

Electronic Supplementary Materials

for

Palladium(II) and Platinum(II) Deprotonated Diaminocarbene Complexes Based on *N*-(2-Pyridyl)ureas with Oxadiazole Periphery

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1. X-ray diffraction data

Table S1. Crystal data and structure refinement parameters for cocrystal **3a**·1,2-DCE, **3b**·1,2-DCE, and **3c**·1½(1,2-DCE).

Cocrystal	3a ·1,2-DCE	3b ·1,2-DCE	3c ·1½(1,2-DCE)
Identification code	SVB-1295	KNS-53	BSC-394
CCDC number	2217791	2217807	2217808
Empirical formula	C ₃₁ H ₃₄ Cl ₃ N ₇ O ₂ Pd	C ₃₁ H ₃₄ Cl ₃ N ₇ O ₂ Pt	C ₆₄ H ₇₂ Cl ₈ N ₁₄ O ₄ Pd ₂
Formula weight	749.40	838.09	1597.75
Temperature, K	100(2)	100(2)	100(2)
Crystal system	triclinic	triclinic	monoclinic
Space group	P-1	P-1	P2/n
a, Å	6.83750(10)	13.5401(4)	22.1071(2)
b, Å	12.39100(10)	13.7525(4)	8.25660(10)
c, Å	19.56780(10)	19.4684(5)	38.6348(3)
α, °	93.7740(10)	83.168(2)	90
β, °	97.6500(10)	83.569(2)	94.9910(10)
γ, °	95.5130(10)	65.673(3)	90
Volume, Å ³	1630.30(3)	3271.93(16)	7025.25(12)
Z	2	4	4
ρ _{calcg} , cm ³	1.527	1.701	1.511
μ, mm ⁻¹	7.183	10.605	7.388
F(000)	764.0	1656.0	3256.0
Crystal size, mm ³	0.18 × 0.15 × 0.12	0.12 × 0.06 × 0.02	0.17 × 0.16 × 0.12
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection, °	4.57 to 154.83	4.582 to 129.97	4.446 to 141.772
Index ranges	−8 ≤ h ≤ 8, −15 ≤ k ≤ 15, −24 ≤ l ≤ 24	−15 ≤ h ≤ 15, −16 ≤ k ≤ 14, −22 ≤ l ≤ 22	−26 ≤ h ≤ 27, −10 ≤ k ≤ 10, −47 ≤ l ≤ 47
Reflections collected	61125	41043	88137
Independent reflections	6817 [R _{int} = 0.0658, R _{sigma} = 0.0277]	11016 [R _{int} = 0.0694, R _{sigma} = 0.0541]	13274 [R _{int} = 0.0523, R _{sigma} = 0.0303]
Data/restraints/parameters	6817/0/404	11016/0/807	13274/0/843
Goodness-of-fit on F ²	1.073	1.054	1.090
Final R indexes [I>=2σ (I)]	R ₁ = 0.0327 wR ₂ = 0.0857	R ₁ = 0.0469 wR ₂ = 0.1147	R ₁ = 0.0496 wR ₂ = 0.1190
Final R indexes [all data]	R ₁ = 0.0334 wR ₂ = 0.0862	R ₁ = 0.0546 wR ₂ = 0.1198	R ₁ = 0.0526 wR ₂ = 0.1206
Largest diff. peak/hole/ eÅ ⁻³	1.19/−1.31	2.88/−1.53	2.25/−2.17

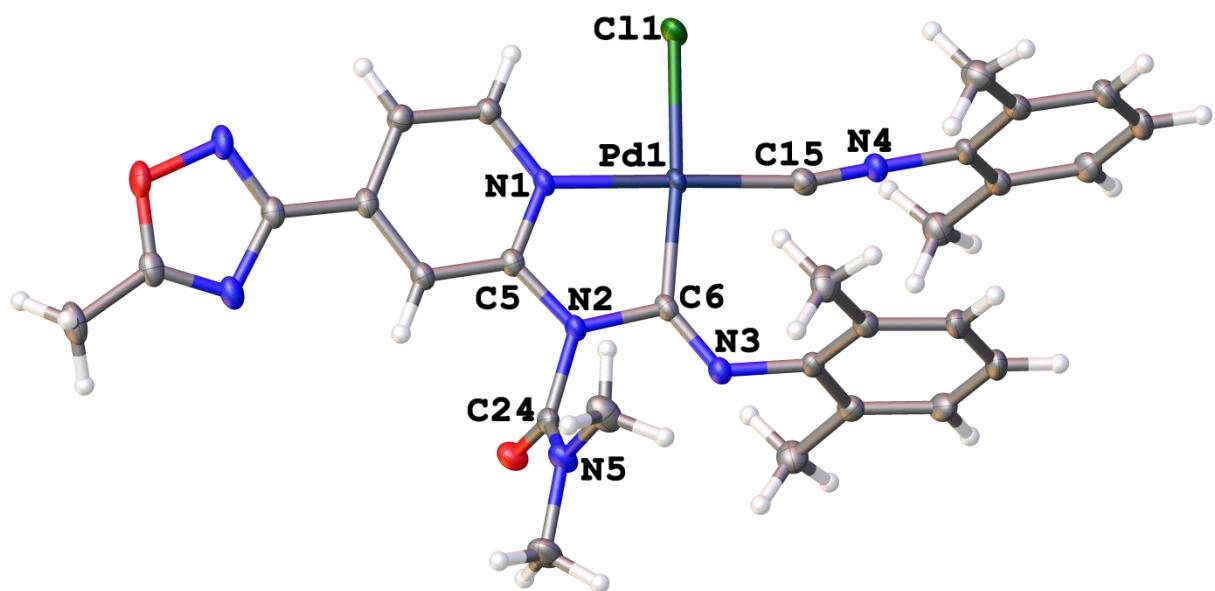


Figure S1. X-ray molecular structure of solvate **3a**·1,2-DCE.

