Supporting Information

IPr*Thia – Wingtip-Flexible, Sterically-Hindered, Modular, N,C/S,C-Chelating Thiazole-Donor N-Heterocyclic Carbene Ligands

Pamela Podchorodecka,[a] Błażej Dziuk,[b] Robert Junga,[c] Roman Szostak,[d] Michal Szostak*,[e] and Elwira Bisz*,[a]

[a]*Department of Chemistry, Opole University, 48 Oleska Street, Opole 45-052, Poland*
[b]*Department of Chemistry, Wroclaw University of Science and Technology, Norwida 4/6, Wroclaw 50-373, Poland*
[c]*Department of Thermal Engineering and Industrial Facilities, Opole University of Technology, 5 Mikołajczyka Street, Opole 45-271, Poland*
[d]*Department of Chemistry, Wroclaw University, F. Joliot-Curie 14, Wroclaw 50-383, Poland*
[e]*Department of Chemistry, Rutgers University, 73 Warren Street, Newark, NJ 07102, USA*

ebisz@uni.opole.pl; michal.szostak@rutgers.edu

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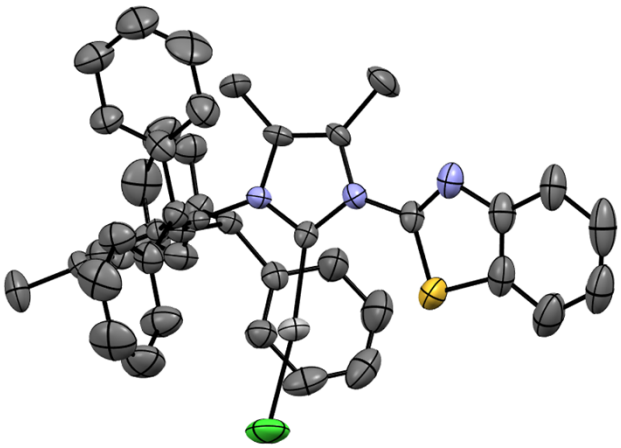
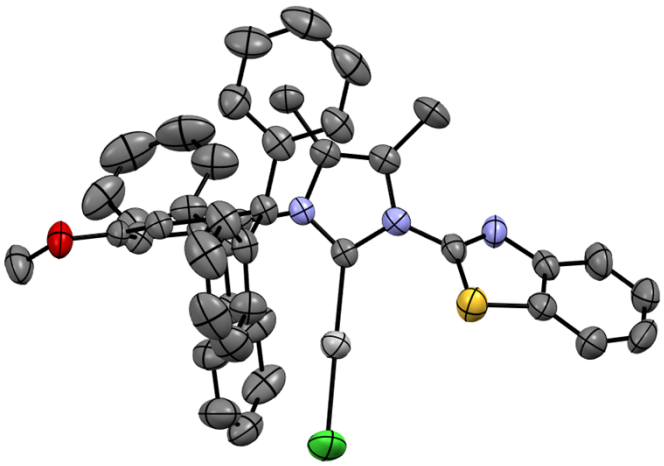
Crystallographic Analysis

Single crystals of Ag and Pd complexes (4a, 4b and 5a) were collected on a Kuma KM4 diffractometer equipped with Eos CCD detector (graphite monochromatic, MoKα radiation, λ = 0.71073 Å) at room temperature. The single crystals of the complexes 5b and 6b were collected on a Rigaku Oxford Diffraction XtaLAB SynergyR DW diffractometer equipped with a HyPix ARC 150° Hybrid Photon Counting (HPC) detector using CuKα (λ = 1.54184 Å) at 100 K. The corrections to the Lorentz and polarization factors were applied to the reflection intensities [1]. Data were processed using the CrysAlisPro software. The structures were solved by direct methods using SHELXS and refined by full-matrix least-squares methods based F^2 using SHELXL [2, 3]. The hydrogen atoms were determined from the geometric concepts and refined in a riding model with isotropic temperature factors of 1.2 times the Ueq value of the parent atom. All non-hydrogen atoms were located from difference Fourier synthesis and refined by least squares method in the full-matrix anisotropic approximation. Disordered solvent was omitted from the refinement of 4a and 5b, using a solvent mask in those structures [4,5]. In structure 5a disorder modeling was used with the atomic occupancy at 50% due to the best divergence coefficient for this model [6]. The crystallographic data for compounds and details of X-ray experiment are collected in the Supplementary information Tables. The structure drawings in ESI were prepared by using Mercury program [7]. The coordinates of atoms and other parameters for structures were deposited with the Cambridge Crystallographic Data Centre: 2354247 for [Ag(IPr*^{Thia})Cl] 4a, 2354248 for [Ag(IPr*^{MeOThia})Cl] 4b, 2354249 for [Pd(IPr*^{Thia})Cl2] 5a, 2354250 for [Pd(IPr*^{MeOThia})Cl_2] 5b, 2372438 for [Se(IPr*^{MeOThia})Cl_2] 6b; 12 Union Road, Cambridge CB2 1EZ, UK (Fax,_44-(1223)336-033, E-mail deposit@ccdc.cam.ac.uk).

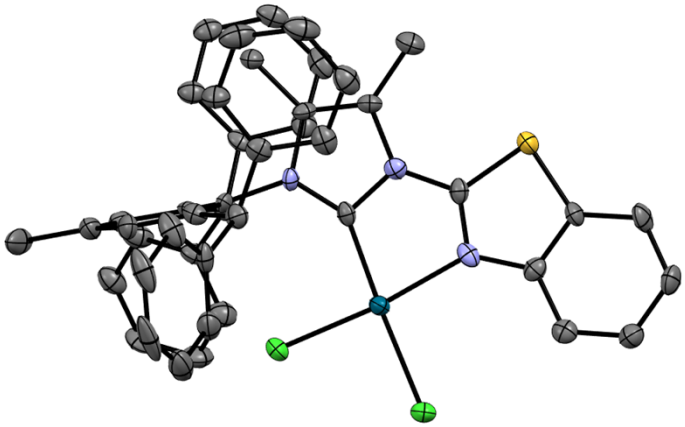
Figure S1. Molecular structures of [Ag(IPr*^{Thia})Cl], [Ag(IPr*^{MeOThia})Cl], [Pd(IPr*^{Thia})Cl_2], [Pd(IPr*^{MeOThia})Cl_2] and [(IPr*^{MeOThia})Se] complexes. Hydrogen atoms and disordered solvent molecules have been omitted for clarity.



[Ag(IPr*^{Thia})Cl]



[Ag(IPr*^{MeOThia})Cl]



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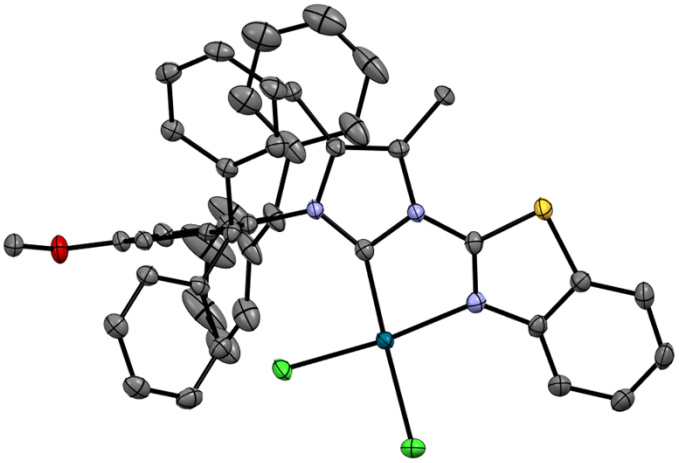

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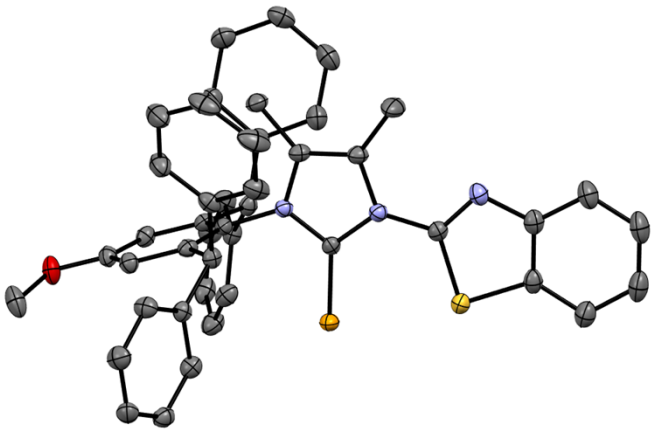


[(IPr*^{MeOThia})Se]

[1] CrysAlis CCD; Oxford Diffraction Ltd: Abingdon, England, 2002. CrysAlis RED; Oxford Diffraction Ltd: Abingdon, England, 2002.

[2] G. M. Sheldrick, A short history of SHELX, Acta Crystallogr. Sect. A 64 (2008) 112−122, https://doi.org/10.1107/S0108767307043930.

[3] G. M. Sheldrick, Crystal structure refinement with SHELXL, Acta Crystallogr. Sect. C 71 (2015) 3–8, https://doi.org/10.1107/S2053229614024218.

[4] A. L. Spek, Acta Cryst. D65 (2009), 148–155, https://doi.org/10.1107/S090744490804362X

[5] A. L. Spek, Acta Cryst. C71 (2015), 9–18, https://doi.org/10.1107/S2053229614024929

[6] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, J. Appl. Cryst. 42(2009) 339−341, https://doi.org/10.1107/S0021889808042726.

[7] C. F. Macrae, I. J. Bruno, J. A. Chisholm, P. R. Edgington, P. McCabe, E. Pidcock, L. Rodriguez-Monge, R. Taylor, J. van de Streek, P. A. Wood, J. Appl. Crystallogr. 41 (2008) 466–470, http://doi.org/10.1107/S0021889807067908.

Table S1. Experimental details for complexes 4a-5b

	[Ag(IPr*^{Thia})Cl]4a	[Ag(IPr*^{MeOThia})Cl] 4b	[Pd(IPr*^{Thia})Cl_2] 5a	[Pd(IPr*^{MeOThia})Cl_2] 5b
		Crystal data		
Chemical formula	$C_{45}H_{37}AgClN_3S$	$C_{45}H_{37}AgClN_3OS$	$C_{47}H_{41}Cl_6N_3PdS$	$C_{45}H_{37}Cl_2N_3OPdS$
M_r	795.15	811.15	998.99	845.13
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, *Cc*	Monoclinic, $P2_1/c$	Orthorhombic, *Pbca*
Temperature (K)	293	293	293	100
a, *b*, *c* (Å)	10.6849 (6), 32.091 (2), 12.6278 (8)	18.9280 (16), 10.7439 (13), 20.2390 (17)	13.466 (3), 11.2456 (11), 28.723 (6)	25.3287 (3), 9.4913 (1), 35.0477 (3)
α, β, γ (°)	90, 104.579 (6), 90	90, 112.350 (11), 90	90, 96.010 (16), 90	90, 90, 90
V (Å^3)	4190.6 (5)	3806.6 (7)	4325.7 (14)	8425.55 (15)
Z	4	4	4	8
Radiation type	Mo *K*α	Mo *K*α	Mo *K*α	Cu *K*α
μ (mm^{-1})	0.63	0.69	0.89	5.46
Crystal size (mm)	0.4 × 0.25 × 0.1	0.4 × 0.3 × 0.2	0.28 × 0.19 × 0.10	0.2 × 0.15 × 0.1
		Data collection		
Diffractometer	KM4, Eos CCD	KM4, Eos CCD	KM4, Eos CCD	Synergy R, DW, HyPix-Arc 150
T_{min}, T_{max}	0.829, 0.939	0.779, 0.870	0.817, 0.915	0.430, 0.579
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18369, 8236, 5007	7542, 5005, 4210	20188, 8474, 5955	33757, 8078, 7670
R_{int}	0.135	0.030	0.079	0.020
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.617	0.617	0.617	0.621
		Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.072, 0.179, 0.99	0.051, 0.106, 1.08	0.062, 0.159, 0.96	0.031, 0.079, 1.12
No. of reflections	8236	5005	8474	8078
No. of parameters	464	473	562	481
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.80, −0.55	0.88, −0.34	1.05, −1.42	0.49, −0.69

Computer programs: CrysAlis CCD (Oxford Diffraction Ltd., 2008), CrysAlis PRO 1.171.42.42a (Rigaku OD, 2022), SHELXS2014/7 (Sheldrick, 2014), SHELXL2014/7 (Sheldrick, 2014), SHELXTL (Sheldrick, 2008). Absorption was corrected for by multi-scan methods, SCALE3 ABSPACK (Rigaku Oxford Diffraction, 2015)

	[Se(IPr*^{MeOThia})Cl_2] 6b
Chemical formula	$C_{45}H_{37}N_3OSSe$
M_r	746.79
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, *b*, *c* (Å)	20.3298 (3), 10.2556 (1), 20.1417 (3)

α, β, γ (°)	90, 118.220 (2), 90
V (Å^3)	3700.28 (11)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.20
Crystal size (mm)	0.38 × 0.29 × 0.22
Data collection	
Diffractometer	XtaLAB Synergy R, DW system, HyPix-Arc 150
T_{min}, T_{max}	0.458, 0.579
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	37461, 7283, 7121
R_{int}	0.020
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.628
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.027, 0.069, 1.06
No. of reflections	7283
No. of parameters	463
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.26, -0.43

Computer programs: CrysAlis CCD (Oxford Diffraction Ltd., 2008), CrysAlis PRO 1.171.42.42a (Rigaku OD, 2022), SHELXS2014/7 (Sheldrick, 2014), SHELXL2014/7 (Sheldrick, 2014), SHELXL 2014/7 (Sheldrick, 2015), Olex2 1.3 (Dolomanov et al., 2009), SHELXTL (Sheldrick, 2008)

Table S2. Selected geometric parameters (Å, º)

[Ag(IPr*Thia)Cl] 4a			
Ag1—C1	2.092 (5)	C21—C22	1.390 (9)
Ag1—Cl1	2.3202 (16)	C21—H21	0.9300
S1—C39	1.727 (6)	C22—H22	0.9300
S1—C41	1.745 (7)	C23—H23A	0.9600
N1—C1	1.359 (6)	C23—H23B	0.9600
N1—C2	1.410 (6)	C23—H23C	0.9600
N1—C4	1.434 (6)	C24—C31	1.519 (7)
N2—C1	1.353 (6)	C24—C25	1.552 (7)
N2—C39	1.405 (7)	C24—H24	0.9800
N2—C3	1.407 (6)	C25—C26	1.372 (8)
N3—C39	1.282 (7)	C25—C30	1.376 (8)
N3—C40	1.390 (7)	C26—C27	1.388 (9)
C2—C3	1.339 (7)	C26—H26	0.9300
C2—C37	1.475 (7)	C27—C28	1.390 (11)
C3—C38	1.505 (7)	C27—H27	0.9300
C4—C5	1.397 (7)	C28—C29	1.366 (10)
C4—C9	1.407 (7)	C28—H28	0.9300
C5—C6	1.382 (7)	C29—C30	1.368 (8)
C5—C10	1.507 (7)	C29—H29	0.9300
C6—C7	1.371 (8)	C30—H30	0.9300
C6—H6	0.9300	C31—C32	1.363 (8)
C7—C8	1.382 (8)	C31—C36	1.377 (8)
C7—C23	1.520 (8)	C32—C33	1.397 (9)
C8—C9	1.375 (8)	C32—H32	0.9300
C8—H8	0.9300	C33—C34	1.366 (10)
C9—C24	1.530 (7)	C33—H33	0.9300
C10—C11	1.534 (7)	C34—C35	1.344 (11)
C10—C17	1.541 (8)	C34—H34	0.9300
C10—H10	0.9800	C35—C36	1.385 (10)
C11—C16	1.364 (8)	C35—H35	0.9300
C11—C12	1.406 (9)	C36—H36	0.9300
C12—C13	1.386 (9)	C37—H37A	0.9600
C12—H12	0.9300	C37—H37B	0.9600
C13—C14	1.341 (10)	C37—H37C	0.9600
C13—H13	0.9300	C38—H38A	0.9600
C14—C15	1.342 (11)	C38—H38B	0.9600
C14—H14	0.9300	C38—H38C	0.9600
C15—C16	1.397 (9)	C40—C41	1.391 (10)
C15—H15	0.9300	C40—C45	1.391 (9)
C16—H16	0.9300	C41—C42	1.377 (9)
C17—C18	1.353 (8)	C42—C43	1.392 (11)
C17—C22	1.367 (8)	C42—H42	0.9300
C18—C19	1.410 (10)	C43—C44	1.366 (12)
C18—H18	0.9300	C43—H43	0.9300
C19—C20	1.295 (11)	C44—C45	1.414 (10)
C19—H19	0.9300	C44—H44	0.9300
C20—C21	1.367 (11)	C45—H45	0.9300

C20—H20	0.9300		
C1—Ag1—Cl1	172.23 (14)	H23A—C23—H23B	109.5
C39—S1—C41	88.2 (3)	C7—C23—H23C	109.5
C1—N1—C2	110.8 (4)	H23A—C23—H23C	109.5
C1—N1—C4	123.1 (4)	H23B—C23—H23C	109.5
C2—N1—C4	126.1 (4)	C31—C24—C9	112.1 (4)
C1—N2—C39	121.6 (4)	C31—C24—C25	112.3 (4)
C1—N2—C3	111.0 (4)	C9—C24—C25	111.2 (4)
C39—N2—C3	127.3 (4)	C31—C24—H24	107.0
C39—N3—C40	110.0 (5)	C9—C24—H24	107.0
N2—C1—N1	104.8 (4)	C25—C24—H24	107.0
N2—C1—Ag1	133.7 (4)	C26—C25—C30	119.5 (5)
N1—C1—Ag1	121.5 (3)	C26—C25—C24	118.2 (5)
C3—C2—N1	106.6 (4)	C30—C25—C24	122.3 (5)
C3—C2—C37	131.8 (5)	C25—C26—C27	120.7 (6)
N1—C2—C37	121.6 (5)	C25—C26—H26	119.6
C2—C3—N2	106.8 (4)	C27—C26—H26	119.6
C2—C3—C38	129.5 (5)	C26—C27—C28	118.9 (7)
N2—C3—C38	123.7 (5)	C26—C27—H27	120.5
C5—C4—C9	121.9 (5)	C28—C27—H27	120.5
C5—C4—N1	119.5 (4)	C29—C28—C27	119.7 (6)
C9—C4—N1	118.6 (4)	C29—C28—H28	120.2
C6—C5—C4	117.3 (5)	C27—C28—H28	120.2
C6—C5—C10	122.1 (5)	C28—C29—C30	121.0 (7)
C4—C5—C10	120.4 (5)	C28—C29—H29	119.5
C7—C6—C5	122.4 (5)	C30—C29—H29	119.5
C7—C6—H6	118.8	C29—C30—C25	120.2 (6)
C5—C6—H6	118.8	C29—C30—H30	119.9
C6—C7—C8	118.8 (5)	C25—C30—H30	119.9
C6—C7—C23	120.9 (5)	C32—C31—C36	118.0 (5)
C8—C7—C23	120.4 (5)	C32—C31—C24	123.5 (5)
C9—C8—C7	122.2 (5)	C36—C31—C24	118.5 (5)
C9—C8—H8	118.9	C31—C32—C33	121.2 (6)
C7—C8—H8	118.9	C31—C32—H32	119.4
C8—C9—C4	117.4 (5)	C33—C32—H32	119.4
C8—C9—C24	123.9 (5)	C34—C33—C32	119.5 (7)
C4—C9—C24	118.5 (5)	C34—C33—H33	120.3
C5—C10—C11	113.5 (5)	C32—C33—H33	120.3
C5—C10—C17	111.3 (4)	C35—C34—C33	119.8 (7)
C11—C10—C17	112.3 (5)	C35—C34—H34	120.1
C5—C10—H10	106.4	C33—C34—H34	120.1
C11—C10—H10	106.4	C34—C35—C36	120.9 (7)
C17—C10—H10	106.4	C34—C35—H35	119.5
C16—C11—C12	117.2 (5)	C36—C35—H35	119.5
C16—C11—C10	123.6 (5)	C31—C36—C35	120.5 (7)
C12—C11—C10	119.1 (5)	C31—C36—H36	119.7
C13—C12—C11	120.5 (7)	C35—C36—H36	119.7
C13—C12—H12	119.7	C2—C37—H37A	109.5

C11—C12—H12	119.7	C2—C37—H37B	109.5
C14—C13—C12	120.8 (7)	H37A—C37—H37B	109.5
C14—C13—H13	119.6	C2—C37—H37C	109.5
C12—C13—H13	119.6	H37A—C37—H37C	109.5
C13—C14—C15	119.7 (7)	H37B—C37—H37C	109.5
C13—C14—H14	120.2	C3—C38—H38A	109.5
C15—C14—H14	120.2	C3—C38—H38B	109.5
C14—C15—C16	121.3 (7)	H38A—C38—H38B	109.5
C14—C15—H15	119.3	C3—C38—H38C	109.5
C16—C15—H15	119.3	H38A—C38—H38C	109.5
C11—C16—C15	120.5 (7)	H38B—C38—H38C	109.5
C11—C16—H16	119.7	N3—C39—N2	122.0 (5)
C15—C16—H16	119.7	N3—C39—S1	117.5 (4)
C18—C17—C22	118.4 (6)	N2—C39—S1	120.5 (4)
C18—C17—C10	120.1 (6)	N3—C40—C41	114.9 (6)
C22—C17—C10	121.6 (5)	N3—C40—C45	124.9 (7)
C17—C18—C19	119.2 (7)	C41—C40—C45	120.2 (6)
C17—C18—H18	120.4	C42—C41—C40	122.0 (7)
C19—C18—H18	120.4	C42—C41—S1	128.6 (7)
C20—C19—C18	122.2 (7)	C40—C41—S1	109.3 (5)
C20—C19—H19	118.9	C41—C42—C43	117.7 (8)
C18—C19—H19	118.9	C41—C42—H42	121.2
C19—C20—C21	119.9 (7)	C43—C42—H42	121.2
C19—C20—H20	120.0	C44—C43—C42	121.5 (7)
C21—C20—H20	120.0	C44—C43—H43	119.2
C20—C21—C22	119.1 (7)	C42—C43—H43	119.2
C20—C21—H21	120.4	C43—C44—C45	121.0 (8)
C22—C21—H21	120.4	C43—C44—H44	119.5
C17—C22—C21	121.1 (6)	C45—C44—H44	119.5
C17—C22—H22	119.4	C40—C45—C44	117.5 (8)
C21—C22—H22	119.4	C40—C45—H45	121.2
C7—C23—H23A	109.5	C44—C45—H45	121.2
C7—C23—H23B	109.5		
C39—N2—C1—N1	175.5 (4)	C22—C17—C18—C19	1.4 (10)
C3—N2—C1—N1	-1.5 (5)	C10—C17—C18—C19	179.8 (6)
C39—N2—C1—Ag1	-1.7 (7)	C17—C18—C19—C20	-1.4 (13)
C3—N2—C1—Ag1	-178.8 (4)	C18—C19—C20—C21	0.8 (14)
C2—N1—C1—N2	0.6 (5)	C19—C20—C21—C22	-0.3 (13)
C4—N1—C1—N2	-179.5 (4)	C18—C17—C22—C21	-0.8 (10)
C2—N1—C1—Ag1	178.3 (3)	C10—C17—C22—C21	-179.3 (6)
C4—N1—C1—Ag1	-1.9 (6)	C20—C21—C22—C17	0.3 (11)
C1—N1—C2—C3	0.5 (6)	C8—C9—C24—C31	-98.0 (6)
C4—N1—C2—C3	-179.3 (5)	C4—C9—C24—C31	77.2 (6)
C1—N1—C2—C37	-178.8 (5)	C8—C9—C24—C25	28.6 (7)
C4—N1—C2—C37	1.4 (7)	C4—C9—C24—C25	-156.1 (4)
N1—C2—C3—N2	-1.4 (6)	C31—C24—C25—C26	-140.0 (5)
C37—C2—C3—N2	177.8 (5)	C9—C24—C25—C26	93.5 (6)
N1—C2—C3—C38	176.1 (6)	C31—C24—C25—C30	39.8 (7)

