

Chelate Palladium(II) Complexes with Saturated N-Phosphanyl-N-Heterocyclic Carbene (NHCP) Ligands: Synthesis and Catalysis

Anatoliy Marchenko,^[a] Georgyi Koidan,^[a] Anastasiia N. Hurieva,^[a] Yurii Vlasenko,

Aleksandr Kostyuk,*^[a] Andrea Biffis *^[b]

^aInstitute of Organic Chemistry National Academy of Sciences of Ukraine, Murmanska 5, Kyiv-94, 02660, Ukraine. Homepage: www.ioch.kiev.ua

^bDipartimento di Scienze Chimiche, Università di Padova, via Marzolo 1, 35131 Padova, Italy.

Supporting Information

Crystallographic parameters of the compounds **3b** and **9a-9c**; copies of spectra of new compounds

Table S1. Main crystallographic parameters of the compounds **3b** and **9a-9c**.

Compound	3b	9a	9b	9c
Cell Parameters				
<i>a</i> [Å]	10.1402(3)	9.4381(2)	7.8616(3)	7.5755(2)
<i>b</i> [Å]	14.3567(4)	12.831(2)	28.4967(10)	29.6946(7)
<i>c</i> [Å]	14.9971(4)	17.115(3)	12.2214(4)	12.1841(3)
α [°]	93.788(1)	90	90	90
β [°]	100.686(1)	90	103.744(2)	101.2660(10)
γ [°]	90.570(1)	90	90	90
V[Å ³]	2140.2(1)	2072.5(6)	2659.56(16)	2688.02(12)
Z	4	4	2	4
D[g·cm ⁻³]	1.075	1.544	1.407	1.453
Crystal system	Triclinic	Orthorhombic	Monoclinic	Monoclinic
Space group	<i>P</i> -1	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ /n	<i>P</i> 2 ₁ /n
μ [cm ⁻¹]	0.133	1.233	0.973	1.043
F(000)	760	984	1162	1216
Indexes	12 \geq <i>h</i> \geq -13 19 \geq <i>k</i> \geq -19 20 \geq <i>l</i> \geq -20	6 \geq <i>h</i> \geq -11 15 \geq <i>k</i> \geq -16 20 \geq <i>l</i> \geq -19	9 \geq <i>h</i> \geq -9 33 \geq <i>k</i> \geq -35 14 \geq <i>l</i> \geq -15	9 \geq <i>h</i> \geq -9 36 \geq <i>k</i> \geq -37 15 \geq <i>l</i> \geq -15
θ_{\max} [°]	29.3	26.5	26.4	26.7
No. of reflections:				
collected	34078	7586	24815	24771
independent	11102	3839	5439	5662
in refinement (<i>I</i> \geq 3 σ (<i>I</i>))	6730	3210	4062	4566
<i>R</i> (int)	0.053	0.042	0.058	0.044
No. of refined parameters	433	217	289	271
Obsd./var.	15.5	14.7	14.1	16.8
Final <i>R</i> indices				
<i>R</i> ₁	0.048	0.046	0.035	0.038
<i>R</i> _w	0.097	0.050	0.032	0.034
GOF	0.9092	1.072	1.094	1.108

Weighting coefficients	11.9 14.7 5.91	4.02 -2.46 3.23	1.21 -1.14 0.607 -0.276	1.13 -1.07 0.622 -0.346
Largest peak/hole [$e \cdot cm^{-3}$]	0.45/-0.30	1.26/-0.64	0.50/-0.56	2.16/-0.78
CCDC deposition number	1437123	1437124	1437122	1437233

