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Electronic Supplementary Information

Double Rollover Cycloplatinated(II) Skeleton: a Versatile Platform for Tuning Emission By Chelating and Non-Chelating Ancillary Ligand Systems

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Table S1. Crystallographic and refinement data for the complexes **2a**, **3a** and **3b**.

	2a.CH_2Cl_2	**3a**	**3b**
Empirical Formula	$C_{21}H_{28}Cl_2N_4Pt_2S_4$	$C_{48}H_{36}N_4P_2Pt_2S_2$	$C_{46}H_{36}N_8P_2Pt_2$
Formula weight	925.79	1185.05	1152.95
Temperature	100(2) K	100(2) K	100(2) K
Wavelength	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Triclinic	Triclinic
Space group	P21	P-1	P-1
Unit cell dimensions	a = 12.4710(7)	a = 9.1906(6)	a = 9.2323(14)
	b = 8.2668(3)	b = 10.0261(7)	b = 9.5583(15)
	c = 14.3476(8)	c = 12.9981(9)	c = 12.8452(19)
	α = 90	α = 112.0030(10)	α = 110.033(2)
	β = 111.524(6)	β = 90.1800(10)	β = 90.129(2)
	γ = 90	γ = 110.3460(10)	γ = 110.867(2)
Volume	1376.02(12)	1028.87(12)	985.1(3)
Z	2	1	1
Density (calculated)	2.234 Mg/m^3	1.913 Mg/m^3	1.944 Mg/m^3
Absorption coefficient	10.672 mm^{-1}	7.011 mm^{-1}	7.221 mm^{-1}
F(000)	872	570	554
Theta range for data collection	2.91 to 30.48	2.30 to 28.71	2.38 to 28.64
Index ranges	-17< h< 17	-11< h< 12	-12< h< 12
	-11< k< 11	-13< k< 13	-12< k< 12
	-19< l< 20	-17< l< 17	-17< l< 16
Reflections collected	12474	9578	11921
Independent reflections	3746 [R(int) = 0.0488]	4728 [R(int) = 0.0179]	4604 [R(int) = 0.0402]
Completeness to theta = 25.00	99.7 %	99.1 %	98.8 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	3746 / 7 / 162	4728 / 0 / 262	4604 / 0 / 262
Goodness-of-fit on F^2	1.026	1.105	1.133
Final R indices [I>2sigma(I)]	R1 = 0.0420, wR2 = 0.0943	R1 = 0.0259, wR2 = 0.0624	R1 = 0.0594, wR2 = 0.1622
R indices (all data)	R1 = 0.0632, wR2 = 0.1049	R1 = 0.0269, wR2 = 0.0629	R1 = 0.0672, wR2 = 0.1669
Largest diff. peak and hole	4.039 and -1.297 e^{-3}	1.823 and -1.043 e^{-3}	5.807 and -1.765 e^{-3}

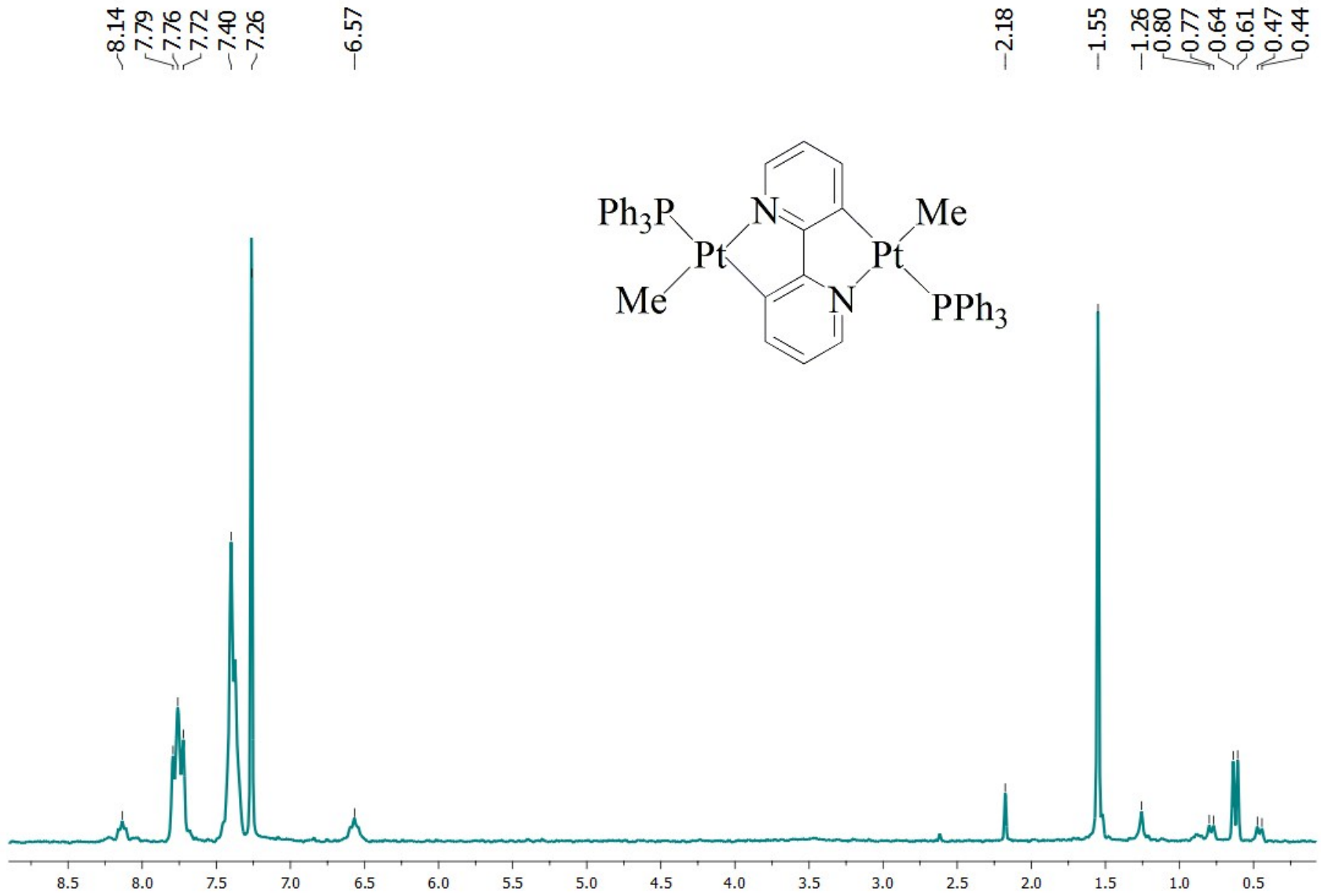

Figure S1. ^{1}HNMR spectrum of the complex **1a** in $CDCl_3$.