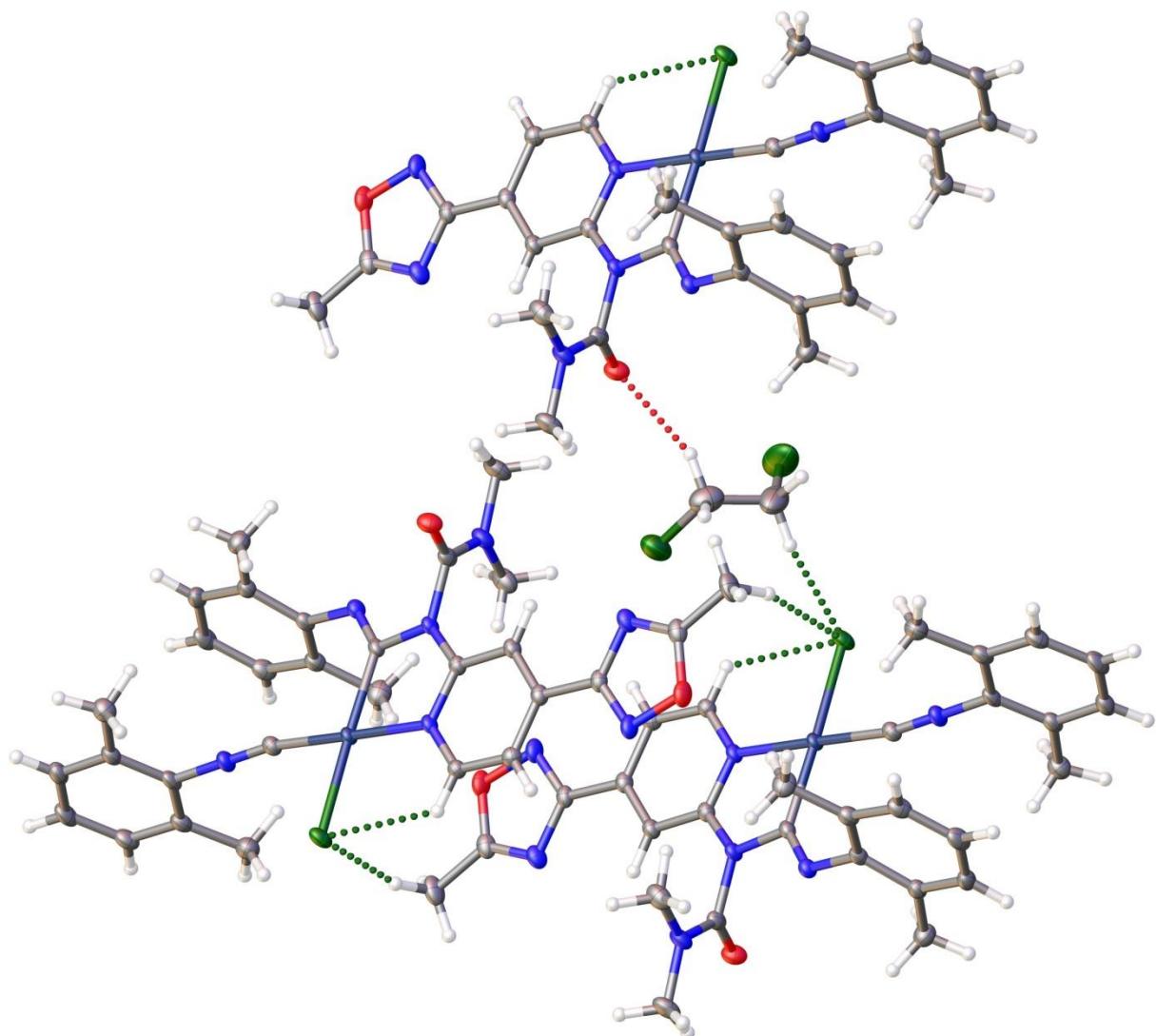


Figure S2. Hydrogen bonding in the solvate **3a**·1,2-DCE.

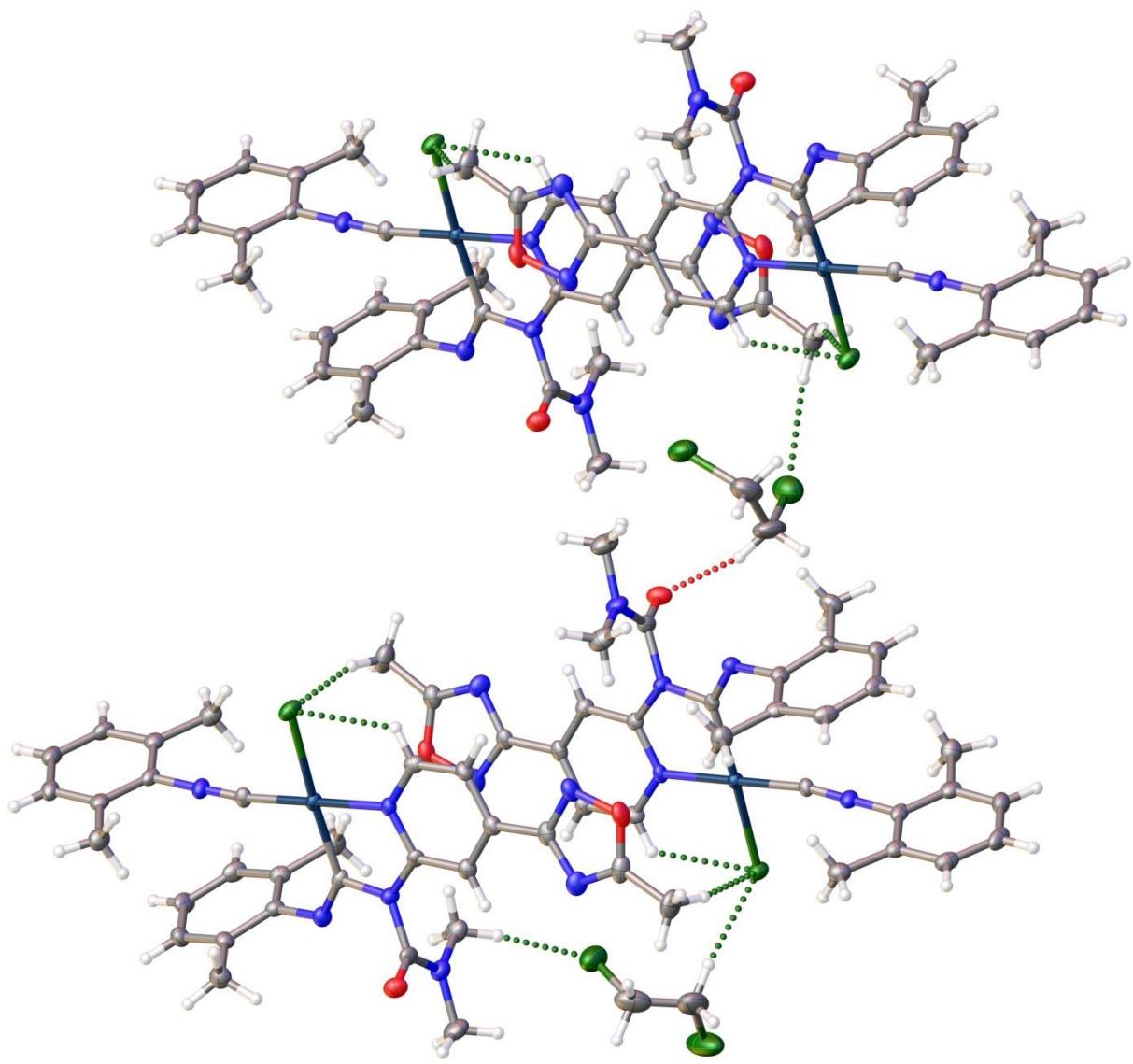


Figure S3. Hydrogen bonding in the solvate **3b**·1,2-DCE.