Figure S1. ^1H NMR spectrum of **2a**

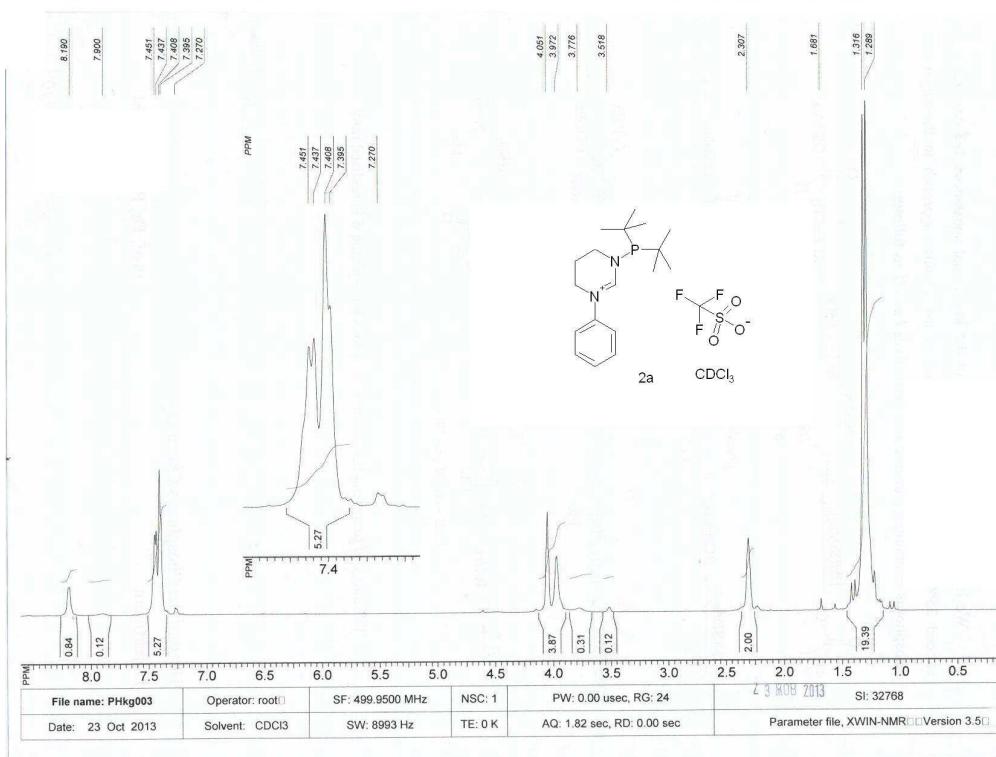


Figure S2. ^{13}C NMR spectrum of **2a**

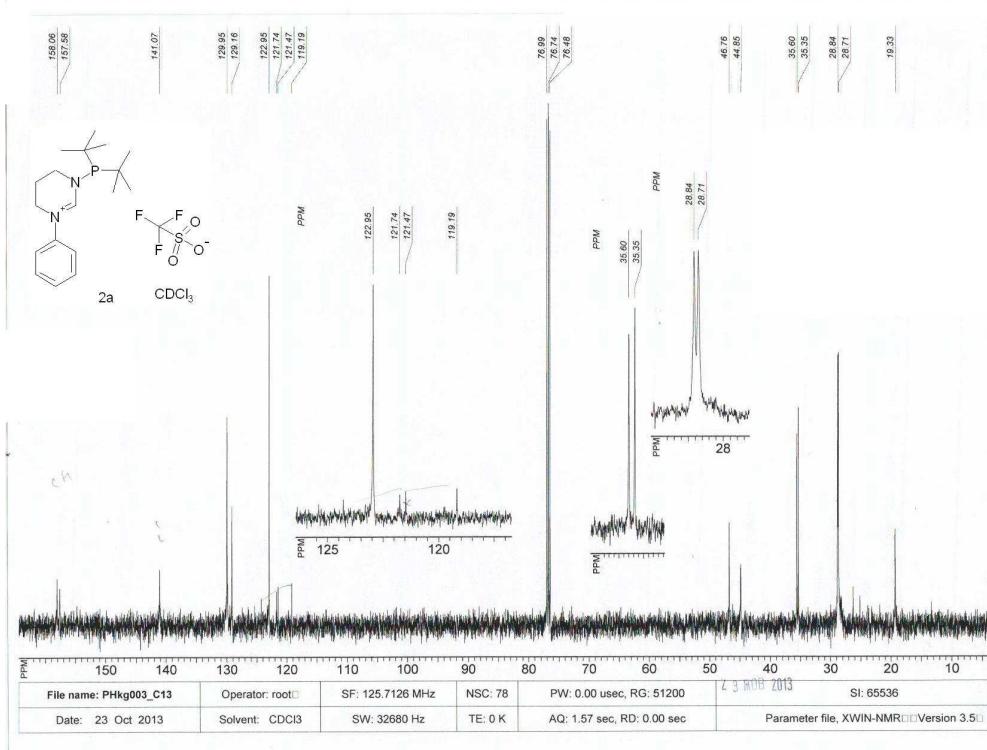


Figure S3. ^{31}P NMR spectrum of **2a**

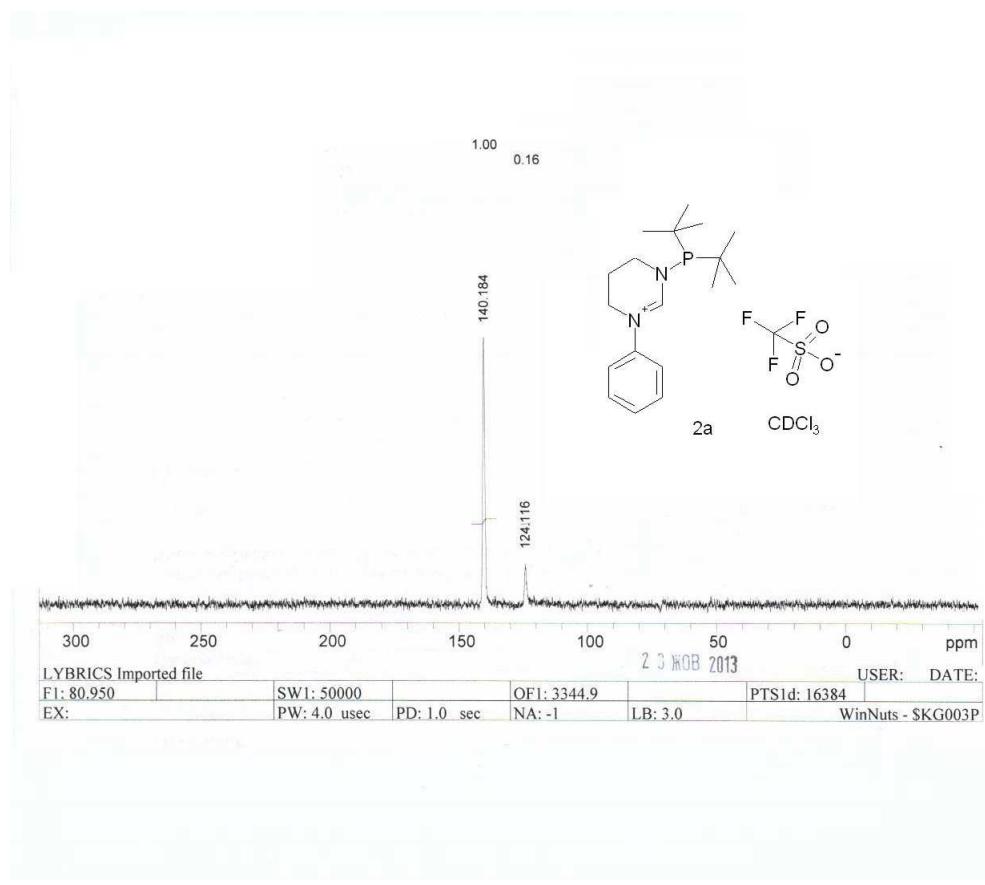


Figure S4. ^1H NMR spectrum of **2b**

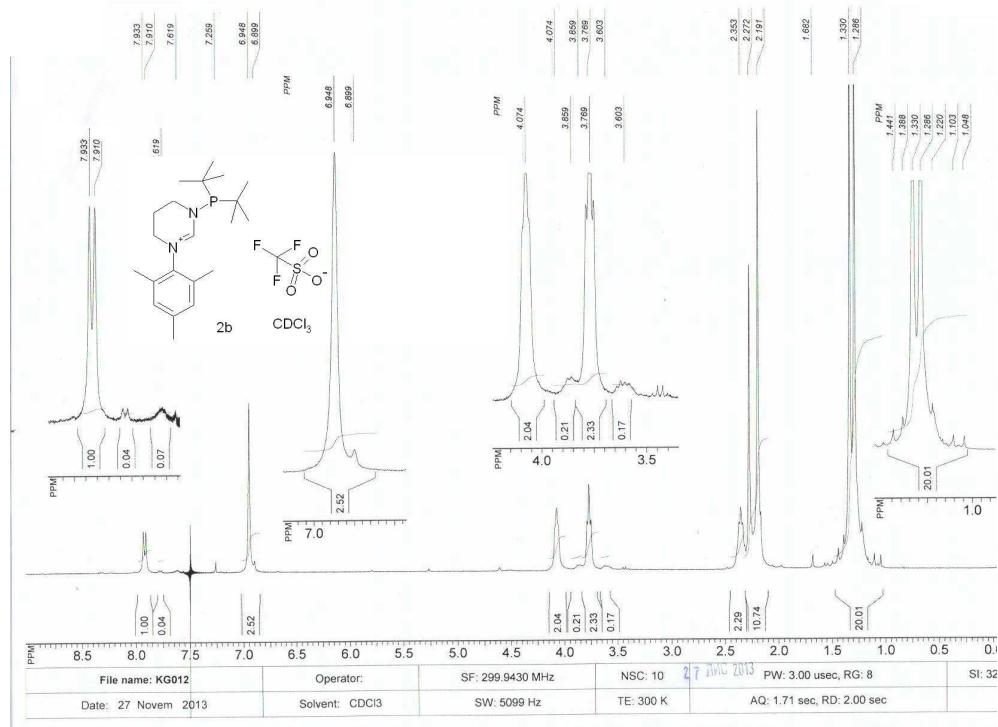


Figure S5. ^{13}C NMR spectrum of **2b**

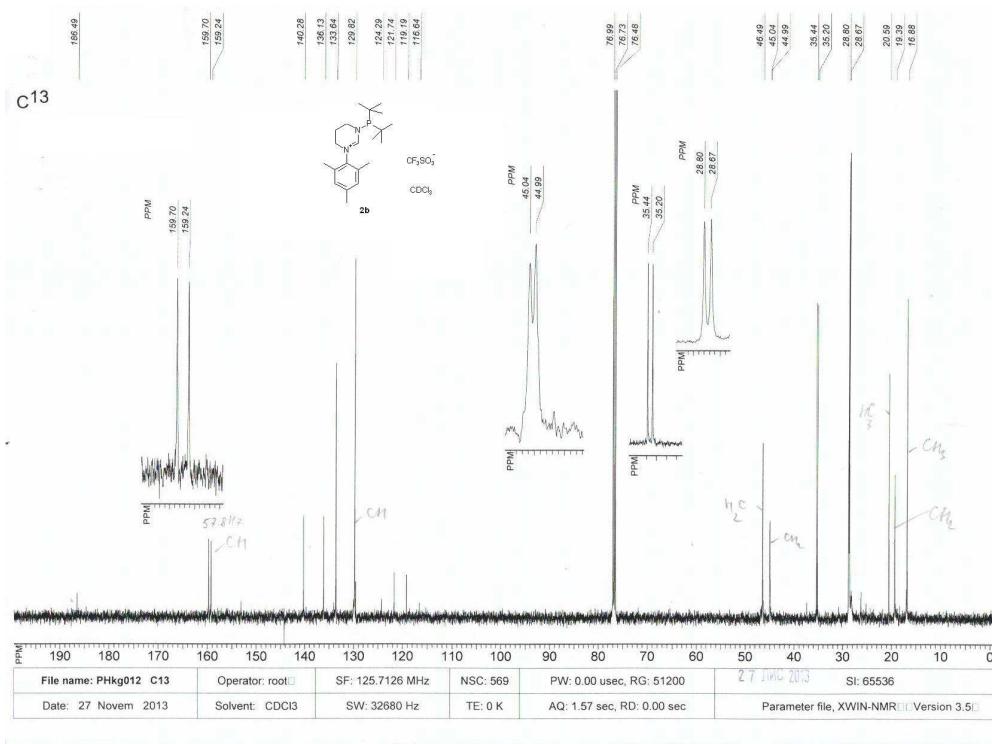


Figure S6. ^{31}P NMR spectrum of **2b**

