A Mesoionic Carbene Stabilized Nickel(II) Hydroxide Complex: A Facile Precursor for C–H Activation Chemistry

- Supporting Information -

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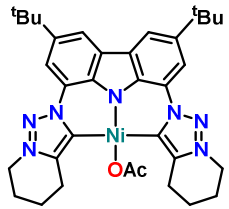
1. NMR spectra



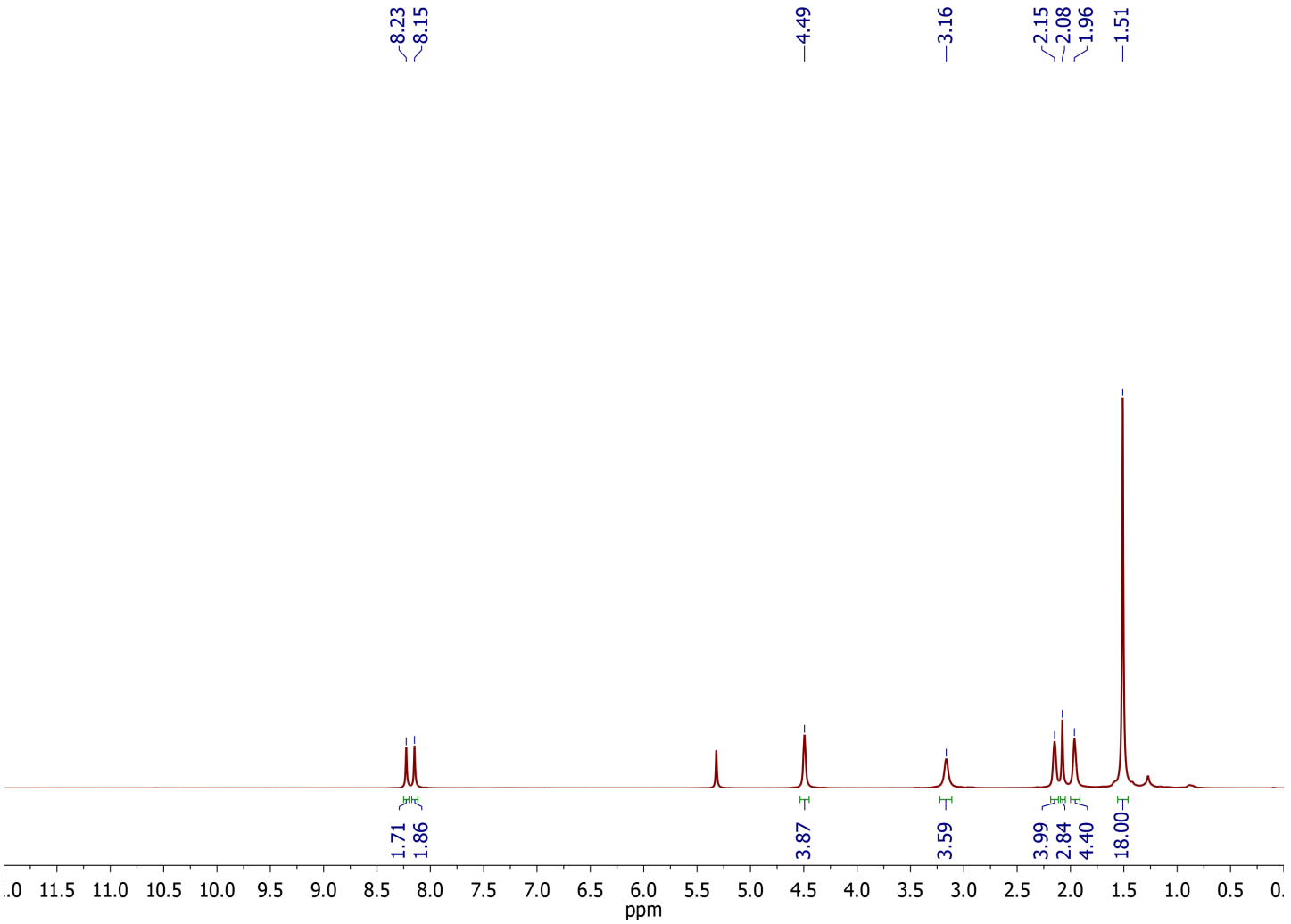
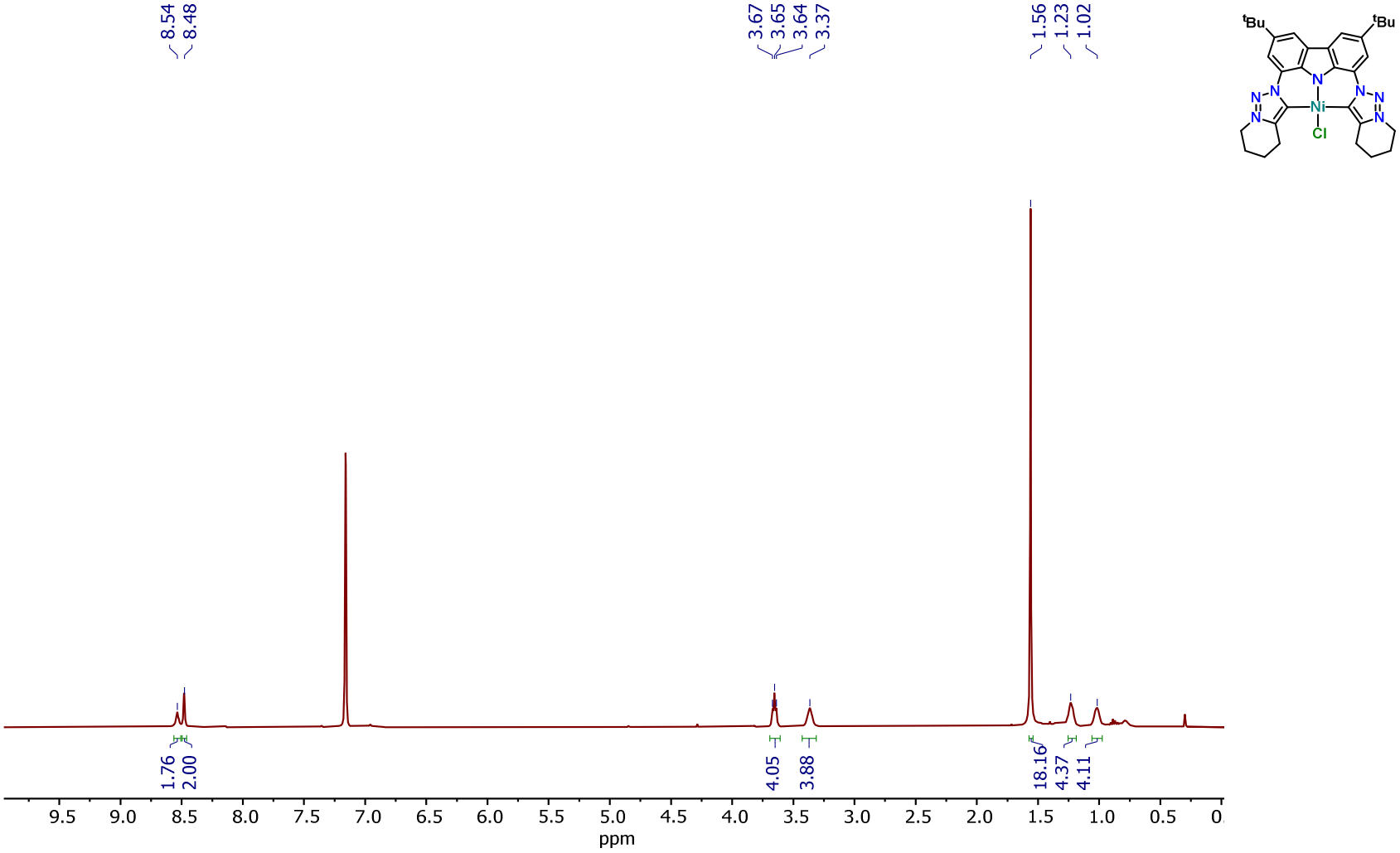


*Figure S 1: ^1H NMR of complex **O** in CD_2Cl_2 at 298 K.*



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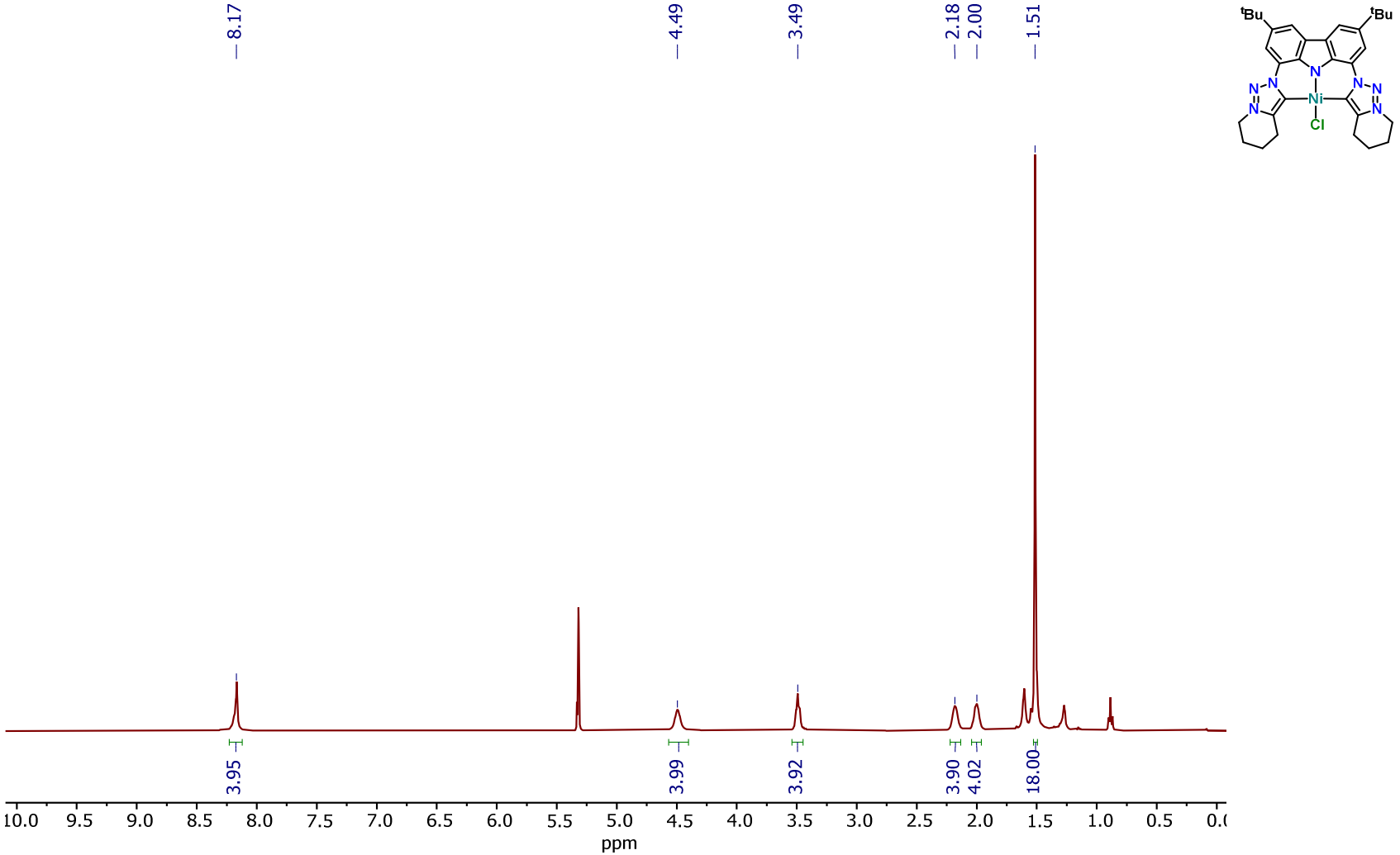

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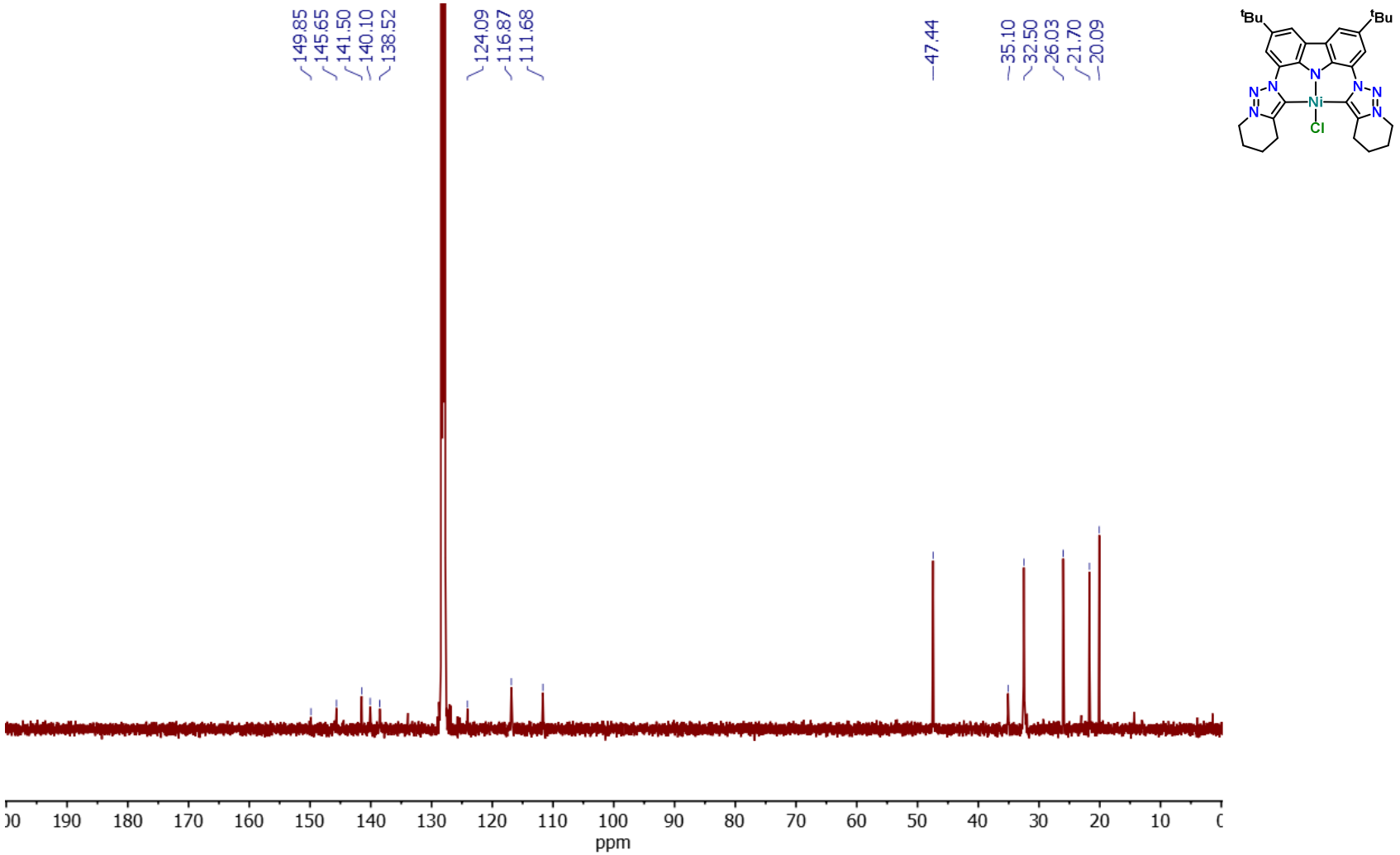

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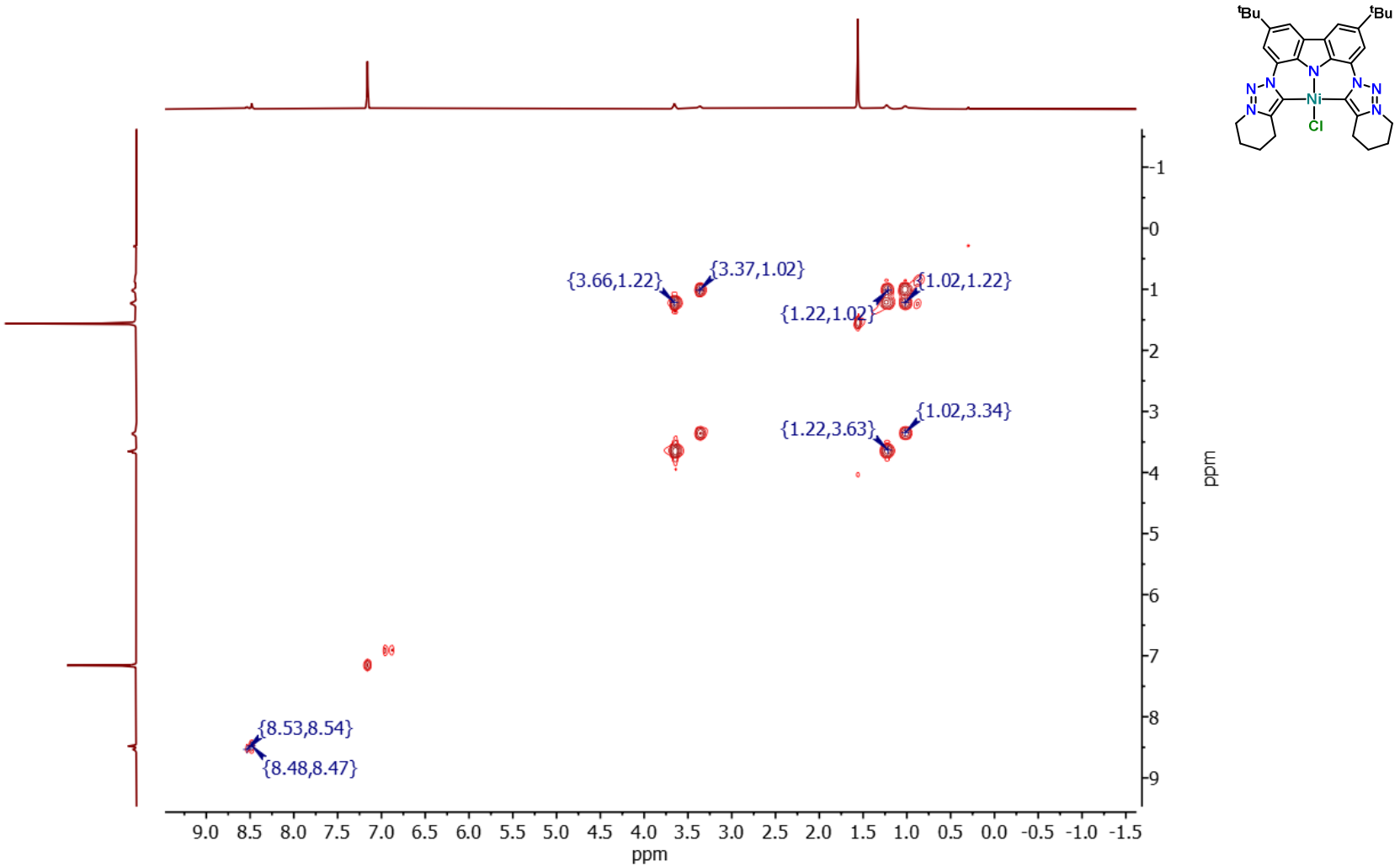

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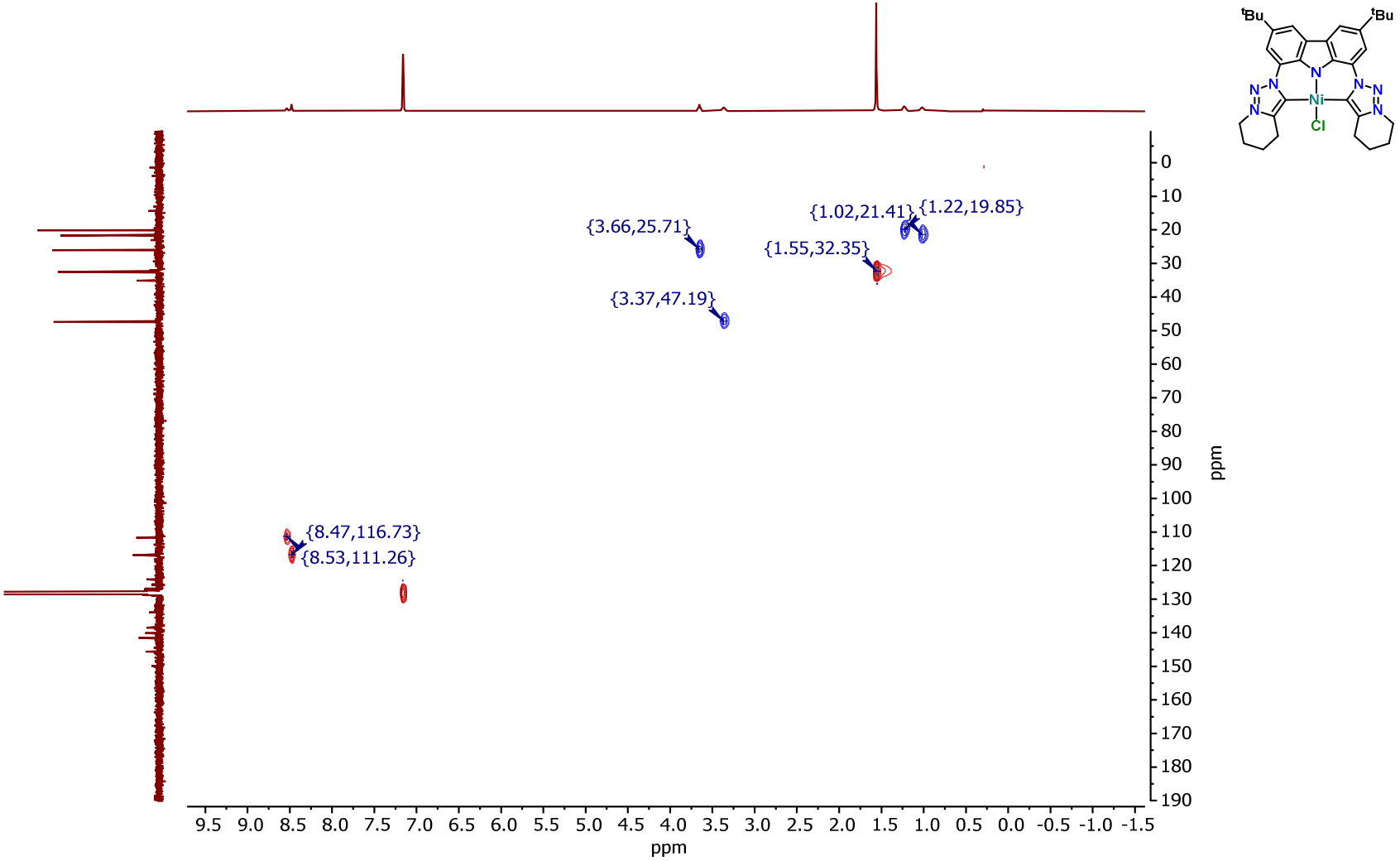

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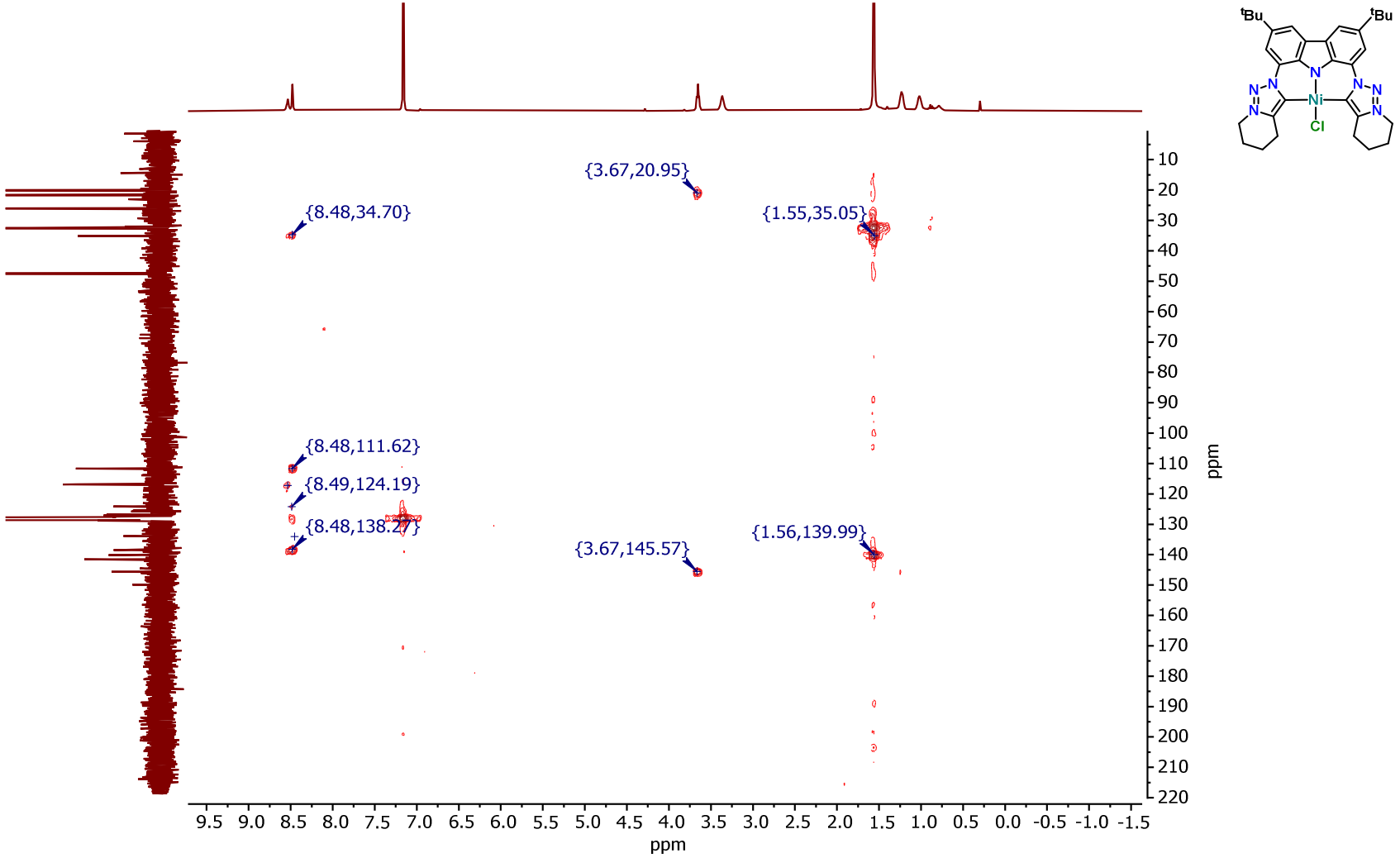

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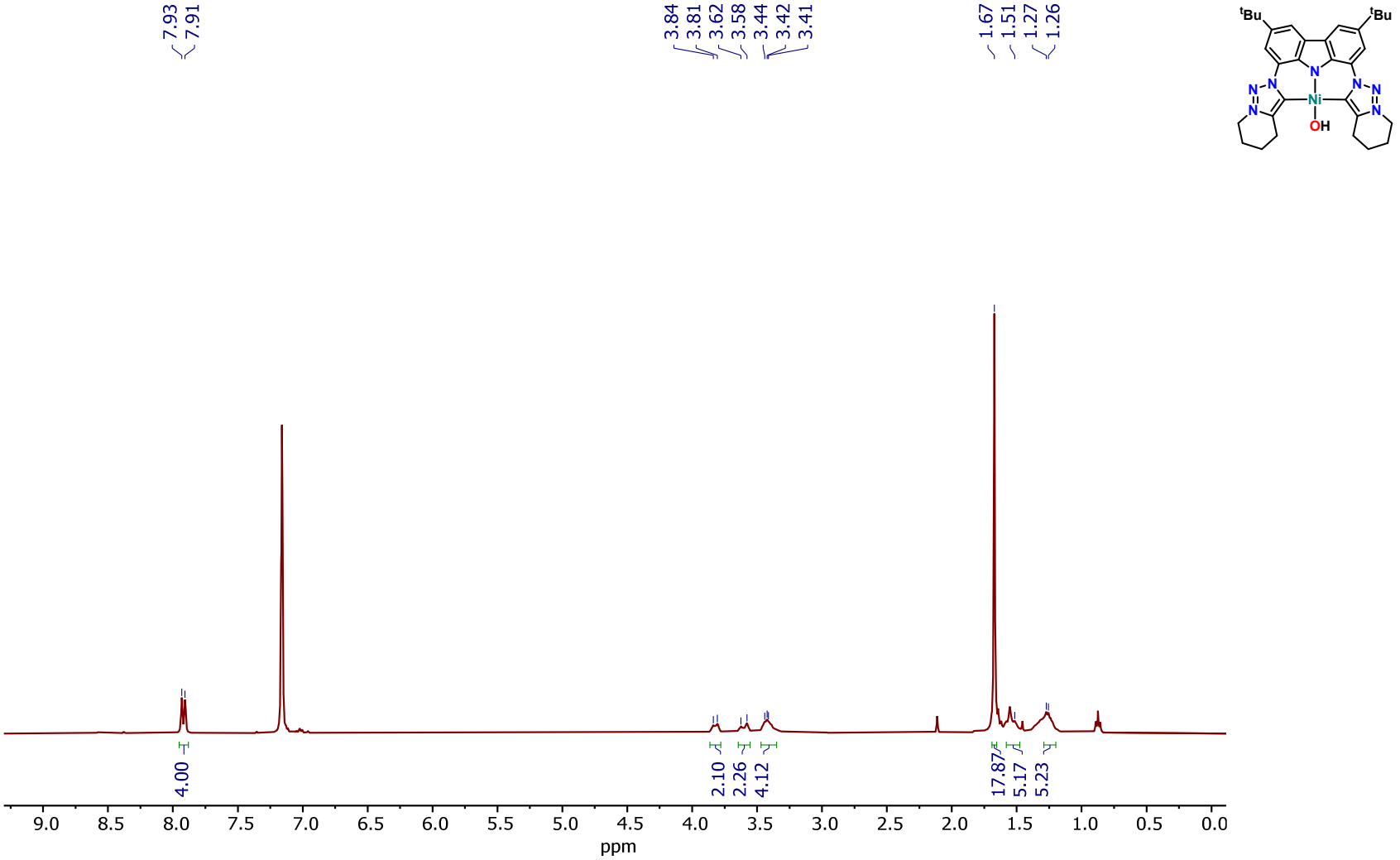

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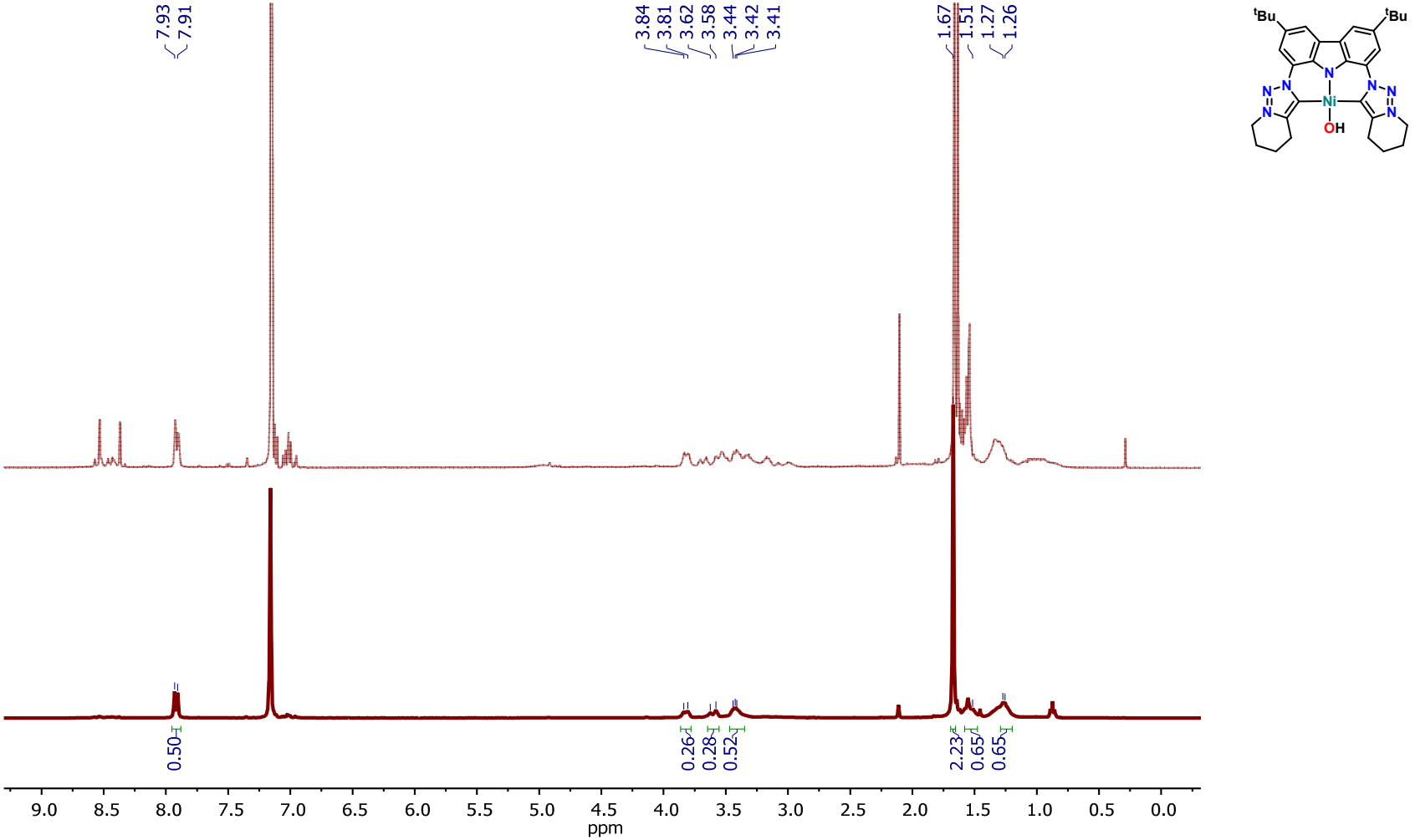

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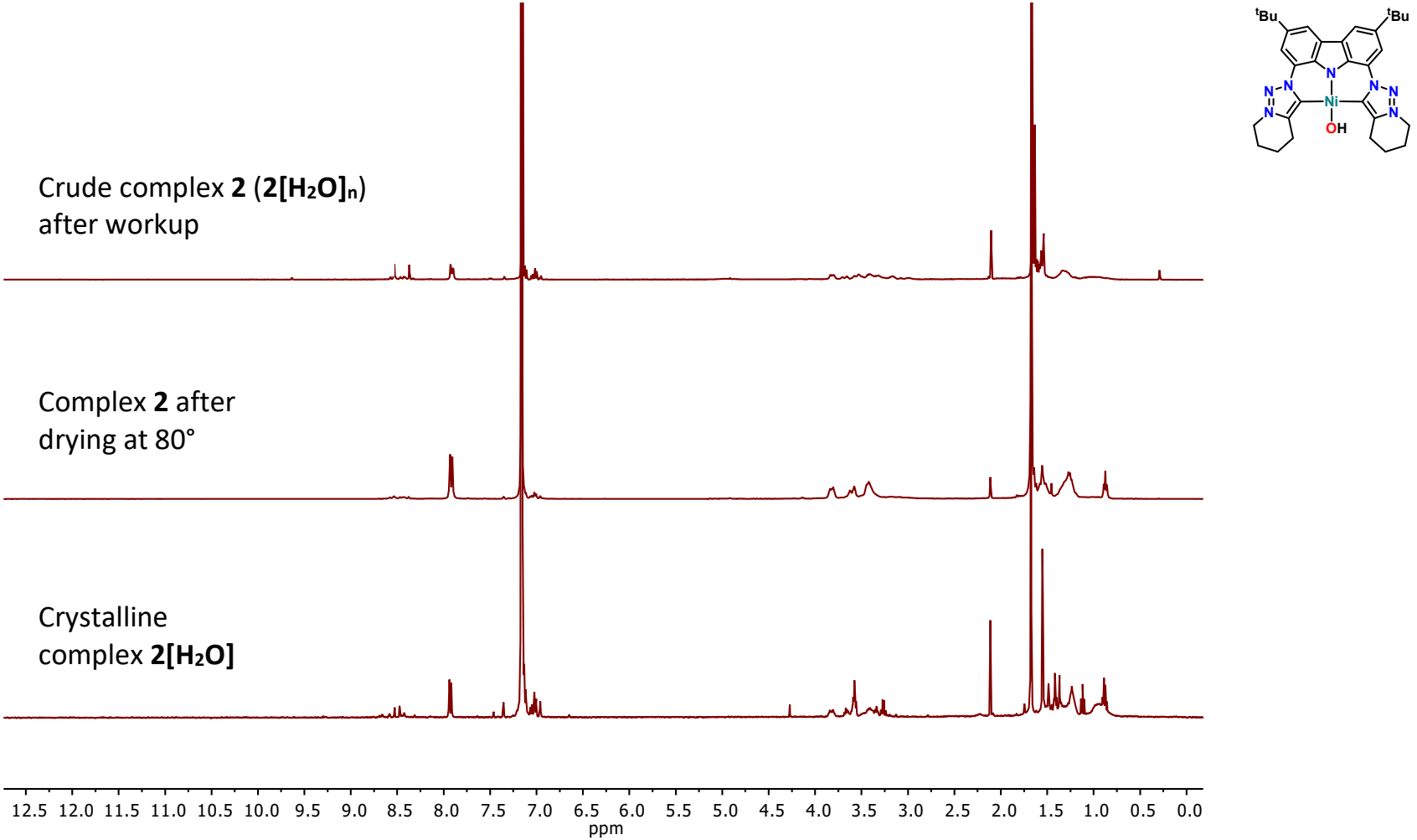

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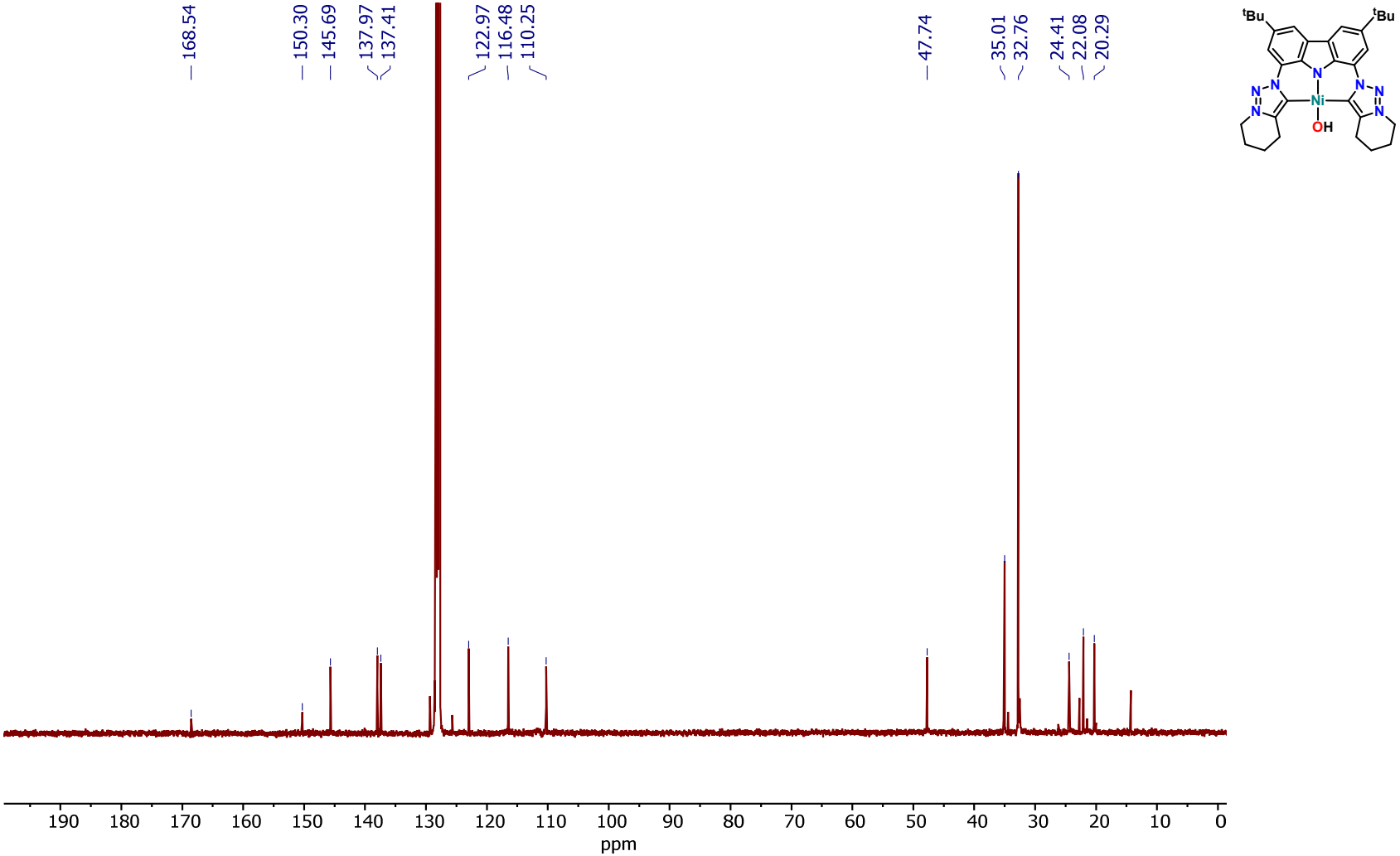

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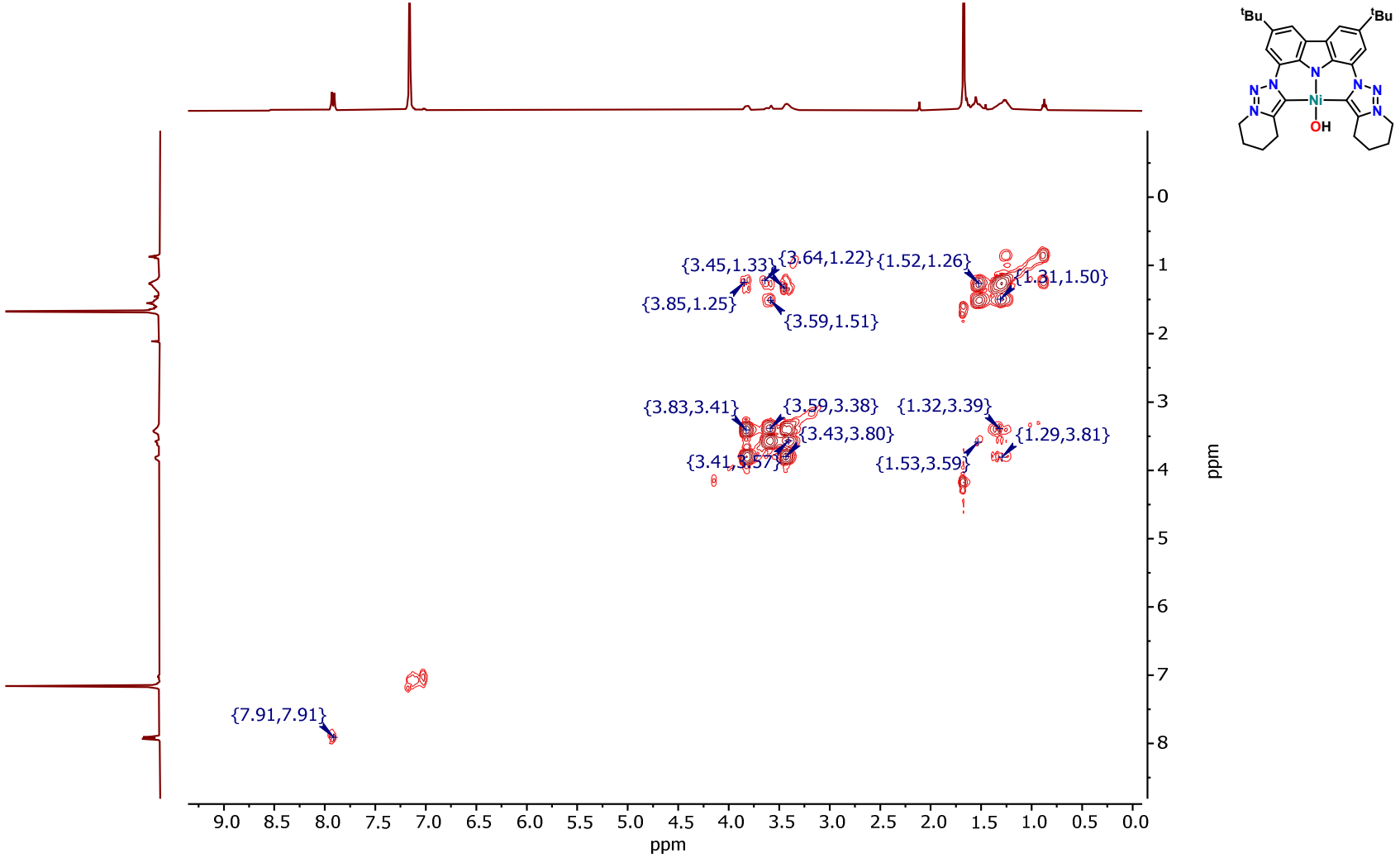

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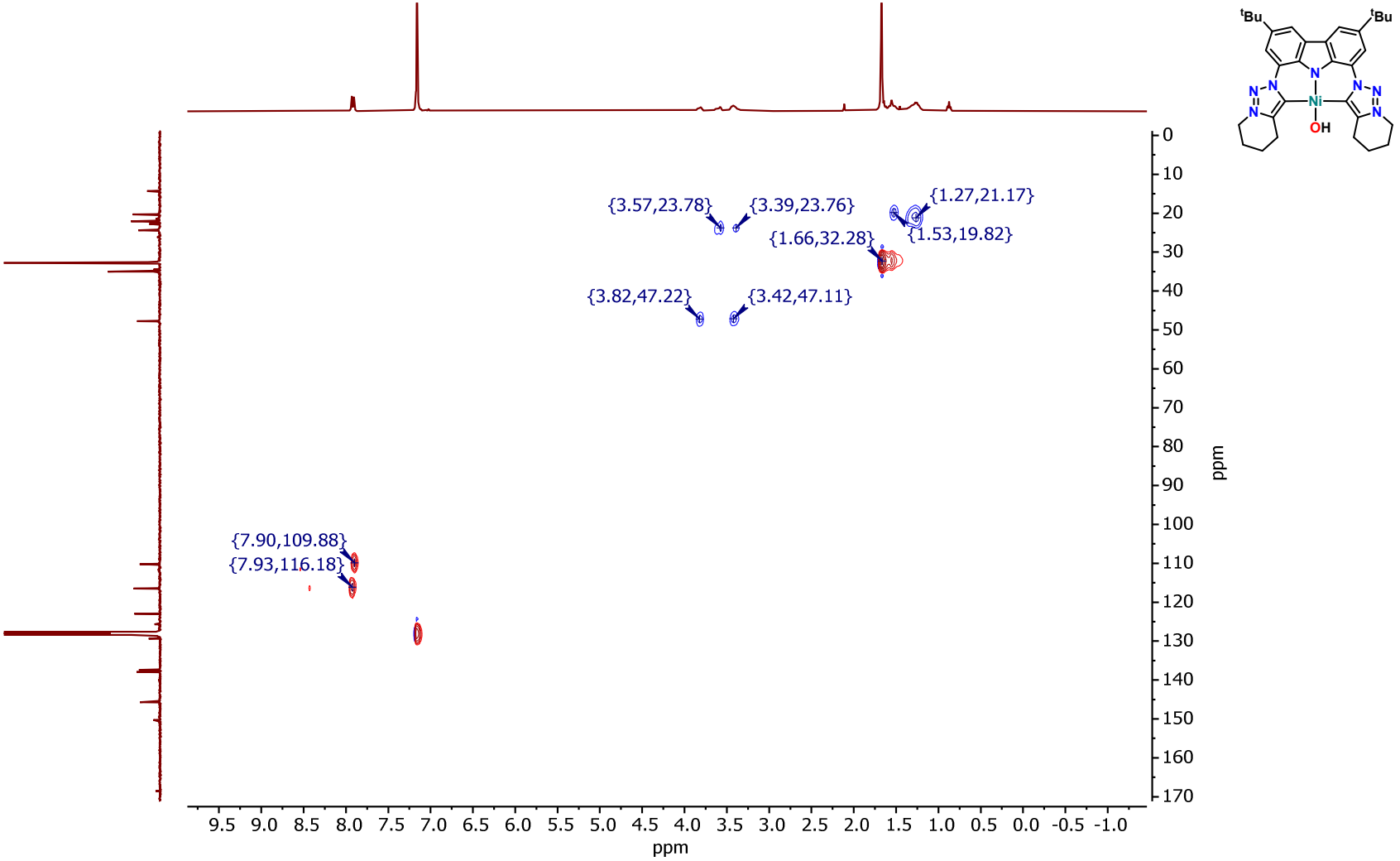

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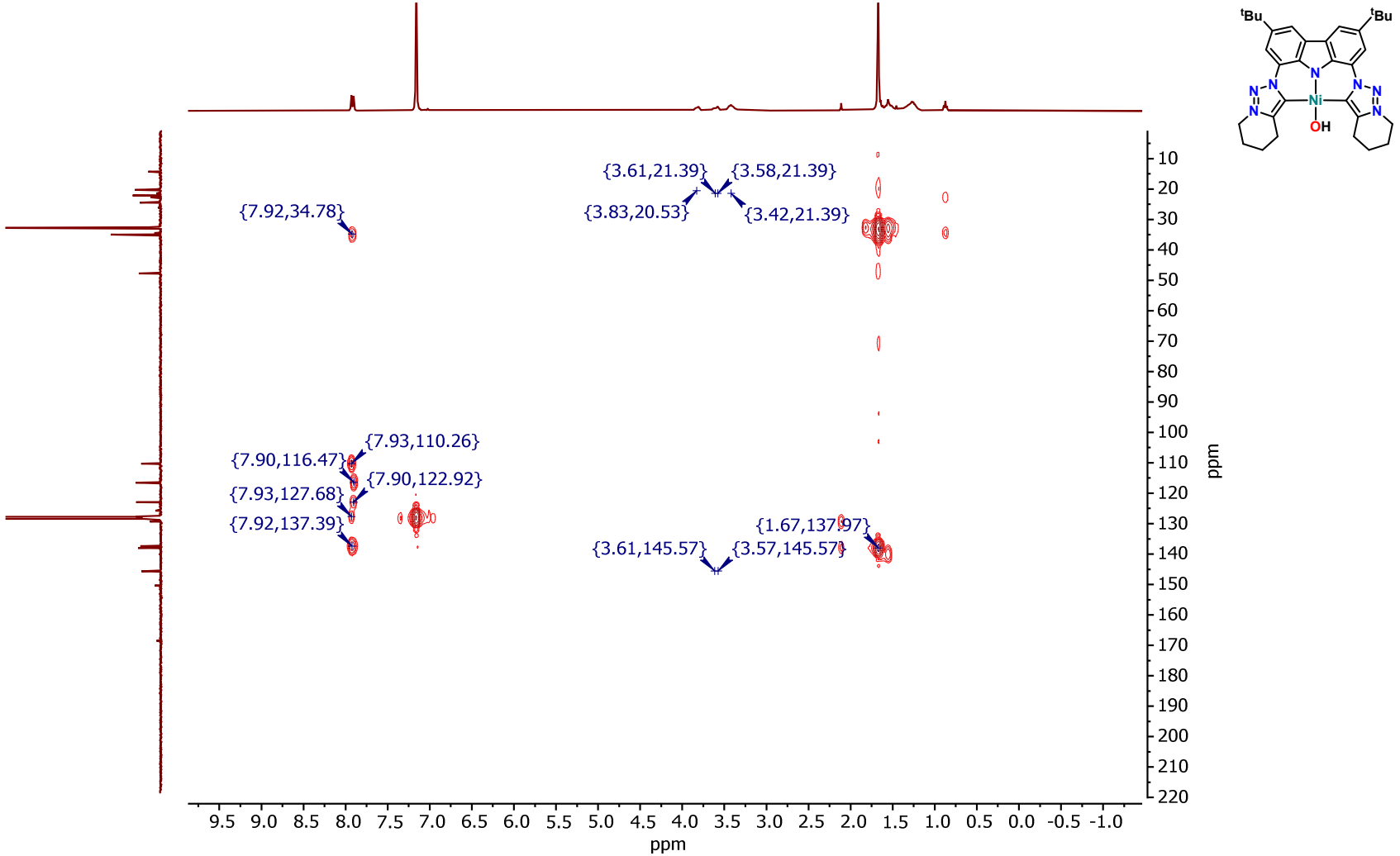

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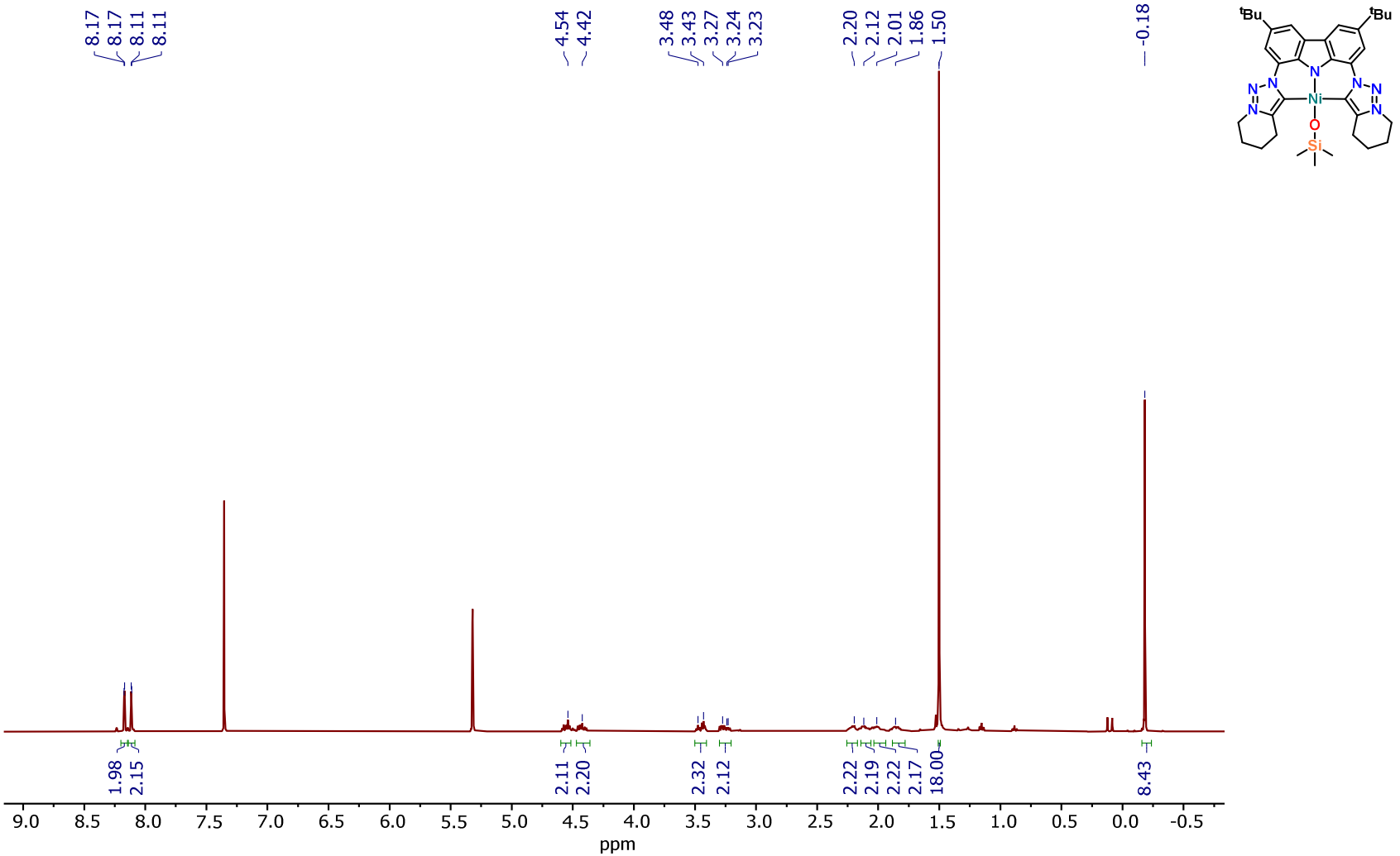

