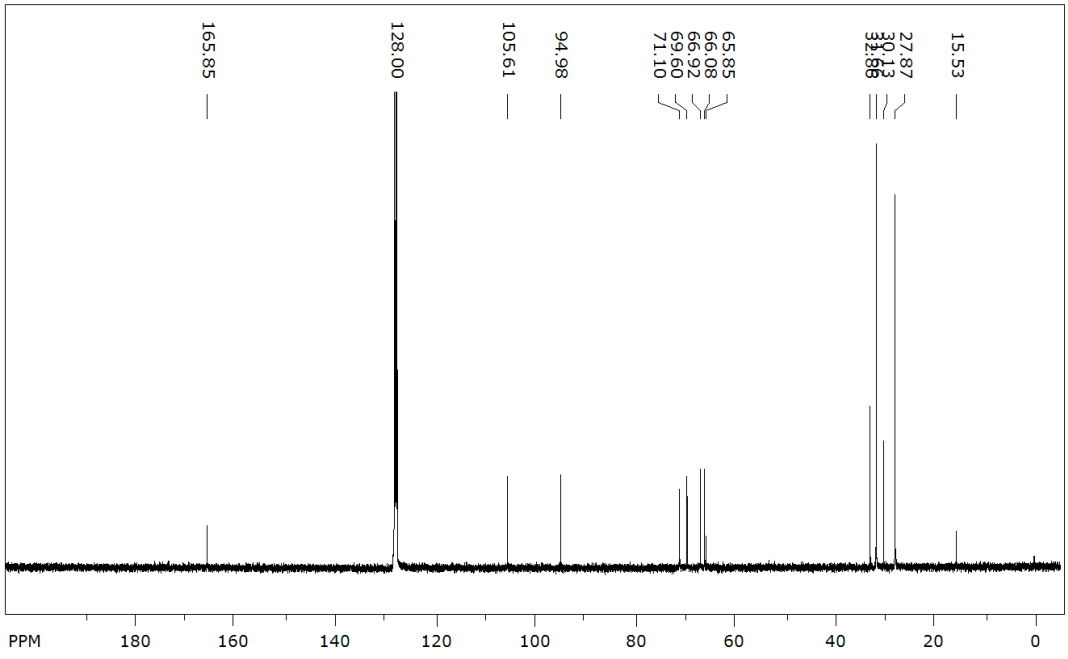

Figure S33. $^{13}C\{^{1}H\}$ NMR spectrum of [**A'-Np**H]BF_4 (C_6D_6, 100.5 MHz).

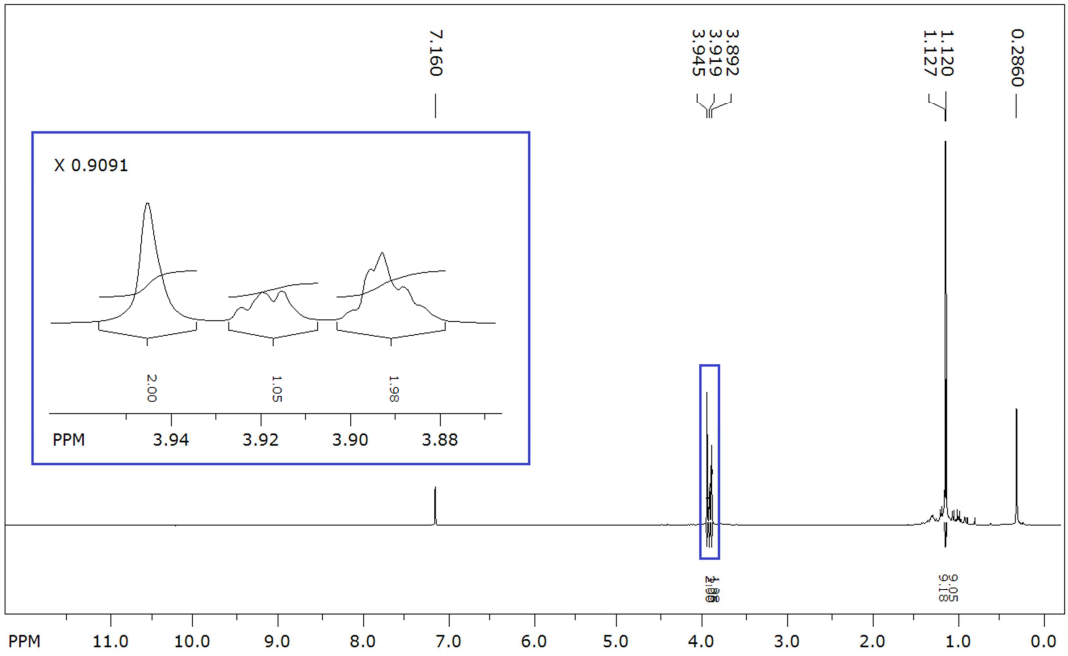

Figure S34. ^{1}H NMR spectrum of **A'-Np** (C_6D_6, 399.9 MHz).

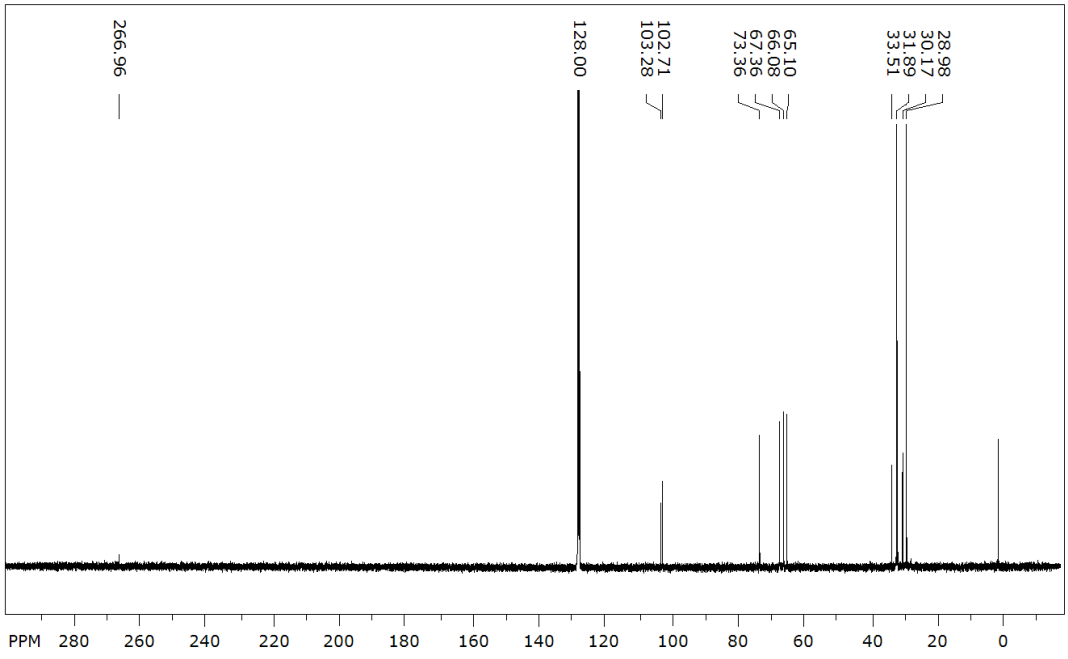

Figure S35. ^{13}C{^{1}H} NMR spectrum of **A'-Np** (C_6D_6, 100.5 MHz).

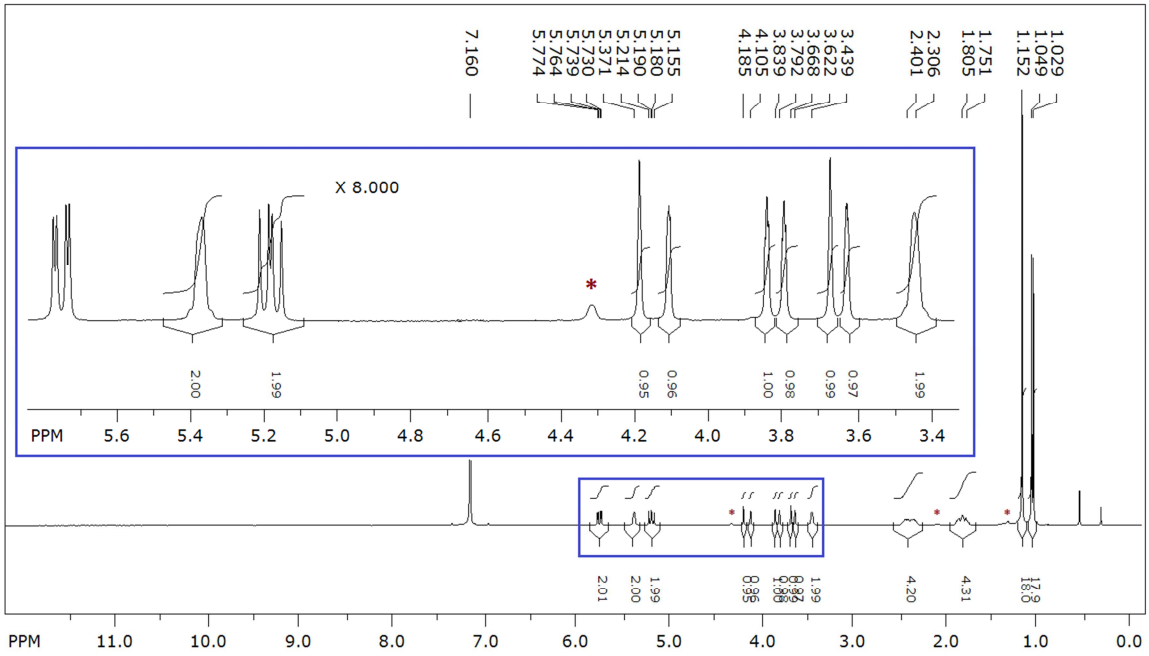

Figure S36. ^{1}H NMR spectrum of *cis*-[RhCl(**A'-Np**)(COD)] (C_6D_6, 399.9 MHz). Signals marked with (*) belong to trace amounts of [{Rh(μ-Cl)(COD)}$_2$].

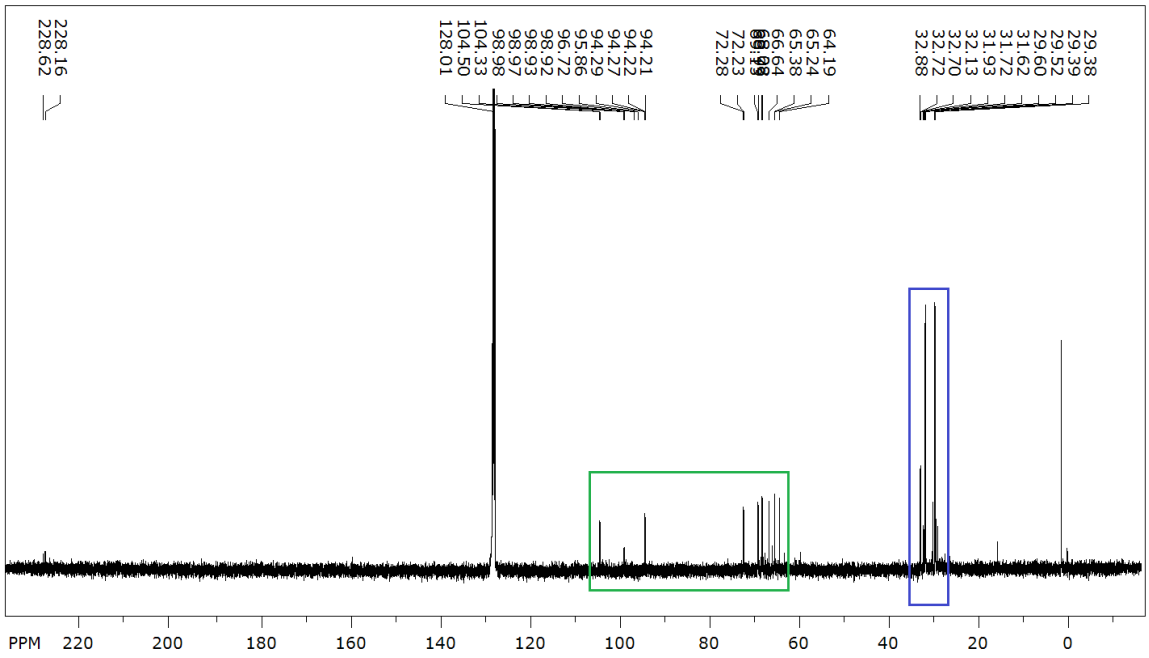

Figure S37. ^{13}C{^{1}H} NMR spectrum of *cis*-[RhCl(**A'-Np**)(COD)] (C_6D_6, 100.5 MHz).