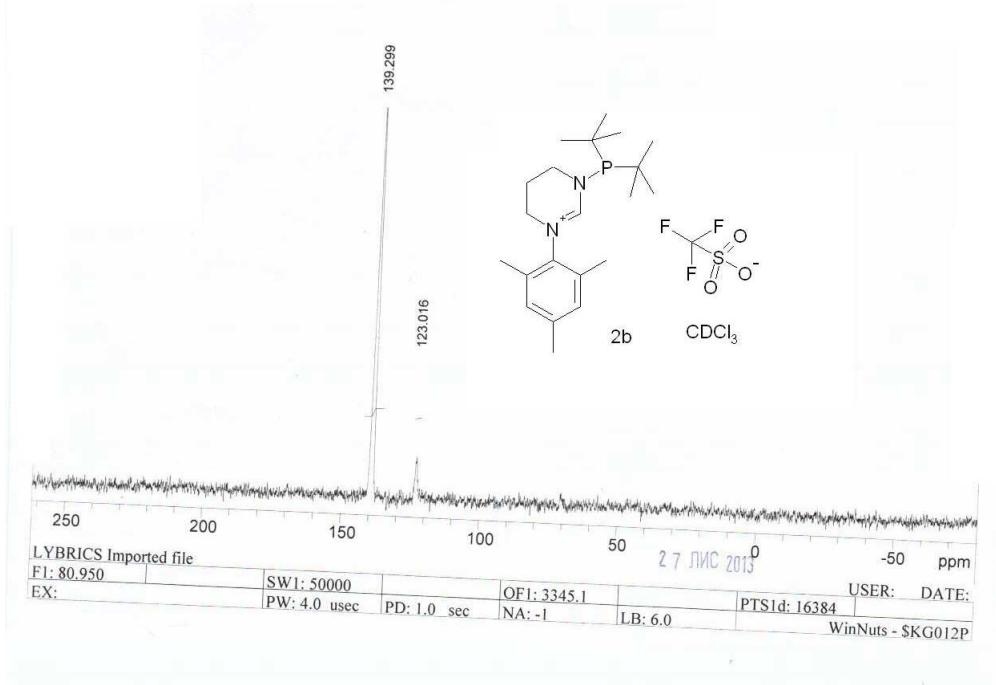


Figure S7. ^1H NMR spectrum of **3a**

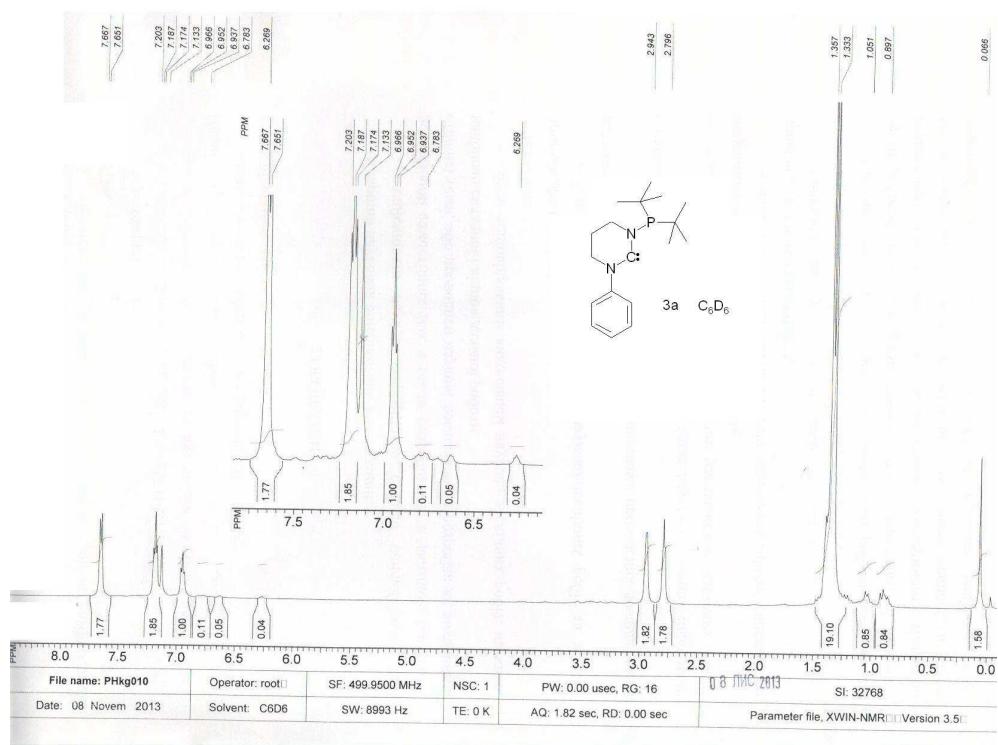


Figure S8. ^{13}C NMR spectrum of **3a**

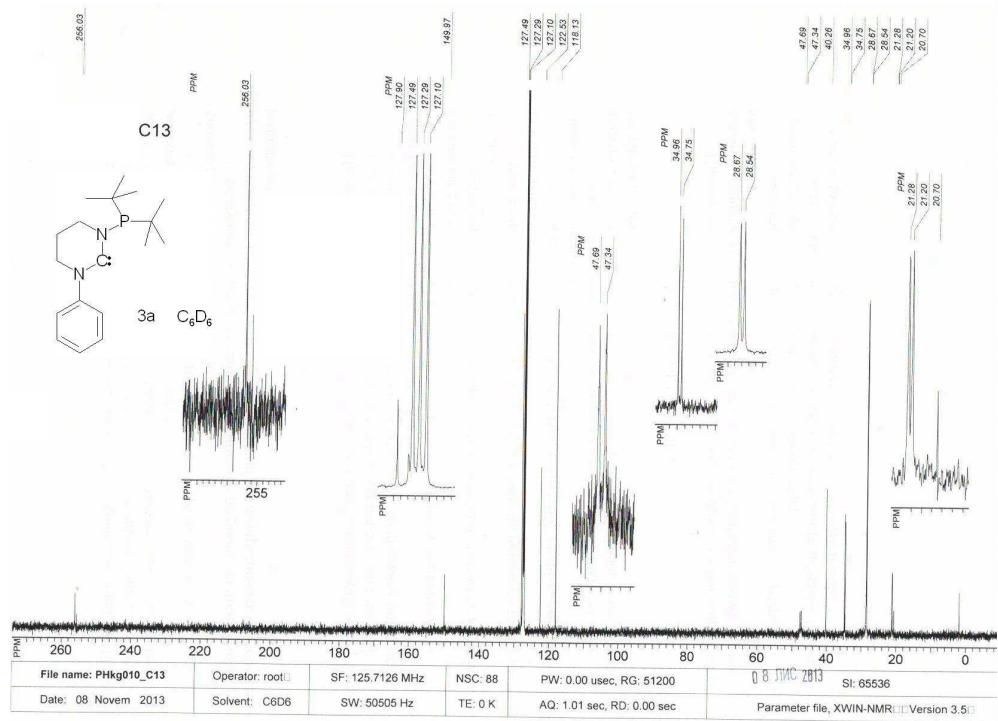


Figure S9. ^1H NMR spectrum of **3b**

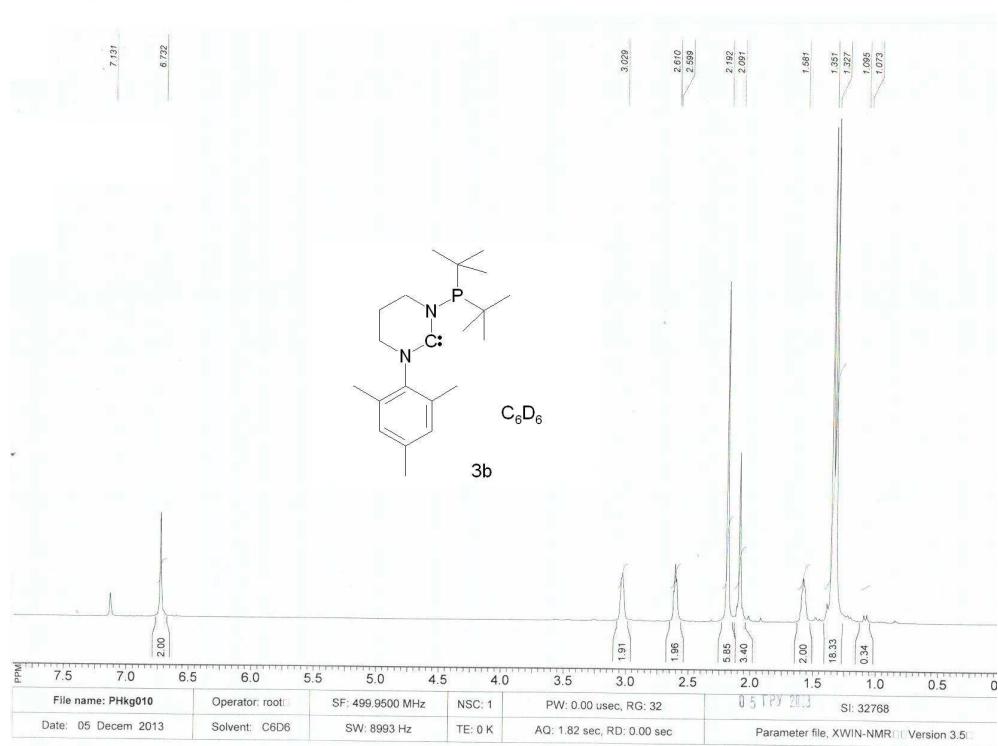


Figure S10. ^{13}C NMR spectrum of **3b**

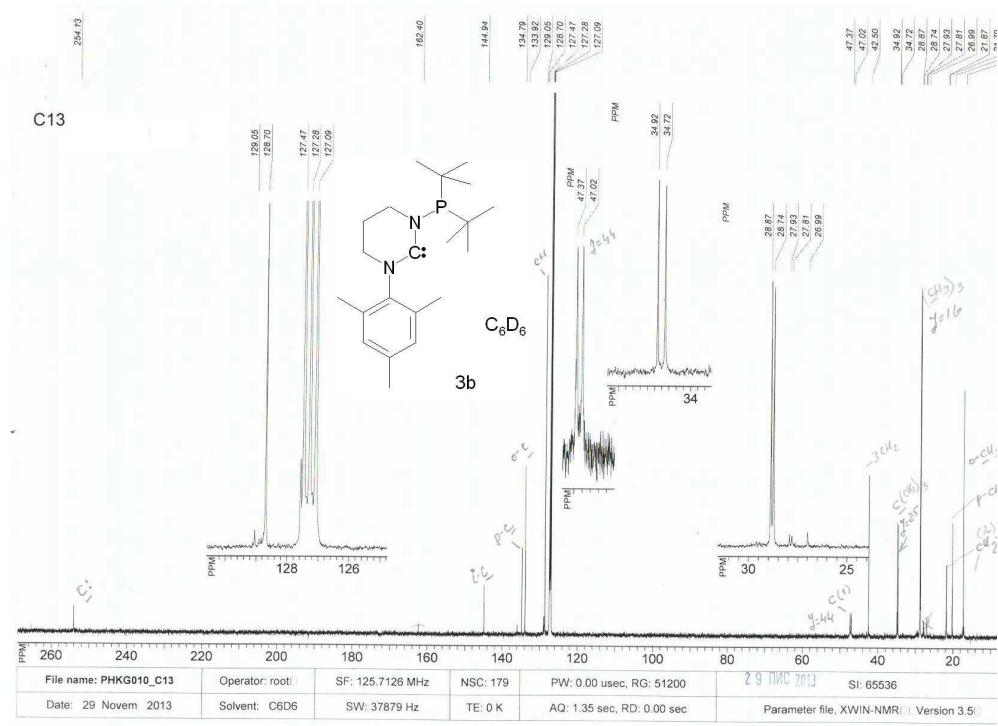


Figure S11. ^1H NMR spectrum of **4a**

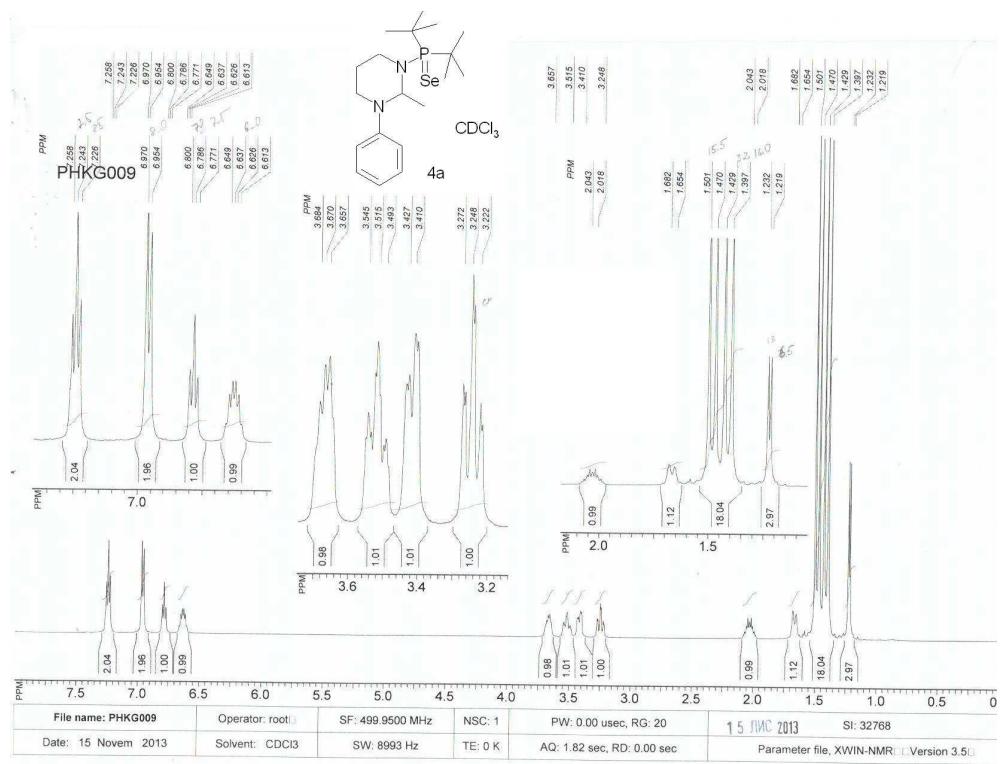