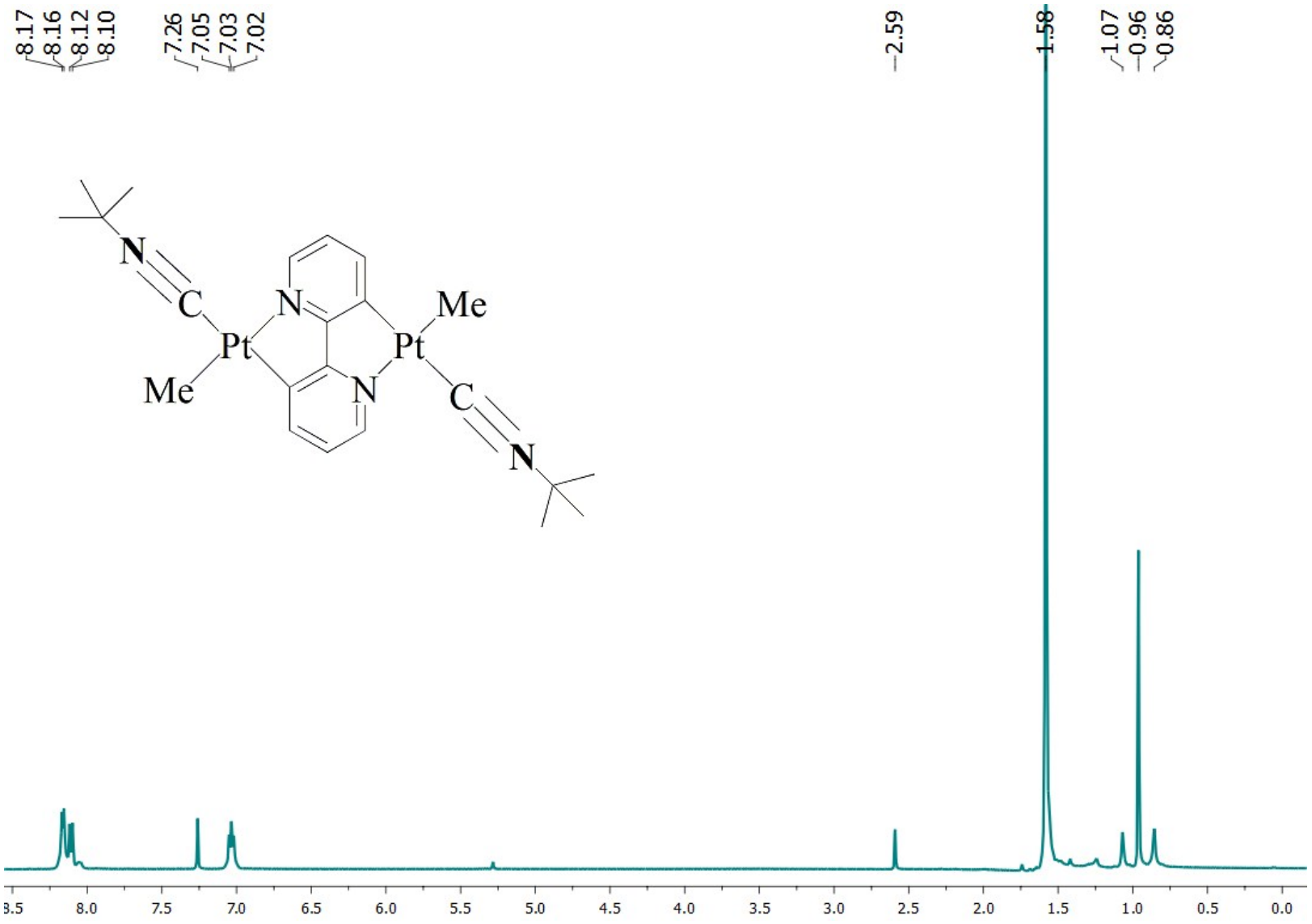

Figure S2. ^{1}HNMR spectrum of the complex **1b** in $CDCl_3$.

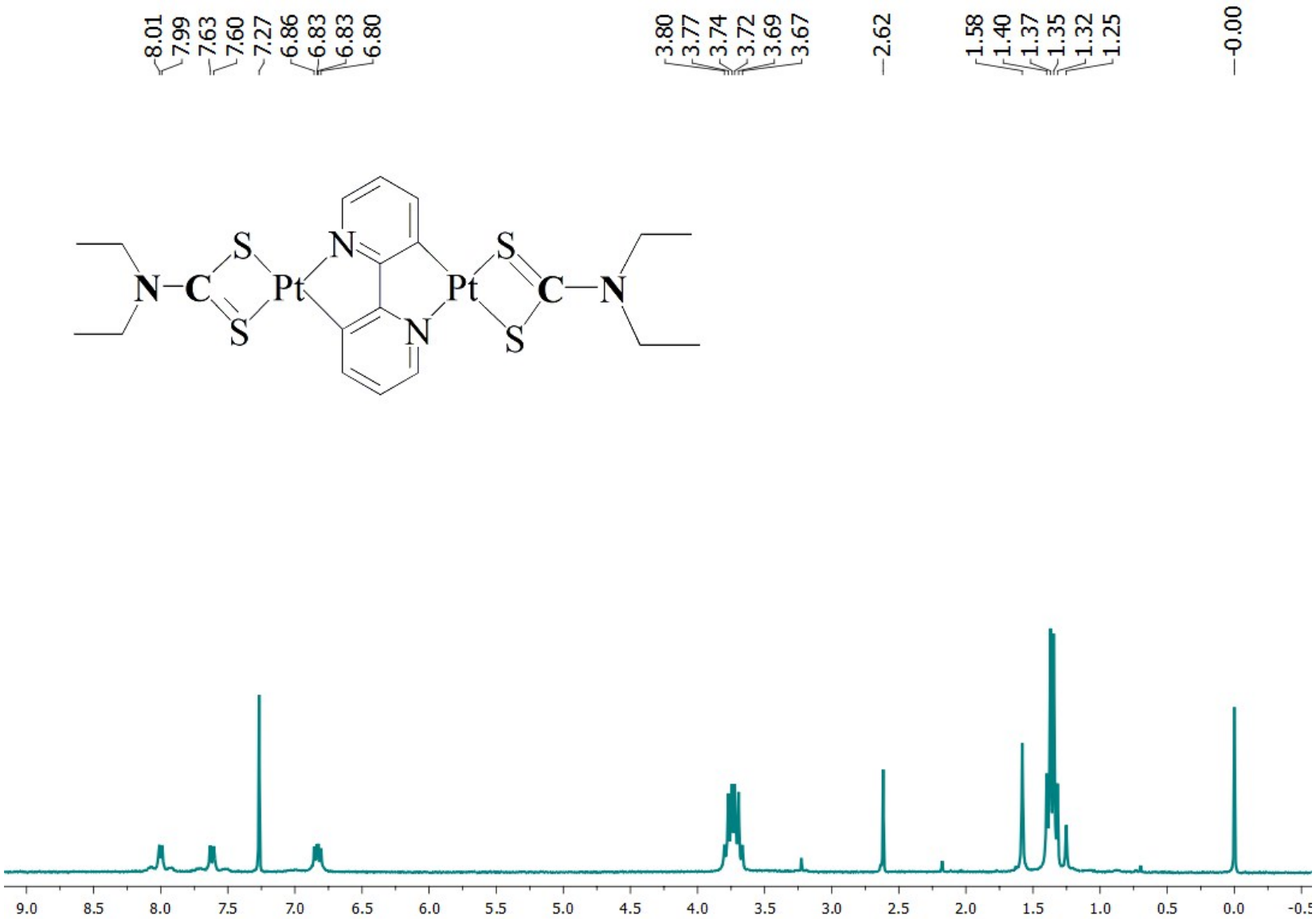

Figure S3. ^{1}HNMR spectrum of the complex **2a** in $CDCl_3$.