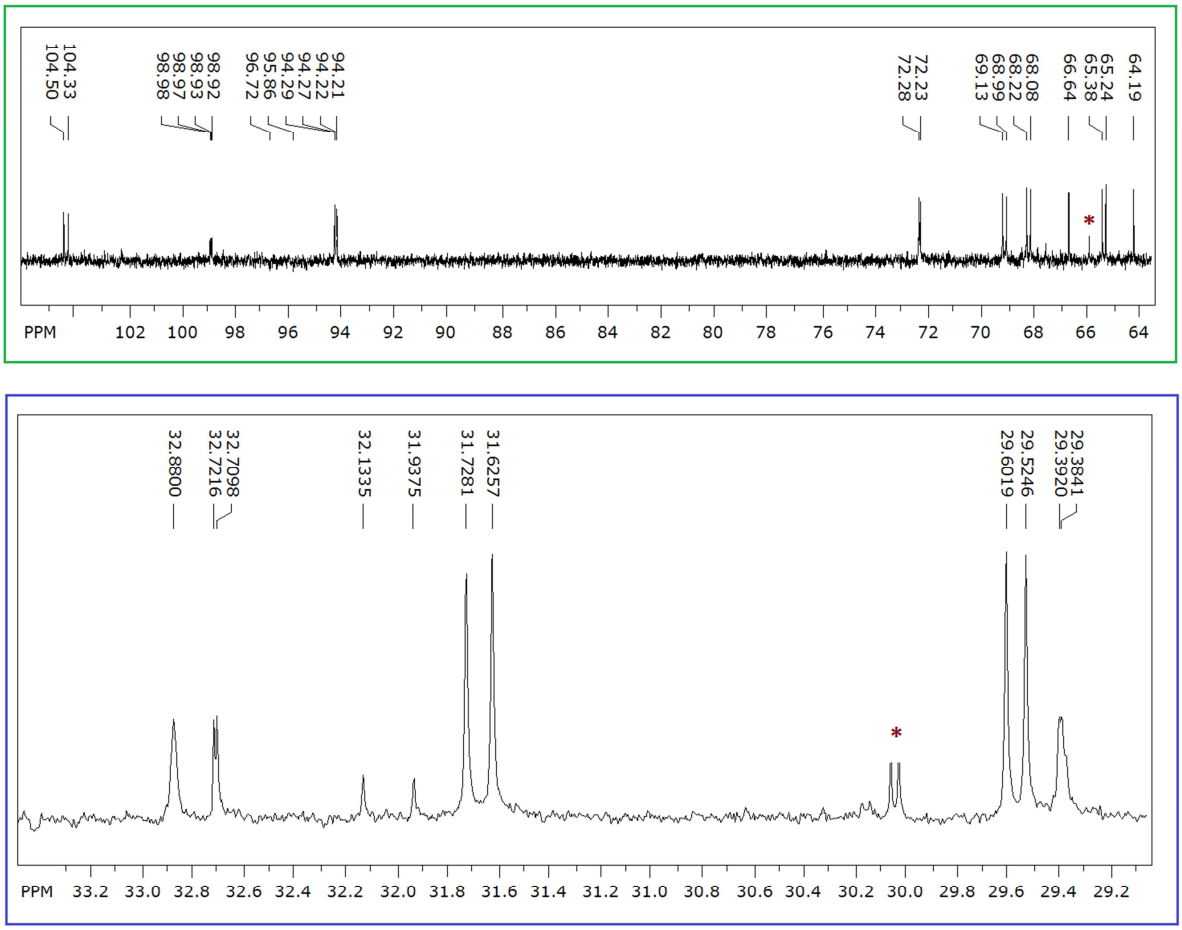

Figure S37 (continued). $^{13}C\{^{1}H\}$ NMR spectrum of *cis*-[RhCl(**A'-Np**)(COD)] (C_6D_6, 100.5 MHz). Signals marked with (*) belong to trace amounts of [{Rh(μ-Cl)(COD)}$_2$].

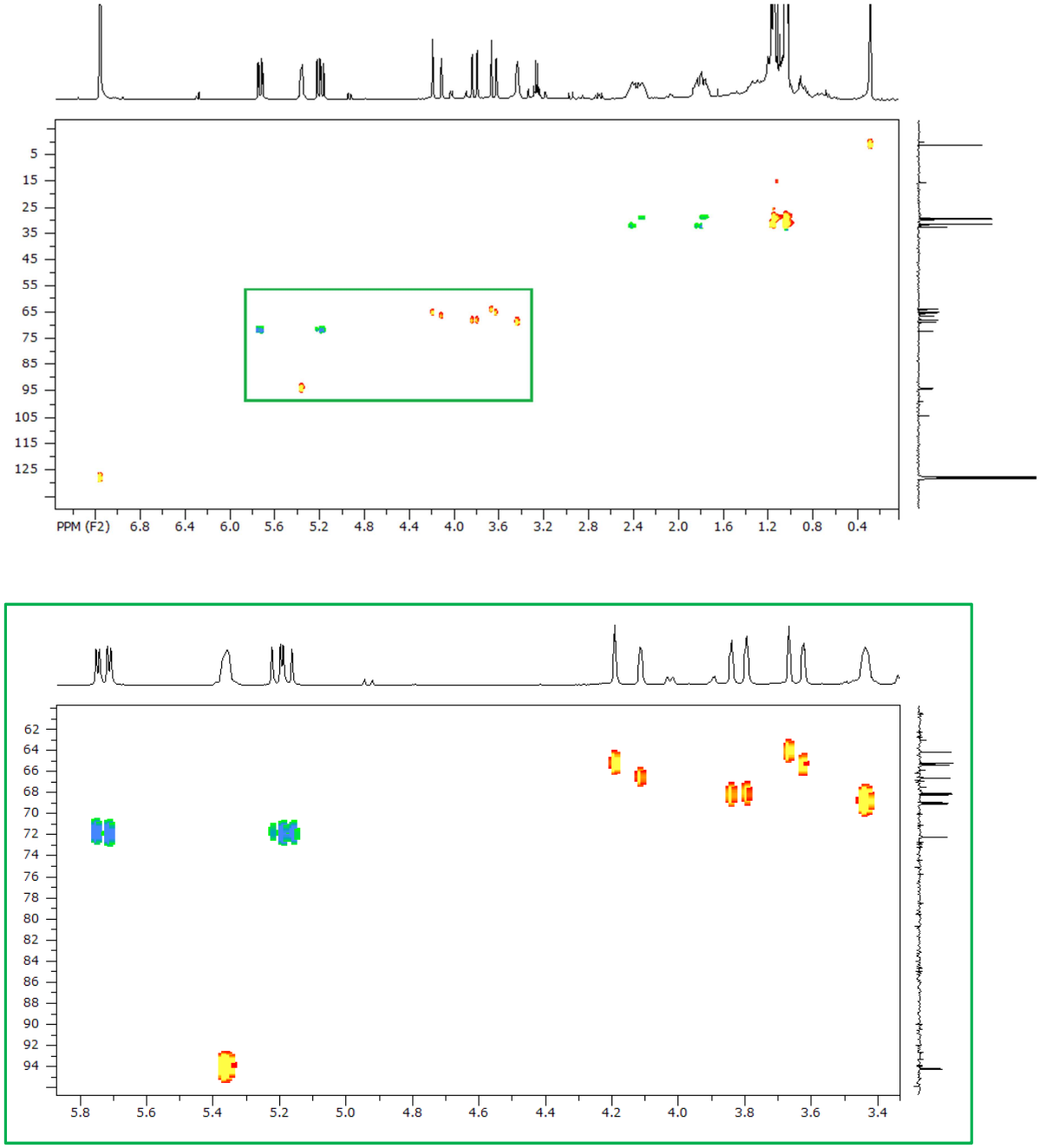

Figure S38. qHSQCad spectrum of *cis*-[RhCl(**A'-Np**)(COD)].

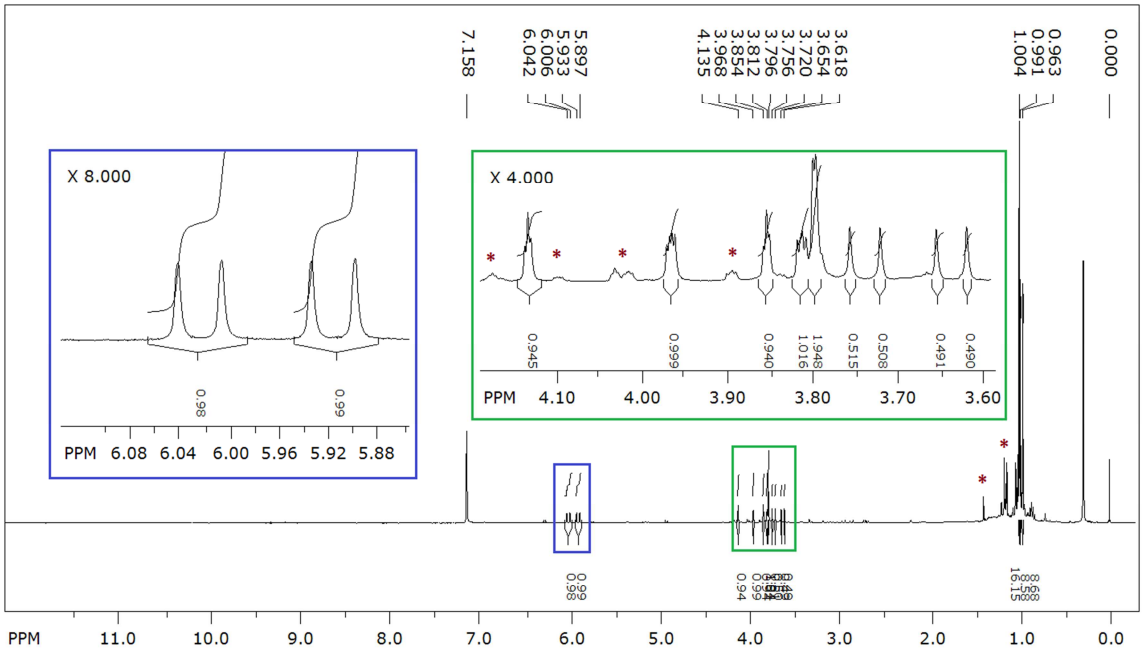

Figure S39. ^{1}H NMR spectrum of *cis*-[RhCl(**A'-Np**)(CO)$_2$] (C_6D_6, 399.9 MHz). Signals marked with (*) belong to trace amounts of [RhCl(**A'-Np**)(COD)].