Figure S12. ^{13}C NMR spectrum of **4a**

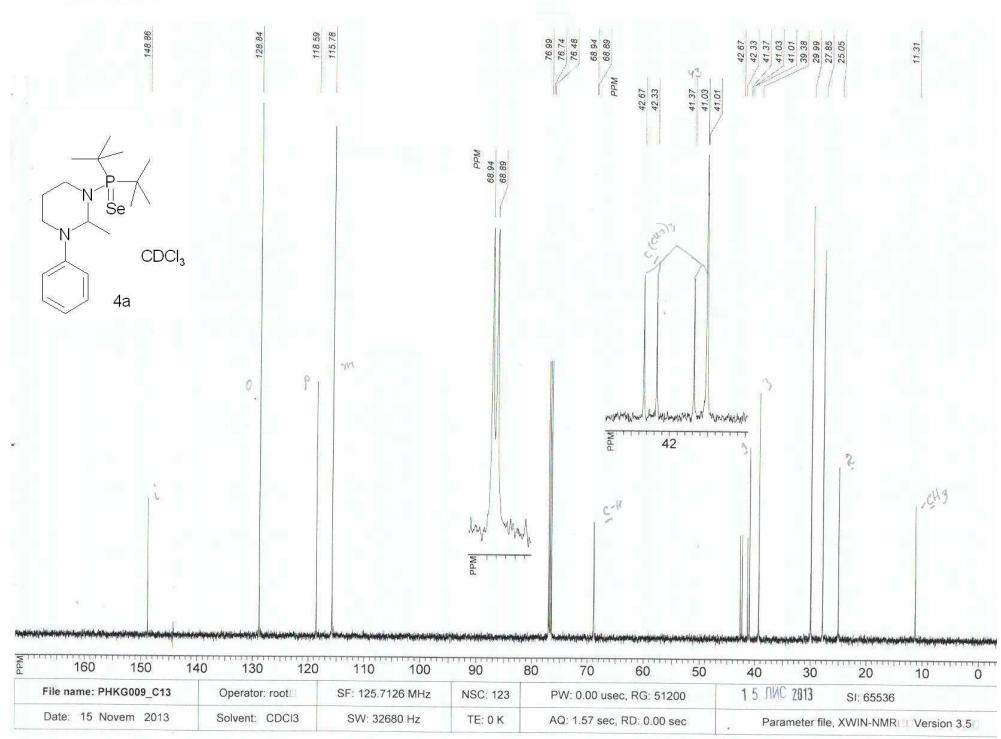


Figure S13. ^1H NMR spectrum of **4b**

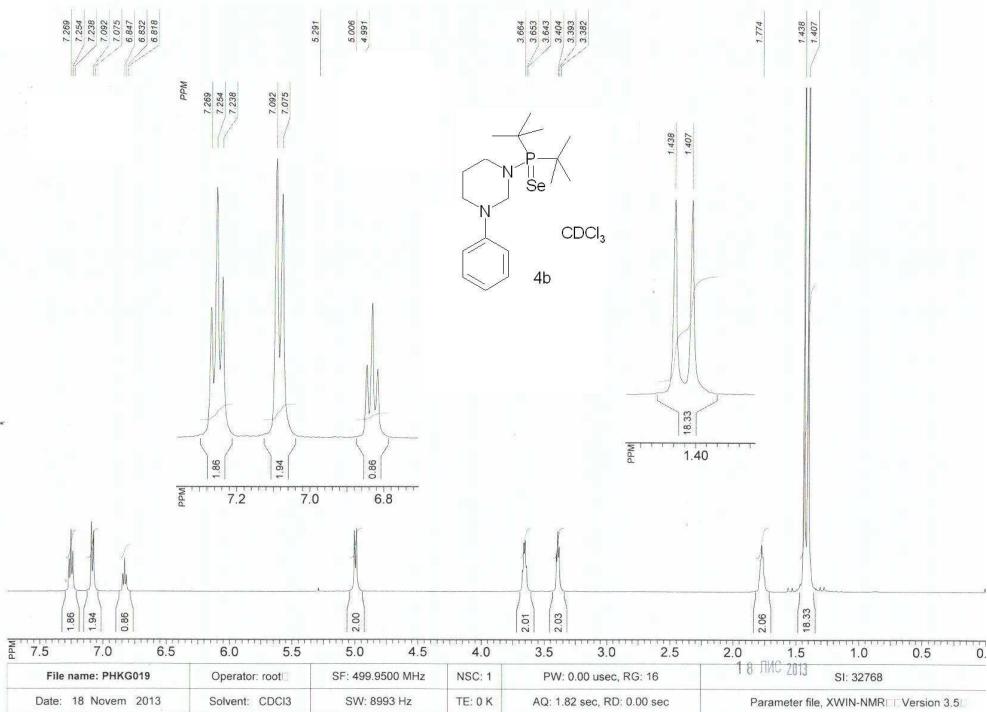


Figure S14. ^{13}C NMR spectrum of **4b**

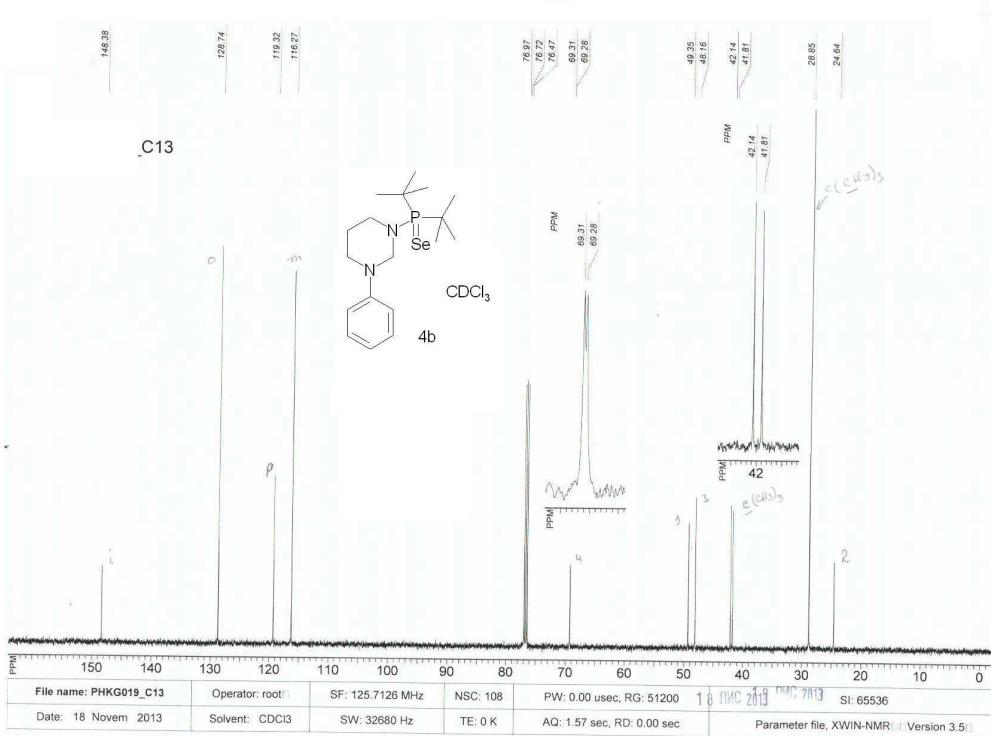


Figure S15. ^1H NMR spectrum of **5a**

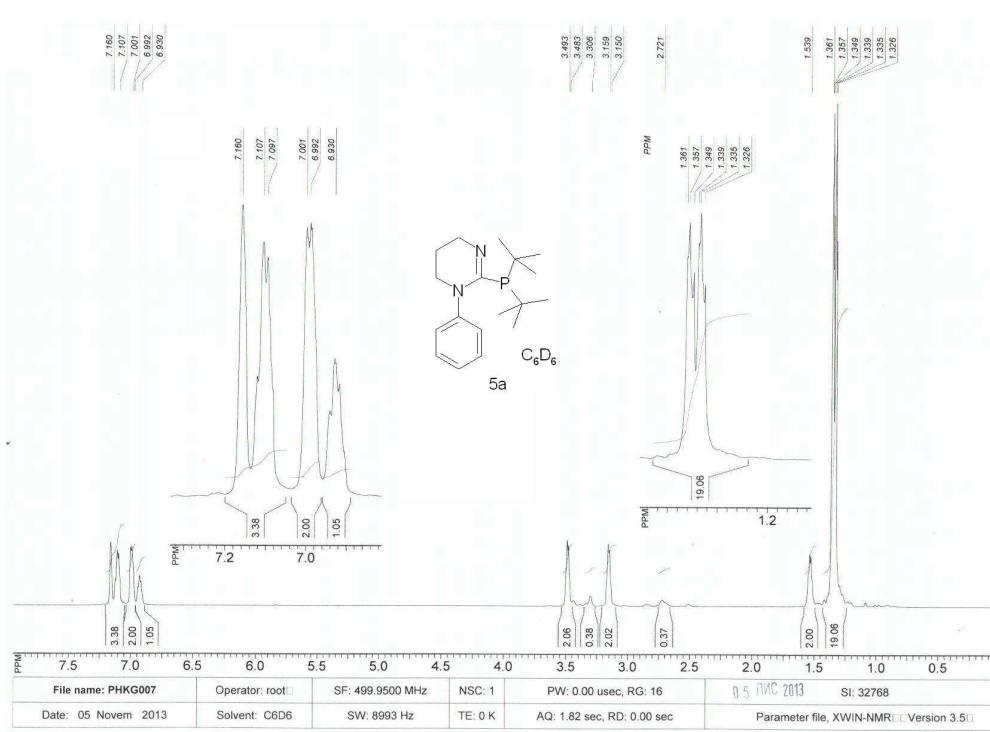


Figure S16. ^{13}C NMR spectrum of **5a**

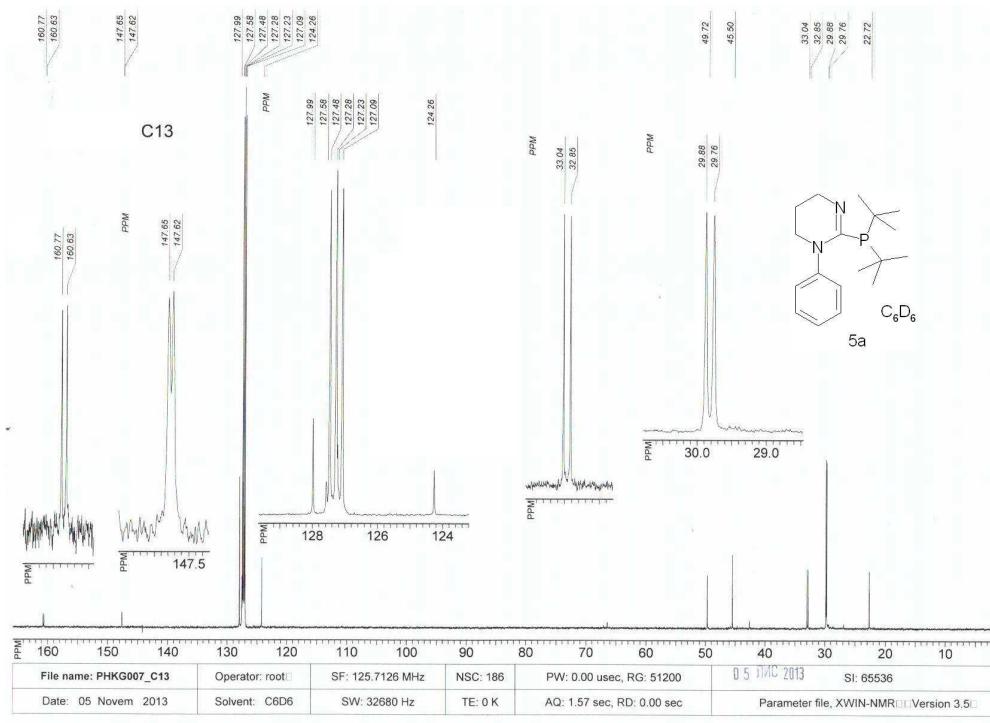


Figure S17. ^1H NMR spectrum of **5b**