C37—C2—C3—C38	-4.7 (10)	C9—C24—C25—C30	-86.7 (6)
C1—N2—C3—C2	1.9 (6)	C30—C25—C26—C27	0.5 (9)
C39—N2—C3—C2	-174.9 (5)	C24—C25—C26—C27	-179.7 (5)
C1—N2—C3—C38	-175.8 (5)	C25—C26—C27—C28	2.1 (10)
C39—N2—C3—C38	7.4 (8)	C26—C27—C28—C29	-2.5 (11)
C1—N1—C4—C5	80.9 (6)	C27—C28—C29—C30	0.2 (12)
C2—N1—C4—C5	-99.3 (6)	C28—C29—C30—C25	2.5 (11)
C1—N1—C4—C9	-98.4 (5)	C26—C25—C30—C29	-2.8 (9)
C2—N1—C4—C9	81.5 (6)	C24—C25—C30—C29	177.4 (6)
C9—C4—C5—C6	0.3 (7)	C9—C24—C31—C32	25.4 (7)
N1—C4—C5—C6	-178.9 (4)	C25—C24—C31—C32	-100.7 (6)
C9—C4—C5—C10	-175.3 (4)	C9—C24—C31—C36	-153.4 (5)
N1—C4—C5—C10	5.5 (7)	C25—C24—C31—C36	80.6 (6)
C4—C5—C6—C7	-0.2 (8)	C36—C31—C32—C33	1.0 (9)
C10—C5—C6—C7	175.3 (5)	C24—C31—C32—C33	-177.7 (6)
C5—C6—C7—C8	-0.1 (9)	C31—C32—C33—C34	0.1 (10)
C5—C6—C7—C23	179.6 (5)	C32—C33—C34—C35	-0.2 (11)
C6—C7—C8—C9	0.3 (9)	C33—C34—C35—C36	-0.7 (13)
C23—C7—C8—C9	-179.4 (6)	C32—C31—C36—C35	-1.9 (10)
C7—C8—C9—C4	-0.2 (8)	C24—C31—C36—C35	176.8 (6)
C7—C8—C9—C24	175.1 (5)	C34—C35—C36—C31	1.8 (13)
C5—C4—C9—C8	-0.1 (7)	C40—N3—C39—N2	179.1 (5)
N1—C4—C9—C8	179.1 (4)	C40—N3—C39—S1	-1.4 (6)
C5—C4—C9—C24	-175.7 (4)	C1—N2—C39—N3	-155.7 (5)
N1—C4—C9—C24	3.5 (6)	C3—N2—C39—N3	20.8 (8)
C6—C5—C10—C11	37.3 (7)	C1—N2—C39—S1	24.8 (6)
C4—C5—C10—C11	-147.3 (5)	C3—N2—C39—S1	-158.6 (4)
C6—C5—C10—C17	-90.5 (6)	C41—S1—C39—N3	1.7 (5)
C4—C5—C10—C17	84.9 (6)	C41—S1—C39—N2	-178.8 (4)
C5—C10—C11—C16	-129.1 (6)	C39—N3—C40—C41	0.2 (8)
C17—C10—C11—C16	-1.7 (8)	C39—N3—C40—C45	179.4 (6)
C5—C10—C11—C12	56.2 (7)	N3—C40—C41—C42	-178.9 (6)
C17—C10—C11—C12	-176.4 (6)	C45—C40—C41—C42	1.9 (10)
C16—C11—C12—C13	-1.3 (11)	N3—C40—C41—S1	1.0 (7)
C10—C11—C12—C13	173.7 (7)	C45—C40—C41—S1	-178.2 (5)
C11—C12—C13—C14	0.6 (13)	C39—S1—C41—C42	178.5 (7)
C12—C13—C14—C15	0.6 (14)	C39—S1—C41—C40	-1.4 (5)
C13—C14—C15—C16	-1.0 (14)	C40—C41—C42—C43	-2.0 (11)
C12—C11—C16—C15	1.0 (10)	S1—C41—C42—C43	178.1 (6)
C10—C11—C16—C15	-173.8 (6)	C41—C42—C43—C44	-0.1 (12)
C14—C15—C16—C11	0.2 (12)	C42—C43—C44—C45	2.4 (12)
C5—C10—C17—C18	-135.5 (6)	N3—C40—C45—C44	-178.8 (6)
C11—C10—C17—C18	96.0 (7)	C41—C40—C45—C44	0.3 (10)
C5—C10—C17—C22	42.9 (7)	C43—C44—C45—C40	-2.4 (11)
C11—C10—C17—C22	-85.6 (7)		
[Ag(IPr*^{MeOThia})Cl] 4b			
Ag1—C1	2.088 (7)	C20—H20	0.9300
Ag1—Cl1	2.314 (2)	C21—C22	1.388 (16)

S1—C40	1.724 (8)	C21—H21	0.9300
S1—C39	1.734 (9)	C22—H22	0.9300
O1—C7	1.360 (9)	C23—H23A	0.9600
O1—C23	1.438 (9)	C23—H23B	0.9600
N1—C1	1.339 (9)	C23—H23C	0.9600
N1—C2	1.399 (9)	C24—C31	1.520 (11)
N1—C4	1.450 (9)	C24—C25	1.527 (11)
C1—N2	1.365 (9)	C24—H24	0.9800
N2—C3	1.417 (9)	C25—C30	1.368 (14)
N2—C39	1.421 (10)	C25—C26	1.372 (12)
C2—C3	1.333 (11)	C26—C27	1.409 (17)
C2—C37	1.488 (11)	C26—H26	0.9300
N3—C39	1.297 (10)	C27—C28	1.40 (2)
N3—C41	1.386 (11)	C27—H27	0.9300
C3—C38	1.489 (11)	C28—C29	1.31 (2)
C4—C9	1.397 (9)	C28—H28	0.9300
C4—C5	1.410 (9)	C29—C30	1.394 (14)
C5—C6	1.374 (9)	C29—H29	0.9300
C5—C10	1.524 (9)	C30—H30	0.9300
C7—C6	1.398 (10)	C31—C36	1.374 (12)
C7—C8	1.399 (10)	C31—C32	1.396 (11)
C6—H6	0.9300	C32—C33	1.383 (14)
C8—C9	1.410 (11)	C32—H32	0.9300
C8—H8	0.9300	C33—C34	1.354 (17)
C9—C24	1.522 (10)	C33—H33	0.9300
C10—C17	1.536 (11)	C34—C35	1.369 (16)
C10—C11	1.539 (12)	C34—H34	0.9300
C10—H10	0.9800	C35—C36	1.375 (13)
C11—C16	1.364 (14)	C35—H35	0.9300
C11—C12	1.375 (12)	C36—H36	0.9300
C12—C13	1.389 (14)	C37—H37A	0.9600
C12—H12	0.9300	C37—H37B	0.9600
C13—C14	1.381 (17)	C37—H37C	0.9600
C13—H13	0.9300	C38—H38A	0.9600
C14—C15	1.356 (19)	C38—H38B	0.9600
C14—H14	0.9300	C38—H38C	0.9600
C16—C15	1.377 (14)	C40—C41	1.400 (12)
C16—H16	0.9300	C40—C45	1.409 (12)
C15—H15	0.9300	C41—C42	1.383 (11)
C17—C22	1.379 (14)	C42—C43	1.333 (14)
C17—C18	1.382 (11)	C42—H42	0.9300
C18—C19	1.371 (14)	C43—C44	1.387 (15)
C18—H18	0.9300	C43—H43	0.9300
C19—C20	1.370 (17)	C44—C45	1.359 (14)
C19—H19	0.9300	C44—H44	0.9300
C20—C21	1.377 (18)	C45—H45	0.9300
C1—Ag1—Cl1	175.8 (2)	O1—C23—H23B	109.5
C40—S1—C39	87.4 (4)	H23A—C23—H23B	109.5

C7—O1—C23	117.6 (6)	O1—C23—H23C	109.5
C1—N1—C2	112.3 (6)	H23A—C23—H23C	109.5
C1—N1—C4	124.0 (6)	H23B—C23—H23C	109.5
C2—N1—C4	123.3 (6)	C31—C24—C9	111.9 (6)
N1—C1—N2	103.8 (6)	C31—C24—C25	111.6 (5)
N1—C1—Ag1	128.9 (5)	C9—C24—C25	114.8 (6)
N2—C1—Ag1	127.3 (5)	C31—C24—H24	105.9
C1—N2—C3	111.1 (6)	C9—C24—H24	105.9
C1—N2—C39	123.6 (6)	C25—C24—H24	105.9
C3—N2—C39	125.4 (6)	C30—C25—C26	117.7 (9)
C3—C2—N1	106.9 (7)	C30—C25—C24	123.0 (8)
C3—C2—C37	130.8 (7)	C26—C25—C24	119.2 (9)
N1—C2—C37	122.3 (7)	C25—C26—C27	120.1 (12)
C39—N3—C41	109.1 (7)	C25—C26—H26	120.0
C2—C3—N2	105.9 (6)	C27—C26—H26	120.0
C2—C3—C38	129.7 (8)	C28—C27—C26	119.7 (13)
N2—C3—C38	124.3 (8)	C28—C27—H27	120.2
C9—C4—C5	122.8 (7)	C26—C27—H27	120.2
C9—C4—N1	118.9 (6)	C29—C28—C27	119.7 (13)
C5—C4—N1	118.2 (6)	C29—C28—H28	120.2
C6—C5—C4	117.9 (6)	C27—C28—H28	120.2
C6—C5—C10	121.7 (6)	C28—C29—C30	120.8 (14)
C4—C5—C10	120.3 (6)	C28—C29—H29	119.6
O1—C7—C6	115.6 (7)	C30—C29—H29	119.6
O1—C7—C8	124.2 (7)	C25—C30—C29	122.0 (12)
C6—C7—C8	120.1 (7)	C25—C30—H30	119.0
C5—C6—C7	121.3 (7)	C29—C30—H30	119.0
C5—C6—H6	119.3	C36—C31—C32	116.7 (8)
C7—C6—H6	119.3	C36—C31—C24	124.6 (7)
C7—C8—C9	120.2 (7)	C32—C31—C24	118.7 (8)
C7—C8—H8	119.9	C33—C32—C31	120.4 (10)
C9—C8—H8	119.9	C33—C32—H32	119.8
C4—C9—C8	117.6 (7)	C31—C32—H32	119.8
C4—C9—C24	121.6 (7)	C34—C33—C32	121.8 (10)
C8—C9—C24	120.5 (6)	C34—C33—H33	119.1
C5—C10—C17	110.2 (6)	C32—C33—H33	119.1
C5—C10—C11	112.6 (6)	C33—C34—C35	118.4 (11)
C17—C10—C11	115.1 (6)	C33—C34—H34	120.8
C5—C10—H10	106.1	C35—C34—H34	120.8
C17—C10—H10	106.1	C34—C35—C36	120.5 (11)
C11—C10—H10	106.1	C34—C35—H35	119.7
C16—C11—C12	118.7 (9)	C36—C35—H35	119.7
C16—C11—C10	121.9 (8)	C31—C36—C35	122.2 (9)
C12—C11—C10	119.4 (8)	C31—C36—H36	118.9
C11—C12—C13	120.2 (10)	C35—C36—H36	118.9
C11—C12—H12	119.9	C2—C37—H37A	109.5
C13—C12—H12	119.9	C2—C37—H37B	109.5
C14—C13—C12	120.3 (10)	H37A—C37—H37B	109.5
C14—C13—H13	119.9	C2—C37—H37C	109.5

C12—C13—H13	119.9	H37A—C37—H37C	109.5
C15—C14—C13	118.9 (11)	H37B—C37—H37C	109.5
C15—C14—H14	120.5	C3—C38—H38A	109.5
C13—C14—H14	120.5	C3—C38—H38B	109.5
C11—C16—C15	121.2 (11)	H38A—C38—H38B	109.5
C11—C16—H16	119.4	C3—C38—H38C	109.5
C15—C16—H16	119.4	H38A—C38—H38C	109.5
C14—C15—C16	120.7 (13)	H38B—C38—H38C	109.5
C14—C15—H15	119.7	N3—C39—N2	122.2 (8)
C16—C15—H15	119.7	N3—C39—S1	118.2 (6)
C22—C17—C18	118.0 (8)	N2—C39—S1	119.5 (6)
C22—C17—C10	118.7 (8)	C41—C40—C45	120.2 (8)
C18—C17—C10	123.4 (8)	C41—C40—S1	110.9 (6)
C19—C18—C17	120.7 (10)	C45—C40—S1	128.9 (7)
C19—C18—H18	119.7	C42—C41—N3	126.6 (9)
C17—C18—H18	119.7	C42—C41—C40	119.0 (9)
C20—C19—C18	120.8 (10)	N3—C41—C40	114.4 (8)
C20—C19—H19	119.6	C43—C42—C41	120.4 (10)
C18—C19—H19	119.6	C43—C42—H42	119.8
C19—C20—C21	119.8 (10)	C41—C42—H42	119.8
C19—C20—H20	120.1	C42—C43—C44	121.2 (9)
C21—C20—H20	120.1	C42—C43—H43	119.4
C20—C21—C22	118.8 (12)	C44—C43—H43	119.4
C20—C21—H21	120.6	C45—C44—C43	121.0 (9)
C22—C21—H21	120.6	C45—C44—H44	119.5
C17—C22—C21	121.8 (11)	C43—C44—H44	119.5
C17—C22—H22	119.1	C44—C45—C40	118.1 (10)
C21—C22—H22	119.1	C44—C45—H45	121.0
O1—C23—H23A	109.5	C40—C45—H45	121.0
C2—N1—C1—N2	-0.3 (7)	C11—C10—C17—C18	19.5 (11)
C4—N1—C1—N2	-173.3 (5)	C22—C17—C18—C19	-0.2 (13)
C2—N1—C1—Ag1	178.0 (5)	C10—C17—C18—C19	179.4 (8)
C4—N1—C1—Ag1	5.0 (9)	C17—C18—C19—C20	1.5 (16)
N1—C1—N2—C3	0.6 (7)	C18—C19—C20—C21	-1.8 (18)
Ag1—C1—N2—C3	-177.7 (5)	C19—C20—C21—C22	0.9 (18)
N1—C1—N2—C39	-178.0 (6)	C18—C17—C22—C21	-0.7 (15)
Ag1—C1—N2—C39	3.6 (9)	C10—C17—C22—C21	179.7 (9)
C1—N1—C2—C3	-0.1 (8)	C20—C21—C22—C17	0.3 (18)
C4—N1—C2—C3	173.0 (6)	C4—C9—C24—C31	94.4 (9)
C1—N1—C2—C37	-179.4 (6)	C8—C9—C24—C31	-80.0 (9)
C4—N1—C2—C37	-6.3 (10)	C4—C9—C24—C25	-137.1 (8)
N1—C2—C3—N2	0.4 (7)	C8—C9—C24—C25	48.5 (10)
C37—C2—C3—N2	179.7 (7)	C31—C24—C25—C30	53.2 (10)
N1—C2—C3—C38	-176.1 (8)	C9—C24—C25—C30	-75.5 (10)
C37—C2—C3—C38	3.1 (14)	C31—C24—C25—C26	-122.0 (8)
C1—N2—C3—C2	-0.7 (7)	C9—C24—C25—C26	109.3 (9)
C39—N2—C3—C2	177.9 (6)	C30—C25—C26—C27	-0.1 (15)
C1—N2—C3—C38	176.1 (7)	C24—C25—C26—C27	175.3 (9)

C39—N2—C3—C38	-5.3 (11)	C25—C26—C27—C28	2.4 (19)
C1—N1—C4—C9	-97.2 (8)	C26—C27—C28—C29	-2 (2)
C2—N1—C4—C9	90.6 (8)	C27—C28—C29—C30	-1 (2)
C1—N1—C4—C5	87.6 (8)	C26—C25—C30—C29	-2.5 (15)
C2—N1—C4—C5	-84.7 (8)	C24—C25—C30—C29	-177.8 (9)
C9—C4—C5—C6	0.9 (11)	C28—C29—C30—C25	2.9 (18)
N1—C4—C5—C6	175.9 (6)	C9—C24—C31—C36	6.4 (11)
C9—C4—C5—C10	177.2 (7)	C25—C24—C31—C36	-123.8 (9)
N1—C4—C5—C10	-7.7 (10)	C9—C24—C31—C32	-173.8 (7)
C23—O1—C7—C6	-163.3 (8)	C25—C24—C31—C32	55.9 (9)
C23—O1—C7—C8	13.2 (13)	C36—C31—C32—C33	-0.8 (12)
C4—C5—C6—C7	-2.5 (11)	C24—C31—C32—C33	179.5 (9)
C10—C5—C6—C7	-178.8 (7)	C31—C32—C33—C34	1.1 (15)
O1—C7—C6—C5	179.8 (7)	C32—C33—C34—C35	-1.6 (17)
C8—C7—C6—C5	3.1 (12)	C33—C34—C35—C36	1.8 (17)
O1—C7—C8—C9	-178.4 (8)	C32—C31—C36—C35	1.0 (13)
C6—C7—C8—C9	-2.0 (13)	C24—C31—C36—C35	-179.3 (9)
C5—C4—C9—C8	0.2 (12)	C34—C35—C36—C31	-1.5 (17)
N1—C4—C9—C8	-174.8 (7)	C41—N3—C39—N2	178.6 (6)
C5—C4—C9—C24	-174.3 (7)	C41—N3—C39—S1	1.1 (9)
N1—C4—C9—C24	10.7 (11)	C1—N2—C39—N3	139.0 (7)
C7—C8—C9—C4	0.3 (12)	C3—N2—C39—N3	-39.4 (10)
C7—C8—C9—C24	174.9 (7)	C1—N2—C39—S1	-43.5 (9)
C6—C5—C10—C17	34.1 (10)	C3—N2—C39—S1	138.1 (6)
C4—C5—C10—C17	-142.1 (7)	C40—S1—C39—N3	-0.4 (7)
C6—C5—C10—C11	-95.9 (8)	C40—S1—C39—N2	-178.0 (6)
C4—C5—C10—C11	87.9 (8)	C39—S1—C40—C41	-0.4 (6)
C5—C10—C11—C16	51.1 (10)	C39—S1—C40—C45	-179.8 (8)
C17—C10—C11—C16	-76.3 (10)	C39—N3—C41—C42	178.0 (8)
C5—C10—C11—C12	-128.5 (7)	C39—N3—C41—C40	-1.5 (10)
C17—C10—C11—C12	104.0 (9)	C45—C40—C41—C42	1.1 (12)
C16—C11—C12—C13	-0.6 (13)	S1—C40—C41—C42	-178.4 (6)
C10—C11—C12—C13	179.1 (7)	C45—C40—C41—N3	-179.4 (7)
C11—C12—C13—C14	-1.0 (14)	S1—C40—C41—N3	1.2 (9)
C12—C13—C14—C15	3.1 (16)	N3—C41—C42—C43	178.5 (9)
C12—C11—C16—C15	0.1 (15)	C40—C41—C42—C43	-2.0 (14)
C10—C11—C16—C15	-179.6 (9)	C41—C42—C43—C44	1.1 (15)
C13—C14—C15—C16	-3.7 (17)	C42—C43—C44—C45	0.7 (16)
C11—C16—C15—C14	2.1 (18)	C43—C44—C45—C40	-1.5 (15)
C5—C10—C17—C22	70.6 (10)	C41—C40—C45—C44	0.7 (13)
C11—C10—C17—C22	-160.8 (8)	S1—C40—C45—C44	180.0 (7)
C5—C10—C17—C18	-109.1 (8)		

[Pd(IPr*^{Thia})Cl_2] 5a

Pd1—C1	1.985 (5)	C20—H20	0.9300
Pd1—N3	2.091 (4)	C21—C22	1.376 (8)
Pd1—Cl1	2.2752 (14)	C21—H21	0.9300
Pd1—Cl2	2.3563 (12)	C22—H22	0.9300
Cl4A—C46	1.83 (2)	C23—H23A	0.9600

Cl3A—C46	1.72 (2)	C23—H23B	0.9600
Cl4B—C46	1.69 (2)	C23—H23C	0.9600
Cl3B—C46	1.816 (16)	C24—C31	1.525 (7)
Cl5A—C47	1.757 (11)	C24—C25	1.530 (7)
Cl6A—C47	1.64 (2)	C24—H24	0.9800
Cl5B—C47	1.623 (11)	C25—C30	1.382 (7)
Cl6B—C47	1.81 (2)	C25—C26	1.396 (8)
S1—C39	1.719 (5)	C26—C27	1.387 (8)
S1—C41	1.737 (5)	C26—H26	0.9300
N1—C1	1.344 (6)	C27—C28	1.384 (8)
N1—C2	1.418 (6)	C27—H27	0.9300
N1—C4	1.440 (6)	C28—C29	1.370 (9)
N2—C1	1.368 (6)	C28—H28	0.9300
N2—C39	1.380 (6)	C29—C30	1.388 (8)
N2—C3	1.424 (6)	C29—H29	0.9300
N3—C39	1.319 (6)	C30—H30	0.9300
N3—C40	1.389 (6)	C31—C32	1.385 (7)
C2—C3	1.341 (7)	C31—C36	1.406 (7)
C2—C37	1.506 (6)	C32—C33	1.385 (8)
C3—C38	1.488 (7)	C32—H32	0.9300
C4—C5	1.394 (7)	C33—C34	1.382 (8)
C4—C9	1.414 (7)	C33—H33	0.9300
C5—C6	1.404 (7)	C34—C35	1.390 (8)
C5—C10	1.522 (8)	C34—H34	0.9300
C6—C7	1.376 (8)	C35—C36	1.397 (7)
C6—H6	0.9300	C35—H35	0.9300
C7—C8	1.384 (8)	C36—H36	0.9300
C7—C23	1.487 (8)	C37—H37A	0.9600
C8—C9	1.398 (7)	C37—H37B	0.9600
C8—H8	0.9300	C37—H37C	0.9600
C9—C24	1.525 (7)	C38—H38A	0.9600
C10—C11	1.503 (8)	C38—H38B	0.9600
C10—C17	1.518 (7)	C38—H38C	0.9600
C10—H10	0.9800	C40—C41	1.391 (7)
C11—C12	1.391 (8)	C40—C45	1.411 (7)
C11—C16	1.405 (7)	C41—C42	1.393 (7)
C12—C13	1.386 (8)	C42—C43	1.398 (8)
C12—H12	0.9300	C42—H42	0.9300
C13—C14	1.402 (8)	C43—C44	1.404 (8)
C13—H13	0.9300	C43—H43	0.9300
C14—C15	1.363 (9)	C44—C45	1.367 (7)
C14—H14	0.9300	C44—H44	0.9300
C15—C16	1.389 (8)	C45—H45	0.9300
C15—H15	0.9300	C46—H46A	0.9700
C16—H16	0.9300	C46—H46B	0.9700
C17—C22	1.392 (8)	C46—H46C	0.9700
C17—C18	1.393 (8)	C46—H46D	0.9700
C18—C19	1.396 (8)	C47—H47A	0.9700
C18—H18	0.9300	C47—H47B	0.9700