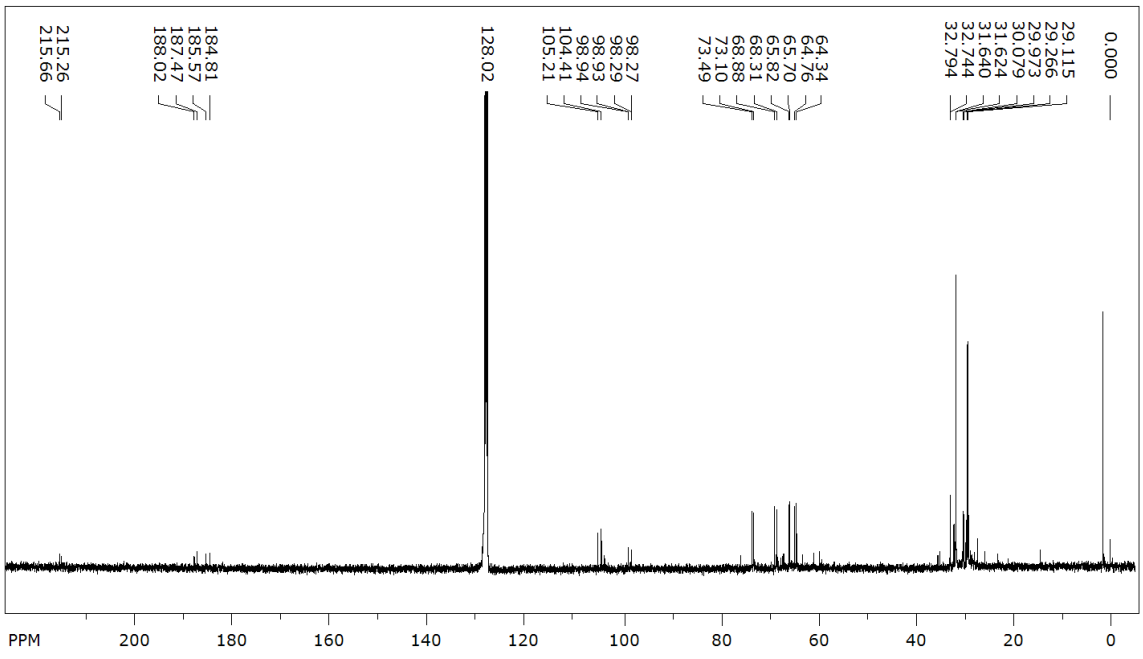

Figure S40. ^{13}C{^{1}H} NMR spectrum of *cis*-[RhCl(**A'-Np**)(CO)$_2$] (C_6D_6, 100.5 MHz).

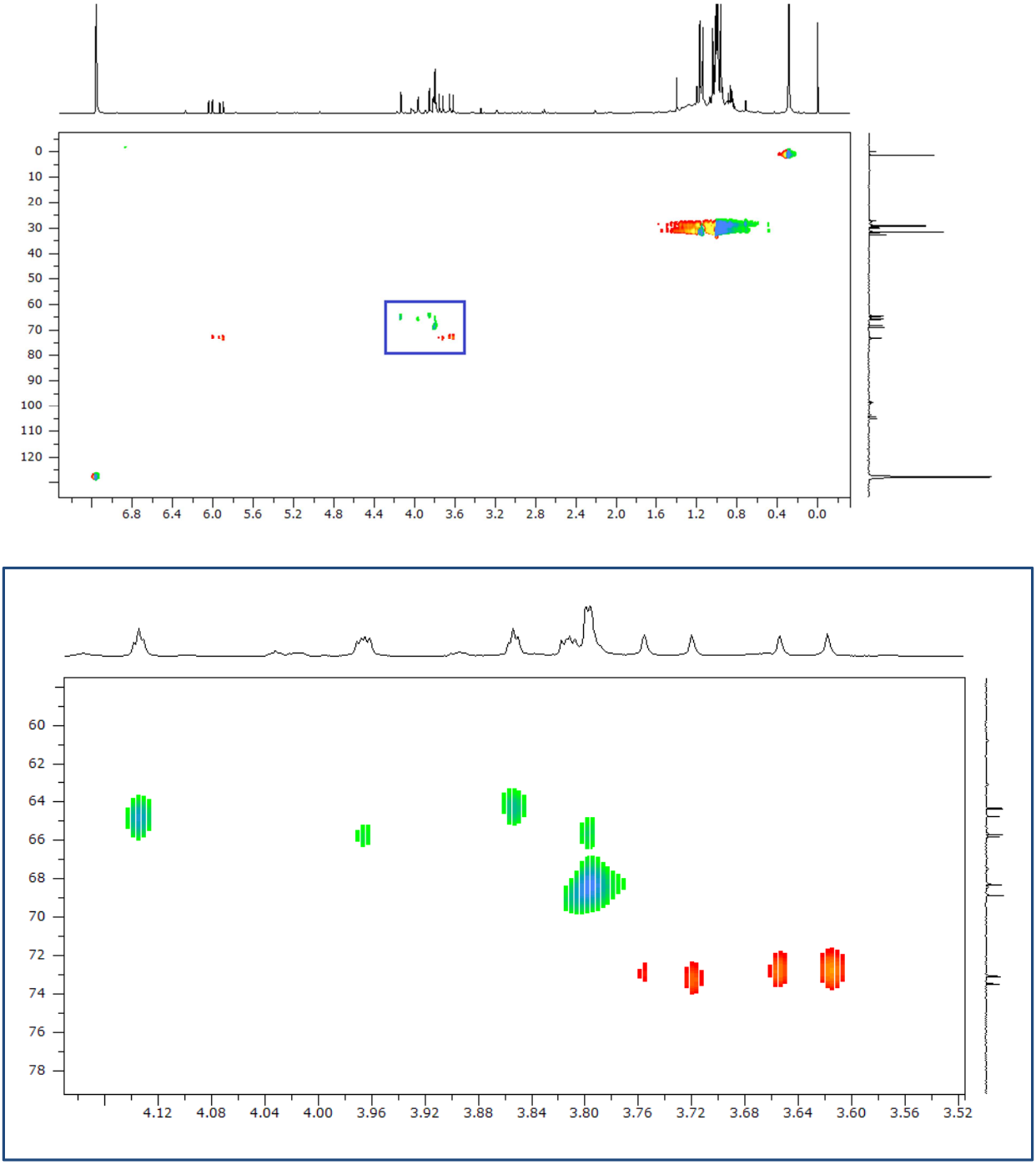

Figure S41. qHSQCad spectrum of *cis*-[RhCl(**A'-Np**)$(CO)_2$].

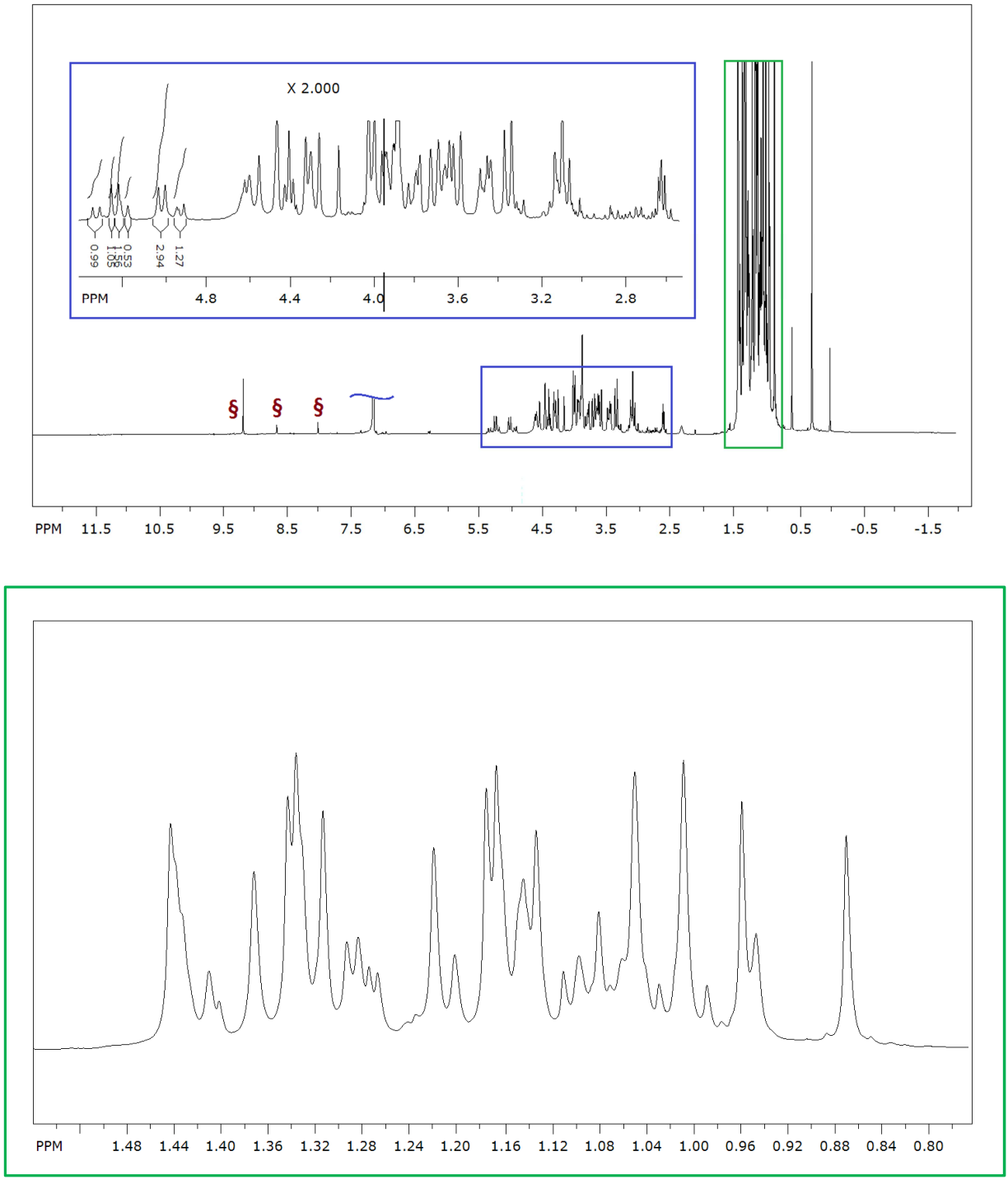

Figure S42. ^{1}H NMR spectrum of the crude carbonylation product of **A'-Np** (C_6D_6, 399.9 MHz). Signals marked with (**§**) belong to trace amounts of unidentified impurities.