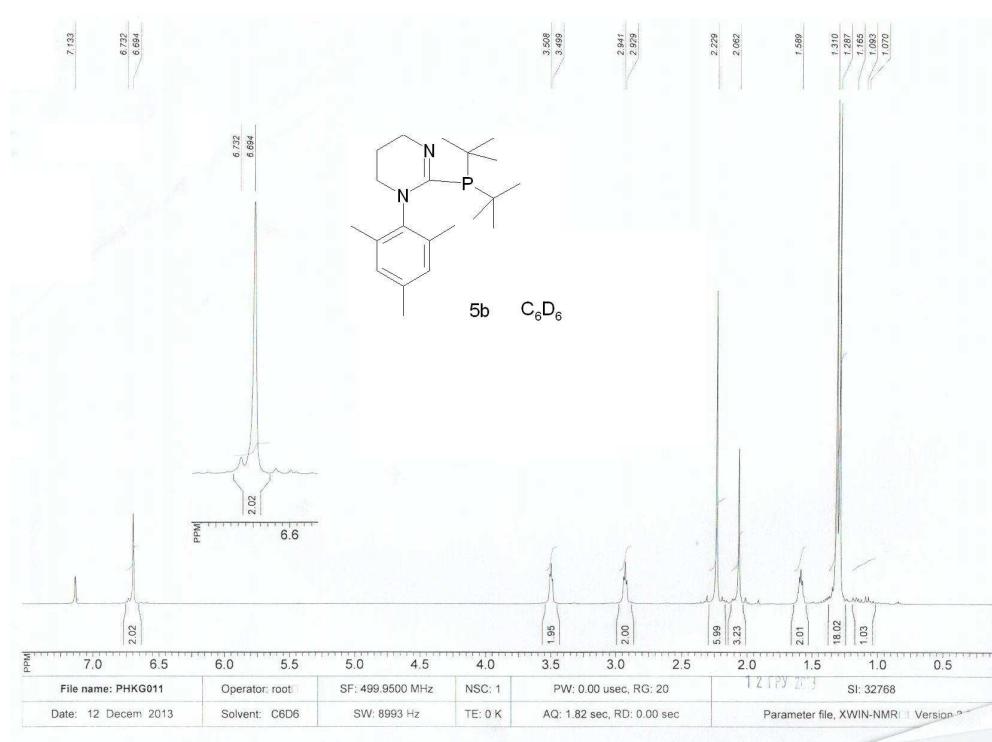


Figure S18. ^{13}C NMR spectrum of **5b**

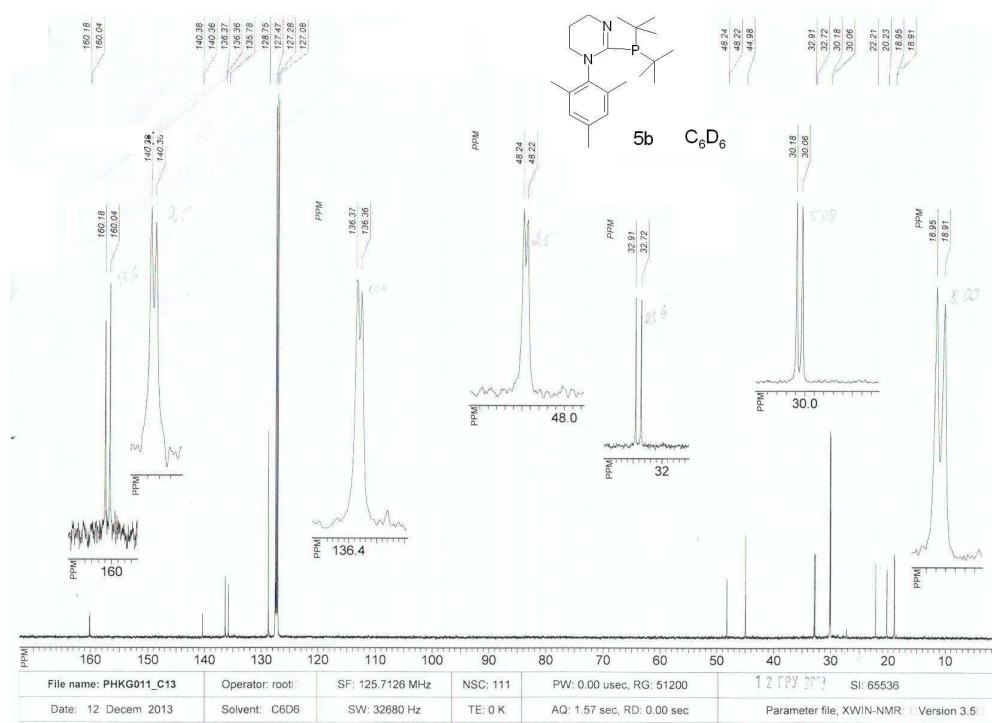


Figure S19. ^1H NMR spectrum of **6a**

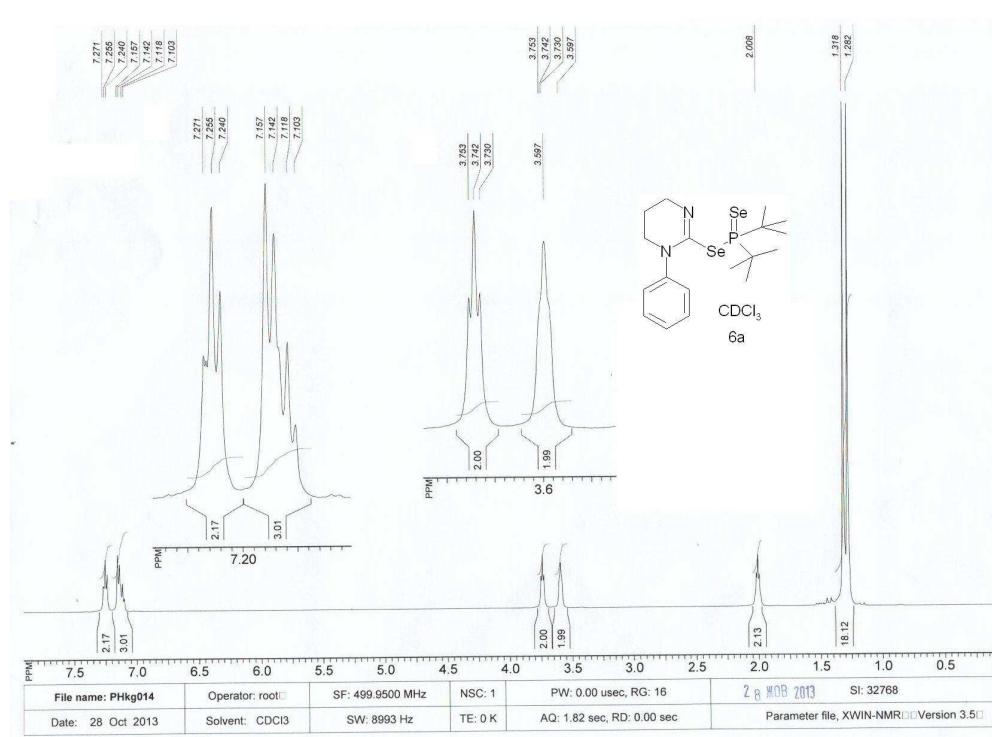


Figure S20. ^{13}C NMR spectrum of **6a**

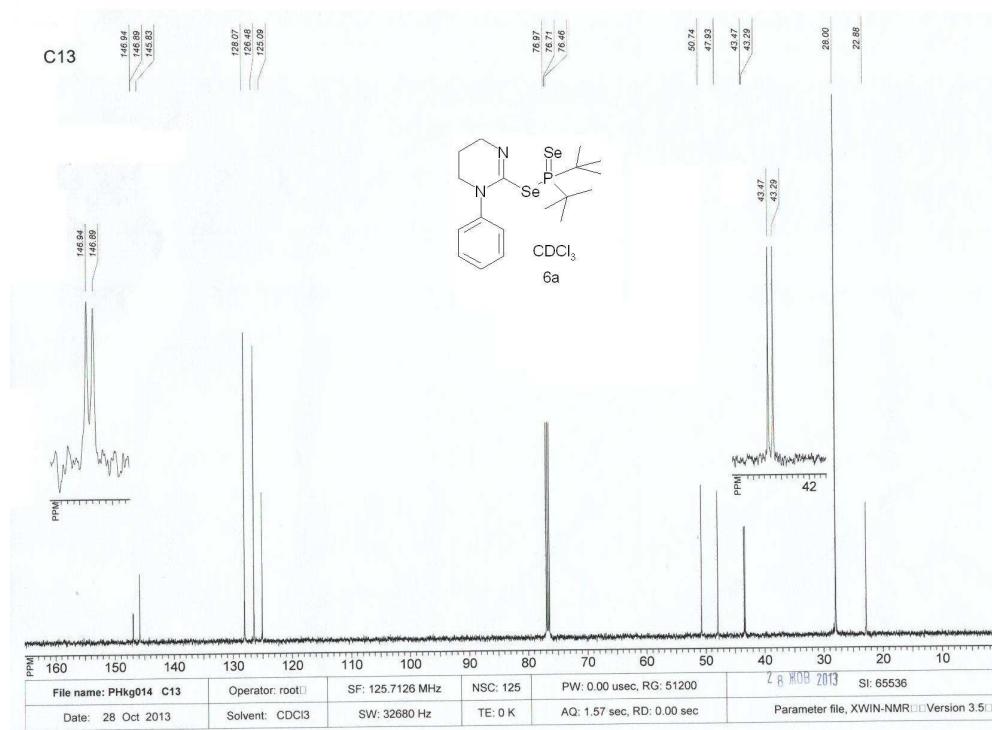


Figure S21. ^{31}P NMR spectrum of **6a**

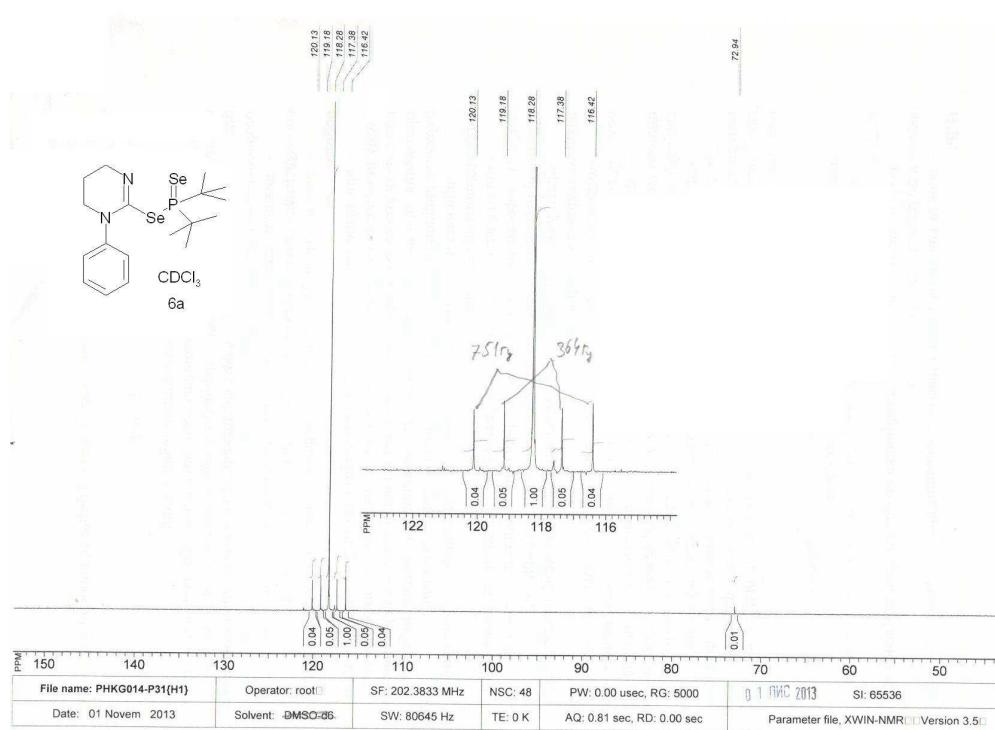


Figure S22. ^1H NMR spectrum of **6b**

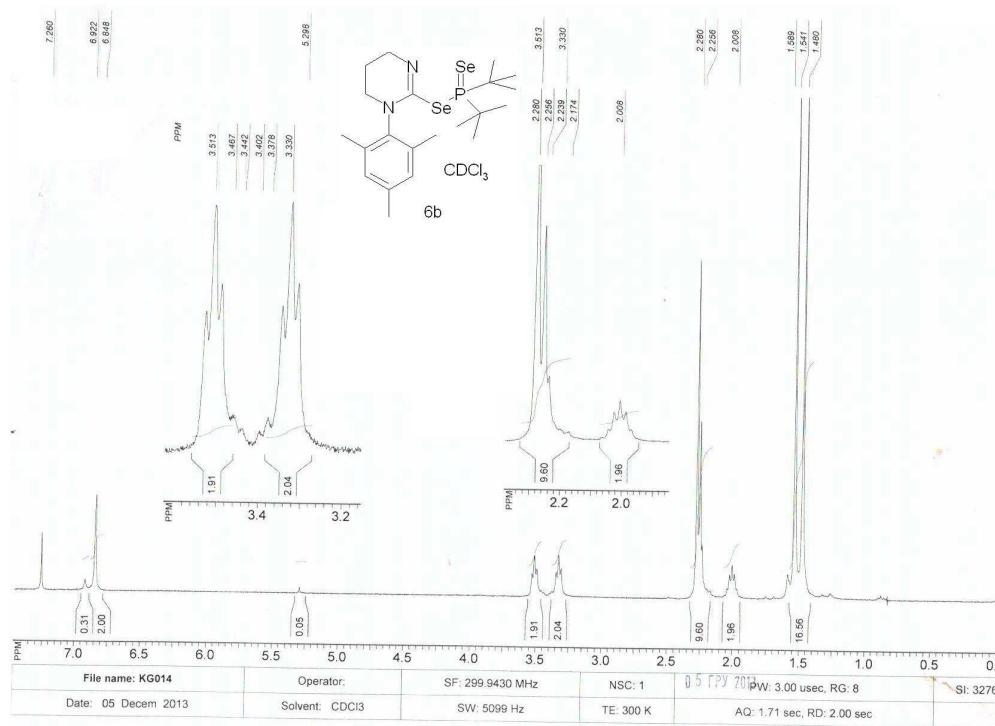