C19—C20	1.390 (10)	C47—H47C	0.9700
C19—H19	0.9300	C47—H47D	0.9700
C20—C21	1.360 (10)		
C1—Pd1—N3	80.42 (18)	C31—C24—H24	105.3
C1—Pd1—Cl1	93.22 (14)	C25—C24—H24	105.3
N3—Pd1—Cl1	173.35 (12)	C30—C25—C26	118.0 (5)
C1—Pd1—Cl2	177.45 (14)	C30—C25—C24	118.5 (5)
N3—Pd1—Cl2	97.09 (12)	C26—C25—C24	123.6 (5)
Cl1—Pd1—Cl2	89.25 (5)	C27—C26—C25	120.3 (5)
C39—S1—C41	88.2 (2)	C27—C26—H26	119.8
C1—N1—C2	110.5 (4)	C25—C26—H26	119.8
C1—N1—C4	128.4 (4)	C28—C27—C26	120.8 (6)
C2—N1—C4	121.1 (4)	C28—C27—H27	119.6
C1—N2—C39	117.6 (4)	C26—C27—H27	119.6
C1—N2—C3	110.9 (4)	C29—C28—C27	119.1 (6)
C39—N2—C3	131.5 (4)	C29—C28—H28	120.4
C39—N3—C40	110.3 (4)	C27—C28—H28	120.4
C39—N3—Pd1	111.0 (3)	C28—C29—C30	120.3 (5)
C40—N3—Pd1	138.4 (3)	C28—C29—H29	119.8
N1—C1—N2	105.3 (4)	C30—C29—H29	119.8
N1—C1—Pd1	141.9 (4)	C25—C30—C29	121.4 (6)
N2—C1—Pd1	112.8 (3)	C25—C30—H30	119.3
C3—C2—N1	107.8 (4)	C29—C30—H30	119.3
C3—C2—C37	128.9 (4)	C32—C31—C36	118.3 (5)
N1—C2—C37	123.2 (4)	C32—C31—C24	119.1 (5)
C2—C3—N2	105.5 (4)	C36—C31—C24	122.7 (5)
C2—C3—C38	130.3 (4)	C33—C32—C31	121.7 (5)
N2—C3—C38	124.2 (4)	C33—C32—H32	119.2
C5—C4—C9	121.5 (4)	C31—C32—H32	119.2
C5—C4—N1	119.5 (5)	C34—C33—C32	119.5 (5)
C9—C4—N1	118.8 (4)	C34—C33—H33	120.2
C4—C5—C6	117.5 (5)	C32—C33—H33	120.2
C4—C5—C10	120.1 (4)	C33—C34—C35	120.6 (5)
C6—C5—C10	122.2 (5)	C33—C34—H34	119.7
C7—C6—C5	122.4 (5)	C35—C34—H34	119.7
C7—C6—H6	118.8	C34—C35—C36	119.4 (5)
C5—C6—H6	118.8	C34—C35—H35	120.3
C6—C7—C8	118.6 (5)	C36—C35—H35	120.3
C6—C7—C23	120.7 (5)	C35—C36—C31	120.5 (5)
C8—C7—C23	120.6 (6)	C35—C36—H36	119.7
C7—C8—C9	122.1 (5)	C31—C36—H36	119.7
C7—C8—H8	119.0	C2—C37—H37A	109.5
C9—C8—H8	119.0	C2—C37—H37B	109.5
C8—C9—C4	117.5 (5)	H37A—C37—H37B	109.5
C8—C9—C24	123.2 (5)	C2—C37—H37C	109.5
C4—C9—C24	119.2 (4)	H37A—C37—H37C	109.5
C11—C10—C17	113.8 (4)	H37B—C37—H37C	109.5
C11—C10—C5	113.4 (4)	C3—C38—H38A	109.5

C17—C10—C5	112.1 (4)	C3—C38—H38B	109.5
C11—C10—H10	105.6	H38A—C38—H38B	109.5
C17—C10—H10	105.6	C3—C38—H38C	109.5
C5—C10—H10	105.6	H38A—C38—H38C	109.5
C12—C11—C16	117.2 (5)	H38B—C38—H38C	109.5
C12—C11—C10	119.9 (5)	N3—C39—N2	118.0 (4)
C16—C11—C10	122.8 (5)	N3—C39—S1	116.8 (4)
C13—C12—C11	121.9 (5)	N2—C39—S1	125.2 (4)
C13—C12—H12	119.0	N3—C40—C41	113.7 (4)
C11—C12—H12	119.0	N3—C40—C45	127.5 (5)
C12—C13—C14	118.9 (6)	C41—C40—C45	118.9 (5)
C12—C13—H13	120.5	C40—C41—C42	122.4 (5)
C14—C13—H13	120.5	C40—C41—S1	111.0 (4)
C15—C14—C13	120.6 (6)	C42—C41—S1	126.5 (4)
C15—C14—H14	119.7	C41—C42—C43	117.6 (5)
C13—C14—H14	119.7	C41—C42—H42	121.2
C14—C15—C16	119.8 (6)	C43—C42—H42	121.2
C14—C15—H15	120.1	C42—C43—C44	120.4 (5)
C16—C15—H15	120.1	C42—C43—H43	119.8
C15—C16—C11	121.5 (6)	C44—C43—H43	119.8
C15—C16—H16	119.3	C45—C44—C43	121.2 (5)
C11—C16—H16	119.3	C45—C44—H44	119.4
C22—C17—C18	118.7 (5)	C43—C44—H44	119.4
C22—C17—C10	119.0 (5)	C44—C45—C40	119.5 (5)
C18—C17—C10	122.3 (5)	C44—C45—H45	120.3
C17—C18—C19	119.2 (6)	C40—C45—H45	120.3
C17—C18—H18	120.4	Cl4B—C46—Cl3B	112.9 (9)
C19—C18—H18	120.4	Cl3A—C46—Cl4A	108.7 (10)
C20—C19—C18	120.7 (6)	Cl3A—C46—H46A	110.0
C20—C19—H19	119.7	Cl4A—C46—H46A	110.0
C18—C19—H19	119.7	Cl3A—C46—H46B	110.0
C21—C20—C19	119.9 (6)	Cl4A—C46—H46B	110.0
C21—C20—H20	120.0	H46A—C46—H46B	108.3
C19—C20—H20	120.0	Cl4B—C46—H46C	109.0
C20—C21—C22	120.0 (6)	Cl3B—C46—H46C	109.0
C20—C21—H21	120.0	Cl4B—C46—H46D	109.0
C22—C21—H21	120.0	Cl3B—C46—H46D	109.0
C21—C22—C17	121.5 (6)	H46C—C46—H46D	107.8
C21—C22—H22	119.2	Cl6A—C47—Cl5A	114.7 (7)
C17—C22—H22	119.2	Cl5B—C47—Cl6B	116.3 (7)
C7—C23—H23A	109.5	Cl6A—C47—H47A	108.6
C7—C23—H23B	109.5	Cl5A—C47—H47A	108.6
H23A—C23—H23B	109.5	Cl6A—C47—H47B	108.6
C7—C23—H23C	109.5	Cl5A—C47—H47B	108.6
H23A—C23—H23C	109.5	H47A—C47—H47B	107.6
H23B—C23—H23C	109.5	Cl5B—C47—H47C	108.2
C9—C24—C31	114.0 (4)	Cl6B—C47—H47C	108.2
C9—C24—C25	112.7 (4)	Cl5B—C47—H47D	108.2
C31—C24—C25	113.1 (4)	Cl6B—C47—H47D	108.2

C9—C24—H24	105.3	H47C—C47—H47D	107.4
C2—N1—C1—N2	-1.0 (5)	C17—C18—C19—C20	0.6 (9)
C4—N1—C1—N2	-178.8 (4)	C18—C19—C20—C21	-1.6 (10)
C2—N1—C1—Pd1	-179.0 (5)	C19—C20—C21—C22	1.3 (10)
C4—N1—C1—Pd1	3.1 (9)	C20—C21—C22—C17	-0.1 (9)
C39—N2—C1—N1	178.5 (4)	C18—C17—C22—C21	-0.9 (8)
C3—N2—C1—N1	1.0 (6)	C10—C17—C22—C21	-179.3 (5)
C39—N2—C1—Pd1	-2.7 (6)	C8—C9—C24—C31	101.4 (6)
C3—N2—C1—Pd1	179.8 (3)	C4—C9—C24—C31	-82.5 (6)
C1—N1—C2—C3	0.5 (6)	C8—C9—C24—C25	-29.3 (6)
C4—N1—C2—C3	178.6 (4)	C4—C9—C24—C25	146.7 (4)
C1—N1—C2—C37	-177.7 (5)	C9—C24—C25—C30	-101.5 (6)
C4—N1—C2—C37	0.3 (7)	C31—C24—C25—C30	127.3 (5)
N1—C2—C3—N2	0.1 (5)	C9—C24—C25—C26	77.9 (6)
C37—C2—C3—N2	178.2 (5)	C31—C24—C25—C26	-53.2 (7)
N1—C2—C3—C38	178.4 (5)	C30—C25—C26—C27	0.6 (8)
C37—C2—C3—C38	-3.4 (10)	C24—C25—C26—C27	-178.8 (5)
C1—N2—C3—C2	-0.7 (6)	C25—C26—C27—C28	-1.0 (8)
C39—N2—C3—C2	-177.8 (5)	C26—C27—C28—C29	-0.4 (9)
C1—N2—C3—C38	-179.2 (5)	C27—C28—C29—C30	2.1 (9)
C39—N2—C3—C38	3.8 (9)	C26—C25—C30—C29	1.1 (8)
C1—N1—C4—C5	85.9 (6)	C24—C25—C30—C29	-179.4 (5)
C2—N1—C4—C5	-91.8 (5)	C28—C29—C30—C25	-2.5 (9)
C1—N1—C4—C9	-98.1 (6)	C9—C24—C31—C32	127.4 (5)
C2—N1—C4—C9	84.3 (6)	C25—C24—C31—C32	-102.0 (6)
C9—C4—C5—C6	-5.6 (7)	C9—C24—C31—C36	-53.2 (7)
N1—C4—C5—C6	170.3 (4)	C25—C24—C31—C36	77.3 (6)
C9—C4—C5—C10	170.4 (4)	C36—C31—C32—C33	1.4 (8)
N1—C4—C5—C10	-13.7 (7)	C24—C31—C32—C33	-179.2 (5)
C4—C5—C6—C7	-0.5 (7)	C31—C32—C33—C34	-1.8 (9)
C10—C5—C6—C7	-176.4 (5)	C32—C33—C34—C35	0.7 (8)
C5—C6—C7—C8	4.8 (8)	C33—C34—C35—C36	0.7 (8)
C5—C6—C7—C23	-179.3 (5)	C34—C35—C36—C31	-1.0 (8)
C6—C7—C8—C9	-3.1 (7)	C32—C31—C36—C35	0.0 (8)
C23—C7—C8—C9	-179.0 (5)	C24—C31—C36—C35	-179.4 (5)
C7—C8—C9—C4	-2.7 (7)	C40—N3—C39—N2	178.2 (4)
C7—C8—C9—C24	173.4 (4)	Pd1—N3—C39—N2	2.9 (6)
C5—C4—C9—C8	7.2 (7)	C40—N3—C39—S1	1.3 (6)
N1—C4—C9—C8	-168.8 (4)	Pd1—N3—C39—S1	-174.1 (2)
C5—C4—C9—C24	-169.1 (4)	C1—N2—C39—N3	-0.2 (7)
N1—C4—C9—C24	15.0 (6)	C3—N2—C39—N3	176.6 (5)
C4—C5—C10—C11	75.3 (6)	C1—N2—C39—S1	176.4 (4)
C6—C5—C10—C11	-108.9 (5)	C3—N2—C39—S1	-6.7 (8)
C4—C5—C10—C17	-154.2 (4)	C41—S1—C39—N3	-1.4 (4)
C6—C5—C10—C17	21.6 (7)	C41—S1—C39—N2	-178.1 (5)
C17—C10—C11—C12	97.2 (6)	C39—N3—C40—C41	-0.4 (6)
C5—C10—C11—C12	-133.2 (5)	Pd1—N3—C40—C41	173.0 (4)
C17—C10—C11—C16	-79.8 (6)	C39—N3—C40—C45	178.5 (5)

C5—C10—C11—C16	49.9 (7)	Pd1—N3—C40—C45	-8.1 (9)
C16—C11—C12—C13	-1.0 (8)	N3—C40—C41—C42	178.3 (5)
C10—C11—C12—C13	-178.2 (5)	C45—C40—C41—C42	-0.7 (8)
C11—C12—C13—C14	2.0 (8)	N3—C40—C41—S1	-0.5 (6)
C12—C13—C14—C15	-1.6 (9)	C45—C40—C41—S1	-179.5 (4)
C13—C14—C15—C16	0.2 (9)	C39—S1—C41—C40	1.0 (4)
C14—C15—C16—C11	0.7 (9)	C39—S1—C41—C42	-177.8 (5)
C12—C11—C16—C15	-0.3 (8)	C40—C41—C42—C43	0.7 (8)
C10—C11—C16—C15	176.7 (5)	S1—C41—C42—C43	179.4 (4)
C11—C10—C17—C22	-152.0 (5)	C41—C42—C43—C44	-0.6 (8)
C5—C10—C17—C22	77.7 (6)	C42—C43—C44—C45	0.5 (9)
C11—C10—C17—C18	29.7 (7)	C43—C44—C45—C40	-0.5 (8)
C5—C10—C17—C18	-100.6 (6)	N3—C40—C45—C44	-178.3 (5)
C22—C17—C18—C19	0.6 (8)	C41—C40—C45—C44	0.6 (8)
C10—C17—C18—C19	178.9 (5)		

[Pd(IPr*^{MeOThia})Cl_2] 5b

Pd1—C1	1.966 (2)	C20—C25	1.397 (3)
Pd1—N3	2.091 (2)	C21—C22	1.391 (3)
Pd1—Cl2	2.2642 (6)	C21—H21	0.9500
Pd1—Cl1	2.3508 (6)	C22—C23	1.382 (4)
S1—C4	1.718 (2)	C22—H22	0.9500
S1—C6	1.743 (3)	C23—C24	1.386 (4)
N1—C1	1.377 (3)	C23—H23	0.9500
N1—C4	1.385 (3)	C24—C25	1.389 (4)
N1—C2	1.402 (3)	C24—H24	0.9500
N2—C1	1.345 (3)	C25—H25	0.9500
N2—C3	1.412 (3)	C26—C27	1.393 (3)
N2—C13	1.455 (3)	C26—C31	1.400 (3)
N3—C4	1.304 (3)	C27—C28	1.389 (4)
N3—C5	1.399 (3)	C27—H27	0.9500
O1—C16	1.368 (3)	C28—C29	1.386 (4)
O1—C32	1.423 (3)	C28—H28	0.9500
C2—C3	1.337 (3)	C29—C30	1.388 (4)
C2—C11	1.493 (3)	C29—H29	0.9500
C3—C12	1.487 (3)	C30—C31	1.389 (3)
C5—C10	1.390 (4)	C30—H30	0.9500
C5—C6	1.404 (4)	C31—H31	0.9500
C6—C7	1.395 (3)	C32—H32A	0.9800
C7—C8	1.382 (4)	C32—H32B	0.9800
C7—H7	0.9500	C32—H32C	0.9800
C8—C9	1.401 (4)	C33—C34	1.530 (3)
C8—H8	0.9500	C33—C40	1.533 (4)
C9—C10	1.379 (4)	C33—H33	1.0000
C9—H9	0.9500	C34—C39	1.379 (5)
C10—H10	0.9500	C34—C35	1.393 (4)
C11—H11A	0.9800	C35—C36	1.391 (4)
C11—H11B	0.9800	C35—H35	0.9500
C11—H11C	0.9800	C36—C37	1.381 (6)
C12—H12A	0.9800	C36—H36	0.9500

C12—H12B	0.9800	C37—C38	1.369 (6)
C12—H12C	0.9800	C37—H37	0.9500
C13—C14	1.390 (3)	C38—C39	1.391 (5)
C13—C18	1.403 (3)	C38—H38	0.9500
C14—C15	1.395 (3)	C39—H39	0.9500
C14—C19	1.538 (3)	C40—C41	1.386 (5)
C15—C16	1.383 (3)	C40—C45	1.392 (4)
C15—H15	0.9500	C41—C42	1.398 (5)
C16—C17	1.397 (3)	C41—H41	0.9500
C17—C18	1.383 (3)	C42—C43	1.381 (6)
C17—H17	0.9500	C42—H42	0.9500
C18—C33	1.531 (3)	C43—C44	1.362 (6)
C19—C26	1.527 (3)	C43—H43	0.9500
C19—C20	1.536 (3)	C44—C45	1.413 (5)
C19—H19	1.0000	C44—H44	0.9500
C20—C21	1.394 (3)	C45—H45	0.9500
C1—Pd1—N3	79.77 (9)	C21—C20—C19	123.0 (2)
C1—Pd1—Cl2	93.61 (7)	C25—C20—C19	118.5 (2)
N3—Pd1—Cl2	173.38 (6)	C22—C21—C20	120.8 (2)
C1—Pd1—Cl1	172.78 (7)	C22—C21—H21	119.6
N3—Pd1—Cl1	97.80 (6)	C20—C21—H21	119.6
Cl2—Pd1—Cl1	88.78 (2)	C23—C22—C21	120.1 (2)
C4—S1—C6	88.06 (12)	C23—C22—H22	119.9
C1—N1—C4	116.5 (2)	C21—C22—H22	119.9
C1—N1—C2	111.6 (2)	C22—C23—C24	119.8 (2)
C4—N1—C2	131.9 (2)	C22—C23—H23	120.1
C1—N2—C3	111.07 (19)	C24—C23—H23	120.1
C1—N2—C13	127.2 (2)	C23—C24—C25	120.2 (2)
C3—N2—C13	121.72 (19)	C23—C24—H24	119.9
C4—N3—C5	110.6 (2)	C25—C24—H24	119.9
C4—N3—Pd1	111.57 (16)	C24—C25—C20	120.6 (2)
C5—N3—Pd1	136.63 (17)	C24—C25—H25	119.7
C16—O1—C32	116.79 (19)	C20—C25—H25	119.7
N2—C1—N1	104.0 (2)	C27—C26—C31	117.8 (2)
N2—C1—Pd1	142.13 (18)	C27—C26—C19	119.5 (2)
N1—C1—Pd1	113.77 (17)	C31—C26—C19	122.6 (2)
C3—C2—N1	105.8 (2)	C28—C27—C26	121.2 (2)
C3—C2—C11	129.5 (2)	C28—C27—H27	119.4
N1—C2—C11	124.5 (2)	C26—C27—H27	119.4
C2—C3—N2	107.5 (2)	C29—C28—C27	120.4 (3)
C2—C3—C12	129.3 (2)	C29—C28—H28	119.8
N2—C3—C12	123.1 (2)	C27—C28—H28	119.8
N3—C4—N1	117.3 (2)	C28—C29—C30	119.1 (2)
N3—C4—S1	117.47 (18)	C28—C29—H29	120.5
N1—C4—S1	125.15 (18)	C30—C29—H29	120.5
C10—C5—N3	127.7 (2)	C29—C30—C31	120.6 (2)
C10—C5—C6	119.3 (2)	C29—C30—H30	119.7
N3—C5—C6	112.9 (2)	C31—C30—H30	119.7

C7—C6—C5	122.3 (2)	C30—C31—C26	120.9 (2)
C7—C6—S1	126.8 (2)	C30—C31—H31	119.6
C5—C6—S1	110.88 (18)	C26—C31—H31	119.6
C8—C7—C6	117.1 (2)	O1—C32—H32A	109.5
C8—C7—H7	121.4	O1—C32—H32B	109.5
C6—C7—H7	121.4	H32A—C32—H32B	109.5
C7—C8—C9	121.0 (2)	O1—C32—H32C	109.5
C7—C8—H8	119.5	H32A—C32—H32C	109.5
C9—C8—H8	119.5	H32B—C32—H32C	109.5
C10—C9—C8	121.5 (3)	C34—C33—C18	111.7 (2)
C10—C9—H9	119.3	C34—C33—C40	113.7 (2)
C8—C9—H9	119.3	C18—C33—C40	110.1 (2)
C9—C10—C5	118.6 (3)	C34—C33—H33	107.0
C9—C10—H10	120.7	C18—C33—H33	107.0
C5—C10—H10	120.7	C40—C33—H33	107.0
C2—C11—H11A	109.5	C39—C34—C35	118.3 (3)
C2—C11—H11B	109.5	C39—C34—C33	123.4 (3)
H11A—C11—H11B	109.5	C35—C34—C33	118.3 (3)
C2—C11—H11C	109.5	C36—C35—C34	120.9 (3)
H11A—C11—H11C	109.5	C36—C35—H35	119.6
H11B—C11—H11C	109.5	C34—C35—H35	119.6
C3—C12—H12A	109.5	C37—C36—C35	119.7 (3)
C3—C12—H12B	109.5	C37—C36—H36	120.2
H12A—C12—H12B	109.5	C35—C36—H36	120.2
C3—C12—H12C	109.5	C38—C37—C36	119.9 (3)
H12A—C12—H12C	109.5	C38—C37—H37	120.0
H12B—C12—H12C	109.5	C36—C37—H37	120.0
C14—C13—C18	122.5 (2)	C37—C38—C39	120.3 (4)
C14—C13—N2	118.7 (2)	C37—C38—H38	119.8
C18—C13—N2	118.7 (2)	C39—C38—H38	119.8
C13—C14—C15	117.9 (2)	C34—C39—C38	120.9 (4)
C13—C14—C19	122.1 (2)	C34—C39—H39	119.6
C15—C14—C19	120.0 (2)	C38—C39—H39	119.6
C16—C15—C14	120.7 (2)	C41—C40—C45	118.5 (3)
C16—C15—H15	119.6	C41—C40—C33	122.3 (3)
C14—C15—H15	119.6	C45—C40—C33	119.2 (3)
O1—C16—C15	124.8 (2)	C40—C41—C42	121.2 (3)
O1—C16—C17	115.0 (2)	C40—C41—H41	119.4
C15—C16—C17	120.2 (2)	C42—C41—H41	119.4
C18—C17—C16	120.6 (2)	C43—C42—C41	119.6 (4)
C18—C17—H17	119.7	C43—C42—H42	120.2
C16—C17—H17	119.7	C41—C42—H42	120.2
C17—C18—C13	118.0 (2)	C44—C43—C42	120.4 (4)
C17—C18—C33	121.1 (2)	C44—C43—H43	119.8
C13—C18—C33	120.9 (2)	C42—C43—H43	119.8
C26—C19—C20	113.21 (19)	C43—C44—C45	120.2 (3)
C26—C19—C14	112.78 (19)	C43—C44—H44	119.9
C20—C19—C14	110.08 (18)	C45—C44—H44	119.9
C26—C19—H19	106.8	C40—C45—C44	120.1 (4)