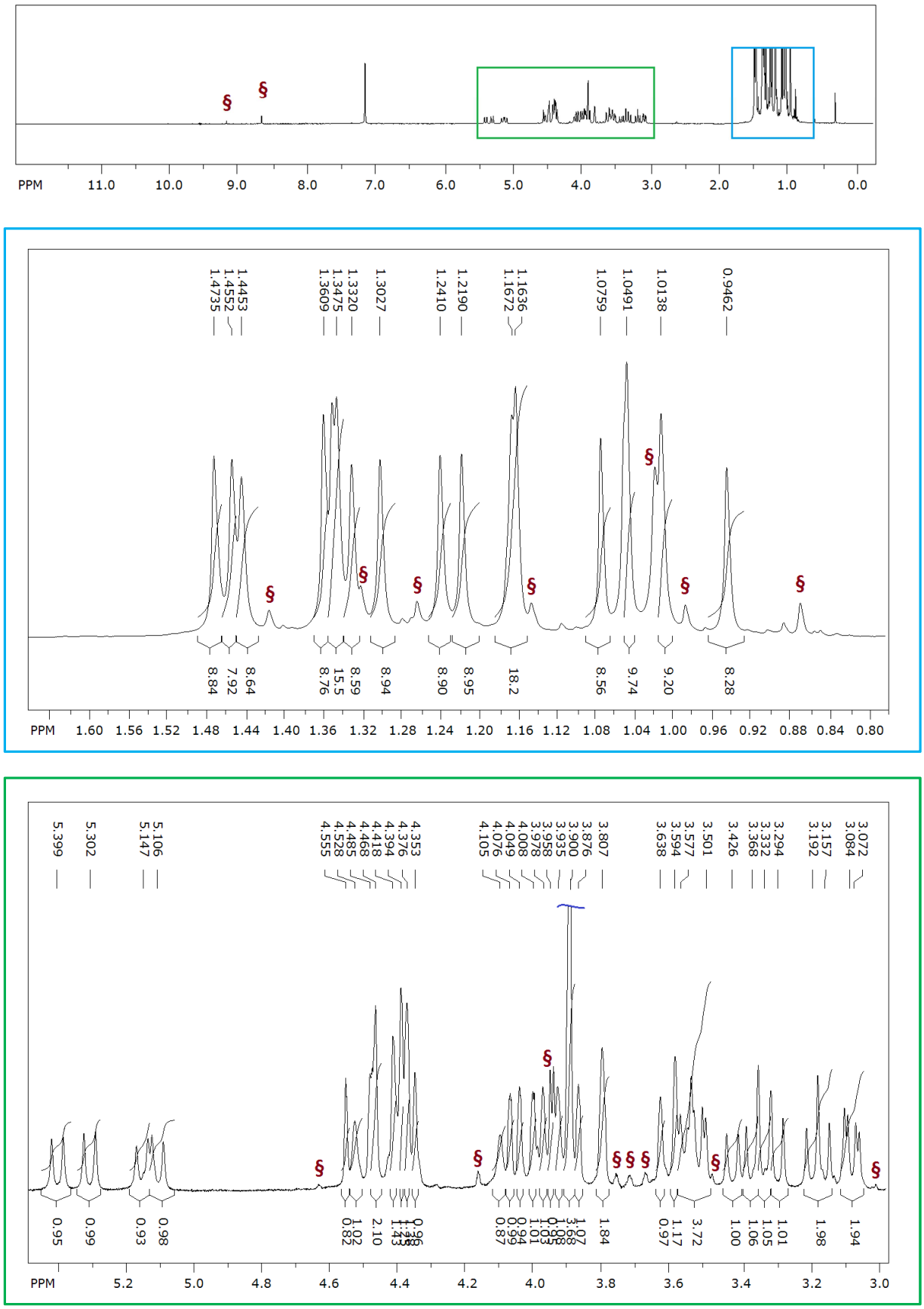

Figure S43. ^{1}H NMR spectrum of the material obtained from the crude carbonylation product by crystallization from hexane (C_6D_6, 399.9 MHz). Resonances marked with (§) belong to unidentified impurities.

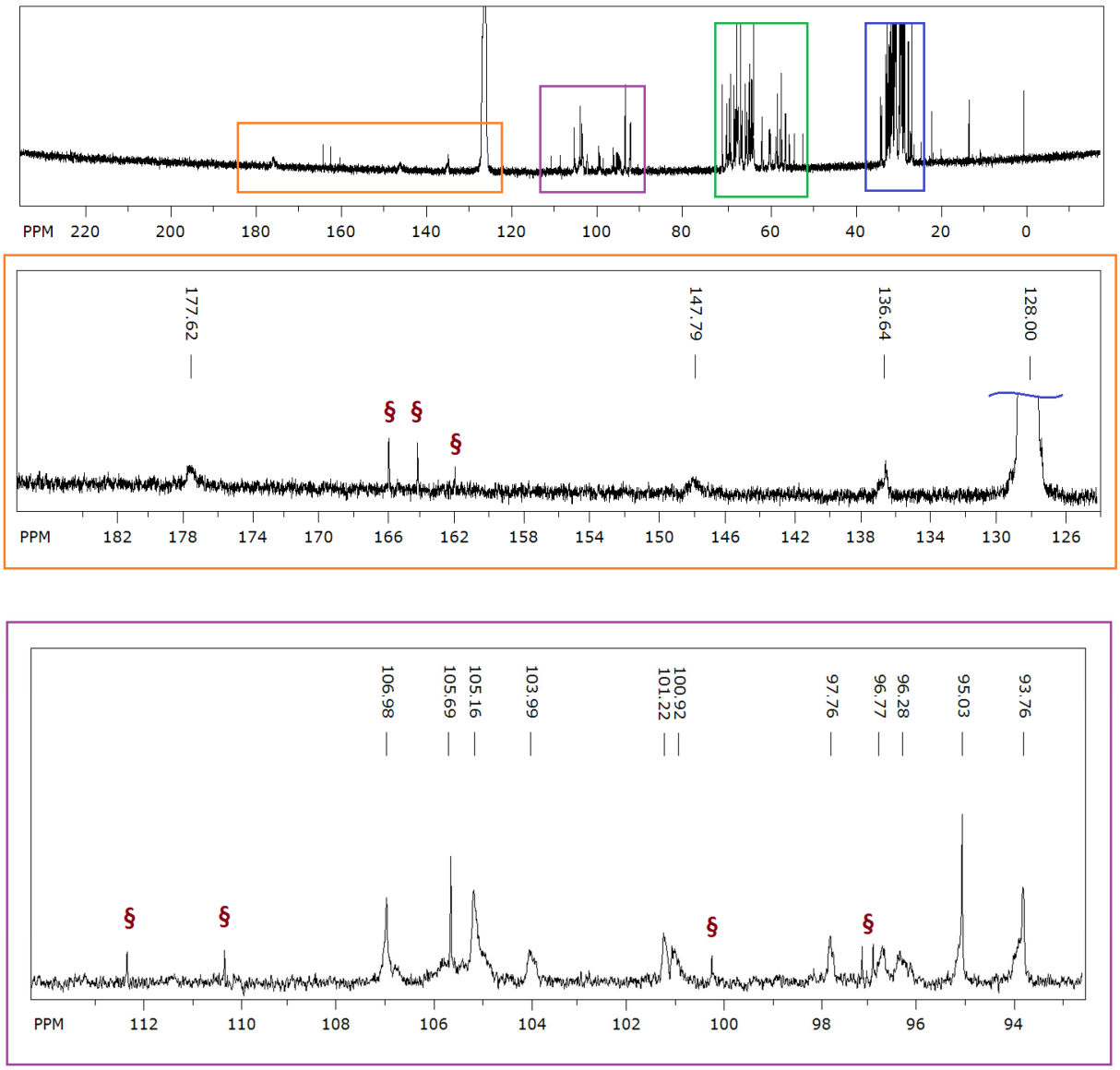

Figure S44. $^{13}C\{^{1}H\}$ NMR spectrum of the material obtained from the crude carbonylation product by crystallization from hexane (C_6D_6, 100.5 MHz). Signals marked with (§) belong to unidentified impurities.

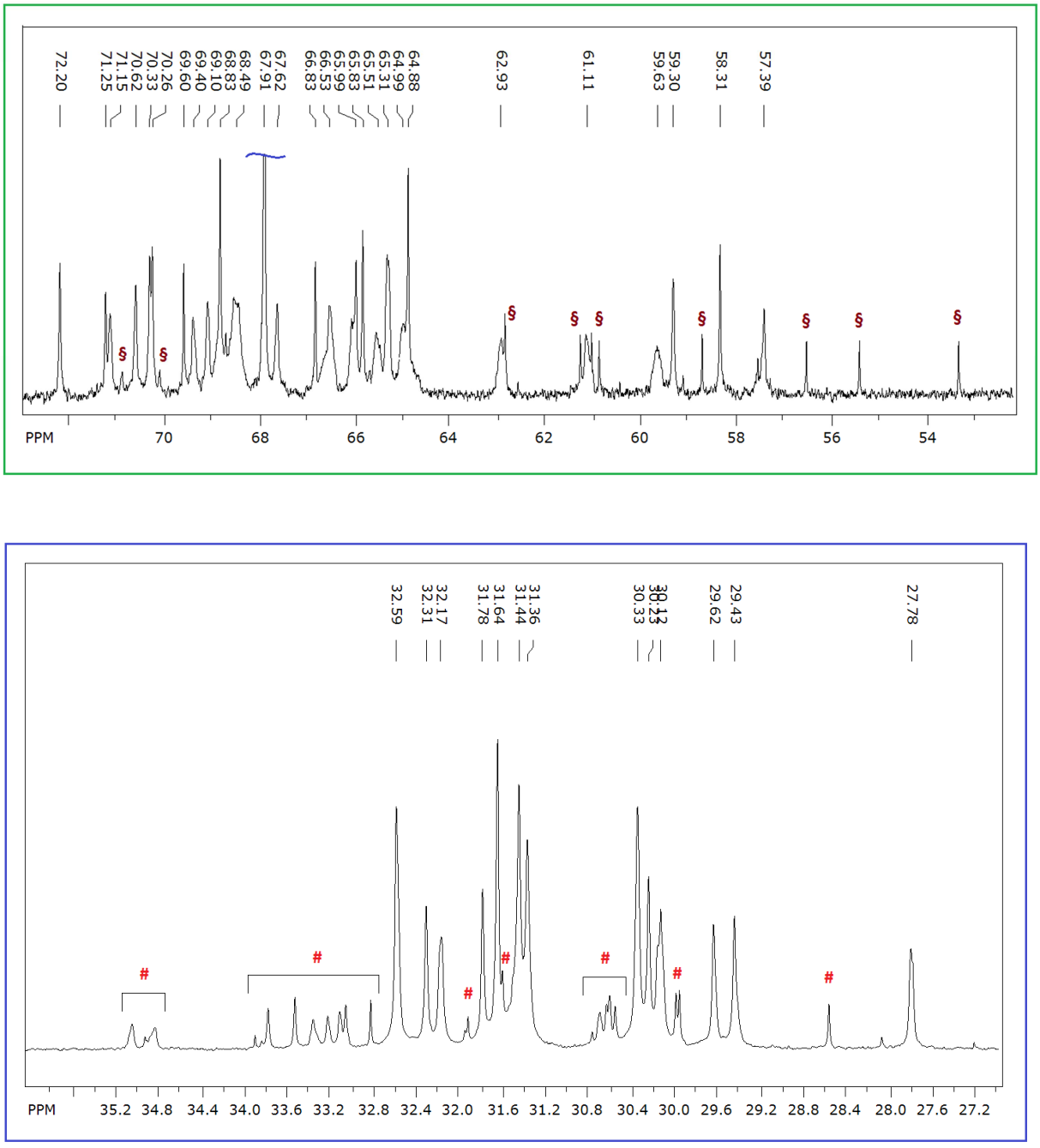

Figure S44 (continued). $^{13}C\{^{1}H\}$ NMR spectrum of the material obtained from the crude carbonylation product by crystallization from hexane (C_6D_6, 100.5 MHz). Signals marked with (**§**) belong to unidentified impurities. Signals with unclear assignment are marked with (**#**).