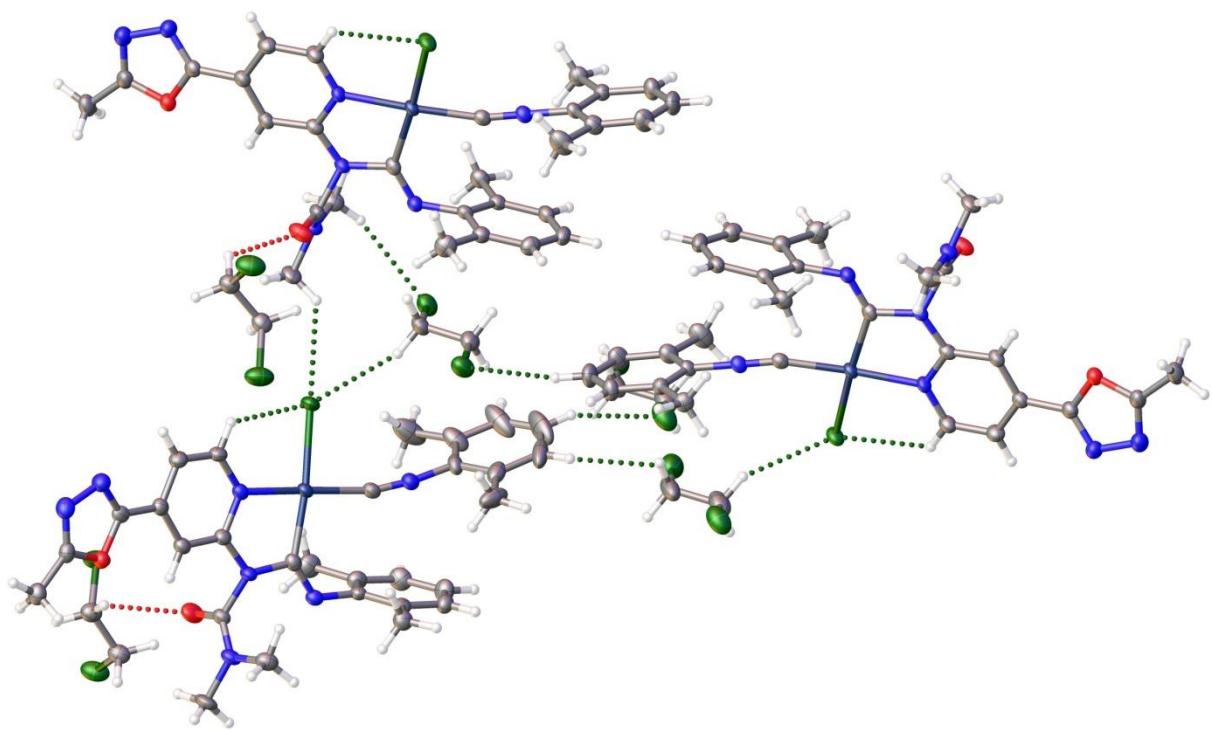


Figure S4. Hydrogen bonding in the solvate **3c**· $\frac{1}{2}$ (1,2-DCE).

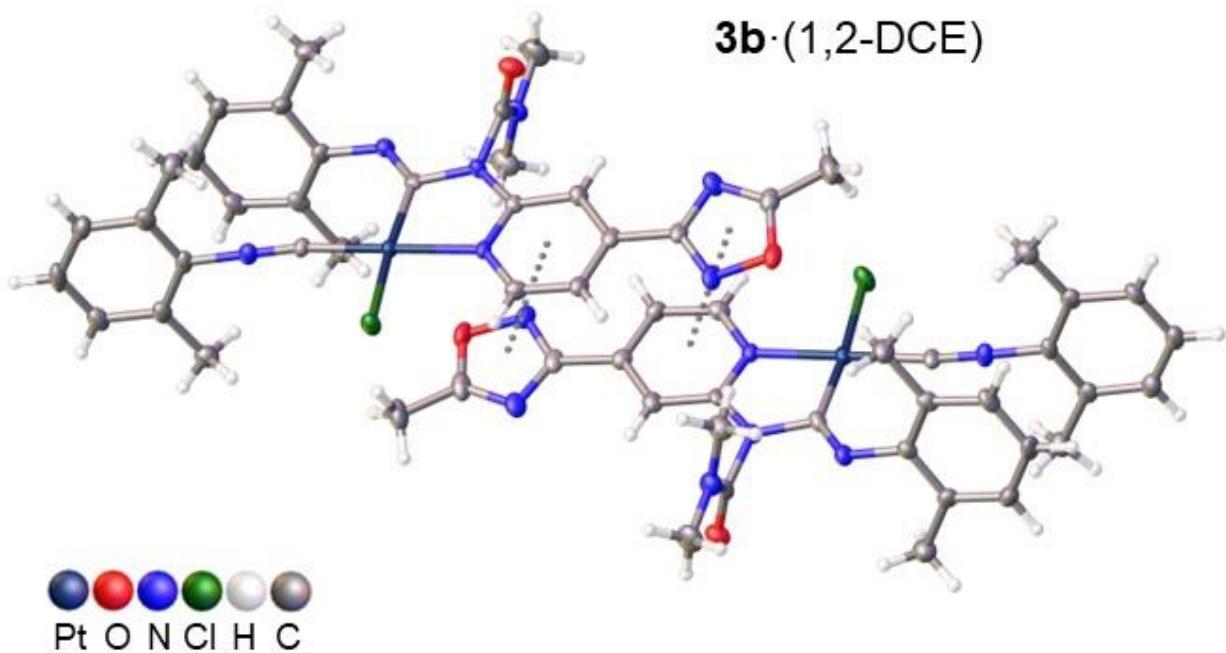
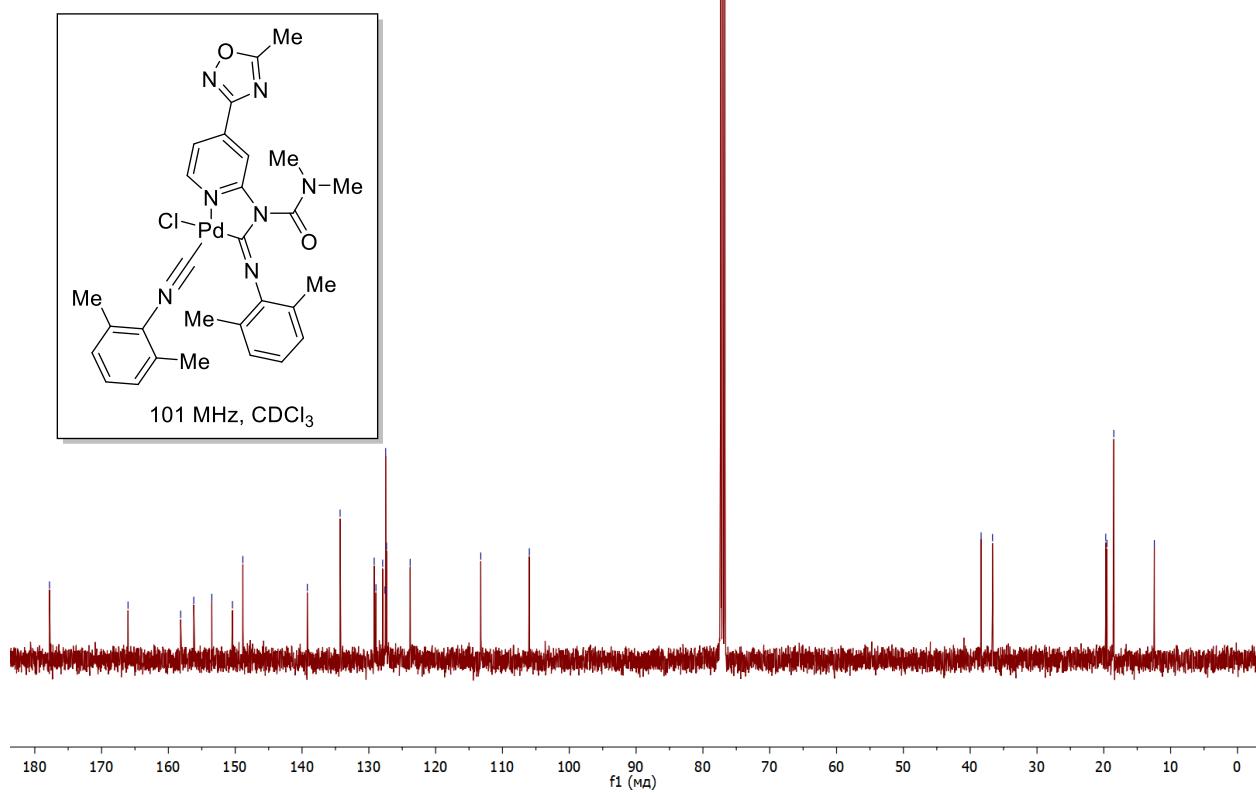
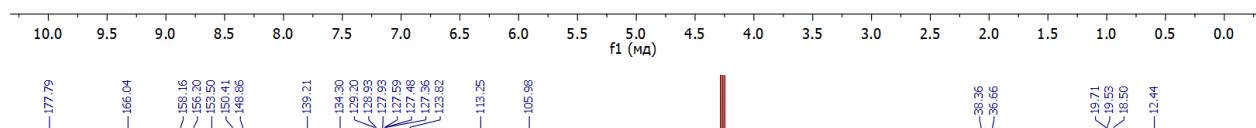
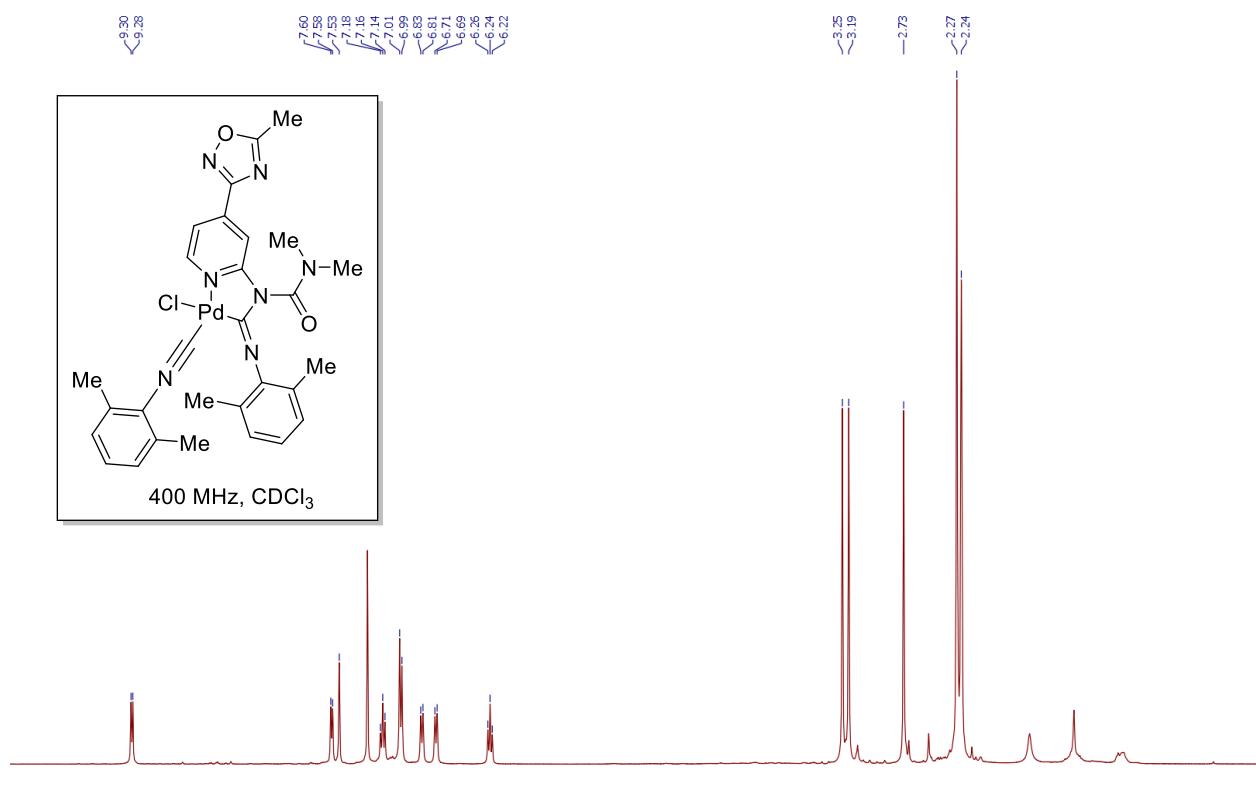