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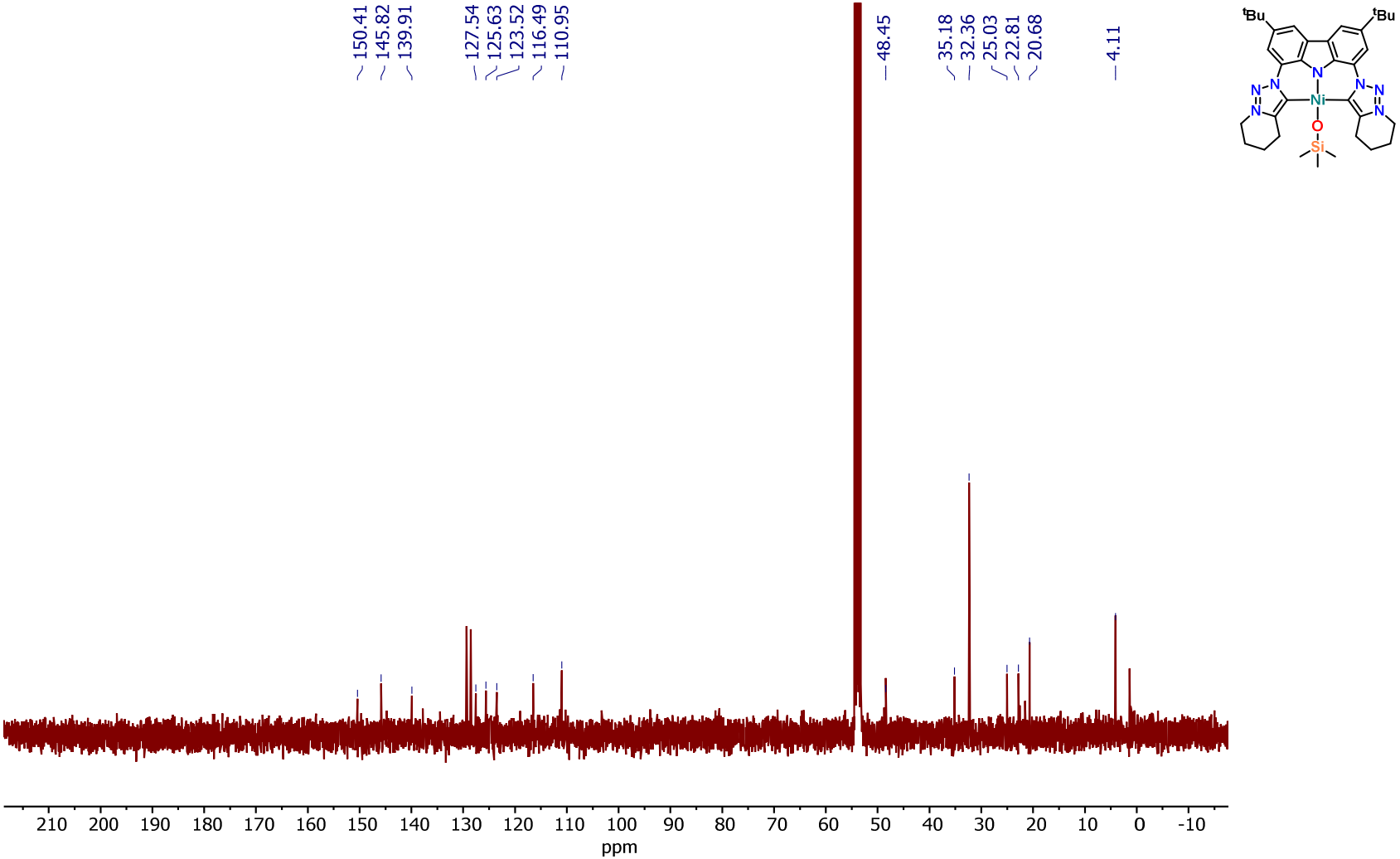

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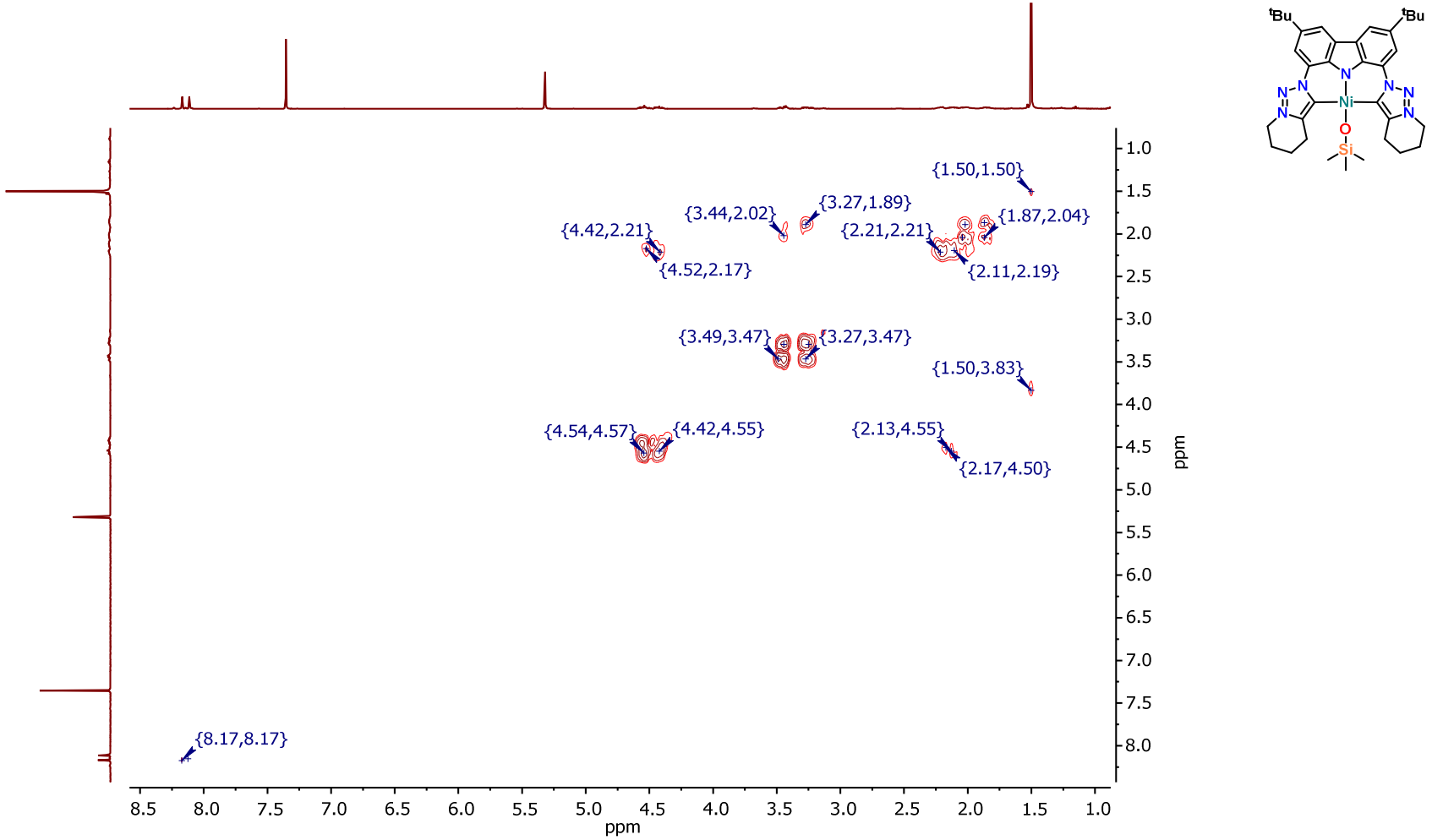

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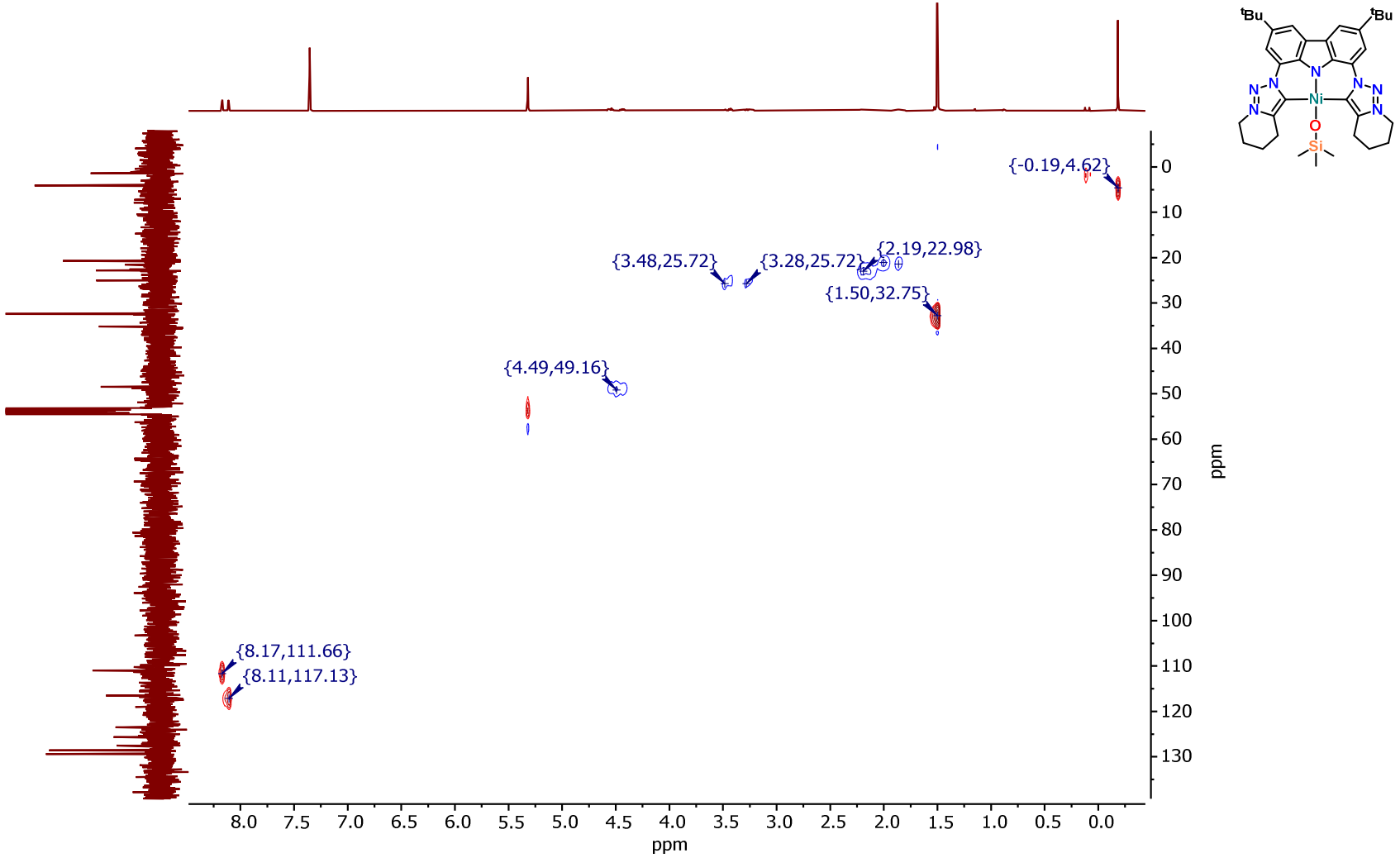

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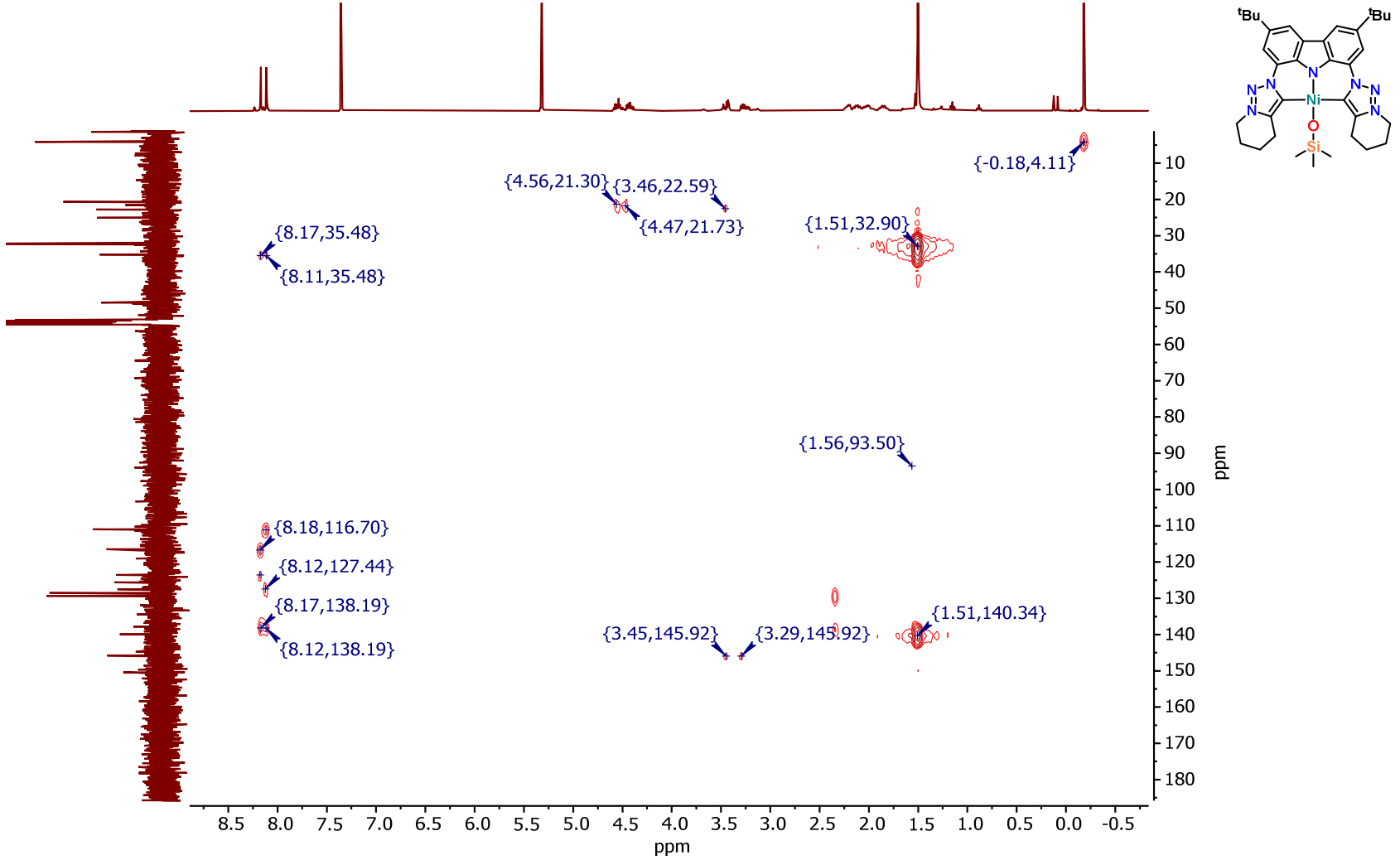

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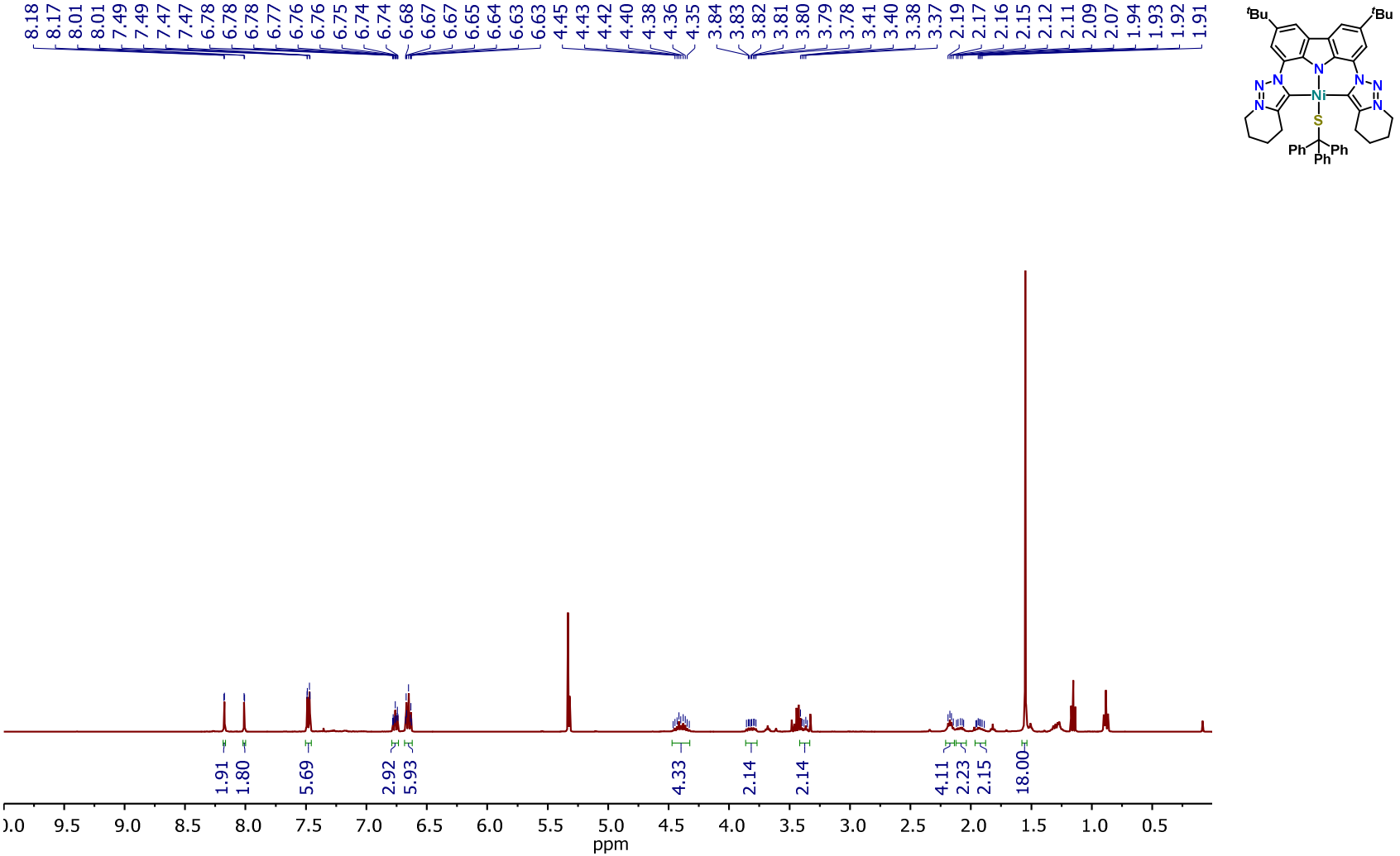

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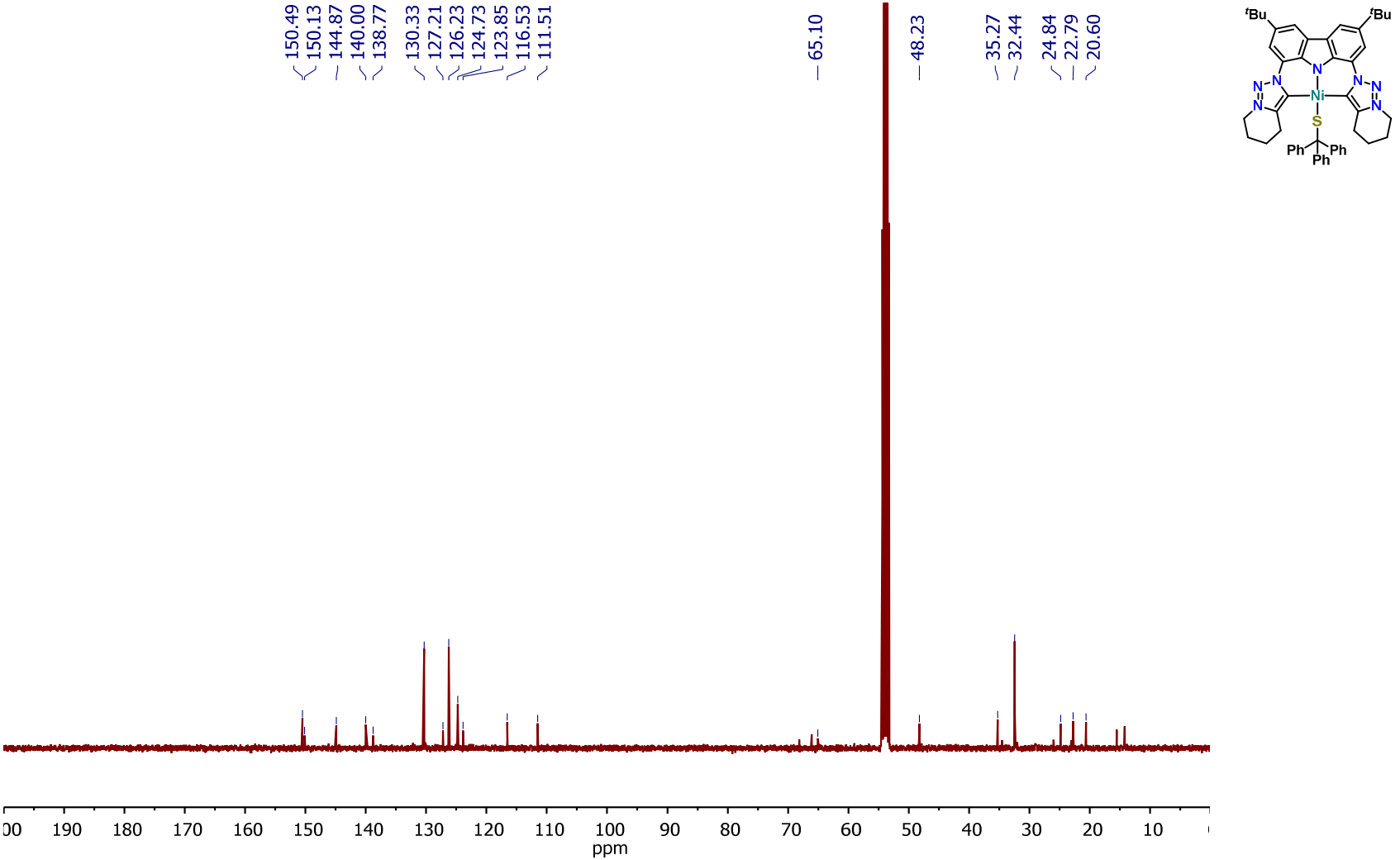

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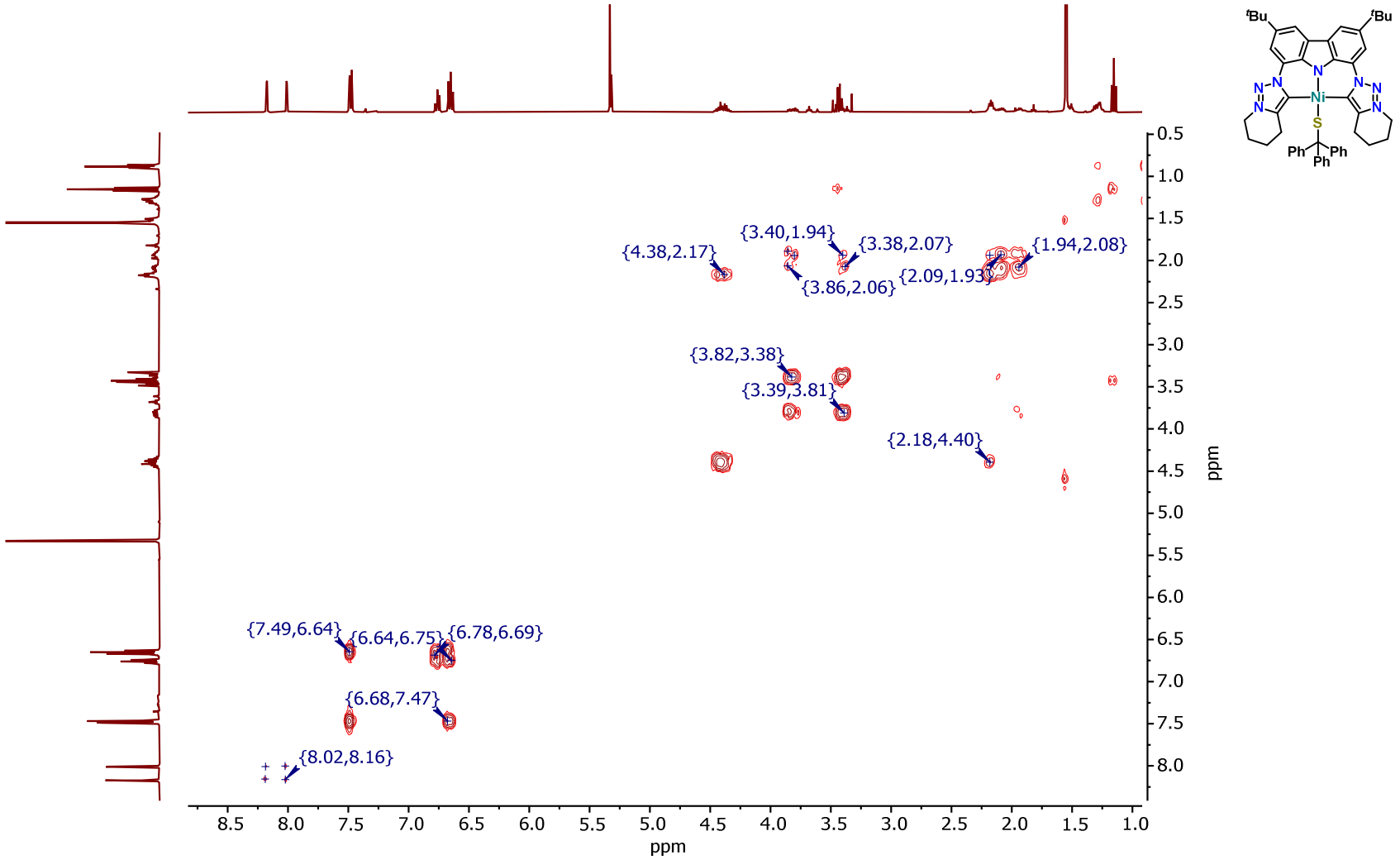

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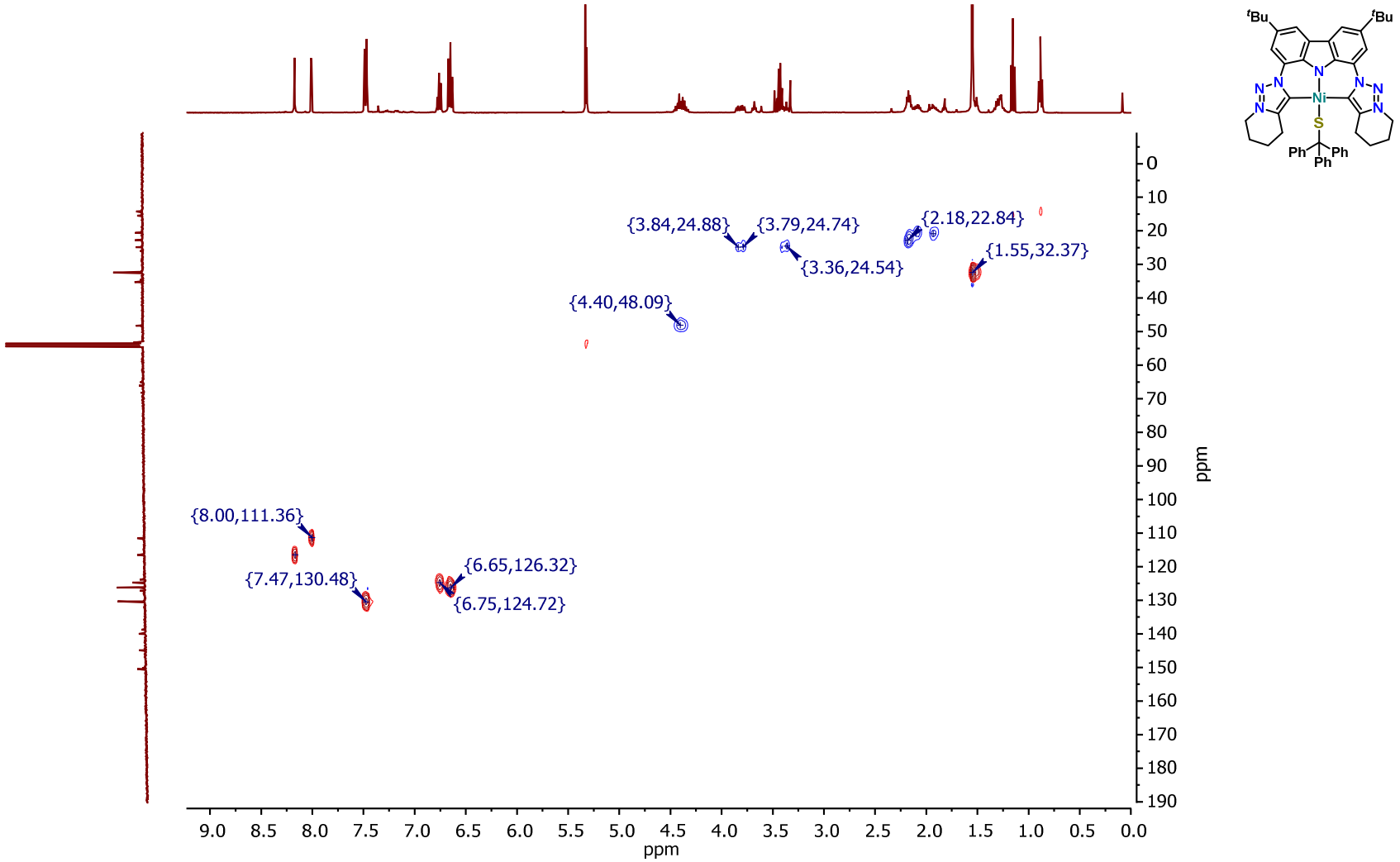

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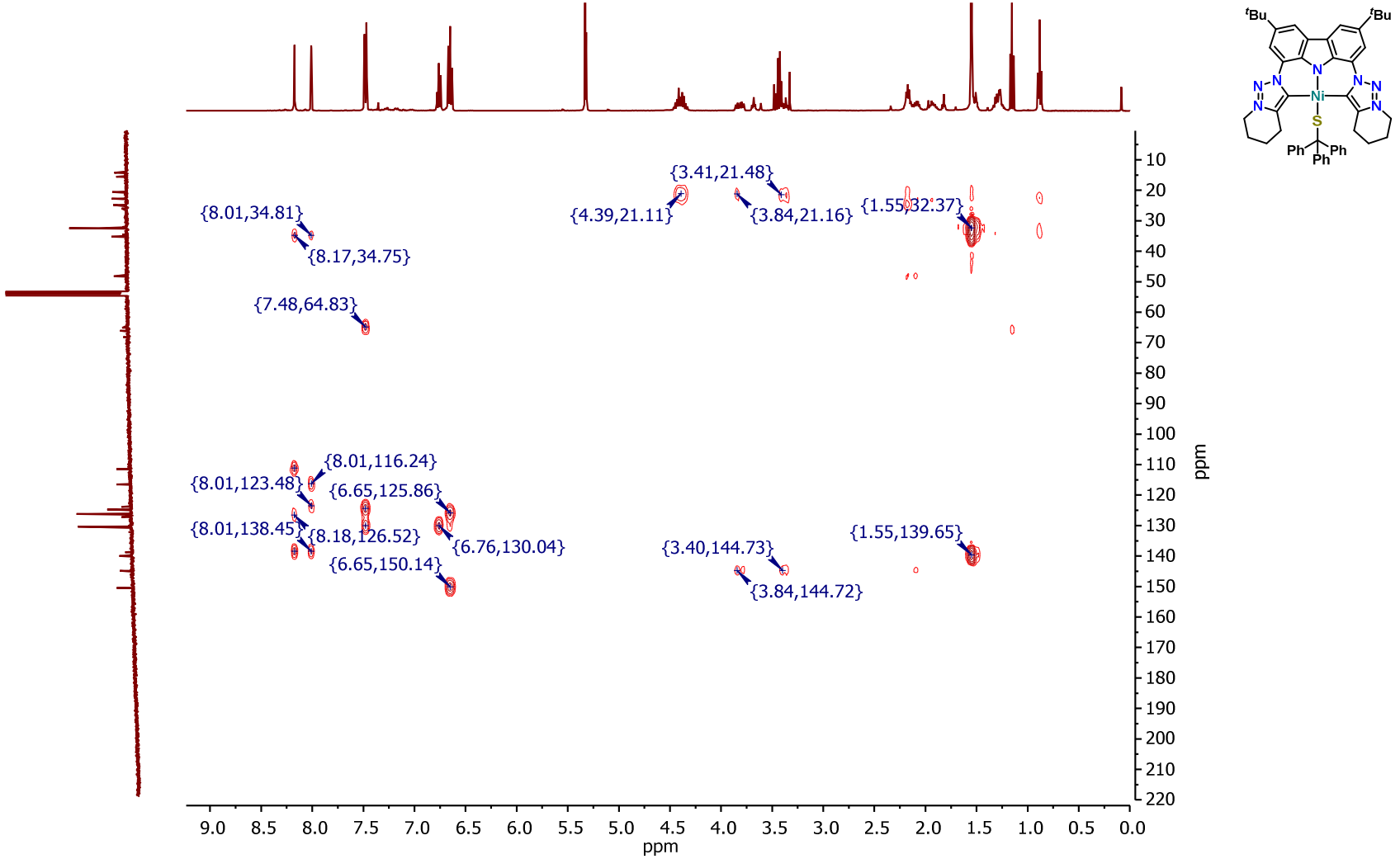

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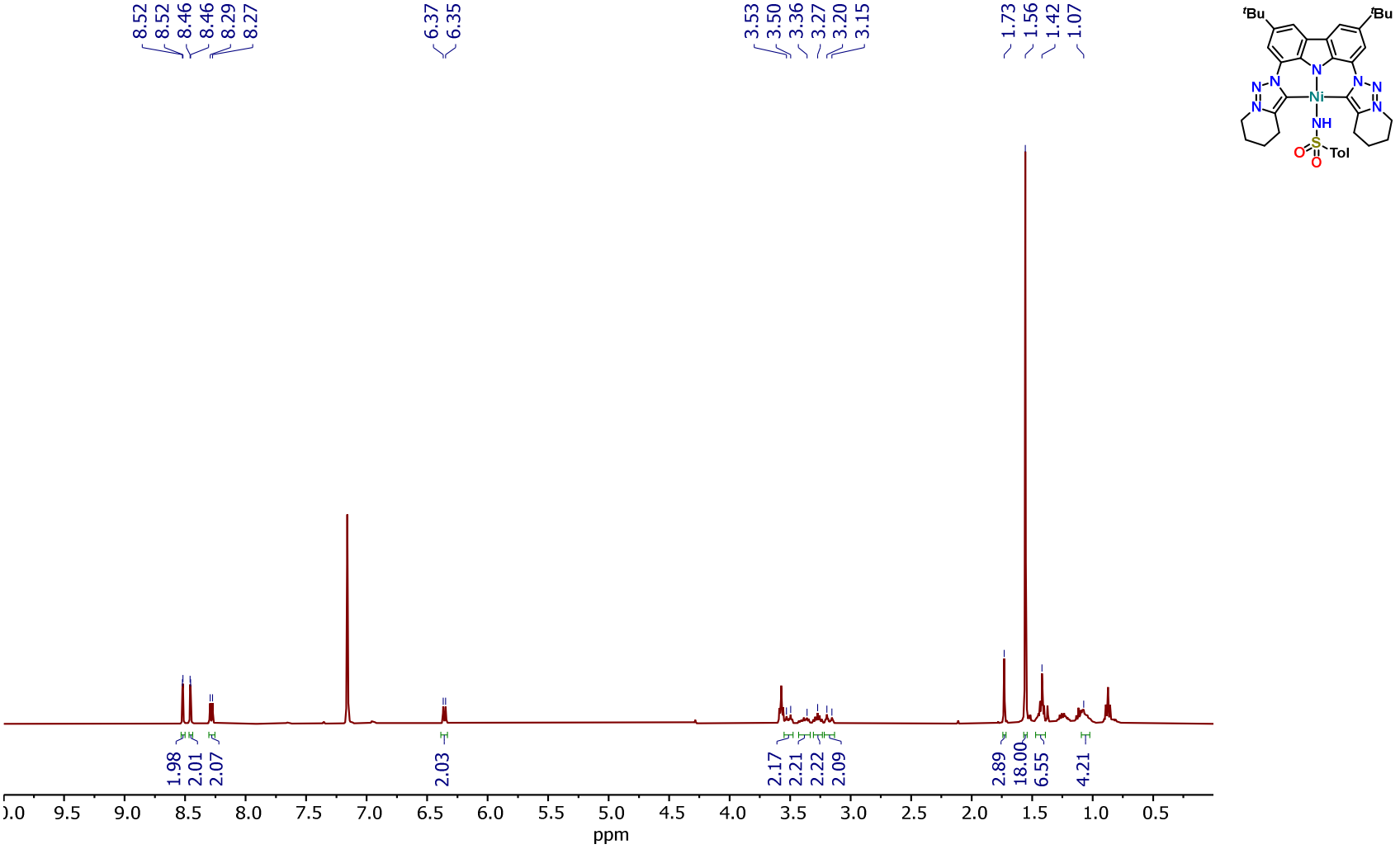

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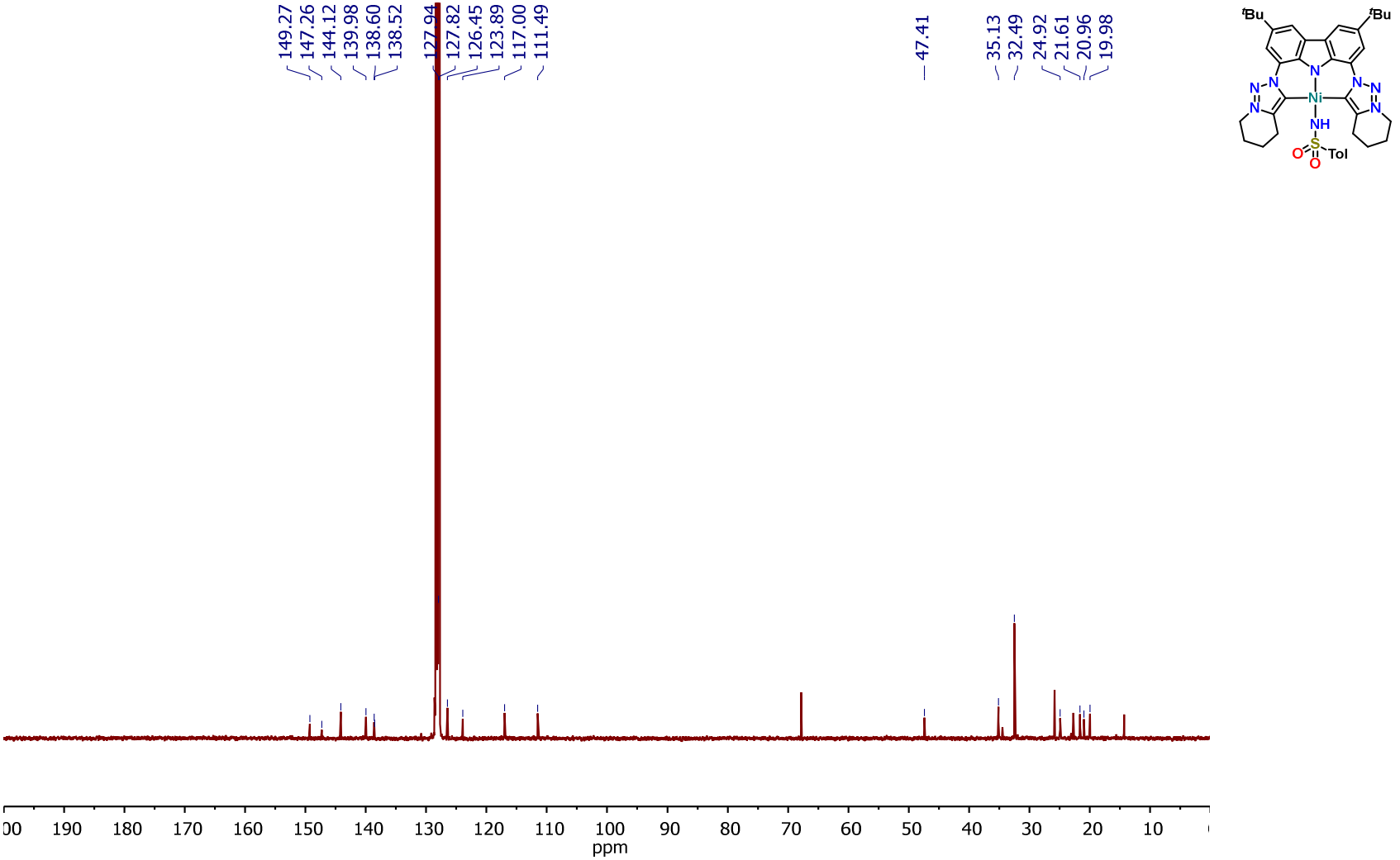

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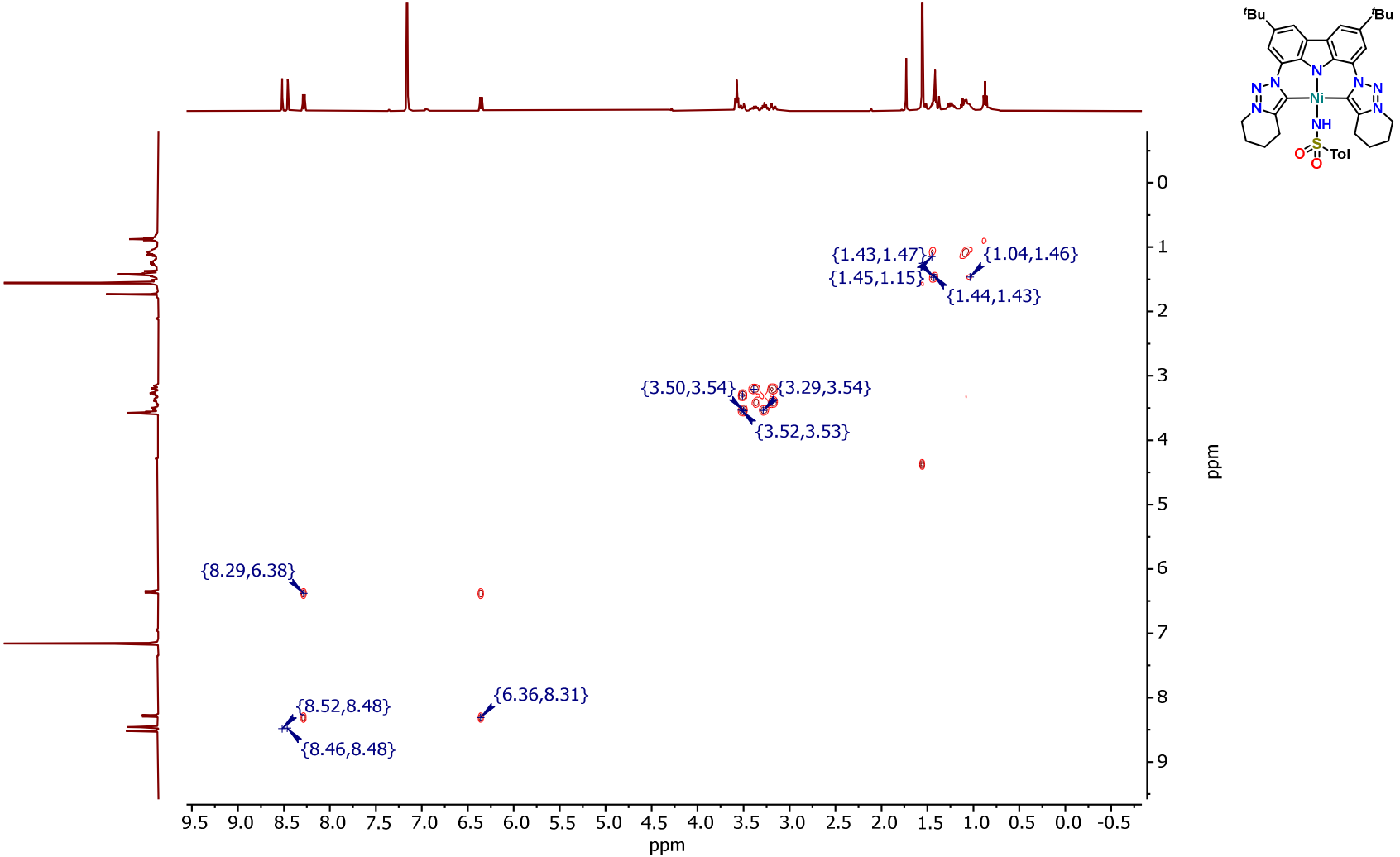

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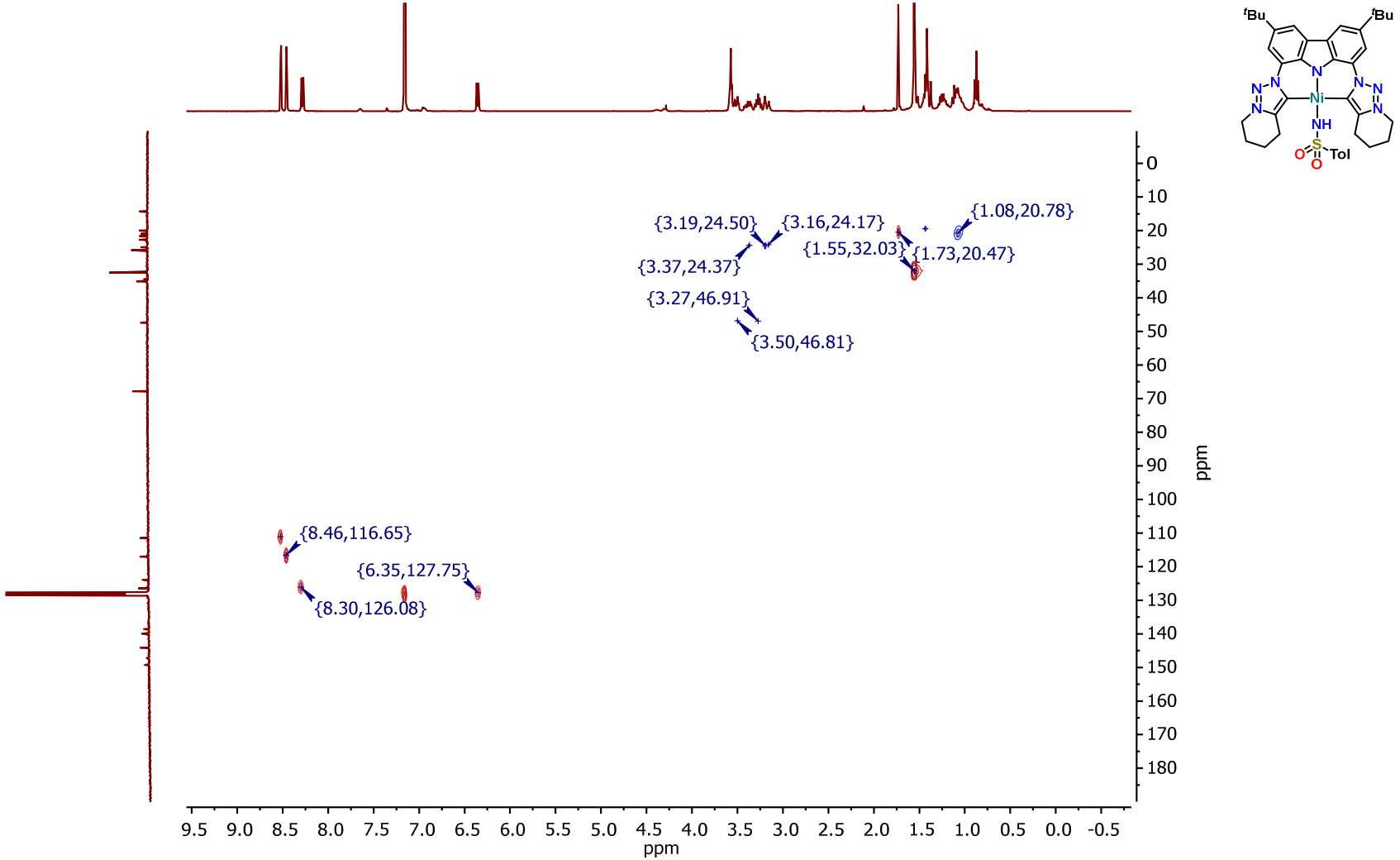

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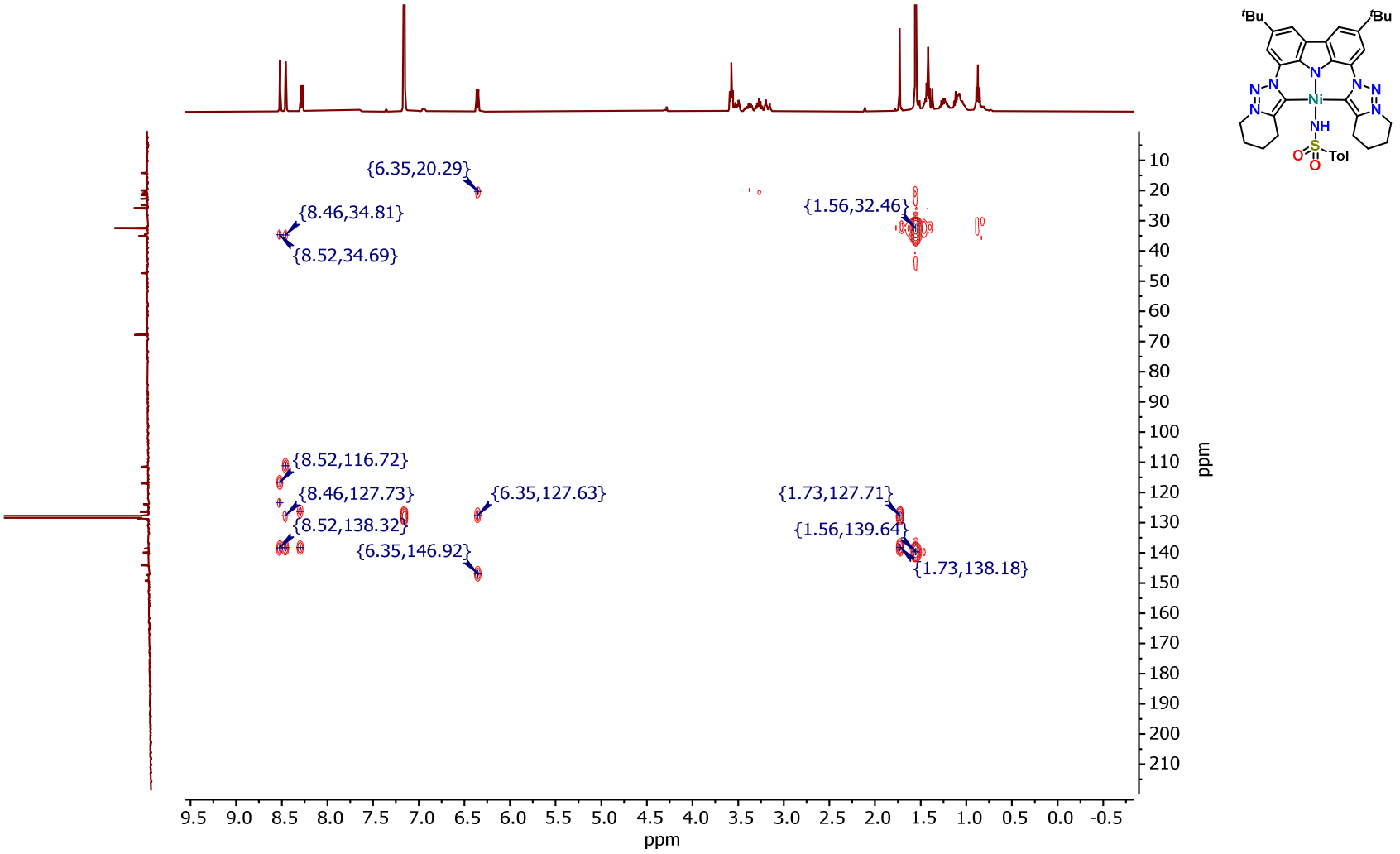