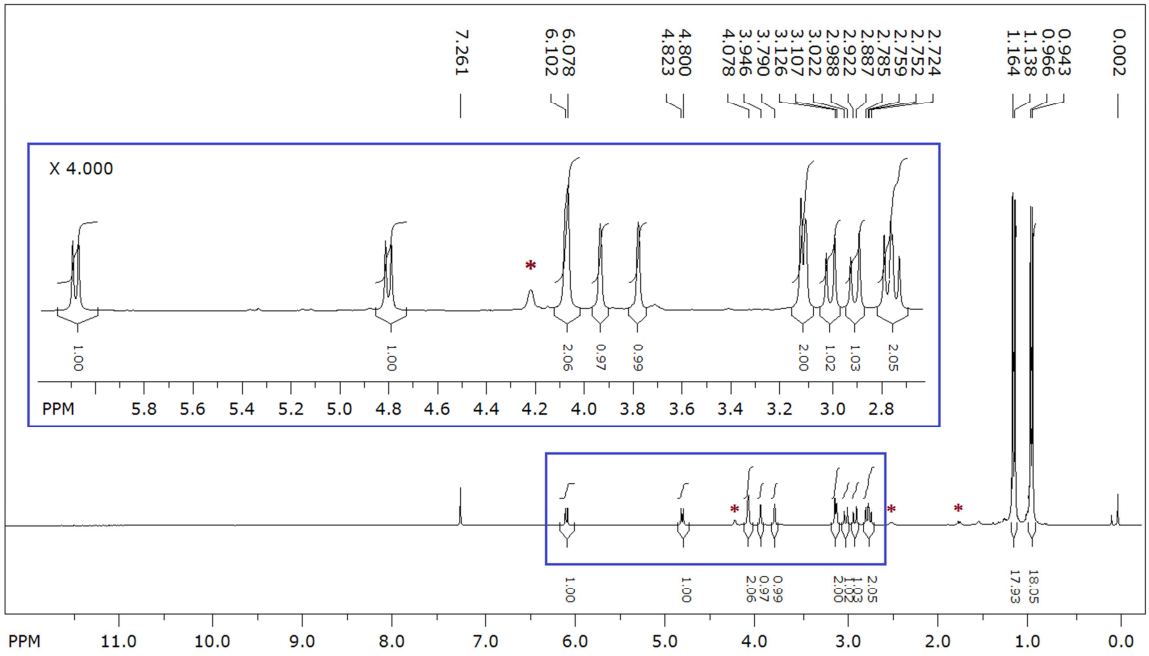

Figure S45. ^{1}H NMR spectrum of **A'-Np**H-$CHCl_2$ ($CDCl_3$, 399.9 MHz). Signals marked with (*) belong to trace amounts of [{Rh(μ-Cl)(COD)}$_2$]

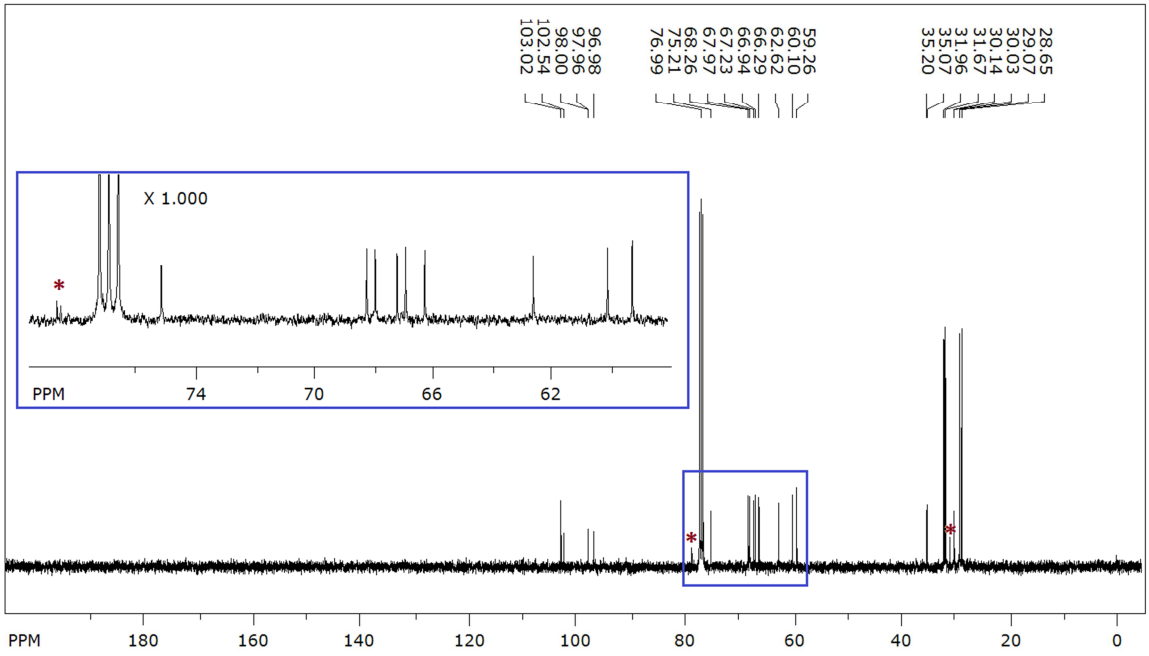

Figure S46. $^{13}C\{^{1}H\}$ NMR spectrum of **A'-Np**H-$CHCl_2$ ($CDCl_3$, 100.5 MHz). Signals marked with (*) belong to trace amounts of [{Rh(μ-Cl)(COD)}$_2$].

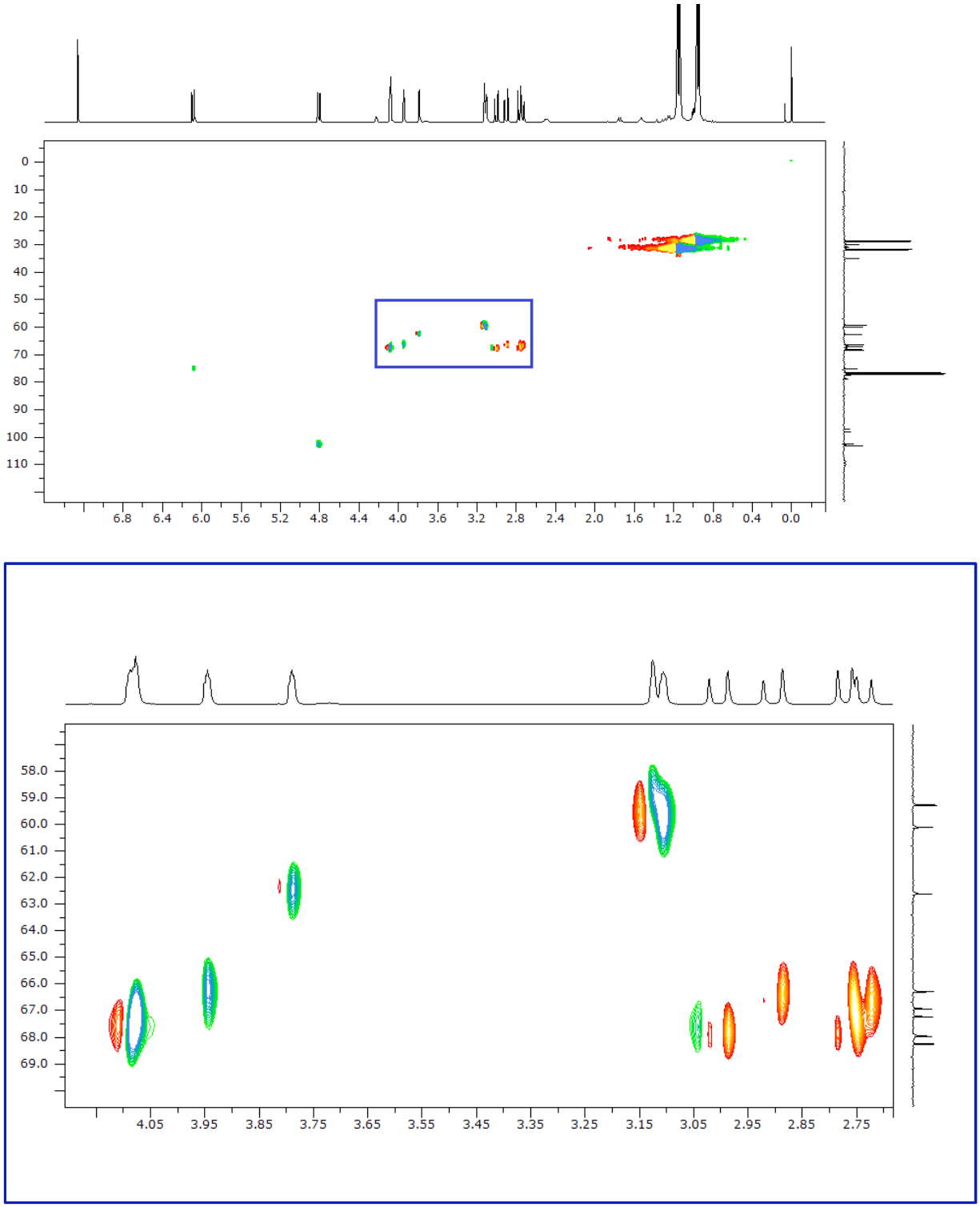

Figure S47. gHSQCad spectrum of **A'-Np**H-$CHCl_2$.

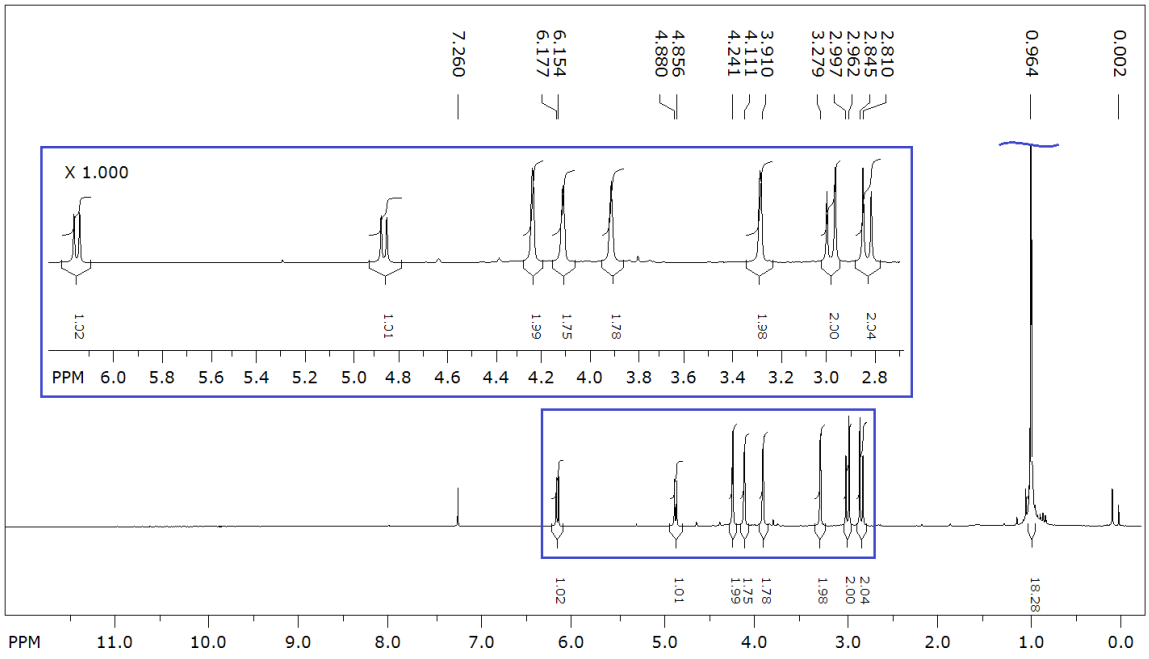

Figure S48. ^{1}H NMR spectrum of **A-Np**H-$CHCl_2$ ($CDCl_3$, 399.9 MHz).

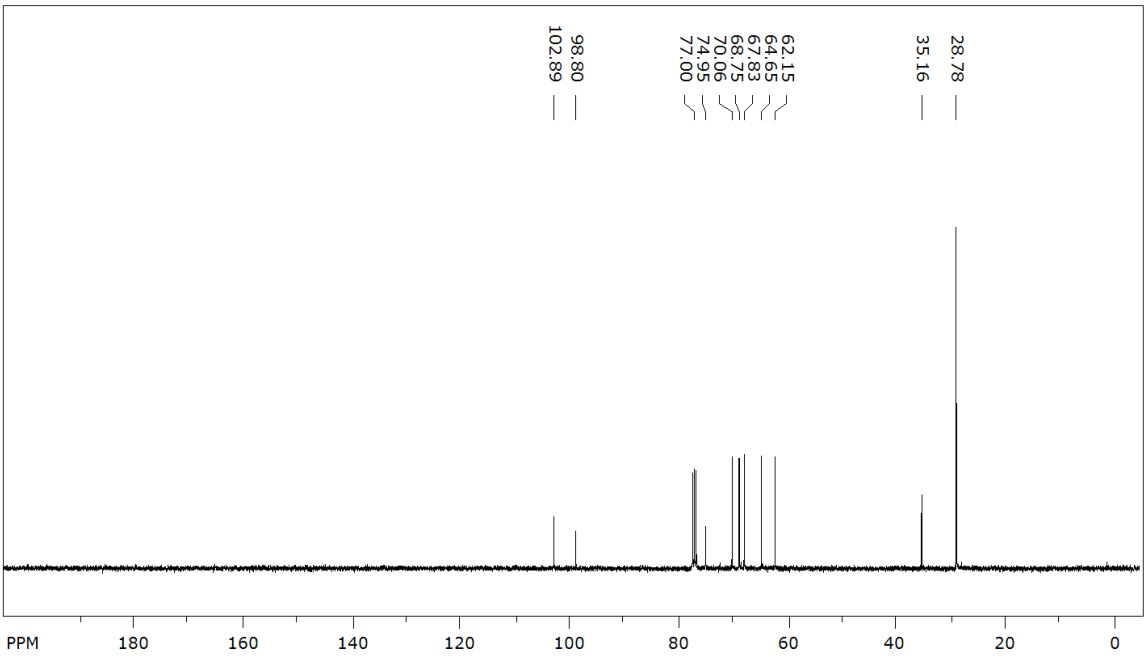

Figure S49. $^{13}C\{^{1}H\}$ NMR spectrum of **A-Np**H-$CHCl_2$ ($CDCl_3$, 100.5 MHz).