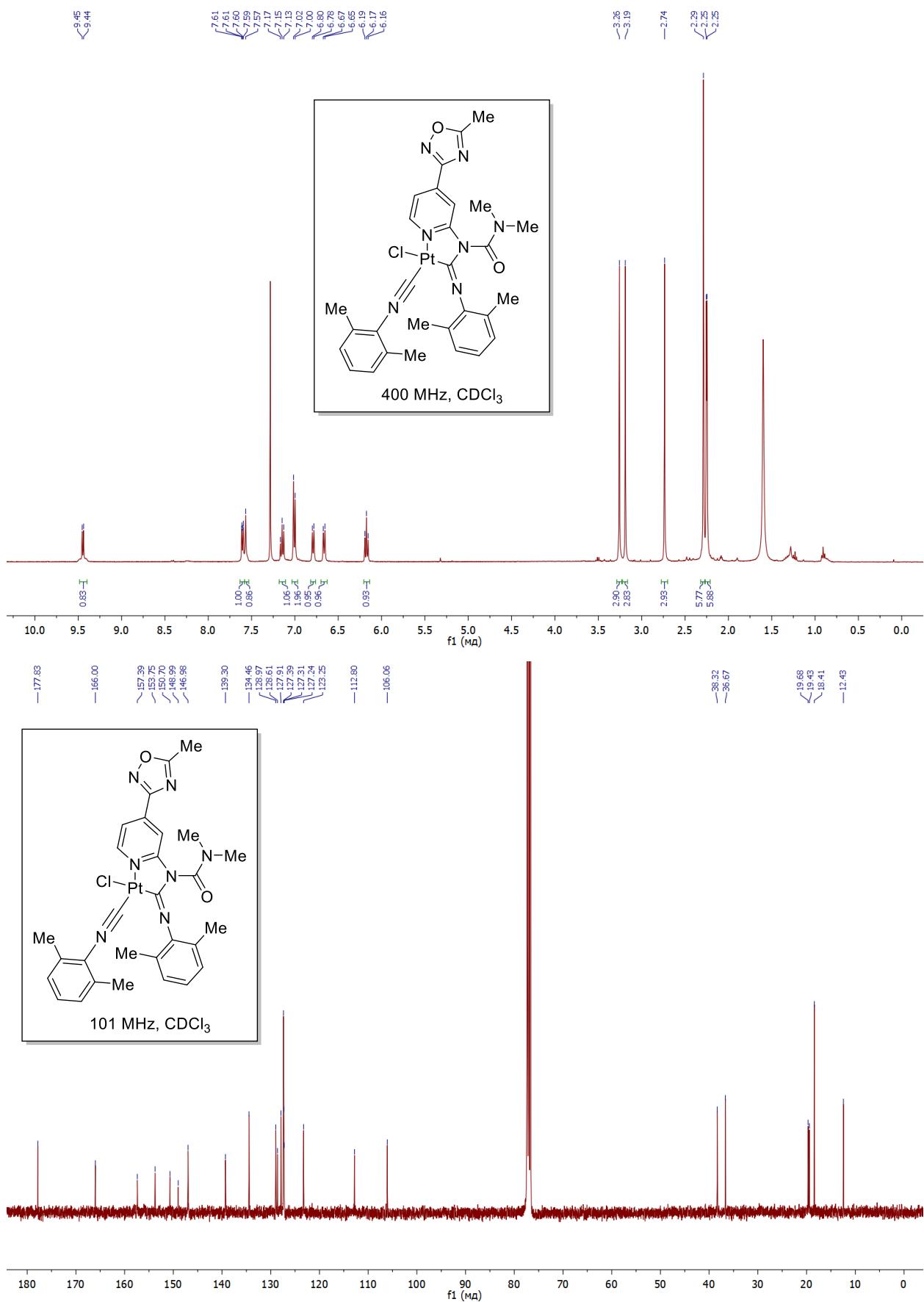
Figure S5. Oxadiazole–pyridine $\pi\cdots\pi$ interactions in the solvate **3b**·(1,2-DCE).