C20—C19—H19	106.8	C40—C45—H45	120.0
C14—C19—H19	106.8	C44—C45—H45	120.0
C21—C20—C25	118.5 (2)		
C3—N2—C1—N1	1.6 (3)	C16—C17—C18—C13	0.6 (4)
C13—N2—C1—N1	178.8 (2)	C16—C17—C18—C33	-178.8 (2)
C3—N2—C1—Pd1	176.7 (2)	C14—C13—C18—C17	1.0 (4)
C13—N2—C1—Pd1	-6.0 (4)	N2—C13—C18—C17	-175.2 (2)
C4—N1—C1—N2	178.08 (19)	C14—C13—C18—C33	-179.6 (2)
C2—N1—C1—N2	-1.8 (3)	N2—C13—C18—C33	4.2 (4)
C4—N1—C1—Pd1	1.3 (3)	C13—C14—C19—C26	95.7 (3)
C2—N1—C1—Pd1	-178.61 (16)	C15—C14—C19—C26	-85.7 (3)
C1—N1—C2—C3	1.4 (3)	C13—C14—C19—C20	-136.8 (2)
C4—N1—C2—C3	-178.5 (2)	C15—C14—C19—C20	41.8 (3)
C1—N1—C2—C11	-173.0 (2)	C26—C19—C20—C21	28.6 (3)
C4—N1—C2—C11	7.1 (4)	C14—C19—C20—C21	-98.6 (3)
N1—C2—C3—N2	-0.4 (3)	C26—C19—C20—C25	-154.9 (2)
C11—C2—C3—N2	173.6 (3)	C14—C19—C20—C25	77.8 (3)
N1—C2—C3—C12	-177.5 (2)	C25—C20—C21—C22	-2.2 (3)
C11—C2—C3—C12	-3.5 (5)	C19—C20—C21—C22	174.3 (2)
C1—N2—C3—C2	-0.7 (3)	C20—C21—C22—C23	1.0 (4)
C13—N2—C3—C2	-178.2 (2)	C21—C22—C23—C24	0.9 (4)
C1—N2—C3—C12	176.6 (2)	C22—C23—C24—C25	-1.4 (4)
C13—N2—C3—C12	-0.9 (3)	C23—C24—C25—C20	0.2 (4)
C5—N3—C4—N1	179.1 (2)	C21—C20—C25—C24	1.6 (4)
Pd1—N3—C4—N1	-11.3 (3)	C19—C20—C25—C24	-175.0 (2)
C5—N3—C4—S1	-2.6 (3)	C20—C19—C26—C27	98.0 (3)
Pd1—N3—C4—S1	167.04 (12)	C14—C19—C26—C27	-136.2 (2)
C1—N1—C4—N3	7.1 (3)	C20—C19—C26—C31	-79.9 (3)
C2—N1—C4—N3	-173.0 (2)	C14—C19—C26—C31	45.9 (3)
C1—N1—C4—S1	-171.06 (18)	C31—C26—C27—C28	0.3 (4)
C2—N1—C4—S1	8.8 (4)	C19—C26—C27—C28	-177.7 (2)
C6—S1—C4—N3	1.1 (2)	C26—C27—C28—C29	-0.1 (4)
C6—S1—C4—N1	179.2 (2)	C27—C28—C29—C30	0.2 (4)
C4—N3—C5—C10	-174.5 (2)	C28—C29—C30—C31	-0.4 (4)
Pd1—N3—C5—C10	19.6 (4)	C29—C30—C31—C26	0.5 (4)
C4—N3—C5—C6	3.1 (3)	C27—C26—C31—C30	-0.5 (4)
Pd1—N3—C5—C6	-162.78 (17)	C19—C26—C31—C30	177.5 (2)
C10—C5—C6—C7	-3.7 (4)	C17—C18—C33—C34	-25.7 (4)
N3—C5—C6—C7	178.5 (2)	C13—C18—C33—C34	154.9 (3)
C10—C5—C6—S1	175.51 (19)	C17—C18—C33—C40	101.7 (3)
N3—C5—C6—S1	-2.3 (3)	C13—C18—C33—C40	-77.7 (3)
C4—S1—C6—C7	179.9 (2)	C18—C33—C34—C39	111.2 (3)
C4—S1—C6—C5	0.77 (19)	C40—C33—C34—C39	-14.2 (4)
C5—C6—C7—C8	0.9 (4)	C18—C33—C34—C35	-68.1 (3)
S1—C6—C7—C8	-178.2 (2)	C40—C33—C34—C35	166.5 (3)
C6—C7—C8—C9	2.3 (4)	C39—C34—C35—C36	-0.6 (5)
C7—C8—C9—C10	-2.7 (4)	C33—C34—C35—C36	178.7 (3)
C8—C9—C10—C5	-0.2 (4)	C34—C35—C36—C37	0.7 (5)

N3—C5—C10—C9	-179.3 (2)	C35—C36—C37—C38	-0.2 (6)
C6—C5—C10—C9	3.3 (4)	C36—C37—C38—C39	-0.5 (7)
C1—N2—C13—C14	100.7 (3)	C35—C34—C39—C38	-0.1 (6)
C3—N2—C13—C14	-82.3 (3)	C33—C34—C39—C38	-179.4 (4)
C1—N2—C13—C18	-83.0 (3)	C37—C38—C39—C34	0.7 (7)
C3—N2—C13—C18	94.0 (3)	C34—C33—C40—C41	77.8 (3)
C18—C13—C14—C15	-1.4 (4)	C18—C33—C40—C41	-48.4 (3)
N2—C13—C14—C15	174.8 (2)	C34—C33—C40—C45	-102.1 (3)
C18—C13—C14—C19	177.3 (2)	C18—C33—C40—C45	131.7 (3)
N2—C13—C14—C19	-6.6 (3)	C45—C40—C41—C42	0.5 (4)
C13—C14—C15—C16	0.1 (3)	C33—C40—C41—C42	-179.5 (3)
C19—C14—C15—C16	-178.5 (2)	C40—C41—C42—C43	-0.8 (5)
C32—O1—C16—C15	11.6 (3)	C41—C42—C43—C44	0.6 (5)
C32—O1—C16—C17	-169.5 (2)	C42—C43—C44—C45	-0.1 (5)
C14—C15—C16—O1	-179.7 (2)	C41—C40—C45—C44	0.1 (4)
C14—C15—C16—C17	1.4 (4)	C33—C40—C45—C44	-180.0 (3)
O1—C16—C17—C18	179.2 (2)	C43—C44—C45—C40	-0.3 (5)
C15—C16—C17—C18	-1.8 (4)		

[Se(IPr*^{MeOThia})Cl_2] 6b

Se1—C1	1.8198 (14)	C21—C22	1.388 (2)
S1—C45	1.7427 (15)	C21—H21	0.9500
S1—C39	1.7545 (15)	C22—H22	0.9500
O1—C7	1.3654 (17)	C23—H23A	0.9800
O1—C23	1.431 (2)	C23—H23B	0.9800
N1—C1	1.3576 (18)	C23—H23C	0.9800
N1—C2	1.3997 (17)	C24—C31	1.520 (2)
N1—C4	1.4432 (17)	C24—C25	1.526 (2)
N2—C1	1.3850 (17)	C24—H24	1.0000
N2—C39	1.4107 (18)	C25—C30	1.387 (2)
N2—C3	1.4250 (18)	C25—C26	1.401 (2)
N3—C39	1.2945 (18)	C26—C27	1.382 (2)
N3—C40	1.391 (2)	C26—H26	0.9500
C2—C3	1.343 (2)	C27—C28	1.390 (2)
C2—C37	1.491 (2)	C27—H27	0.9500
C3—C38	1.492 (2)	C28—C29	1.375 (2)
C4—C5	1.392 (2)	C28—H28	0.9500
C4—C9	1.4019 (19)	C29—C30	1.394 (2)
C5—C6	1.397 (2)	C29—H29	0.9500
C5—C10	1.5300 (19)	C30—H30	0.9500
C6—C7	1.389 (2)	C31—C32	1.390 (2)
C6—H6	0.9500	C31—C36	1.391 (2)
C7—C8	1.396 (2)	C32—C33	1.388 (2)
C8—C9	1.386 (2)	C32—H32	0.9500
C8—H8	0.9500	C33—C34	1.387 (3)
C9—C24	1.528 (2)	C33—H33	0.9500
C10—C11	1.520 (2)	C34—C35	1.384 (2)
C10—C17	1.528 (2)	C34—H34	0.9500
C10—H10	1.0000	C35—C36	1.392 (2)

C11—C16	1.390 (2)	C35—H35	0.9500
C11—C12	1.391 (2)	C36—H36	0.9500
C12—C13	1.390 (2)	C37—H37A	0.9800
C12—H12	0.9500	C37—H37B	0.9800
C13—C14	1.381 (3)	C37—H37C	0.9800
C13—H13	0.9500	C38—H38A	0.9800
C14—C15	1.384 (3)	C38—H38B	0.9800
C14—H14	0.9500	C38—H38C	0.9800
C15—C16	1.393 (2)	C40—C45	1.396 (2)
C15—H15	0.9500	C40—C41	1.399 (2)
C16—H16	0.9500	C41—C42	1.382 (3)
C17—C18	1.391 (2)	C41—H41	0.9500
C17—C22	1.394 (2)	C42—C43	1.395 (3)
C18—C19	1.392 (2)	C42—H42	0.9500
C18—H18	0.9500	C43—C44	1.385 (2)
C19—C20	1.381 (2)	C43—H43	0.9500
C19—H19	0.9500	C44—C45	1.395 (2)
C20—C21	1.386 (2)	C44—H44	0.9500
C20—H20	0.9500		
C45—S1—C39	87.69 (7)	H23A—C23—H23B	109.5
C7—O1—C23	116.86 (12)	O1—C23—H23C	109.5
C1—N1—C2	110.93 (11)	H23A—C23—H23C	109.5
C1—N1—C4	123.98 (11)	H23B—C23—H23C	109.5
C2—N1—C4	124.80 (12)	C31—C24—C25	114.01 (12)
C1—N2—C39	126.08 (12)	C31—C24—C9	112.04 (12)
C1—N2—C3	109.30 (11)	C25—C24—C9	112.25 (12)
C39—N2—C3	124.46 (12)	C31—C24—H24	105.9
C39—N3—C40	109.88 (13)	C25—C24—H24	105.9
N1—C1—N2	105.29 (11)	C9—C24—H24	105.9
N1—C1—Se1	124.93 (10)	C30—C25—C26	118.24 (14)
N2—C1—Se1	129.77 (10)	C30—C25—C24	123.62 (14)
C3—C2—N1	107.66 (12)	C26—C25—C24	118.12 (13)
C3—C2—C37	129.55 (13)	C27—C26—C25	121.09 (14)
N1—C2—C37	122.78 (13)	C27—C26—H26	119.5
C2—C3—N2	106.81 (12)	C25—C26—H26	119.5
C2—C3—C38	126.83 (14)	C26—C27—C28	120.09 (15)
N2—C3—C38	126.21 (13)	C26—C27—H27	120.0
C5—C4—C9	121.94 (13)	C28—C27—H27	120.0
C5—C4—N1	118.68 (12)	C29—C28—C27	119.30 (15)
C9—C4—N1	119.37 (12)	C29—C28—H28	120.3
C4—C5—C6	118.53 (13)	C27—C28—H28	120.3
C4—C5—C10	121.07 (12)	C28—C29—C30	120.85 (15)
C6—C5—C10	120.35 (13)	C28—C29—H29	119.6
C7—C6—C5	120.09 (13)	C30—C29—H29	119.6
C7—C6—H6	120.0	C25—C30—C29	120.42 (15)
C5—C6—H6	120.0	C25—C30—H30	119.8
O1—C7—C6	123.64 (13)	C29—C30—H30	119.8
O1—C7—C8	115.75 (13)	C32—C31—C36	118.57 (14)
C6—C7—C8	120.57 (13)	C32—C31—C24	119.47 (13)

C9—C8—C7	120.33 (13)	C36—C31—C24	121.96 (13)
C9—C8—H8	119.8	C33—C32—C31	121.14 (15)
C7—C8—H8	119.8	C33—C32—H32	119.4
C8—C9—C4	118.39 (13)	C31—C32—H32	119.4
C8—C9—C24	122.12 (13)	C34—C33—C32	119.78 (15)
C4—C9—C24	119.40 (12)	C34—C33—H33	120.1
C11—C10—C17	113.19 (12)	C32—C33—H33	120.1
C11—C10—C5	112.90 (12)	C35—C34—C33	119.73 (15)
C17—C10—C5	110.48 (11)	C35—C34—H34	120.1
C11—C10—H10	106.6	C33—C34—H34	120.1
C17—C10—H10	106.6	C34—C35—C36	120.26 (15)
C5—C10—H10	106.6	C34—C35—H35	119.9
C16—C11—C12	118.45 (15)	C36—C35—H35	119.9
C16—C11—C10	122.04 (13)	C31—C36—C35	120.52 (15)
C12—C11—C10	119.47 (14)	C31—C36—H36	119.7
C13—C12—C11	120.94 (17)	C35—C36—H36	119.7
C13—C12—H12	119.5	C2—C37—H37A	109.5
C11—C12—H12	119.5	C2—C37—H37B	109.5
C14—C13—C12	120.20 (16)	H37A—C37—H37B	109.5
C14—C13—H13	119.9	C2—C37—H37C	109.5
C12—C13—H13	119.9	H37A—C37—H37C	109.5
C13—C14—C15	119.46 (16)	H37B—C37—H37C	109.5
C13—C14—H14	120.3	C3—C38—H38A	109.5
C15—C14—H14	120.3	C3—C38—H38B	109.5
C14—C15—C16	120.36 (17)	H38A—C38—H38B	109.5
C14—C15—H15	119.8	C3—C38—H38C	109.5
C16—C15—H15	119.8	H38A—C38—H38C	109.5
C11—C16—C15	120.56 (16)	H38B—C38—H38C	109.5
C11—C16—H16	119.7	N3—C39—N2	120.18 (13)
C15—C16—H16	119.7	N3—C39—S1	117.19 (11)
C18—C17—C22	118.73 (14)	N2—C39—S1	122.63 (10)
C18—C17—C10	123.09 (13)	N3—C40—C45	115.02 (13)
C22—C17—C10	118.17 (13)	N3—C40—C41	125.09 (15)
C17—C18—C19	120.17 (15)	C45—C40—C41	119.89 (15)
C17—C18—H18	119.9	C42—C41—C40	118.63 (17)
C19—C18—H18	119.9	C42—C41—H41	120.7
C20—C19—C18	120.73 (15)	C40—C41—H41	120.7
C20—C19—H19	119.6	C41—C42—C43	121.01 (16)
C18—C19—H19	119.6	C41—C42—H42	119.5
C19—C20—C21	119.47 (15)	C43—C42—H42	119.5
C19—C20—H20	120.3	C44—C43—C42	121.17 (16)
C21—C20—H20	120.3	C44—C43—H43	119.4
C20—C21—C22	120.05 (14)	C42—C43—H43	119.4
C20—C21—H21	120.0	C43—C44—C45	117.75 (16)
C22—C21—H21	120.0	C43—C44—H44	121.1
C21—C22—C17	120.82 (14)	C45—C44—H44	121.1
C21—C22—H22	119.6	C44—C45—C40	121.53 (14)
C17—C22—H22	119.6	C44—C45—S1	128.23 (13)
O1—C23—H23A	109.5	C40—C45—S1	110.21 (11)

O1—C23—H23B	109.5		
C2—N1—C1—N2	-0.14 (15)	C5—C10—C17—C22	63.60 (16)
C4—N1—C1—N2	-174.17 (12)	C22—C17—C18—C19	-0.1 (2)
C2—N1—C1—Se1	179.36 (10)	C10—C17—C18—C19	178.60 (14)
C4—N1—C1—Se1	5.34 (19)	C17—C18—C19—C20	-0.7 (2)
C39—N2—C1—N1	-175.02 (12)	C18—C19—C20—C21	0.7 (2)
C3—N2—C1—N1	0.65 (15)	C19—C20—C21—C22	0.2 (2)
C39—N2—C1—Se1	5.5 (2)	C20—C21—C22—C17	-1.0 (2)
C3—N2—C1—Se1	-178.82 (11)	C18—C17—C22—C21	1.0 (2)
C1—N1—C2—C3	-0.45 (16)	C10—C17—C22—C21	-177.80 (13)
C4—N1—C2—C3	173.52 (13)	C8—C9—C24—C31	102.64 (15)
C1—N1—C2—C37	178.32 (13)	C4—C9—C24—C31	-80.86 (15)
C4—N1—C2—C37	-7.7 (2)	C8—C9—C24—C25	-27.15 (18)
N1—C2—C3—N2	0.82 (16)	C4—C9—C24—C25	149.35 (13)
C37—C2—C3—N2	-177.84 (14)	C31—C24—C25—C30	-3.9 (2)
N1—C2—C3—C38	-174.91 (16)	C9—C24—C25—C30	124.84 (15)
C37—C2—C3—C38	6.4 (3)	C31—C24—C25—C26	174.75 (13)
C1—N2—C3—C2	-0.94 (16)	C9—C24—C25—C26	-56.49 (17)
C39—N2—C3—C2	174.82 (13)	C30—C25—C26—C27	-0.6 (2)
C1—N2—C3—C38	174.83 (16)	C24—C25—C26—C27	-179.38 (14)
C39—N2—C3—C38	-9.4 (2)	C25—C26—C27—C28	0.8 (2)
C1—N1—C4—C5	89.29 (17)	C26—C27—C28—C29	-0.1 (2)
C2—N1—C4—C5	-83.91 (17)	C27—C28—C29—C30	-0.6 (3)
C1—N1—C4—C9	-89.76 (16)	C26—C25—C30—C29	-0.1 (2)
C2—N1—C4—C9	97.04 (16)	C24—C25—C30—C29	178.57 (15)
C9—C4—C5—C6	-3.6 (2)	C28—C29—C30—C25	0.7 (3)
N1—C4—C5—C6	177.40 (12)	C25—C24—C31—C32	-100.24 (16)
C9—C4—C5—C10	173.89 (13)	C9—C24—C31—C32	130.89 (14)
N1—C4—C5—C10	-5.13 (19)	C25—C24—C31—C36	78.98 (18)
C4—C5—C6—C7	0.3 (2)	C9—C24—C31—C36	-49.89 (18)
C10—C5—C6—C7	-177.17 (13)	C36—C31—C32—C33	-0.2 (2)
C23—O1—C7—C6	-10.0 (2)	C24—C31—C32—C33	179.05 (15)
C23—O1—C7—C8	167.67 (14)	C31—C32—C33—C34	0.1 (3)
C5—C6—C7—O1	179.65 (13)	C32—C33—C34—C35	0.0 (3)
C5—C6—C7—C8	2.1 (2)	C33—C34—C35—C36	-0.1 (3)
O1—C7—C8—C9	-179.04 (13)	C32—C31—C36—C35	0.1 (2)
C6—C7—C8—C9	-1.3 (2)	C24—C31—C36—C35	-179.09 (14)
C7—C8—C9—C4	-1.9 (2)	C34—C35—C36—C31	0.0 (3)
C7—C8—C9—C24	174.67 (13)	C40—N3—C39—N2	-179.08 (12)
C5—C4—C9—C8	4.3 (2)	C40—N3—C39—S1	0.60 (16)
N1—C4—C9—C8	-176.63 (12)	C1—N2—C39—N3	173.13 (13)
C5—C4—C9—C24	-172.29 (13)	C3—N2—C39—N3	-1.9 (2)
N1—C4—C9—C24	6.73 (19)	C1—N2—C39—S1	-6.5 (2)
C4—C5—C10—C11	86.23 (16)	C3—N2—C39—S1	178.42 (11)
C6—C5—C10—C11	-96.35 (16)	C45—S1—C39—N3	-0.86 (12)
C4—C5—C10—C17	-145.89 (13)	C45—S1—C39—N2	178.81 (12)
C6—C5—C10—C17	31.53 (18)	C39—N3—C40—C45	0.09 (18)
C17—C10—C11—C16	-84.34 (17)	C39—N3—C40—C41	179.42 (15)

C5—C10—C11—C16	42.1 (2)	N3—C40—C41—C42	-177.42 (15)
C17—C10—C11—C12	93.35 (17)	C45—C40—C41—C42	1.9 (2)
C5—C10—C11—C12	-140.20 (14)	C40—C41—C42—C43	-0.7 (3)
C16—C11—C12—C13	1.4 (2)	C41—C42—C43—C44	-0.6 (3)
C10—C11—C12—C13	-176.34 (15)	C42—C43—C44—C45	0.6 (3)
C11—C12—C13—C14	-0.9 (3)	C43—C44—C45—C40	0.6 (2)
C12—C13—C14—C15	-0.6 (3)	C43—C44—C45—S1	178.46 (13)
C13—C14—C15—C16	1.4 (3)	N3—C40—C45—C44	177.53 (14)
C12—C11—C16—C15	-0.6 (2)	C41—C40—C45—C44	-1.8 (2)
C10—C11—C16—C15	177.12 (15)	N3—C40—C45—S1	-0.71 (17)
C14—C15—C16—C11	-0.8 (3)	C41—C40—C45—S1	179.92 (12)
C11—C10—C17—C18	12.61 (19)	C39—S1—C45—C44	-177.27 (15)
C5—C10—C17—C18	-115.11 (15)	C39—S1—C45—C40	0.82 (11)
C11—C10—C17—C22	-168.68 (13)		

Full information from Platon program (version 2021.2) using SQUEEZE option

4amask.log
Miller array info: C:\Users\Blazej\Desktop\CIFY GOTOWE\B128_a.hkl:Iobs,SigIobs
Observation type: xray.intensity
Type of data: double, size=19523
Type of sigmas: double, size=19523
Number of Miller indices: 19523
Anomalous flag: False
Unit cell: (10.6849, 32.0913, 12.6278, 90, 104.579, 90)
Space group: P 1 21/c 1 (No. 14)
Systematic absences: 234
Systematic absences not included in following:
Centric reflections: 19289
Resolution range: 11.421 0.771579

use_set_completion: True
solvent_radius: 1.20
shrink_truncation_radius: 1.20
van der Waals radii:

Ag	C	Cl	H	N	S
1.72	1.70	1.75	1.09	1.55	1.80

Total solvent accessible volume / cell = 672.1 Ang^3 [16.0%]
Total electron count / cell = 169.6

gridding: (60,180,72)

Void	#Grid points	Vol/A^3	Vol/%	Centre of mass (frac)	Eigenvectors (frac)
1	52871	284.9	6.8	(-0.000,-0.000, 0.000)	1 (0.705,-0.093, 0.703)
					2 (-0.701, 0.059, 0.711)
					3 (0.108, 0.994, 0.024)
2	52871	284.9	6.8	(-0.000, 0.500, 0.500)	1 (0.705, 0.093, 0.703)
					2 (-0.701,-0.059, 0.711)
					3 (-0.108, 0.994,-0.024)
3	3040	16.4	0.4	(0.232, 0.089, 0.576)	1 (0.741,-0.049, 0.669)

				2	(-0.656, 0.156, 0.738)
				3	(0.140, 0.987,-0.084)
4	3040	16.4	0.4	(0.232, 0.411, 0.076) 1	(0.741, 0.049, 0.669)
				2	(-0.656,-0.156, 0.738)
				3	(-0.140, 0.987, 0.084)
5	1702	9.2	0.2	(0.217, 0.650, 0.951) 1	(0.901, 0.009, 0.434)
				2	(-0.434, 0.040, 0.900)
				3	(0.009, 0.999,-0.040)
6	1702	9.2	0.2	(0.217, 0.850, 0.451) 1	(0.901,-0.009, 0.434)
				2	(-0.434,-0.040, 0.900)
				3	(-0.009, 0.999, 0.040)
7	3040	16.4	0.4	(0.768, 0.589, 0.924) 1	(0.741, 0.049, 0.669)
				2	(-0.656,-0.156, 0.738)
				3	(-0.140, 0.987, 0.084)
8	3040	16.4	0.4	(0.768, 0.911, 0.424) 1	(0.741,-0.049, 0.669)
				2	(-0.656, 0.156, 0.738)
				3	(0.140, 0.987,-0.084)
9	1702	9.2	0.2	(0.783, 0.150, 0.549) 1	(0.901,-0.009, 0.434)
				2	(-0.434,-0.040, 0.900)
				3	(-0.009, 0.999, 0.040)
10	1702	9.2	0.2	(0.783, 0.350, 0.049) 1	(0.901, 0.009, 0.434)
				2	(-0.434, 0.040, 0.900)
				3	(0.009, 0.999,-0.040)

Void	Vol/Ang^3	#Electrons
1	284.9	84.8
2	284.9	84.8
3	16.4	0.0
4	16.4	0.0
5	9.2	0.0
6	9.2	0.0
7	16.4	0.0
8	16.4	0.0
9	9.2	0.0
10	9.2	0.0

5bmask.log

Miller array info: C:\Users\Blazej\Desktop\CIFY GOTOWE\PdBenzotiazol_auto_a.hkl:Iobs,SigIobs

Observation type: xray.intensity

Type of data: double, size=36247

Type of sigmas: double, size=36247

Number of Miller indices: 36247

Anomalous flag: False

Unit cell: (25.3287, 9.4913, 35.0477, 90, 90, 90)

Space group: P b c a (No. 61)

Systematic absences: 2471

Systematic absences not included in following:

Centric reflections: 33776

Resolution range: 17.5238 0.805477

use_set_completion: True

solvent_radius: 1.20

shrink_truncation_radius: 1.20

van der Waals radii:

C	Cl	H	N	O	Pd	S
1.70	1.75	1.09	1.55	1.52	1.63	1.80

Total solvent accessible volume / cell = 1347.5 Ang^3 [16.0%]

Total electron count / cell = 439.2

gridding: (128,48,180)

Void	#Grid points	Vol/A^3	Vol/%	Centre of mass (frac)	Eigenvectors (frac)
1	88438	673.8	8.0	(-0.997,-0.049,-0.000)	1 (-0.079, 0.086, 0.993)
					2 (-0.576, 0.809,-0.115)
					3 (0.814, 0.581, 0.015)
2	88438	673.8	8.0	(-0.104,-0.819, 0.500)	1 (-0.365, 0.775, 0.516)
					2 (0.181,-0.485, 0.856)
					3 (0.913, 0.406, 0.036)

Void	Vol/Ang^3	#Electrons
1	673.8	219.6
2	673.8	219.6

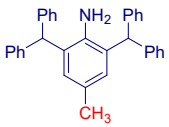
Computational Methods

Computational Methods. All of the calculations were performed using Gaussian 09 suite of programs. All of the geometry optimizations were performed at the B3LYP level of theory in the gas phase with the 6-311++G(d,p) basis set. For geometry optimizations, we employed the X-ray structures of 1-(benzo[*d*]thiazol-2-yl)-3-(2,6-dibenzhydryl-4-methylphenyl)-4,5-dimethyl-1*H*-imidazol-3-ium or its linear metal complexes as the starting geometry and performed full optimization. The absence of imaginary frequencies was used to characterize the structures as minima on the potential energy surface. All of the optimized geometries were verified as minima (no imaginary frequencies). Energetic parameters were calculated under standard conditions (298.15 K and 1 atm). Structural representations were generated using CYLview software (Legault, C. Y. CYLview version 1.0 BETA, University of Sherbrooke). All other representations were generated using GaussView (GaussView, version 5, Dennington, R.; Keith, T.; Millam, J. Semichem Inc., Shawnee Mission, KS, 2009) or ChemCraft software (Andrienko, G. L. ChemCraft version b562a, https://www.chemcraftprog.com).