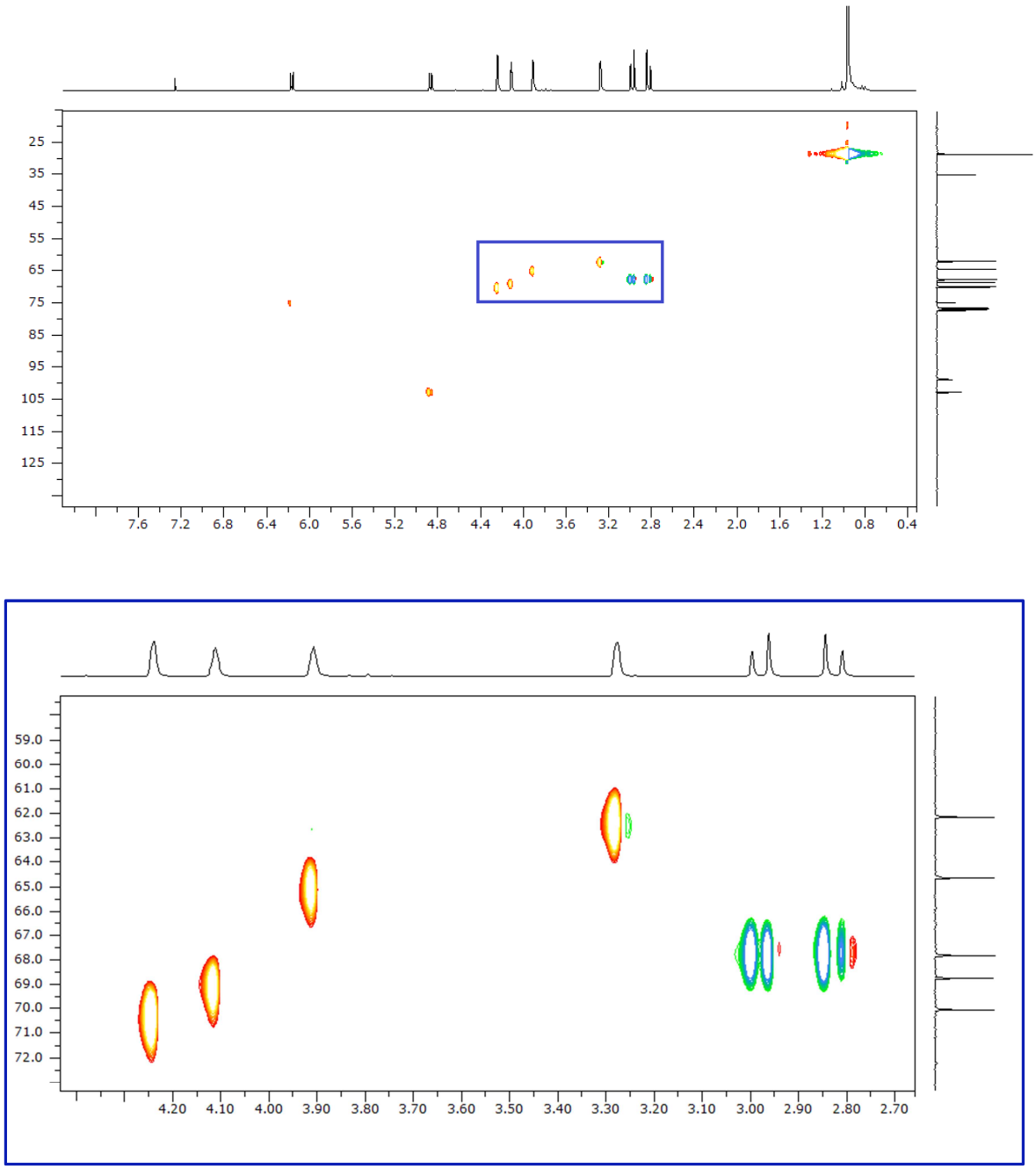

Figure S50. gHSQCad spectrum of **A'-Np**H-$CHCl_2$.

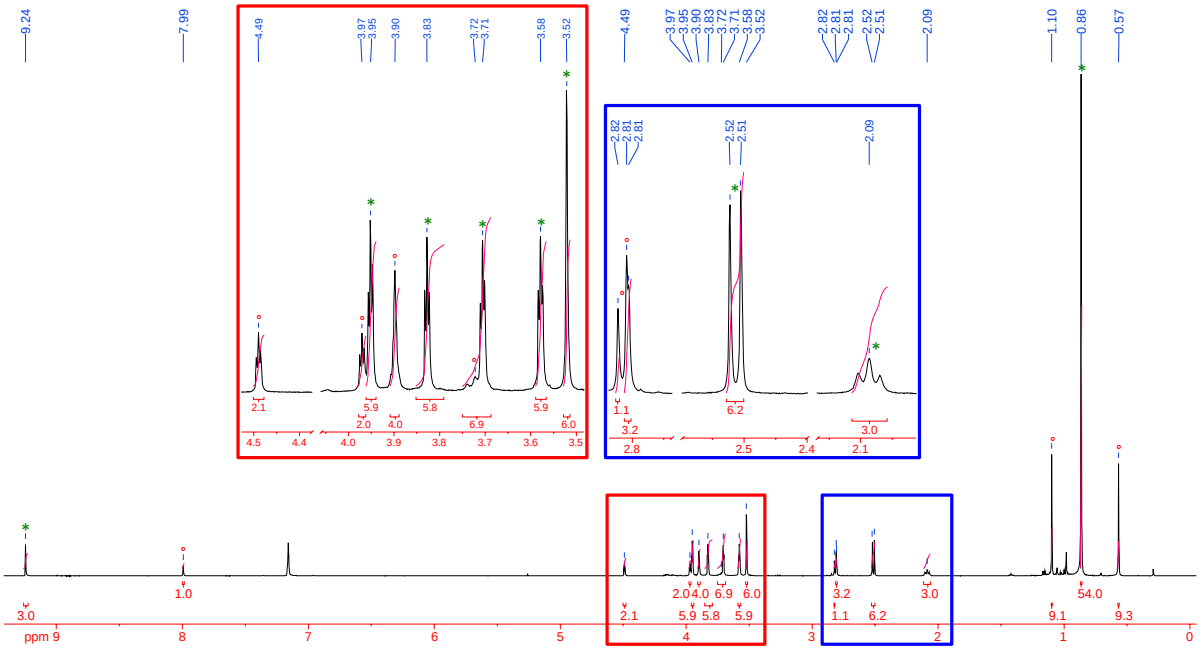

Figure S51. ^{1}H NMR spectrum of **A-Np**(H_2O) (C_6D_6, 399.9 MHz). Signals marked with (*) are due to the major isomer. Signals marked with (°) are due to the minor isomer.

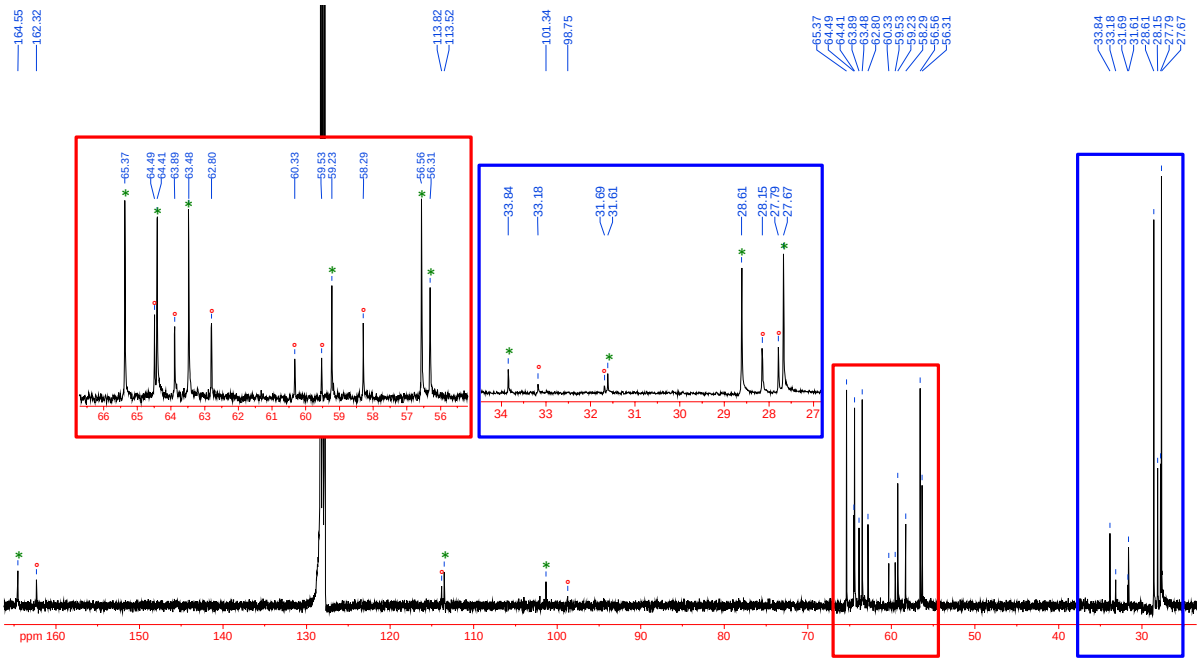

Figure S52. $^{13}C\{^{1}H\}$ NMR spectrum of **A-Np**(H_2O) (C_6D_6, 399.9 MHz). Signals marked with (*) are due to the major isomer. Signals marked with (°) are due to the minor isomer.

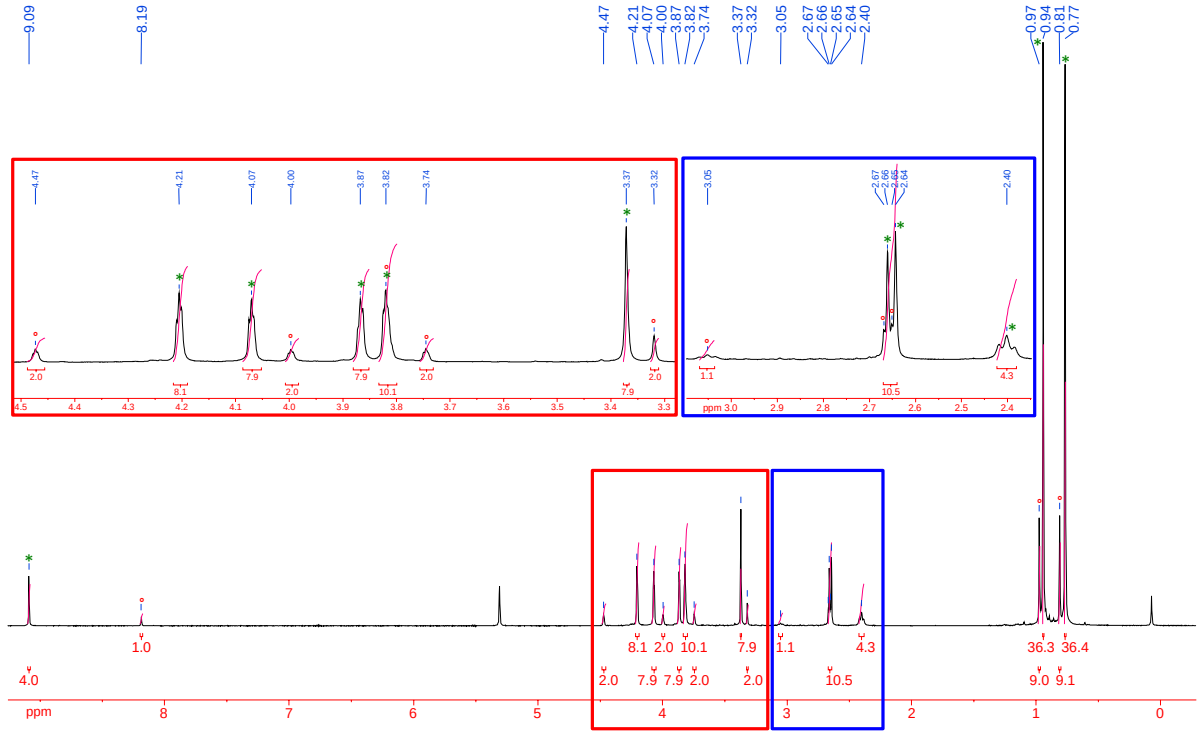

Figure S53. ^{1}H NMR spectrum of **A-Np**(H_2O) (CD_2Cl_2, 399.9 MHz). Signals marked with (*) are due to the major isomer. Signals marked with (°) are due to the minor isomer.