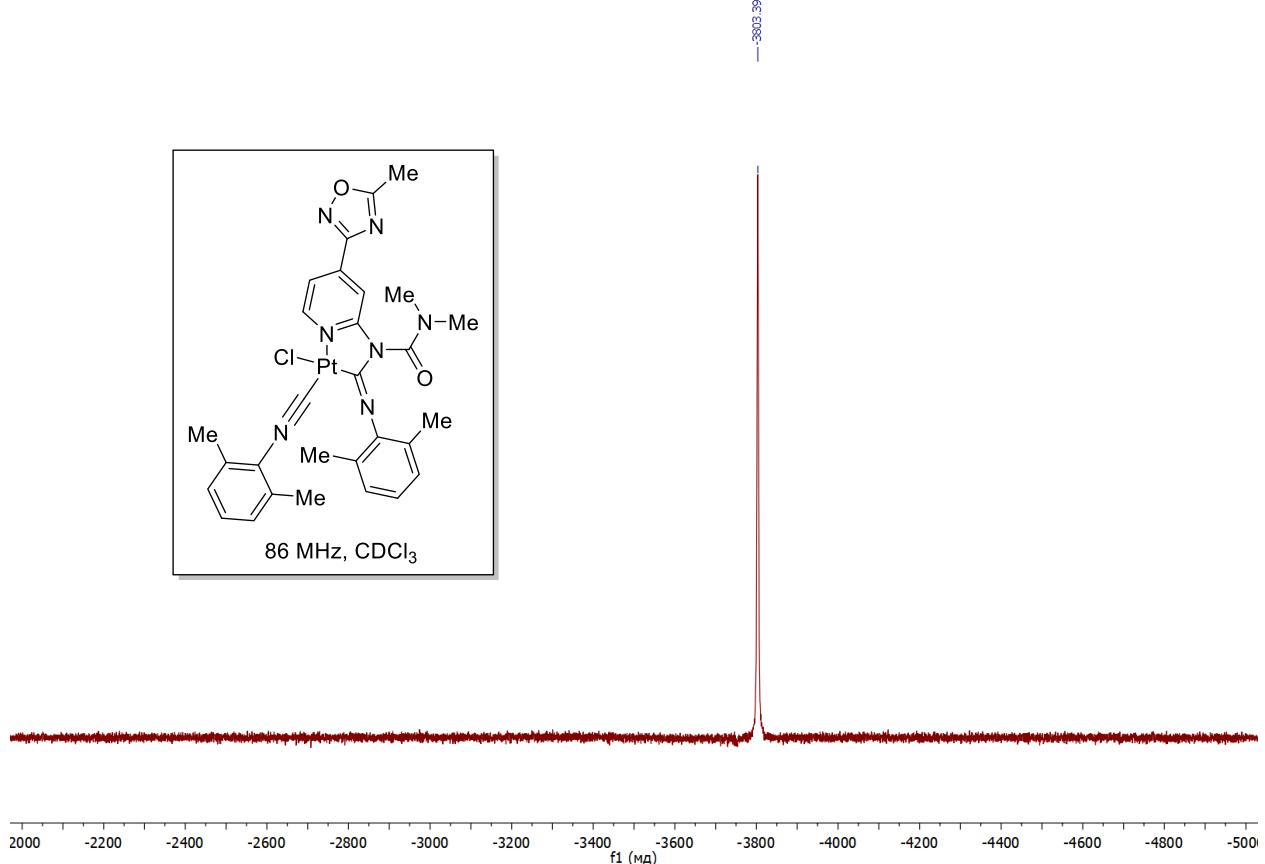
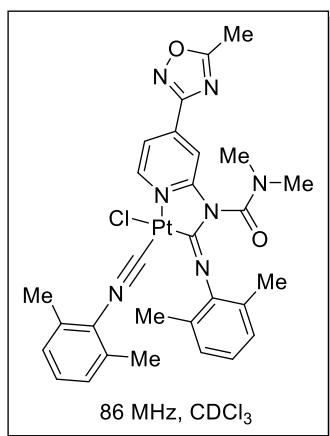
2. Copies of NMR spectra of complexes 3a–d