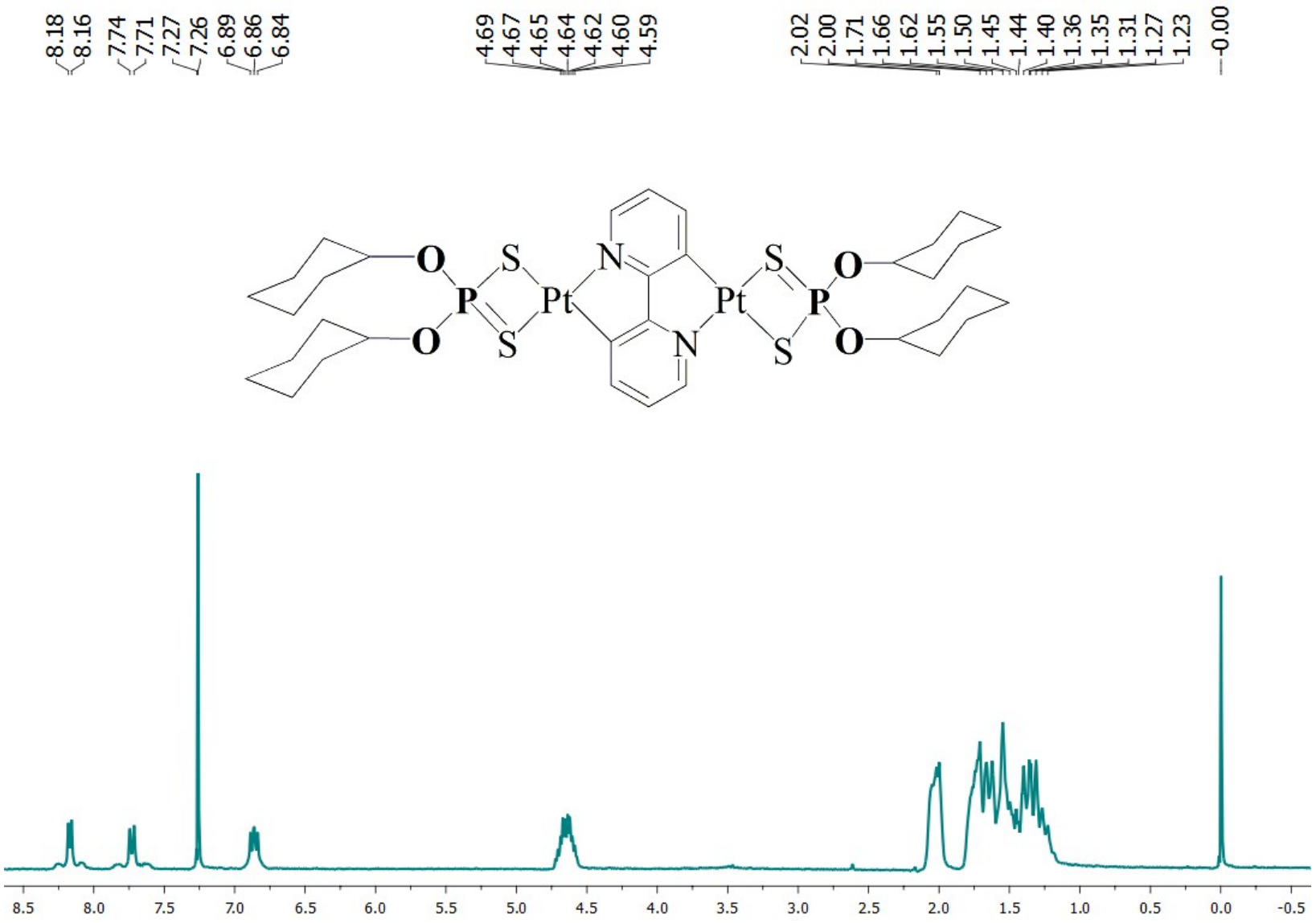

Figure S4. ^{1}HNMR spectrum of the complex **2b** in $CDCl_3$.

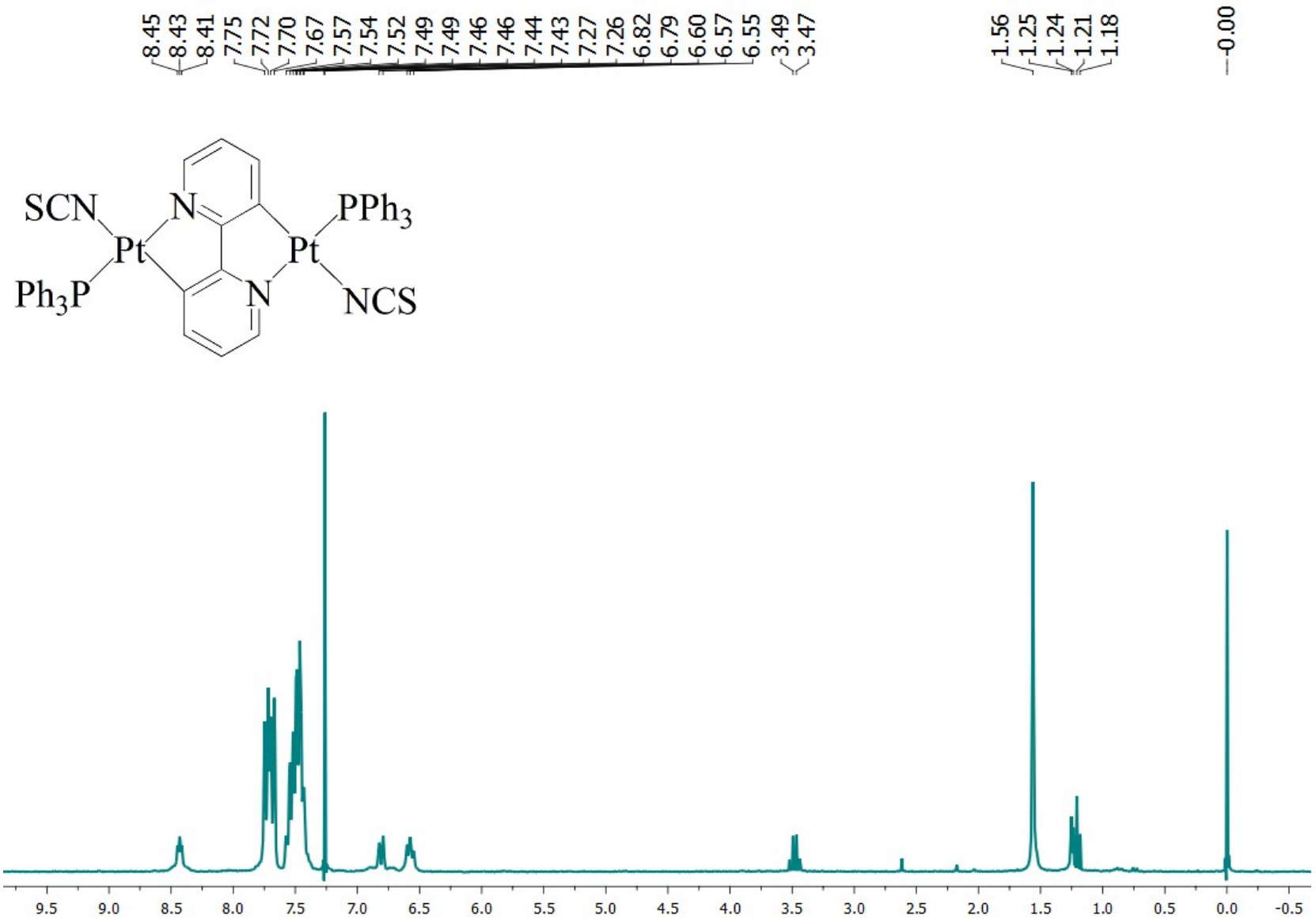

Figure S5. ^{1}HNMR spectrum of the complex **3a** in $CDCl_3$.

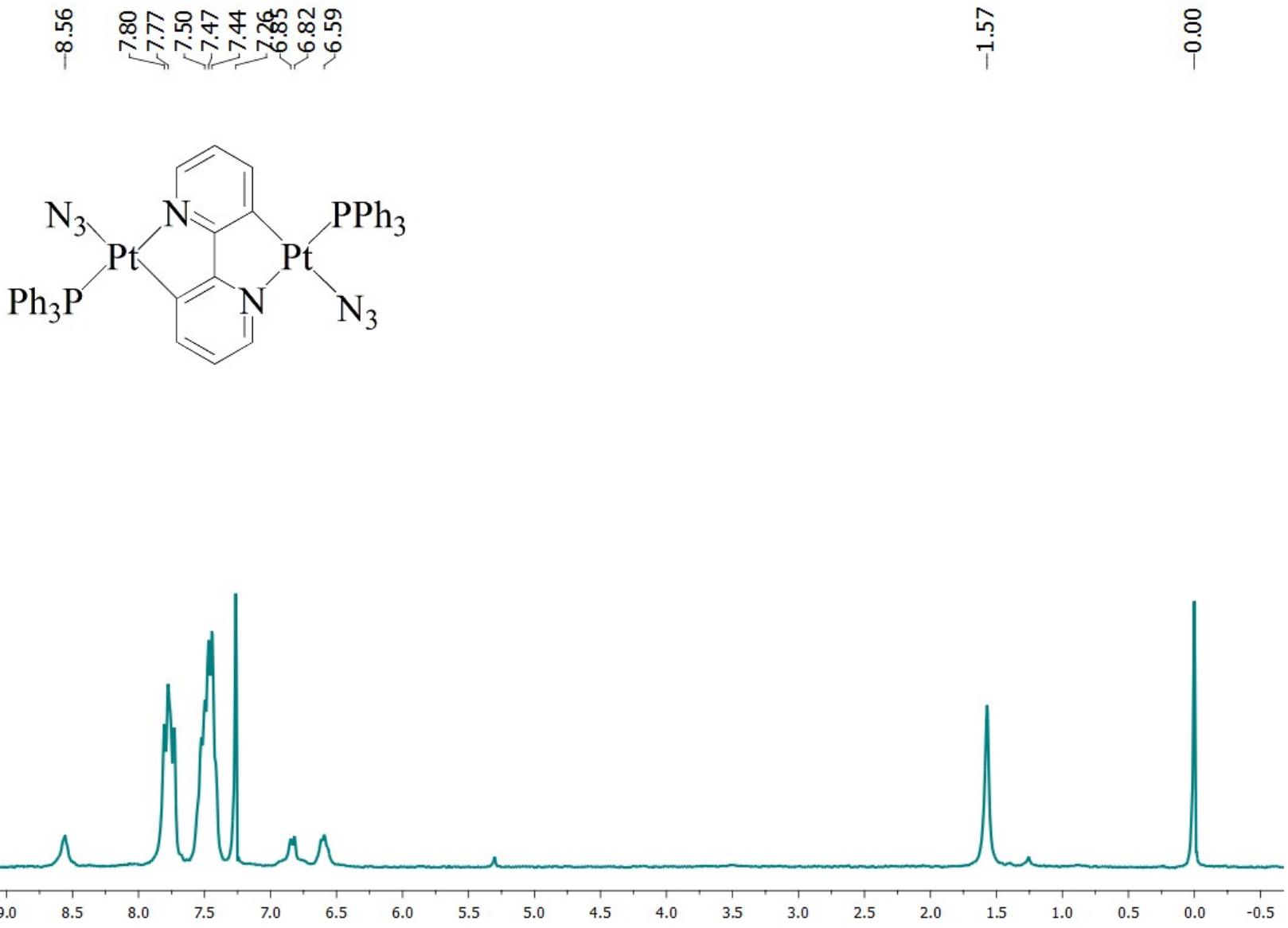

Figure S6. ^{1}HNMR spectrum of the complex **3b** in $CDCl_3$.