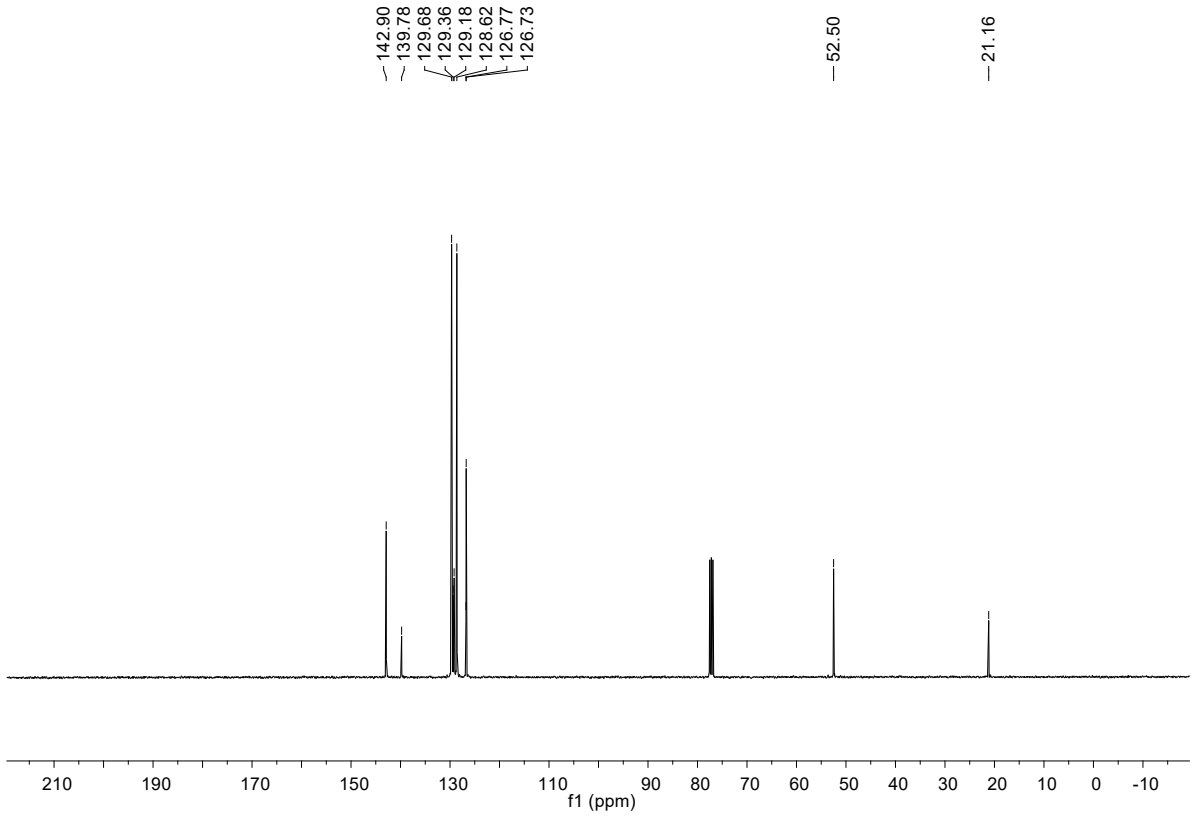
Full Reference for Gaussian 09

Gaussian 09, Revision D.01, 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, Inc., Wallingford CT, 2009.