^1H and ^{13}C NMR spectra of complex 3a

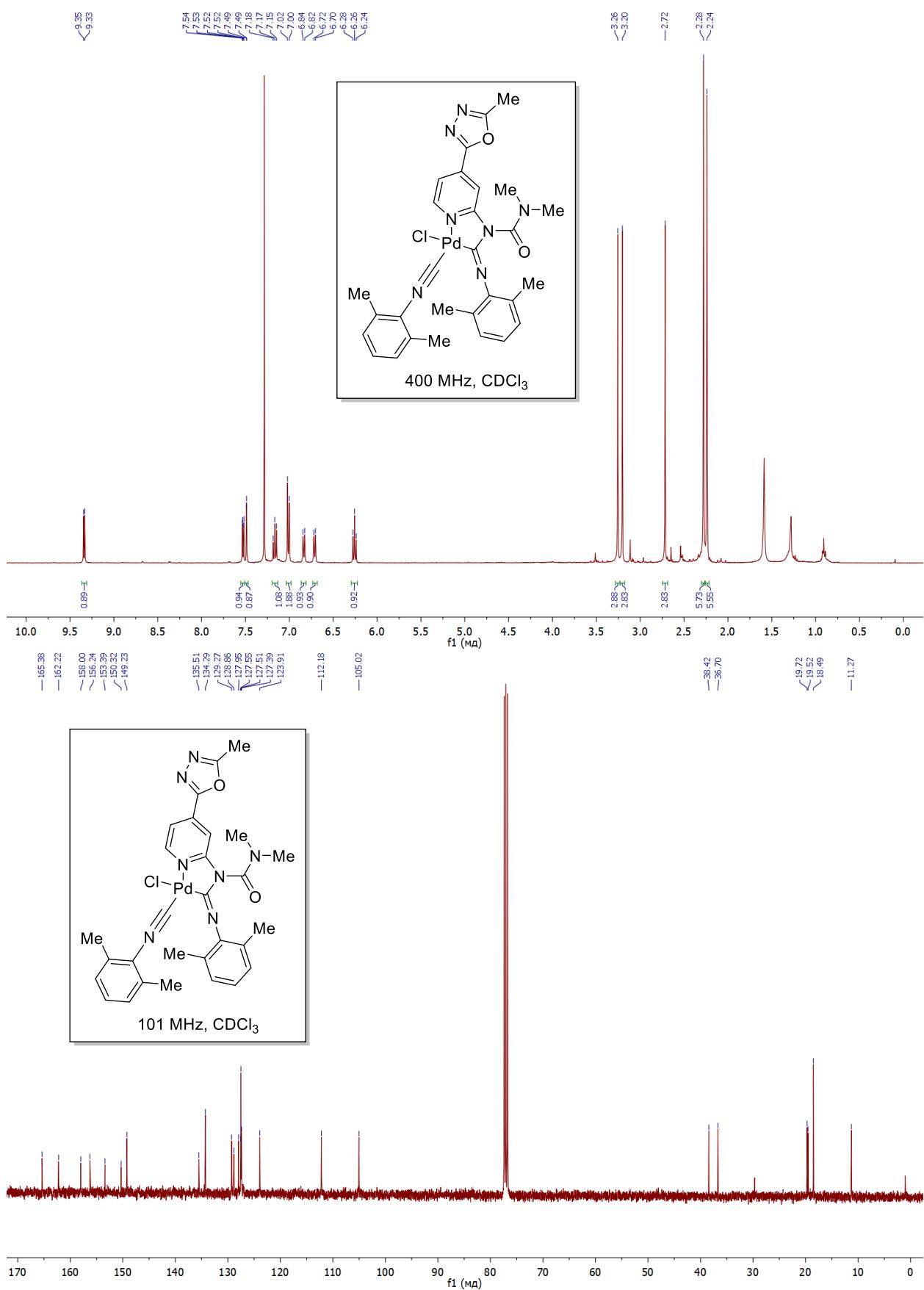


¹H, ¹³C, and ¹⁹⁵Pt NMR spectra of complex **3b**

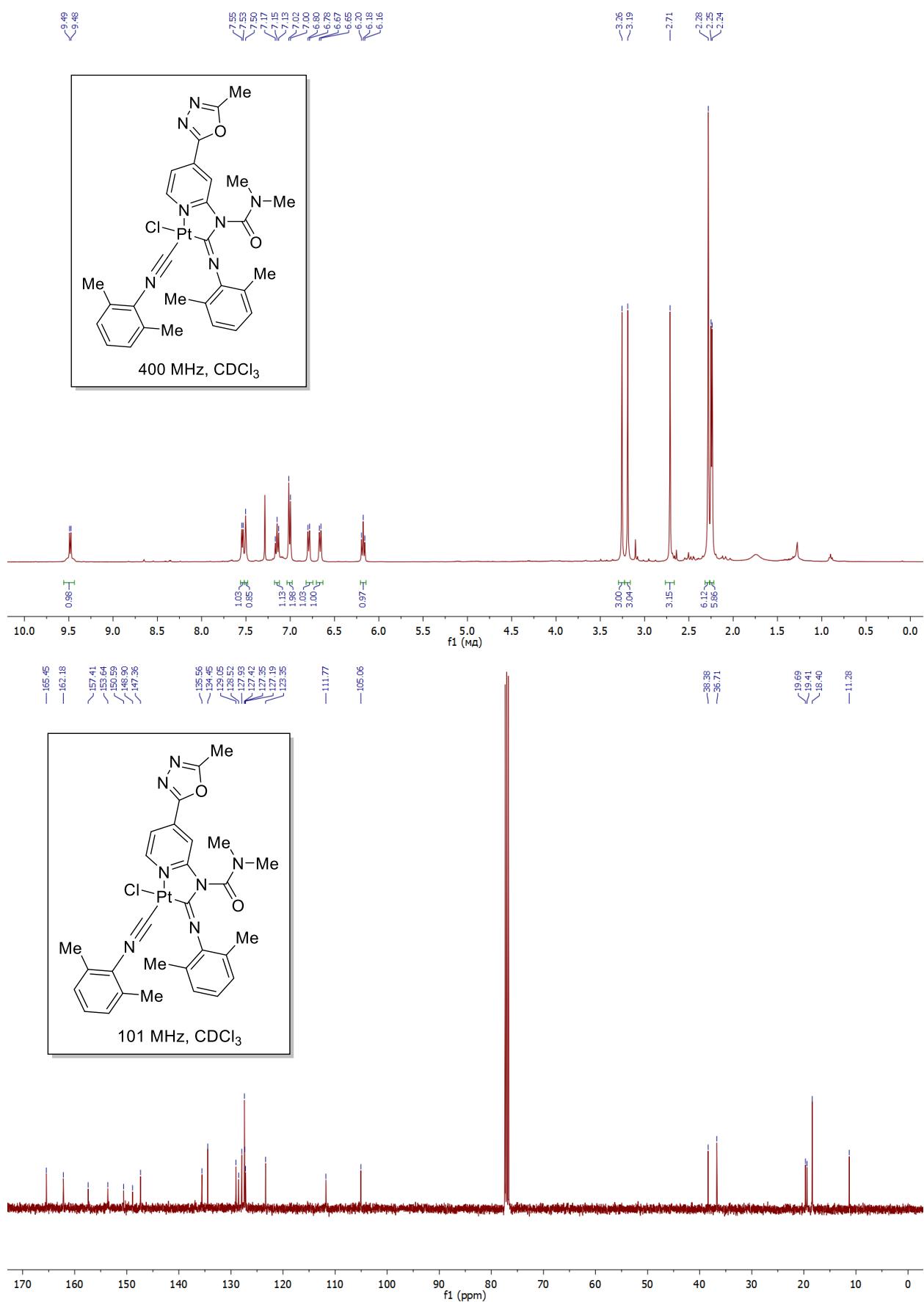


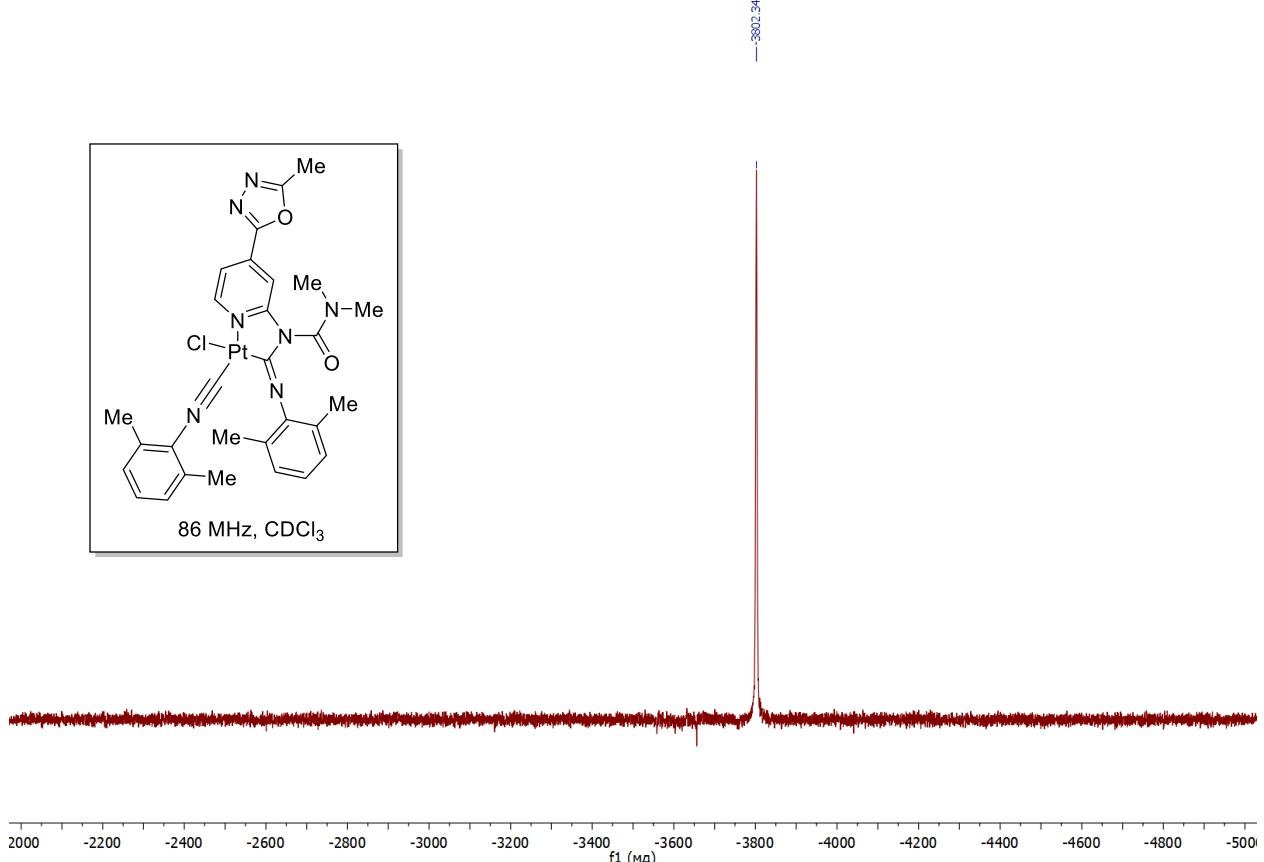