Figure S23. ^{13}C NMR spectrum of **6b**

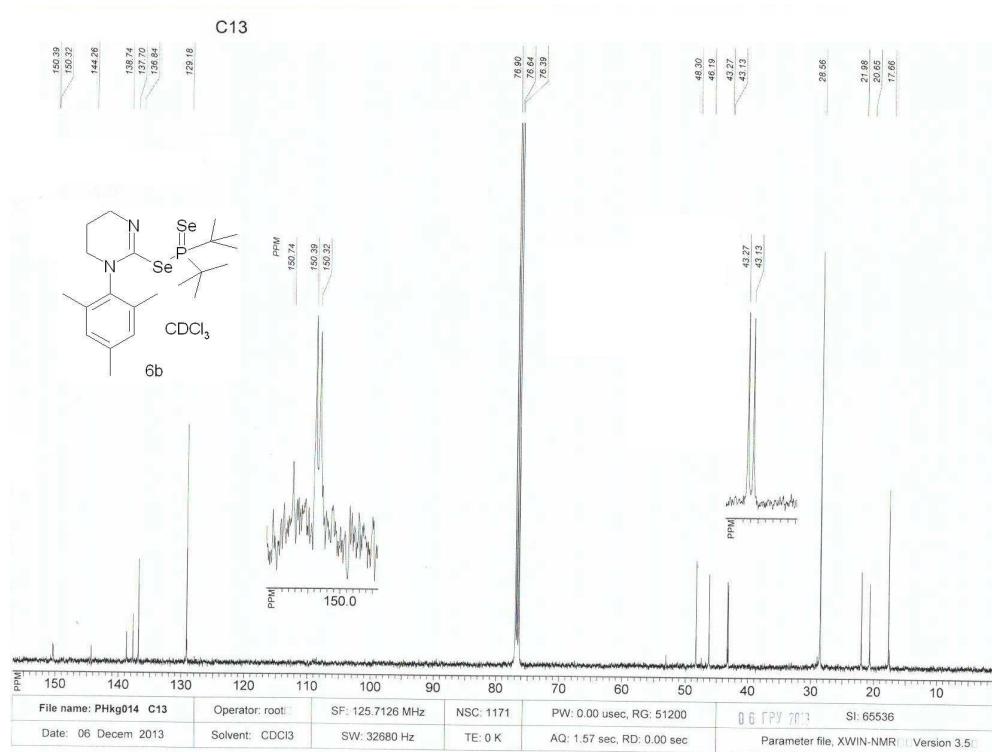


Figure S24. ^{31}P NMR spectrum of **6b**

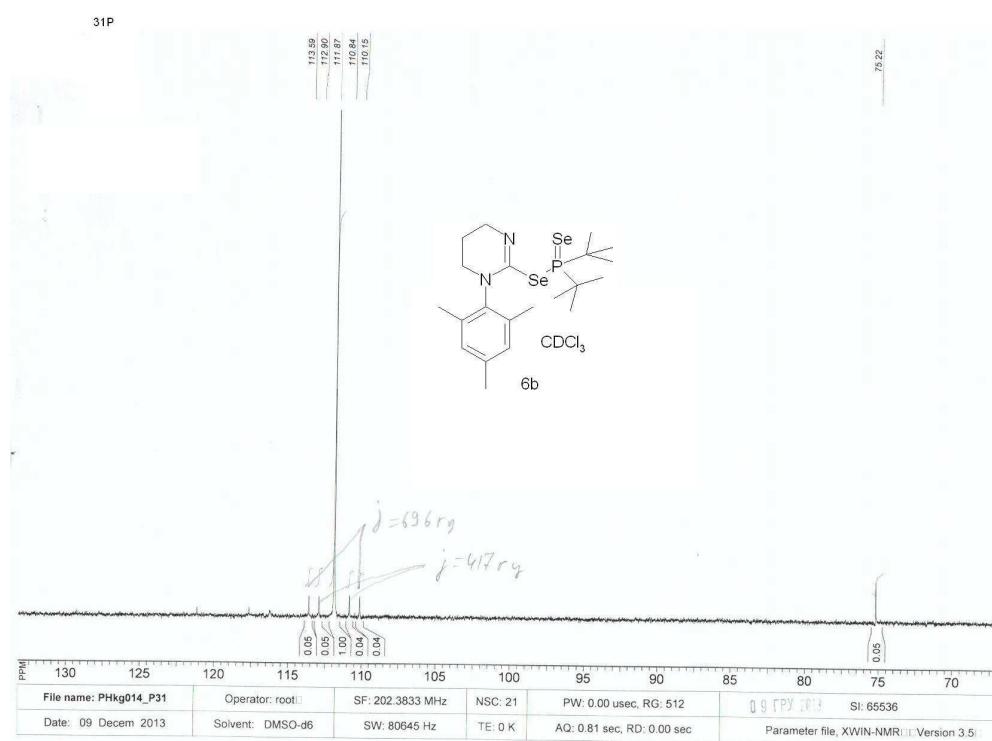


Figure S25. ^1H NMR spectrum of **7a**

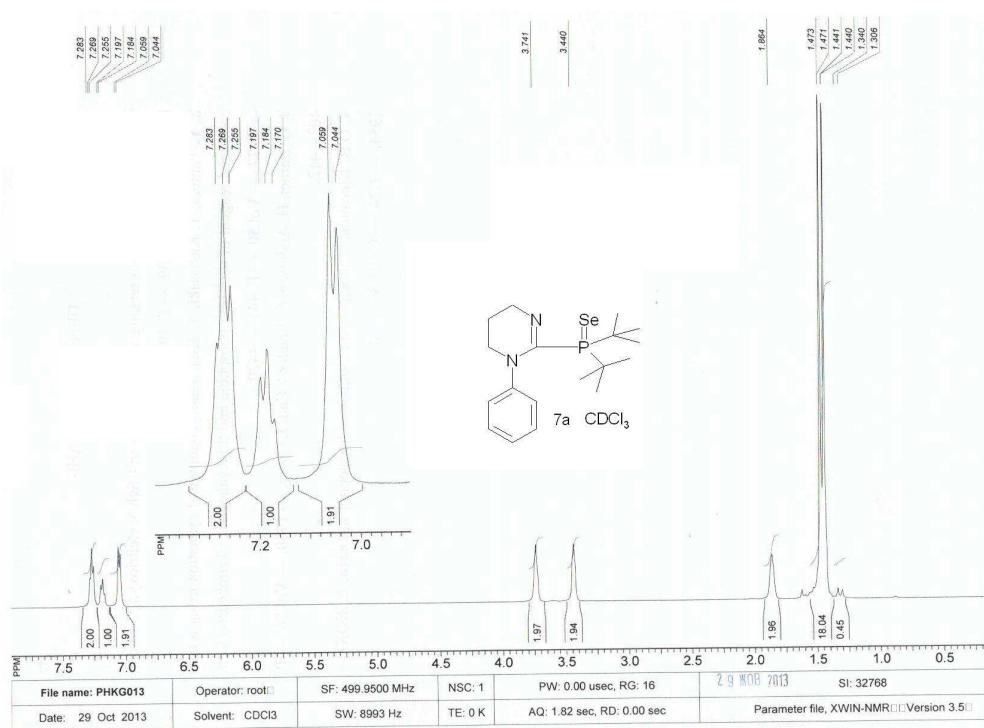


Figure S26. ^{13}C NMR spectrum of **7a**

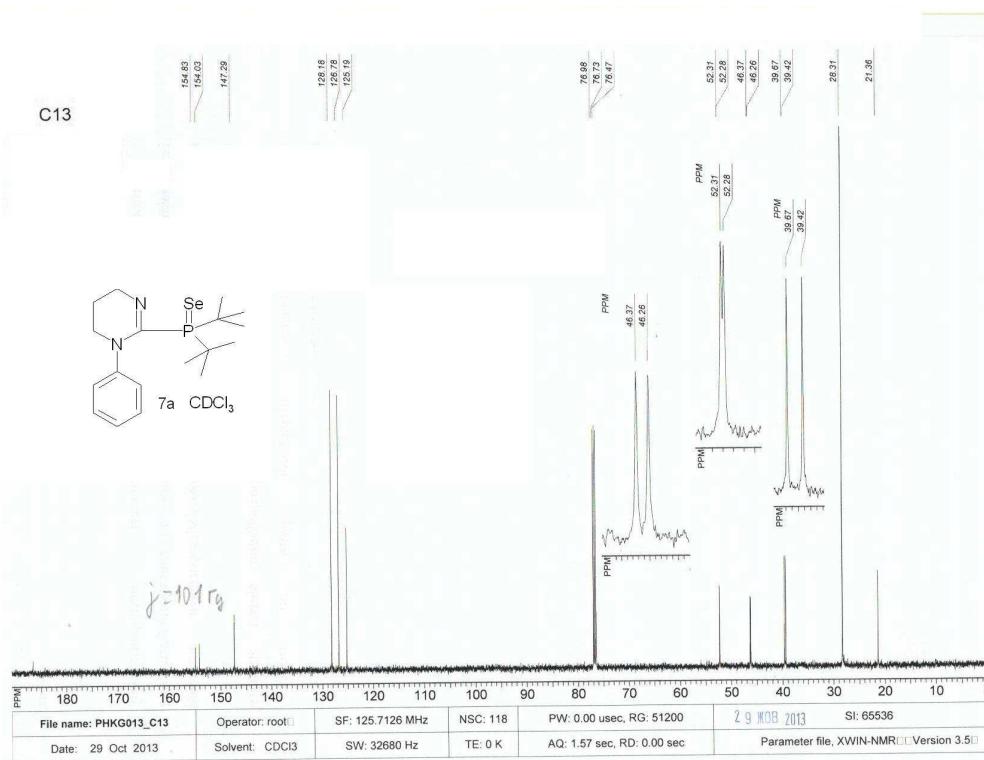


Figure S27. ^{31}P NMR spectrum of **7a**

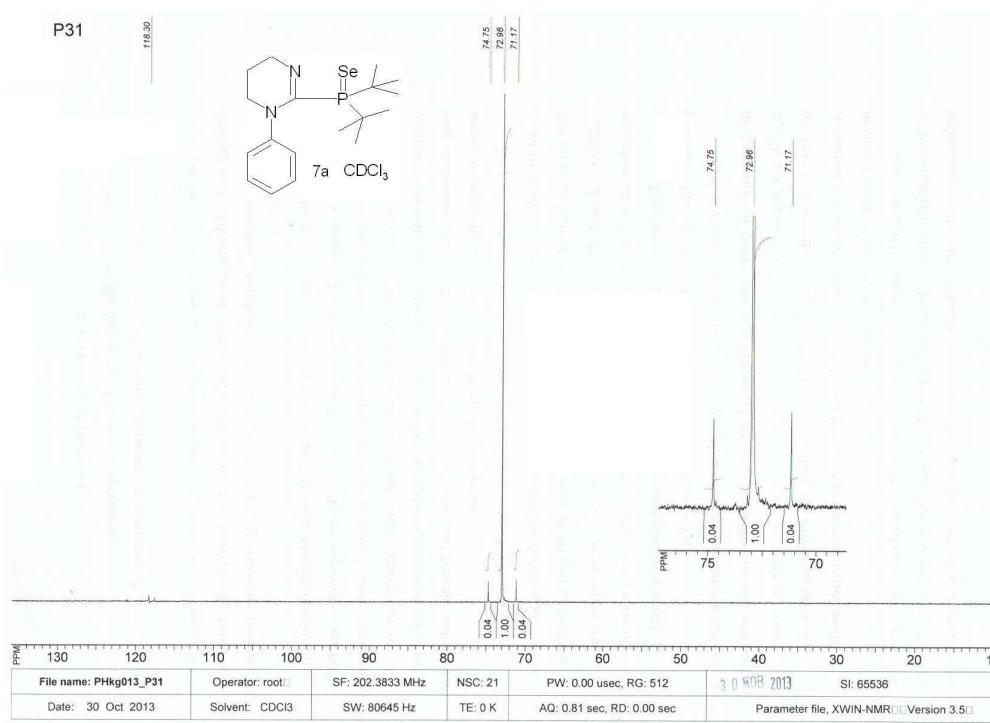


Figure S28. ^1H NMR spectrum of **7b**