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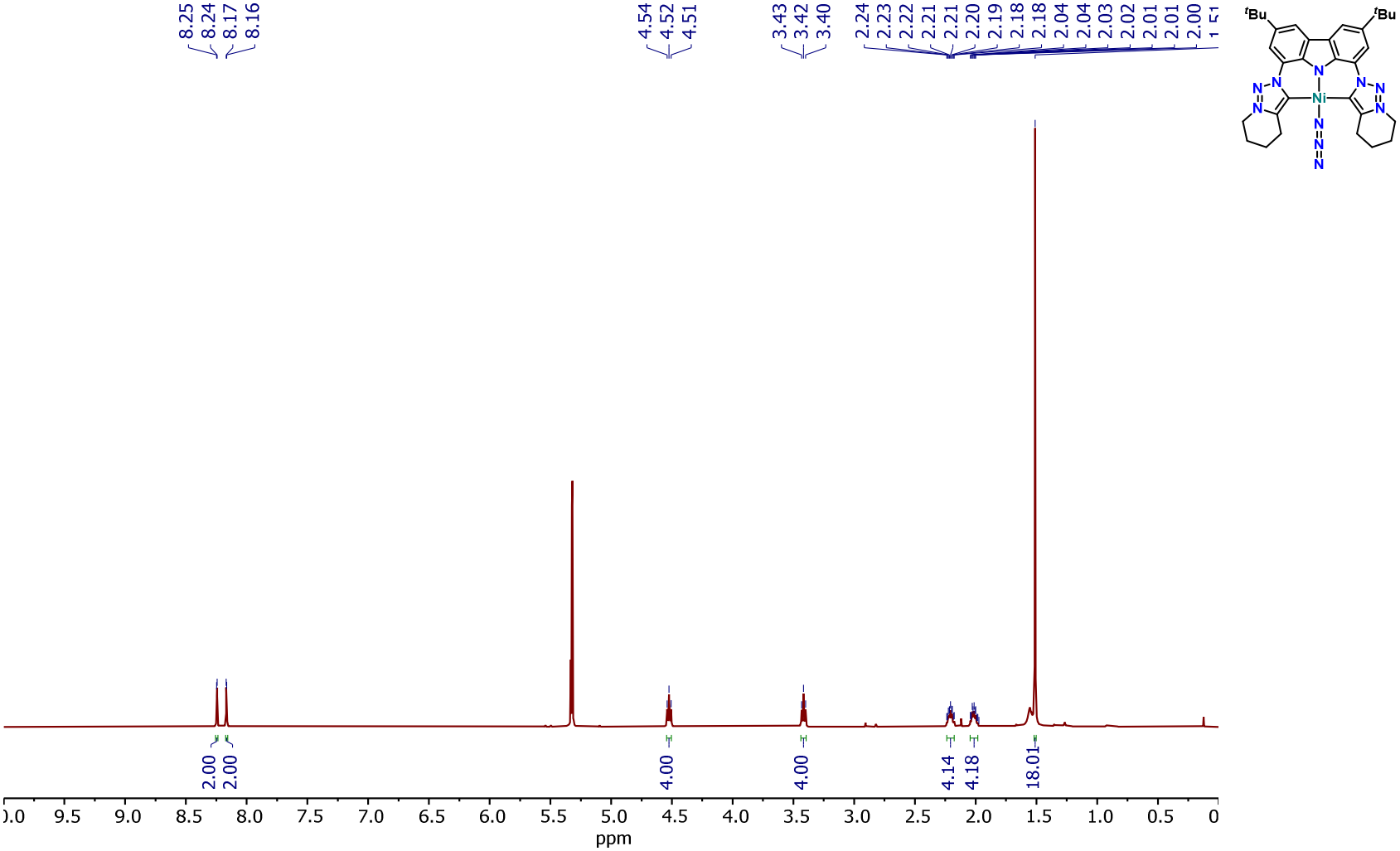

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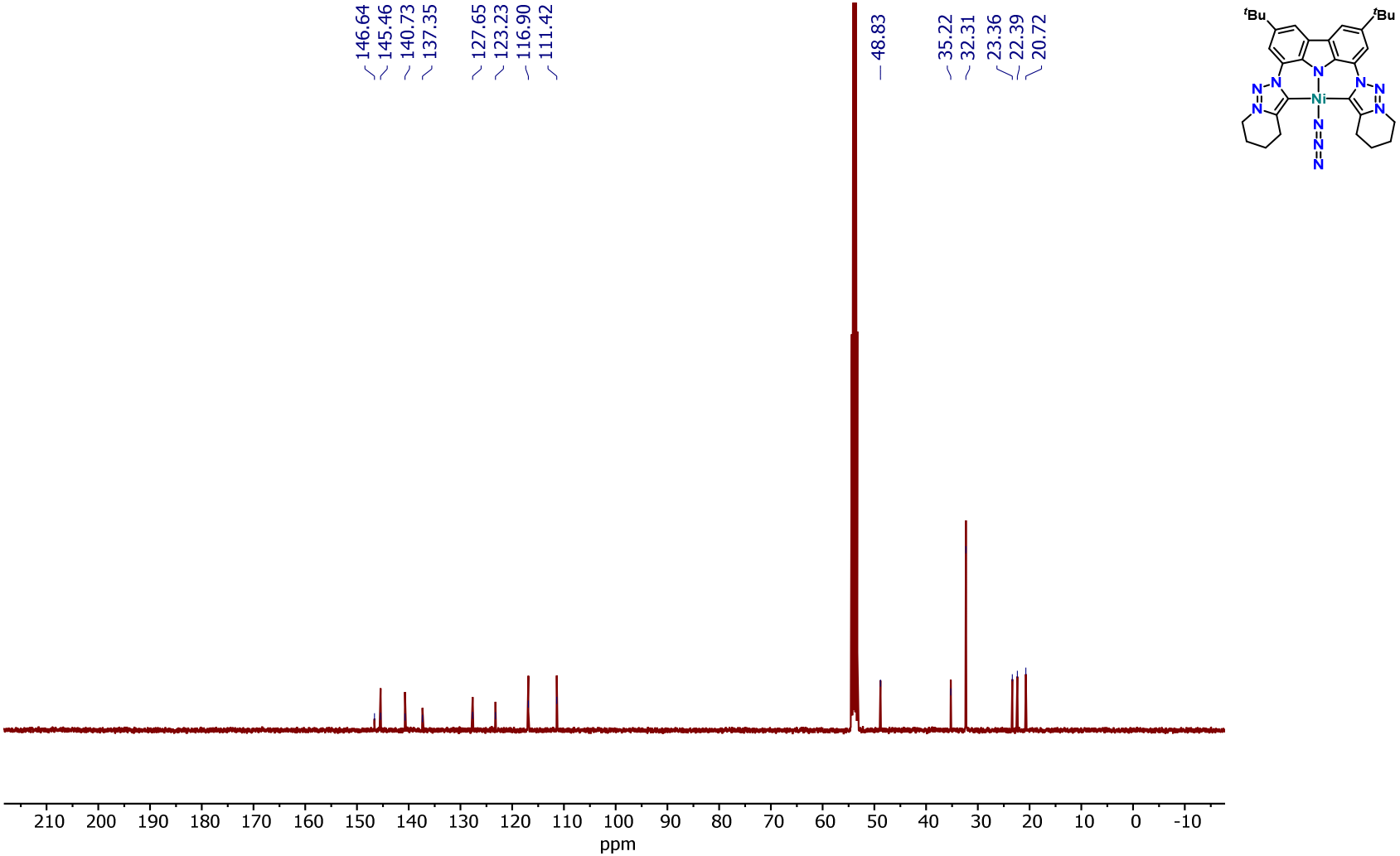

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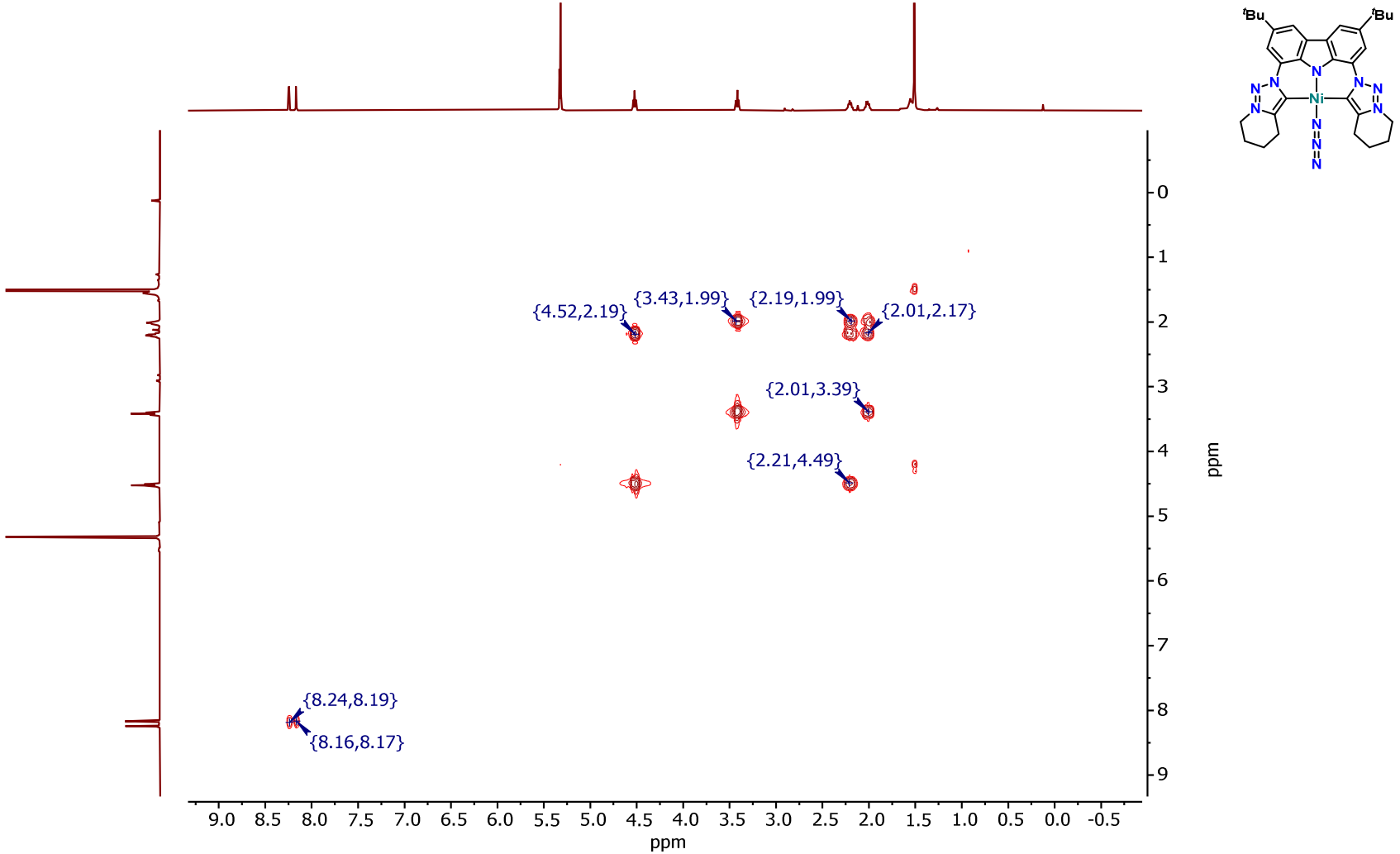

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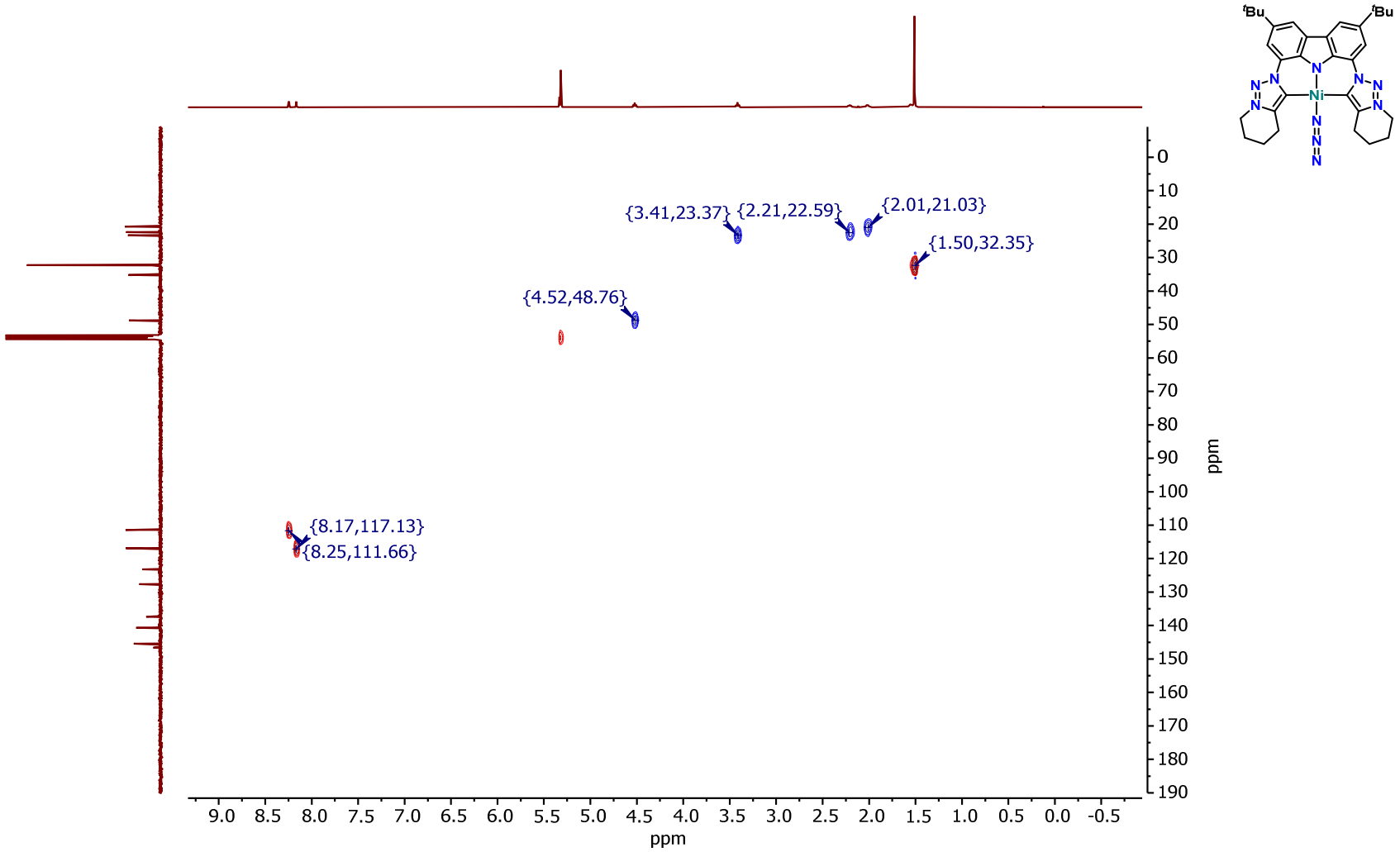

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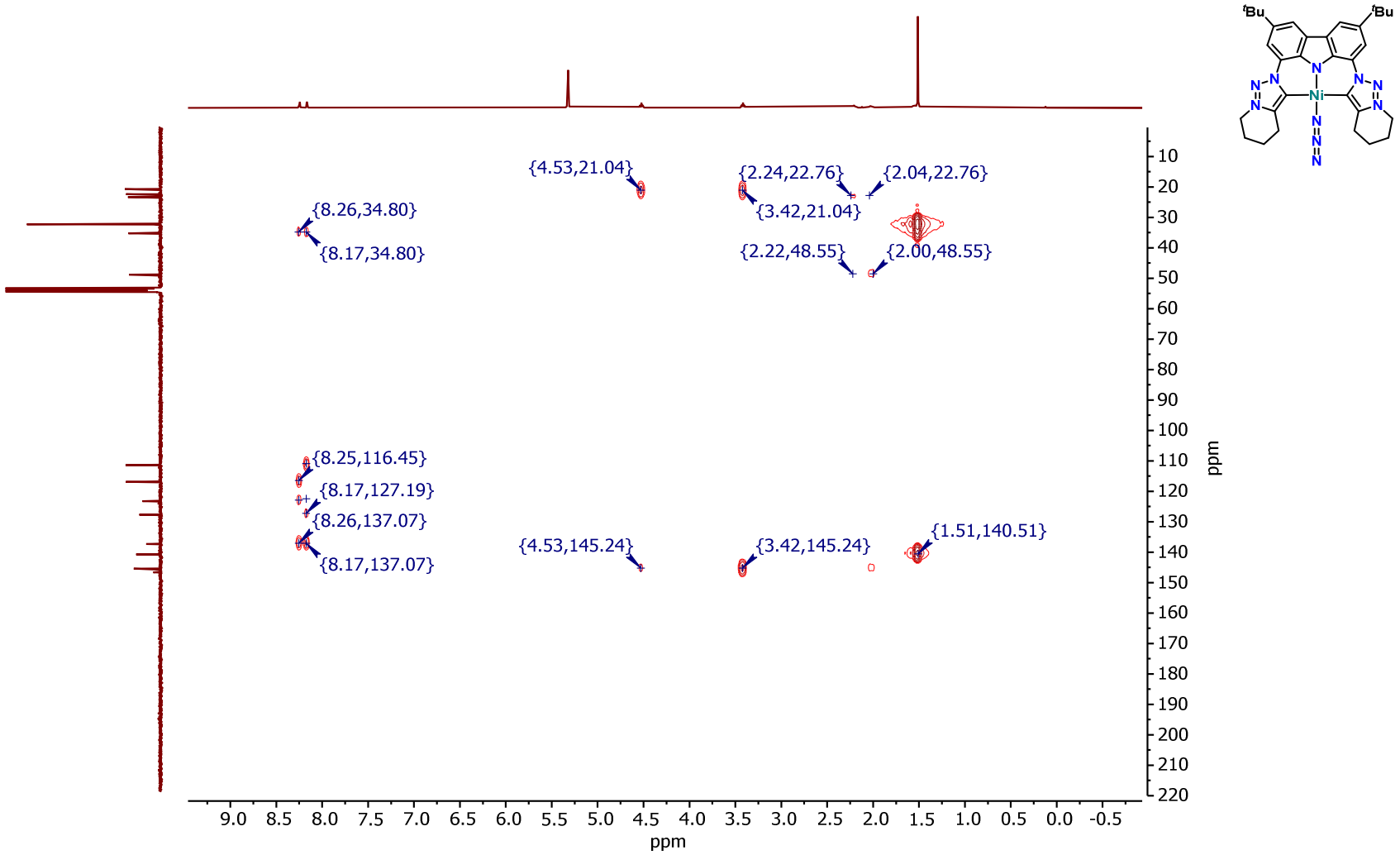

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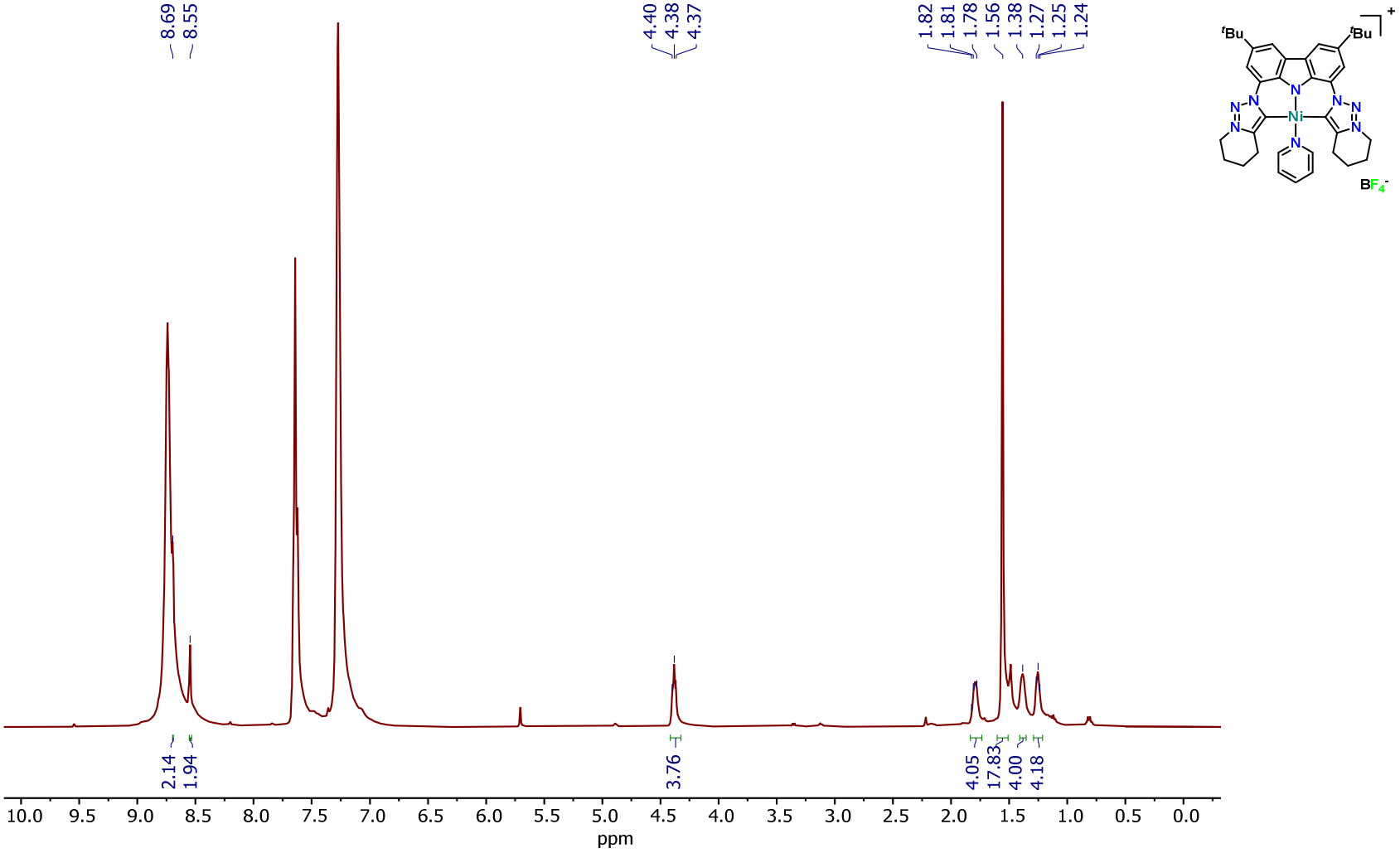

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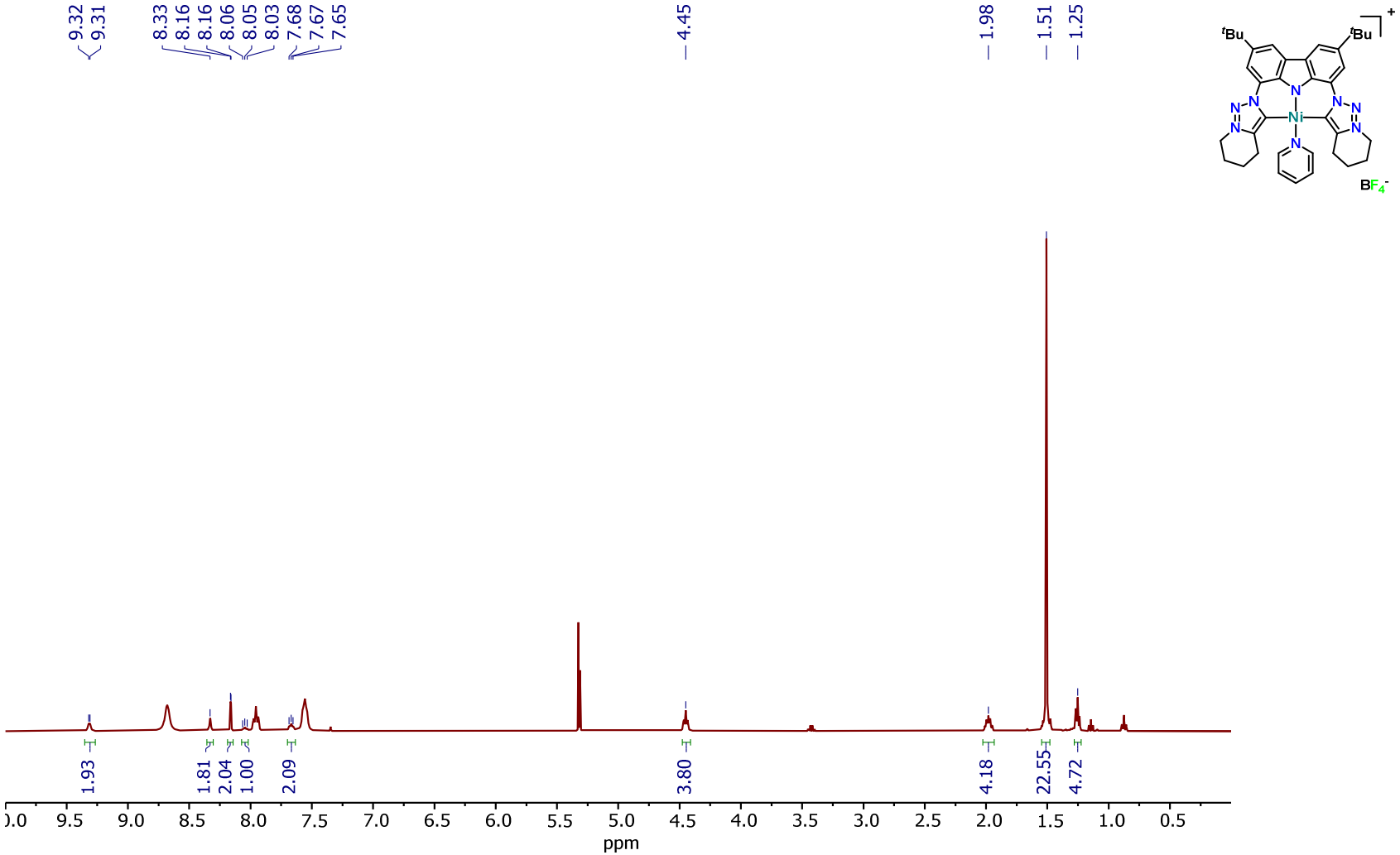

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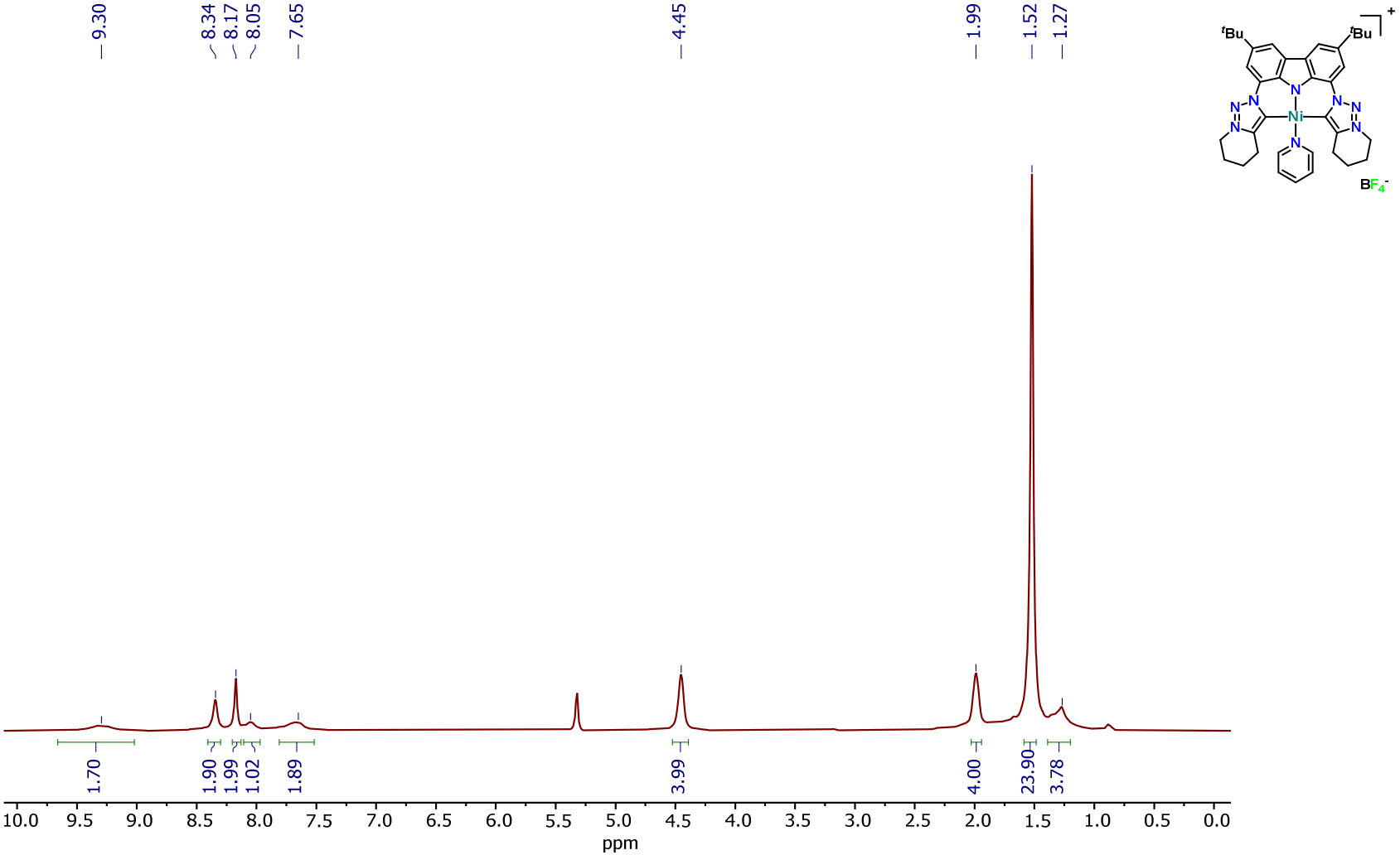

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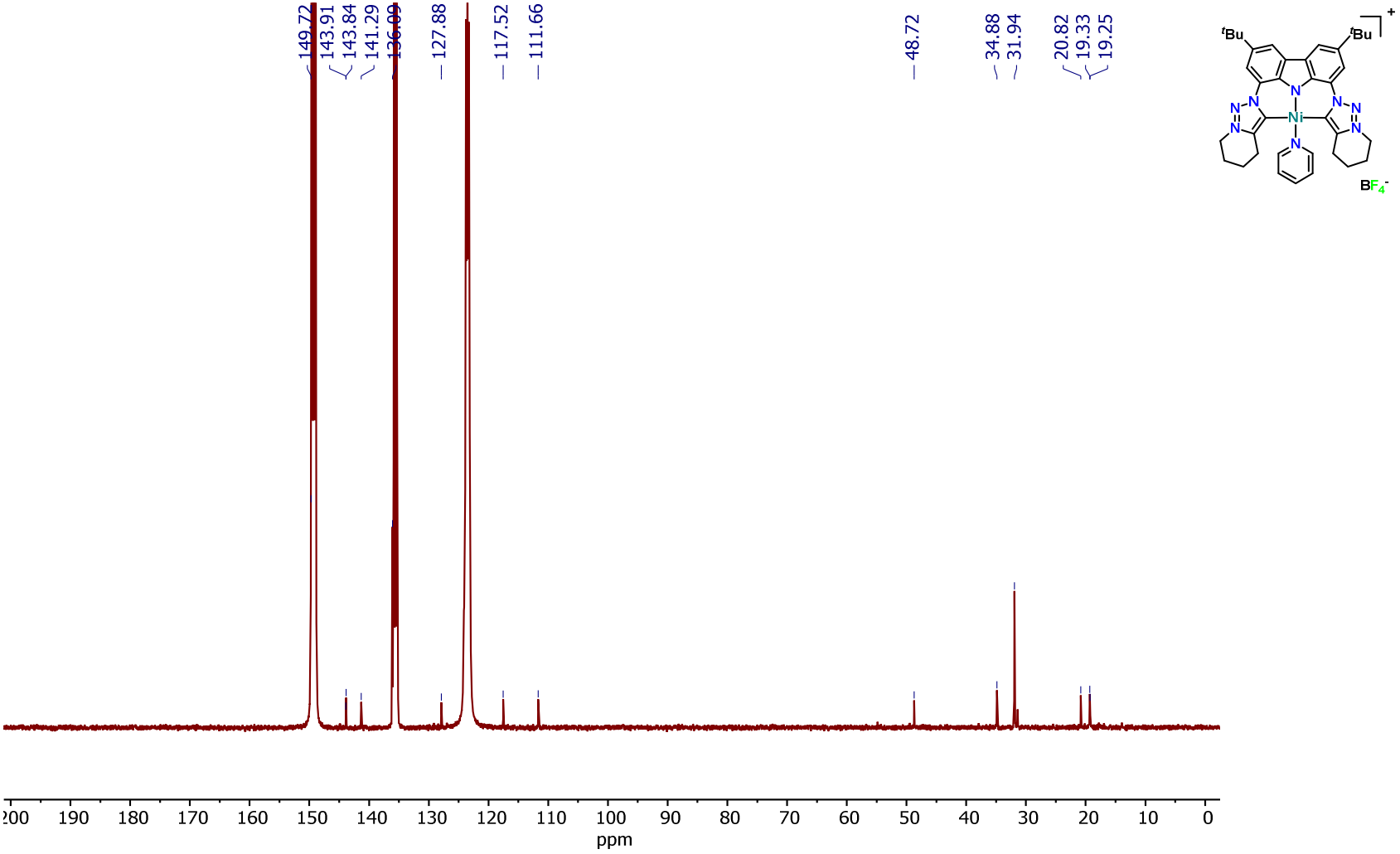

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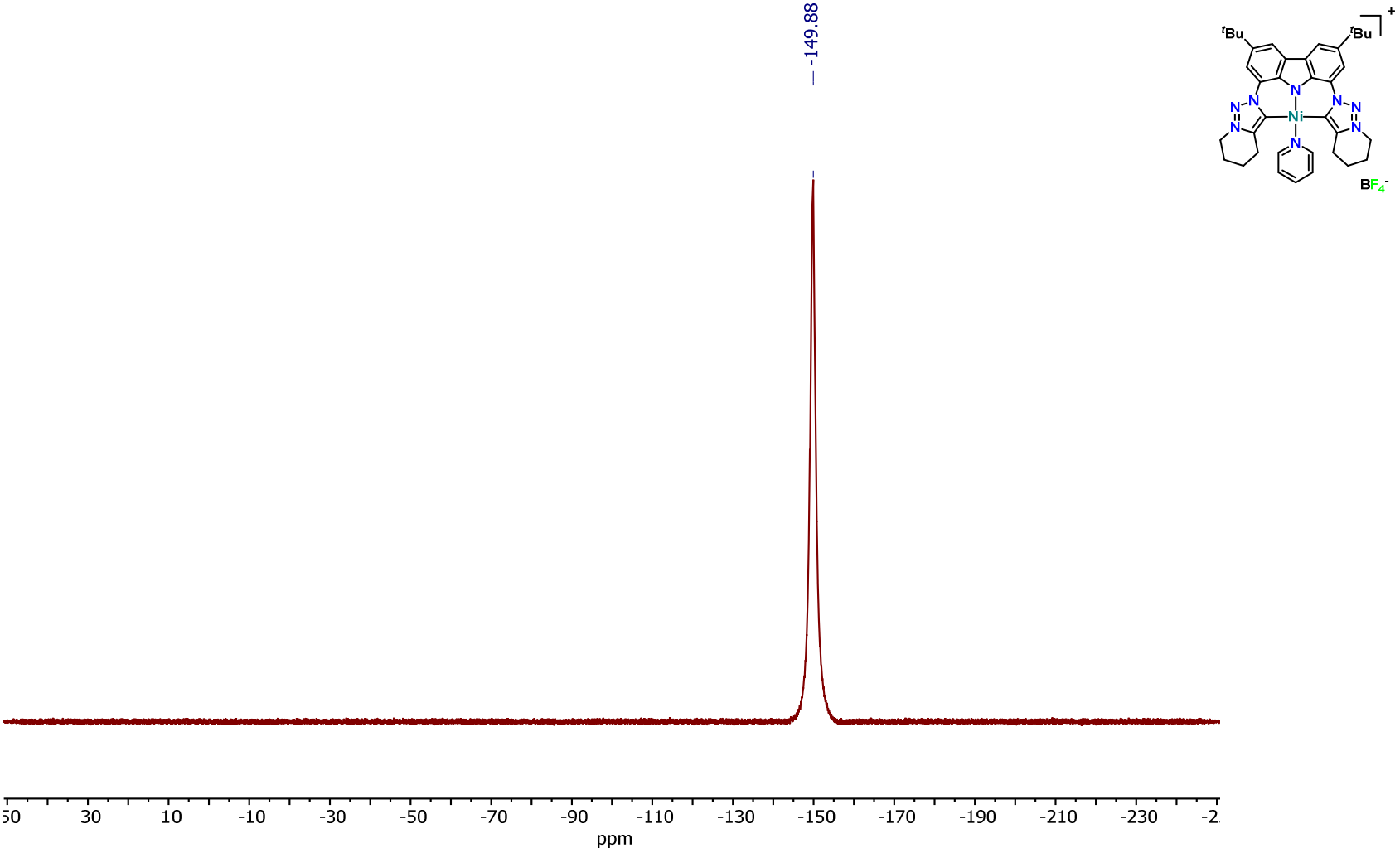

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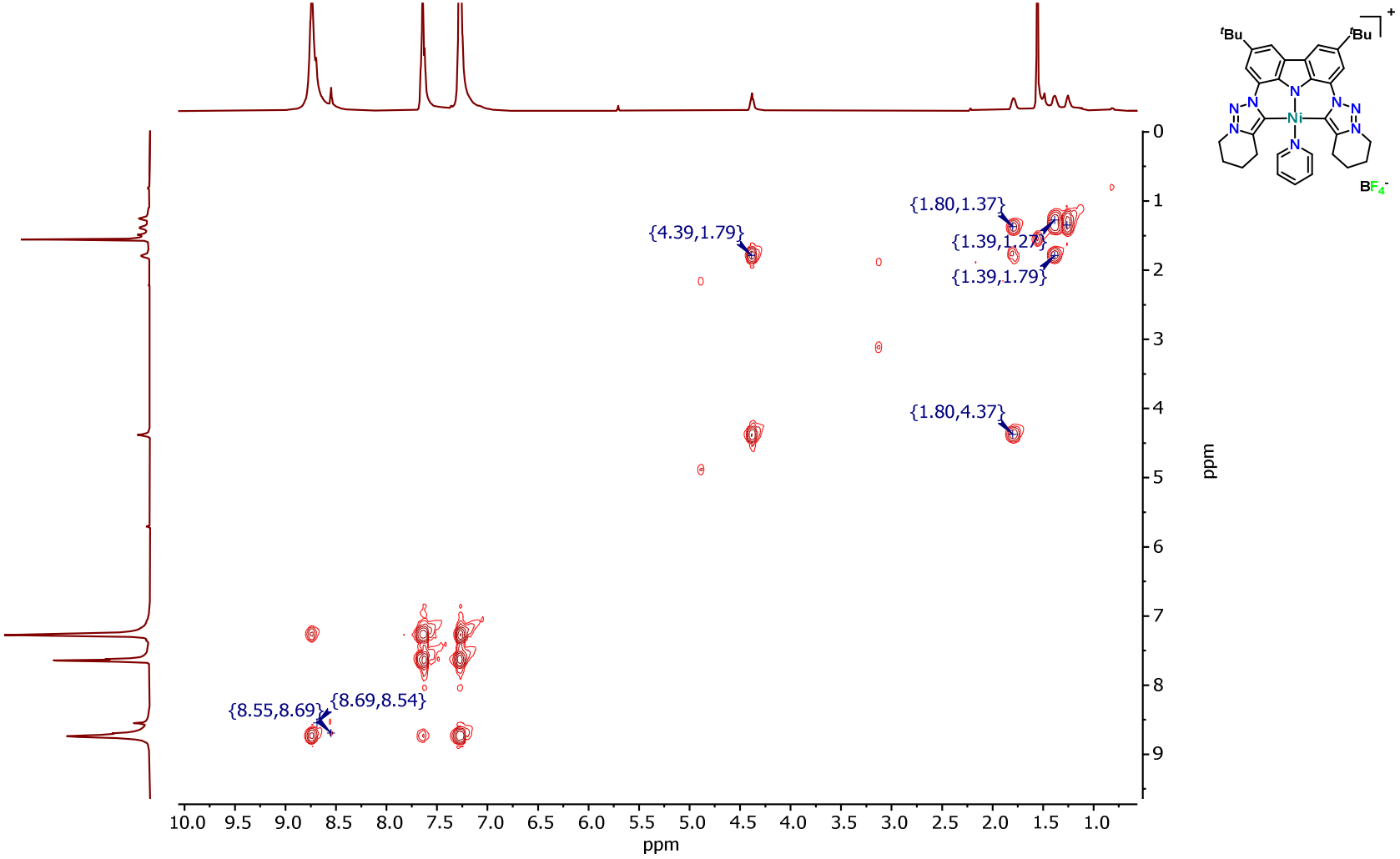

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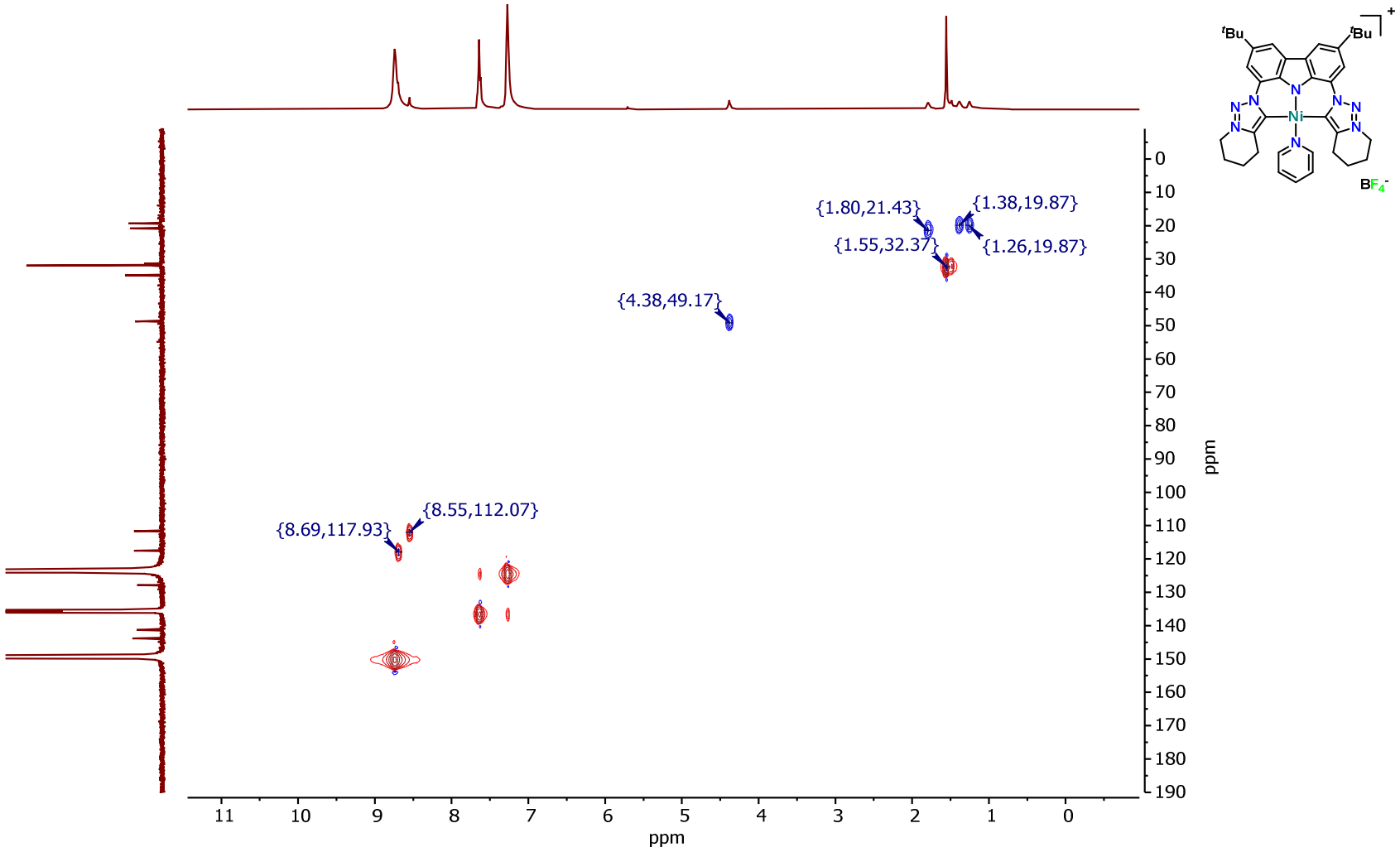

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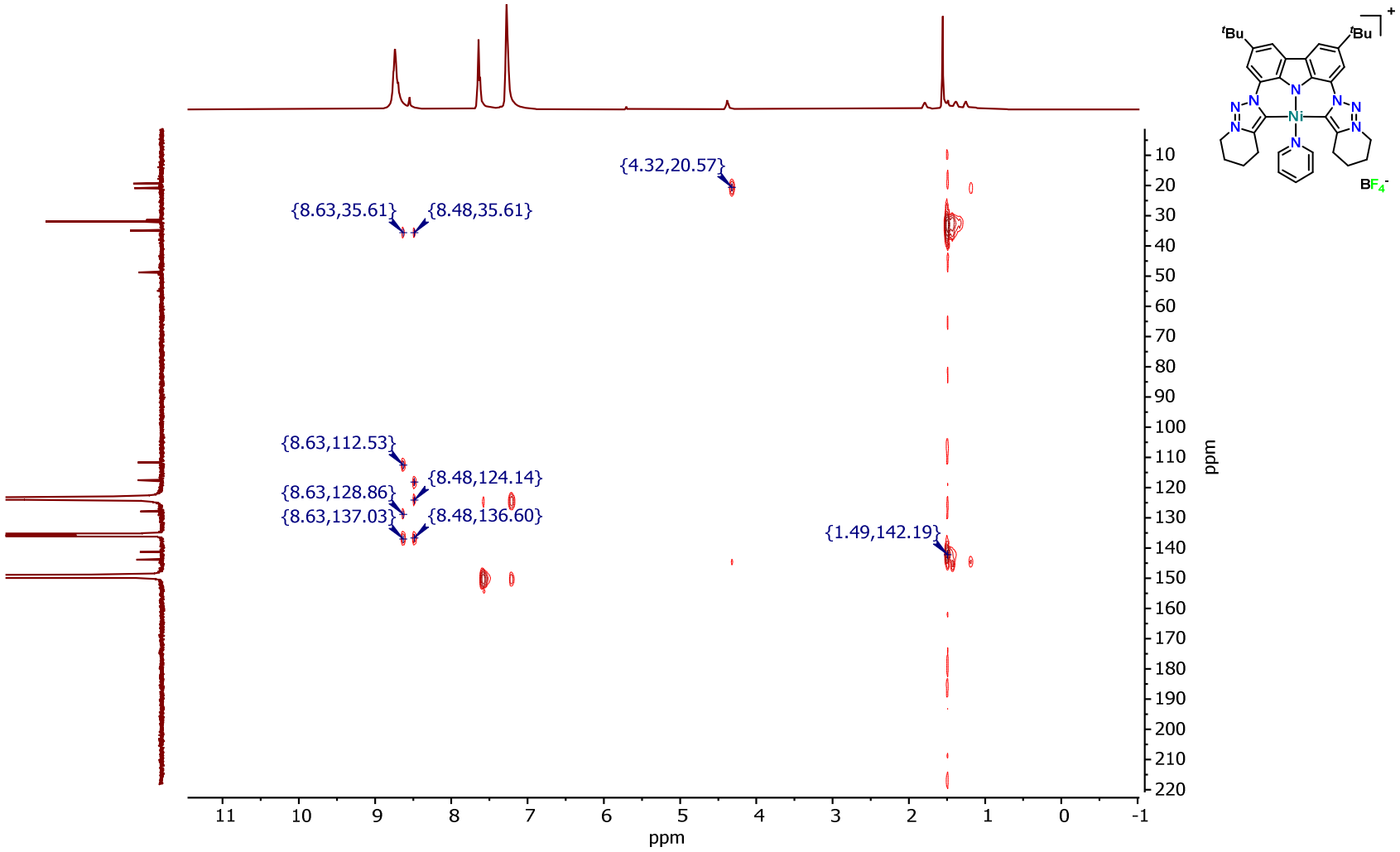

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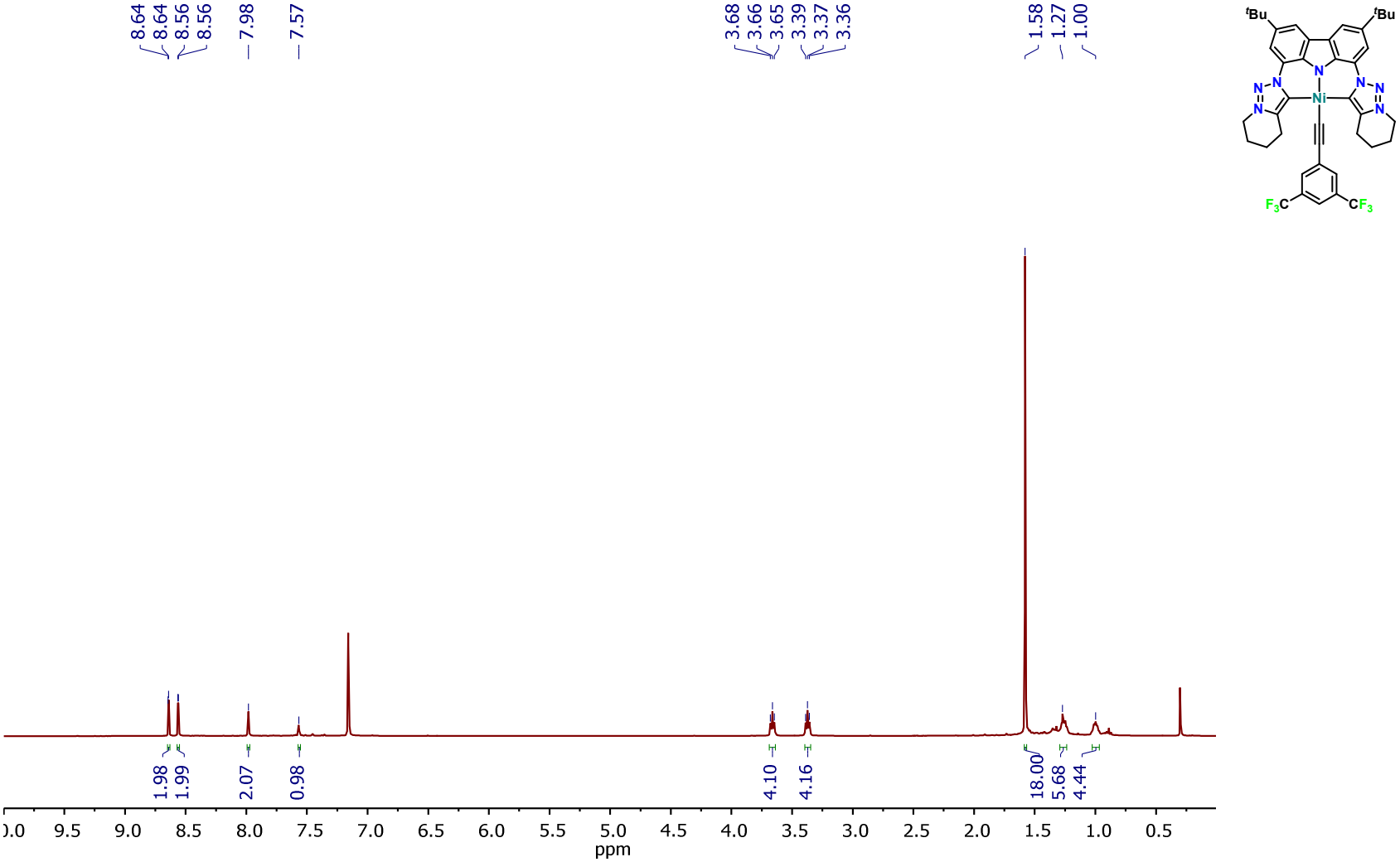

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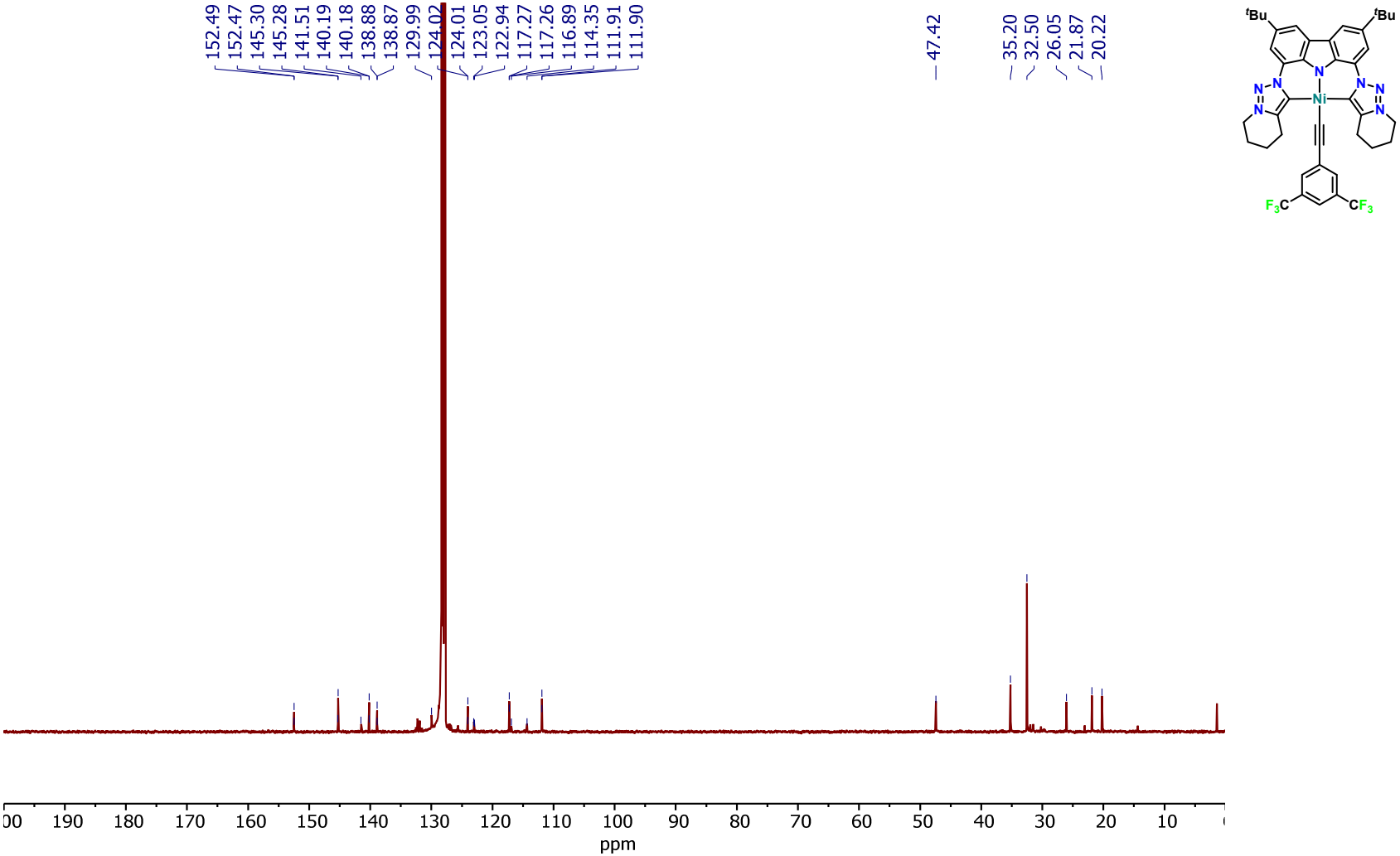