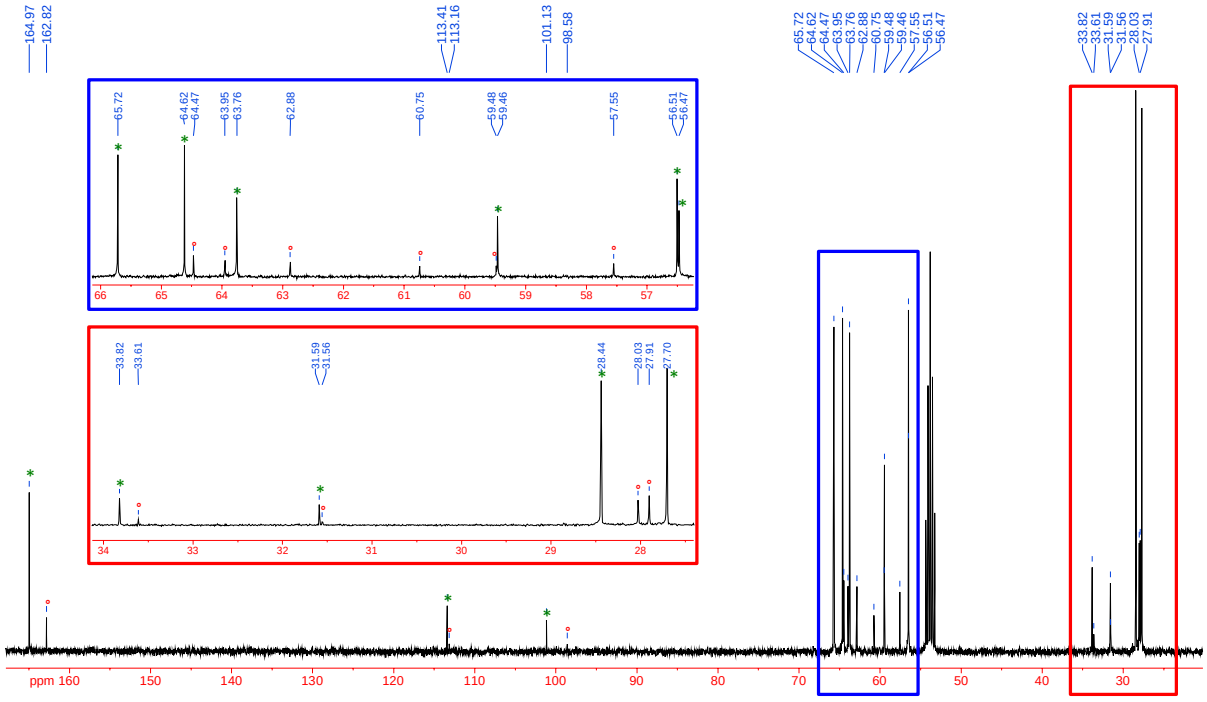

Figure S54. $^{13}C\{^{1}H\}$ NMR spectrum of **A-Np**(H_2O) (CD_2Cl_2, 399.9 MHz). Signals marked with (*) are due to the major isomer. Signals marked with (°) are due to the minor isomer.

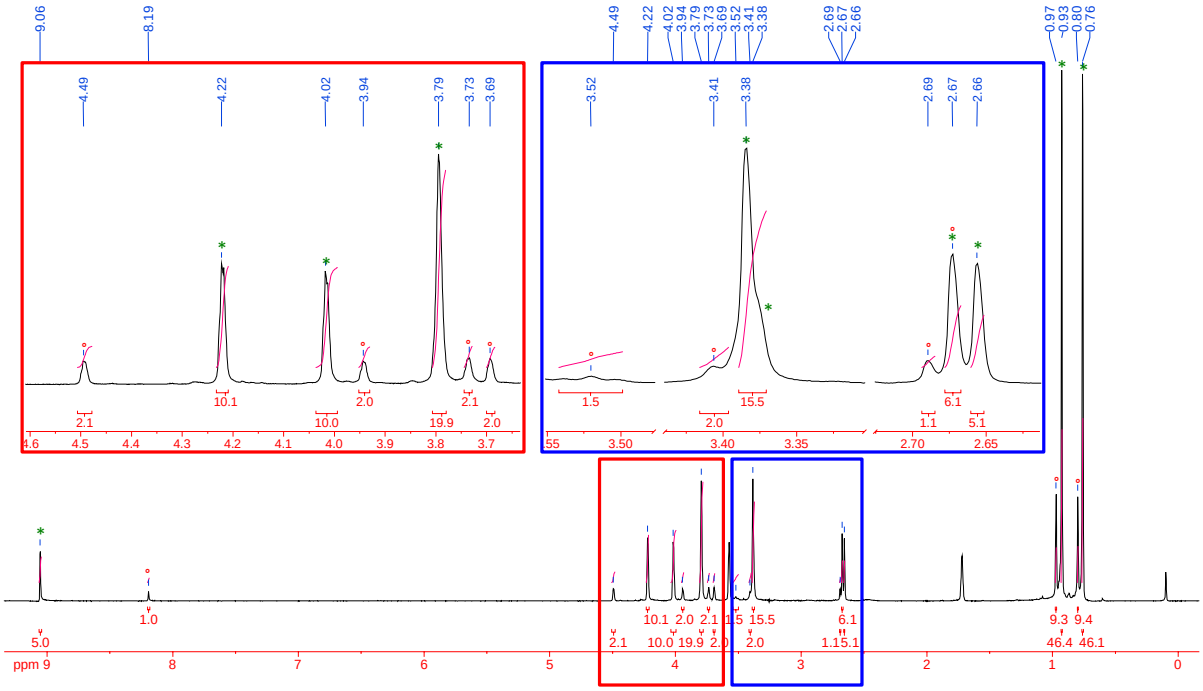

Figure S55. ^{1}H NMR spectrum of **A-Np**(H_2O) (THF-d_8, 399.9 MHz). Signals marked with (*) are due to the major isomer. Signals marked with (°) are due to the minor isomer.

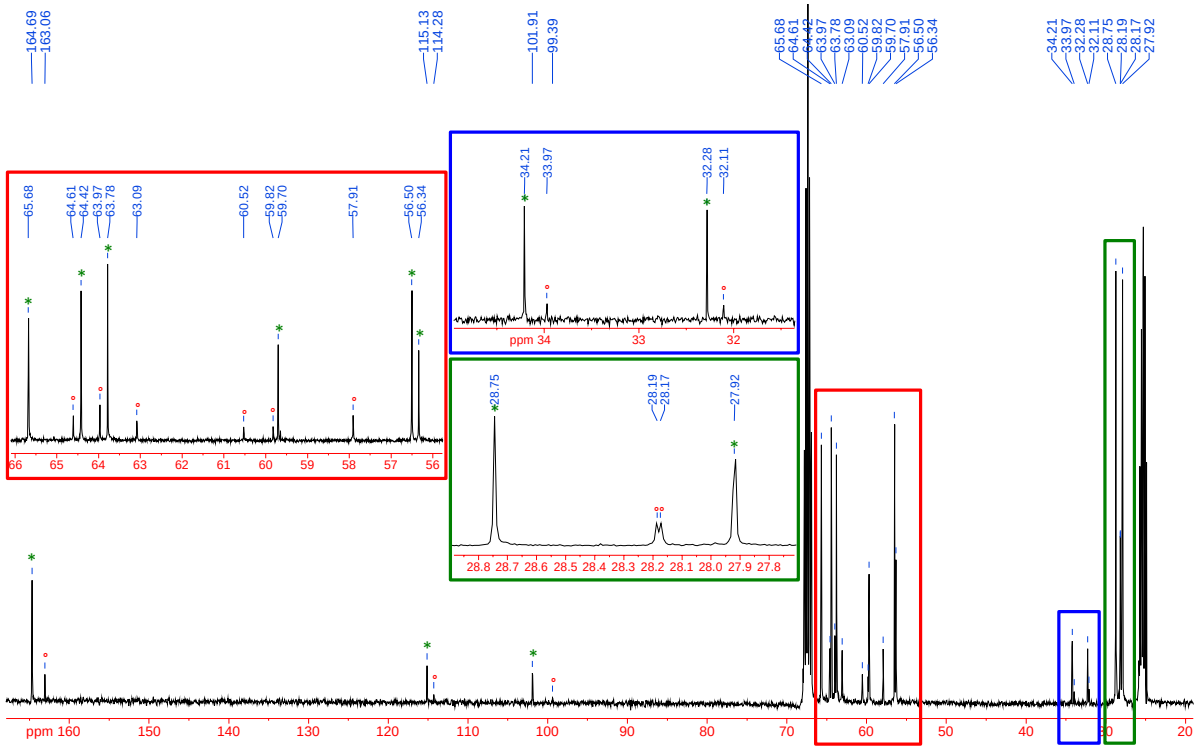

Figure S56. $^{13}C\{^{1}H\}$ NMR spectrum of **A-Np**(H_2O) (THF-d_8, 399.9 MHz). Signals marked with (*) are due to the major isomer. Signals marked with (°) are due to the minor isomer.

5. Computational Details

The geometry optimizations were performed at the BP86 level of theory, using Becke's exchange functional[S1] and Perdew's correlation functional.[S2] Ahlrich's def2-SVP basis set was used.[S3] The Gaussian09 program package was used for all calculations.[S4] Stationary points were characterized with frequency calculations at BP86/def2-SVP.

Table S2. Cartesian coordinates and energies at BP86/def2-SVP of the calculated molecules

A-Np

A-Np, singlet carbene; Cartesian coordinates in Å.

E(BP86/def2-SVP) = -2190.881538 a.u.