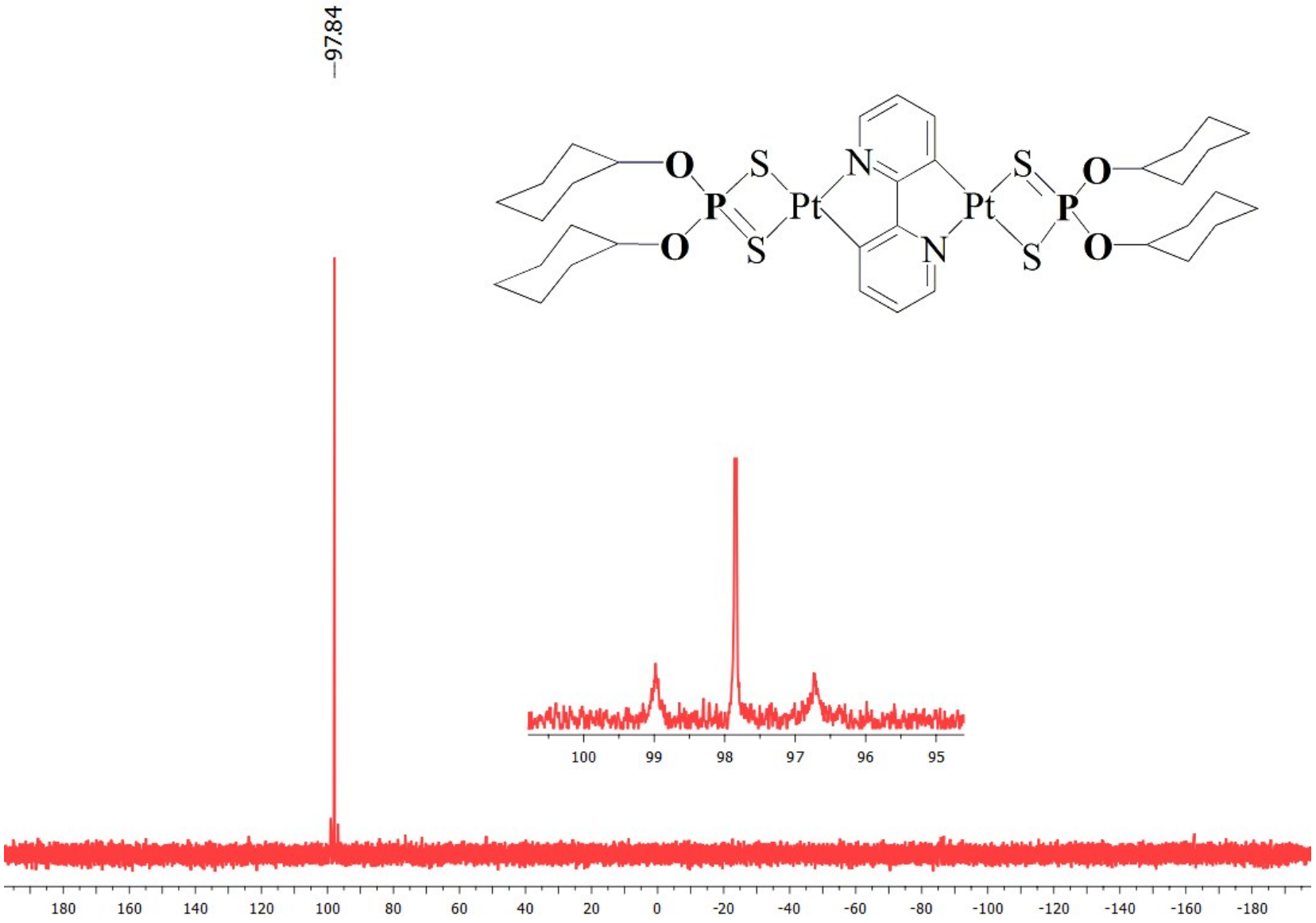

Figure S7. $^{31}P\{H\}$NMR spectrum of the complex **2b** in $CDCl_3$.

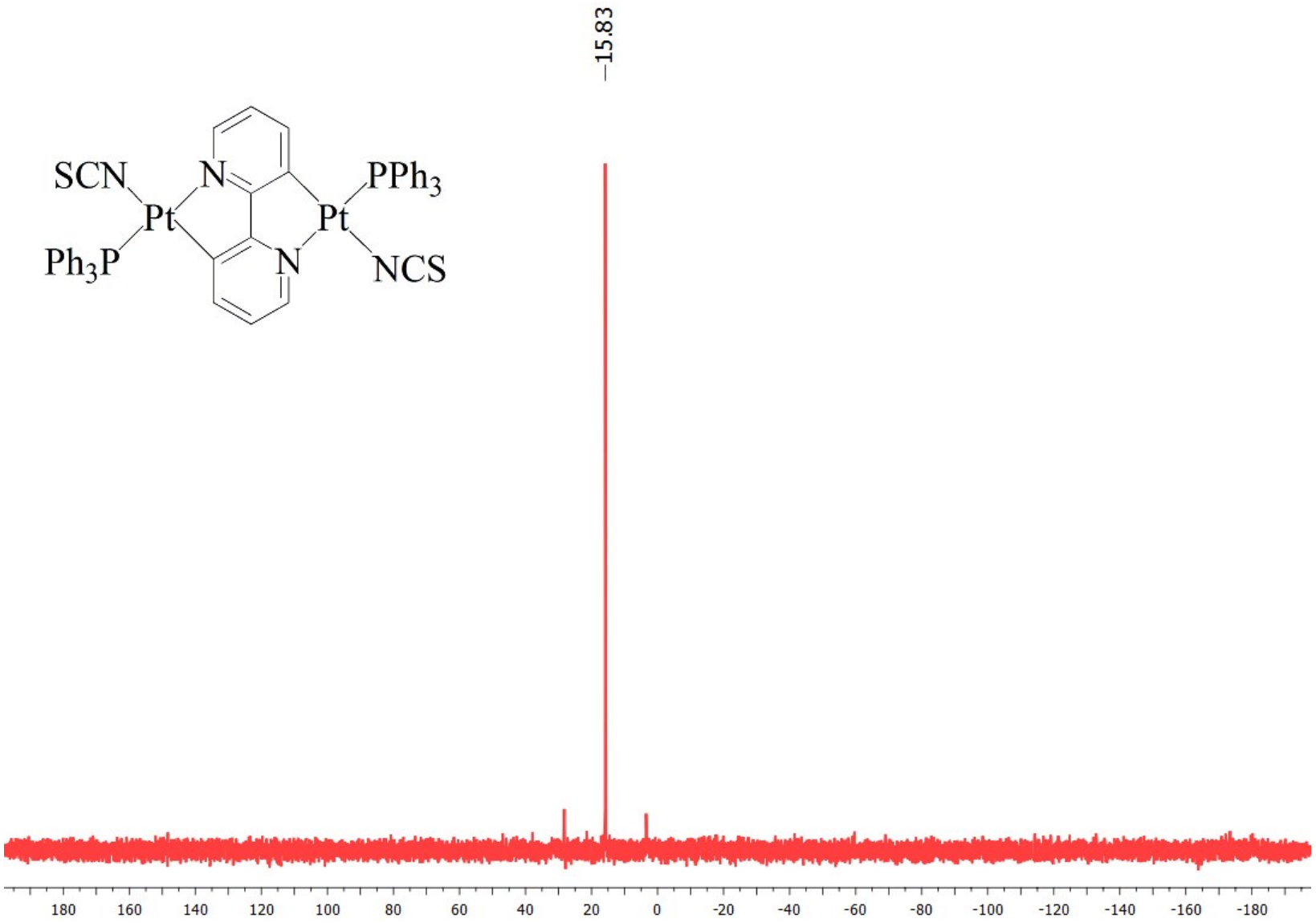

Figure S8. $^{31}P\{H\}$NMR spectrum of the complex **3a** in $CDCl_3$.