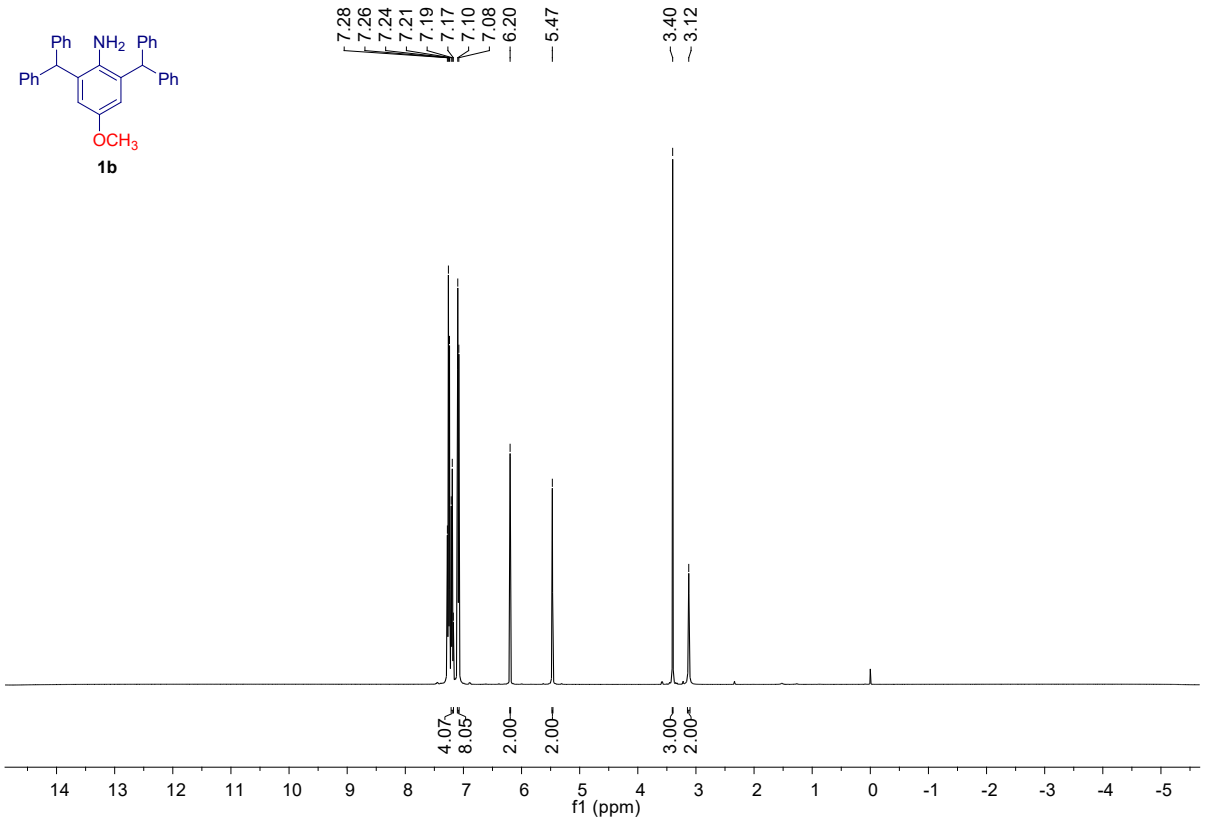
1a 2,6-Dibenzhydryl-4-methylaniline

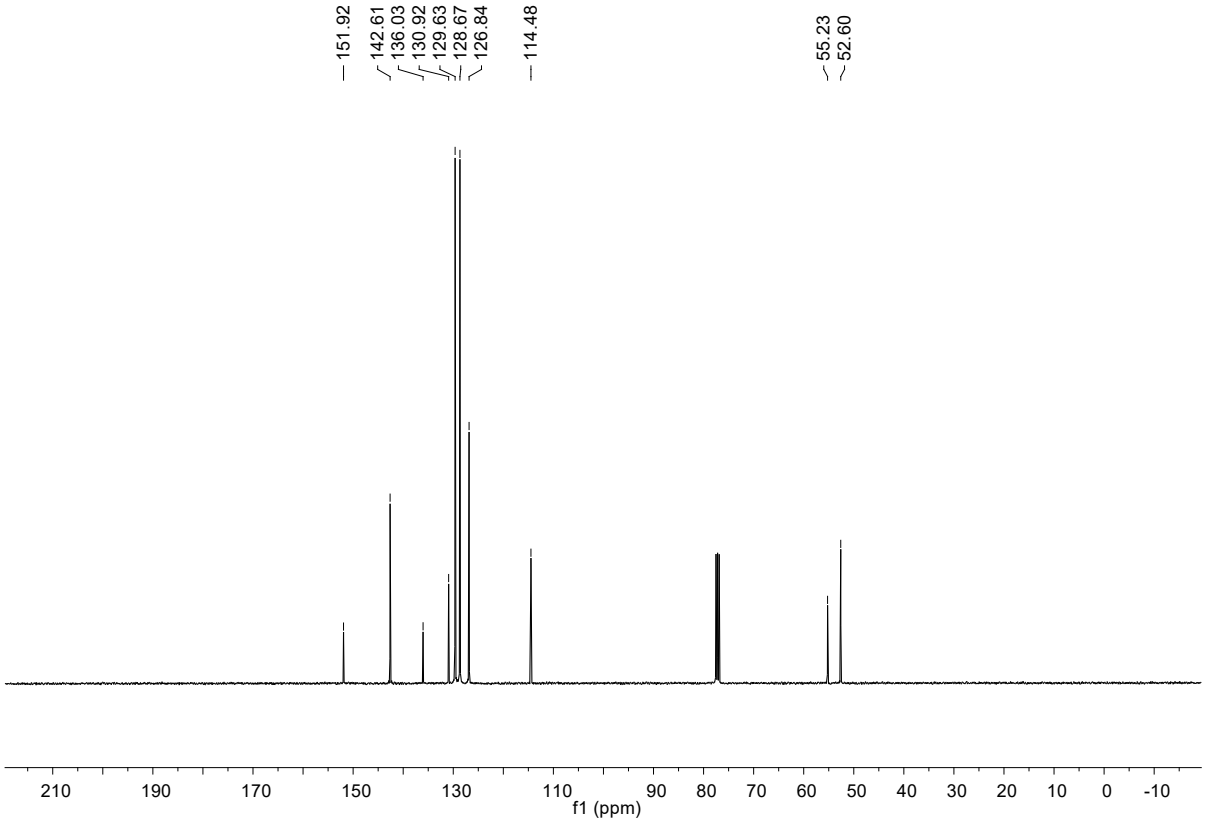


1a

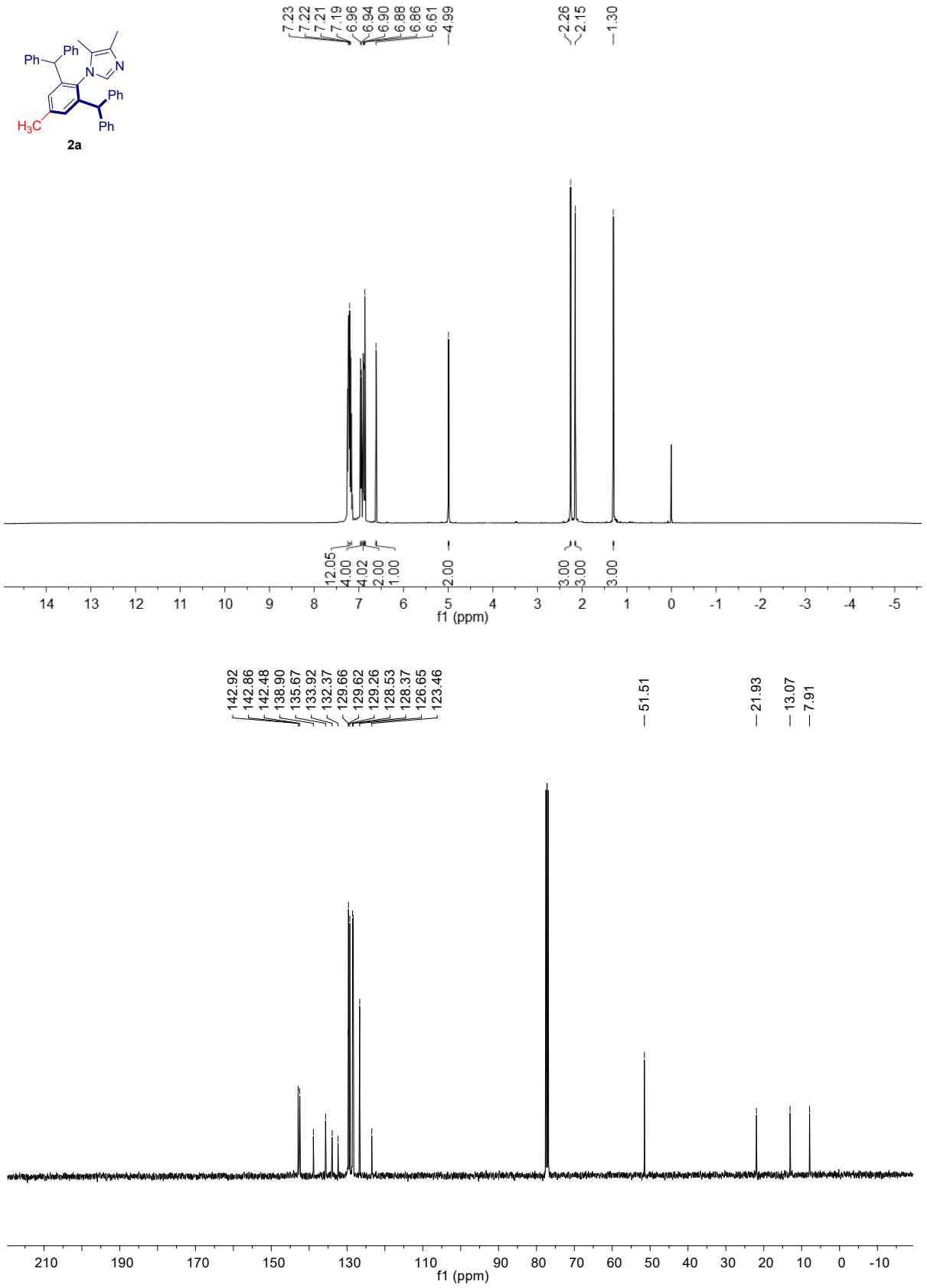


1b 4-Methoxy-2,6-bis(diphenylmethyl)aniline

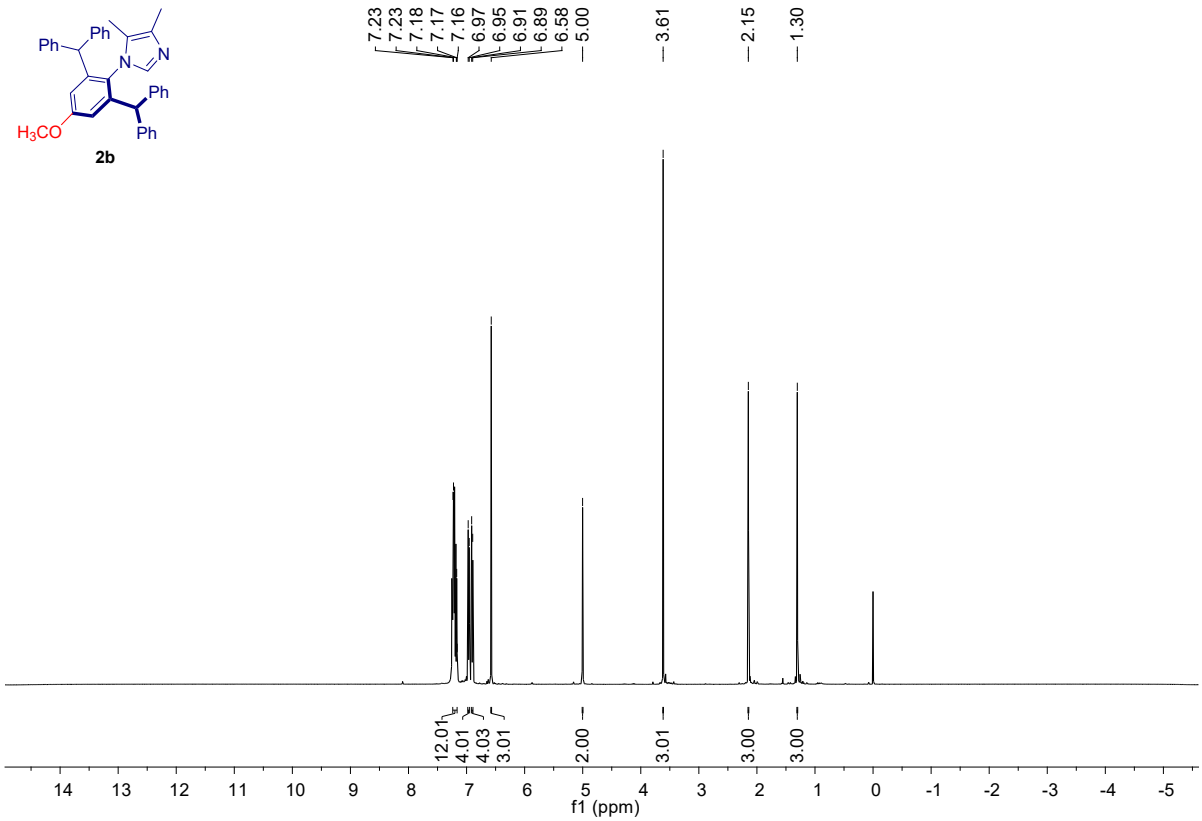


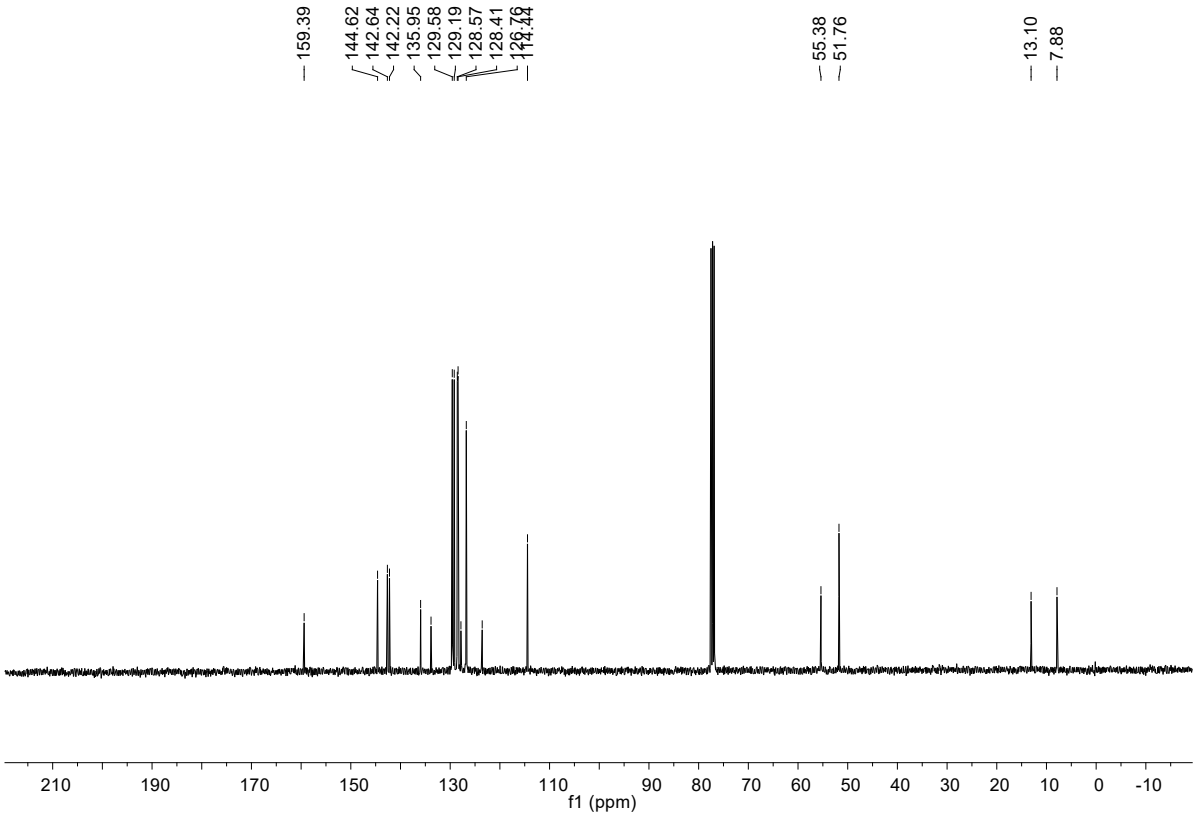


2a 1-(2,6-Dibenzhydryl-4-methylphenyl)-4,5-dimethyl-1*H*-imidazole

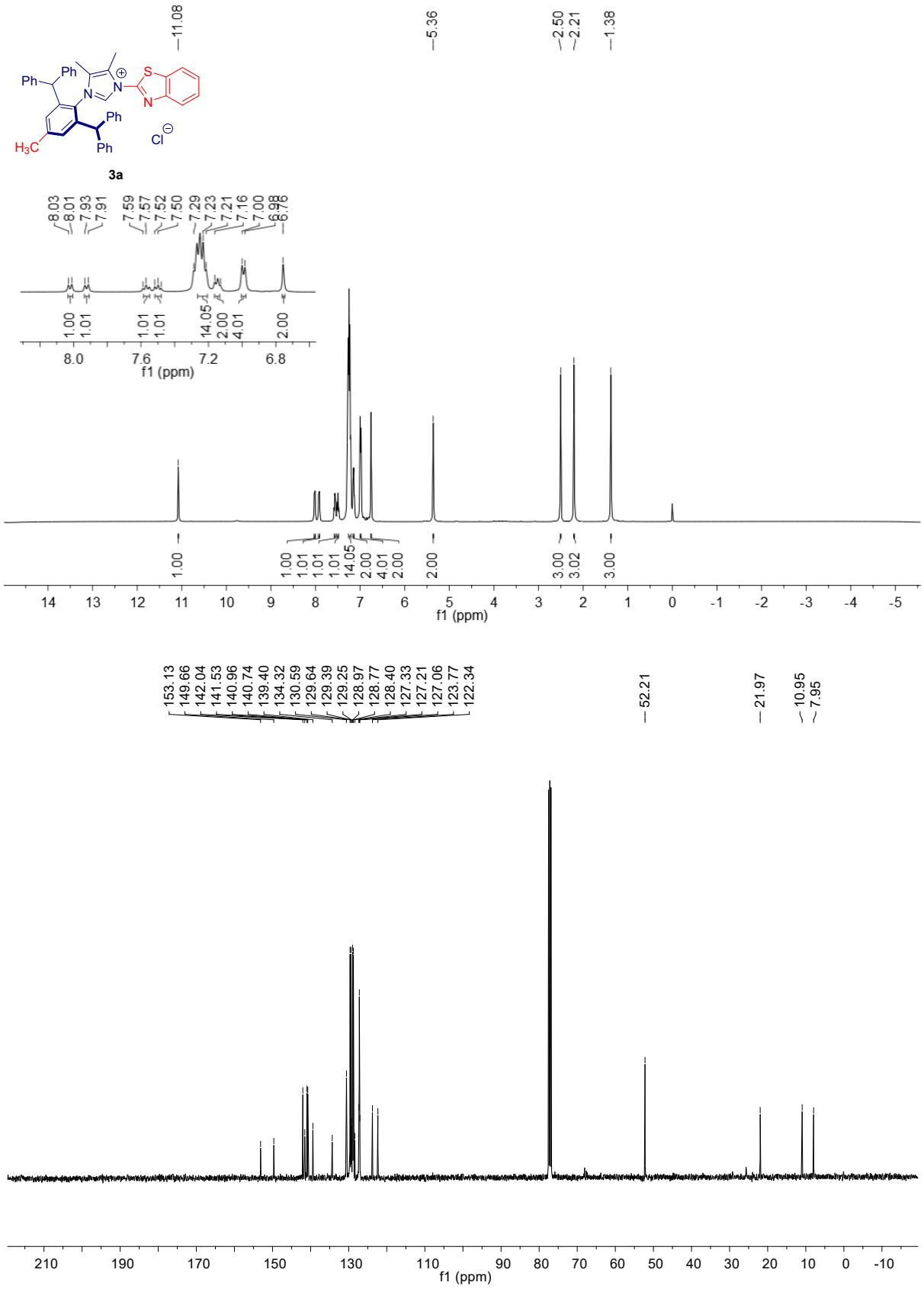


2b 1-(2,6-Dibenzhydryl-4-methoxyphenyl)-4,5-dimethyl-1*H*-imidazole

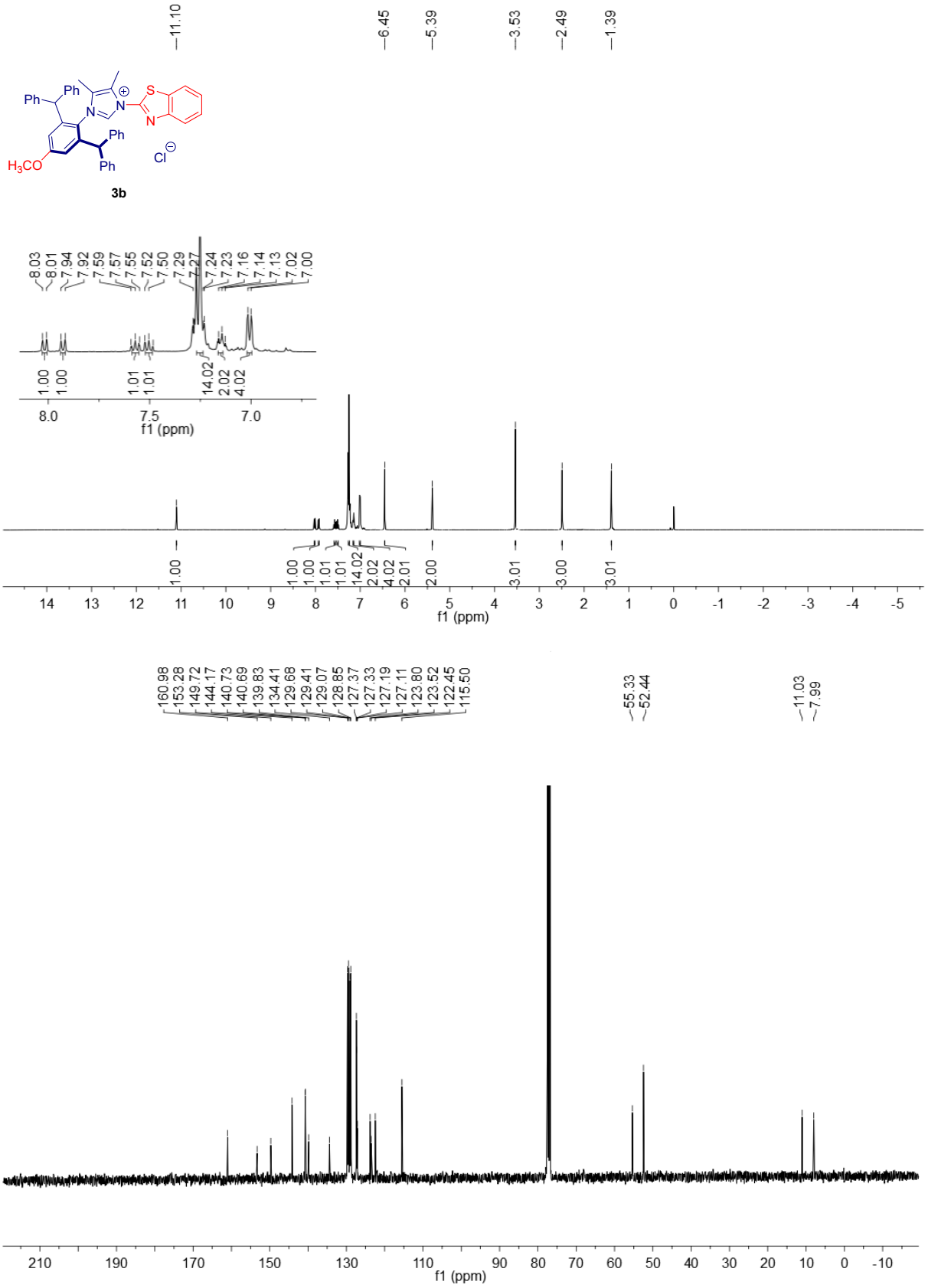




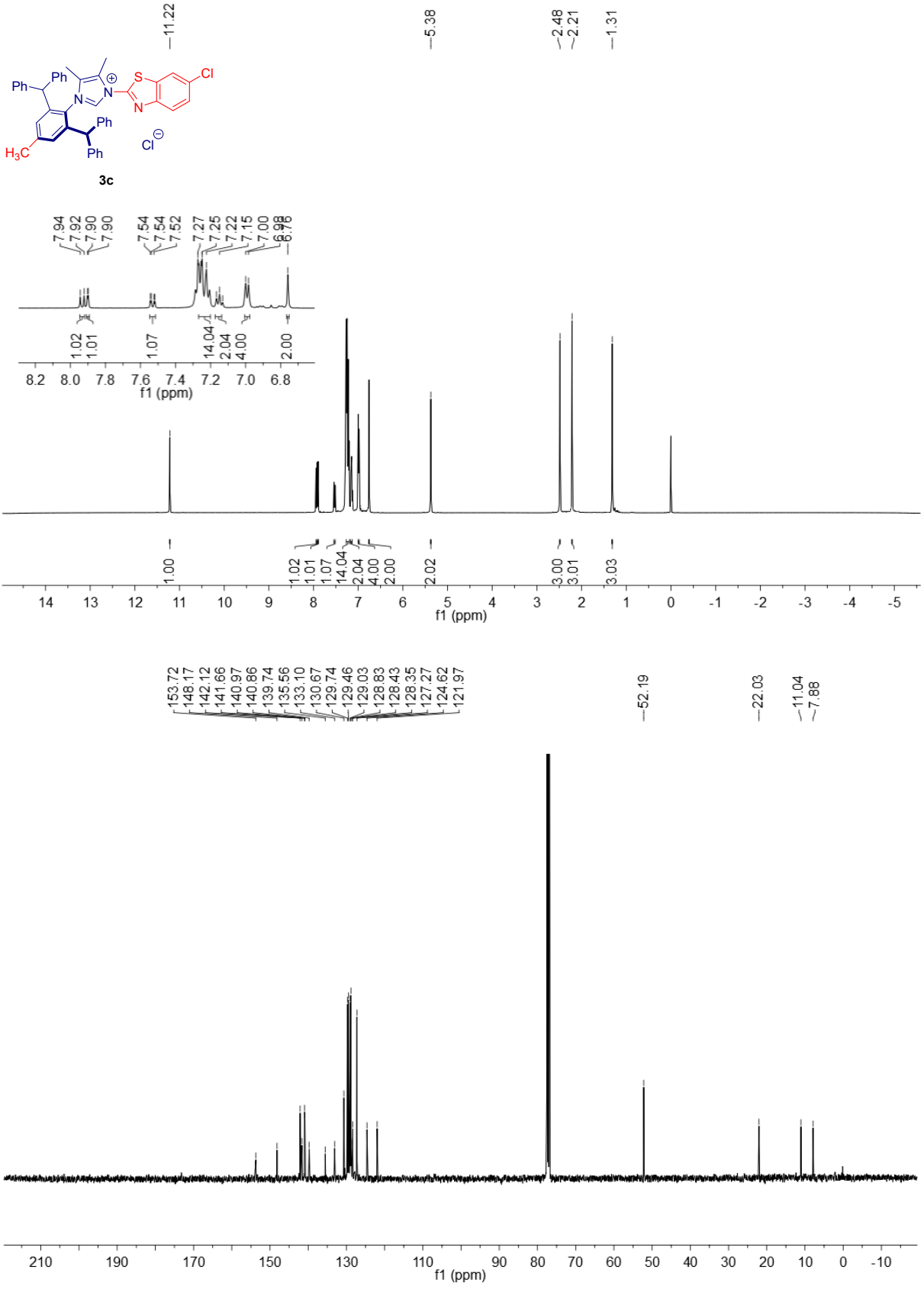
3a 1-(Benzo[*d*]thiazole)-3-(2,6-dibenzhydryl-4-methylphenyl)-4,5-dimethyl-1*H*-imidazol-3-ium chloride



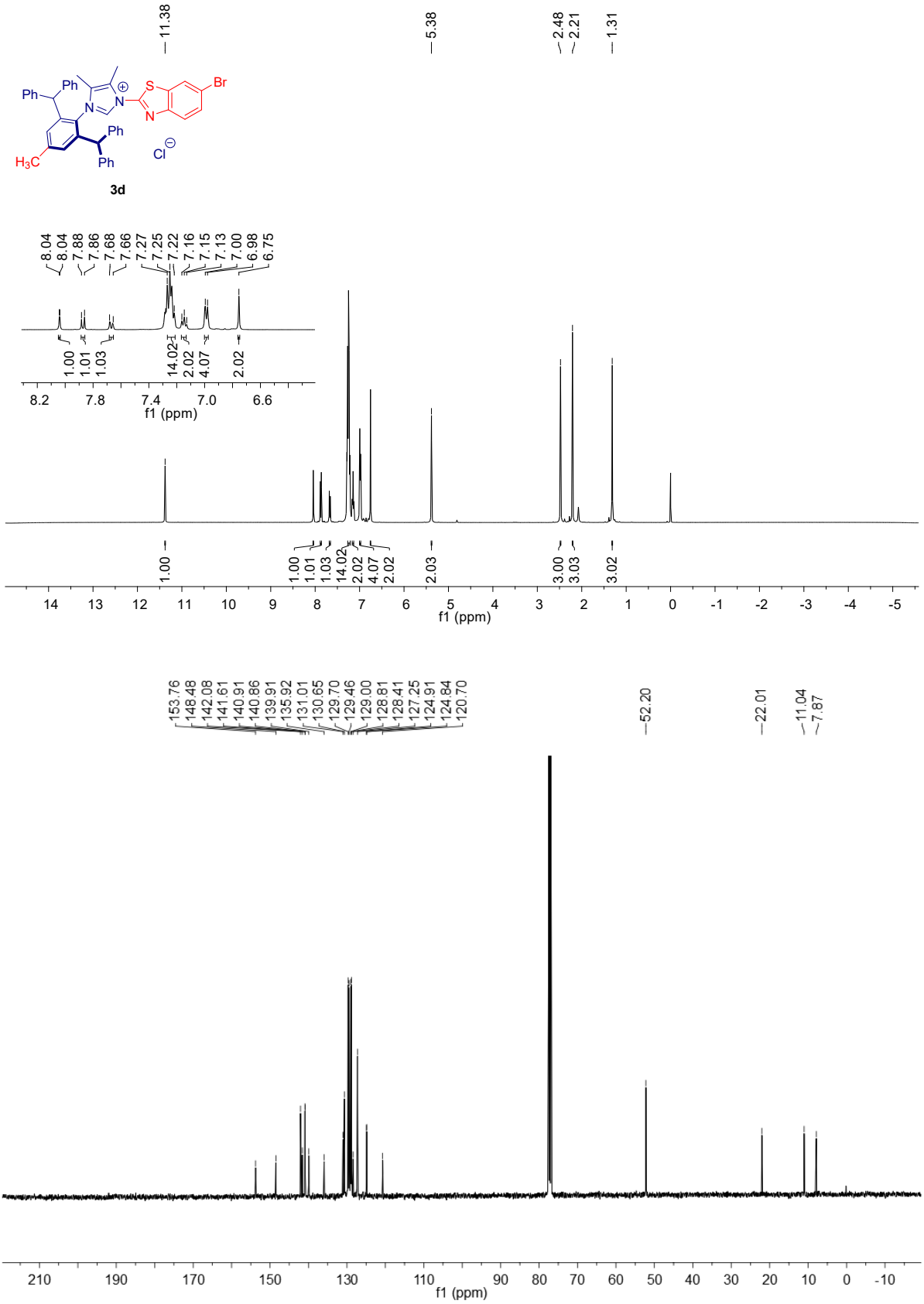
3b 1-(Benzo[*d*]thiazole)-3-(2,6-dibenzhydryl-4-methoxyphenyl)-4,5-dimethyl-1*H*-imidazol-3-ium chloride



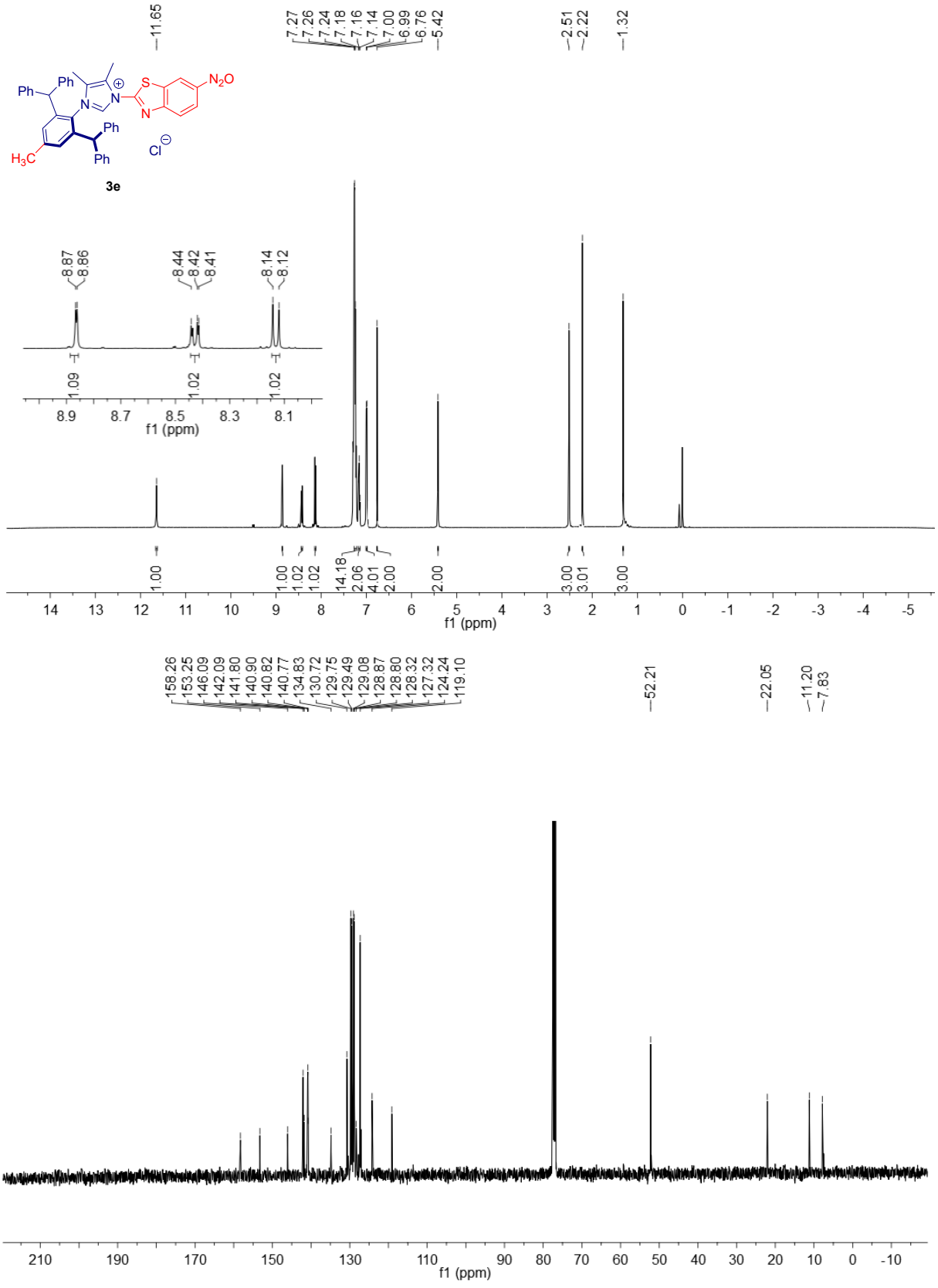
3c 6-Chloro-1-(Benzothiazol-2-yl)-3-(2,6-dibenzhydryl-4-methylphenyl)-4,5-dimethyl-1*H*-imidazol-3-ium chloride



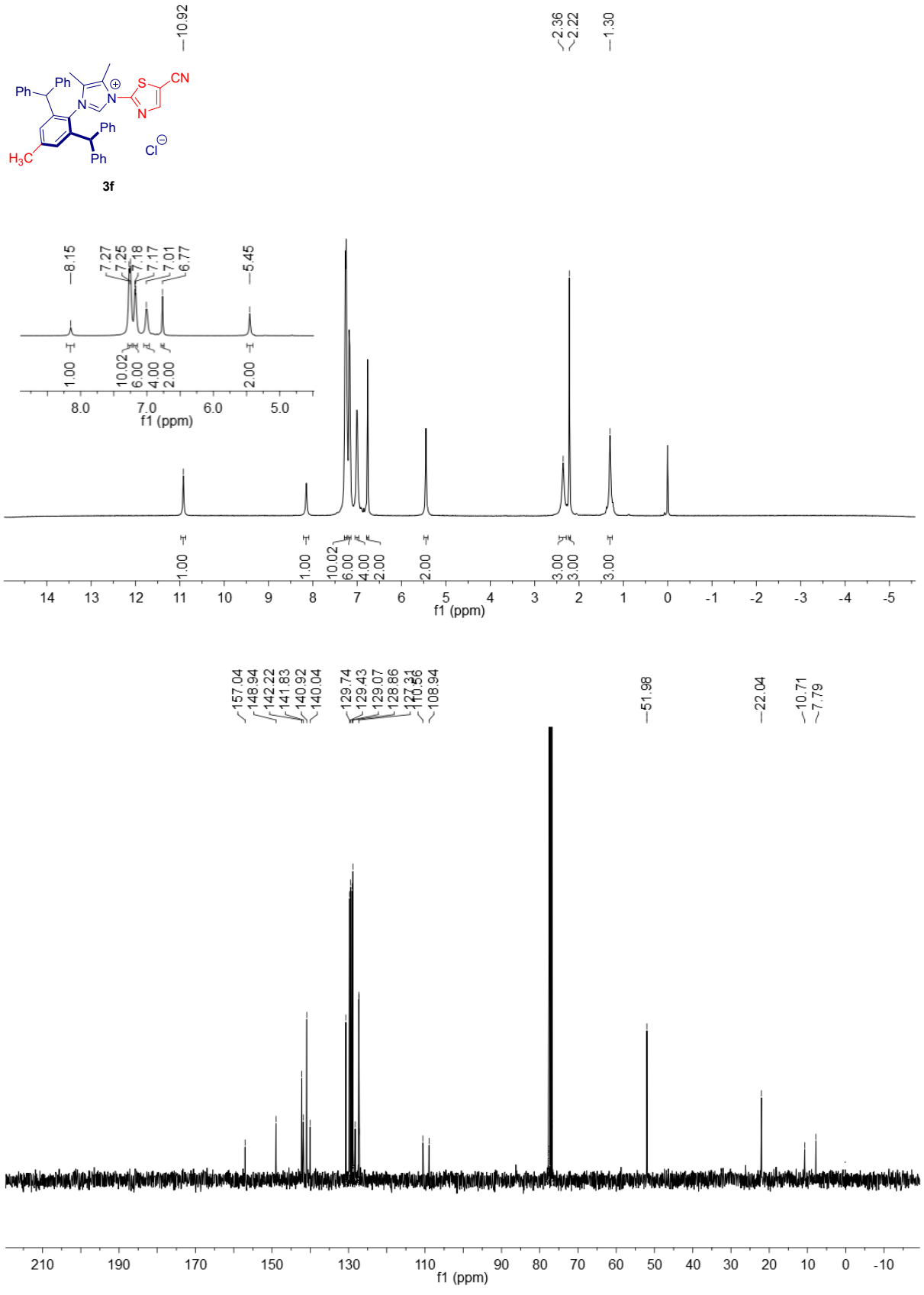
3d 6-Bromo-1-(Benzothiazol-2-yl)-3-(2,6-dibenzhydryl-4-methylphenyl)-4,5-dimethyl-1*H*-imidazol-3-ium chloride



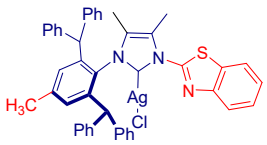
3e 6-(Oxidaneyl)diazenyl-1-(Benzothiazol-2-yl)-3-(2,6-dibenzhydryl-4-methylphenyl)-4,5-dimethyl-1*H*-imidazol-3-ium chloride



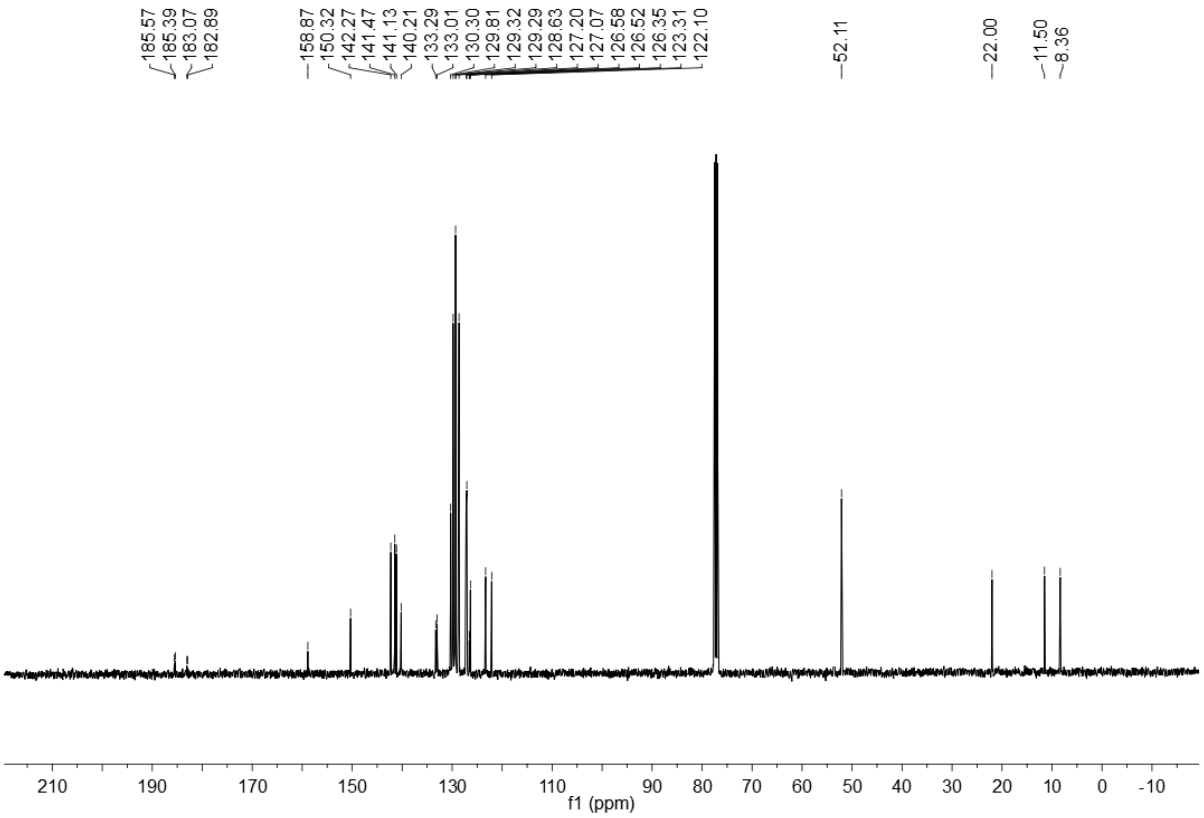
3f 5-Carbonitrile-1-(thiazol-2-yl)-3-(2,6-dibenzhydryl-4-methylphenyl)-4,5-dimethyl-1*H*-imidazol-3-ium chloride