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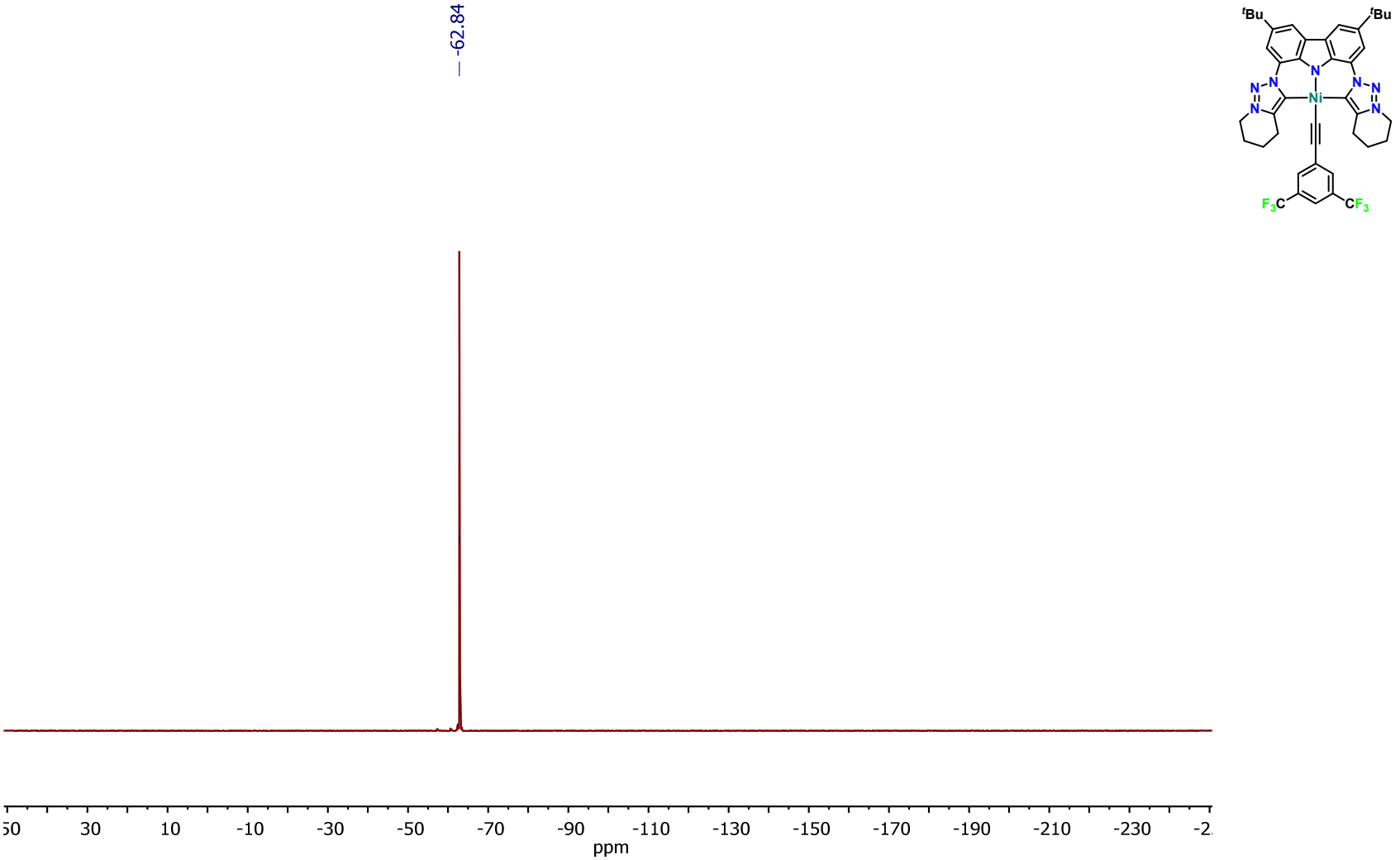

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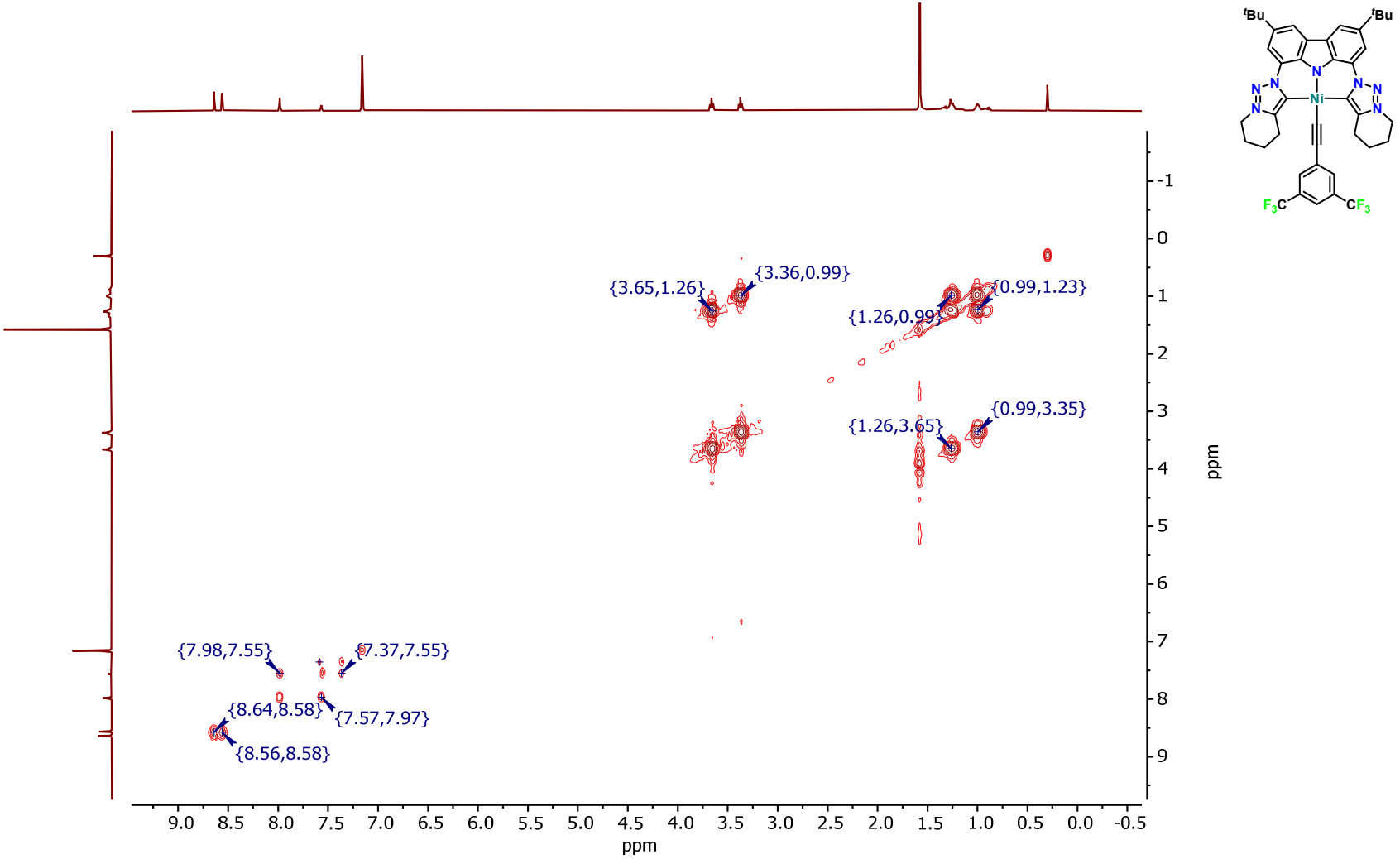

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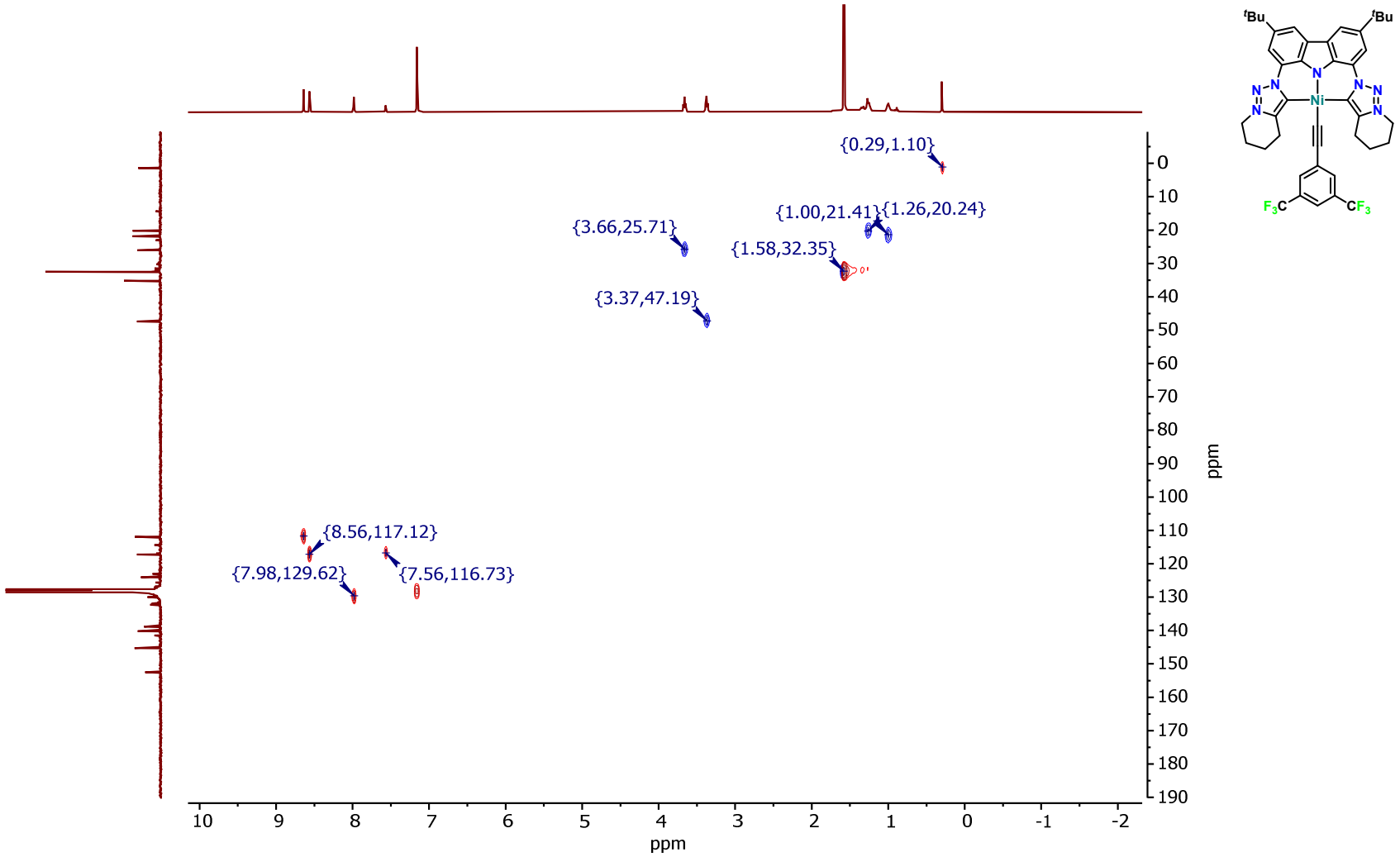

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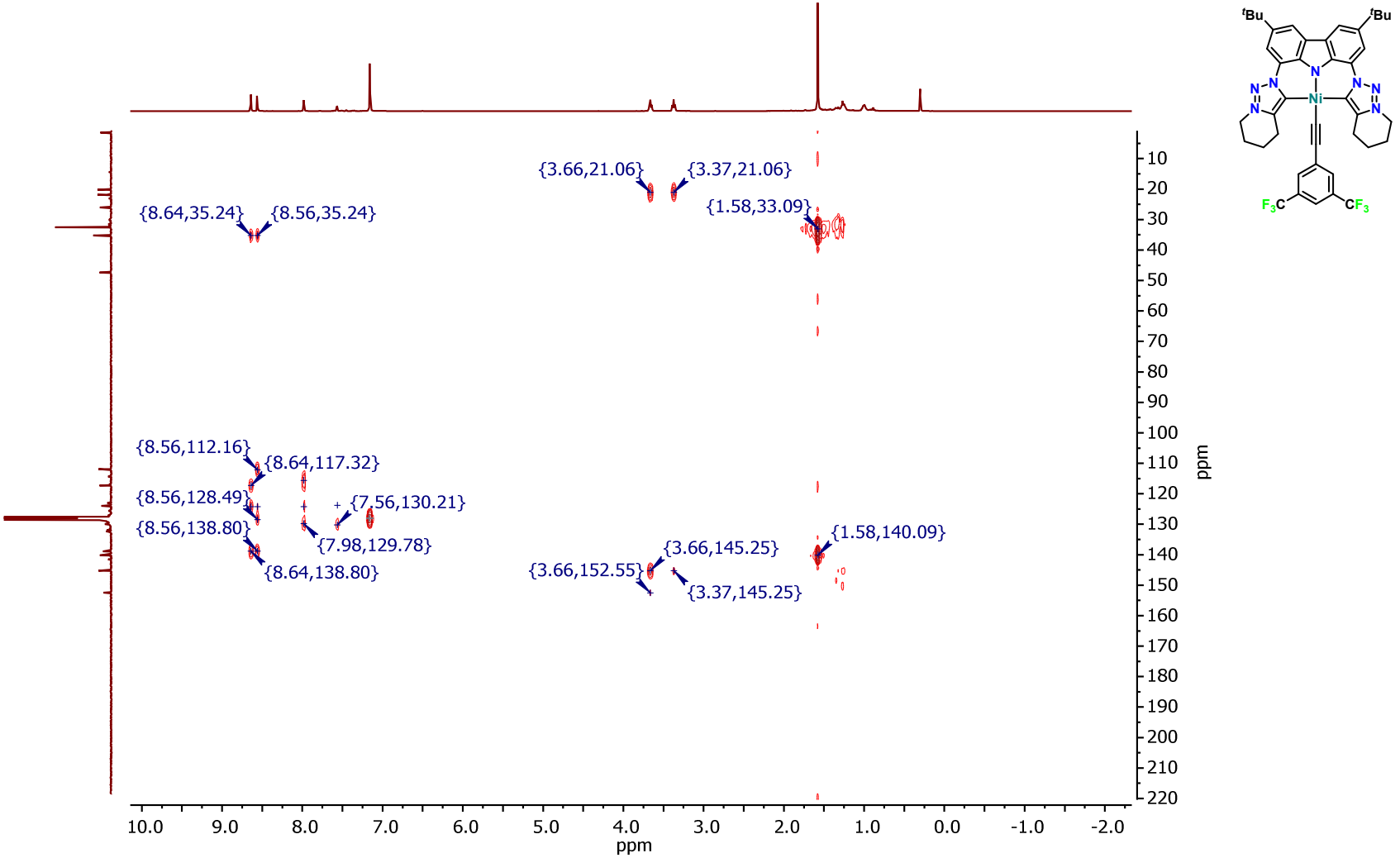

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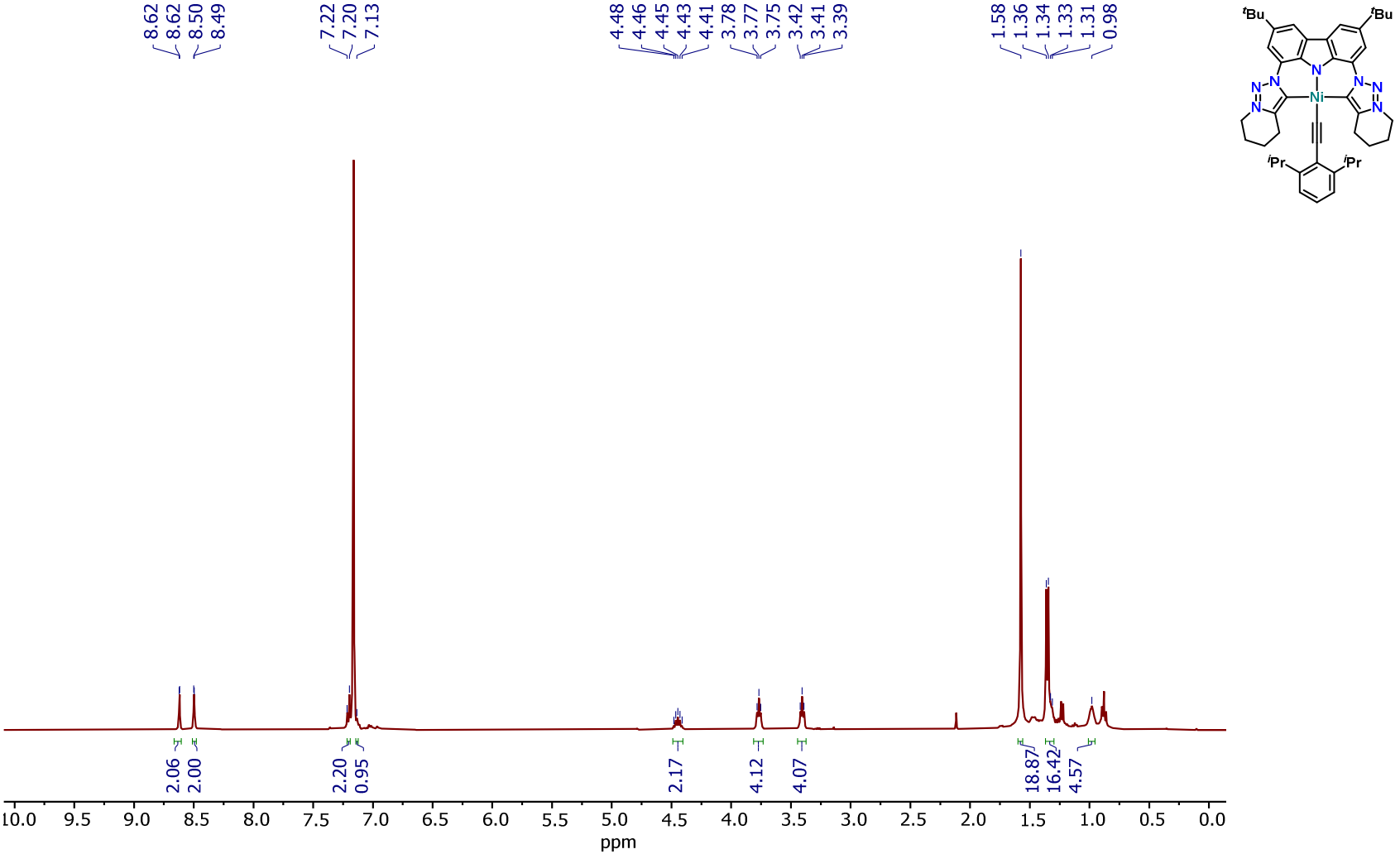