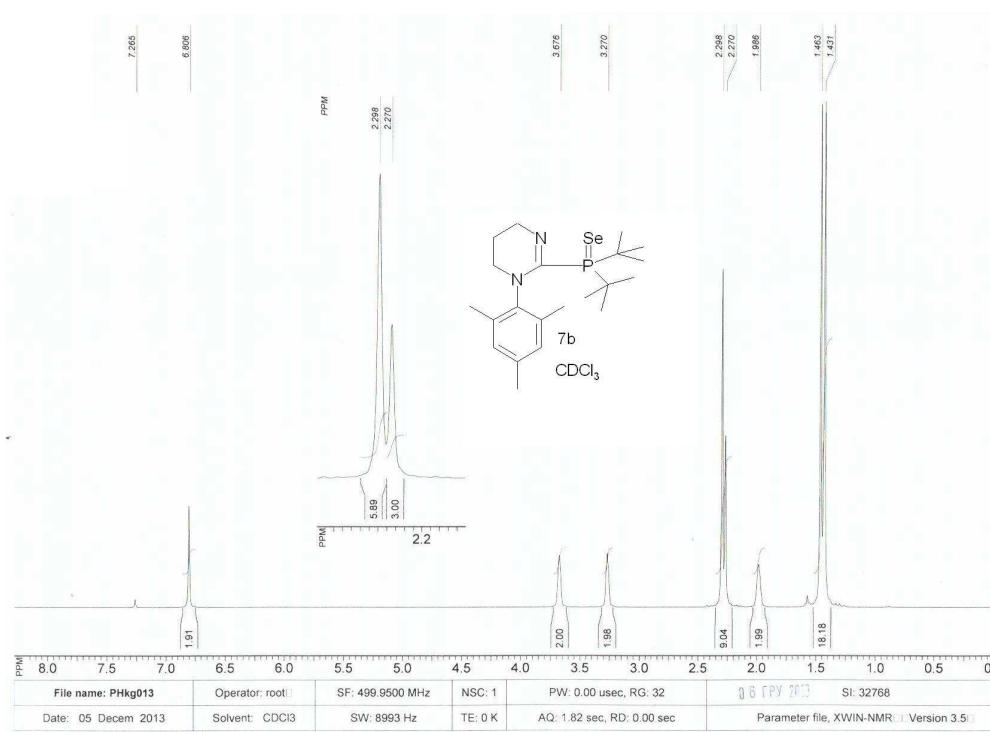


Figure S29. ^{13}C NMR spectrum of **7b**

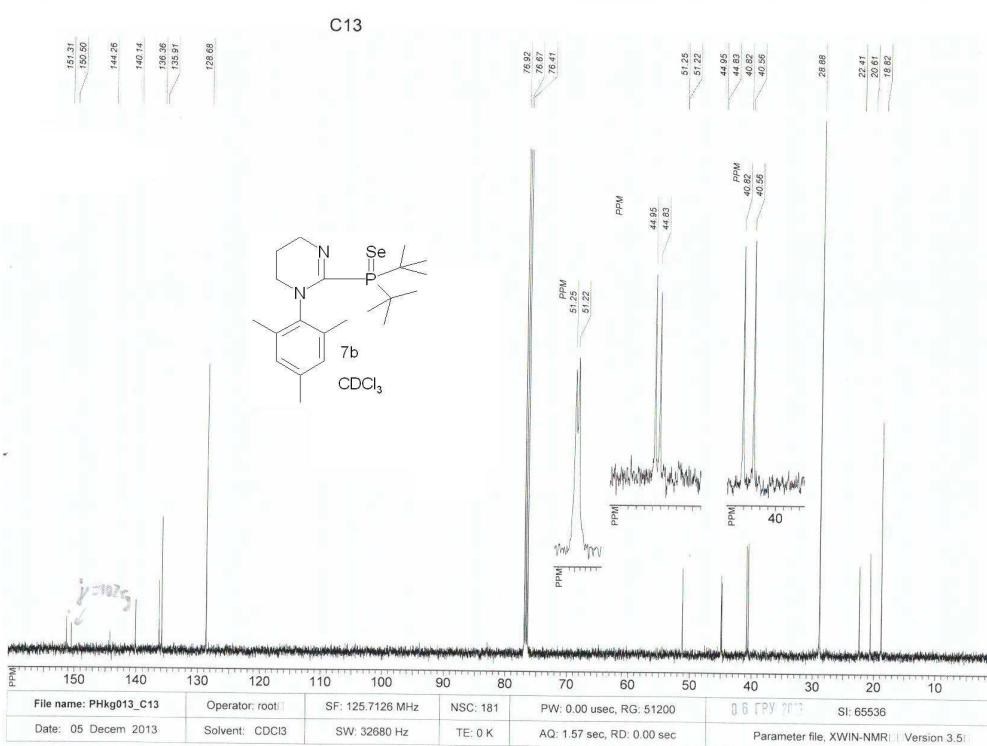


Figure S30. ^{31}P NMR spectrum of **7b**

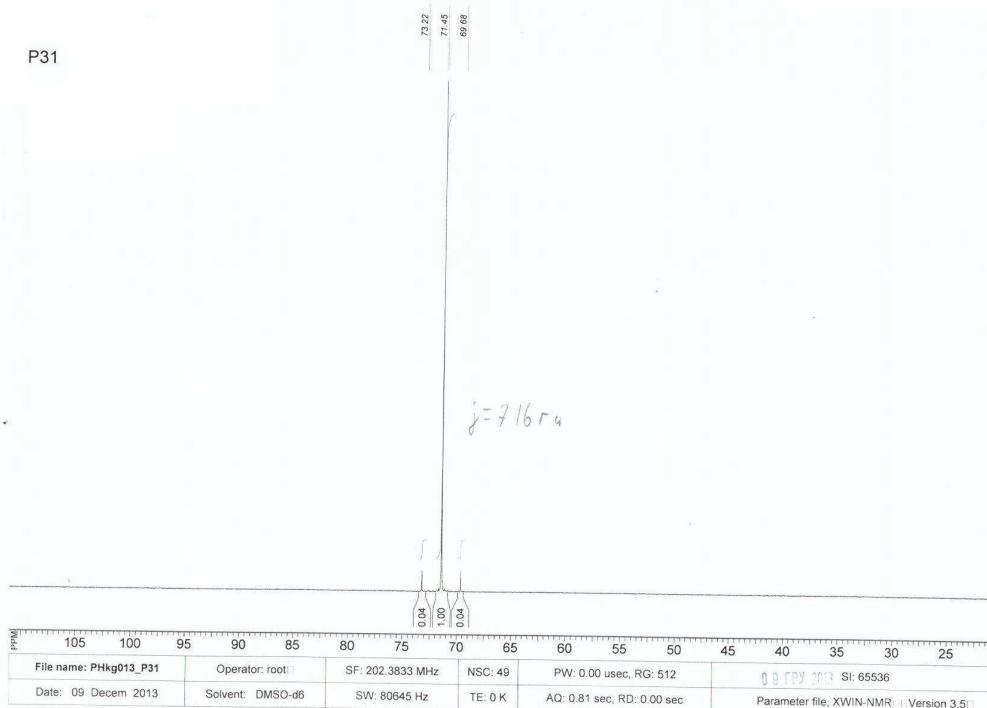


Figure S31. ^1H NMR spectrum of **8**

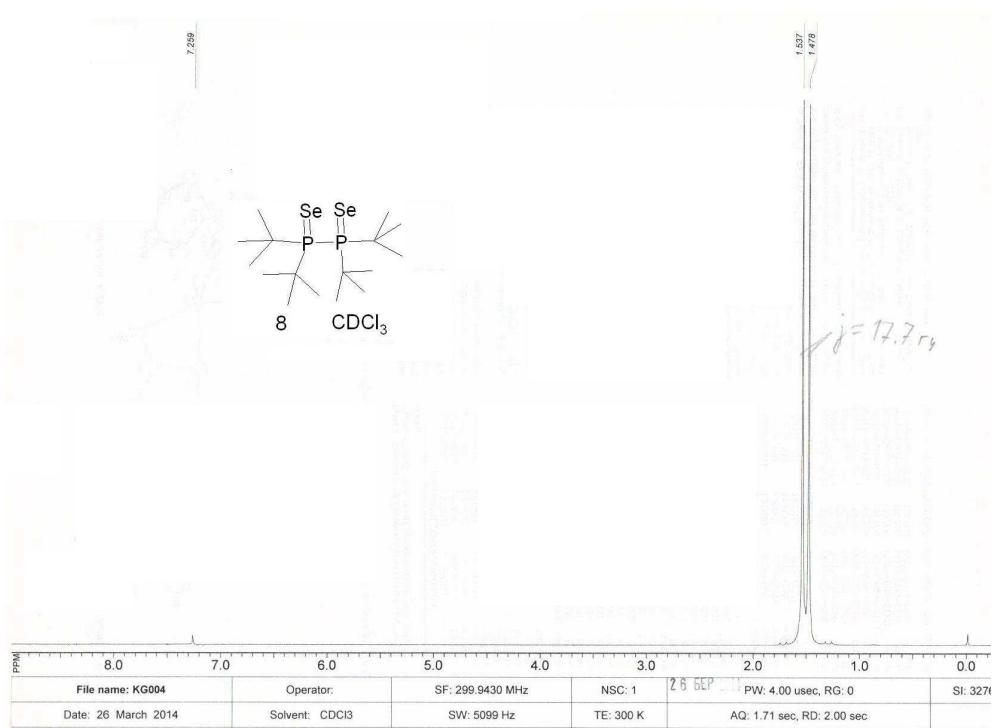


Figure S32. ^{13}C NMR spectrum of **8**

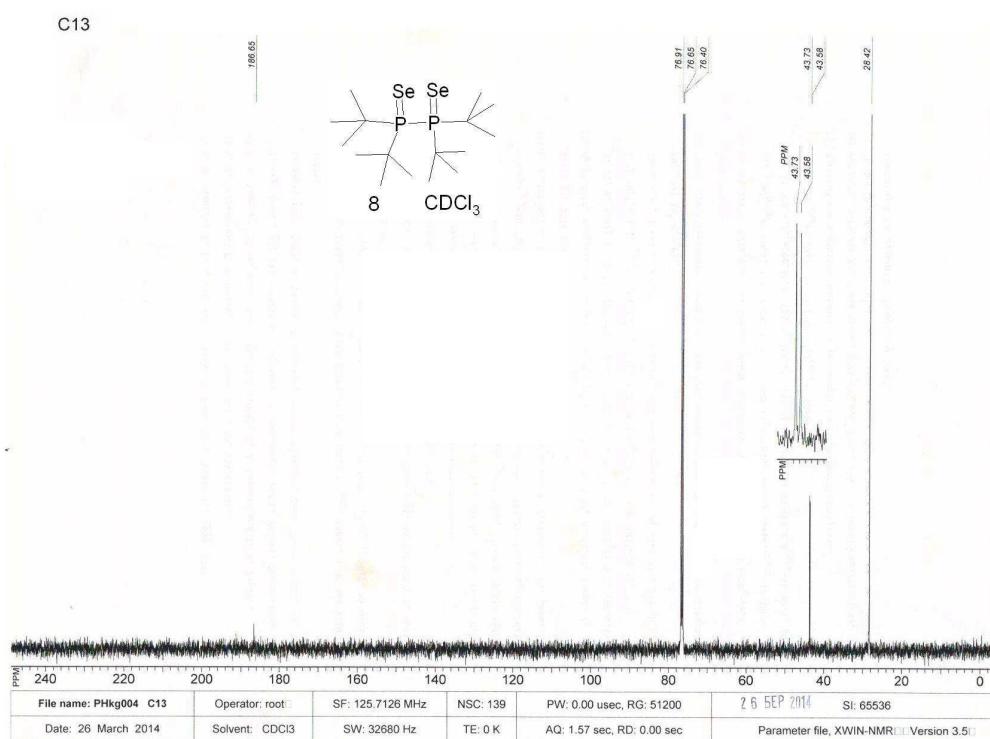


Figure S33. ^{31}P NMR spectrum of **8**

P31

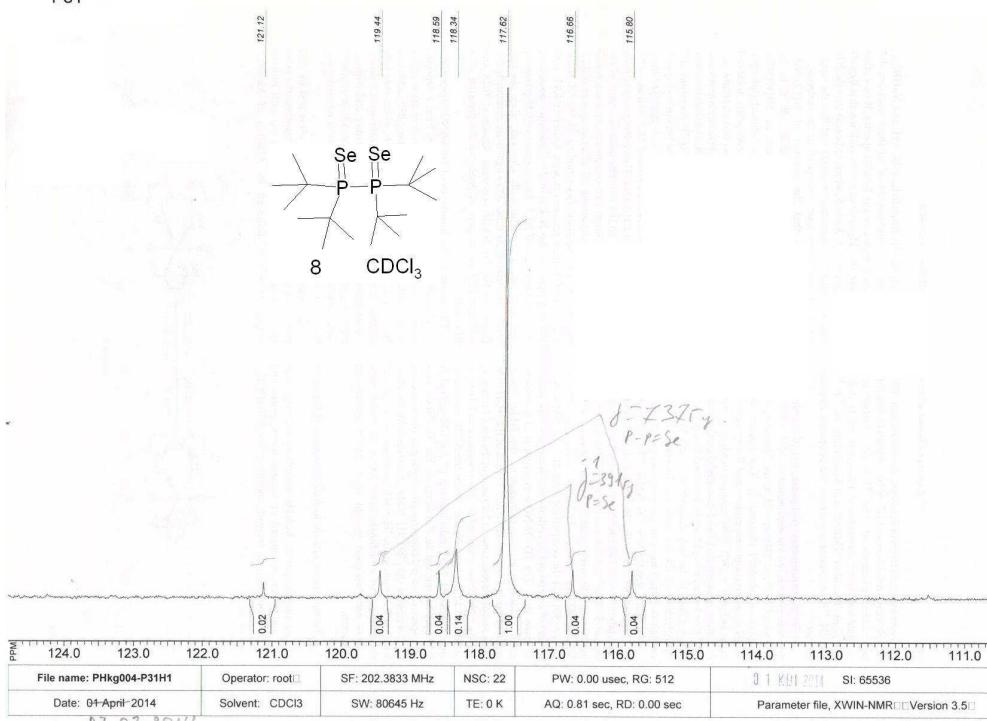