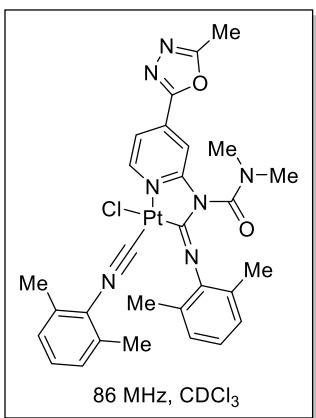


¹H and ¹³C NMR spectra of complex **3c**



¹H, ¹³C, and ¹⁹⁵Pt NMR spectra of complex **3d**





3. TG/DTG data

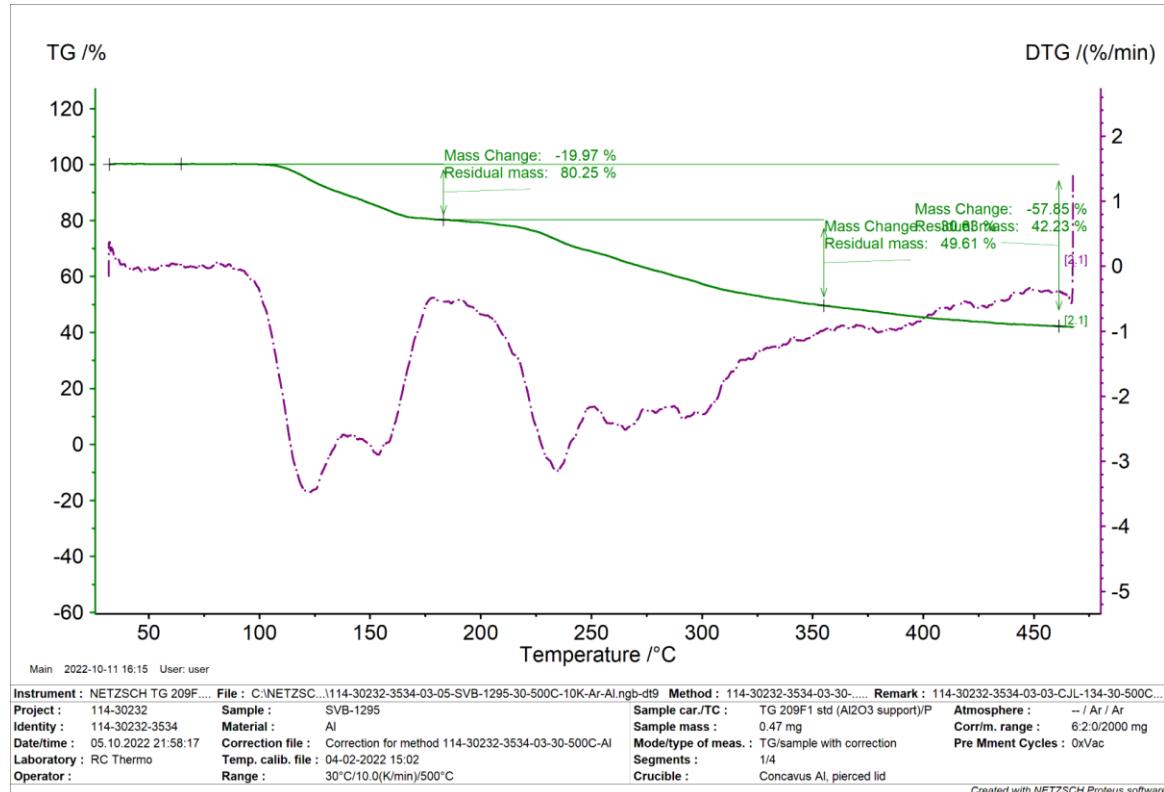


Figure S6. TG/DTG curves of complex 3a.