*Figure S 49: ^{1}H NMR of **9** in C_6D_6 at 298K.*

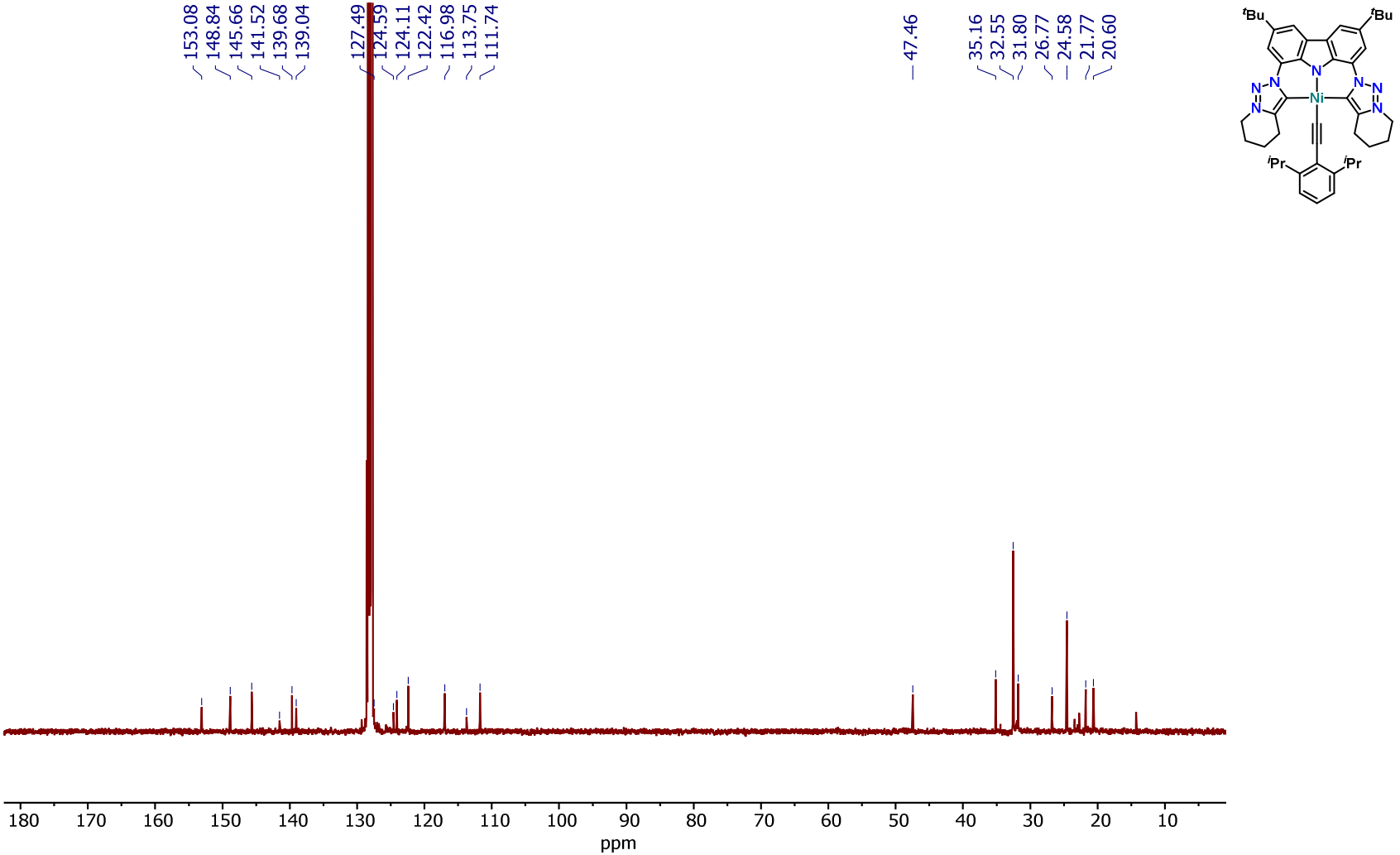


*Figure S 50: ^{13}C NMR of **9** in C_6D_6 at 298K.*

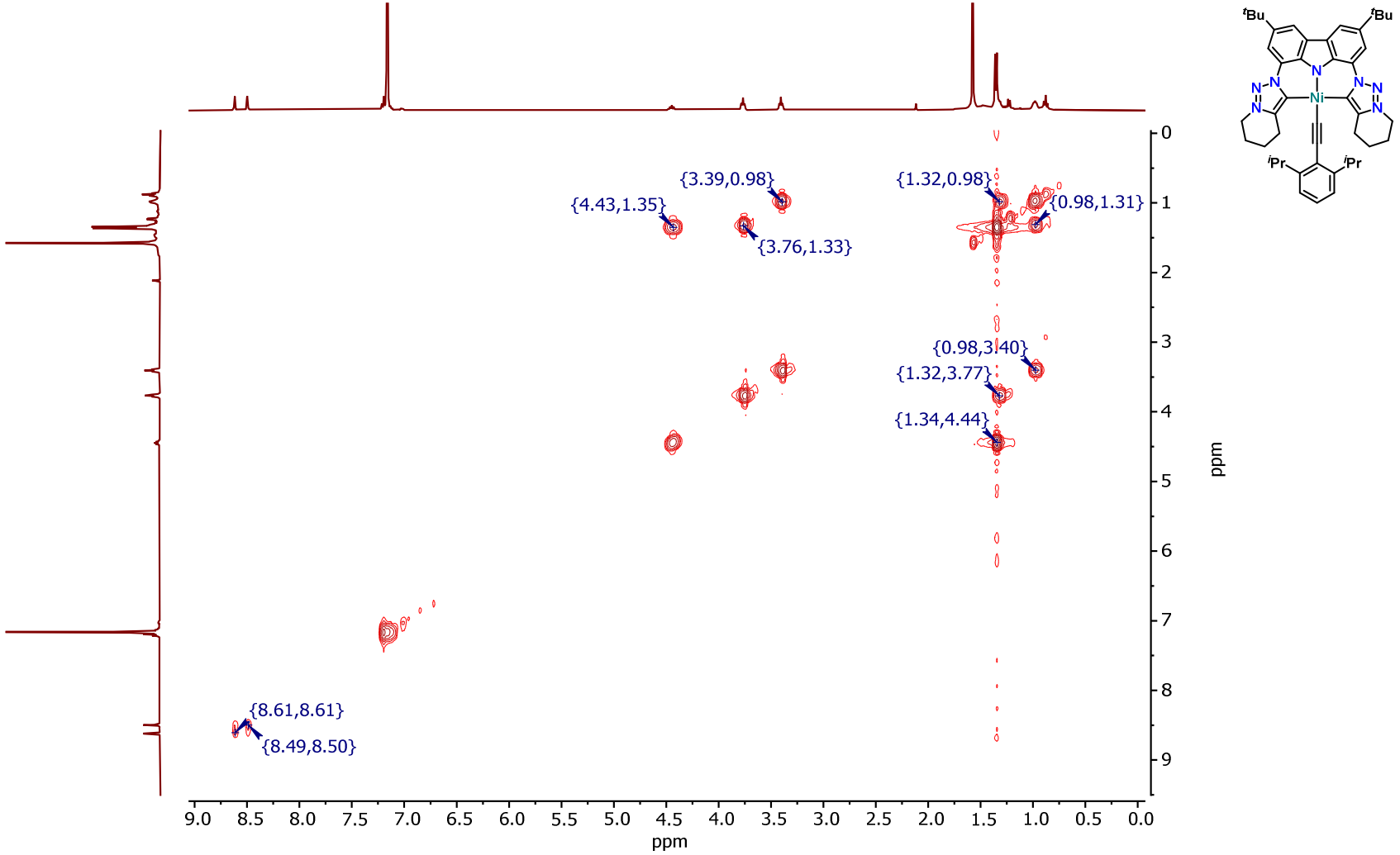


*Figure S 51: $^{1}H - {}^{1}H$ COSY of **9** in C_6D_6 at 298K.*

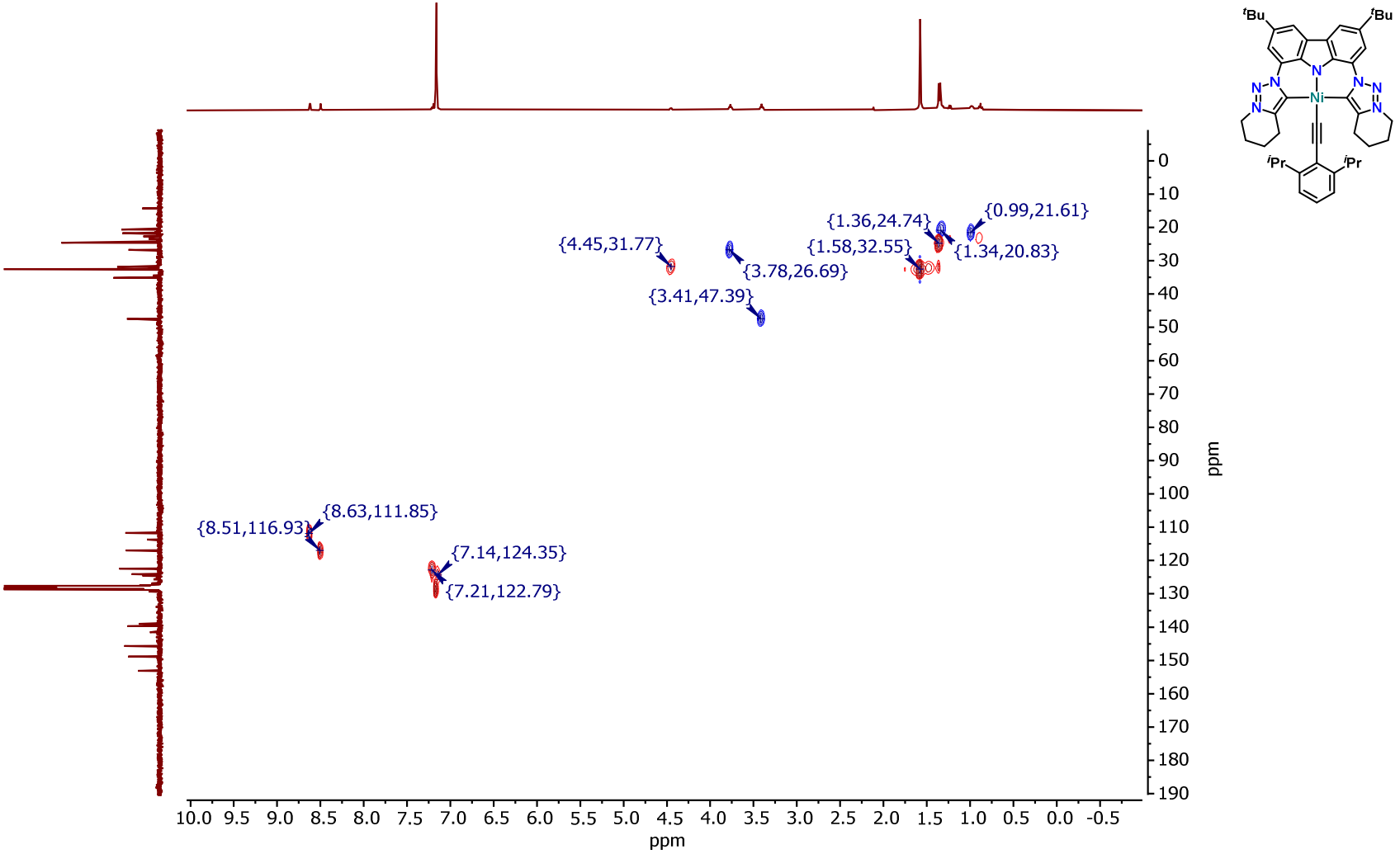


*Figure S 52: $^{1}H - ^{13}C$ HSQC of **9** in C_6D_6 at 298K.*

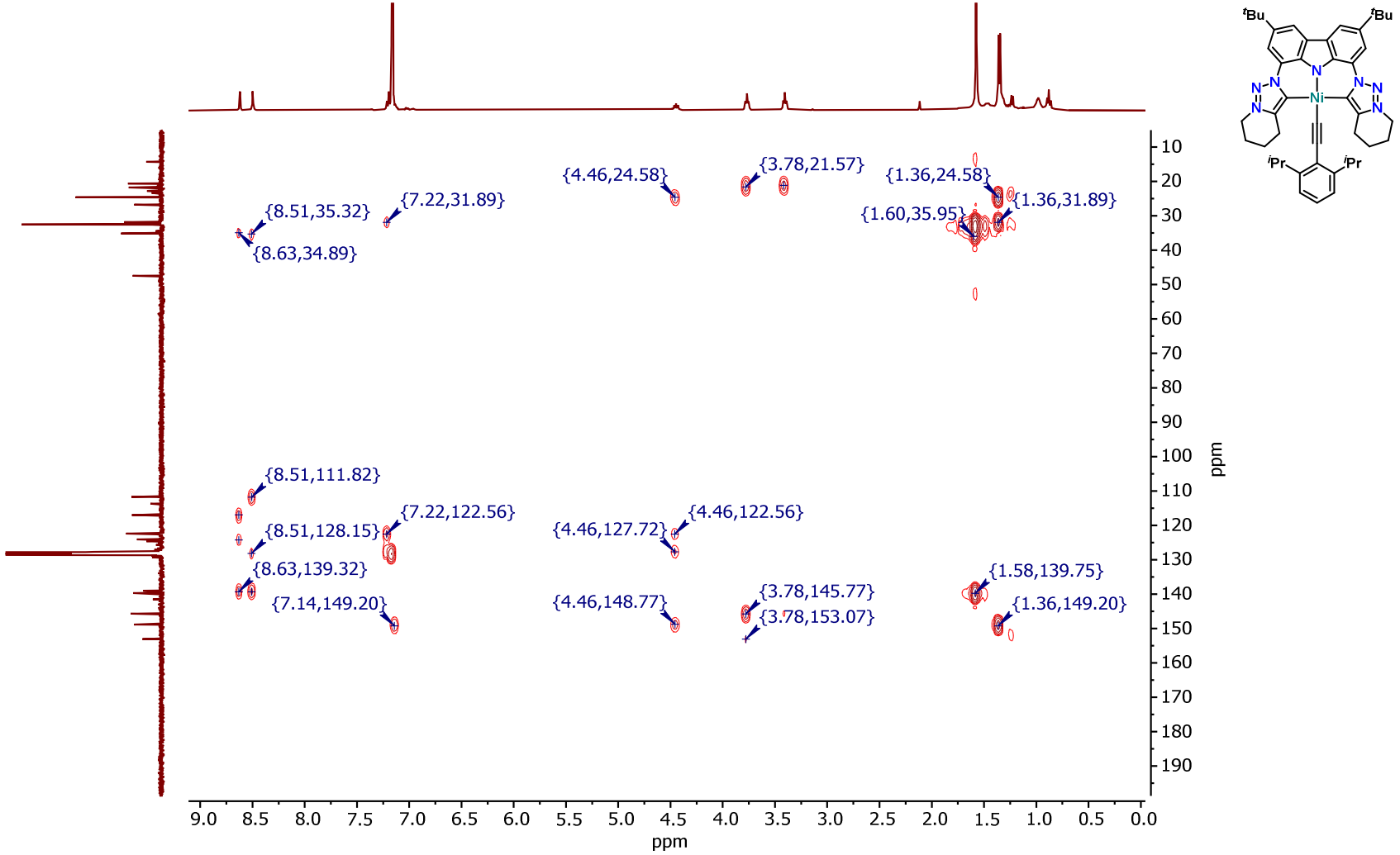


*Figure S 53: $^{1}H - ^{13}C$ HMBC of **9** in C_6D_6 at 298K.*

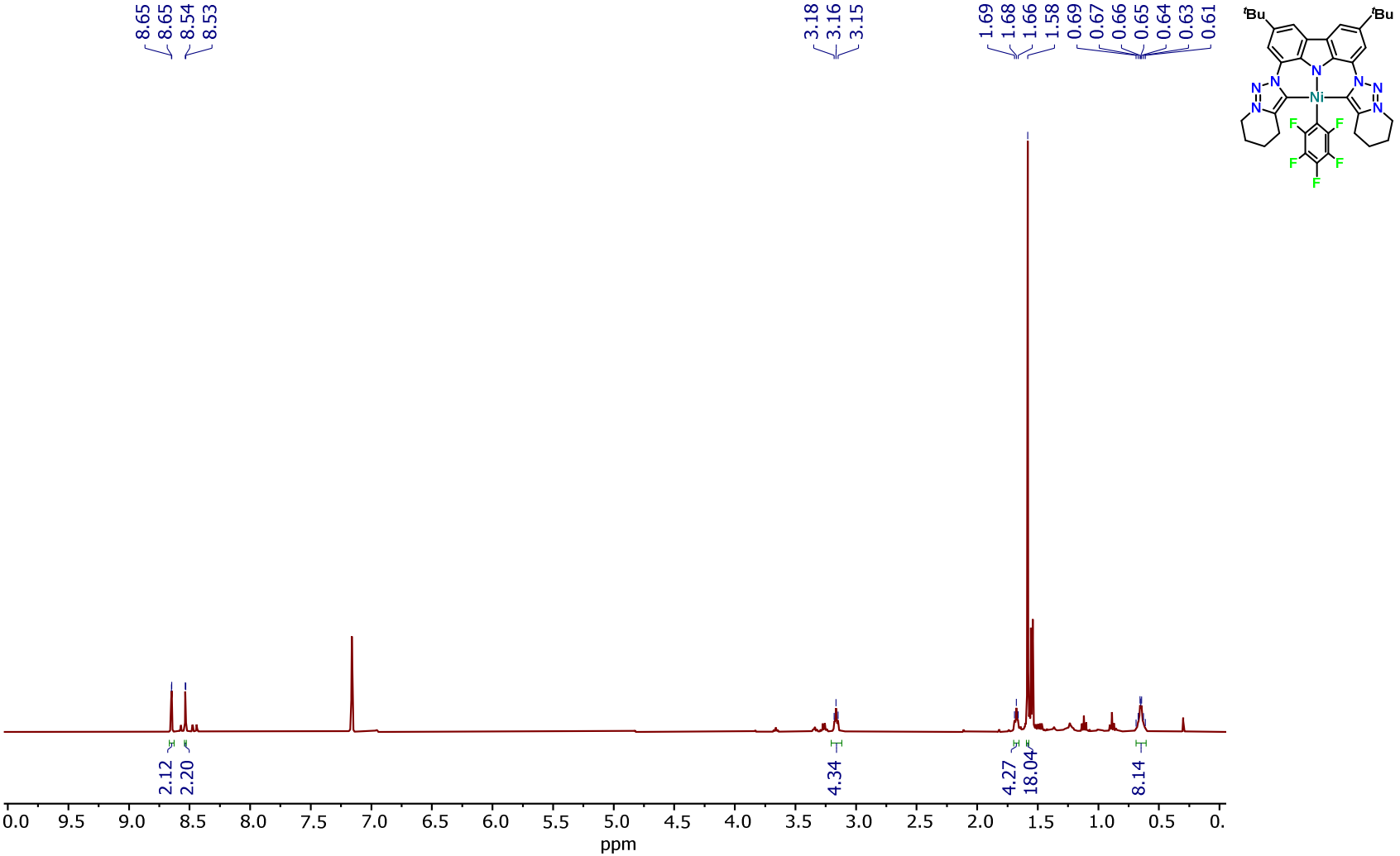


*Figure S 54: ^{1}H NMR of **10** in C_6D_6 at 298K.*

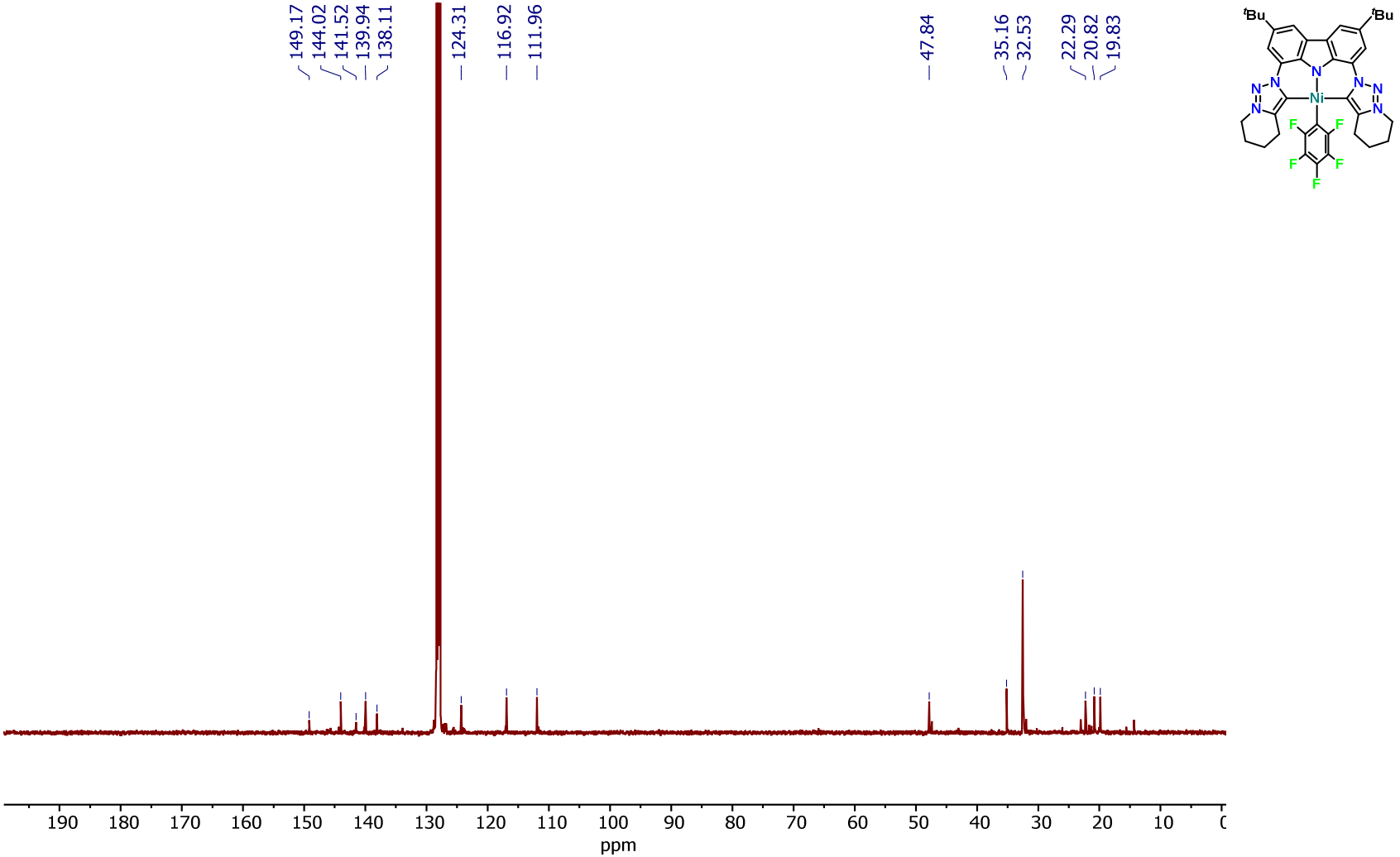


*Figure S 55: ^{13}C NMR of **10** in C_6D_6 at 298K.*

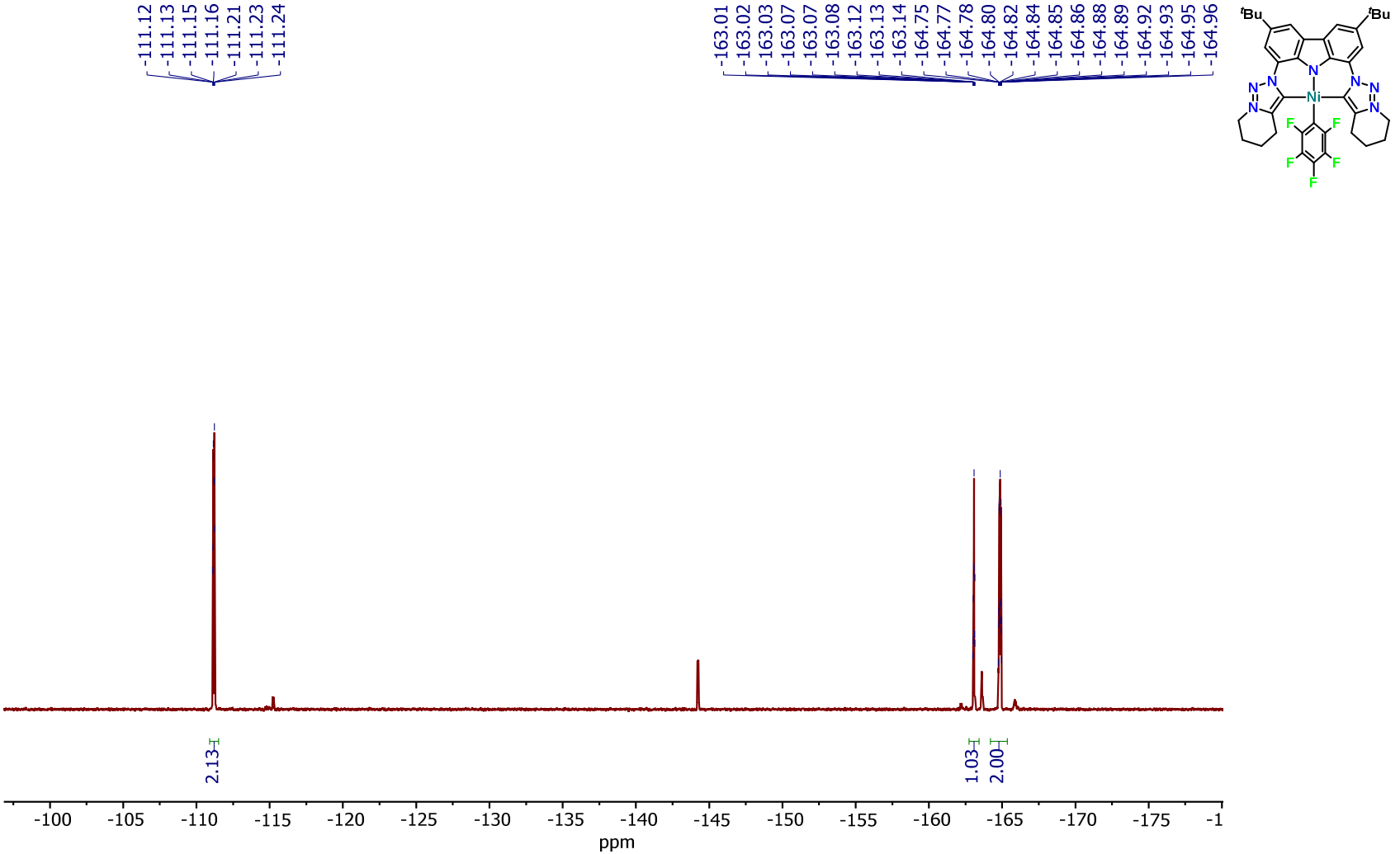


*Figure S 56: ^{19}F NMR of **10** in C_6D_6 at 298K.*

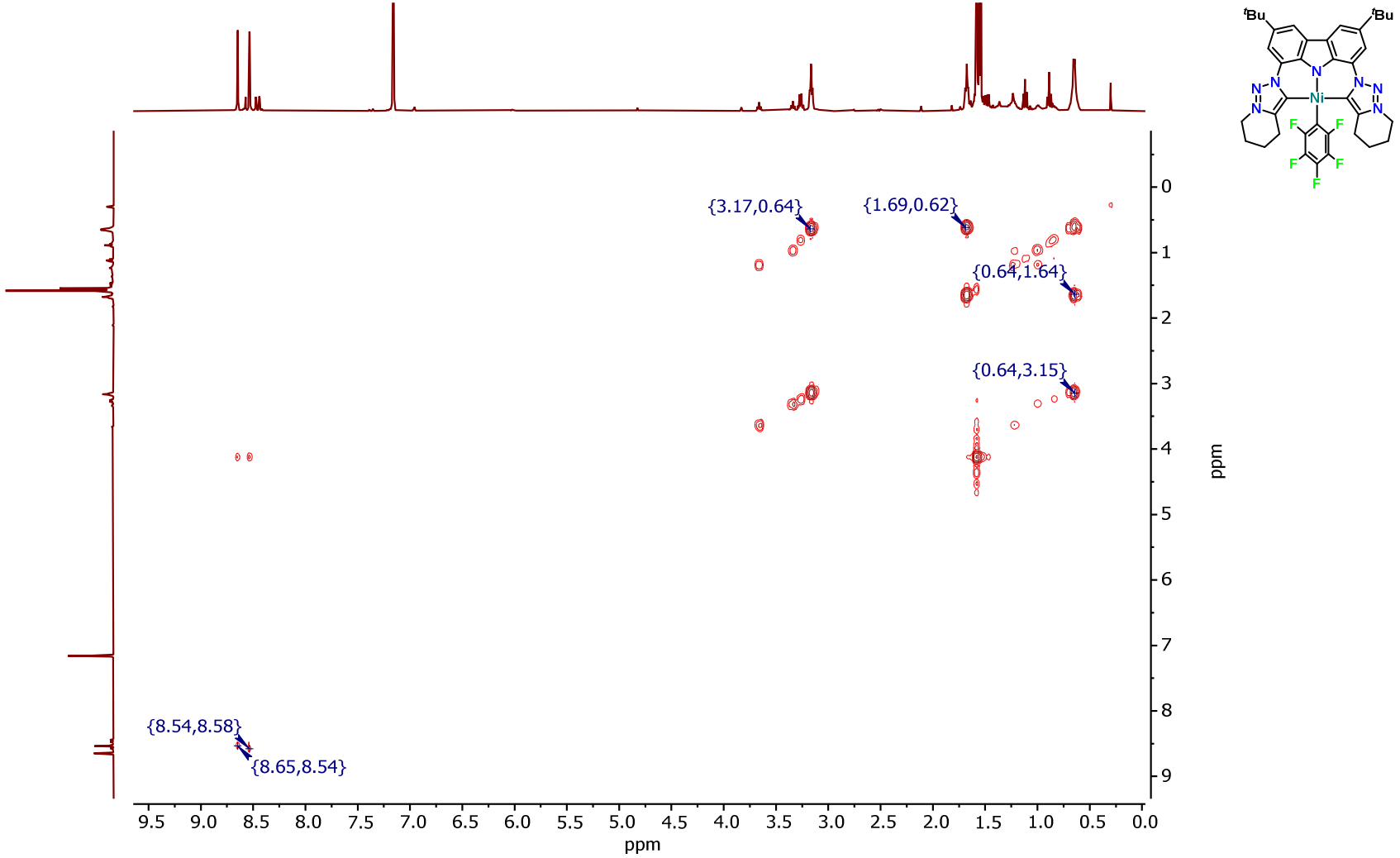


*Figure S 57: $^{1}H - ^{1}H$ COSY of **10** in C_6D_6 at 298K.*

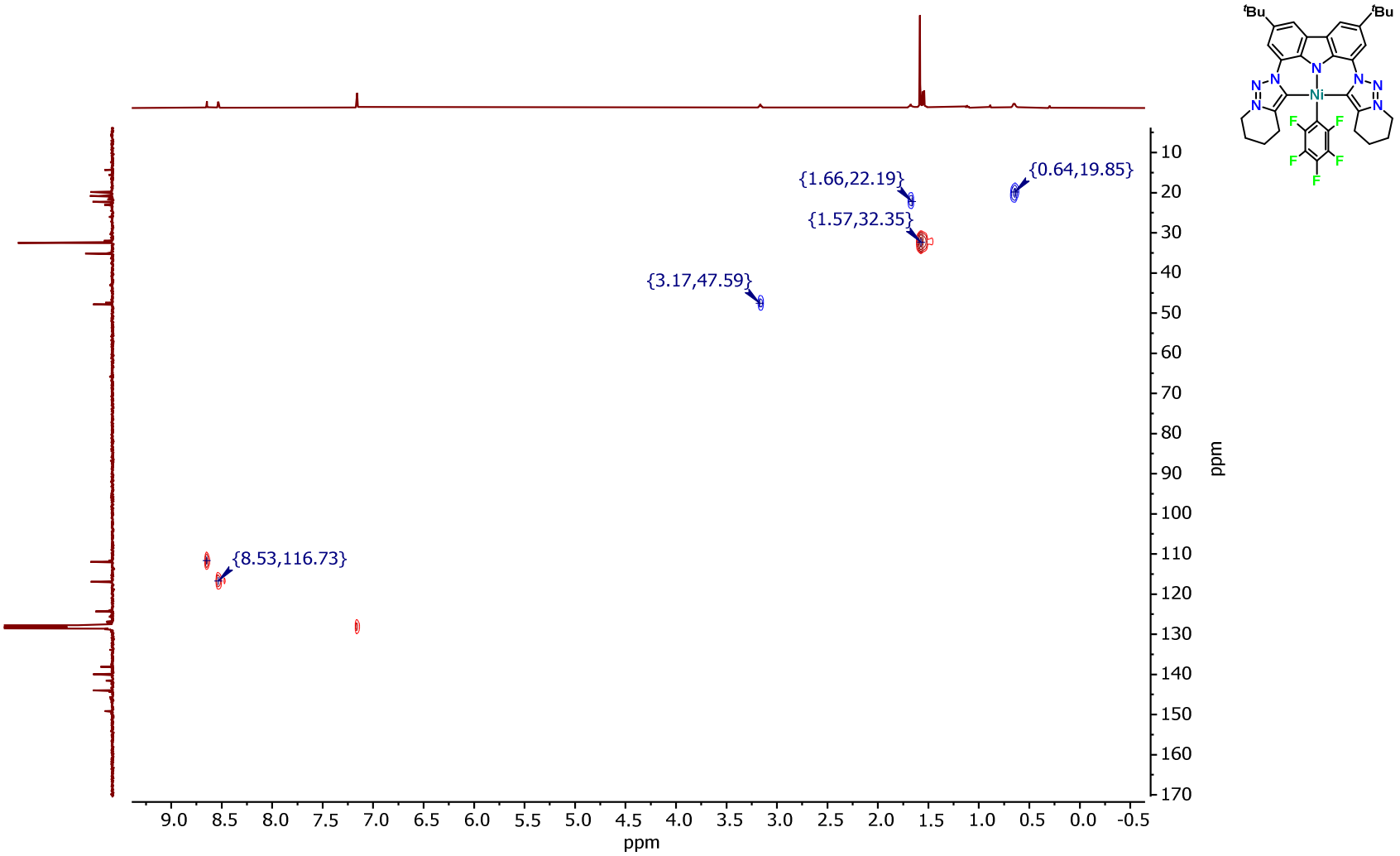


*Figure S 58: $^{1}H - ^{13}C$ HSQC of **10** in C_6D_6 at 298K.*

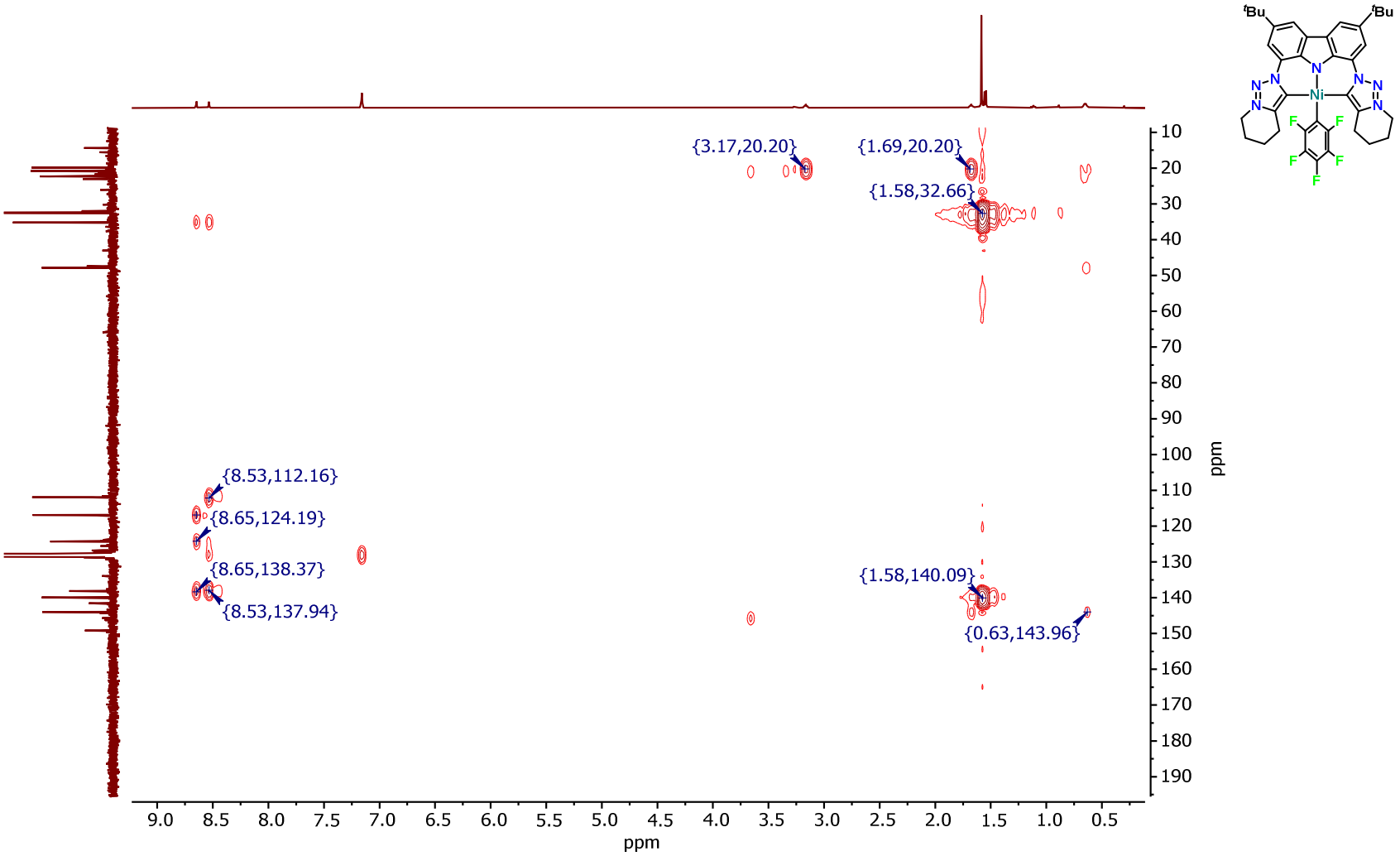


*Figure S 59: $^{1}H - ^{13}C$ HMBC of **10** in C_6D_6 at 298K.*

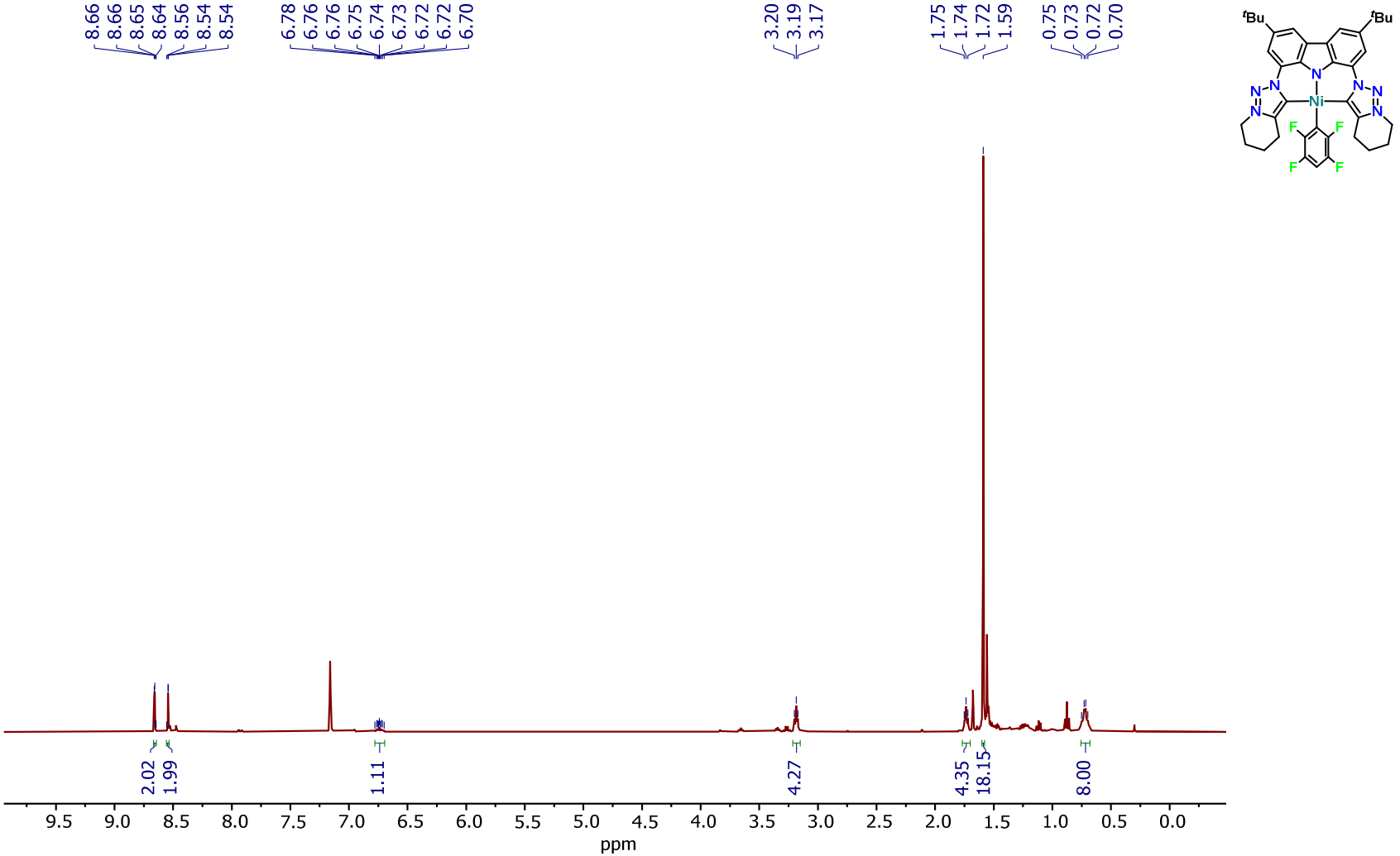


*Figure S 60: ^{1}H NMR of **11** in C_6D_6 at 298K.*

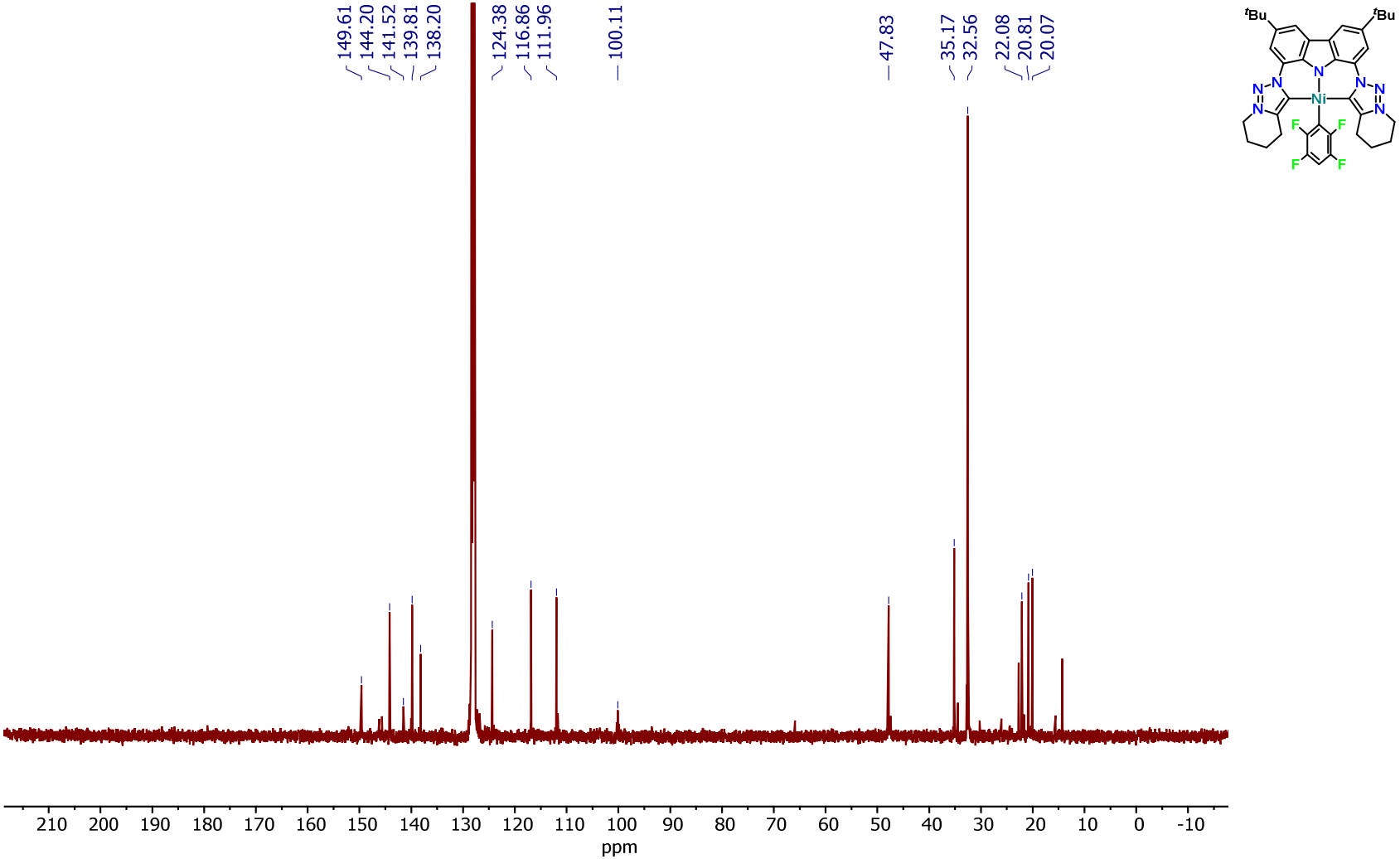


*Figure S 61: ^{13}C NMR of **11** in C_6D_6 at 298K.*

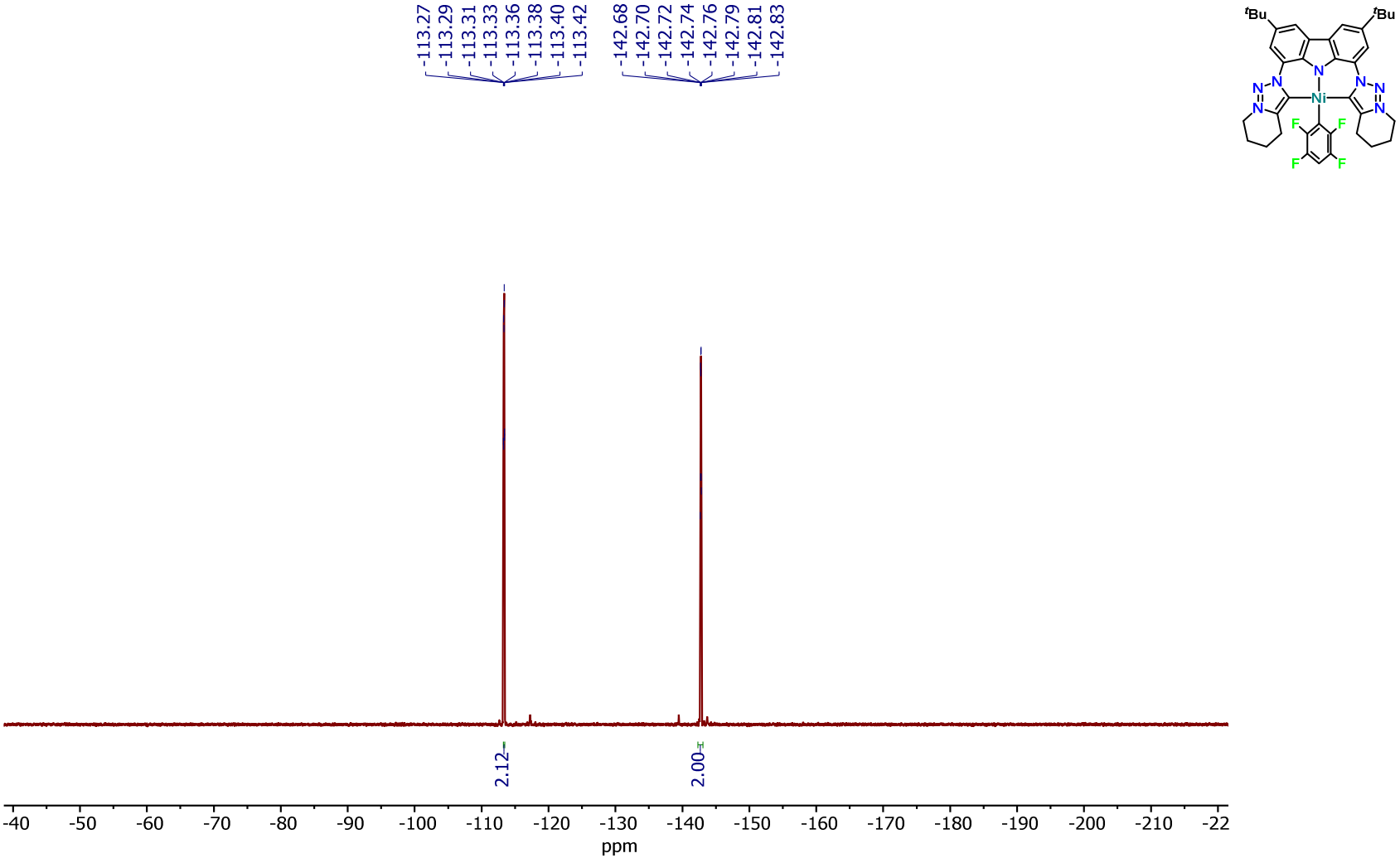


*Figure S 62: ^{19}F NMR of **11** in C_6D_6 at 298K.*

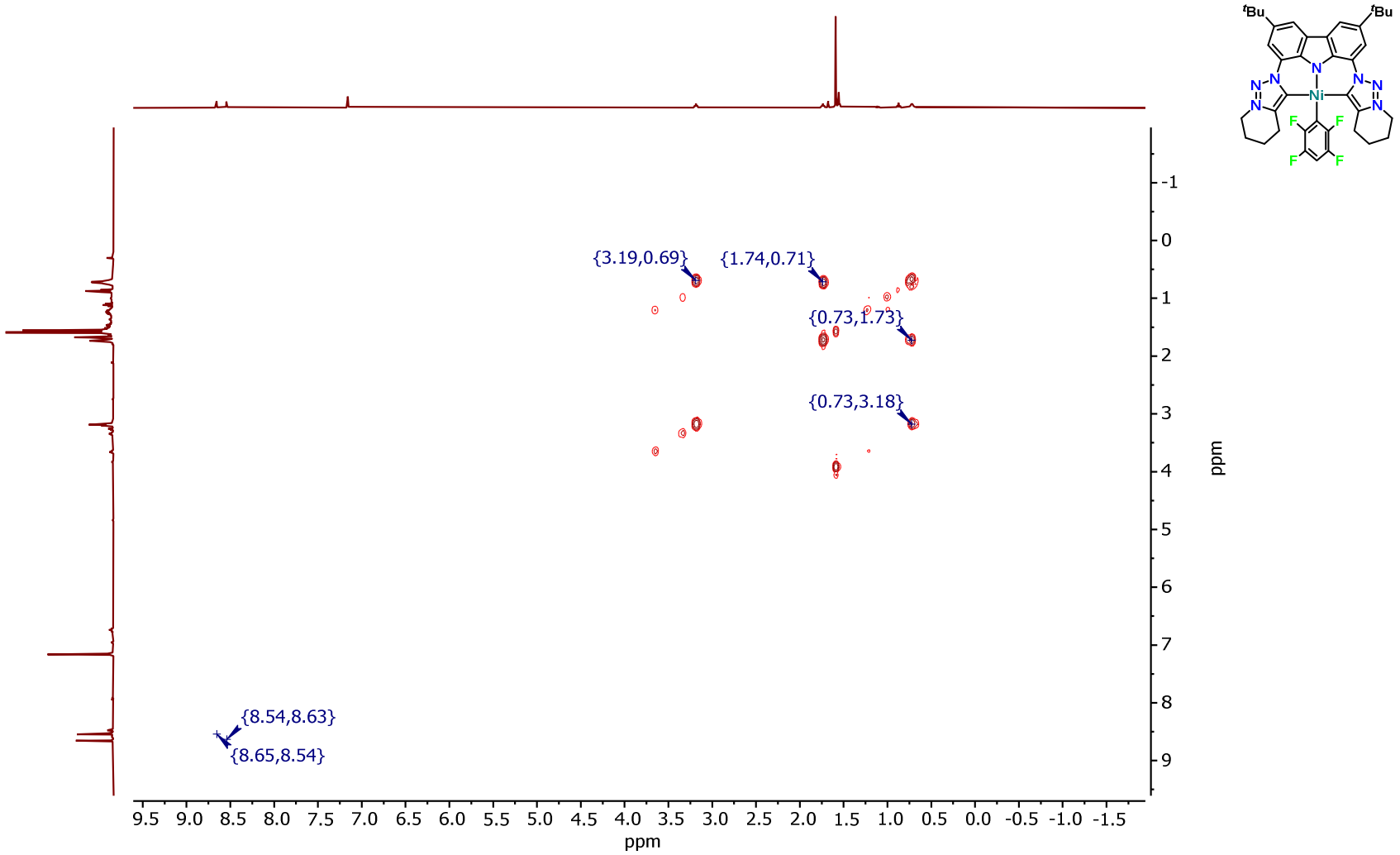


*Figure S 63: $^{1}H - ^{1}H$ COSY of **11** in C_6D_6 at 298K.*

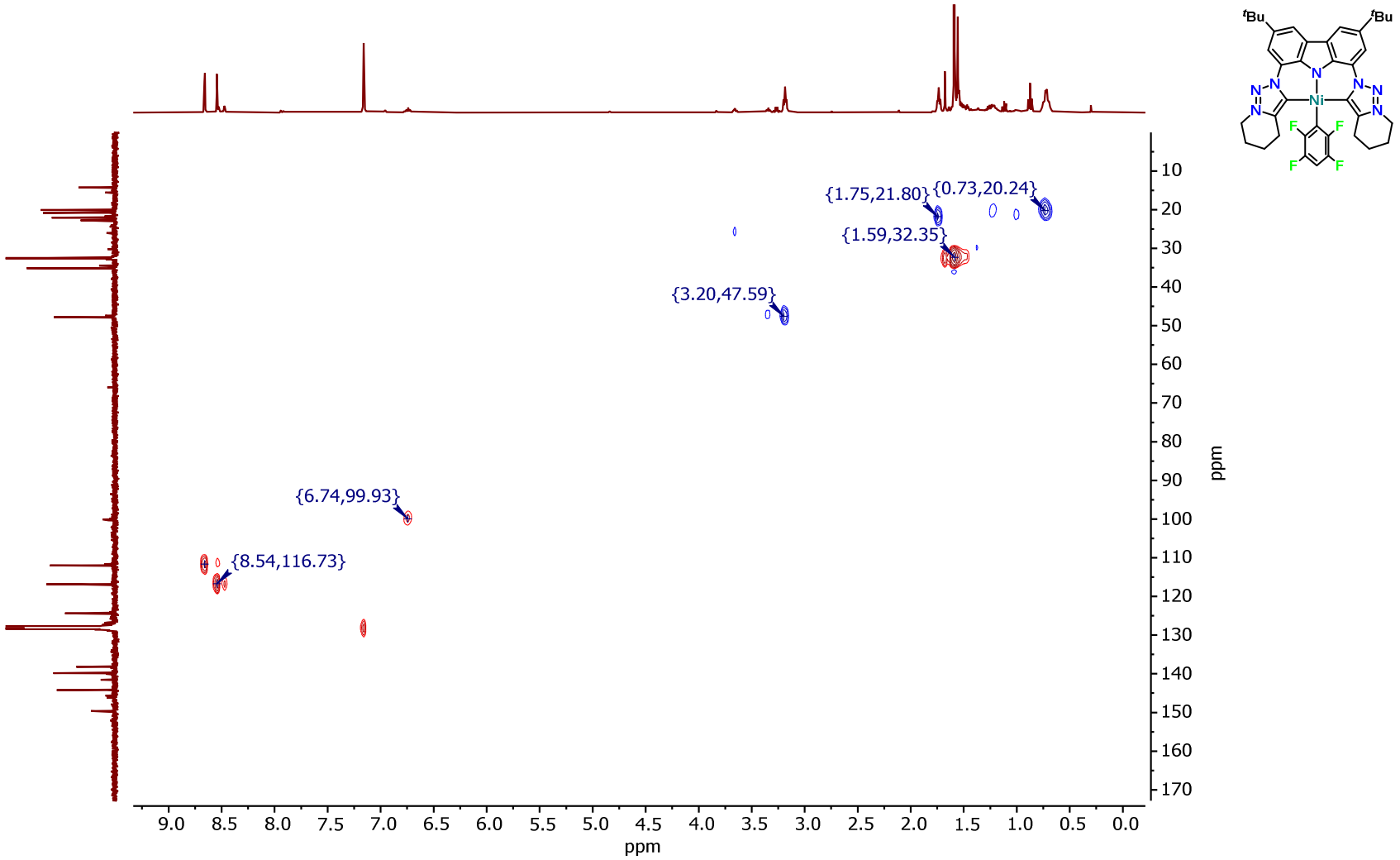


*Figure S 64: $^{1}H - ^{13}C$ HSQC of **11** in C_6D_6 at 298K.*

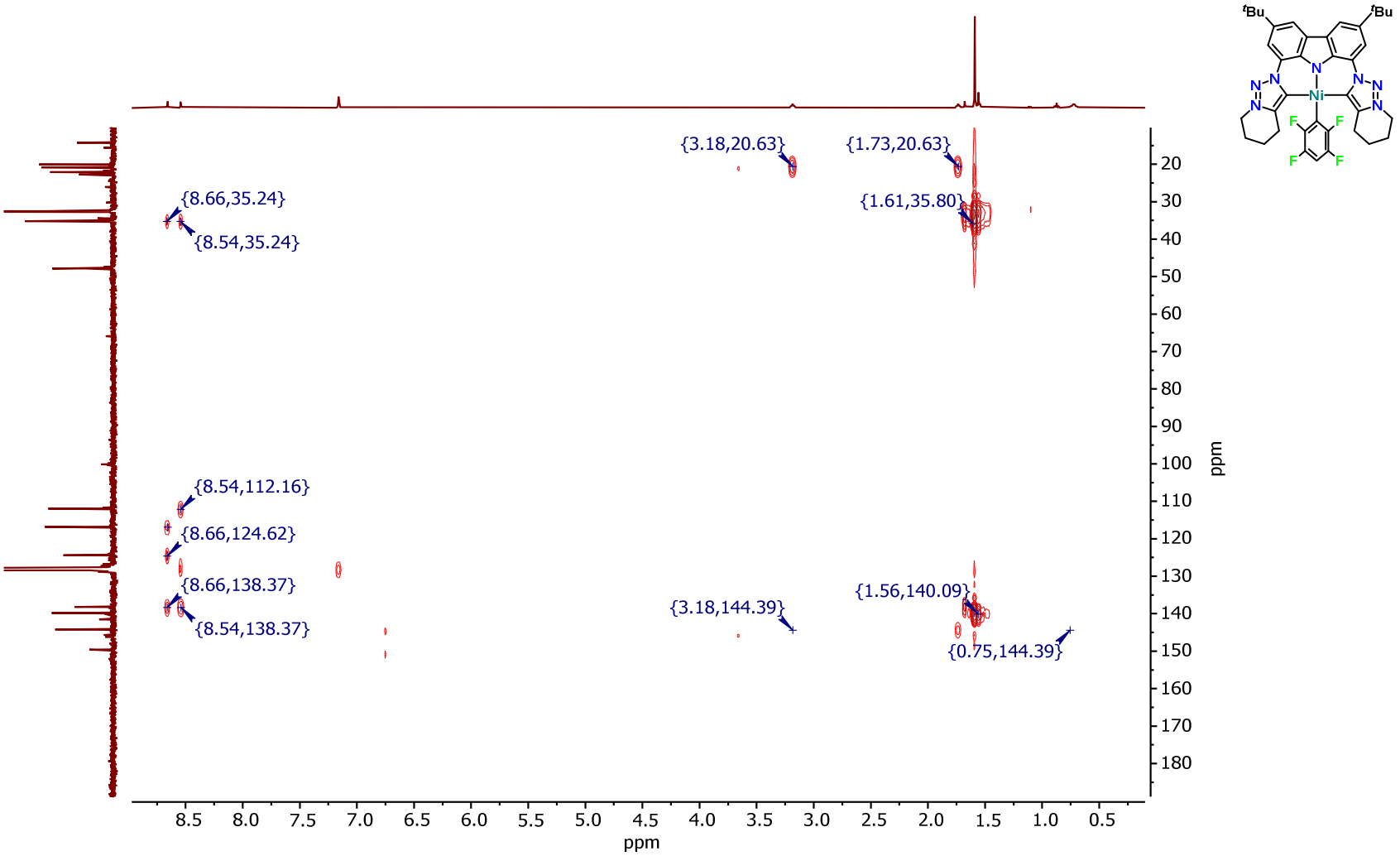


*Figure S 65: $^{1}H - ^{13}C$ HMBC of **11** in C_6D_6 at 298K.*

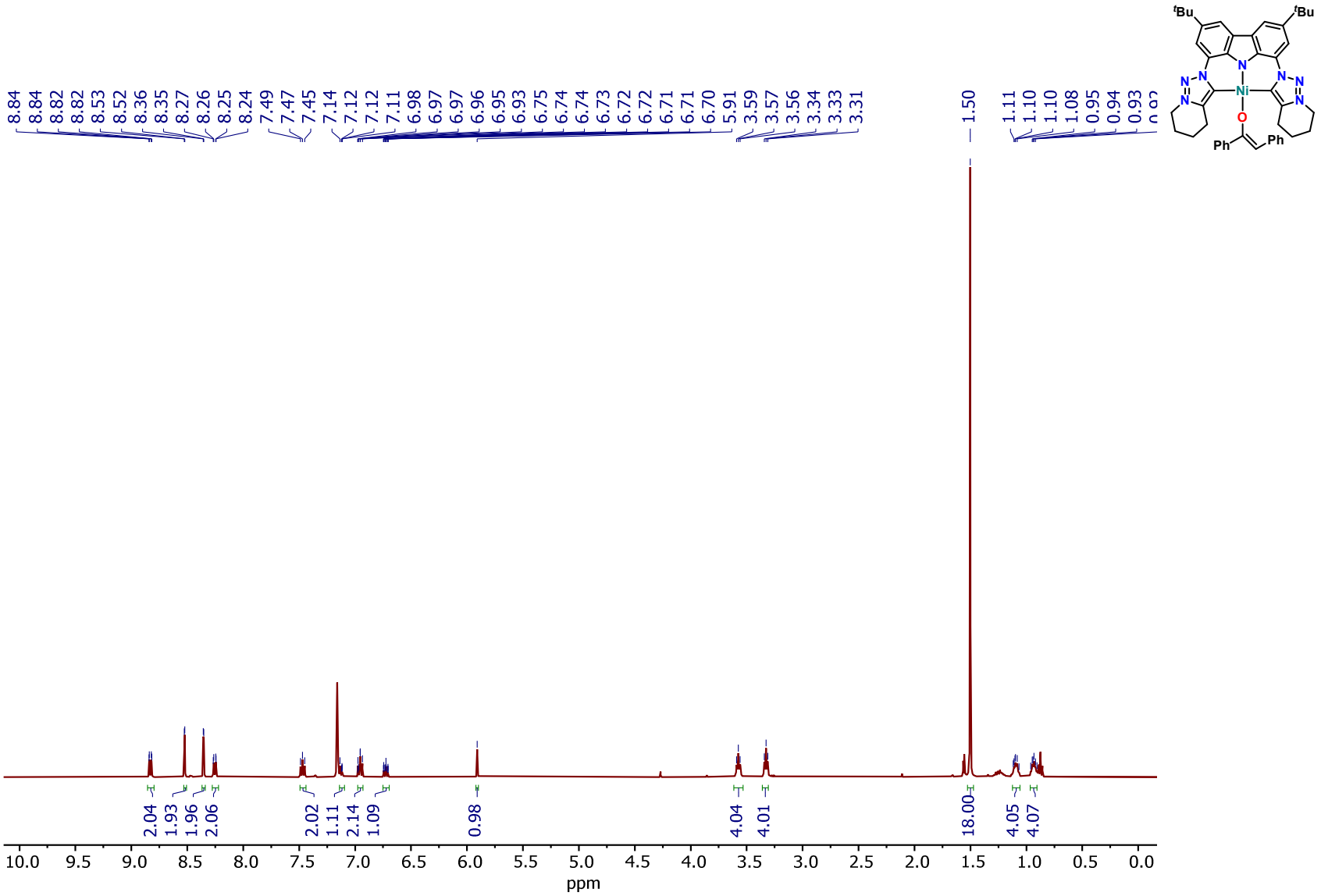