C	-1.862052	-3.050966	0.106738
C	-1.259812	-2.984461	1.415292
C	-0.950688	-1.607449	1.698572
C	-1.324743	-0.815165	0.539356
C	-1.925131	-1.717255	-0.429721
Fe	-0.000095	-2.167305	0.000002
C	1.861760	-3.051178	-0.106725
C	1.259530	-2.984616	-1.415280
C	0.950563	-1.607571	-1.698571
C	1.324707	-0.815320	-0.539360
C	1.924990	-1.717471	0.429724
N	1.116809	0.605169	-0.393829
C	2.253076	1.435872	-0.873516
C	3.106101	2.194228	0.190063
N	-1.116687	0.605300	0.393813
C	-2.252864	1.436125	0.873507
C	-3.105917	2.194455	-0.190068
C	0.000101	1.275513	-0.000005
H	-1.853939	2.177749	1.597234
H	1.854229	2.177478	-1.597304
H	2.308400	-1.430000	1.415772
H	2.218765	-3.961664	0.392500
H	1.077460	-3.836123	-2.084213
H	0.469153	-1.215137	-2.603839
H	-2.308512	-1.429747	-1.415769
H	-2.219161	-3.961414	-0.392479
H	-1.077837	-3.835983	2.084231
H	-0.469232	-1.215063	2.603836
H	2.923378	0.751073	-1.436261
H	-2.923181	0.751398	1.436322
C	4.362893	2.710869	-0.547414
C	2.331133	3.396004	0.771006
C	3.536959	1.255064	1.334328
C	-4.362668	2.711131	0.547451
C	-2.330979	3.396205	-0.771107
C	-3.536846	1.255242	-1.334265
H	4.195952	1.791738	2.049262
H	2.656761	0.889610	1.902718
H	4.098002	0.374524	0.955215
H	4.993004	3.322943	0.131986
H	4.988811	1.874352	-0.926933
H	4.089809	3.350752	-1.413940
H	2.941172	3.917638	1.540162
H	2.082635	4.129880	-0.024992
H	1.369732	3.071877	1.216859
H	-4.195940	1.791865	-2.049144
H	-2.656688	0.889823	-1.902739
H	-4.097803	0.374679	-0.955074
H	-2.941071	3.917811	-1.540241

H	-2.082428	4.130109	0.024848
H	-1.369607	3.072067	-1.217009
H	-4.992843	3.323123	-0.131964
H	-4.988538	1.874634	0.927094
H	-4.089537	3.351104	1.413896

A-Np-t, triplet carbene; Cartesian Coordinates in Å.
E(BP86/def2-SVP) = -2190.822136 a.u.

C	-2.021816	-3.023607	0.380336
C	-1.313172	-2.894953	1.630533
C	-0.984439	-1.526991	1.840671
C	-1.320500	-0.818424	0.626981
C	-2.050363	-1.740454	-0.250891
Fe	-0.053945	-2.224626	-0.099224
C	2.006765	-3.017529	-0.289365
C	1.464507	-2.880868	-1.614426
C	1.011286	-1.540065	-1.771467
C	1.328135	-0.818337	-0.529744
C	2.024073	-1.731902	0.341721
N	1.113965	0.599403	-0.339122
C	2.240416	1.447009	-0.814963
C	3.104618	2.176974	0.258726
N	-1.133136	0.597303	0.411842
C	-2.288933	1.433923	0.834092
C	-3.090448	2.187943	-0.272279
C	-0.009788	1.262662	0.039054
H	-1.920902	2.180171	1.569941
H	1.824720	2.208760	-1.507520
H	2.390465	-1.510076	1.350195
H	2.418164	-3.942208	0.137475
H	1.348122	-3.694826	-2.342703
H	0.558738	-1.087757	-2.663268
H	-2.546746	-1.467936	-1.189036
H	-2.456369	-3.953209	-0.010804
H	-1.112303	-3.717297	2.330676
H	-0.421178	-1.108509	2.684137
H	2.905170	0.782461	-1.407801
H	-2.985385	0.755880	1.372070
C	4.322233	2.765490	-0.490591
C	2.317569	3.326313	0.923176
C	3.597824	1.196263	1.341207
C	-4.369594	2.726599	0.409177
C	-2.282298	3.375334	-0.837551
C	-3.486659	1.239831	-1.421738
H	4.261914	1.717086	2.063166
H	2.746399	0.776162	1.915419
H	4.171430	0.352090	0.902640
H	4.965287	3.347798	0.202684
H	4.949574	1.968014	-0.944095
H	4.003572	3.451805	-1.304355
H	2.945683	3.835356	1.686127
H	2.007774	4.082815	0.171710
H	1.389593	2.954341	1.401152
H	-4.097937	1.778780	-2.176283
H	-2.589035	0.843802	-1.940454
H	-4.086448	0.379688	-1.055614
H	-2.858747	3.894112	-1.634087
H	-2.054258	4.115688	-0.041434
H	-1.308865	3.036637	-1.245066
H	-4.966454	3.335317	-0.302346
H	-5.018288	1.901631	0.775245
H	-4.123423	3.375473	1.277045

A’-Np

A’-Np, singlet carbene; Cartesian coordinates in Å.

E(BP86/def2-SVP) = -2505.148845 a.u.

C	-0.535999	1.918361	-0.349644
C	-1.900927	1.908300	0.121166
C	-1.892513	1.259058	1.416775
C	-0.542709	0.878996	1.741774
C	0.307082	1.262042	0.629739
Fe	-1.073324	-0.004525	-0.003351
C	-0.540147	-1.931094	0.334035
C	-1.909849	-1.915001	-0.122965
C	-1.912214	-1.263067	-1.417254
C	-0.564638	-0.886952	-1.755502
C	0.294421	-1.274665	-0.652605
N	1.717974	-1.060293	-0.557513
C	2.397945	-0.013676	-0.019719
N	1.728727	1.038887	0.522751
C	2.561185	2.082145	1.178032
C	3.320951	3.099604	0.272689
C	2.370167	3.764135	-0.742453
C	3.891805	4.178811	1.221954
C	4.483917	2.420119	-0.480054
C	2.534215	-2.129847	-1.192036
C	3.352180	-3.080900	-0.263482
C	2.479900	-3.618083	0.888400
C	3.815598	-4.261285	-1.148757
C	4.591461	-2.365501	0.315364
H	3.234542	-1.649935	-1.907979
H	3.303524	1.566180	1.822106
H	-0.185148	2.315197	-1.308990
C	-3.069979	2.647601	-0.531782
H	-2.766276	1.098024	2.061454
H	-0.208349	0.353932	2.646294
H	-0.179228	-2.332034	1.288042
C	-3.074805	-2.651822	0.539874
H	-2.792215	-1.096609	-2.052057
H	-0.237747	-0.361296	-2.662380
H	1.880540	2.652781	1.846121
H	1.827115	-2.747360	-1.786293
H	2.902978	4.552788	-1.315230
H	1.989725	3.022828	-1.474804
H	1.497658	4.237184	-0.243585
H	4.501320	4.915950	0.658197
H	3.083631	4.736475	1.742845
H	4.546877	3.728285	1.998384
H	5.009406	3.155351	-1.127541
H	5.224664	1.994816	0.229723
H	4.118387	1.577394	-1.100003
H	3.049539	-4.352249	1.496807
H	2.164614	-2.797058	1.565016
H	1.567961	-4.127428	0.510373
H	5.148768	-3.042410	0.998785
H	5.283450	-2.053216	-0.495865
H	4.295633	-1.444798	0.856868
H	4.469952	-4.950171	-0.574123
H	2.954128	-4.851569	-1.529731
H	4.396989	-3.904160	-2.025912
C	-2.896237	-2.697851	2.073857
C	-4.425319	-1.981035	0.213530
C	-3.081077	-4.102081	-0.015735
H	-3.757623	-3.213767	2.547718
H	-1.980243	-3.250813	2.367476

H	-2.828212	-1.675276	2.498818
H	-3.904427	-4.694024	0.438779
H	-3.221823	-4.107186	-1.116637
H	-2.124254	-4.619947	0.203625
H	-5.259985	-2.551714	0.672450
H	-4.459514	-0.945228	0.606144
H	-4.615820	-1.940993	-0.878918
C	-3.074236	4.095231	0.030521
C	-2.899692	2.700995	-2.066481
C	-4.418292	1.974218	-0.201763
H	-3.899553	4.689094	-0.417877
H	-3.210383	4.095259	1.132003
H	-2.118415	4.614198	-0.190546
H	-3.764770	3.217054	-2.533393
H	-1.986624	3.257494	-2.362508
H	-2.831792	1.680500	-2.496466
H	-5.255911	2.548005	-0.651361
H	-4.454671	0.941314	-0.601747
H	-4.602030	1.926089	0.891512

A’-Np-t, triplet carbene; Cartesian coordinates in Å.
E(BP86/def2-SVP) = -2505.090340 a.u.

C	-0.478280	-2.071698	0.285240
C	-1.791585	-2.142691	-0.288770
C	-1.724171	-1.548391	-1.606319
C	-0.417429	-1.015654	-1.809697
C	0.359680	-1.303617	-0.599257
Fe	-1.114669	-0.002421	-0.126063
C	-0.654529	2.016886	-0.259103
C	-1.974141	2.003773	0.299490
C	-1.894734	1.263588	1.542174
C	-0.536146	0.930368	1.820387
C	0.233545	1.292173	0.656586
N	1.663405	1.149128	0.503127
C	2.379751	0.090483	0.048502
N	1.768135	-1.021633	-0.433232
C	2.663147	-2.064514	-1.003881
C	3.469036	-2.961373	-0.014497
C	2.547874	-3.575959	1.057848
C	4.089771	-4.093290	-0.865816
C	4.600895	-2.167186	0.670837
C	2.446226	2.296977	1.037152
C	3.236170	3.186292	0.026808
C	2.345069	3.617381	-1.155000
C	3.683242	4.440564	0.813383
C	4.486262	2.456734	-0.509244
H	3.161311	1.904325	1.791272
H	3.381393	-1.563196	-1.686440
H	-0.184166	-2.432359	1.276606
C	-2.979051	-2.914558	0.290432
H	-2.558849	-1.476829	-2.316291
H	-0.027706	-0.527157	-2.712260
H	-0.328432	2.514947	-1.178643
C	-3.208502	2.724595	-0.245515
H	-2.741765	1.056237	2.209965
H	-0.165135	0.359378	2.680904
H	2.018994	-2.724521	-1.623611
H	1.720853	2.942222	1.577104
H	3.118307	-4.274592	1.706108
H	2.118112	-2.789451	1.712077
H	1.708655	-4.143685	0.602604
H	4.727669	-4.751414	-0.238769
H	3.308839	-4.728596	-1.337011

H	4.728909	-3.684059	-1.677601
H	5.160755	-2.819938	1.375364
H	5.320312	-1.772353	-0.077395
H	4.198622	-1.291762	1.218197
H	2.905713	4.290195	-1.837926
H	2.014718	2.739032	-1.747522
H	1.442340	4.164350	-0.809341
H	5.035437	3.103902	-1.227305
H	5.180412	2.196714	0.318231
H	4.207614	1.504559	-1.002696
H	4.306149	5.102692	0.175616
H	2.813062	5.033954	1.168752
H	4.291741	4.166201	1.701846
C	-3.038364	3.034685	-1.749105
C	-4.483002	1.872574	-0.051473
C	-3.364854	4.058749	0.533660
H	-3.948032	3.530781	-2.147701
H	-2.182694	3.716558	-1.933575
H	-2.867889	2.106825	-2.334310
H	-4.242495	4.631572	0.163557
H	-3.508267	3.874940	1.618765
H	-2.463808	4.695670	0.415509
H	-5.375946	2.423685	-0.415374
H	-4.415797	0.918704	-0.614188
H	-4.659448	1.626533	1.016099
C	-2.889527	-4.374995	-0.230375
C	-2.929380	-2.921577	1.834452
C	-4.319845	-2.297154	-0.163198
H	-3.731265	-4.983679	0.164302
H	-2.931743	-4.407514	-1.338886
H	-1.939981	-4.853871	0.086268
H	-3.806376	-3.463656	2.246457
H	-2.019721	-3.428817	2.216452
H	-2.940169	-1.887672	2.237236
H	-5.170885	-2.872498	0.258340
H	-4.410370	-1.246574	0.180579
H	-4.431122	-2.308271	-1.267187

6. References

(S1) Becke, A. D. *Phys. Rev. A* **1988**, *38*, 3098−3100.
(S2) Perdew, J. P. *Phys. Rev. B* **1986**, *33*, 8822−8824.
(S3) Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297−3305.
(S4) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, M. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09*, Revision D.01; Gaussian, Inc.: Wallingford, CT, 2013.