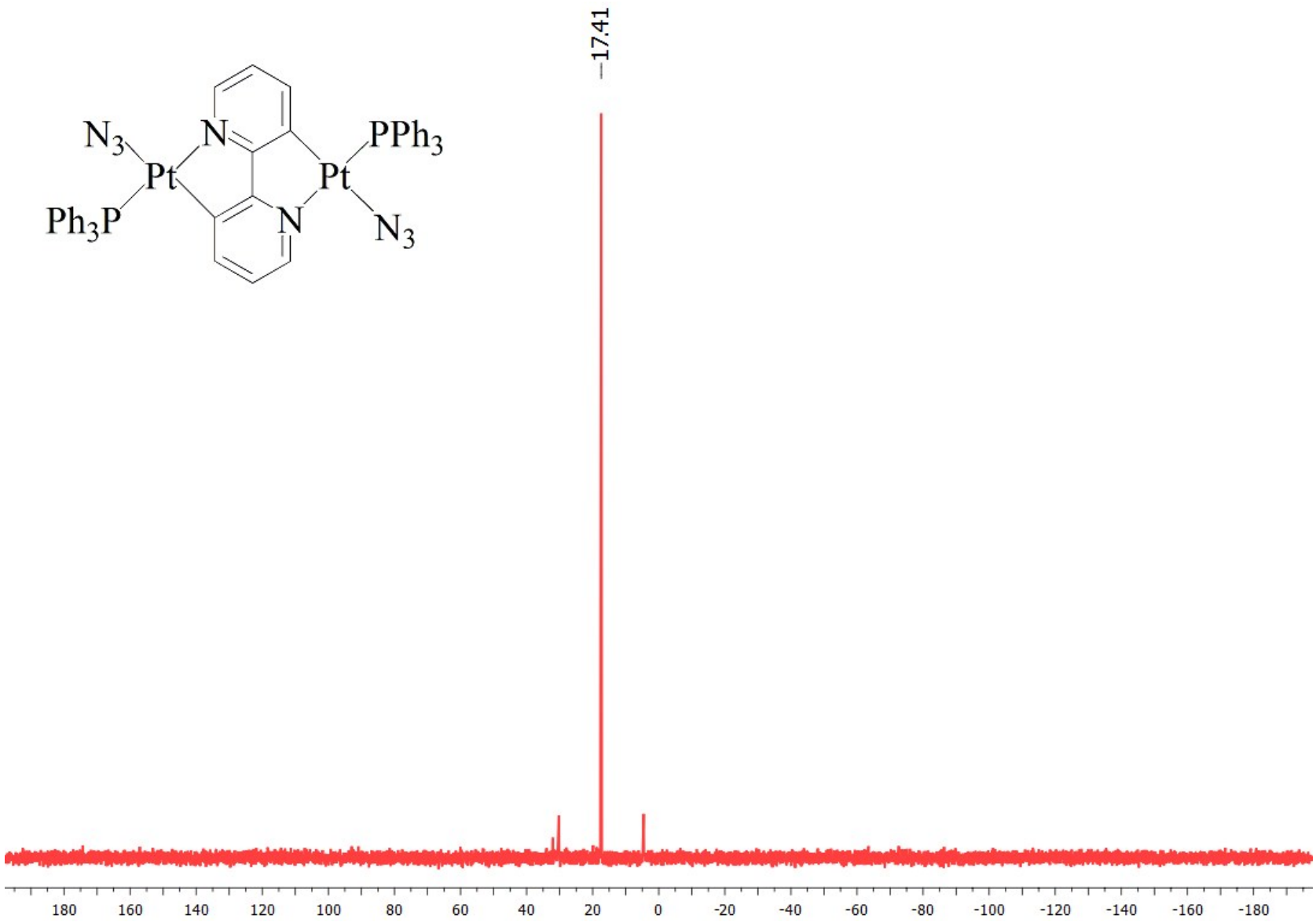

Figure S9. $^{31}P\{H\}$NMR spectrum of the complex **3b** in $CDCl_3$.

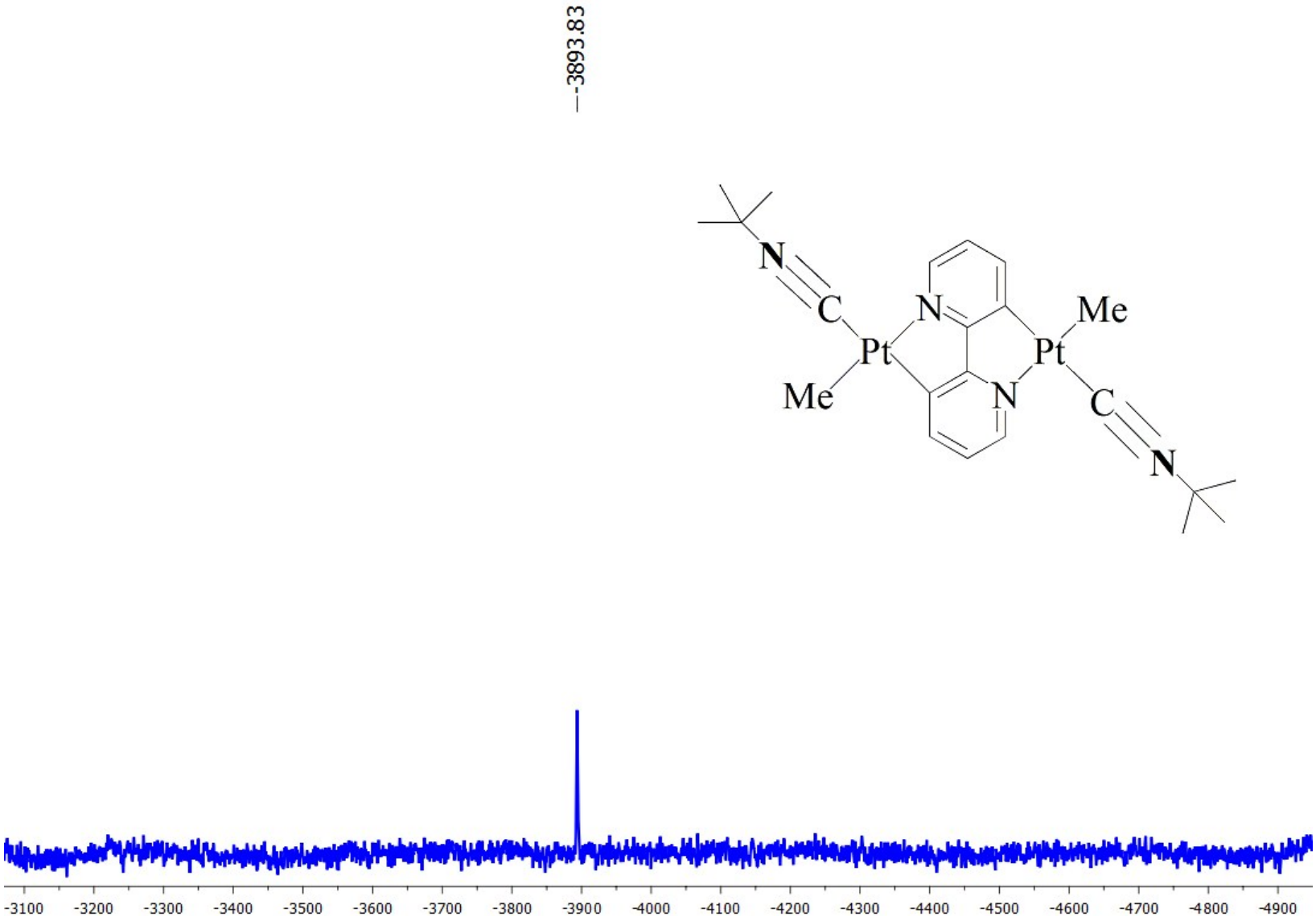

Figure S10. $^{195}Pt\{H\}$NMR spectrum of the complex **1b** in CD_2Cl_2.