*Figure S 66: ^{1}H NMR of **12** in C_6D_6 at 298K.*

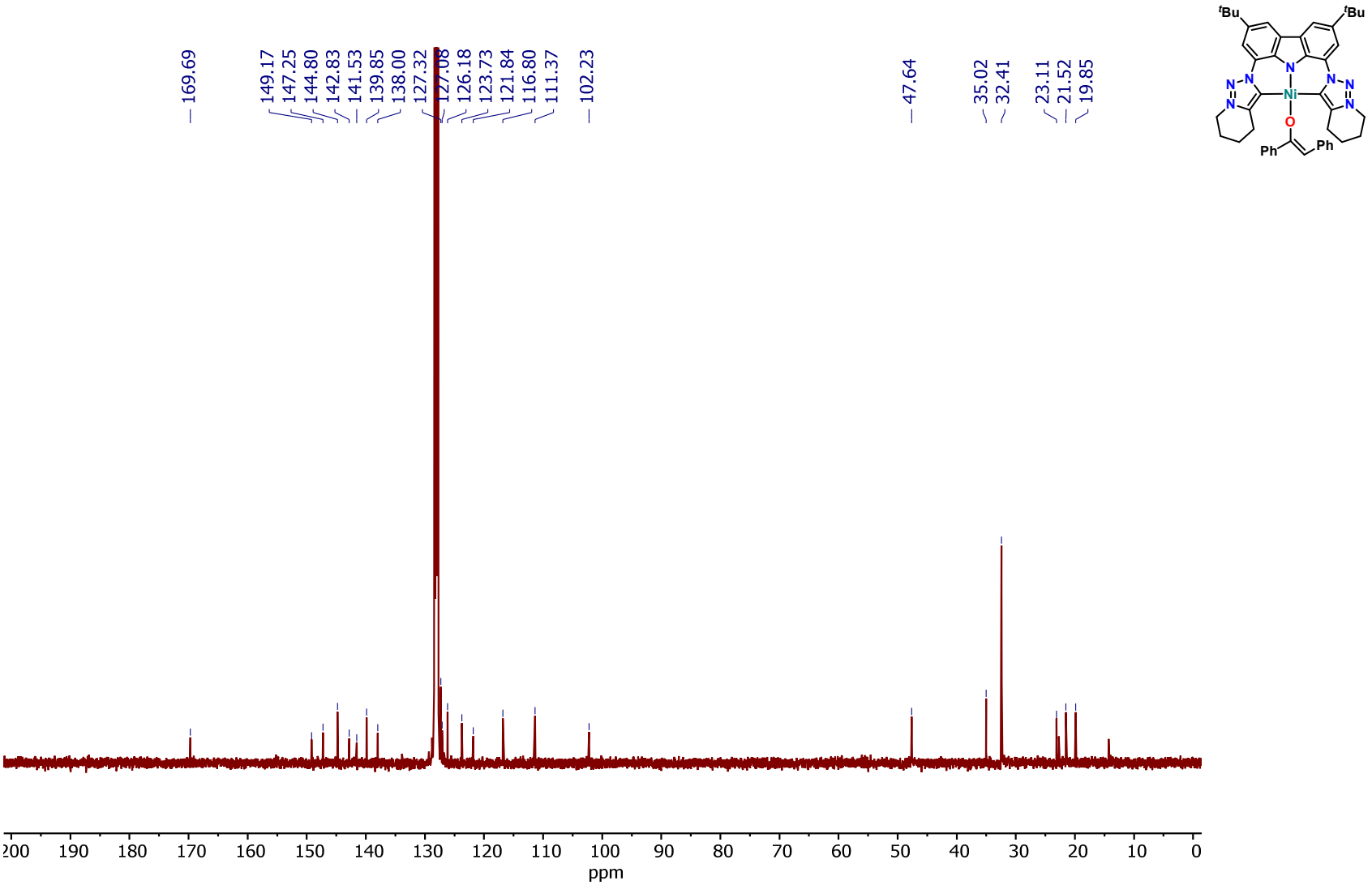


*Figure S 67: ^{13}C NMR of **12** in C_6D_6 at 298K.*

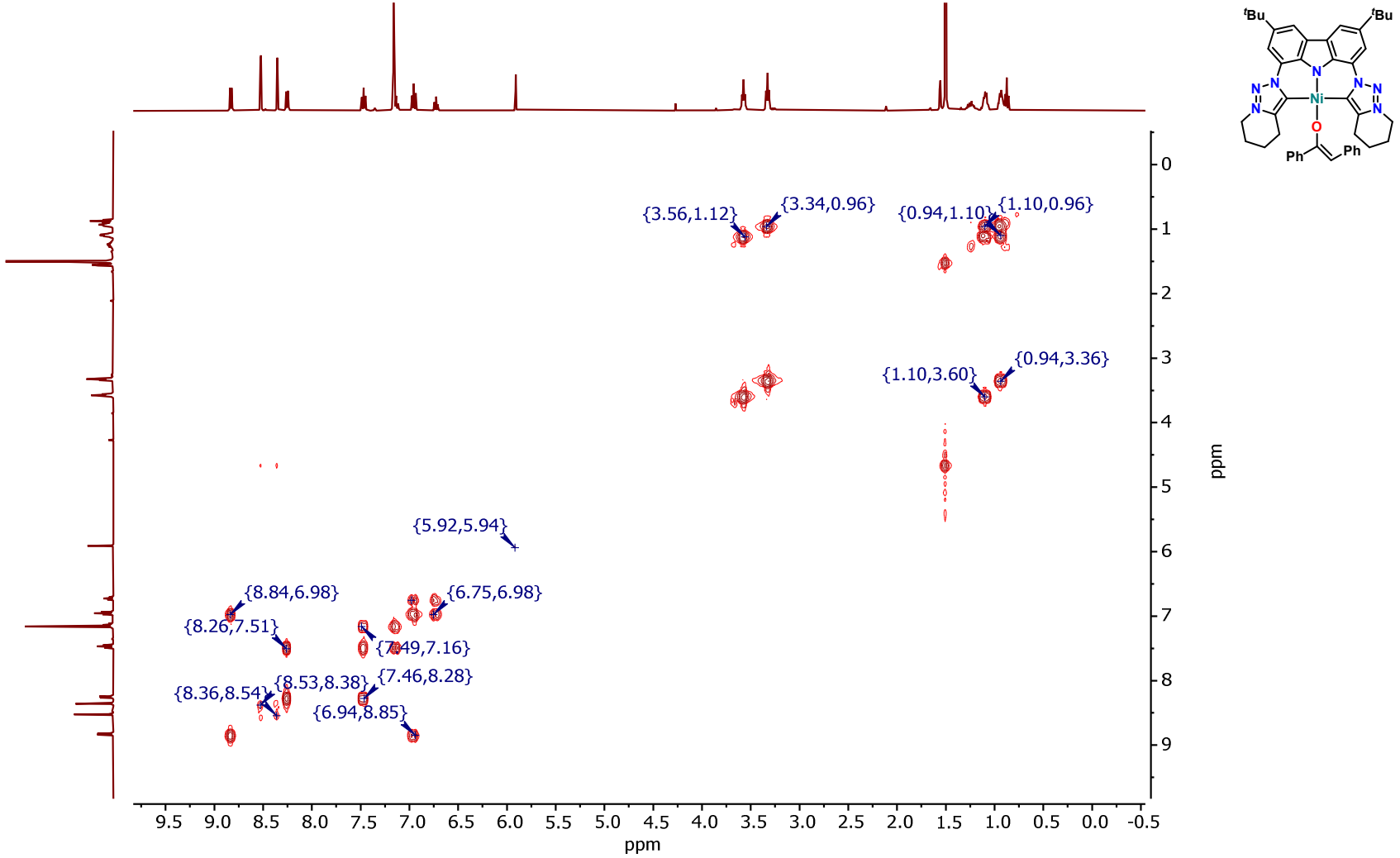


*Figure S 68: $^{1}H - ^{1}H$ COSY of **12** in C_6D_6 at 298K.*

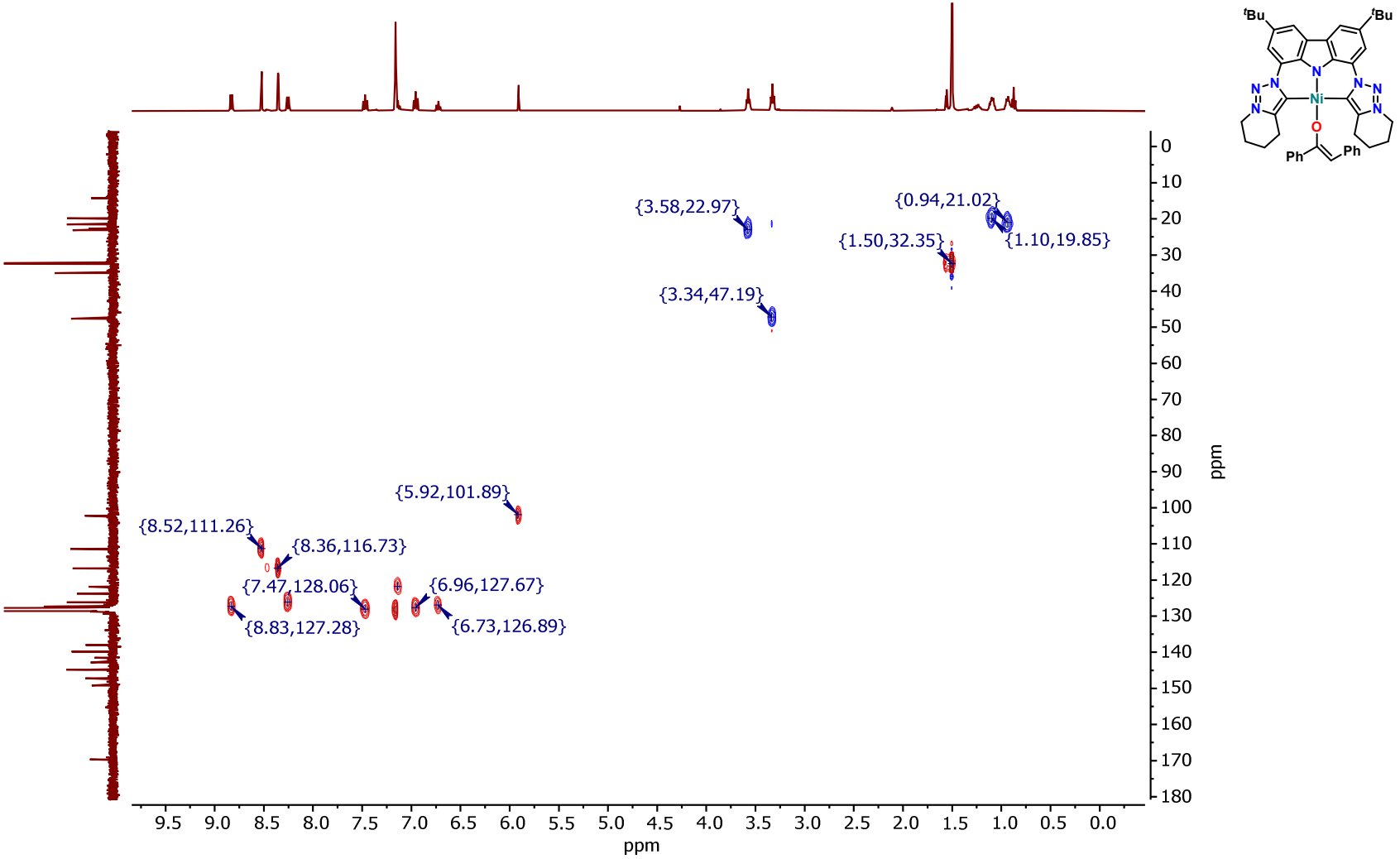


*Figure S 69: $^{1}H - ^{13}C$ HSQC of **12** in C_6D_6 at 298K.*

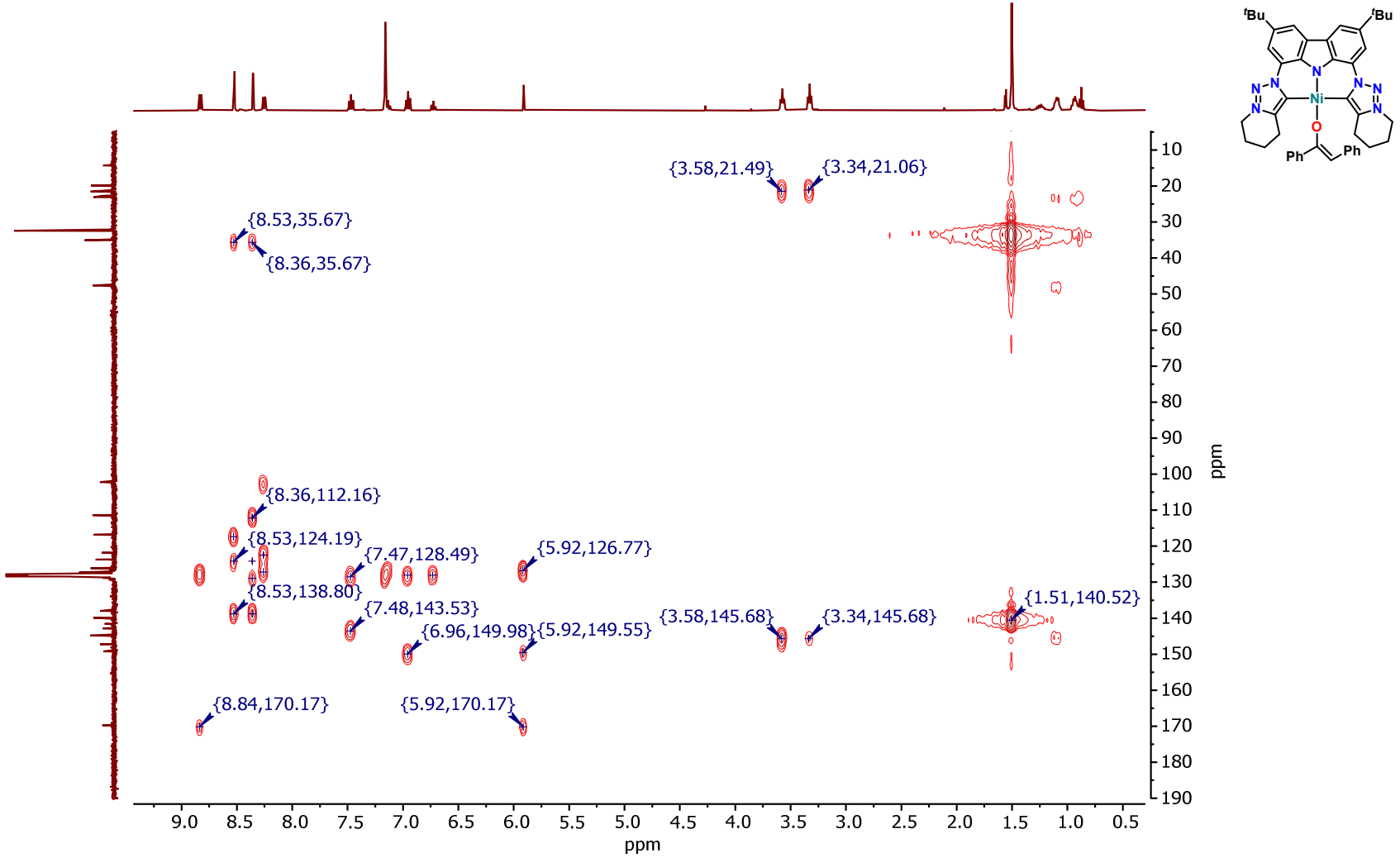


*Figure S 70: $^{1}H - ^{13}C$ HMBC of **12** in C_6D_6 at 298K.*

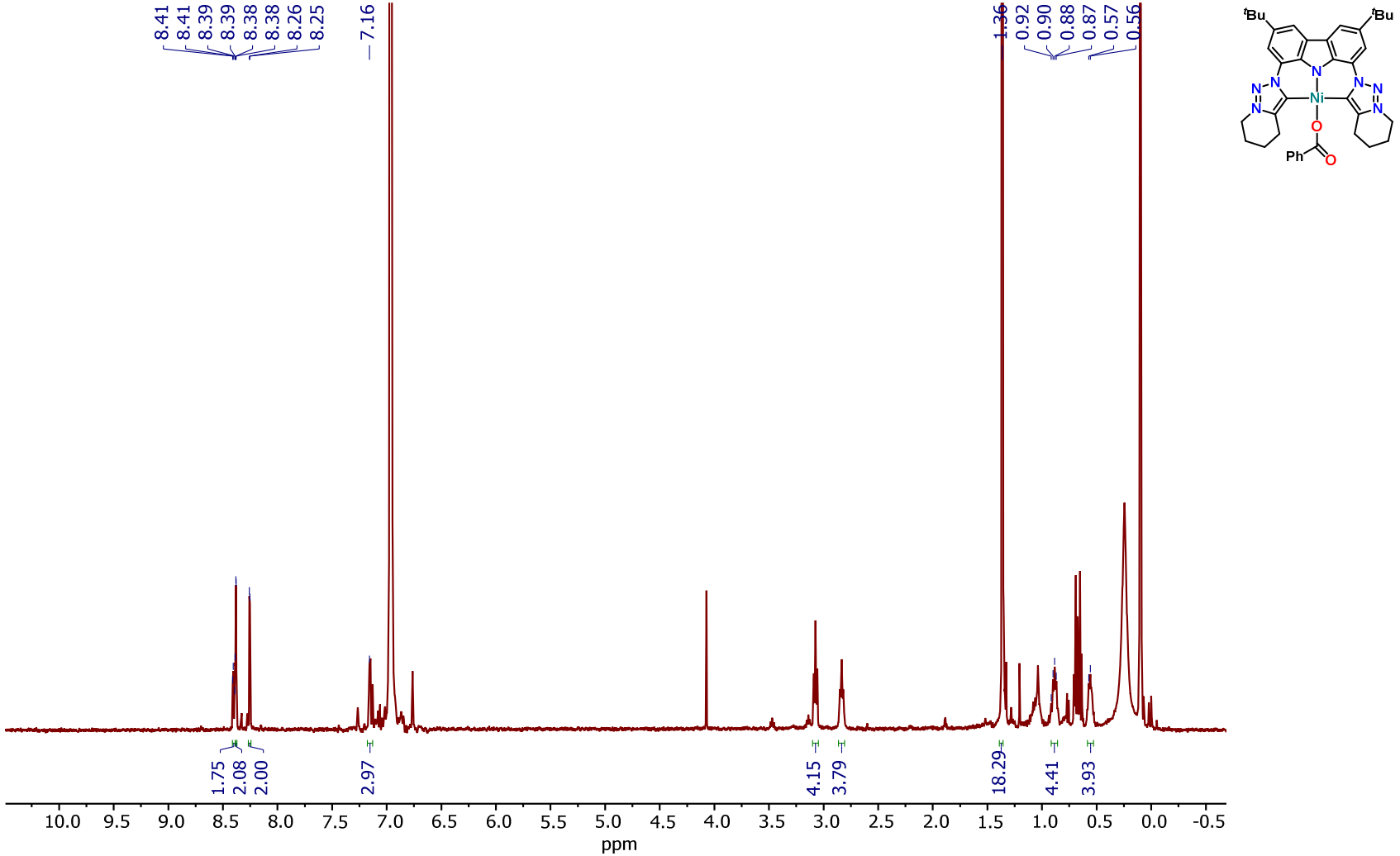


*Figure S 71: ^{1}H NMR of **12'** (crystals) in C_6D_6 at 298K.*

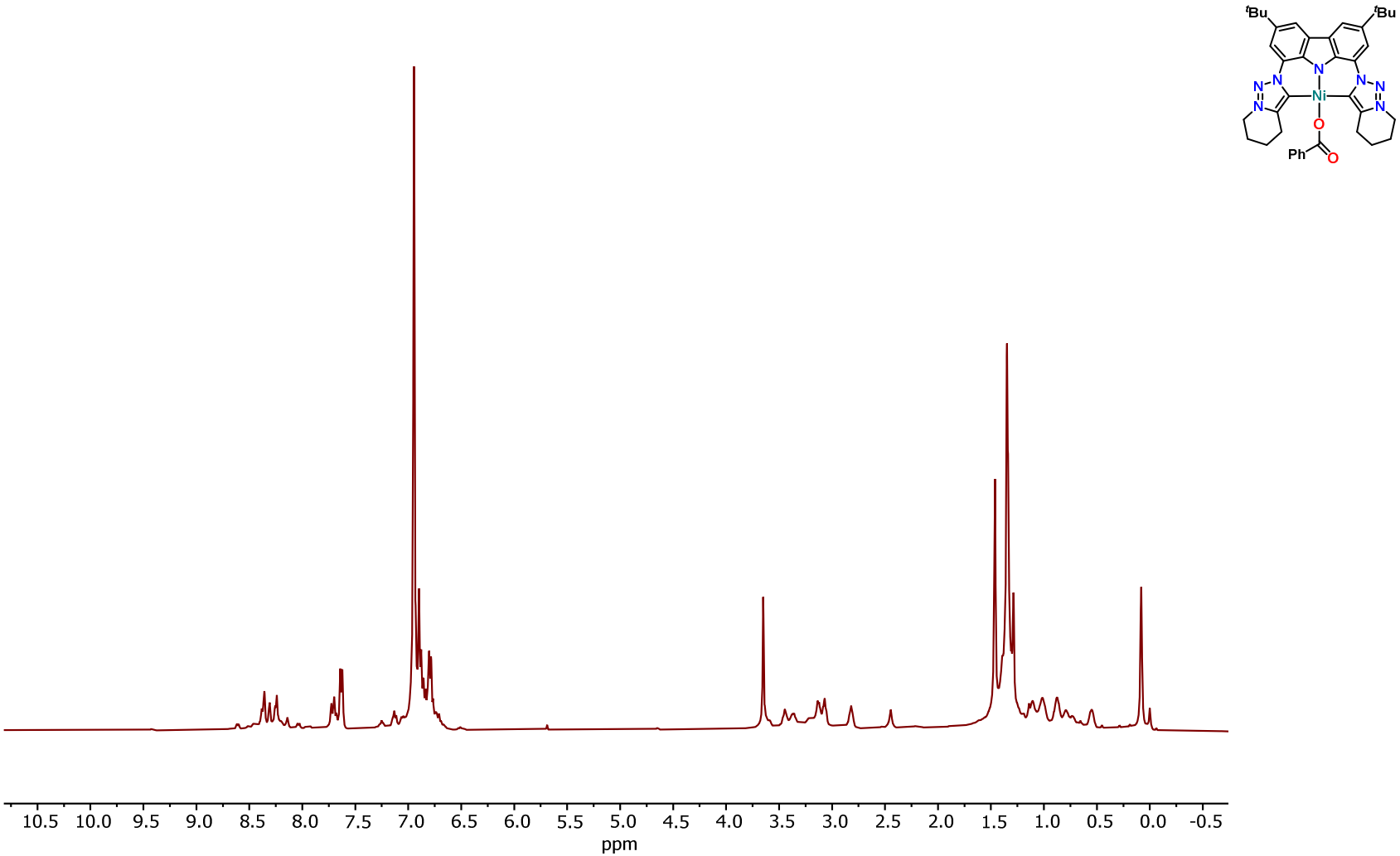


*Figure S 72: ^{1}H NMR of **12'** (crude) in C_6D_6 at 298K.*

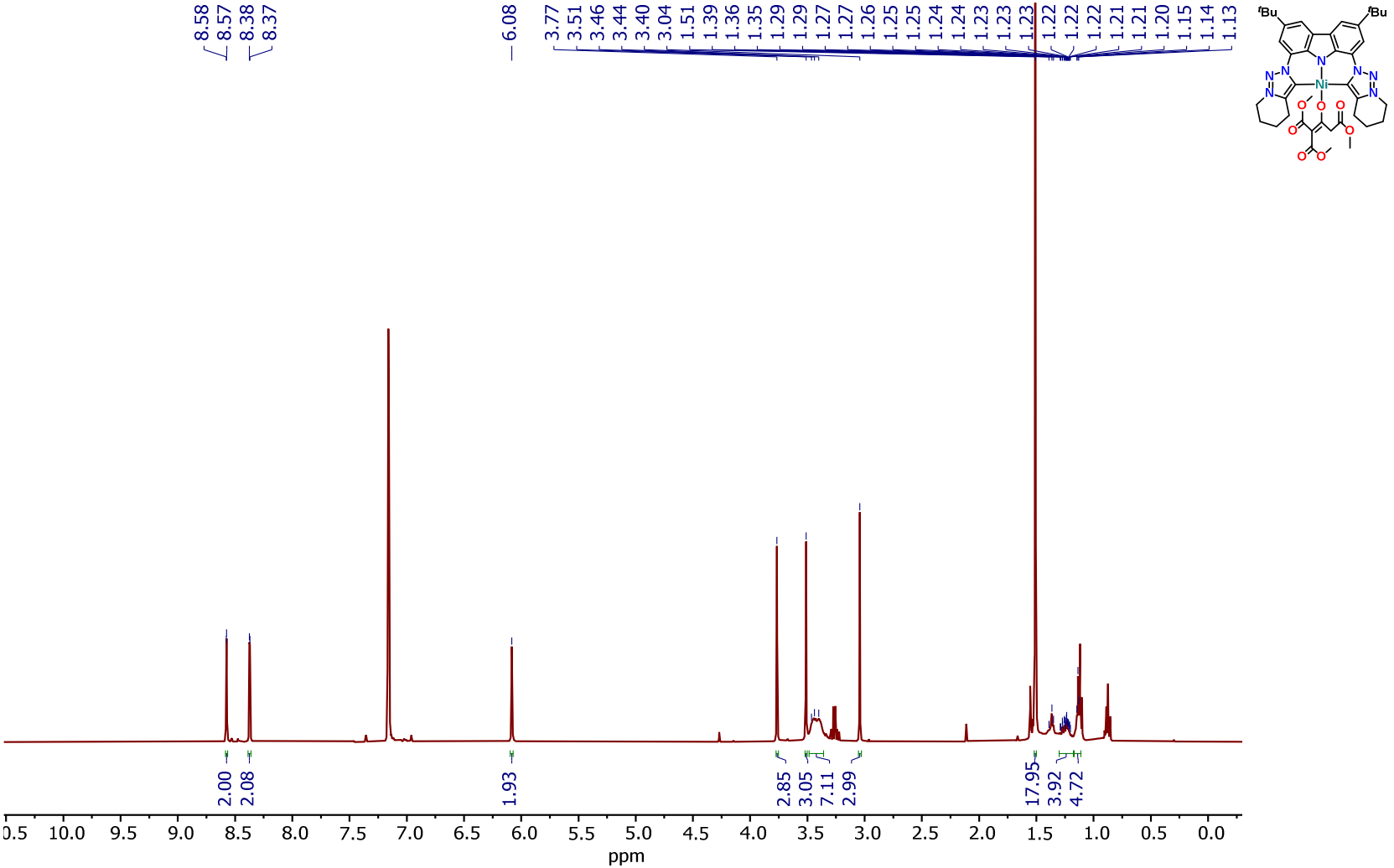


*Figure S 73: ^{1}H NMR of **13** in C_6D_6 at 298K.*

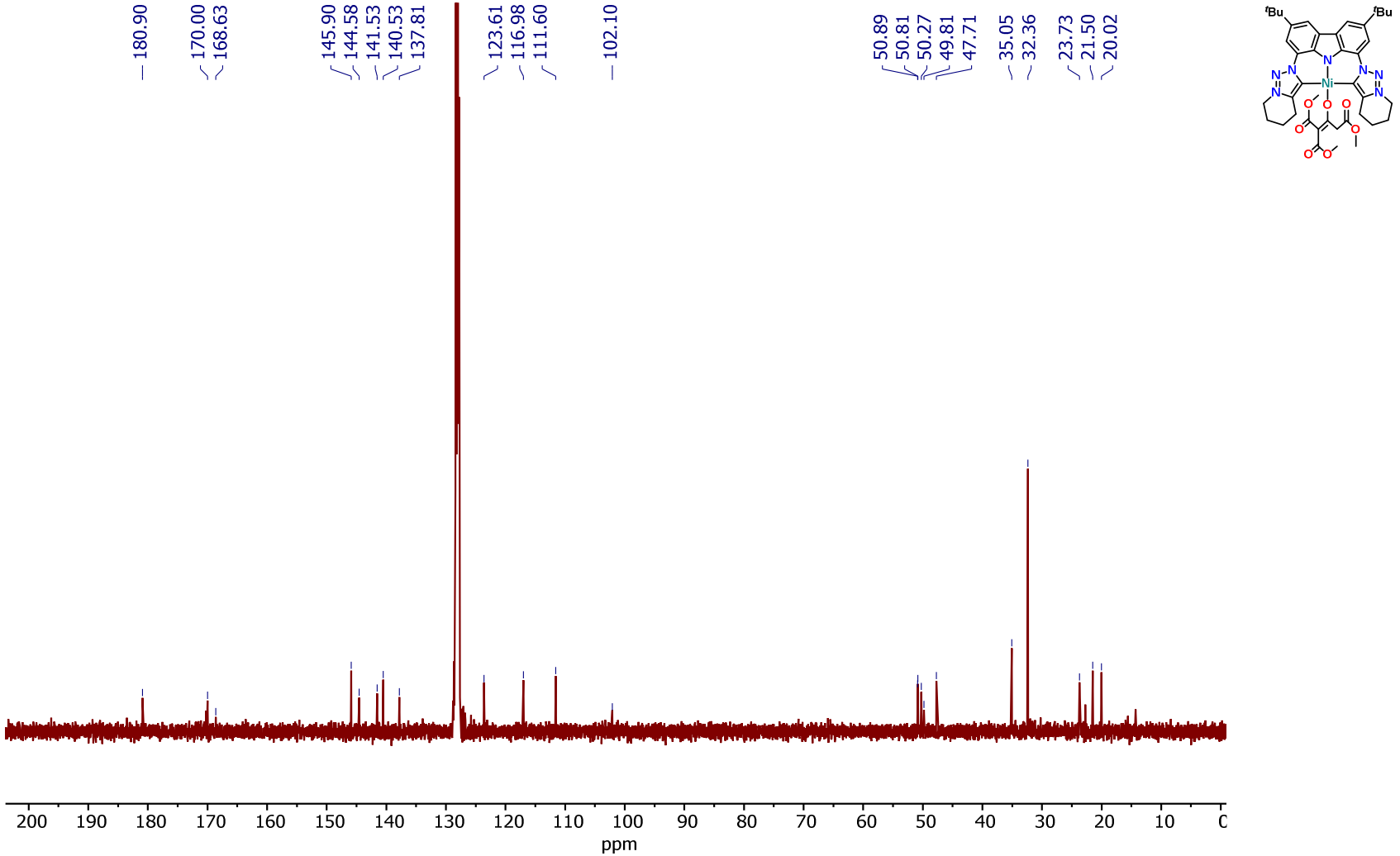


*Figure S 74: ^{13}C NMR of **13** in C_6D_6 at 298K.*

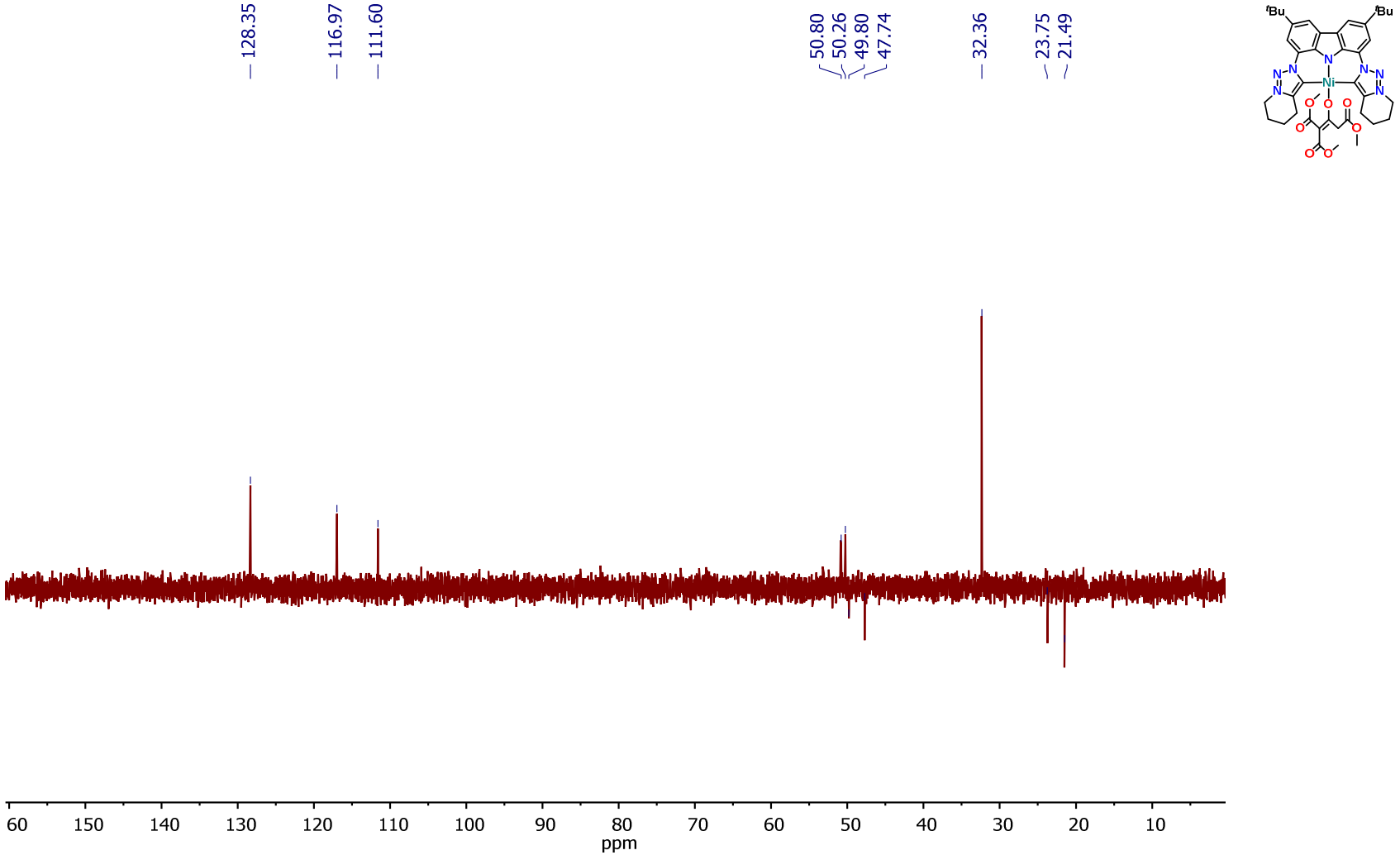


*Figure S 75: 135-DEPT ^{13}C NMR of **13** in C_6D_6 at 298K.*

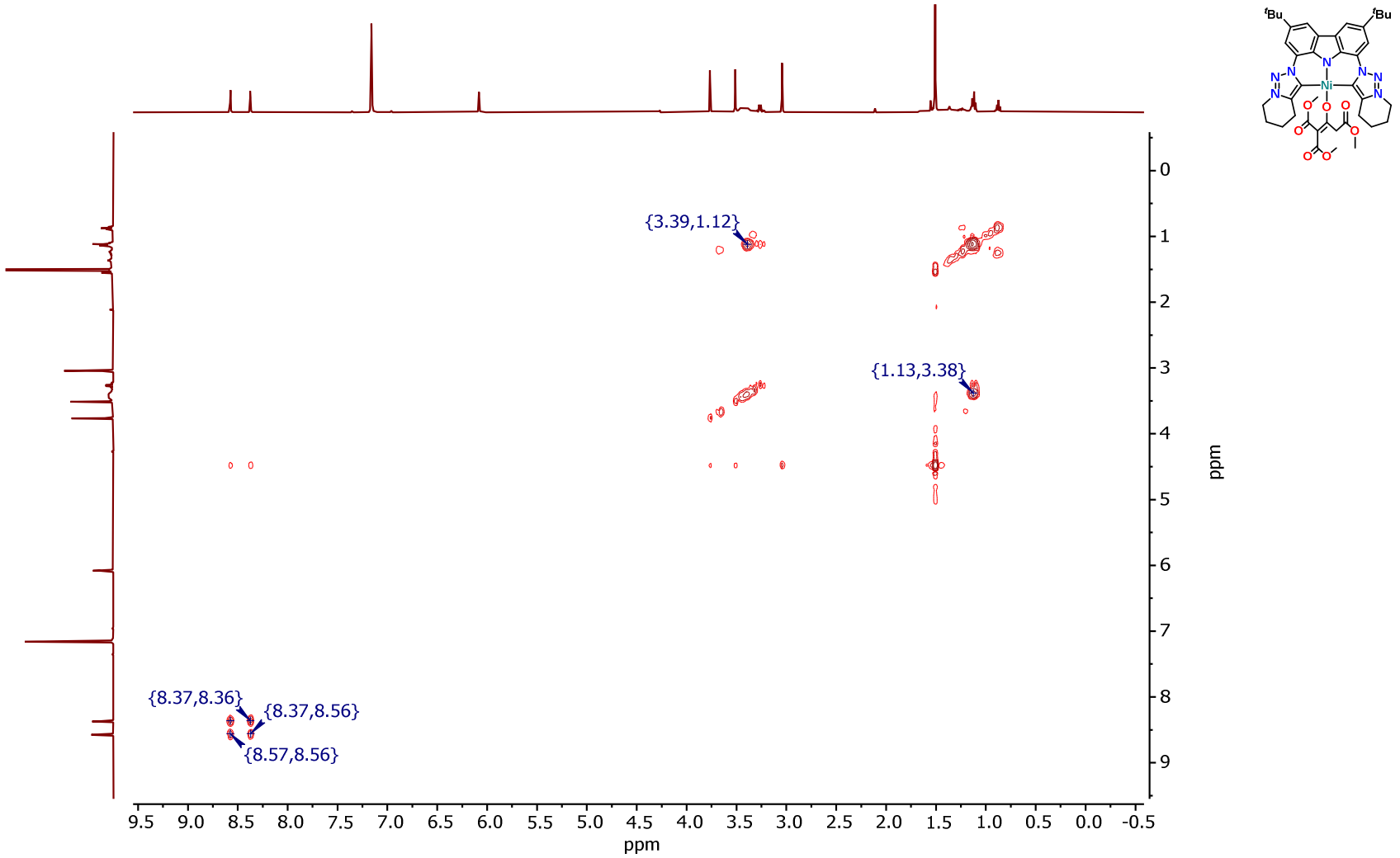


*Figure S 76: $^{1}H - ^{1}H$ COSY of **13** in C_6D_6 at 298K.*

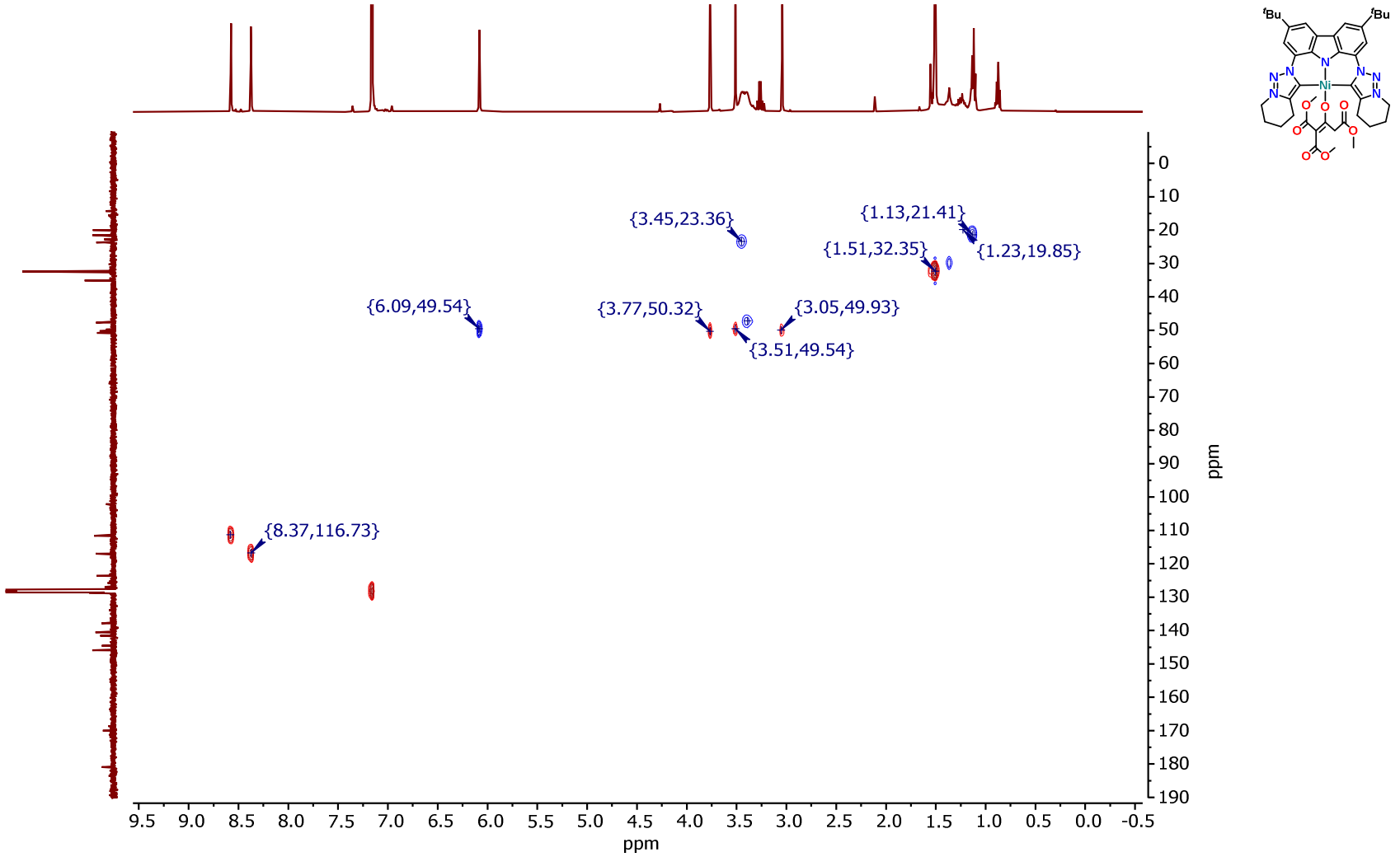


*Figure S 77: $^{1}H - ^{13}C$ HSQC of **13** in C_6D_6 at 298K.*

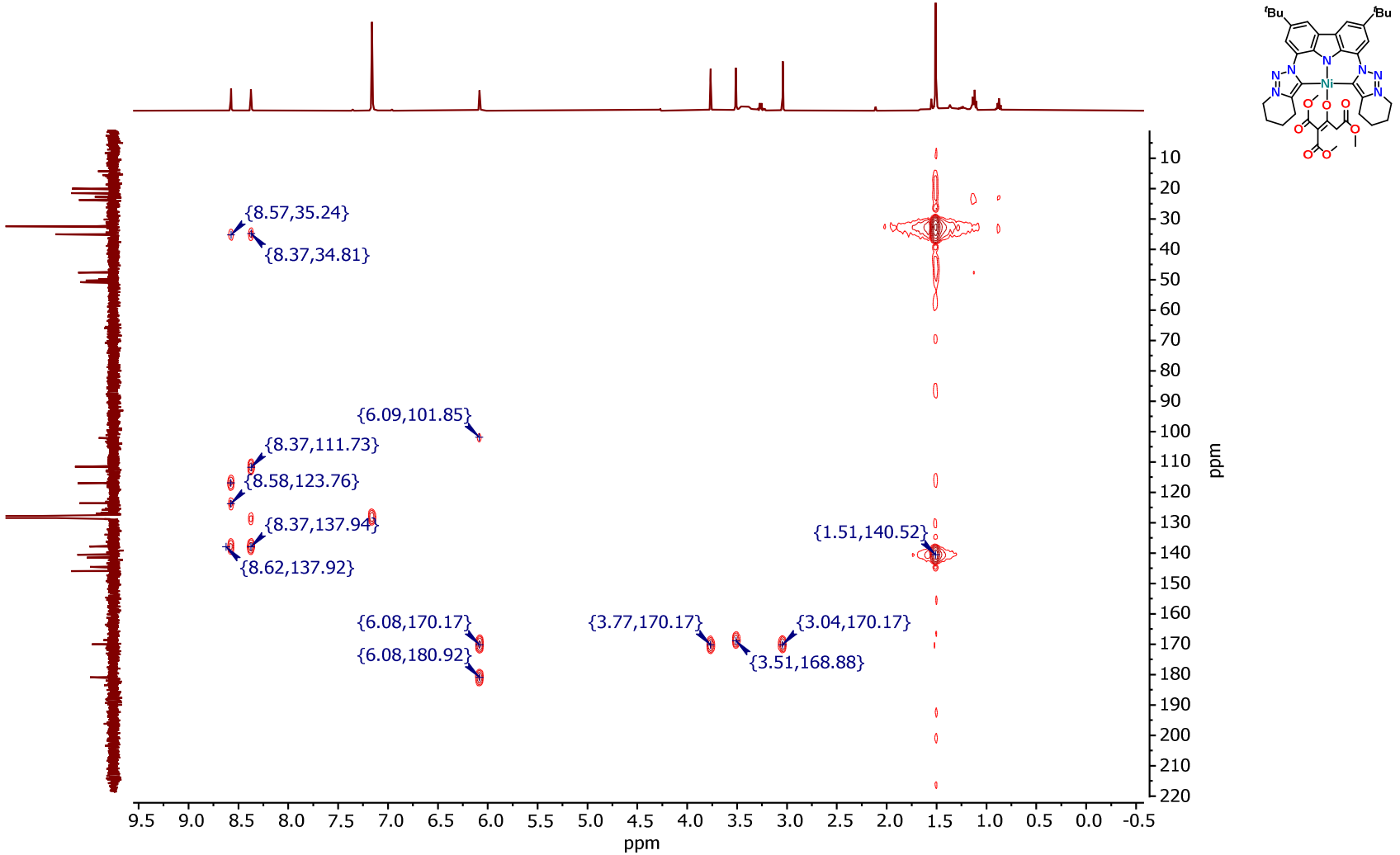


*Figure S 78: $^{1}H - ^{13}C$ HMBC of **13** in C_6D_6 at 298K.*

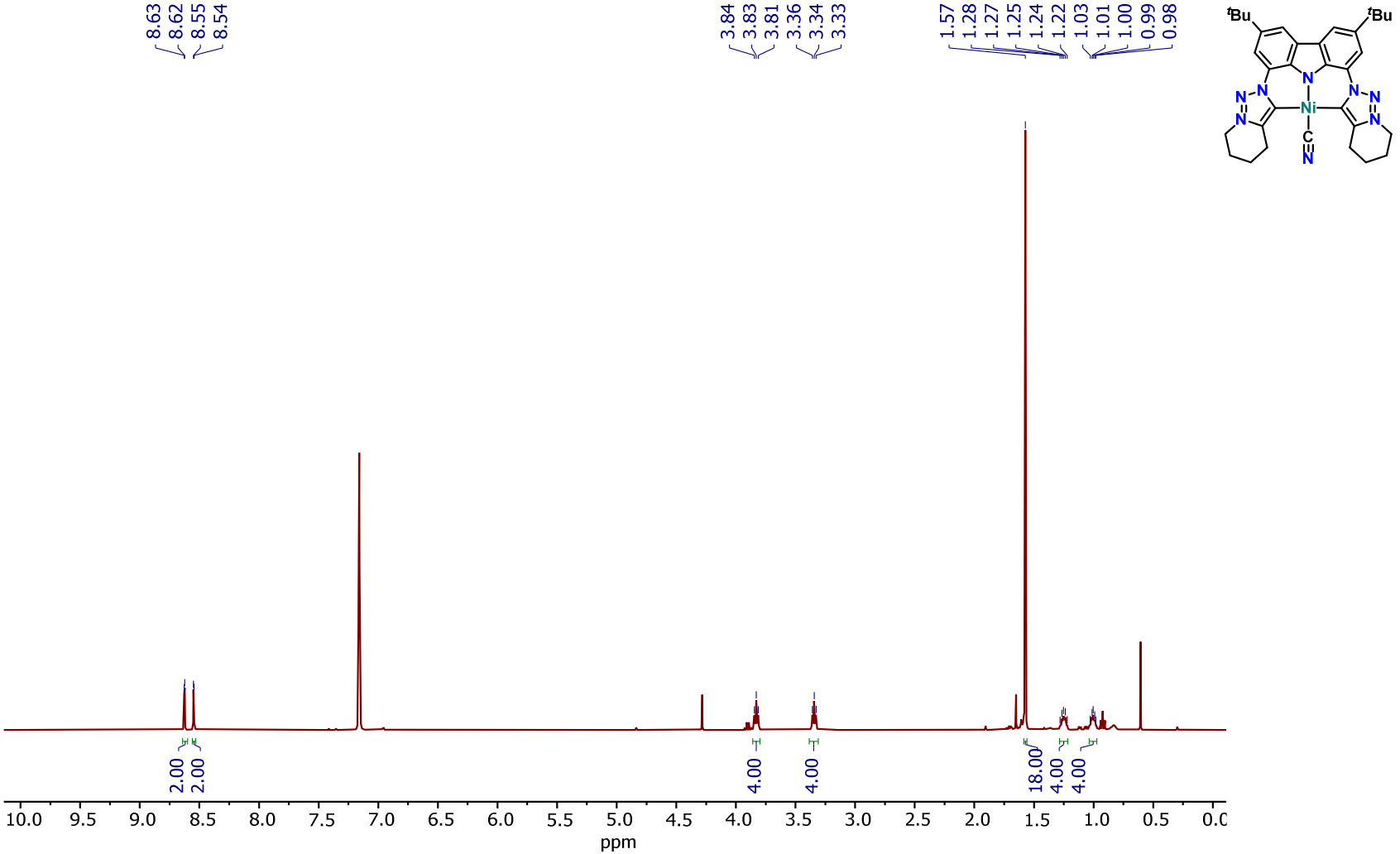


*Figure S 79: ^{1}H NMR of **14** in C_6D_6 at 298K.*

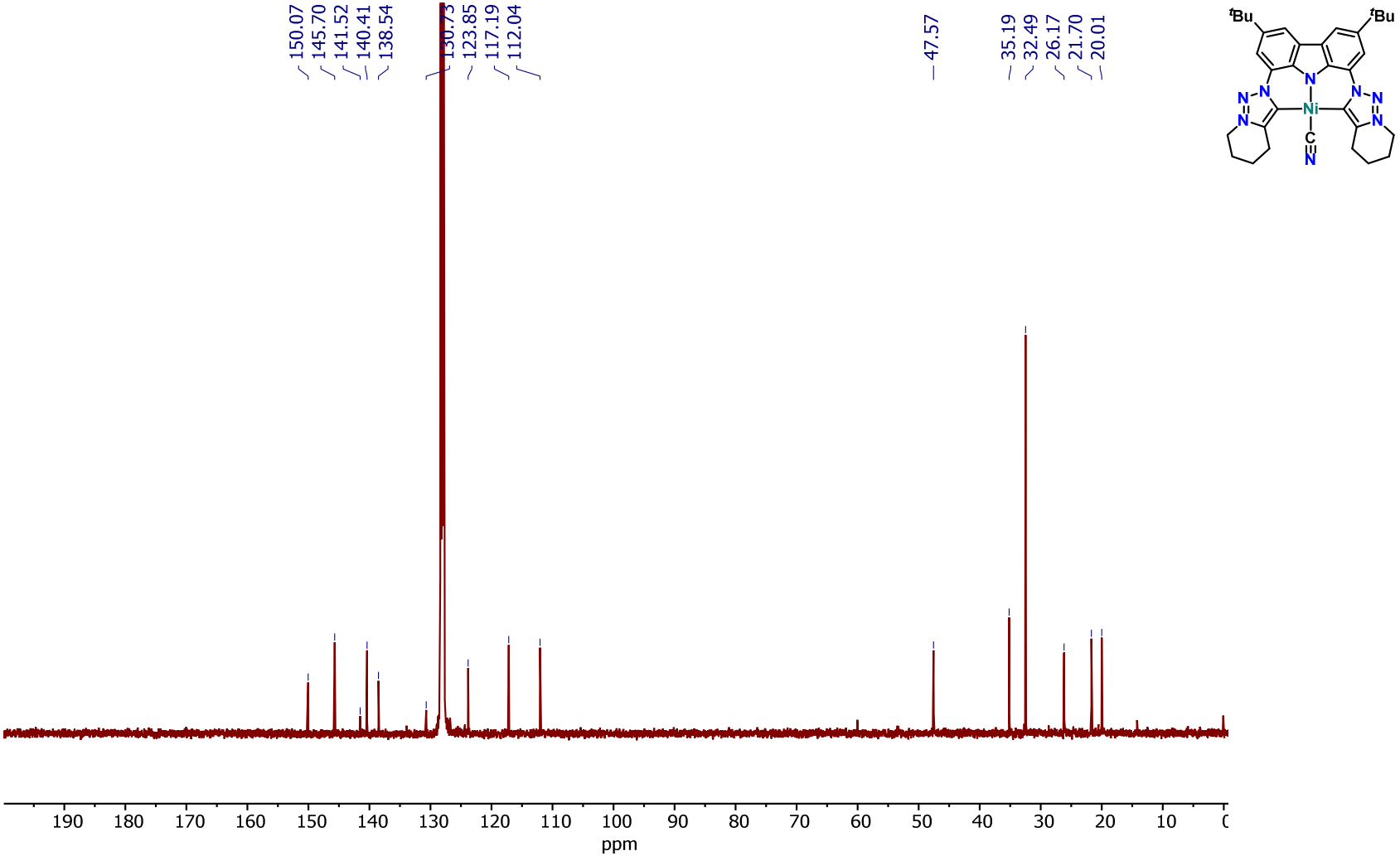


Figure S 80: ^{13}C NMR of **14** *in C_6D_6 at 298K.*

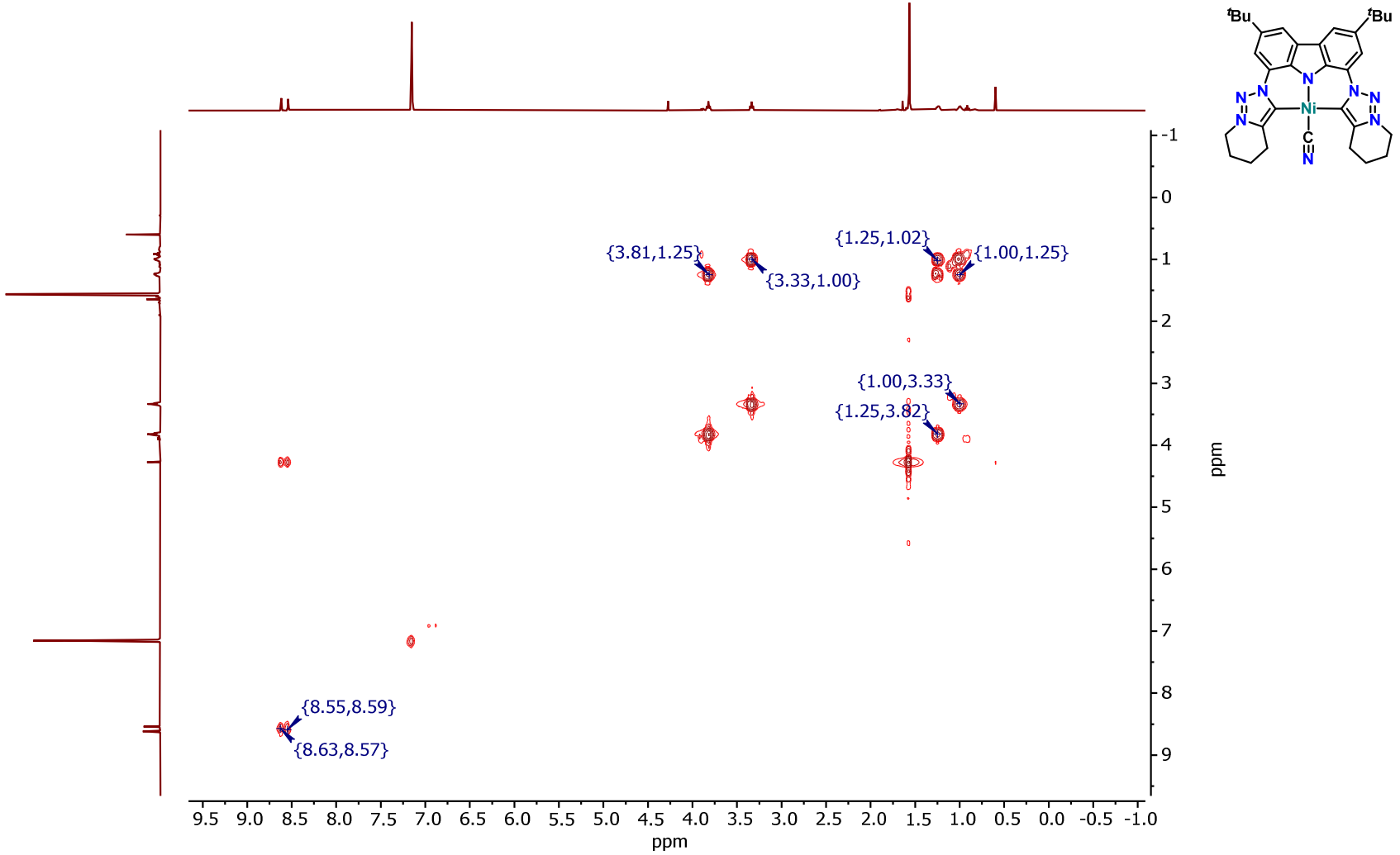


*Figure S 81: $^{1}H - {}^{1}H$ COSY of **14** in C_6D_6 at 298K.*

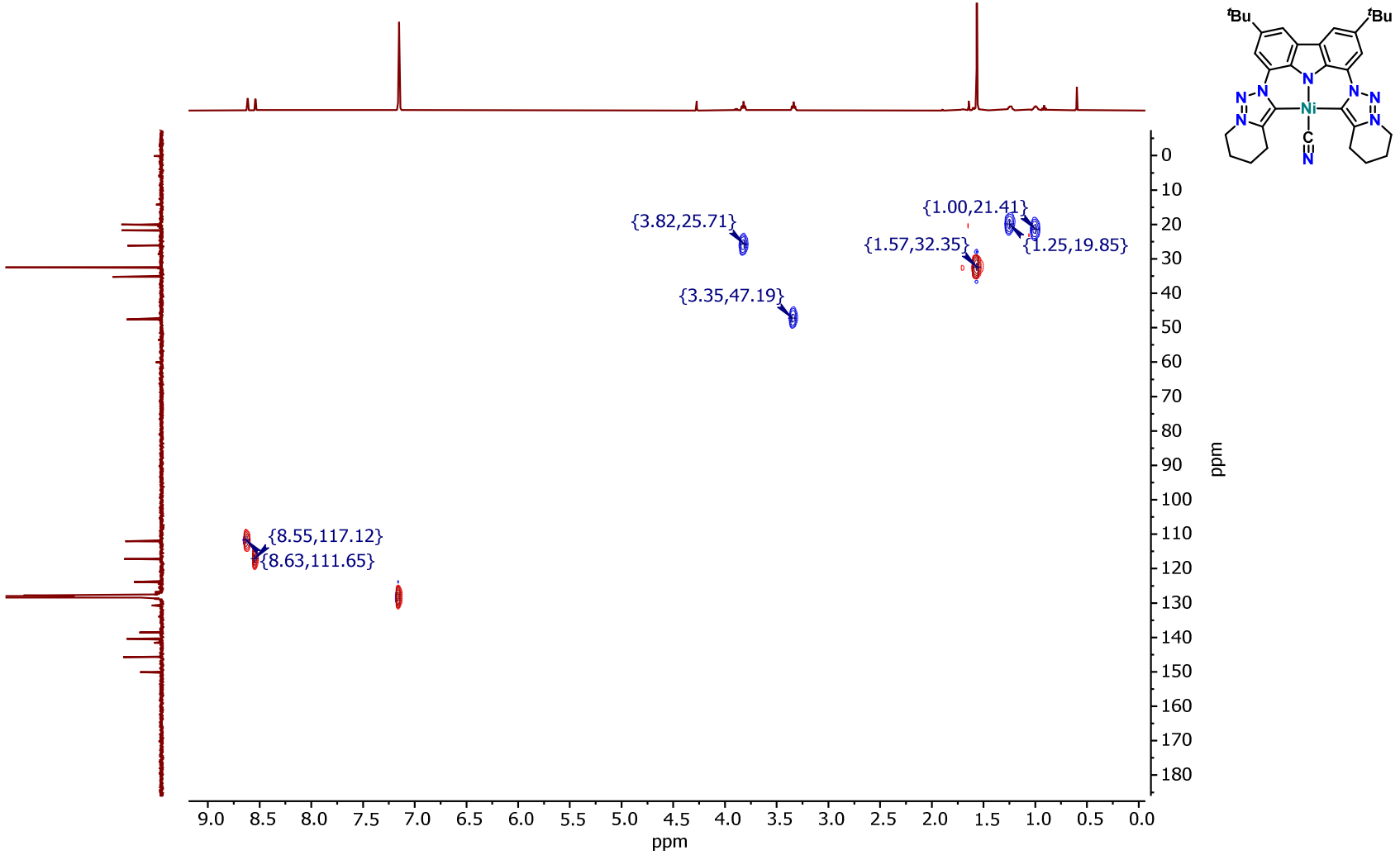


*Figure S 82: $^{1}H - ^{13}C$ HSQC of **14** in C_6D_6 at 298K.*

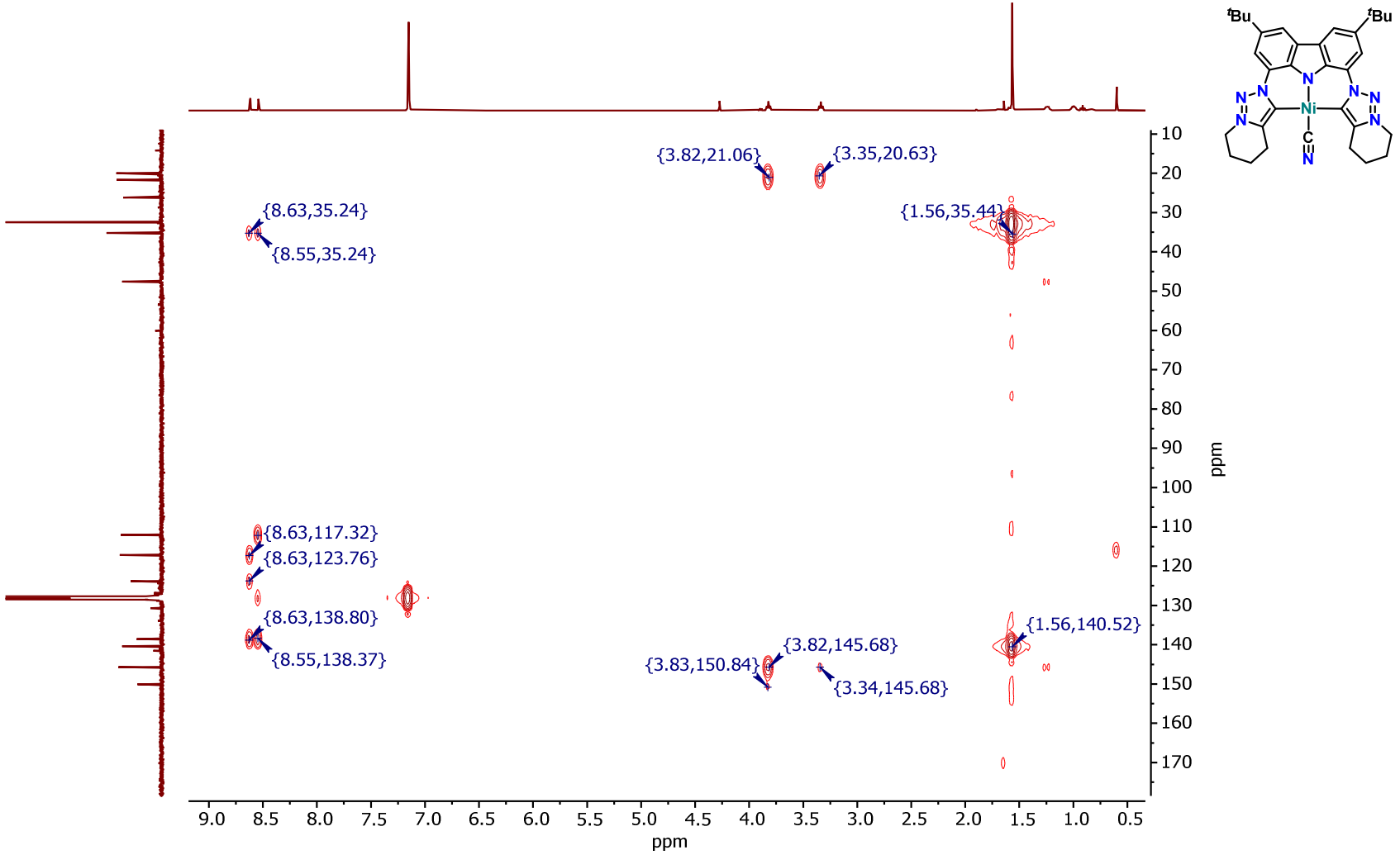