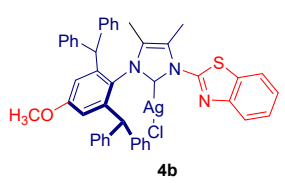
4a 1-(Benzo[*d*]thiazol-2-yl)-3-(2,6-dibenzhydryl-4-methylphenyl)-4,5-dimethylimidazol-2-ylidene)silver(I) chloride



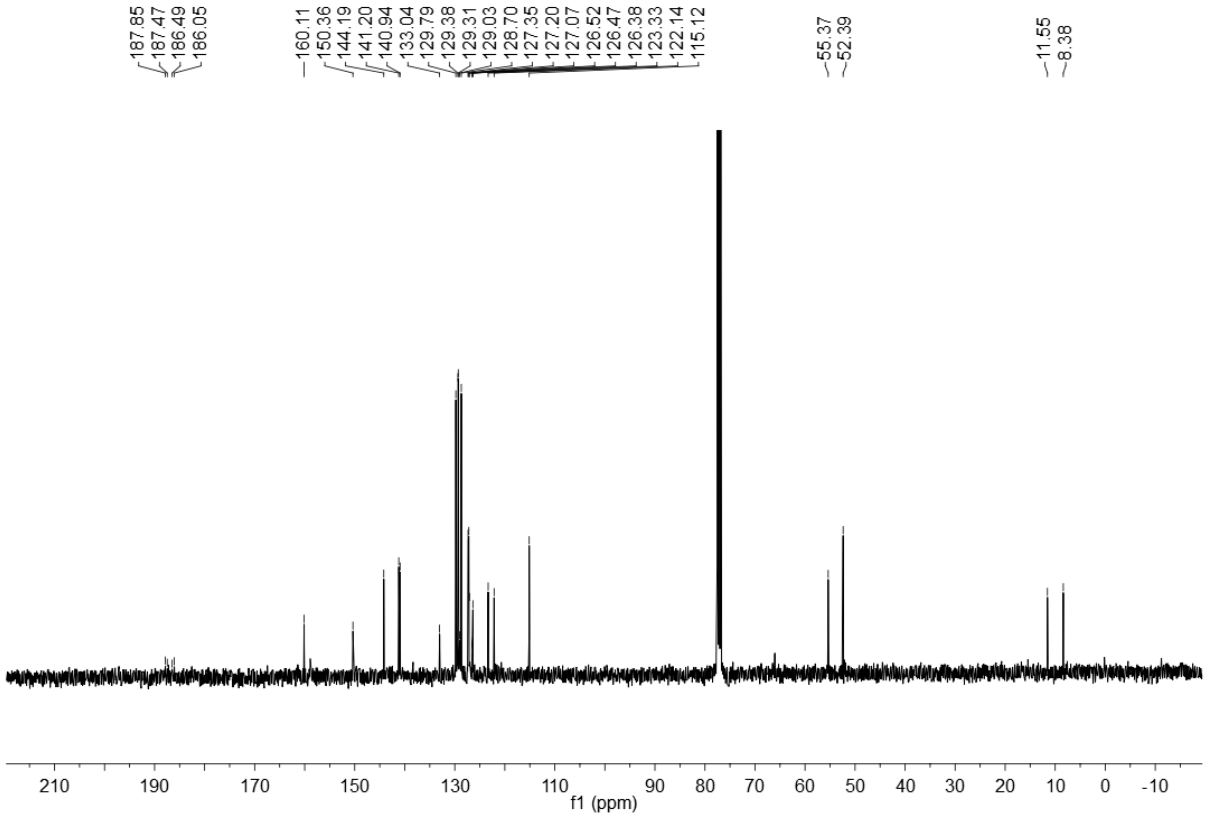
4a



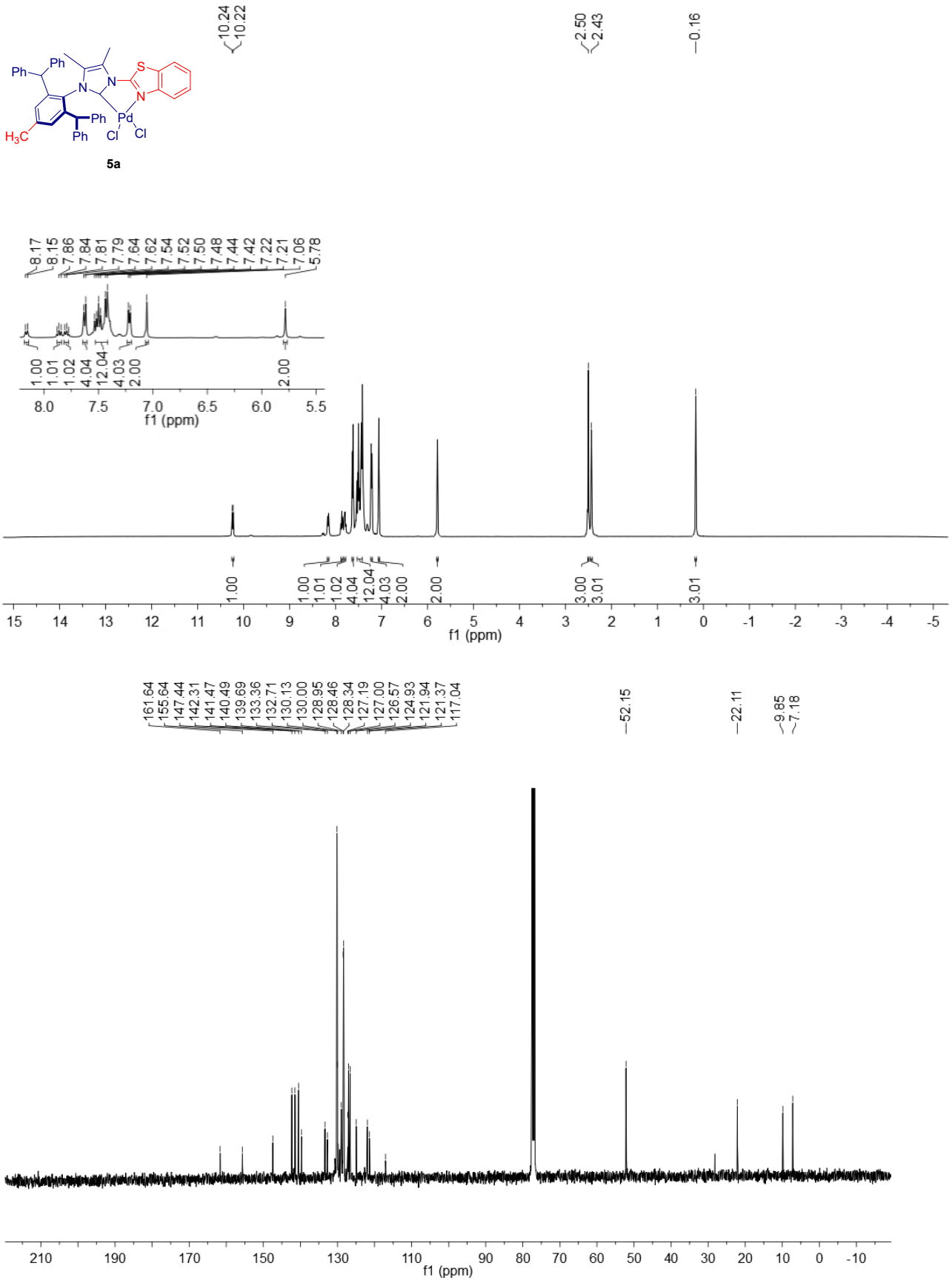
4b 1-(Benzo[*d*]thiazol-2-yl)-3-(2,6-dibenzhydryl-4-methoxyphenyl)-4,5-dimethylimidazol-2-ylidene)silver(I) chloride



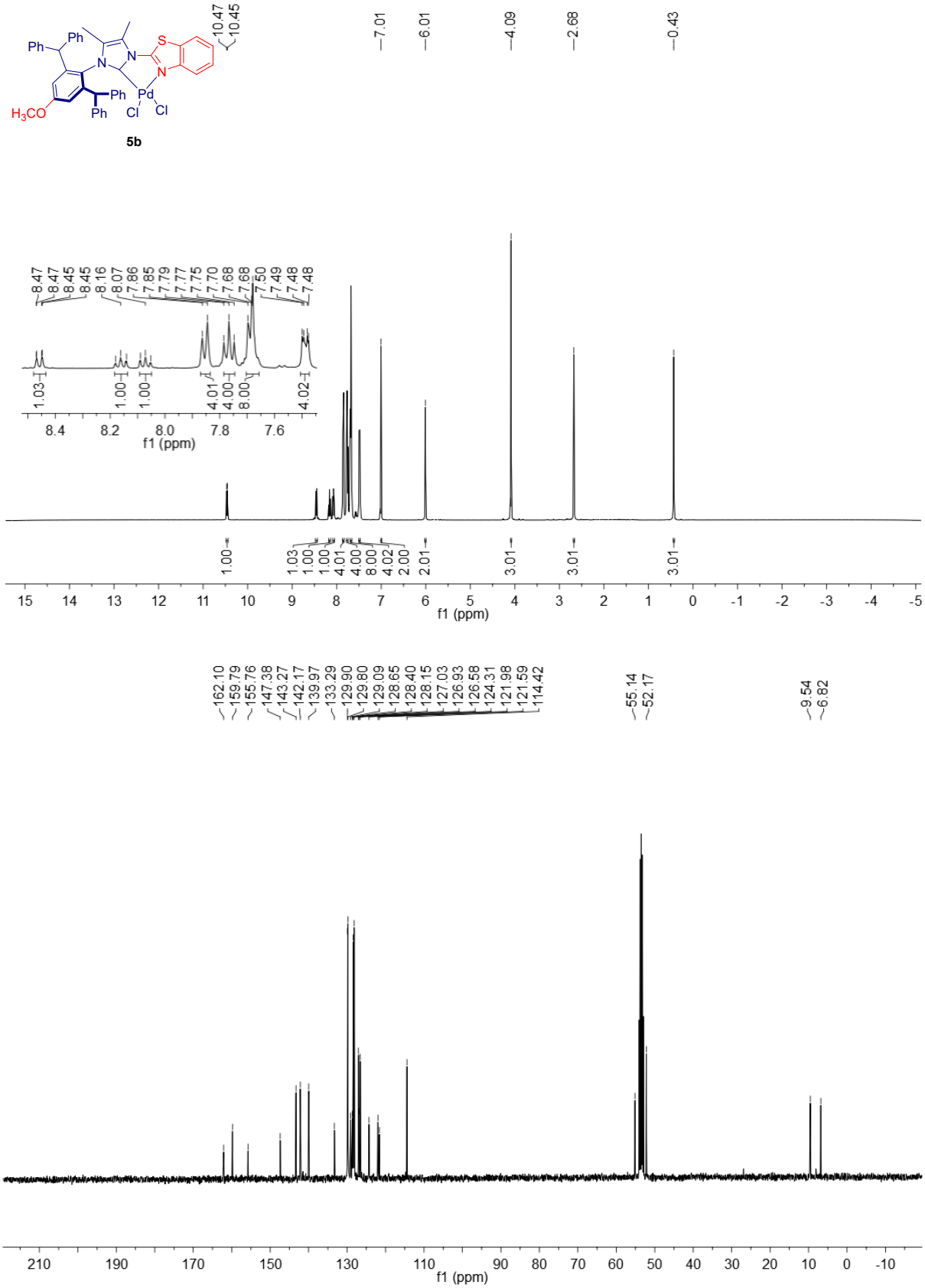
4b



5a Dichloro(1-(benzo[*d*]thiazol-2-yl)-3-(2,6-dibenzhydryl-4-methylphenyl)-4,5-dimethylimidazol-2-ylidene)palladium(II)

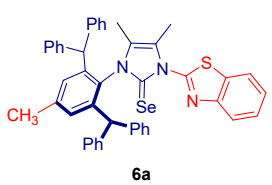


5b Dichloro(1-(benzo[*d*]thiazol-2-yl)-3-(2,6-dibenzhydryl-4-methoxyphenyl)-4,5-dimethylimidazol-2-ylidene)palladium(II)

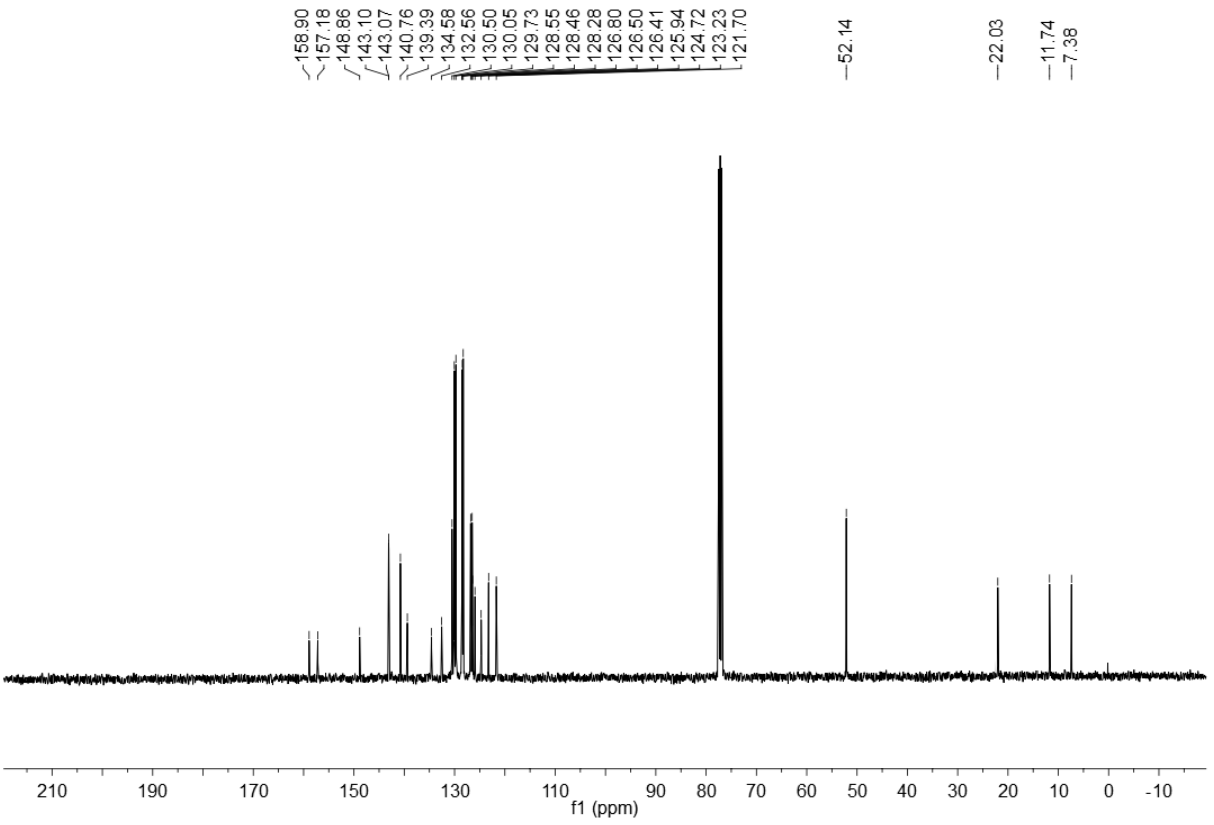


5b

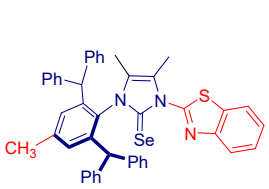
6a (1-(Benzo[*d*]thiazol-2-yl)-3-(2,6-dibenzhydryl-4-methylphenyl)-4,5-dimethylimidazol-2-ylidene)selenone



6a

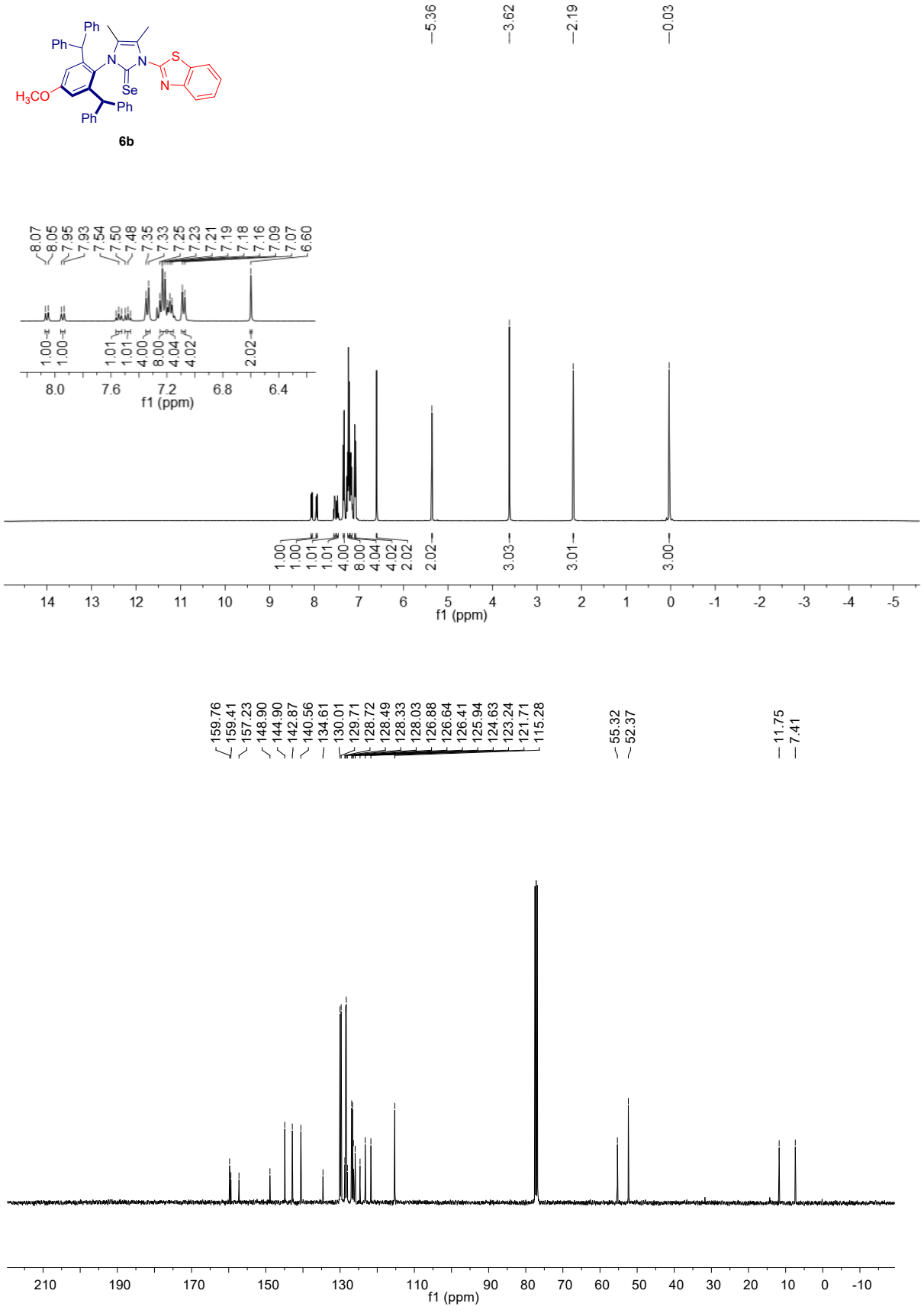


6a (1-(Benzo[*d*]thiazol-2-yl)-3-(2,6-dibenzhydryl-4-methylphenyl)-4,5-dimethylimidazol-2-ylidene)selenone, **^{77}Se NMR**

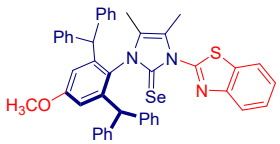


6a

6b (1-(Benzo[*d*]thiazol-2-yl)-3-(2,6-dibenzhydryl-4-methoxyphenyl)-4,5-dimethylimidazol-2-ylidene)selenone

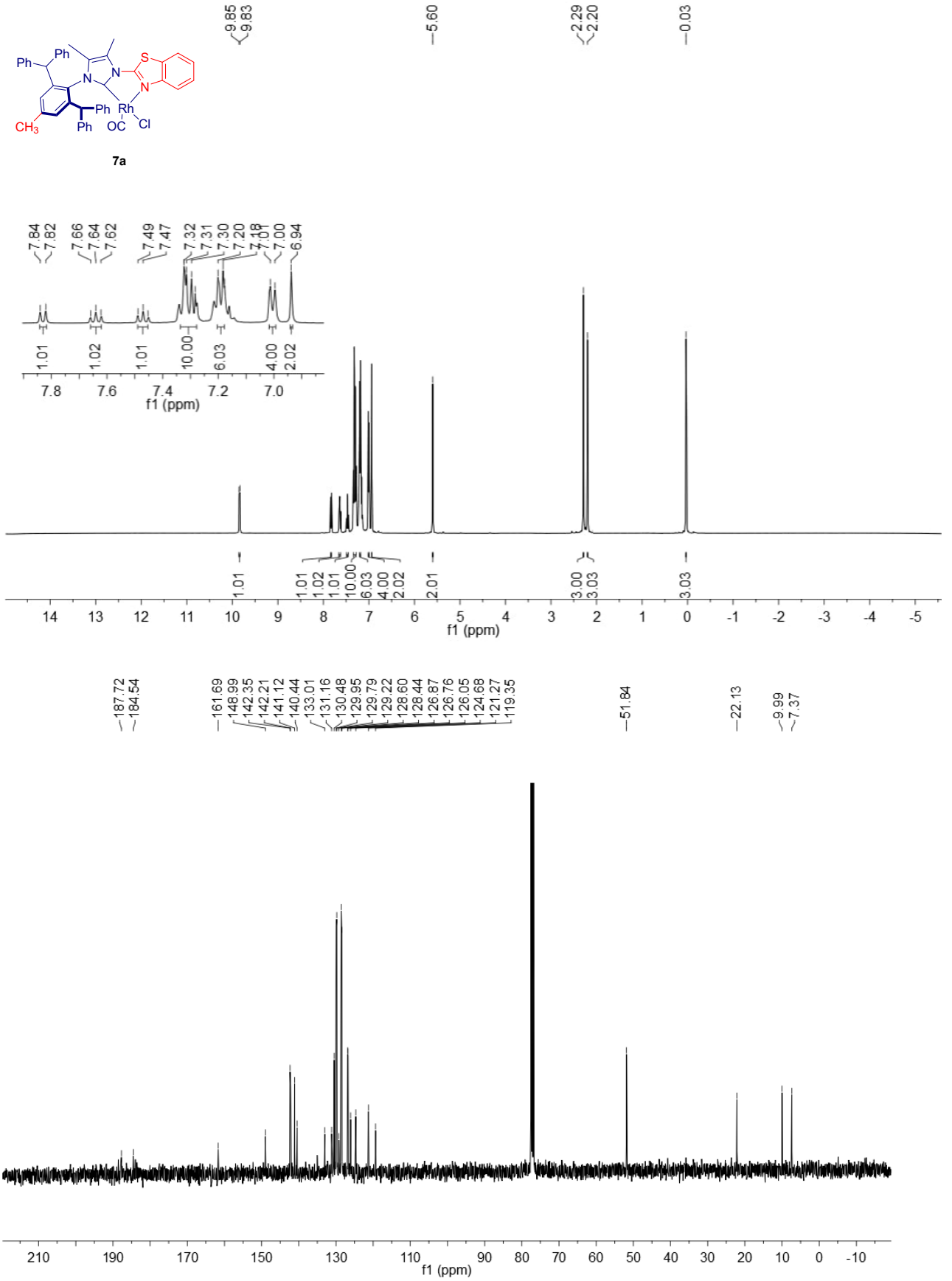


6b (1-(Benzo[*d*]thiazol-2-yl)-3-(2,6-dibenzhydryl-4-methoxyphenyl)-4,5-dimethylimidazol-2-ylidene)selenone, **^{77}Se NMR**