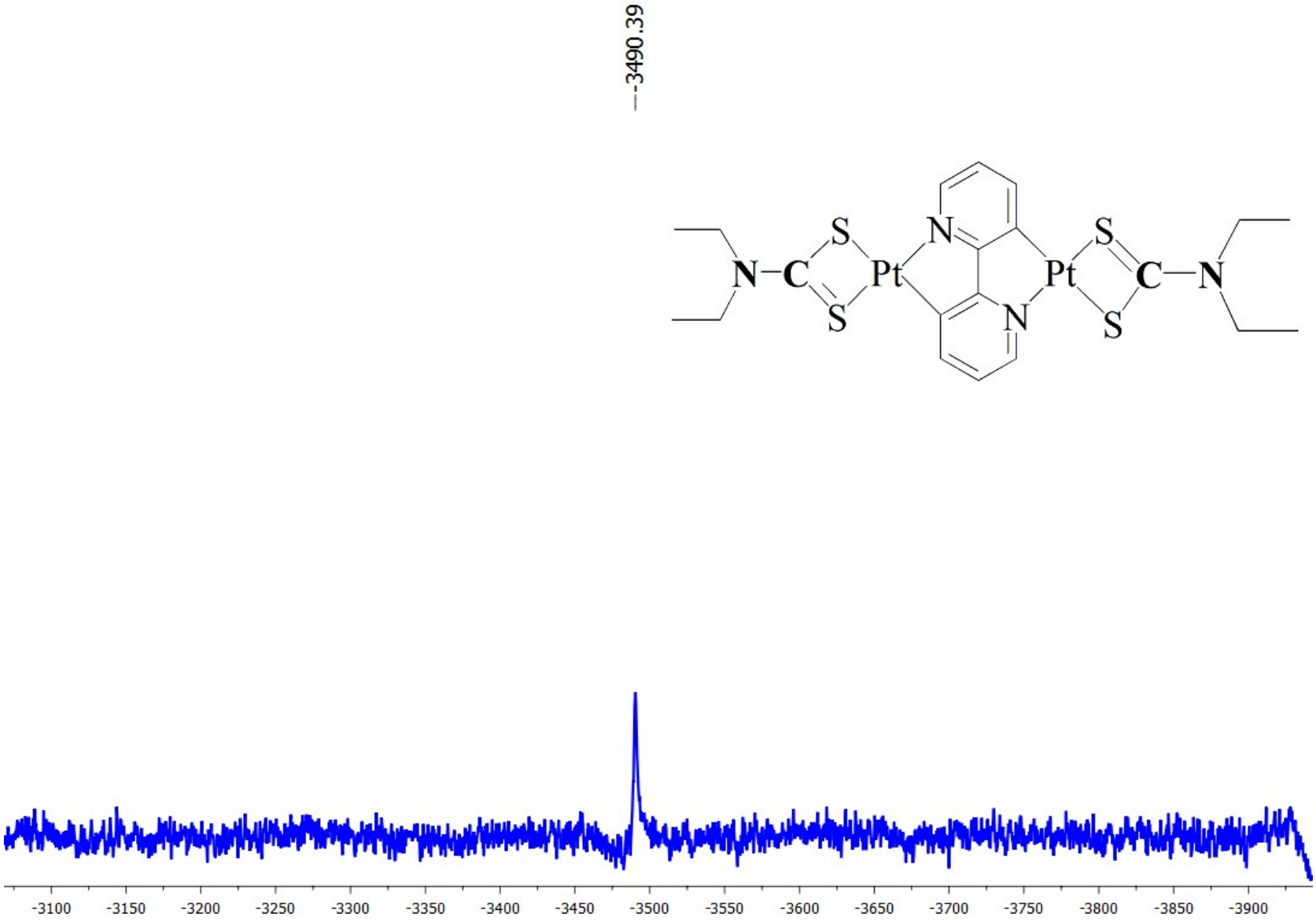

Figure S11. $^{195}Pt\{H\}$NMR spectrum of the complex **2a** in CD_2Cl_2.

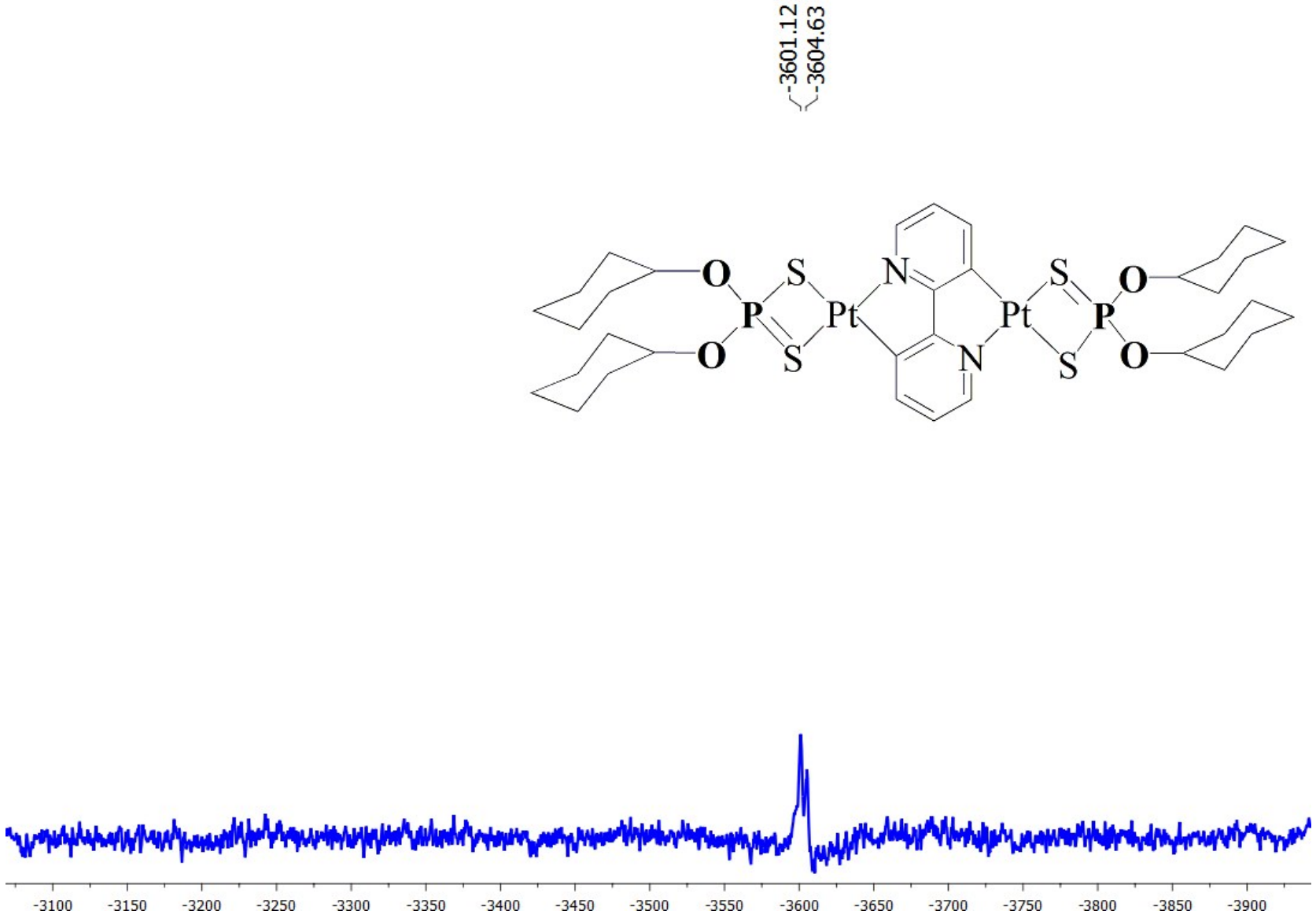

Figure S12. $^{195}Pt\{H\}$NMR spectrum of the complex **2b** in CD_2Cl_2.