*Figure S 83: $^{1}H - ^{13}C$ HMBC of **14** in C_6D_6 at 298K.*

2. IR spectra

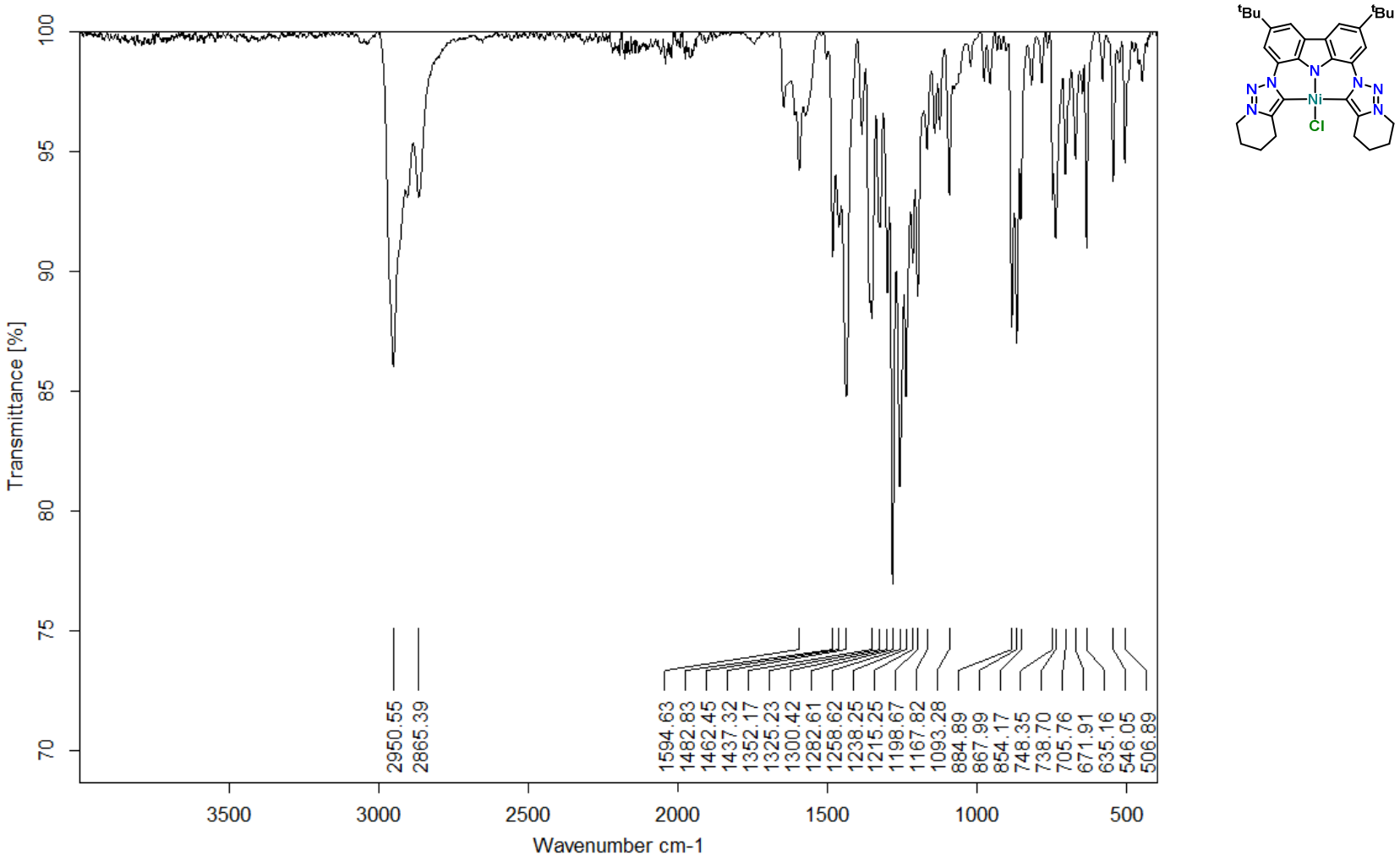


*Figure S 84: IR spectrum of **1** at 298K.*

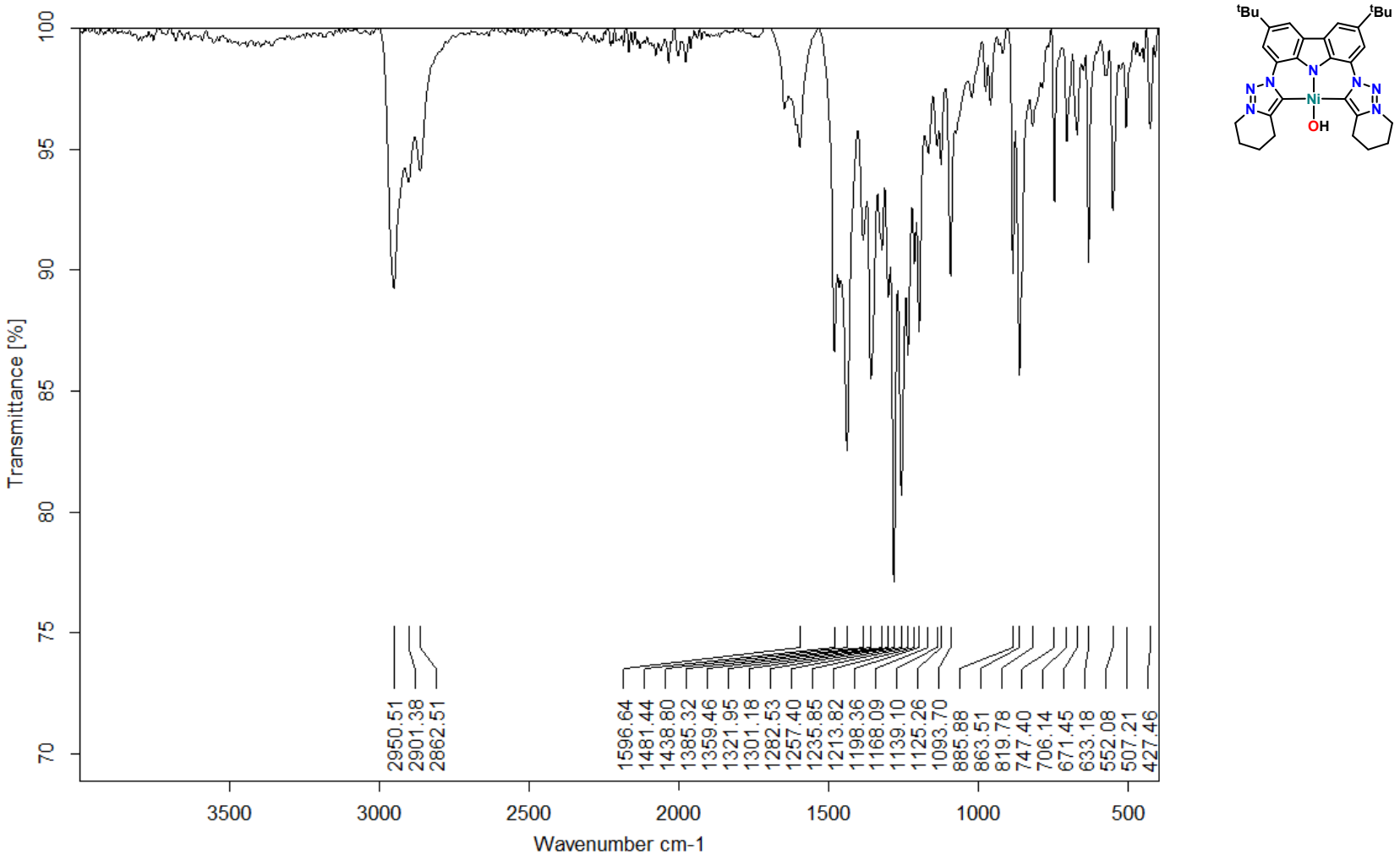


*Figure S 85: IR spectrum of **2** at 298K.*

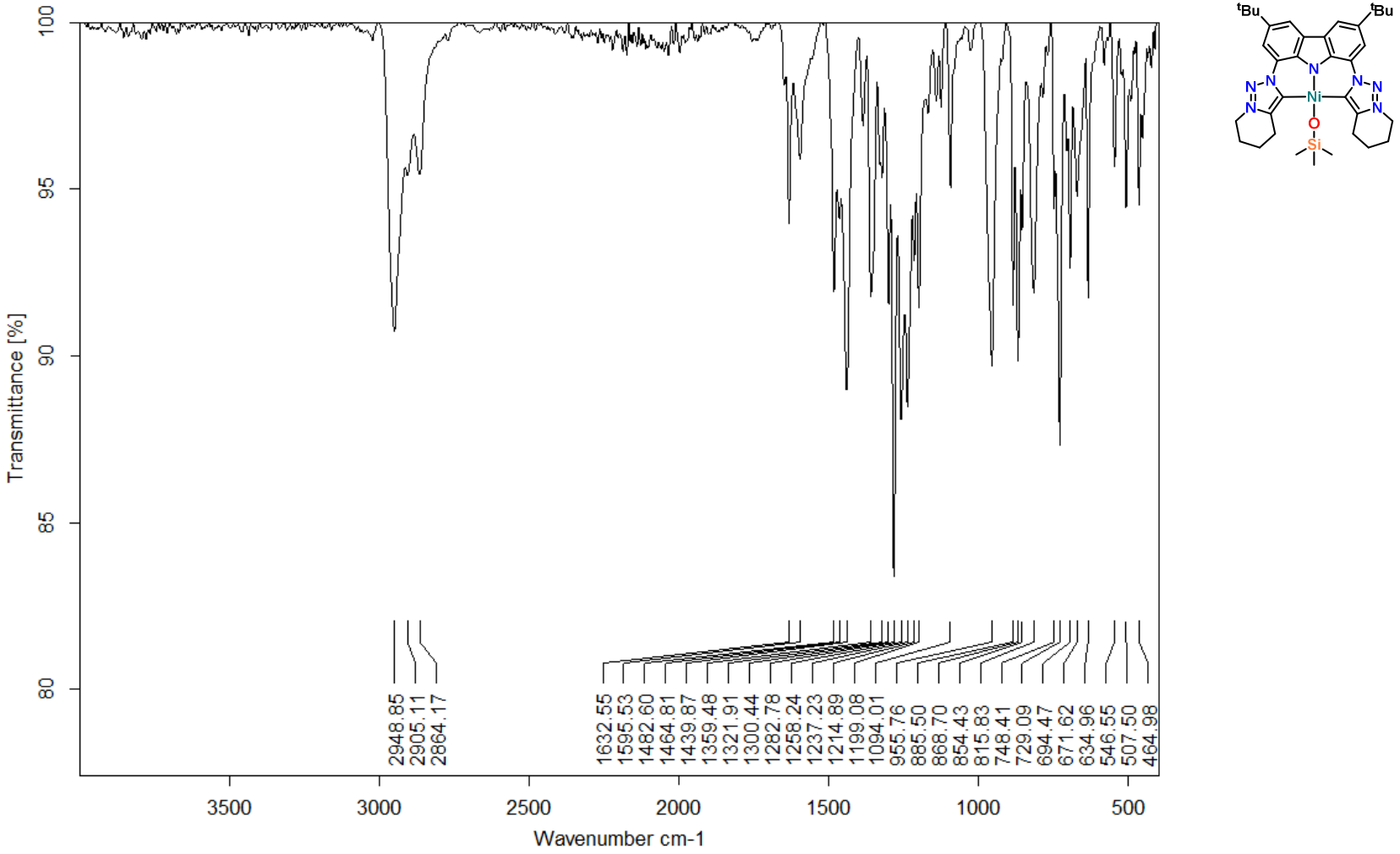


*Figure S 86: IR spectrum of **3** at 298K.*

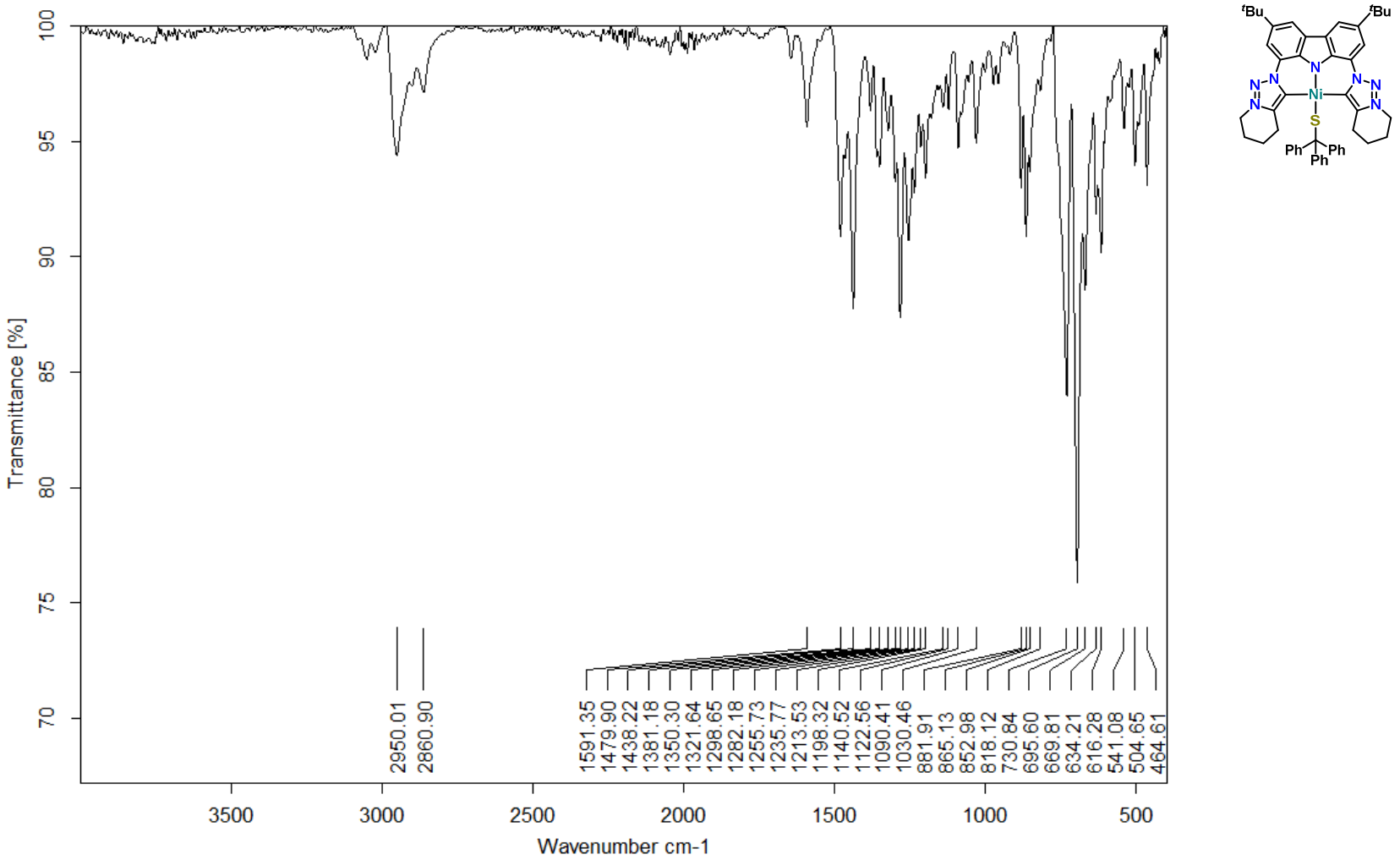


*Figure S 87: IR spectrum of **4** at 298K.*

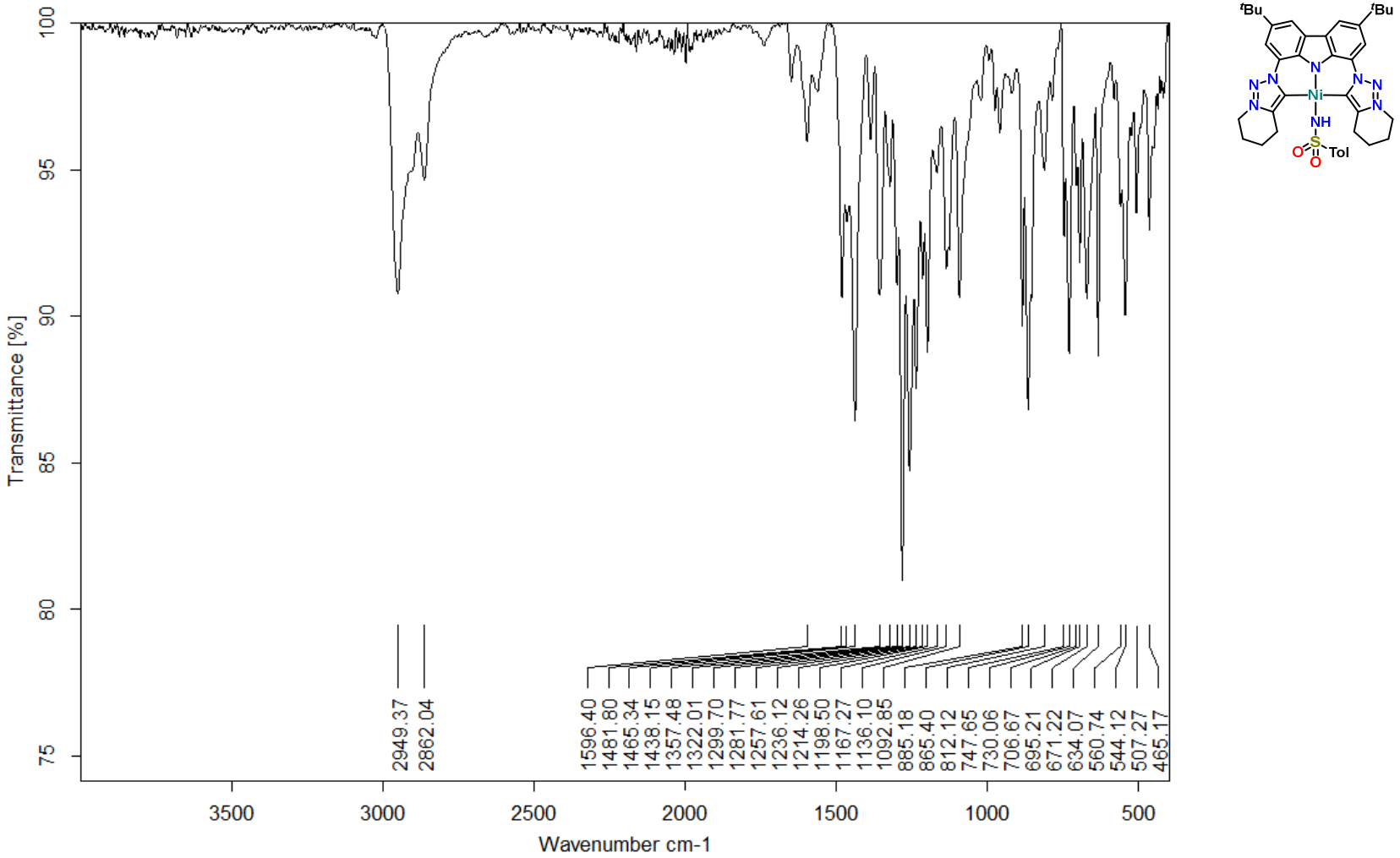


*Figure S 88: IR spectrum of **5** at 298K.*

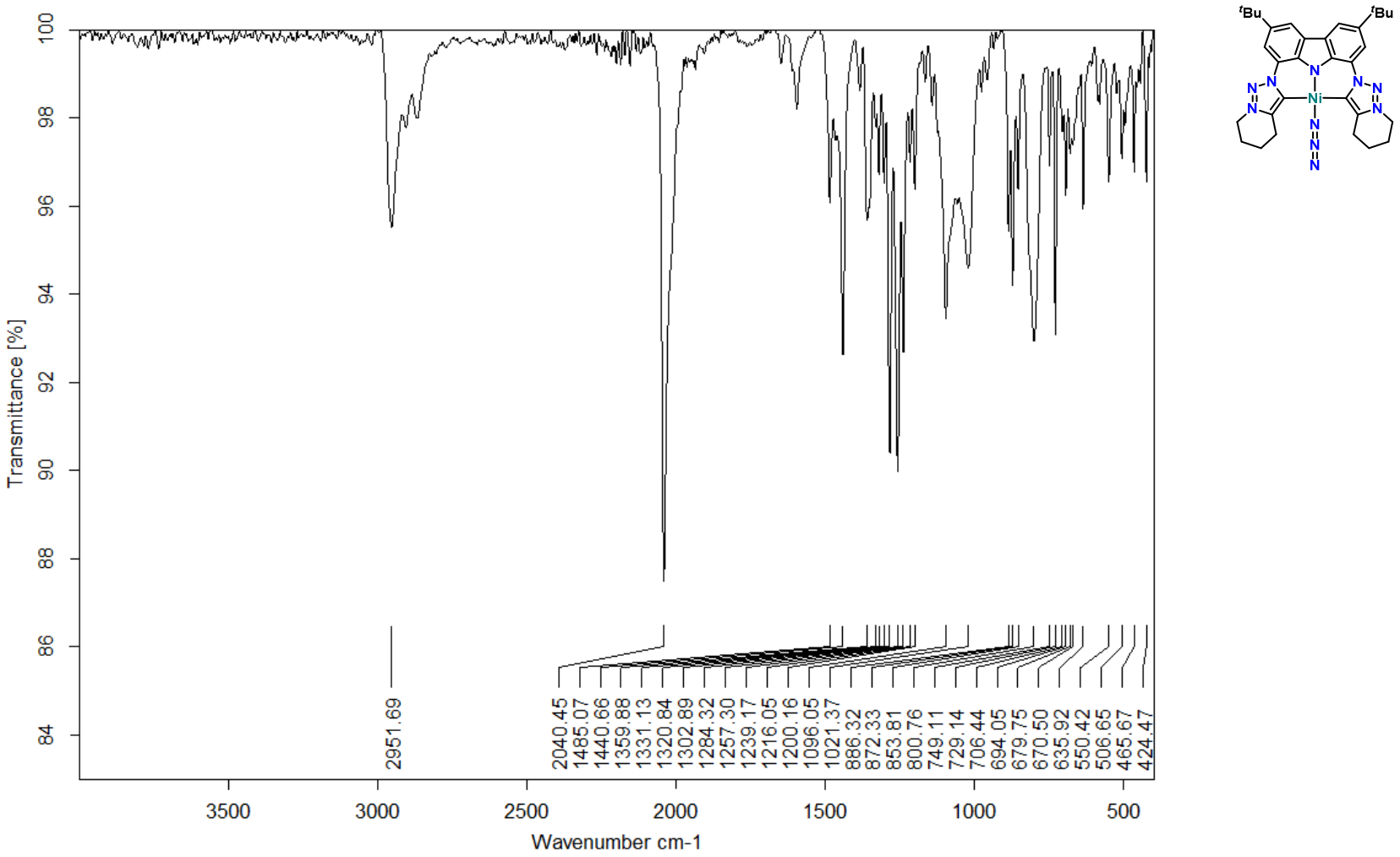


*Figure S 89: IR spectrum of **6** at 298K.*

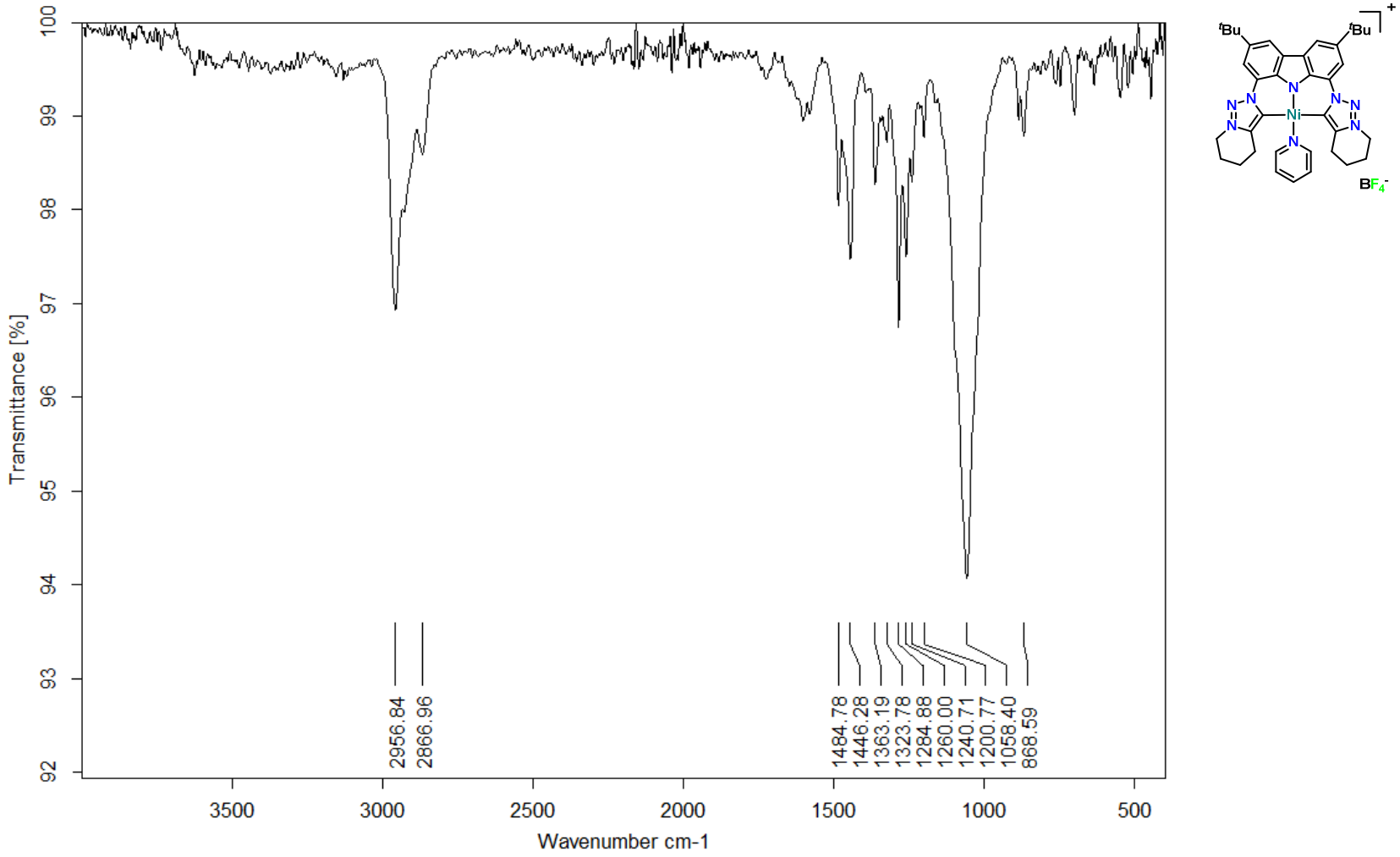


*Figure S 90: IR spectrum of **7** at 298K.*

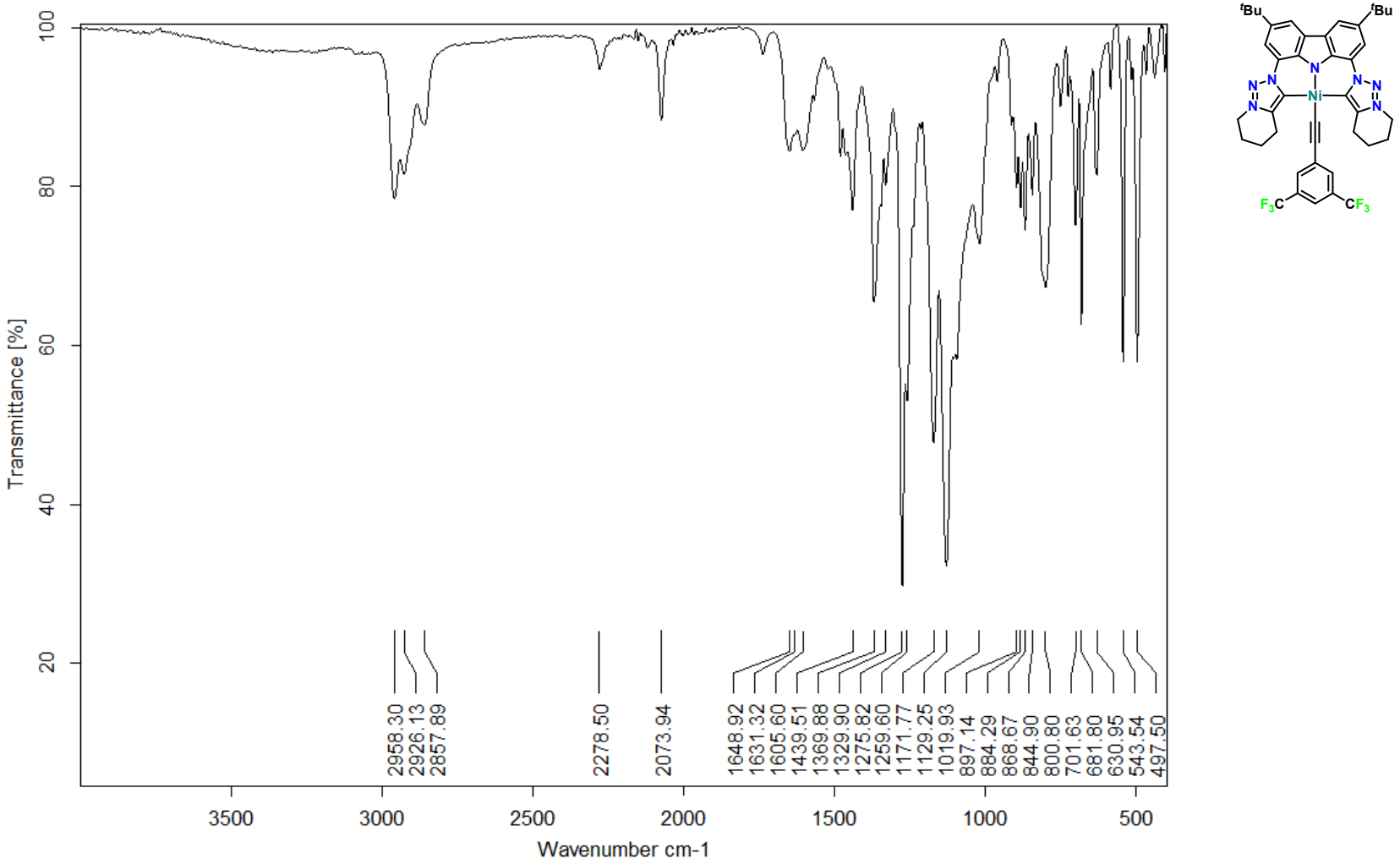


*Figure S 91: IR spectrum of **8** at 298K.*

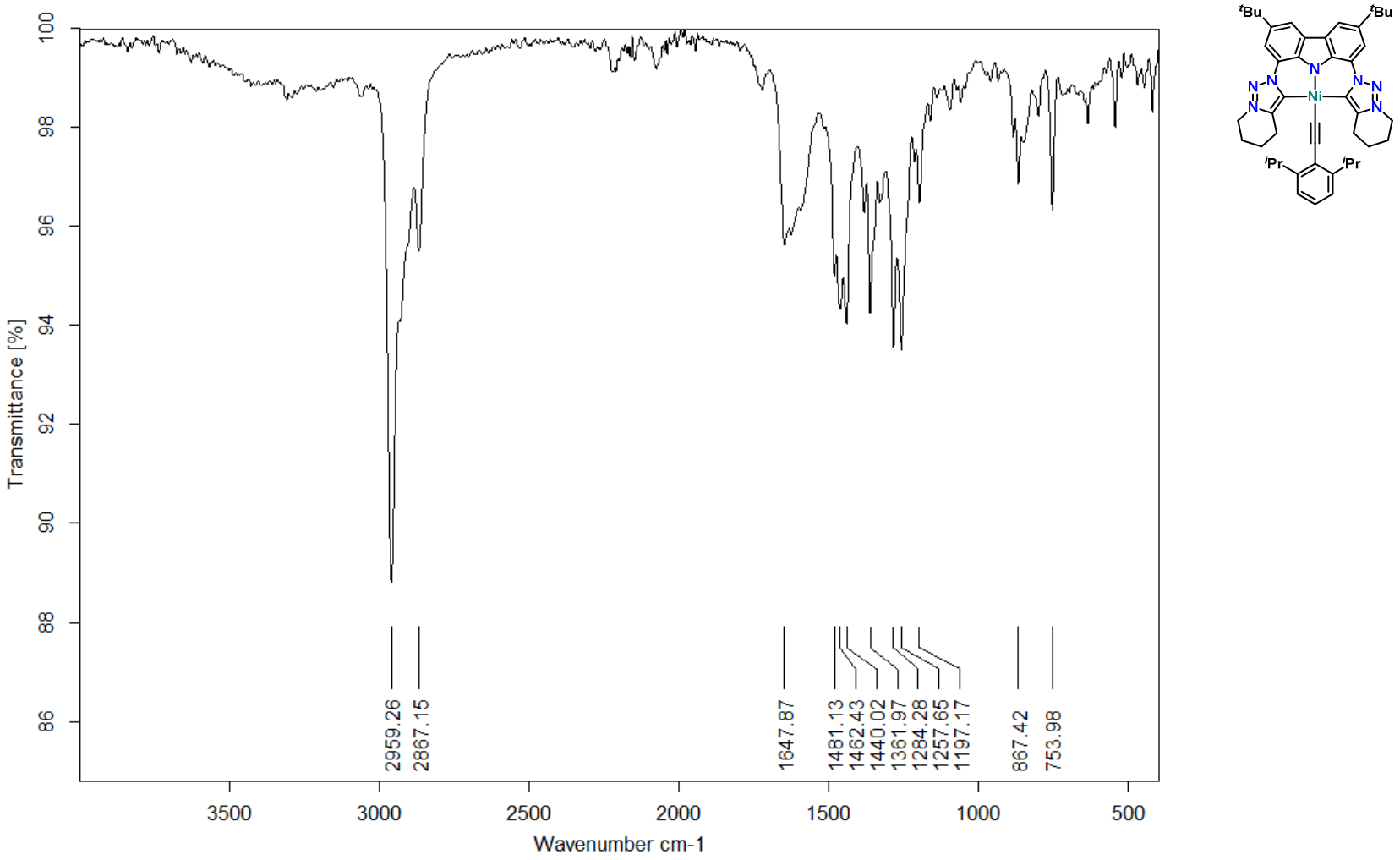


*Figure S 92: IR spectrum of **9** at 298K.*

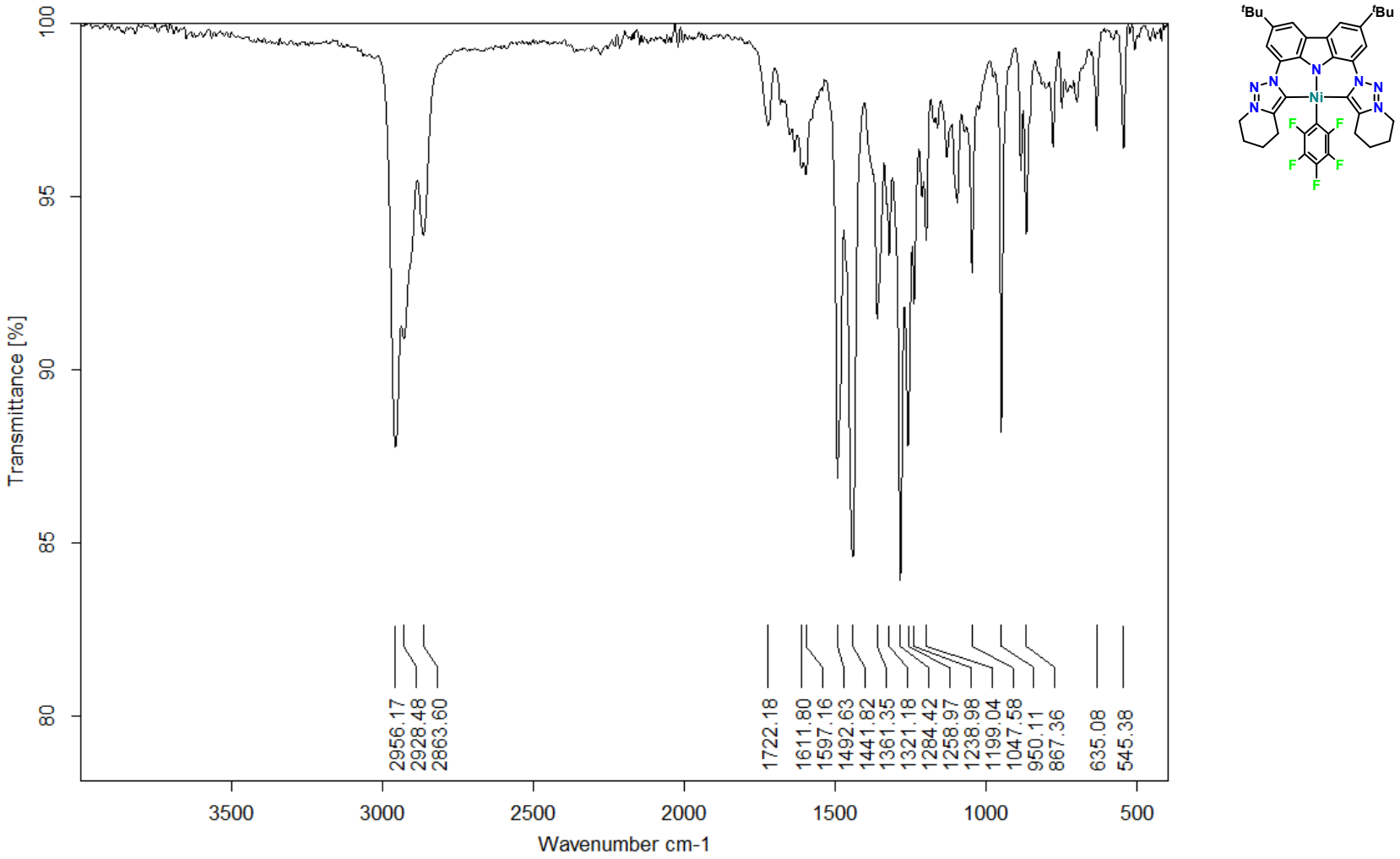


*Figure S 93: IR spectrum of **10** at 298K.*

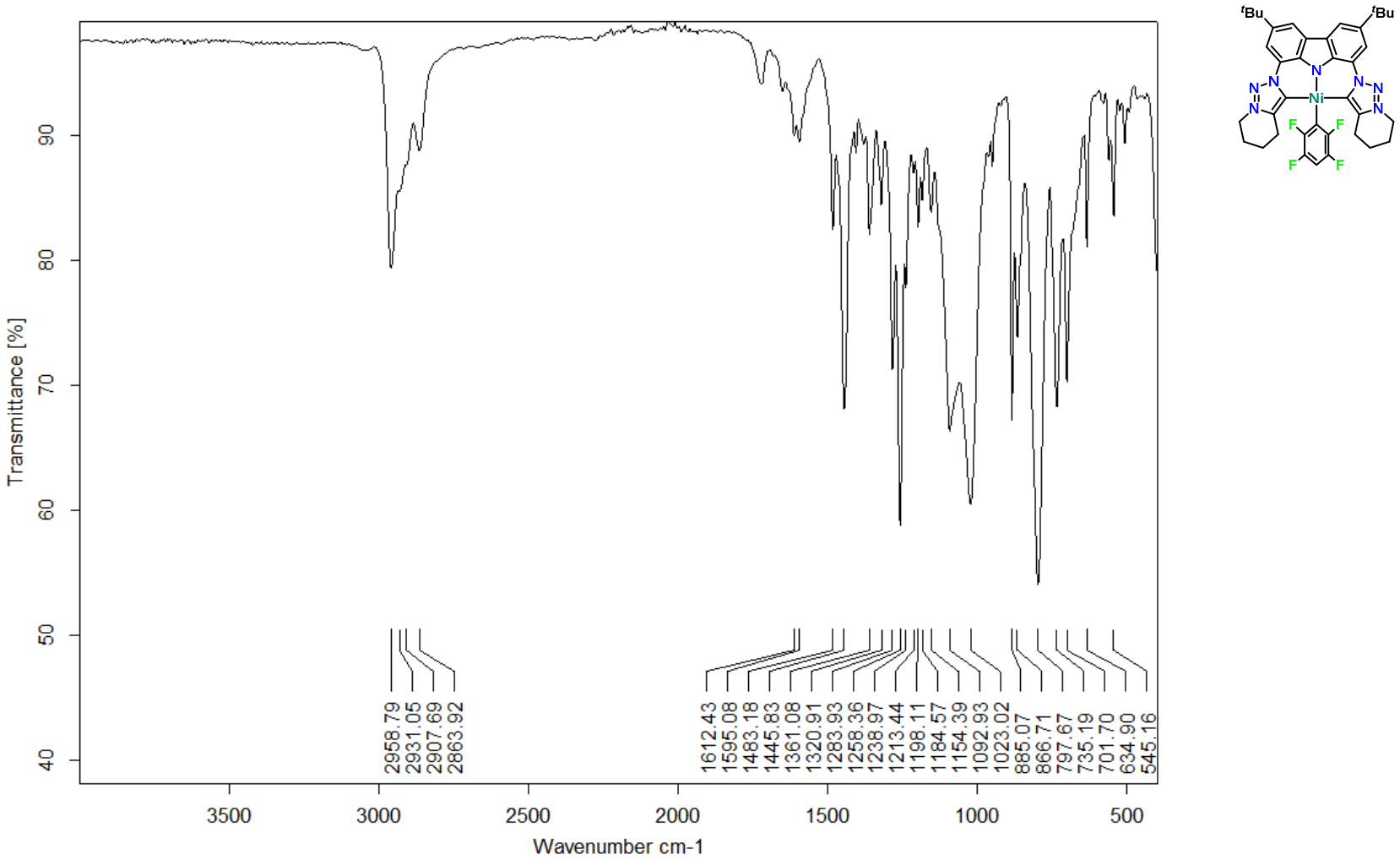


*Figure S 94: IR spectrum of **11** at 298K.*

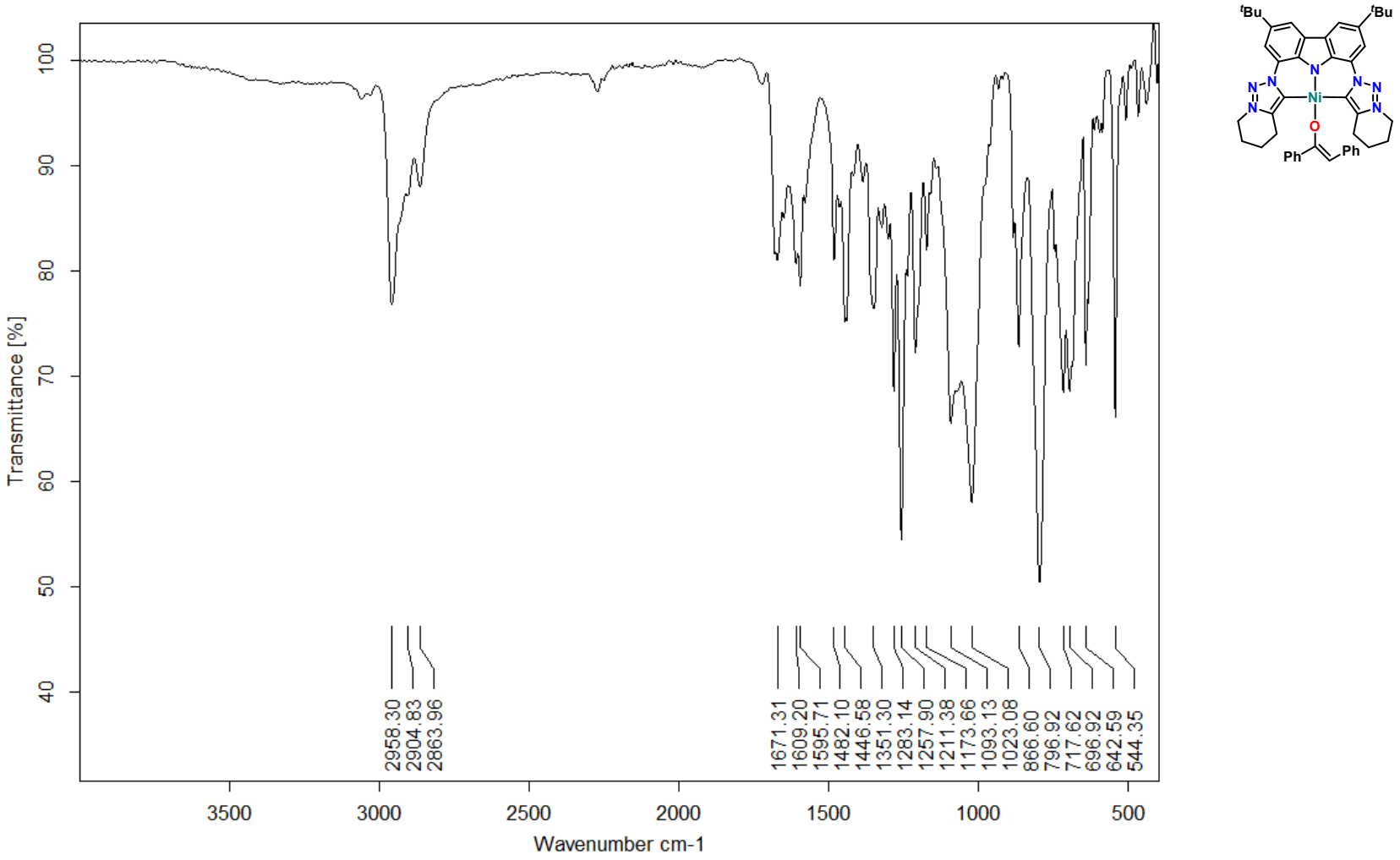


*Figure S 95: IR spectrum of **12** at 298K.*

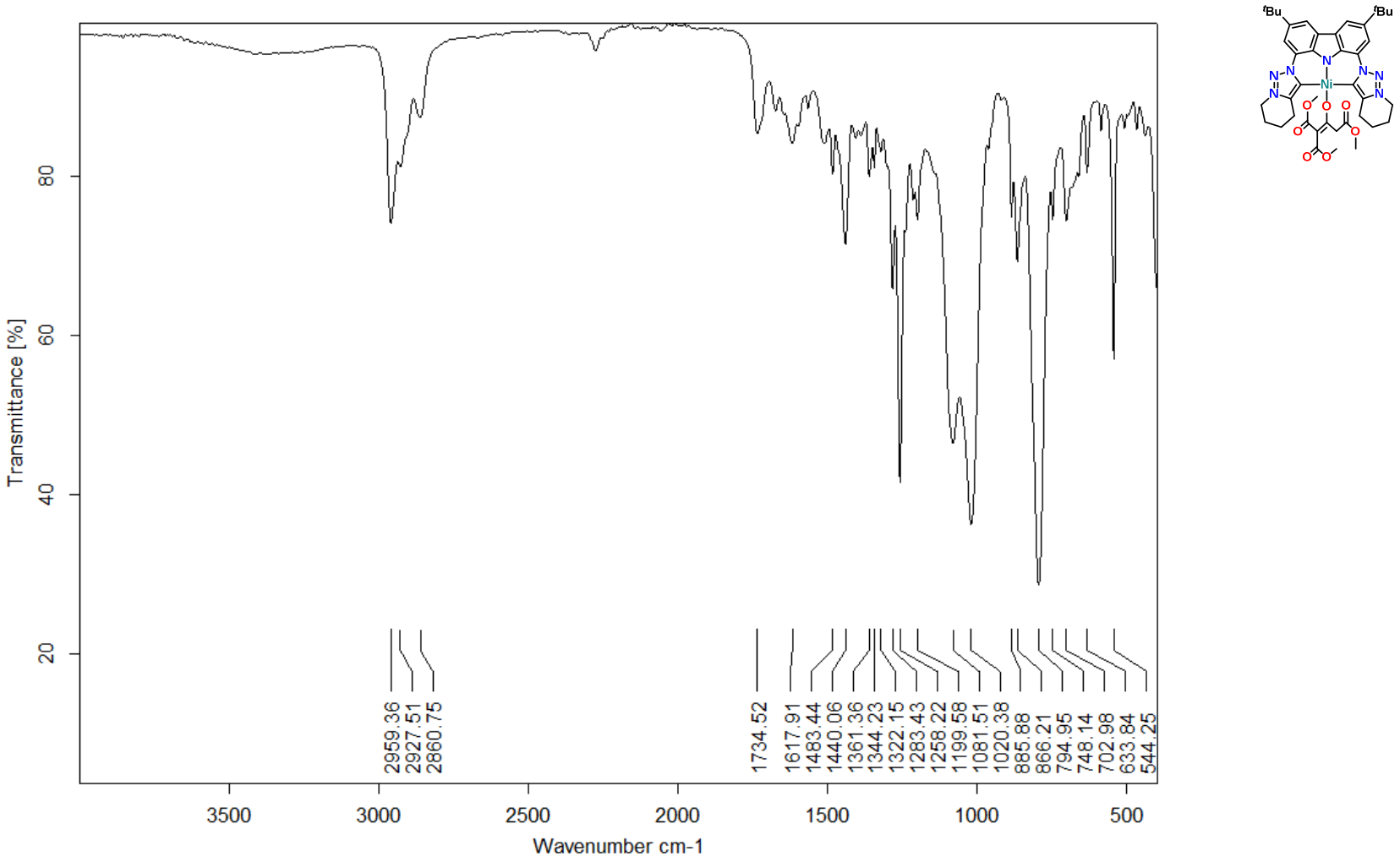


*Figure S 96: IR spectrum of **13** at 298K.*

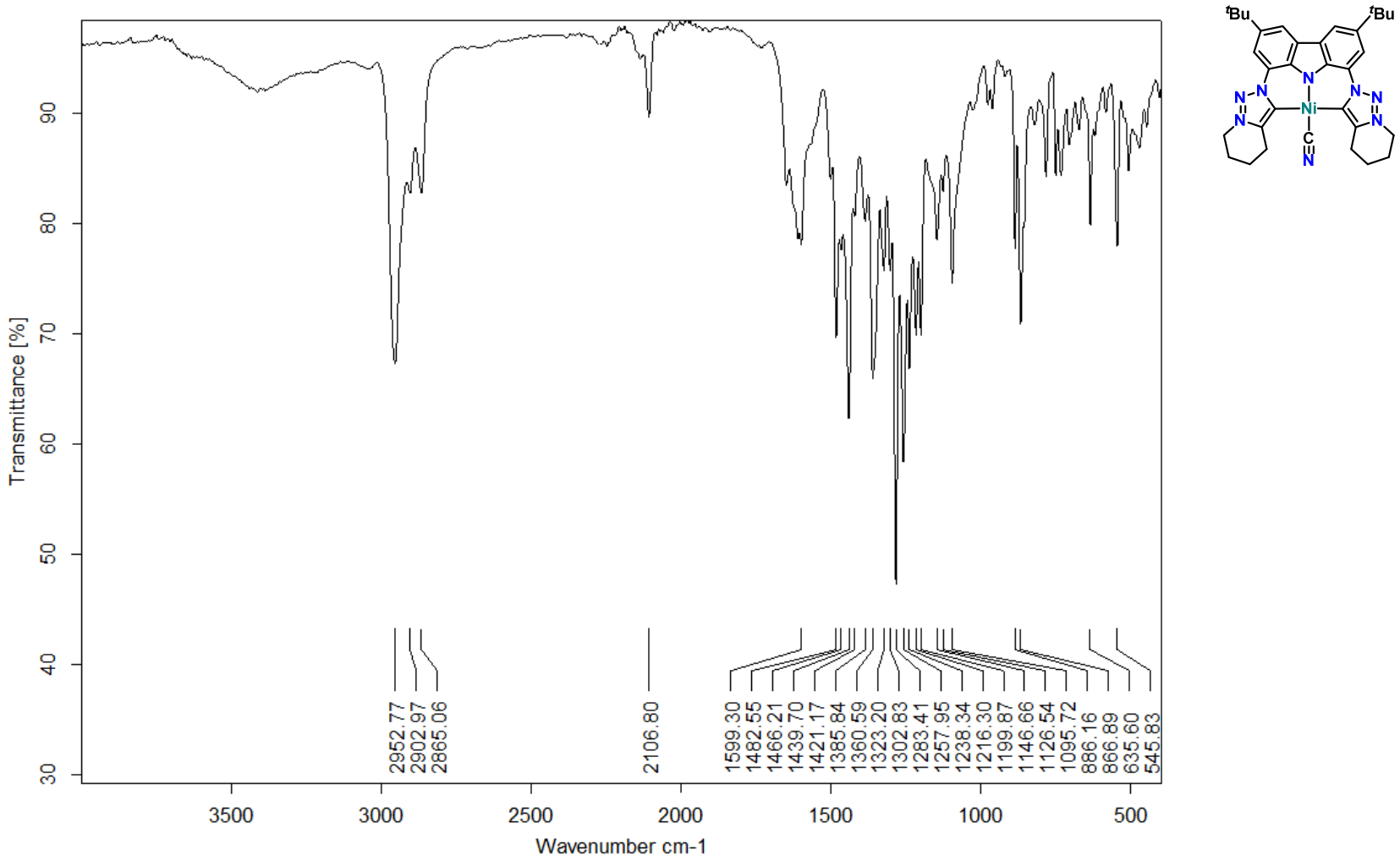


*Figure S 97: IR spectrum of **14** at 298K.*

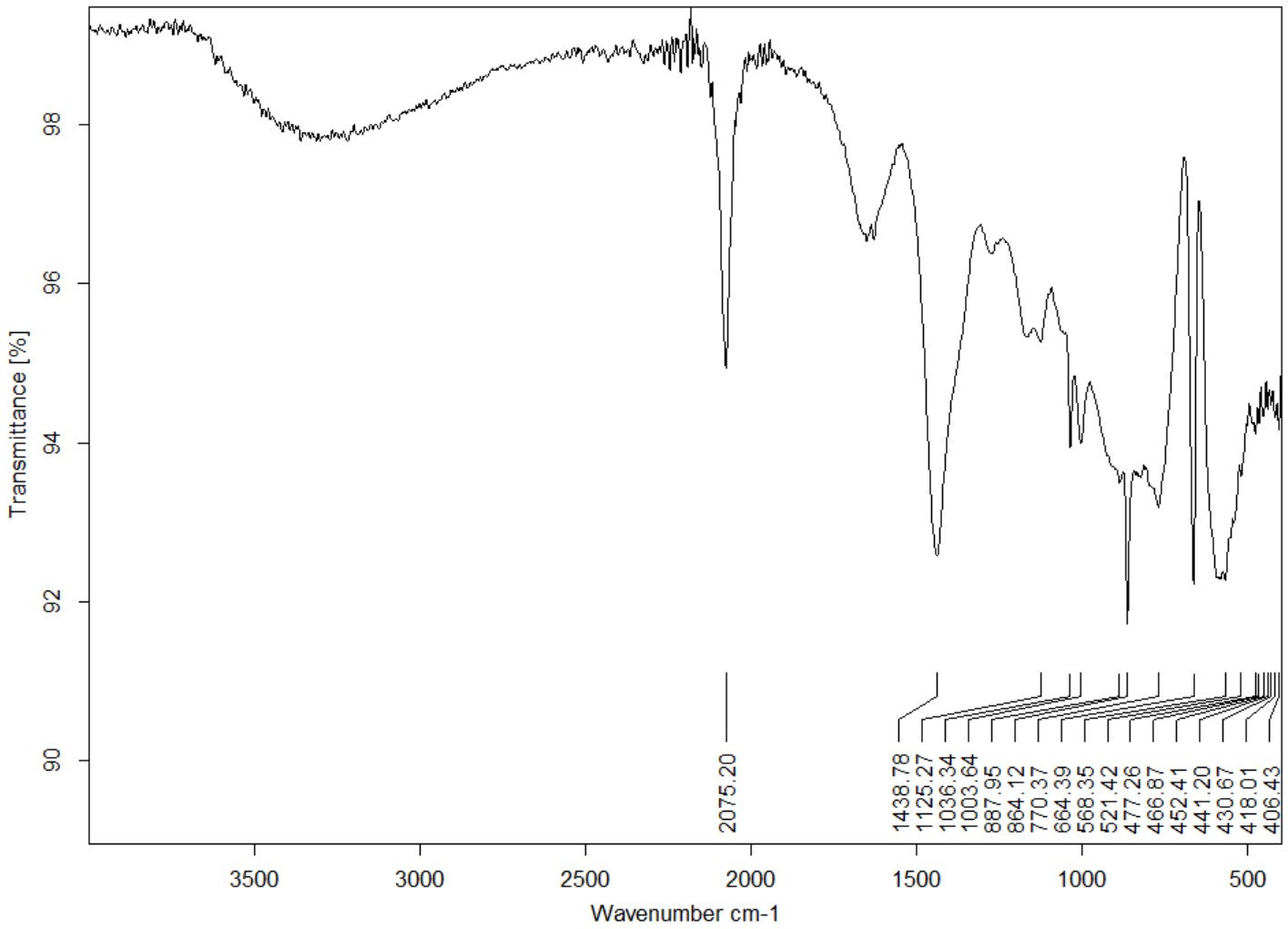
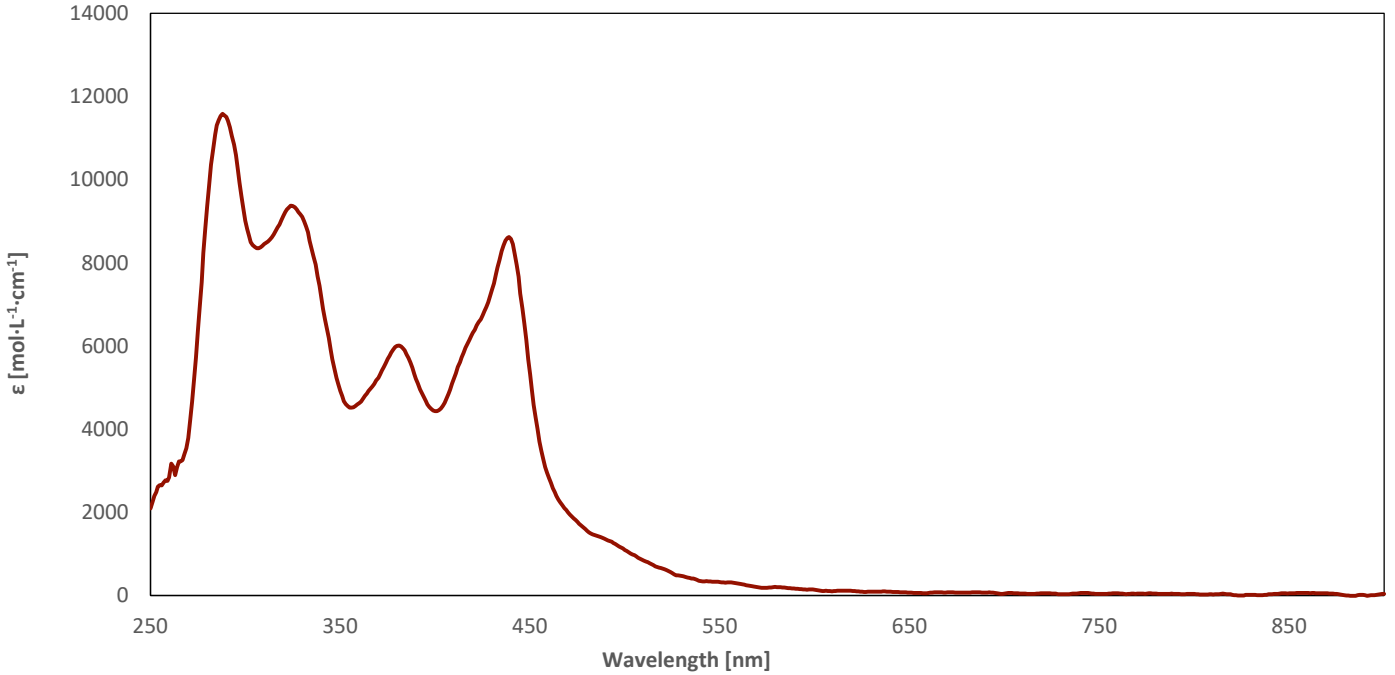


Figure S 98: ATR-IR spectra of solid KCN at 298 K.

3. UV-VIS spectra



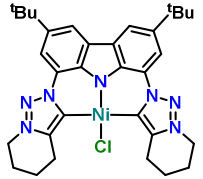


*Figure S 99: UV-VIS spectrum of **1** at 298K.*

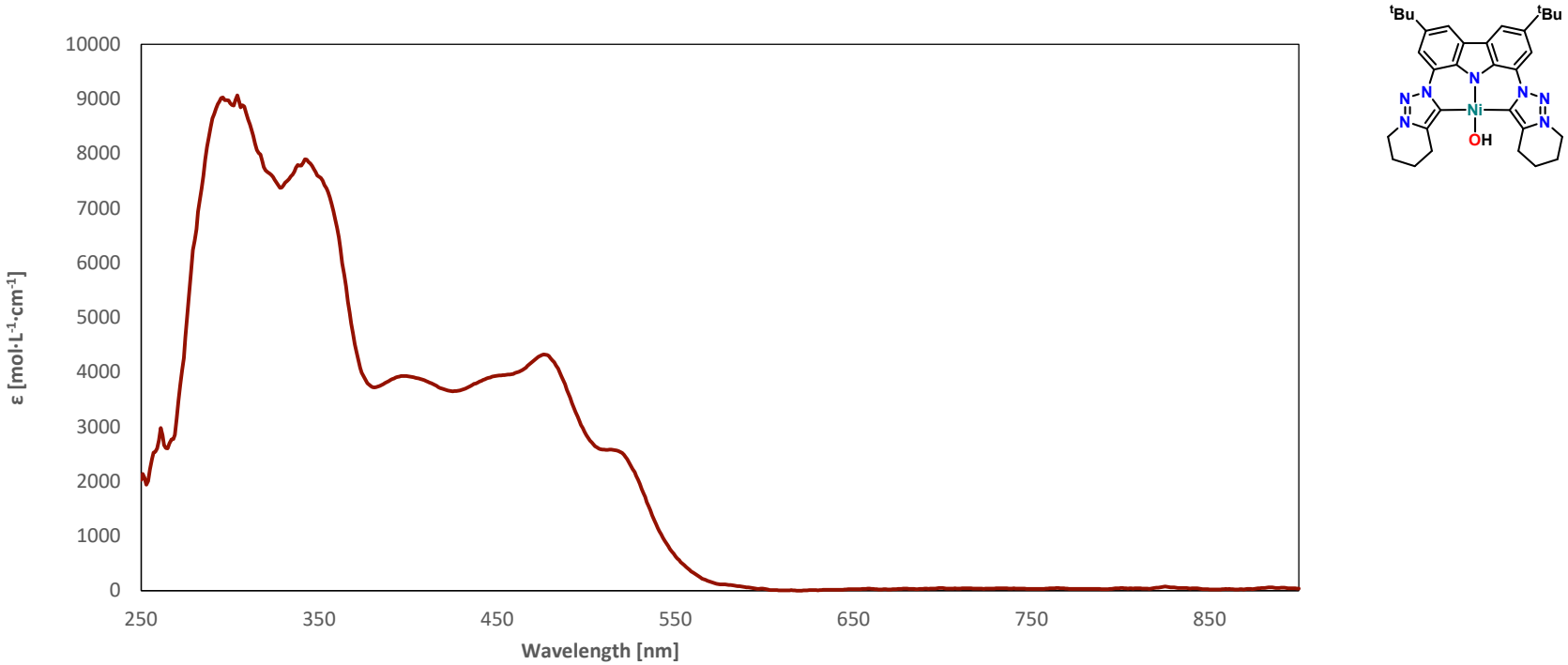


*Figure S 100: UV-VIS spectrum of **2** at 298K.*

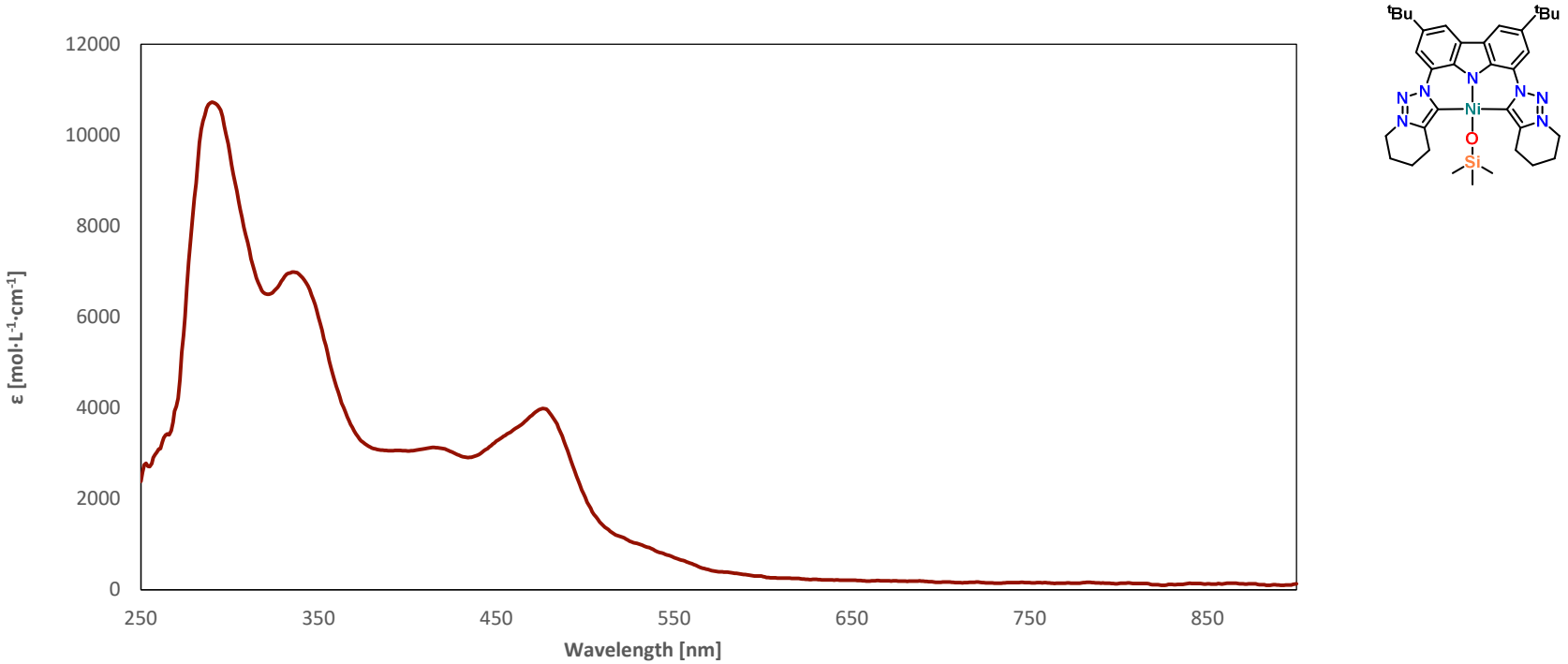
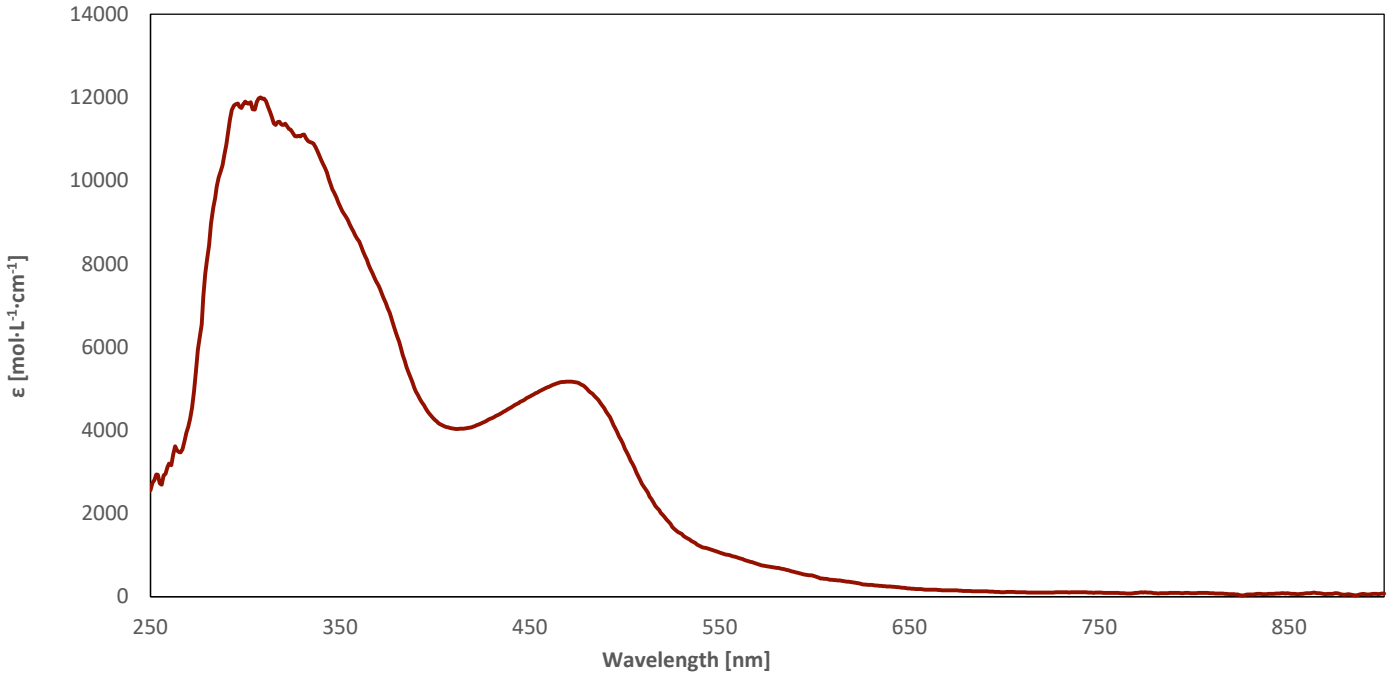