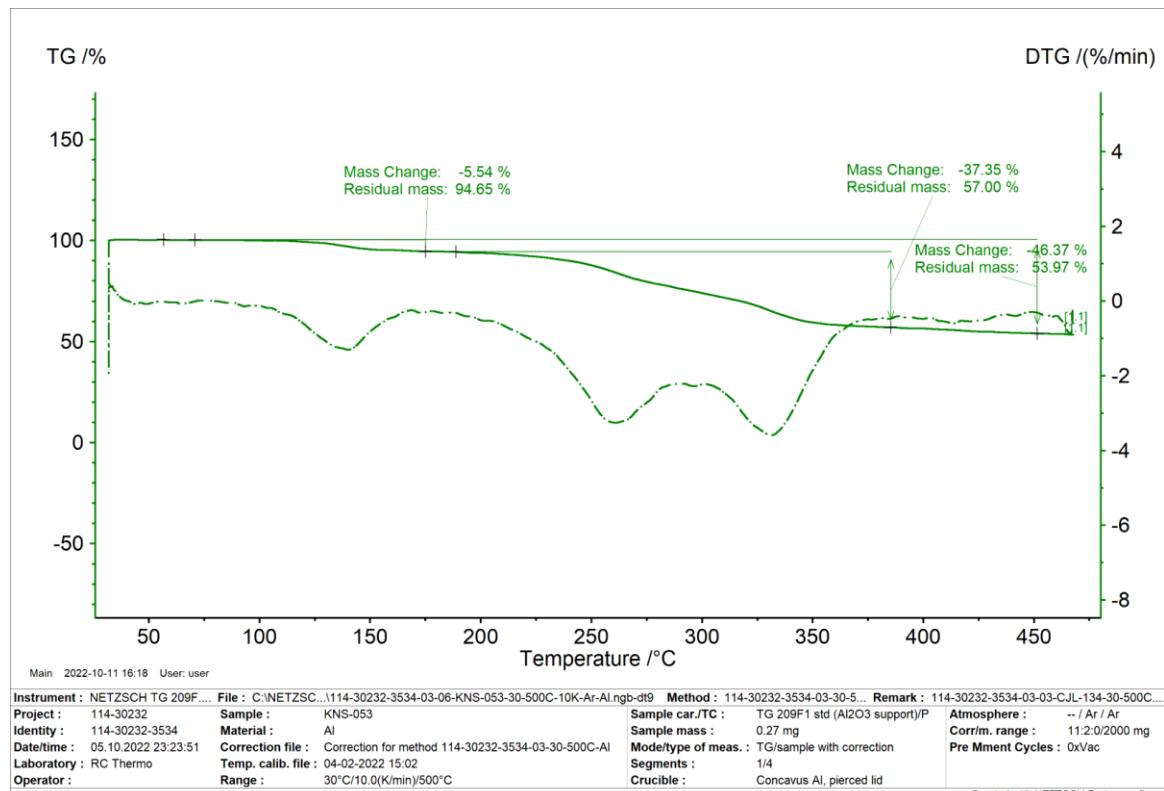


Figure S7. TG/DTG curves of complex 3b.

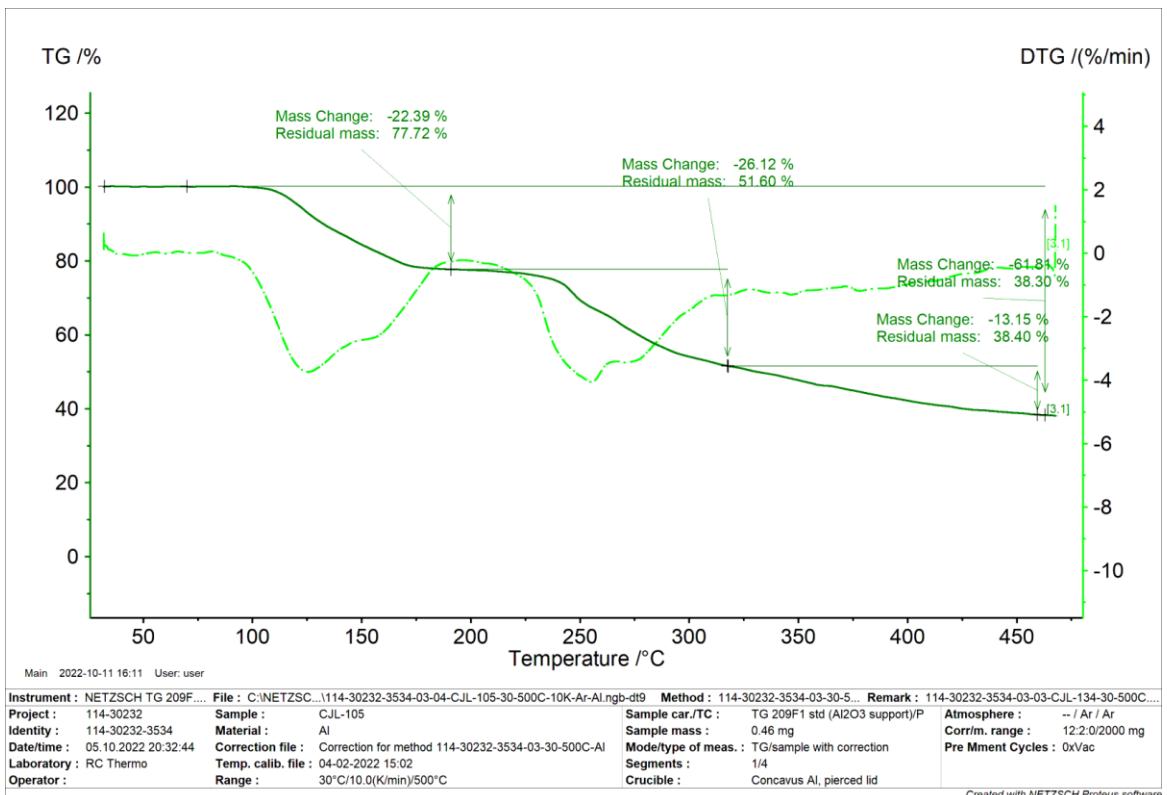


Figure S8. TG/DTG curves of complex 3c.

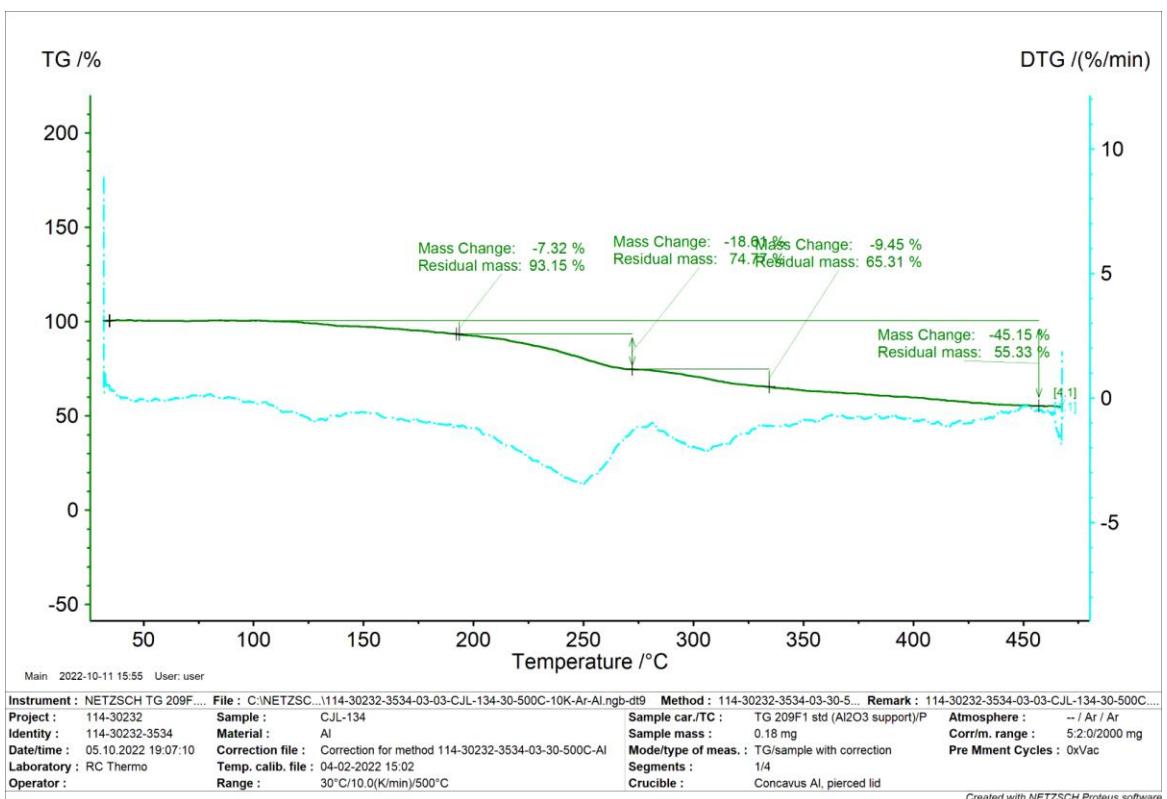


Figure S9. TG/DTG curves of complex 3d.