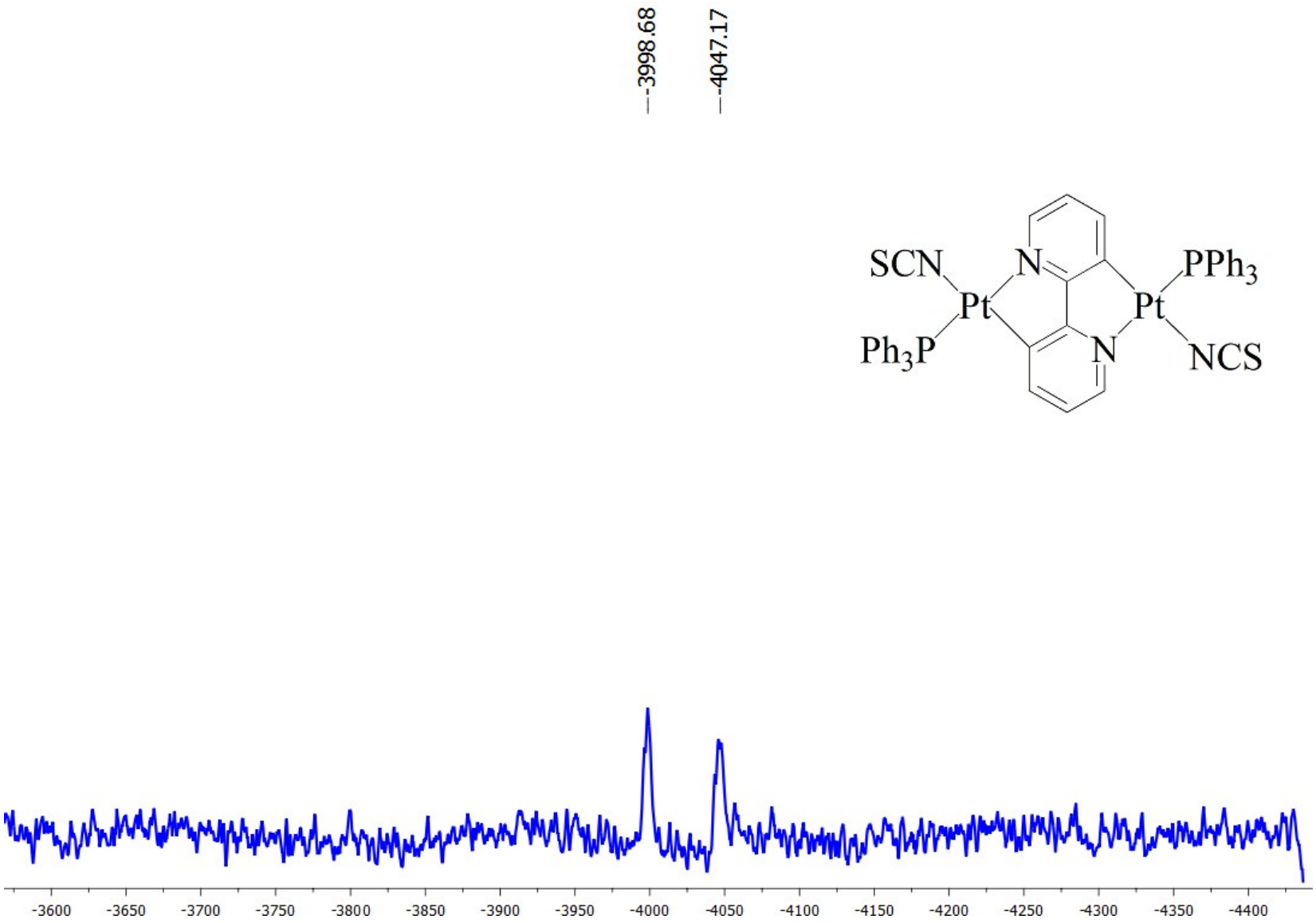

Figure S13. $^{195}Pt\{H\}$NMR spectrum of the complex **3a** in CD_2Cl_2.

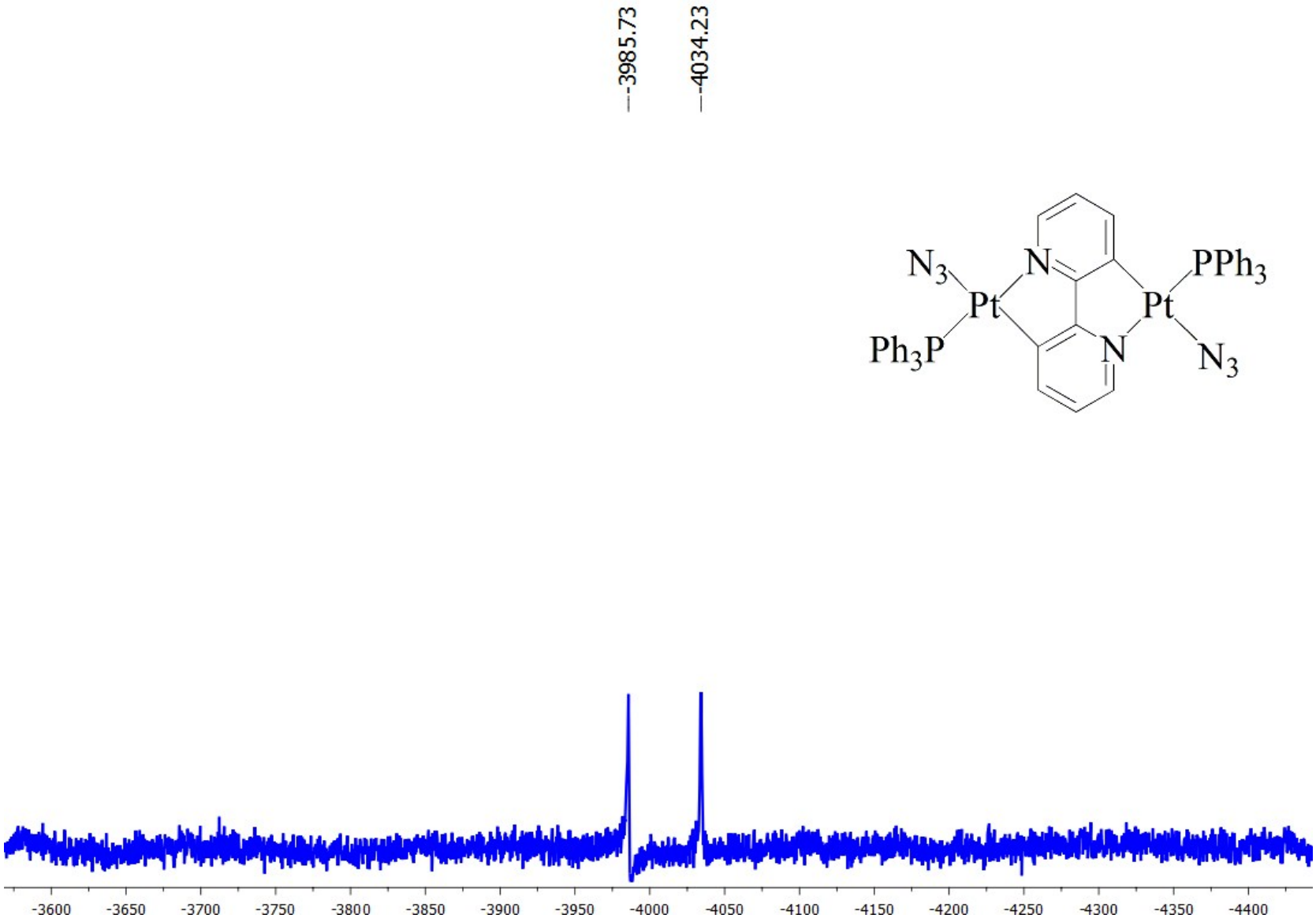

Figure S14. $^{195}Pt\{H\}$NMR spectrum of the complex **3b** in CD_2Cl_2.