*Figure S 101: UV-VIS spectrum of **3** at 298K.*



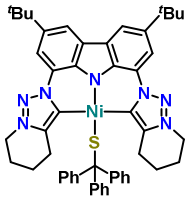


*Figure S 102: UV-VIS spectrum of **4** at 298K.*

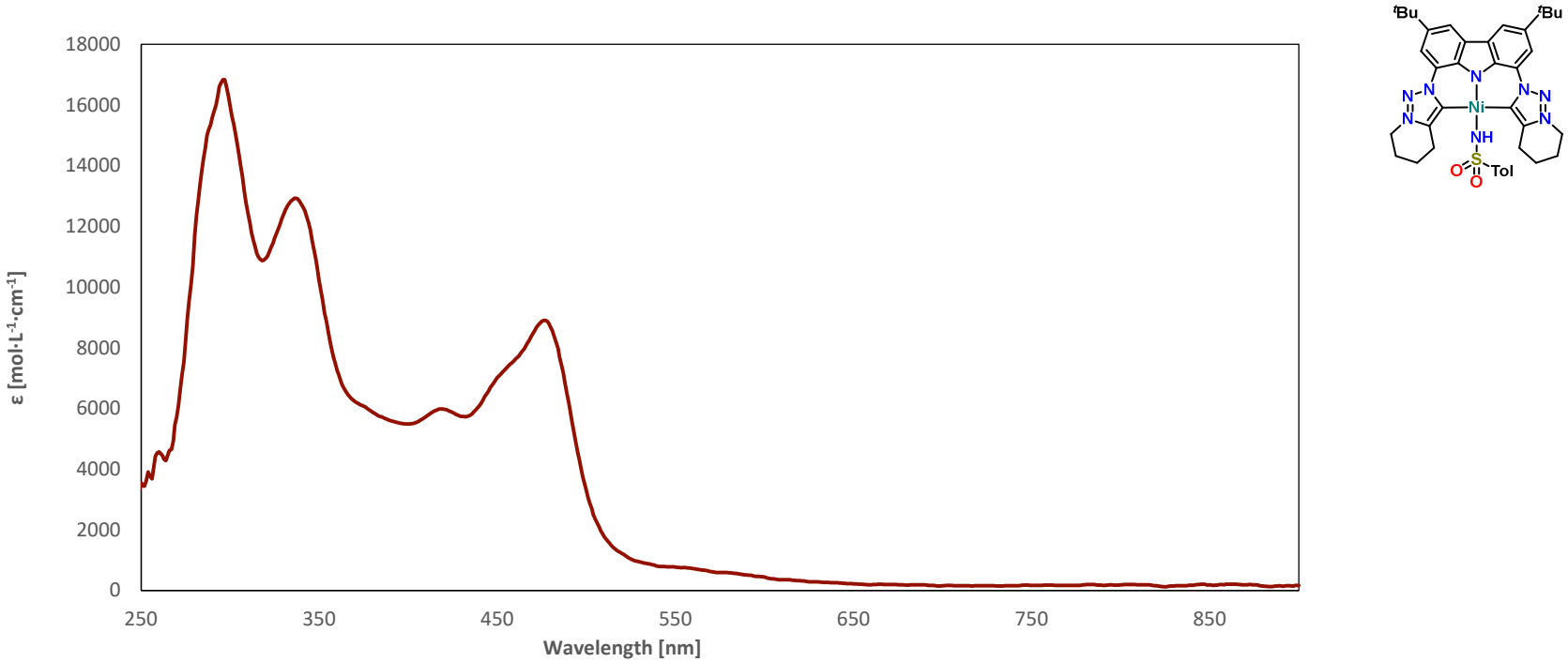


*Figure S 103: UV-VIS spectrum of **5** at 298K.*

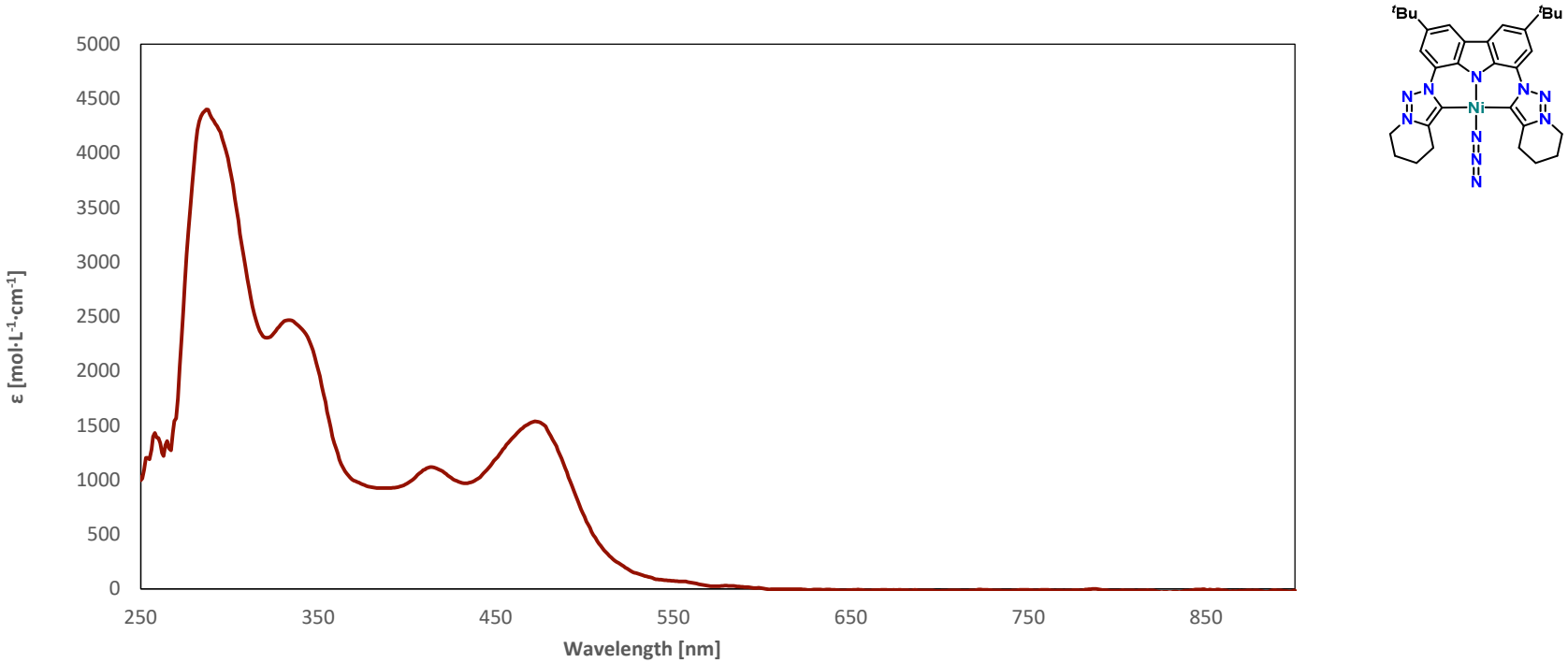


*Figure S 104: UV-VIS spectrum of **6** at 298K.*

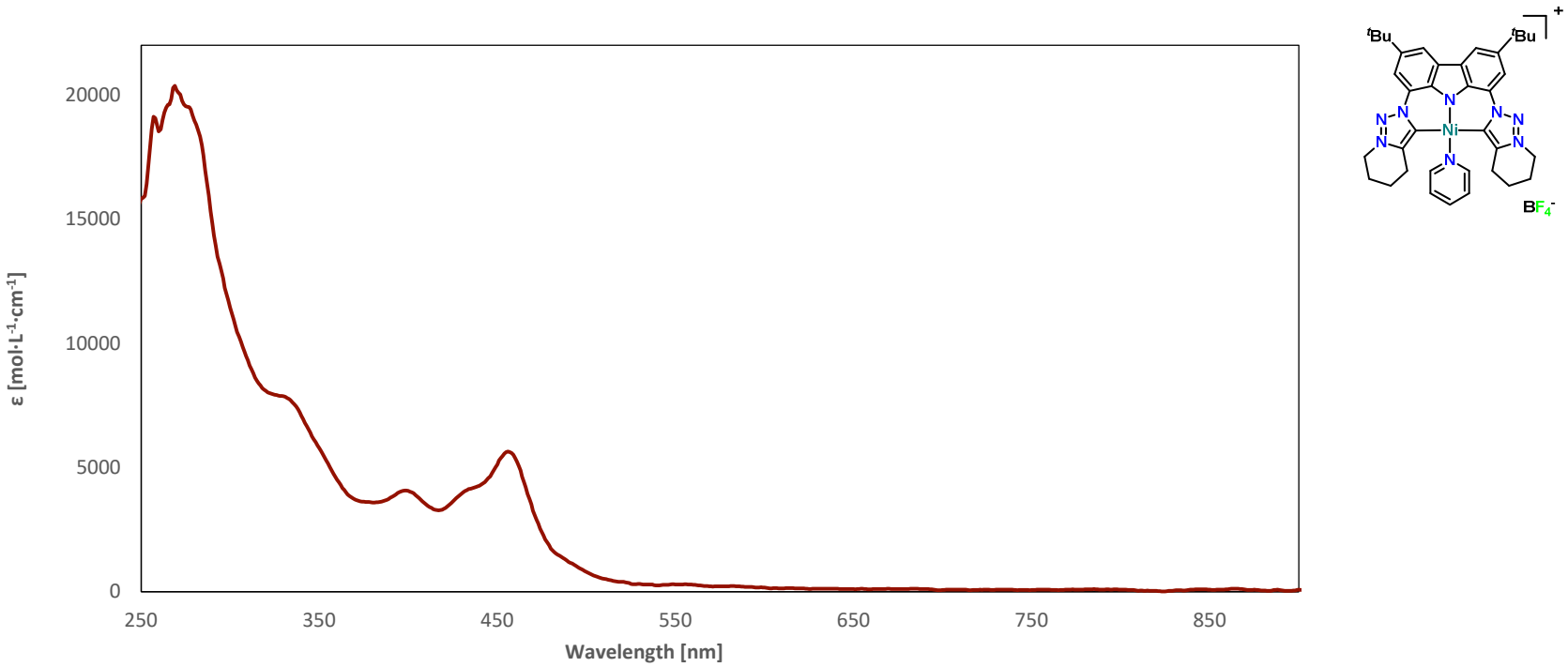


*Figure S 105: UV-VIS spectrum of **7** at 298K.*

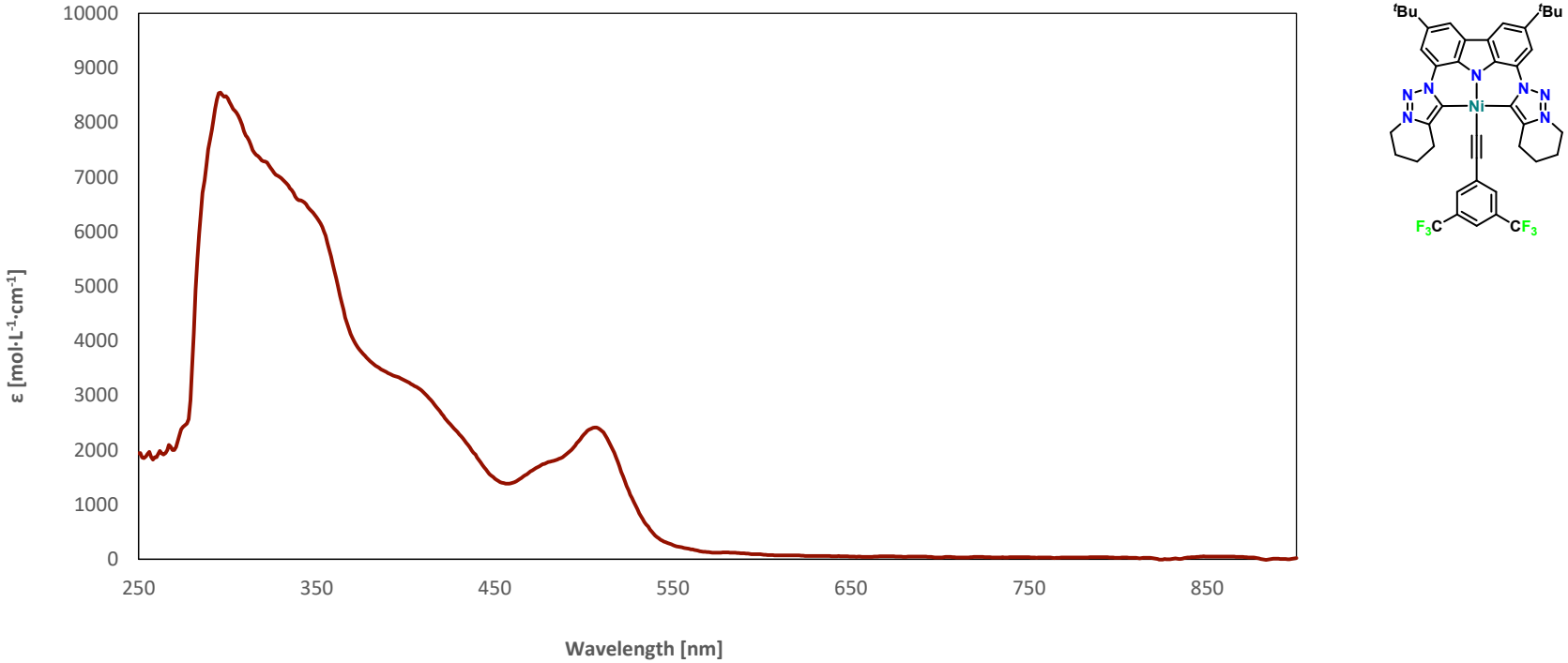
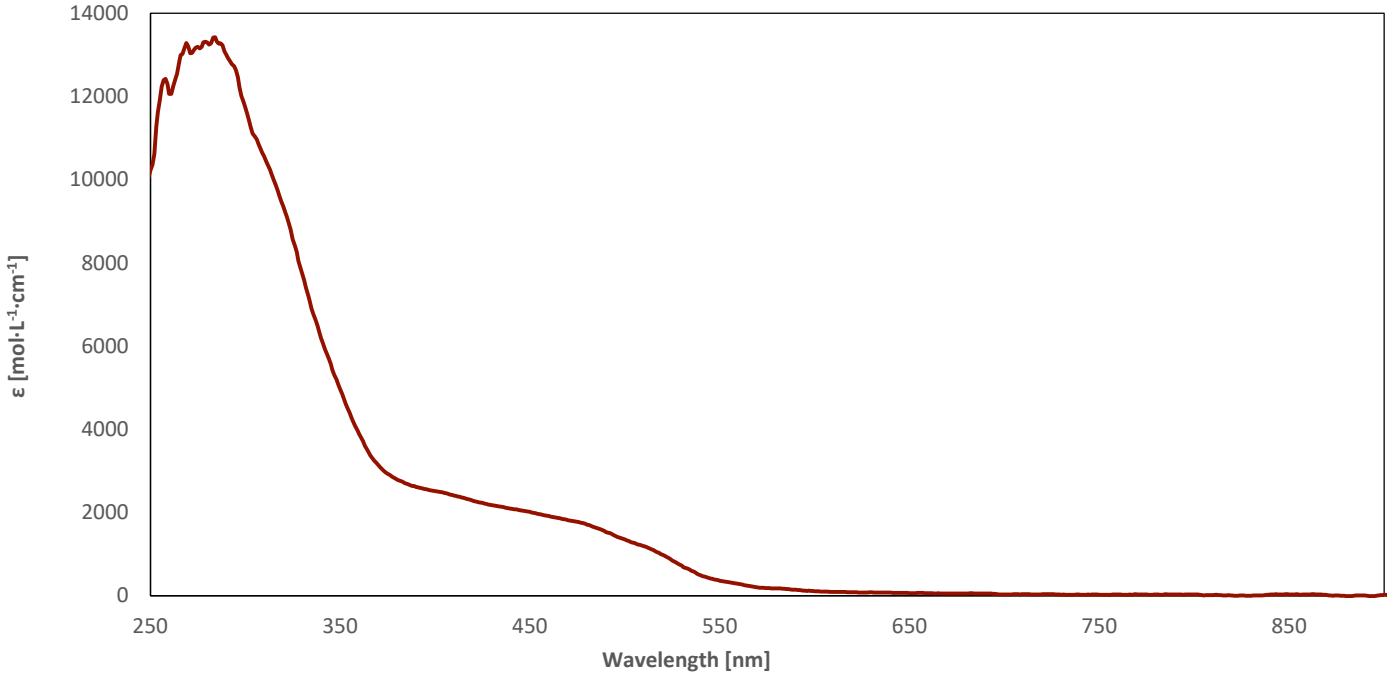


*Figure S 106: UV-VIS spectrum of **8** at 298K.*



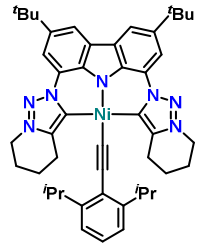


*Figure S 107: UV-VIS spectrum of **9** at 298K.*

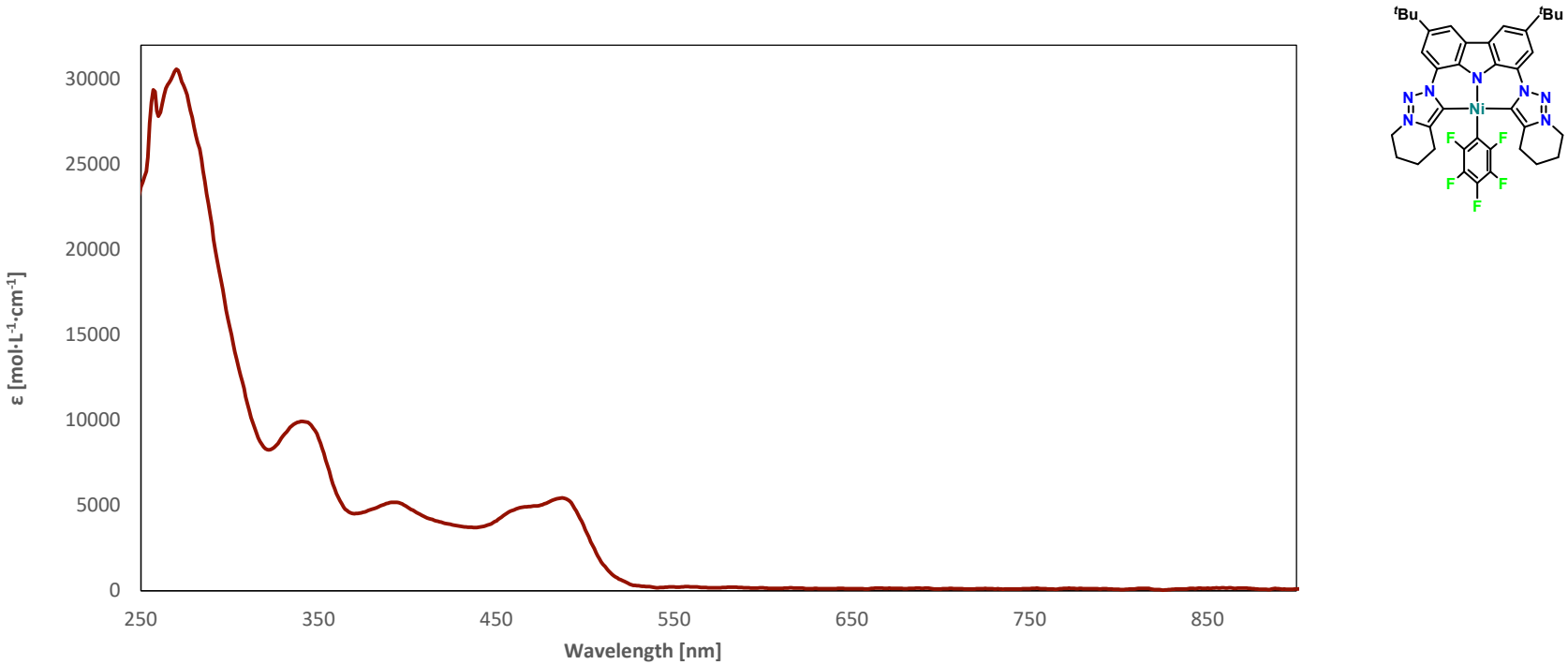
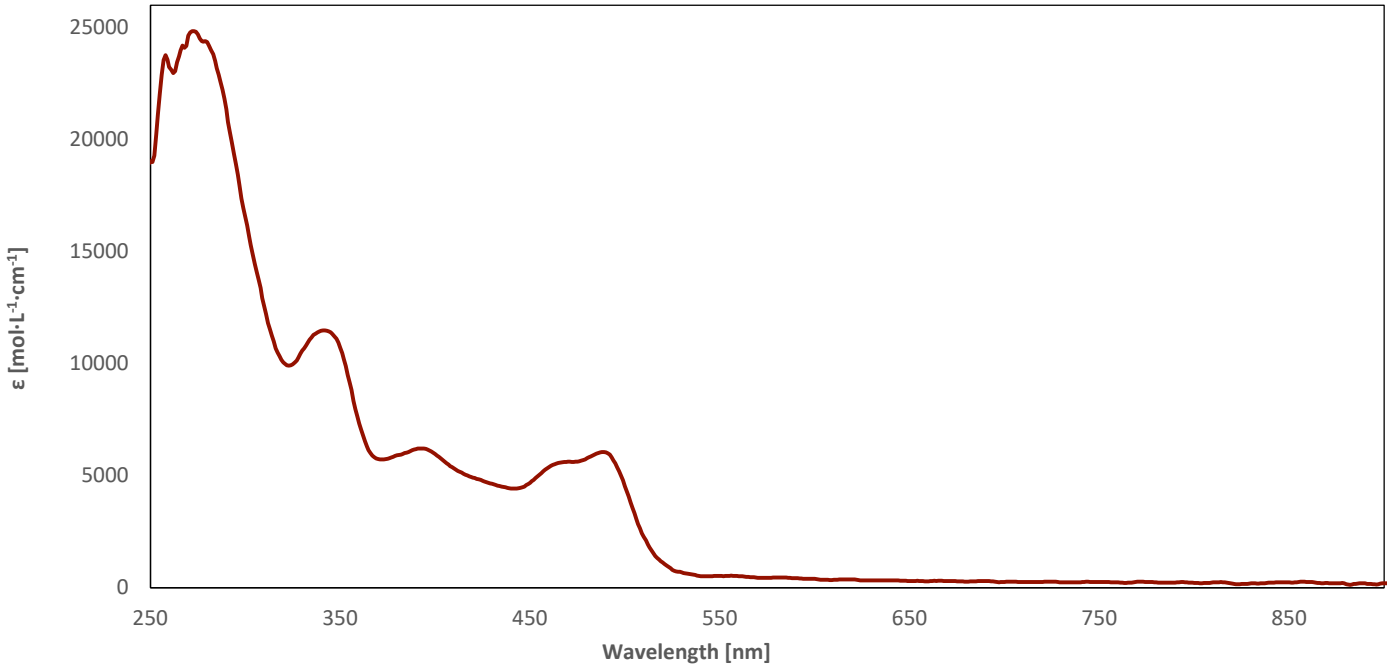


*Figure S 108: UV-VIS spectrum of **10** at 298K.*



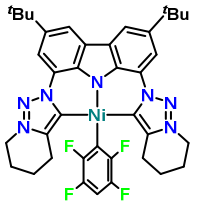


*Figure S 109: UV-VIS spectrum of **11** at 298K.*

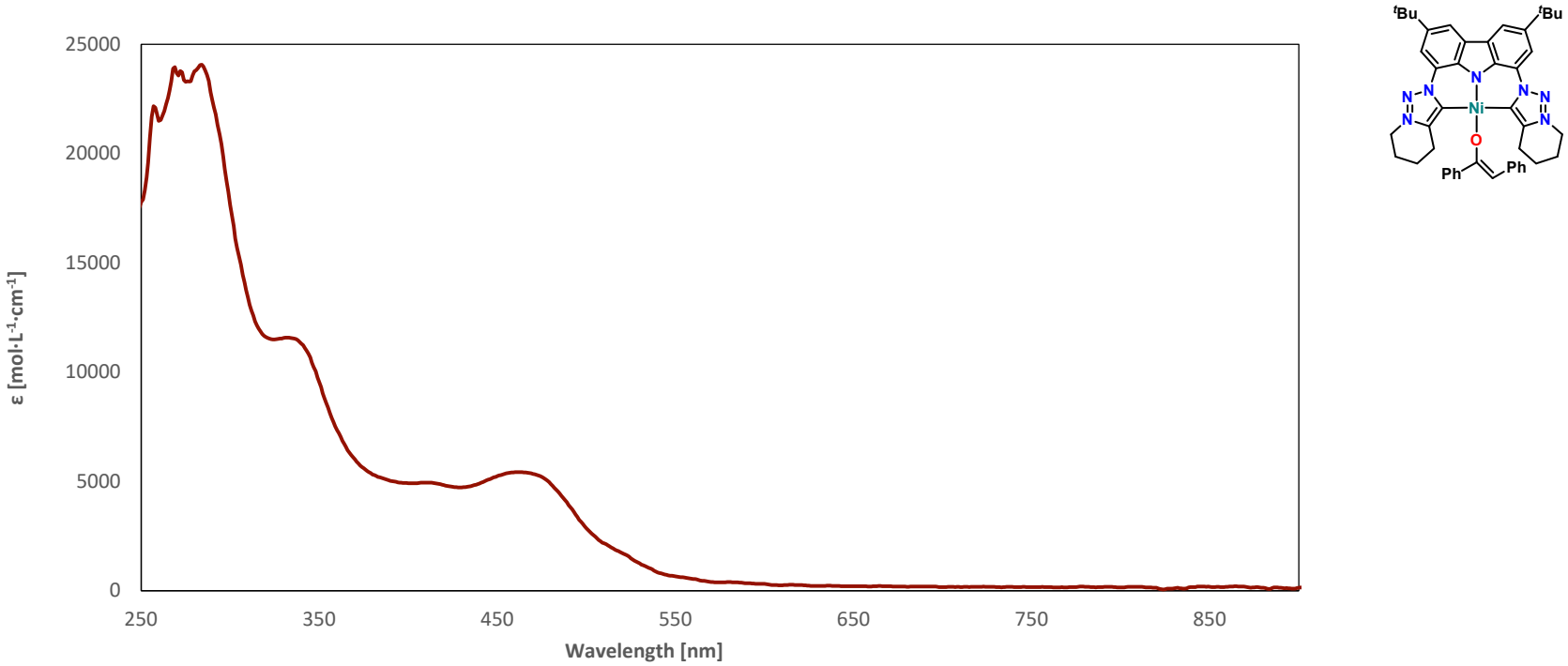


*Figure S 110: UV-VIS spectrum of **12** at 298K.*

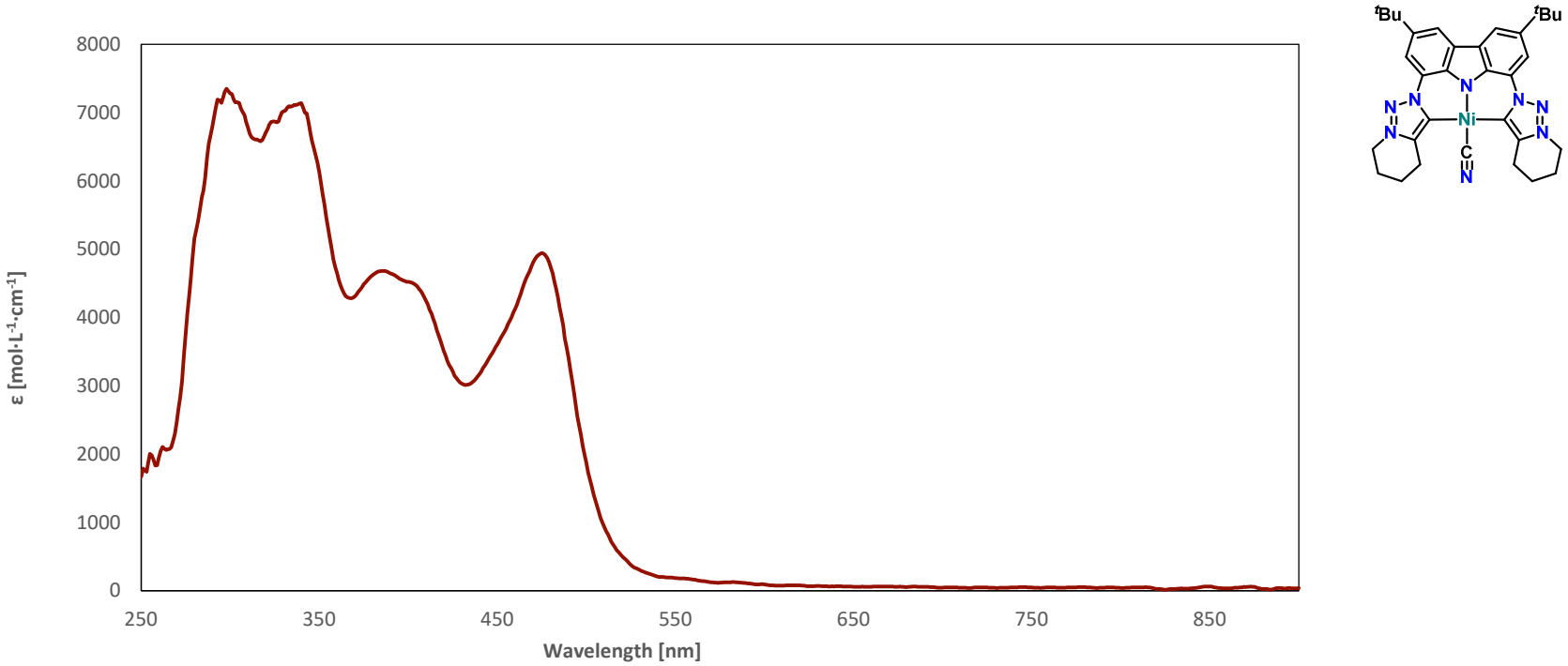


*Figure S 111: UV-VIS spectrum of **14** at 298K.*

4. Crystallographic details

*Table S1: Crystallographic data for complexes **1 – 8***

	1	**2[H_2O]**	**3**	**4***	**5**	**6****	**7****	**8**
Chemical formula	$C_{32}H_{38}N_7Cl_1Ni_1$ CH_2Cl_2	$C_{32}H_{39}N_7O_1Ni_1$ H_2O $C_4H_8O_1$	$C_{35}H_{47}N_7O_1Si_1Ni_1$ CH_2Cl_2	$C_{51}H_{53}N_7S_1Ni_1$ $2(C_7H_8)$	$C_{39}H_{46}N_8O_2S_1Ni_1$ C_6H_6	$C_{32}H_{38}N_{10}Ni_1$ CH_2Cl_2	$C_{37}H_{43}N_8Ni_1$ B_1F_4	$C_{42}H_{41}N_7F_6Ni_1$ $2(C_7H_8)$
M_r	699.78	686.53	753.52	1039.04	827.71	706.36	745.31	1000.73
Crystal system	Triclinic	Triclinic	Triclinic	Monoclinic	Monoclinic	Triclinic	Monoclinic	Triclinic
Space group	*P*-1	*P*-1	*P*-1	$P2_1/c$	$P2_1/c$	*P*-1	$P2_1/c$	*P*-1
a (Å)	7.6503(5)	7.7434(4)	11.4300(8)	15.78(5)	16.3158(15)	7.7265(16)	11.8809(6)	9.6617(5)
b (Å)	13.2697(8)	13.6237(7)	13.2816(11)	17.42(5)	21.3714(16)	13.252(2)	10.3569(4)	15.7074(8)
c (Å)	16.4268(11)	16.4176(9)	13.6078(12)	20.19(6)	12.1193(11)	16.223(3)	27.9319(13)	18.8918(10)
α (°)	77.840(3)	83.877(2)	72.352(3)	90	90	77.721(7)	90	67.512(2)
β (°)	86.166(3)	85.612(2)	70.181(3)	103.02(12)	96.097(3)	85.348(7)	93.247(2)	75.835(2)
γ (°)	79.990(3)	77.880(2)	74.277(3)	90	90	79.973(7)	90	77.315(2)
V (Å^3)	1604.58(18)	1681.08(15)	1819.1(3)	5408(28)	4202.0(6)	1596.7(5)	3431.5(3)	2542.9(2)
Z	2	2	2	4	4	2	4	2
Densitiy (g cm^{-3})	1.448	1.356	1.376	1.276	1.308	1.469	1.443	1.307
F(000)	732	732	796	2208	1752	740	1560	1048
Radiation Type	MoK_α	MoK_α	MoK_α	MoK_α	MoK_α	MoK_α	MoK_α	MoK_α
μ (mm^{-1})	0.891	0.625	0.753	0.446	0.559	0.818	0.629	0.448
Crystal size (mm)	0.15x0.07x0.02	0.10x0.09x0.02	0.08x0.07x0.06	0.10x0.04x0.02	0.40x0.12x0.03	0.15x0.14x0.01	0.20x0.18x0.02	0.15x0.14x0.03
Meas. Refl.	41628	57462	71977	9661	95811	5579	7067	79947
Indep. Refl.	6590	6442	7147	9661	7819	5579	7069	9039
Obsvd. [$I > 2\sigma(I)$]	5130	4964	5590	7424	5626	5098	6390	7166
R_{int}	0.0884	0.1129	0.1079	0.1968	0.1362	0.0975	0.0858	0.1121
R_1 [$I > 2\sigma(I)$]	0.0437	0.0486	0.0746	0.1073	0.0528	0.0694	0.0694	0.0703
$wR_2(F^2)$	0.1088	0.1256	0.2093	0.2301	0.0760	0.1116	0.1490	0.2077
GooF	1.036	1.032	1.031	1.165	1.019	1.226	1.199	1.053
$\Delta\rho_{max}$ (e Å^{-3})	0.523	0.580	3.854	0.878	0.557	0.501	0.643	1.073
$\Delta\rho_{min}$ (e Å^{-3})	-0.431	-0.459	-0.719	-0.549	-0.638	-0.476	-0.412	-0.601
CCDC	2294436	2294437	2294438	2294435	2294440	2294434	2294433	2294439

*The structure of **4** was heavily twinned, which explains the rather high ESD values obtained.

** Refined as a two component twin.

*Table S2: Crystallographic data for complexes **9**, **11**, **12'**, **13** and **14**.*

	9	**11**	**12'**	**13**	**14**
Chemical formula	$C_{46}H_{55}N_7Ni_1$ C_6H_6 C_5H_{12}	$C_{38}H_{39}N_7F_4Ni_1$ 0.8 C_6H_6	$C_{39}H_{43}N_7O_2Ni_1$ 2(C_6H_6)	$C_{39.92}H_{47.28}O_{6.16}Cl_{0.12}N_7Ni_1$	$C_{33}H_{38}N_8Ni_1$ 0.471(C_7H_8) 0.487(C_2H_3N)
M_r	914.93	790.96	856.73	786.69	668.84
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	P-1	$C2$	$P2_1/n$	$P2_1/n$
a (Å)	10.2341(10)	7.8623(11)	15.1996(9)	12.26757(15)	12.5534(4)
b (Å)	11.5523(14)	14.8825(18)	16.7302(8)	13.99843(13)	11.2678(4)
c (Å)	41.346(4)	17.700(2)	17.9276(10)	22.5929(2)	23.8559(10)
α (°)	90	77.464(4)	90	90	90
β (°)	96.430(3)	79.327(5)	107.549(2)	97.2879(11)	100.0500(10)
γ (°)	90	85.883(5)	90	90	90
V (Å^3)	4857.5(9)	1985.7(4)	4346.7(4)	3848.46(7)	3322.6
Z	4	2	4	4	4
Densitiy (g cm^{-3})	1.251	1.323	1.309	1.358	1.337
F(000)	1968	827	1816	1660	1417
Radiation Type	MoK_α	MoK_α	MoK_α	CuK_α	MoK_α
μ (mm^{-1})	0.445	0.547	0.496	1.269	0.625
Crystal size (mm)	0.14x0.12x0.02	0.15x0.14x0.02	0.35x.011x0.09	0.08.x0.058x0.015	0.45x0.40x0.35
Meas. Refl.	73579	79172	44884	47663	74517
Indep. Refl.	8681	7072	4623	7565	7637
Obsvd. [$I > 2\sigma(I)$]	7116	5113	3641	6505	6760
R_{int}	0.0509	0.1240	0.0991	0.0329	0.0424
R_1 [$I > 2\sigma(I)$]	0.0675	0.0741	0.0525	0.0638	0.0344
$wR_2(F^2)$	0.1761	0.2194	0.1379	0.1682	0.0971
GooF	1.069	1.031	1.045	1.123	1.047
$\Delta\rho_{max}$ (e Å^{-3})	1.088	2.245	0.475	0.719	0.505
$\Delta\rho_{min}$ (e Å^{-3})	-0.650	-0.486	-0.290	-0.365	-0.369
CCDC	2295617	2296517	2294782	2306311	2294579

*Table S3: Selected bond lengths and angles for complexes **1 – 10***

	1	**2[H_2O]**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
Ni1 – N10	1.862(2)	1.857(2)	1.858(3)	1.892(9)	1.862(3)	1.872(4)	1.862(3)	1.871(3)	1.881(3)
Ni1 – C1	1.916(3)	1.929(3)	1.926(4)	1.907(10)	1.921(3)	1.954(5)	1.989(4)	1.913(4)	1.947(4)
Ni1 – C2	1.946(3)	1.919(3)	1.934(4)	1.906(10)	1.907(3)	1.925(5)	1.986(4)	1.914(4)	1.938(4)
Ni1 – X	2.2007(8)	1.848(2)	1.874(3)	2.243(6)	1.937(3)	1.913(5)	1.893(3)	1.846(4)	1.849(4)
N10 – Ni1 – X	158.69(7)	165.86(10)	168.36(15)	154.1(2)	156.20(12)	168.4(2)	179.55(14)	160.62(16)	164.72(15)
C1 – Ni1 – C2	165.61(11)	167.12(12)	169.91(18)	157.2(3)	163.83(13)	169.2(2)	176.11(16)	163.05(16)	169.69(15)
N10 – Ni1 – C1	89.75(10)	91.84(11)	91.31(16)	90.7(4)	91.80(12)	91.9(2)	91.62(15)	92.12(15)	92.13(13)
C1 – Ni1 – X	89.14(8)	88.98(11)	89.76(15)	97.9(3)	90.94(12)	91.8(2)	88.01(14)	91.15(17)	91.12(15)
X – Ni1 – C2	93.66(8)	91.44(10)	88.86(16)	90.7(3)	92.47(12)	87.7(2)	88.25(15)	91.32(17)	88.42(15)
C2 – Ni1 – N10	92.68(10)	90.89(11)	92.06(17)	90.6(3)	91.43(12)	90.7(2)	92.12(15	91.09(15)	91.00(13)
τ_4'	0.27	0.19	0.16	0.35	0.30	0.16	0.04	0.26	0.16

X = Cl1, O1, S1, N1, C40, N40, N11

*Table S4: Selected bond lengths and angles for complexes **11 – 14***

	11	**12'**	**13**	**14**
Ni1 – N10	1.871(4)	1.857(3)	1.866(2)	1.8718(13)
Ni1 – C1	1.972(4)	1.936(2)	1.951(3)	1.9340(15)
Ni1 – C2	1.977(4)	-	1.938(3)	1.9290(16)
Ni1 – X	1.867(4)	1.906(3)	1.913(2)	1.8501(18)
N10 – Ni1 – X	179.78(18)	169.96(14)	170.80(11)	158.93(7)
C1 – Ni1 – C2	176.24(17)	168.17(15)	170.12(15)	167.96(6)
N10 – Ni1 – C1	91.99(16)	91.65(7)	90.84(12)	92.47(6)
C1 – Ni1 – X	88.13(16)	89.36(7)	88.86(12)	89.98(7)
X – Ni1 – C2	91.72(16)	-	90.01(12)	90.35(7)
C2 – Ni1 – N10	88.17(17)	-	91.83(12)	91.55(6)
τ_4'	0.04	0.15	0.14	0.26

X = Cl1, O1, S1, N1, C40, N40, N11

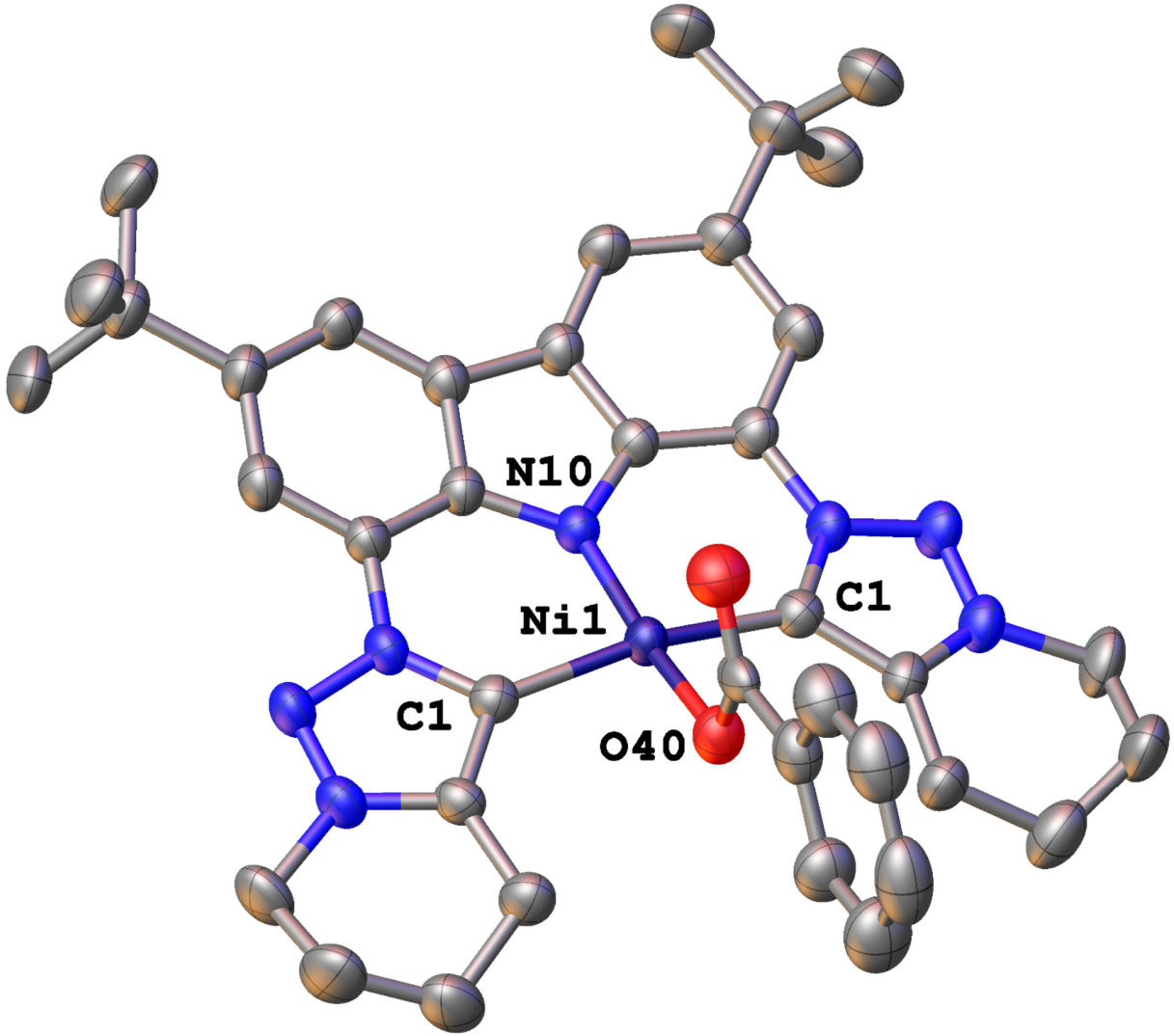


*Figure S 112: Molecular structure of **12'**. Hydrogen atoms and lattice solvents have been omitted for clarity. Ellipsoids are shown at a probability level of 50%.*

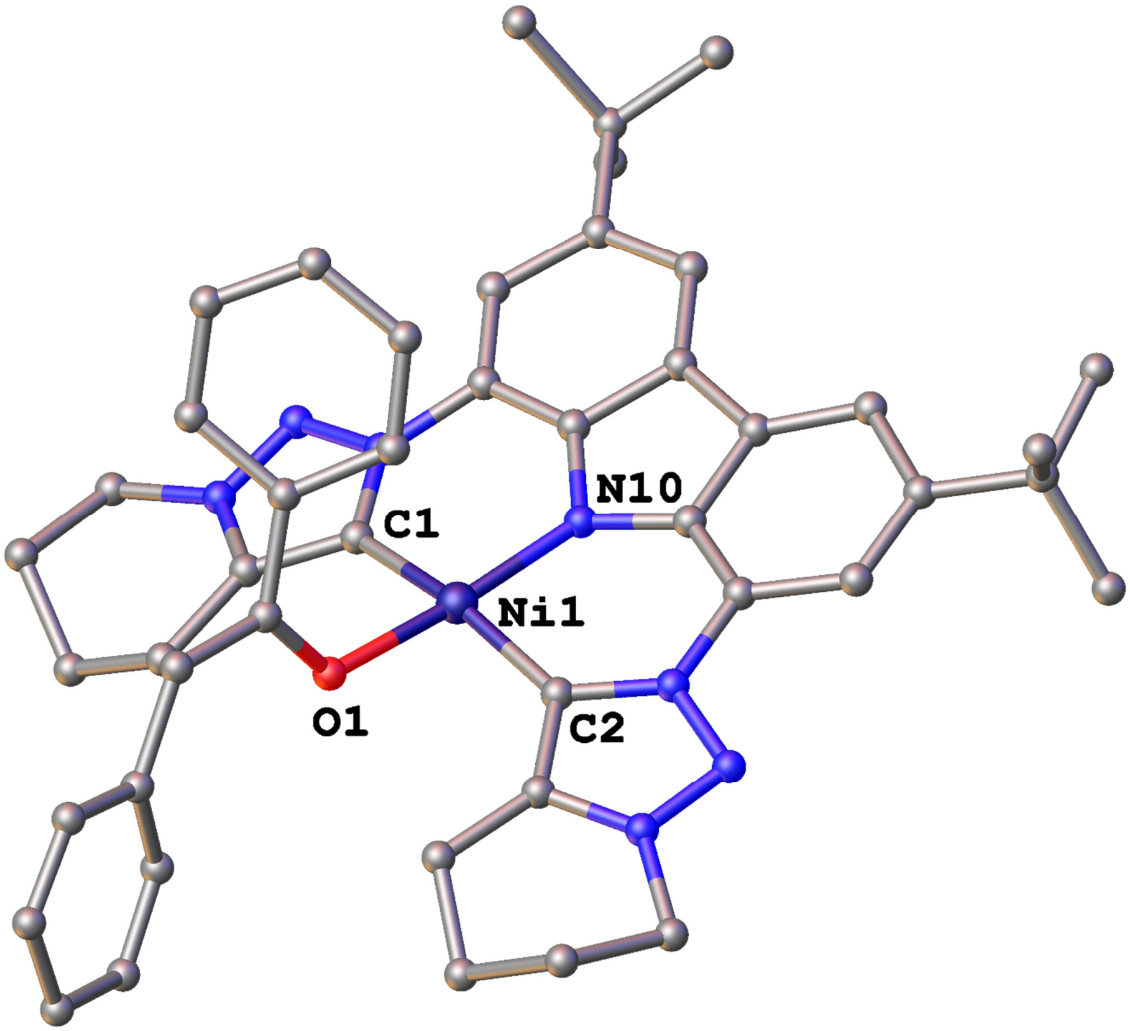


*Figure S 113: Molecular structure of complex **12**. The structure is heavily twinned with many overlying spots, wherefore the twin component could not be cleanly separated leading to R1 values of 15 % lowest. In addition to this unresolvable twinnig, a full molecule disorder is present with a second complex molecule stand perpendicular to the shown being only occupied by 20%. Although the quality of the crystal structure is low, the connectivity can unambiguously be determined from the data set.*

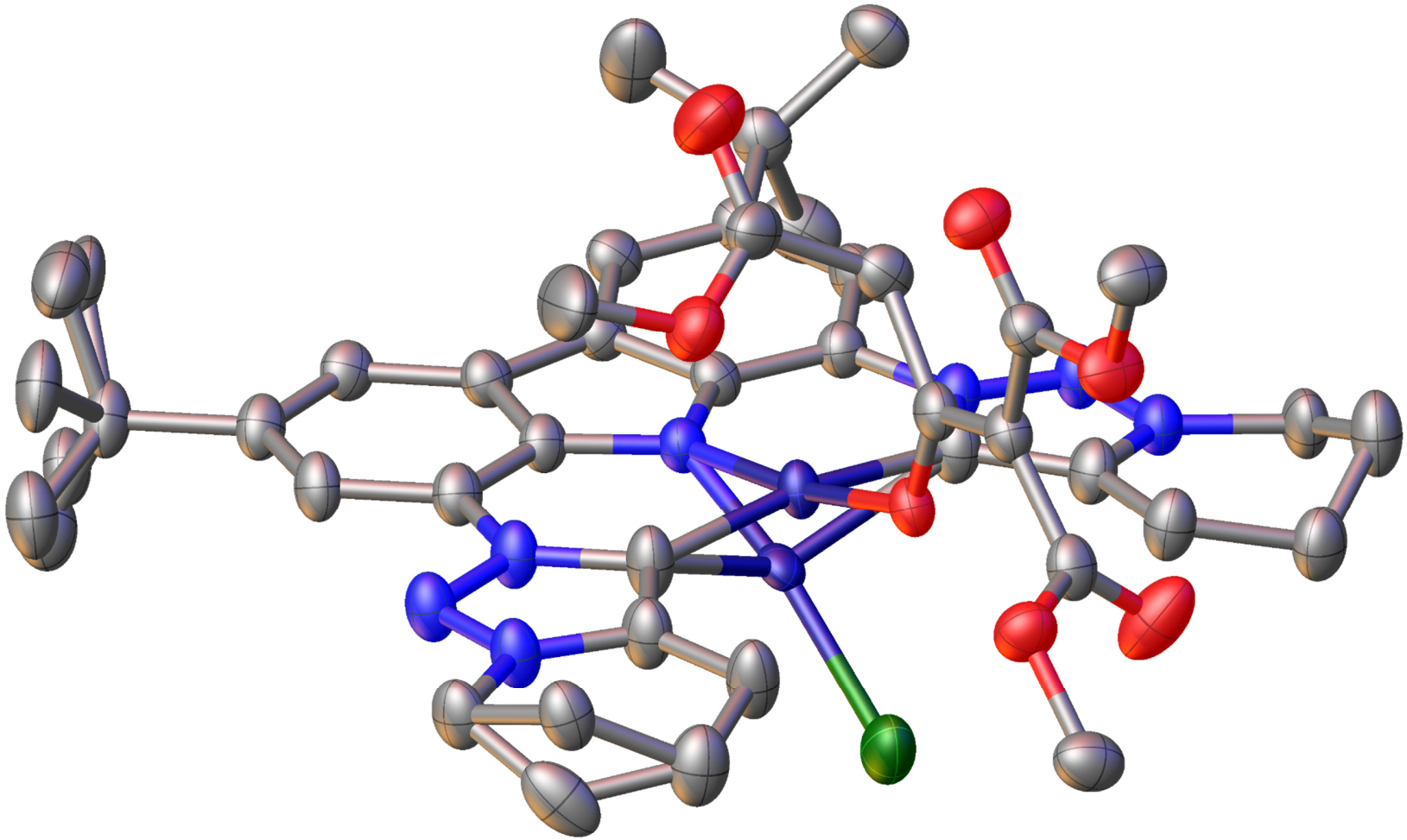


*Figure S 114: Full molecular structure of **13**, containing all disorders and the impurity with compound 1. Note that the occupation of the Ni and Cl center are only 12 %. Hydrogen atoms have been omitted for clarity. Ellipsoids are shown at a probability level of 50%.*

5. Computational details

Computations were performed with ORCA 5.0[1] program package, geometry optimizations and frequency calculations were carried out with density functional theory (DFT) using the B3LYP[2] functional, Grimme's D3 dispersion correction[3] and 6-31G** basis set[4,5]. The calculated structure was verified as true minimum by the absence of negative eigenvalues in the harmonic vibrational frequency analysis.

*Table S5: XYZ Coordinates Compound **2**.*

At.	x	y	z	At.	x	y	z
Ni	-0.105941000	-1.518939000	0.174024000	H	-2.987540000	-4.022613000	0.844083000
O	-0.473265000	-3.244613000	0.732614000	H	-2.108531000	-4.128004000	-0.639594000
H	0.203239000	-3.475204000	1.379872000	C	4.621750000	5.022355000	0.169333000
N	0.202627000	0.310321000	-0.134566000	H	4.106097000	5.327392000	-0.747023000
N	-2.691228000	-0.114436000	-0.340712000	H	5.552667000	5.595137000	0.233159000
N	2.819243000	-0.996355000	-0.047442000	H	3.998312000	5.303981000	1.024174000
N	-4.162117000	-1.560120000	-0.567048000	C	-3.299031000	4.839609000	-0.370898000
N	-3.996059000	-0.248624000	-0.601860000	H	5.324688000	3.450318000	-1.981771000
C	-0.742481000	1.307097000	-0.197183000	C	2.963665000	-5.424827000	-0.940809000
C	-1.997300000	-1.295291000	-0.140342000	H	2.691892000	-6.478511000	-0.825655000
C	1.777733000	-1.904467000	0.079970000	H	2.890546000	-5.188188000	-2.010494000
C	1.408315000	0.962382000	-0.055008000	C	-2.529954000	6.170719000	-0.322593000
C	-2.133063000	1.187674000	-0.295675000	H	-1.950606000	6.269460000	0.601089000
C	2.448723000	-3.119573000	-0.120279000	H	-3.235703000	7.006751000	-0.363533000
C	-0.162592000	2.609613000	-0.158792000	H	-1.844762000	6.272275000	-1.170538000
C	-3.013984000	-2.247402000	-0.303098000	C	-4.269575000	4.801456000	0.830212000
C	3.802252000	1.253213000	0.081084000	H	-4.879932000	3.893551000	0.828020000
C	1.992266000	-4.545969000	-0.141216000	H	-4.948718000	5.661687000	0.803334000
H	0.963632000	-4.568317000	-0.505177000	H	-3.717488000	4.829732000	1.775173000
H	1.945616000	-4.925188000	0.889950000	C	-4.111021000	4.801875000	-1.684796000

C	-2.922524000	2.332615000	-0.348584000	H	-3.444184000	4.831164000	-2.552623000
H	-3.995543000	2.206972000	-0.420576000	H	-4.788207000	5.662067000	-1.742354000
C	-2.359844000	3.625155000	-0.311060000	H	-4.716289000	3.893687000	-1.759990000
C	-0.968179000	3.748910000	-0.215438000	N	4.019578000	-1.527298000	-0.299049000
H	-0.502813000	4.727250000	-0.182211000	N	3.764676000	-2.824097000	-0.327943000
C	2.694223000	0.414124000	0.005979000	H	4.783145000	0.796959000	0.130125000
C	-5.545571000	-3.572312000	-0.422412000	H	-5.626197000	-3.608808000	0.671046000
H	-6.456031000	-4.022634000	-0.830751000	C	5.844413000	3.218234000	-1.046505000
C	1.262638000	2.381579000	-0.062628000	C	5.703038000	3.187296000	1.470272000
C	4.938945000	3.517521000	0.168827000	C	4.402142000	-5.191553000	-0.458629000
C	3.669123000	2.656607000	0.085168000	C	4.834235000	-3.747818000	-0.718224000
C	2.384040000	3.209885000	0.008000000	H	6.138411000	2.165030000	-1.081252000
H	2.248542000	4.285250000	0.003518000	H	6.759450000	3.820542000	-1.003074000
C	-5.479851000	-2.116994000	-0.882982000	H	5.999718000	2.134997000	1.508367000
H	-5.622418000	-2.044765000	-1.967110000	H	6.612170000	3.794930000	1.546505000
H	-6.228609000	-1.486422000	-0.398600000	H	5.079356000	3.390134000	2.346944000
C	-4.290196000	-4.330502000	-0.873155000	H	5.109178000	-5.856063000	-0.965197000
H	-4.206516000	-4.270622000	-1.966902000	H	4.466582000	-5.408909000	0.614823000
H	-4.376771000	-5.391431000	-0.618854000	H	5.032610000	-3.586695000	-1.783444000
C	-3.034618000	-3.741714000	-0.213880000	H	5.732453000	-3.473052000	-0.160407000

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