Figure S34. ^1H NMR spectrum of **9a**

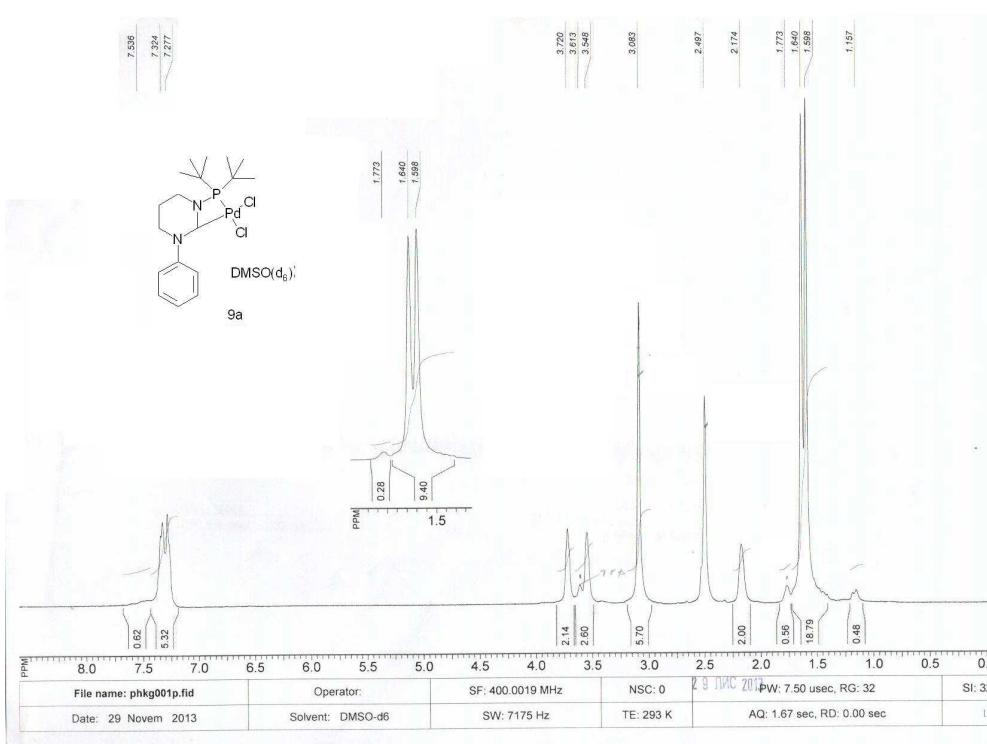


Figure S35. ^{13}C NMR spectrum of **9a**

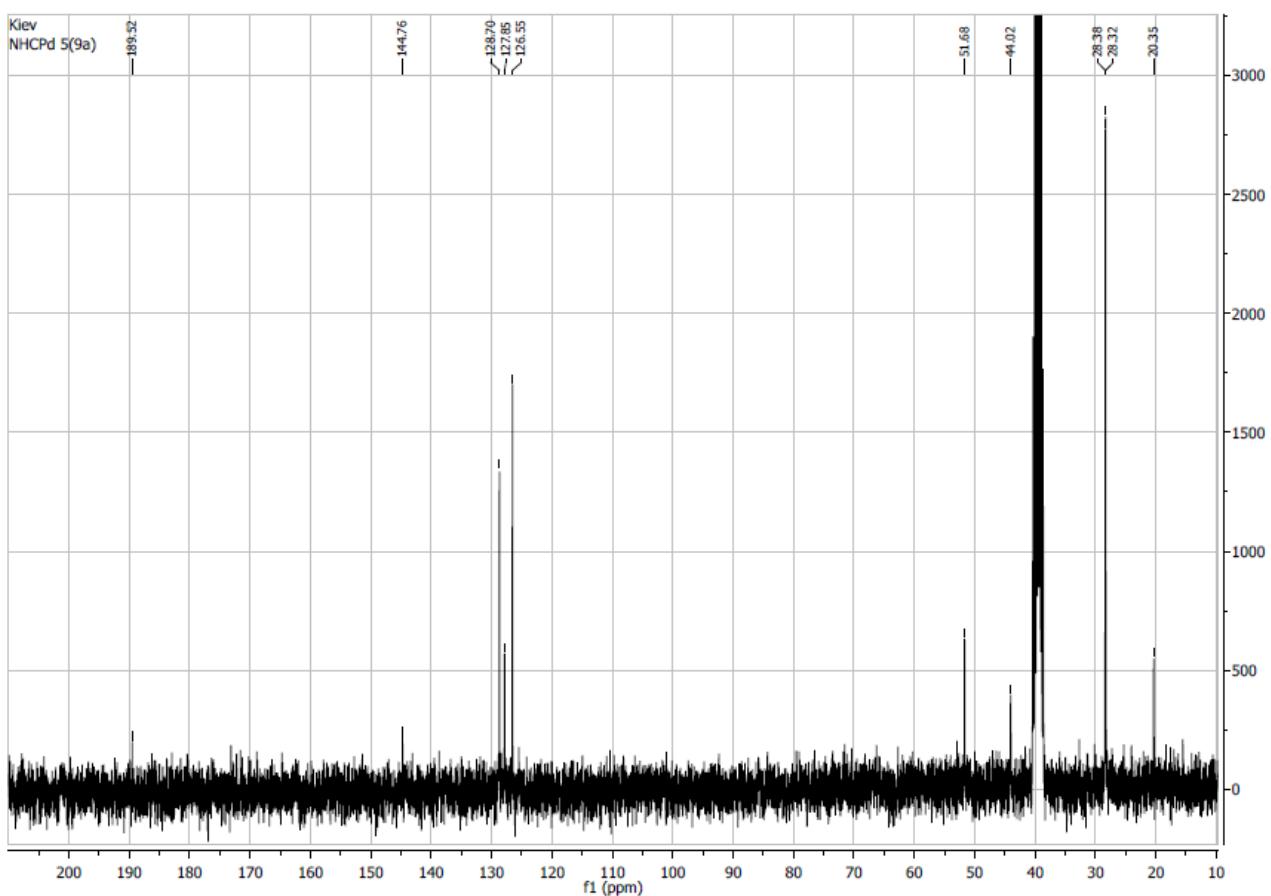


Figure S36. ^1H NMR spectrum of **9b**

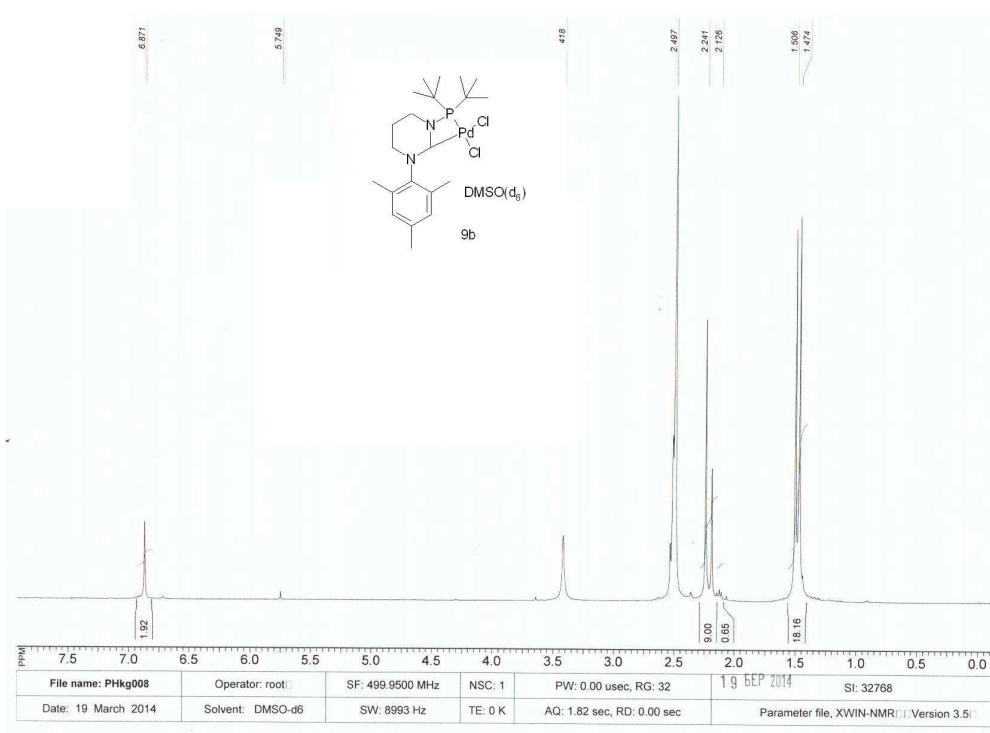


Figure S37. ^{13}C NMR spectrum of **9b**

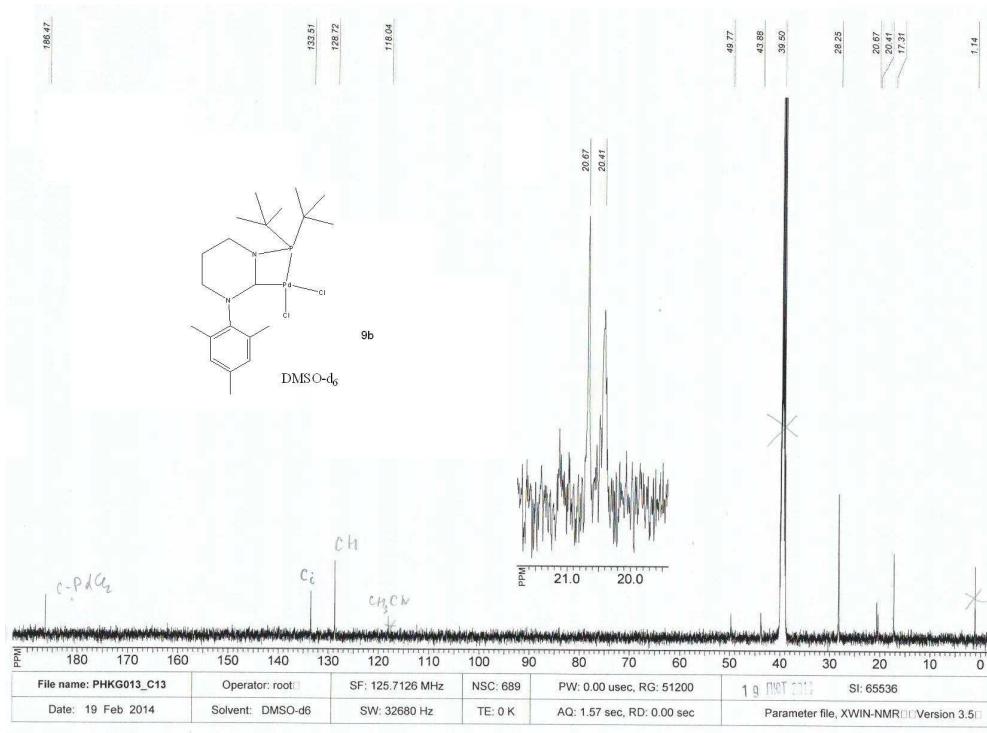


Figure S38. ^1H NMR spectrum of **9c**

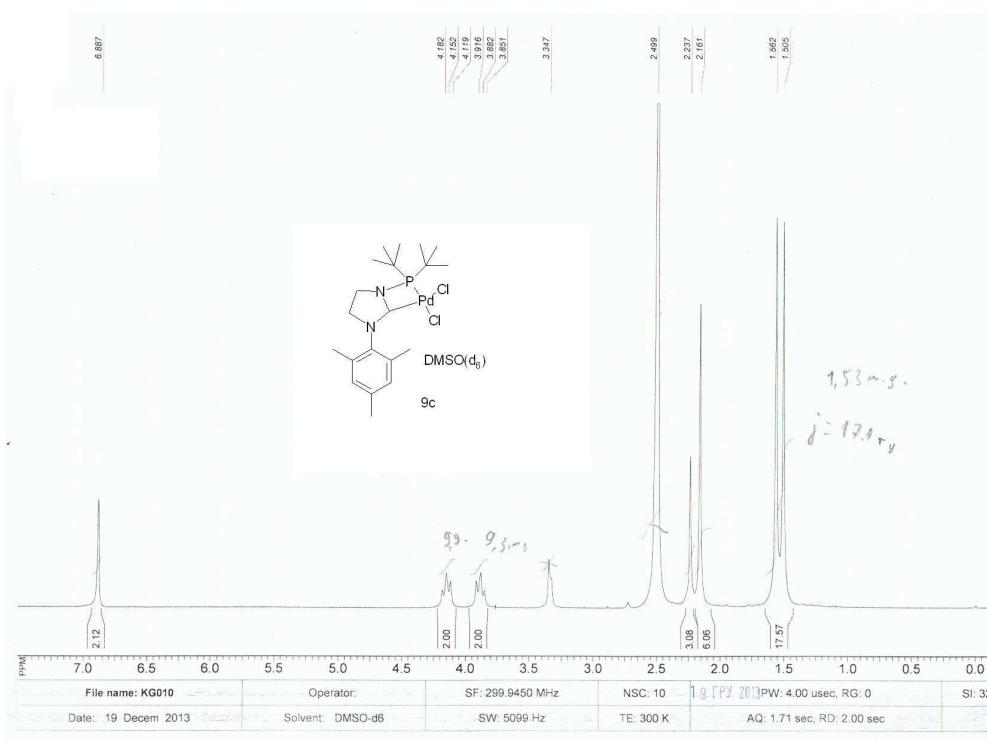


Figure S39. ^{13}C NMR spectrum of **9c**