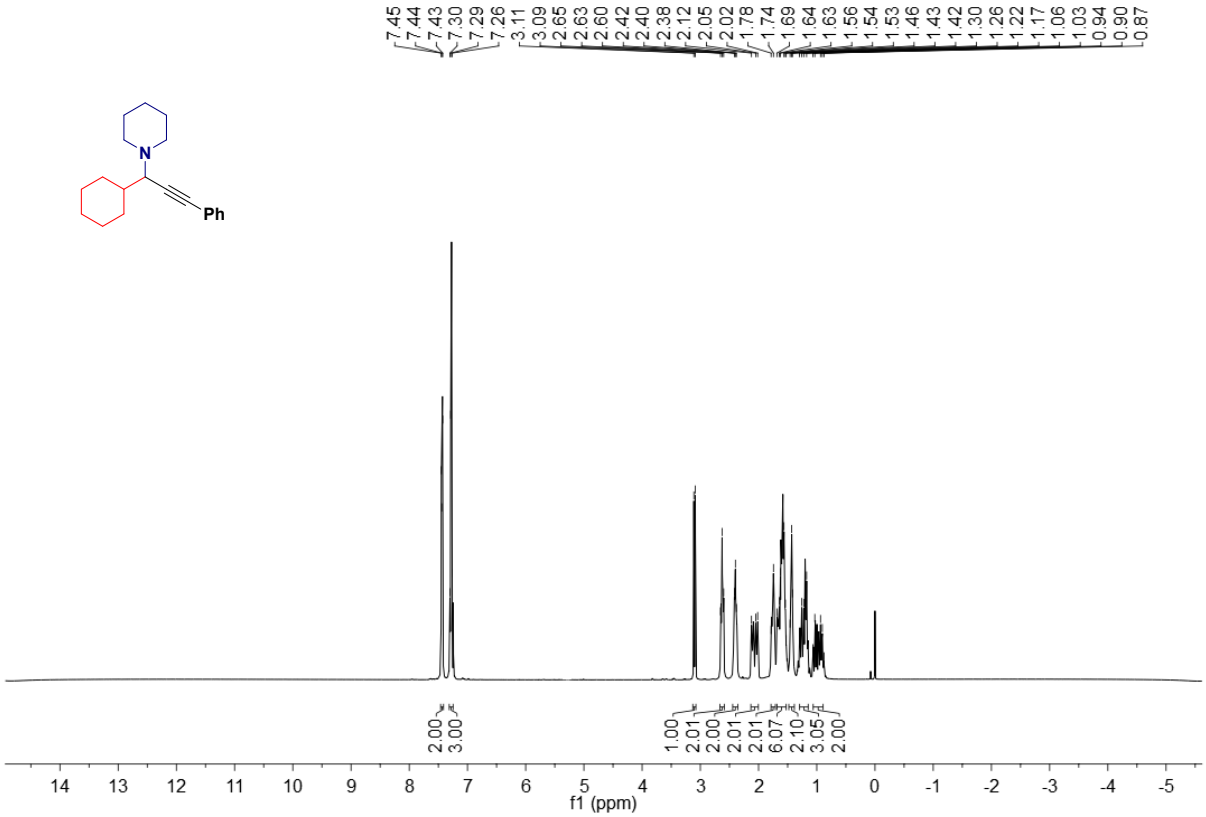


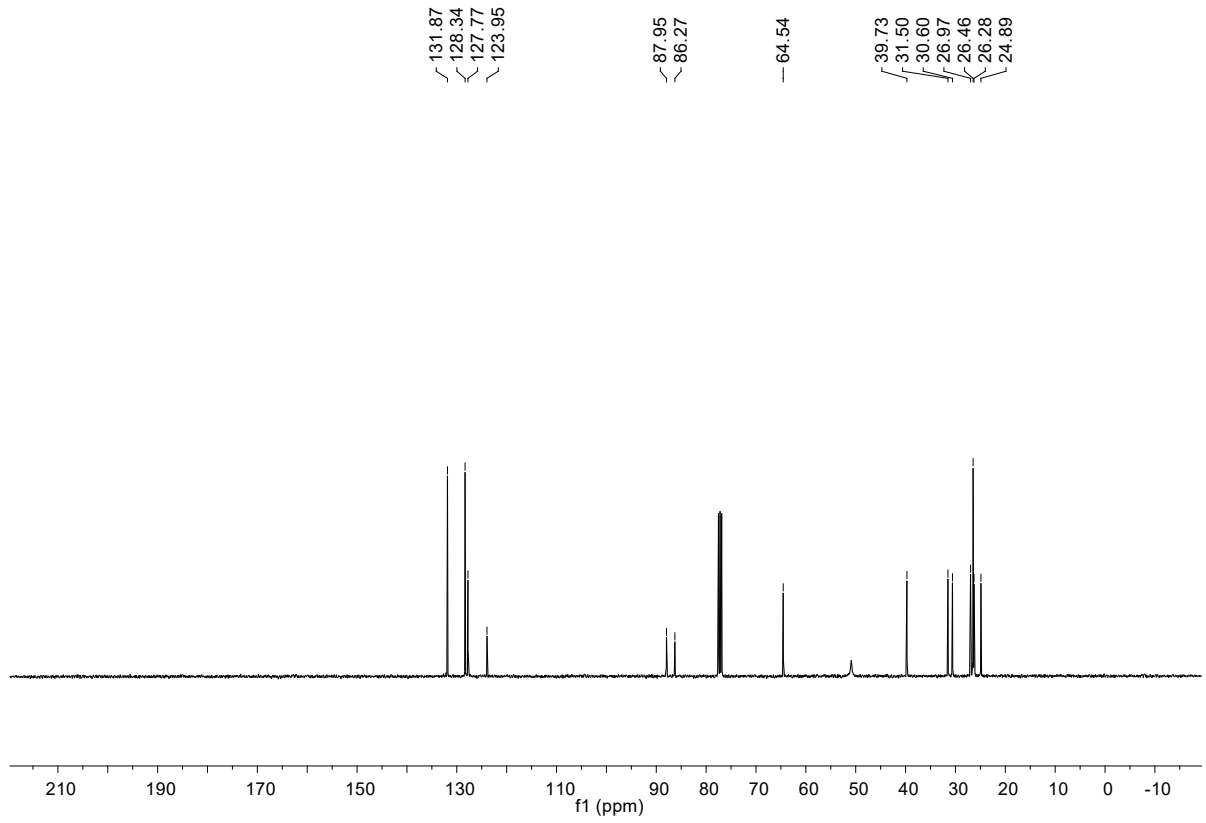
6b

7a Chlorocarbonyl(1-(benzo[*d*]thiazol-2-yl)-3-(2,6-dibenzhydryl-4-methylphenyl)-4,5-dimethylimidazol-2-ylidene)rhodium(I)

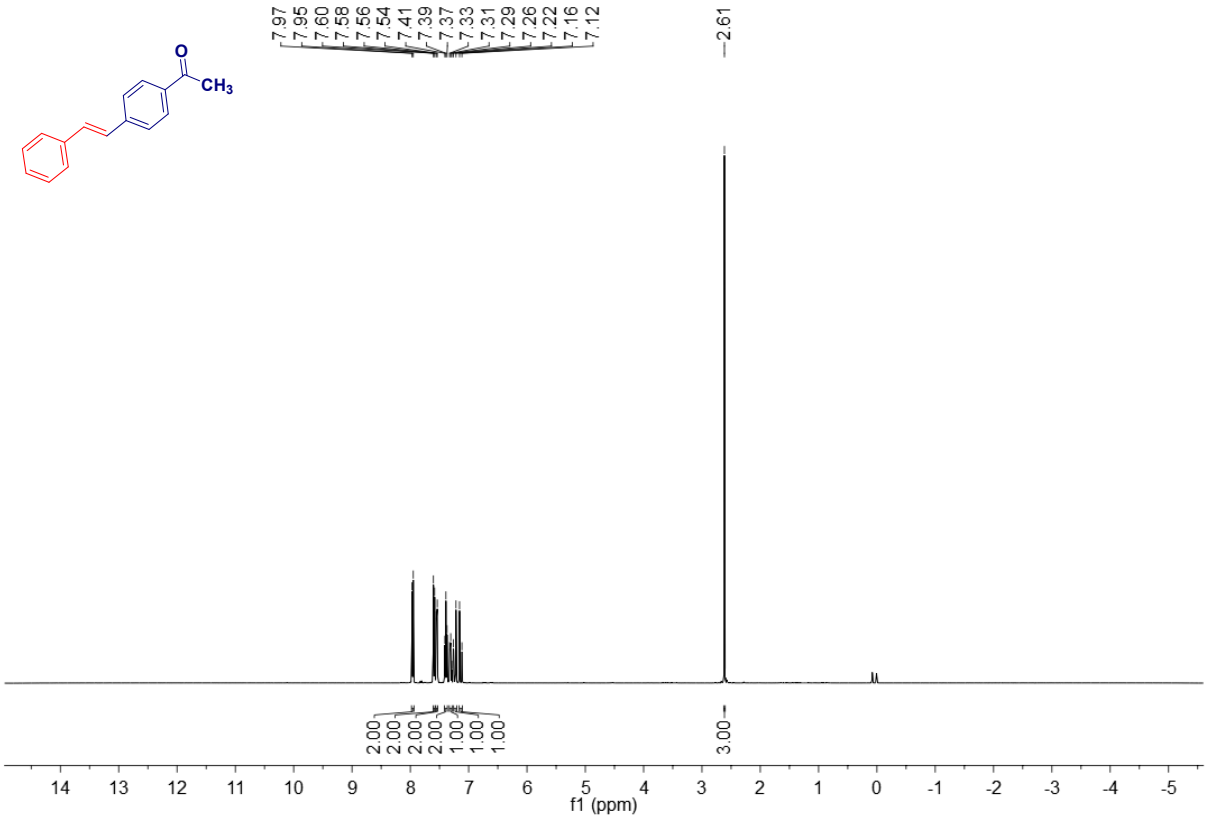


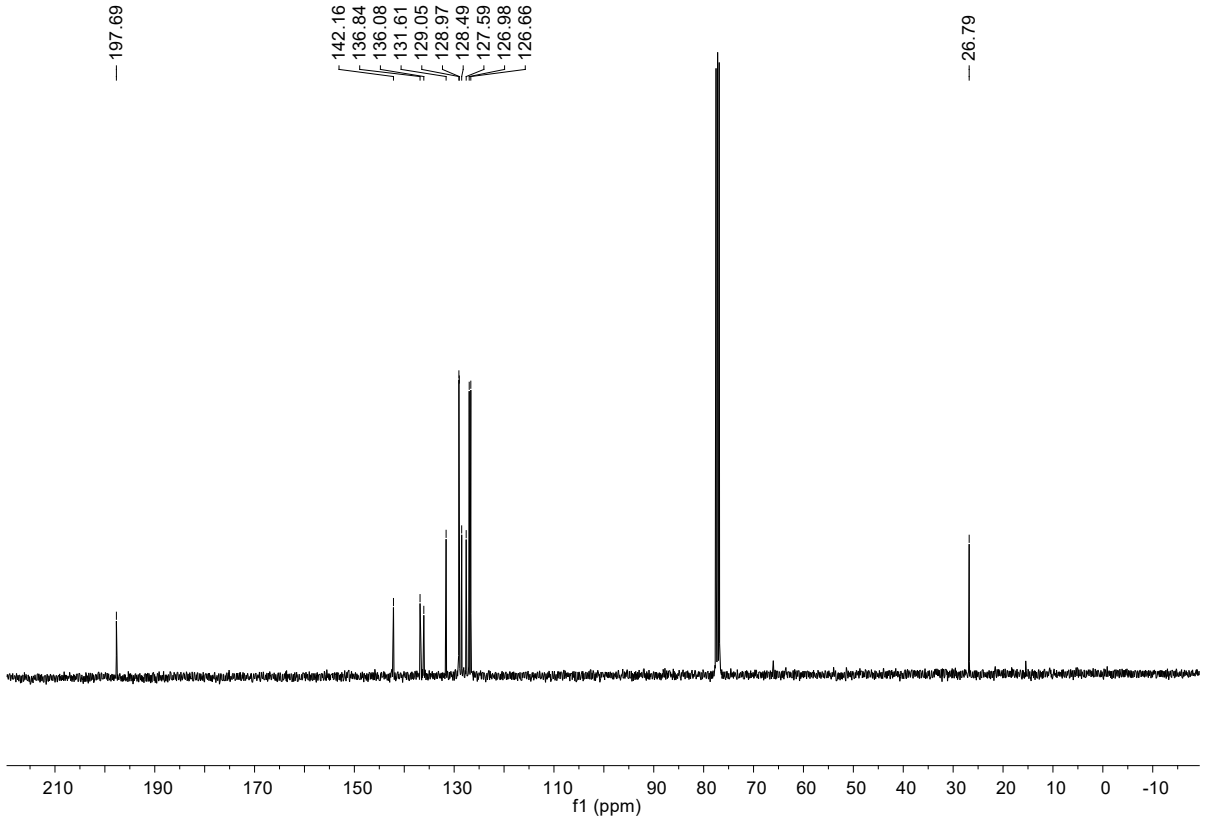
Ag(I)–NHC-catalyzed three component coupling: 1-(1-Cyclohexyl-3-phenylprop-2-yn-1-yl)piperidine



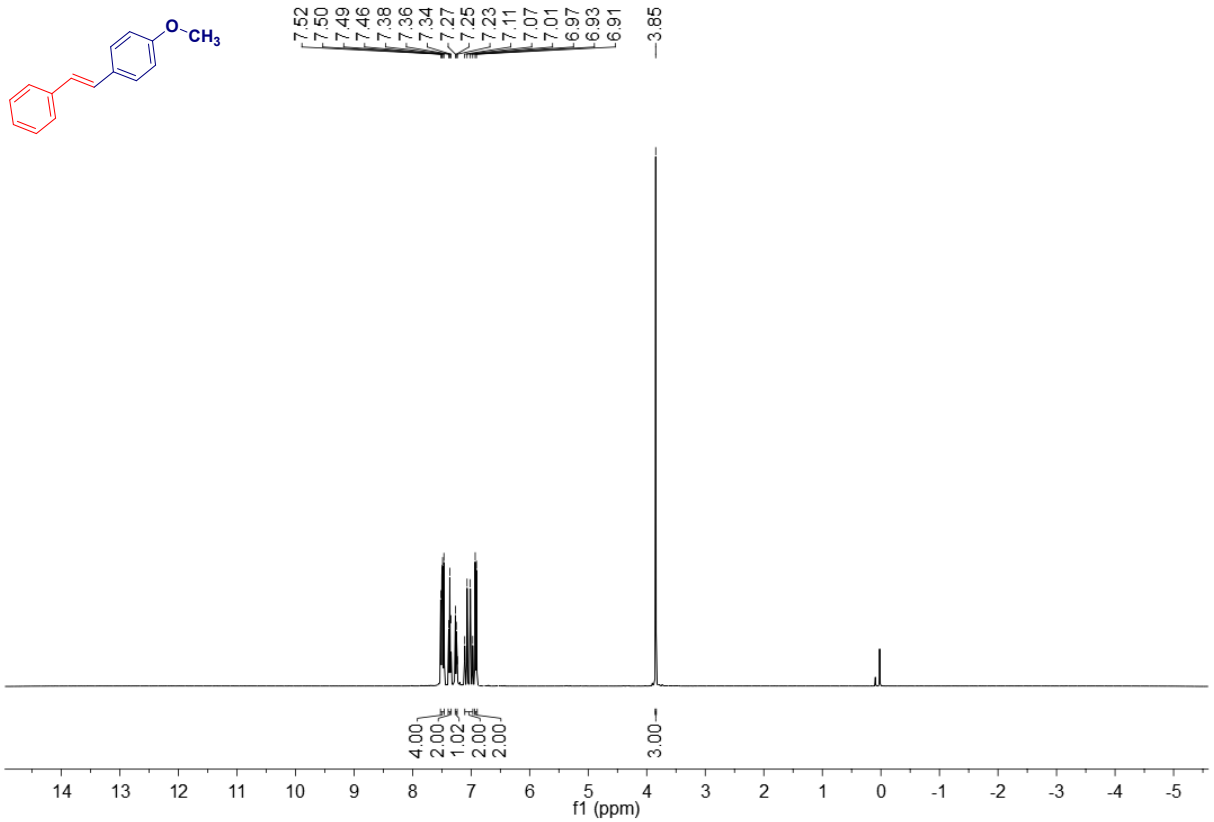


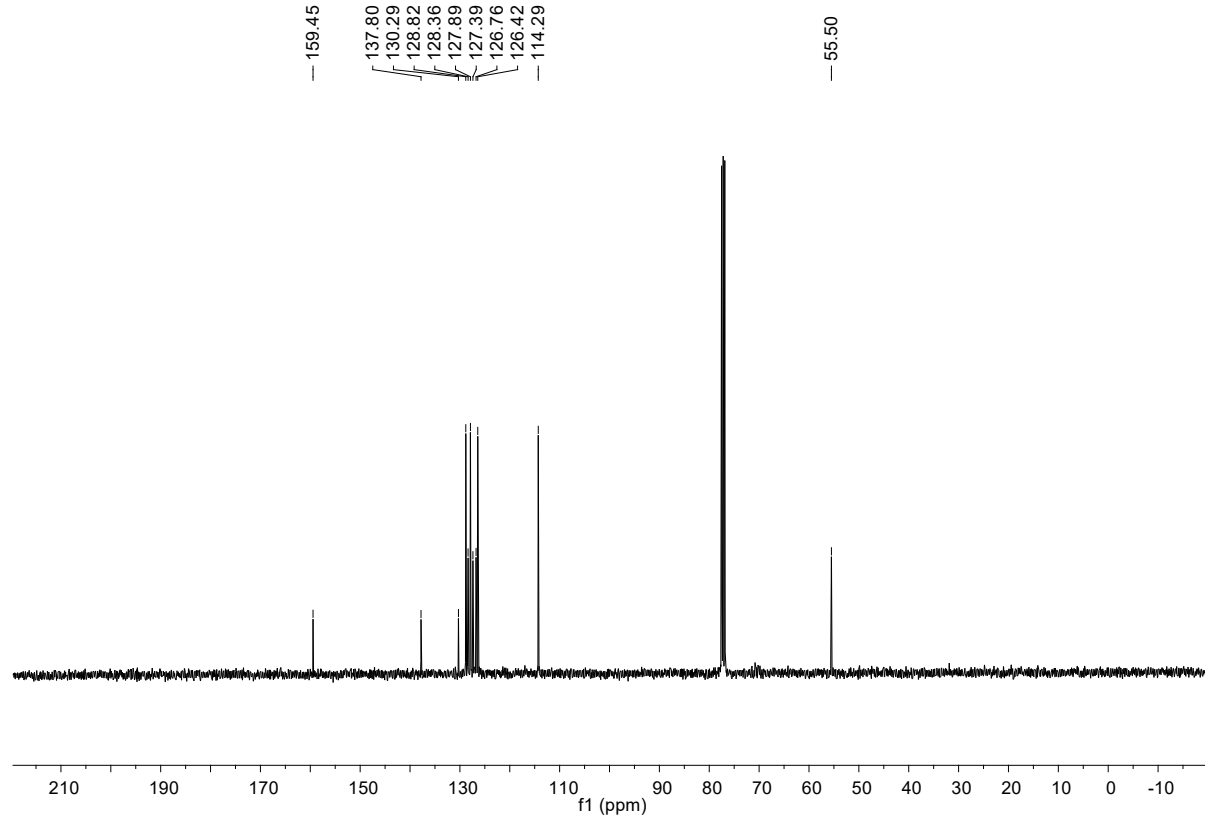
Pd–NHC-catalyzed Heck coupling reaction: (*E*)-1-(4-Styrylphenyl)ethenone





Pd–NHC-catalyzed Heck coupling reaction: (*E*)-1-Methoxy-4-styrylbenzene





IPr*Thia

Energy: -2299.998373 au

Sum of electronic and thermal Energies: -2299.262336 au

Geometry:

N	-0.00112800	0.00000100	0.51322900
N	2.11254000	0.00000800	0.76080100
C	1.13992000	0.00000200	-0.21442900
C	0.22971300	0.00000300	1.90947900
C	1.57752100	0.00000800	2.07447100
C	-0.86879700	0.00000300	2.91716200
H	-1.50343200	-0.88398200	2.81630000
H	-1.50343900	0.88398200	2.81629100
H	-0.45302800	0.00000900	3.92505500
C	2.38260900	0.00001200	3.33024300
H	3.03140200	-0.87593300	3.39369200
H	1.71139500	0.00001300	4.19031800
H	3.03140000	0.87595900	3.39368700
C	-1.29747300	-0.00000400	-0.11910200
C	-1.89999100	1.22535400	-0.45555800
C	-3.13462200	1.19665300	-1.10746900
H	-3.58789400	2.13463600	-1.40880000
C	-3.77497700	-0.00001500	-1.42776500
C	-3.13461100	-1.19667700	-1.10747000
H	-3.58787500	-2.13466500	-1.40880200
C	-1.89998100	-1.22536800	-0.45555800
C	-5.11877200	-0.00002100	-2.11590100

H	-5.24330500	0.88480300	-2.74416900
H	-5.93450900	-0.00001500	-1.38432000
H	-5.24330500	-0.88485400	-2.74415500
C	-1.20888600	2.56105700	-0.16577500
H	-0.14794900	2.33856500	-0.04212400
C	-1.65367000	3.22194500	1.14130700
C	-2.94070000	3.08960300	1.67100000
H	-3.66951400	2.46612600	1.16732900
C	-3.29954600	3.74086200	2.85261700
H	-4.30356800	3.62282100	3.24562400
C	-2.37508900	4.53354000	3.52759500
H	-2.65267100	5.03635700	4.44717900
C	-1.08617900	4.67024700	3.01191500
H	-0.35464600	5.28068800	3.52996000
C	-0.73330000	4.02089800	1.83228300
H	0.27151300	4.13511400	1.43820200
C	-1.28612100	3.50390300	-1.37432400
C	-0.47265600	3.23117000	-2.48252700
H	0.19316700	2.37424800	-2.45427500
C	-0.51199900	4.04190300	-3.61271800
H	0.12841000	3.81653500	-4.45849100
C	-1.36835800	5.14298300	-3.65712000
H	-1.39885700	5.77655000	-4.53653800
C	-2.17666100	5.42545200	-2.55972200
H	-2.84011000	6.28331600	-2.57949400
C	-2.13311600	4.61335500	-1.42461100

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H	-0.14792700	-2.33856500	-0.04213400
C	-1.28610100	-3.50391500	-1.37432300
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C	-0.51200000	-4.04190800	-3.61272600
H	0.12839400	-3.81653200	-4.45850900
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H	-1.39884300	-5.77657100	-4.53653000
C	-2.17662600	-5.42548100	-2.55970500
H	-2.84006200	-6.28335500	-2.57946600
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H	-2.75584500	-4.85649700	-0.57167500
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C	-2.94066500	-3.08962400	1.67100500
H	-3.66948800	-2.46615900	1.16733300
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H	-4.30352200	-3.62285300	3.24563500
C	-2.37503000	-4.53354500	3.52760600
H	-2.65260400	-5.03636100	4.44719300
C	-1.08612000	-4.67023700	3.01192400
H	-0.35457800	-5.28066600	3.52997100
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H	0.27156200	-4.13509300	1.43820600
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C	3.45848300	0.00001000	0.39209400
C	5.54063700	0.00001600	-0.88357800
C	5.65505600	0.00001800	0.52366800
C	6.92191400	0.00002400	1.11646000
H	7.00564800	0.00002500	2.19667300
C	8.04651400	0.00002600	0.30054000
H	9.03354300	0.00003000	0.74847800
C	7.92214800	0.00002400	-1.09630900
H	8.81241000	0.00002600	-1.71465100
C	6.66883800	0.00001900	-1.70211000
H	6.57722300	0.00001800	-2.78187100
S	3.84076300	0.00000900	-1.34191000