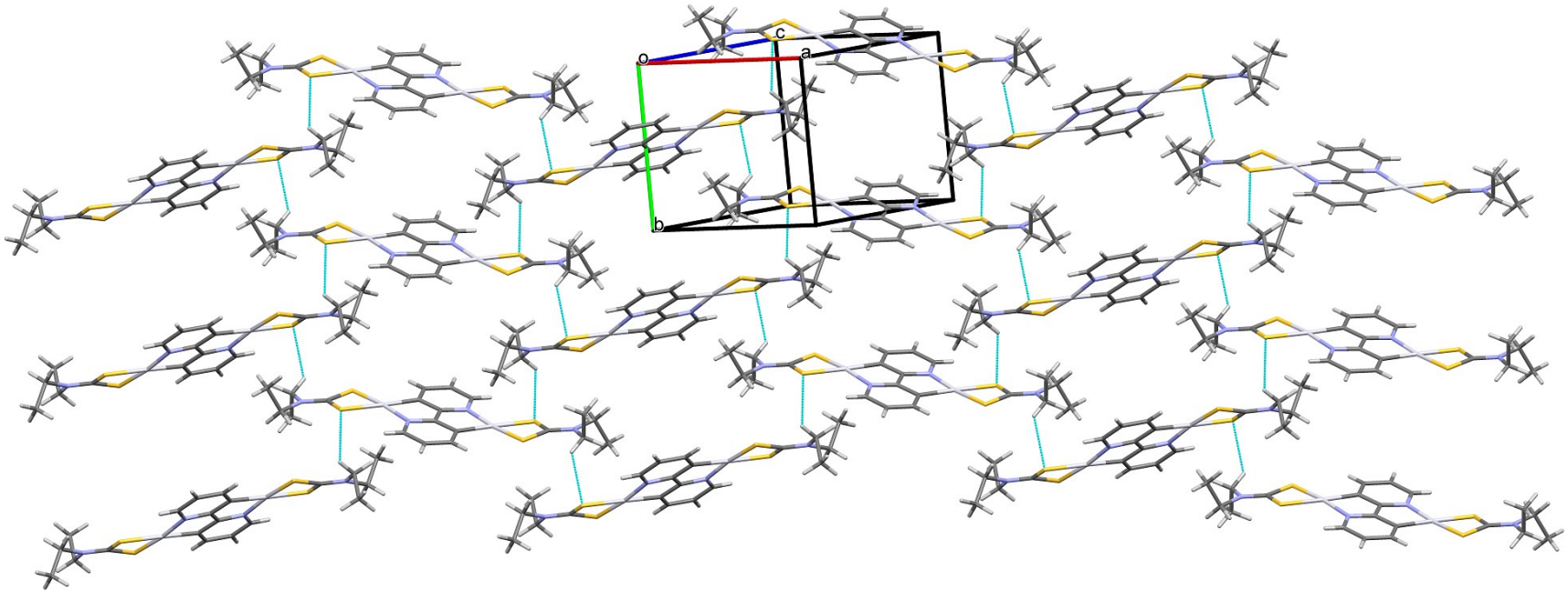

Figure S15. Crystal packing for the complex **2a**.

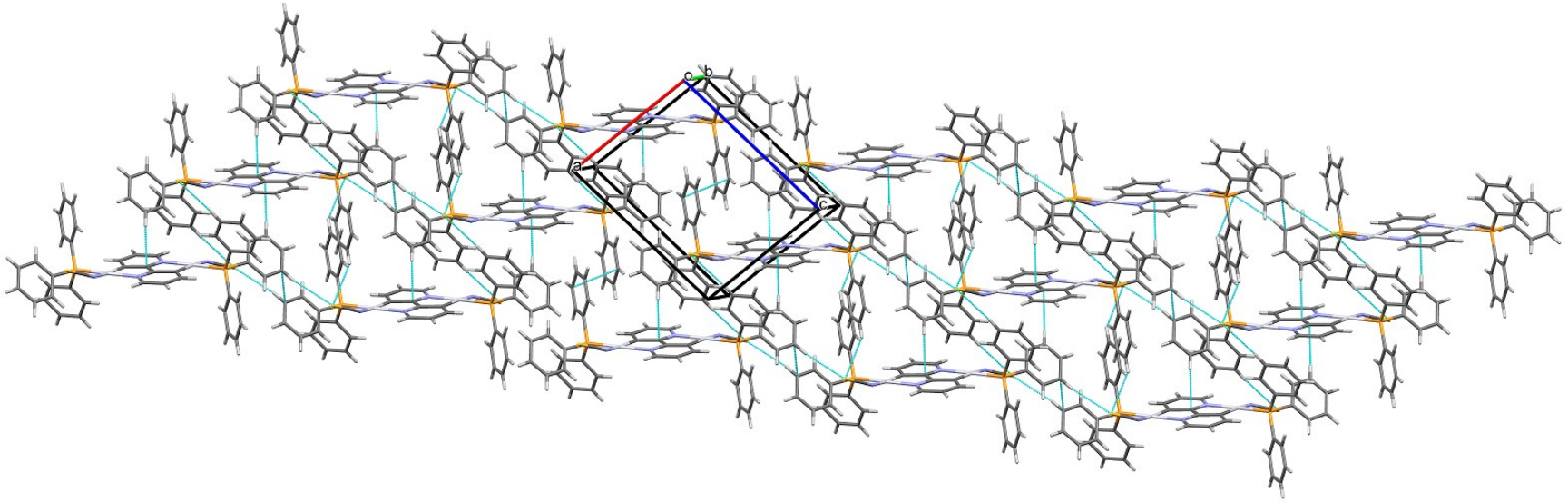

Figure S16. Crystal packing for the complex **3a**.

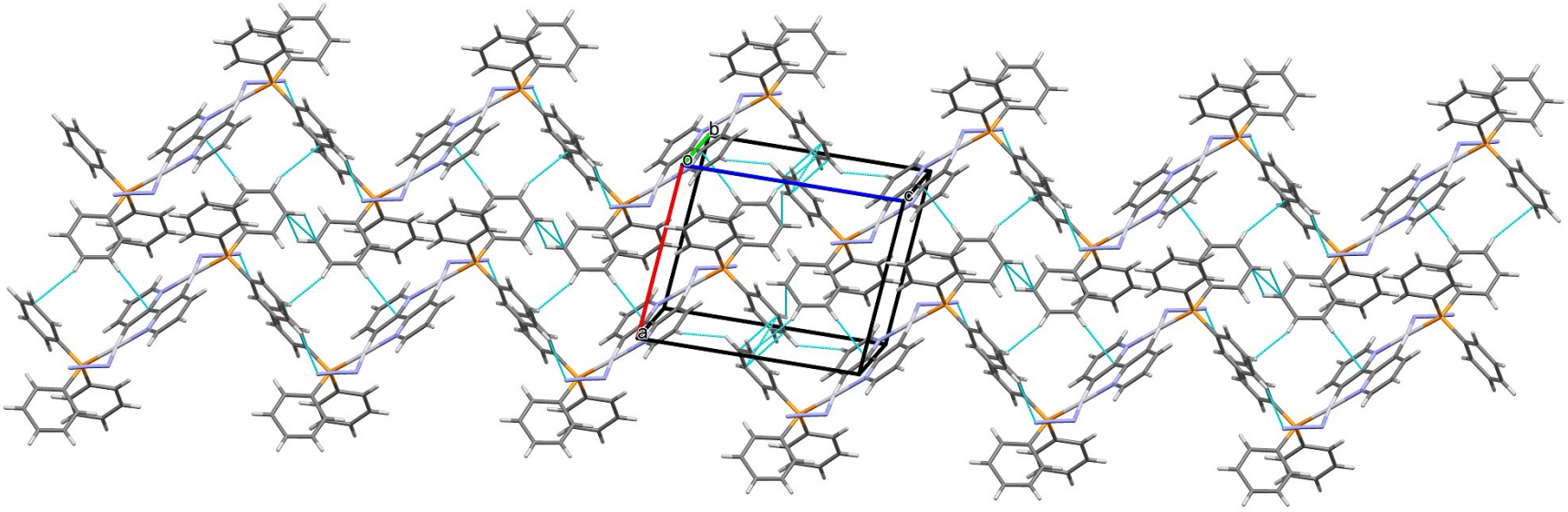

Figure S17. Crystal packing for the complex **3b**.

Table S2. Selected bonds (Å) and angles (°) for the crystal structures of complexes **2a**, **3a** and **3b**.

2a	**3a**	**3b**
Pt(1)-N(1) 2.033(6)	Pt(1)-C(1) 2.011(4)	Pt(1)-C(1) 2.016(13)
Pt(1)-C(1) 2.045(6)	Pt(1)-N(1) 2.038(4)	Pt(1)-N(2) 2.074(12)
Pt(1)-S(1) 2.3226(18)	Pt(1)-N(2) 2.091(3)	Pt(1)-N(1) 2.096(9)
Pt(1)-S(2) 2.3348(19)	Pt(1)-P(1) 2.2367(11)	Pt(1)-P(1) 2.230(3)
S(1)-C(10) 1.732(7)	P(1)-C(20) 1.819(4)	P(1)-C(40) 1.810(12)
N(1)-C(5) 1.372(9)	P(1)-C(40) 1.820(4)	P(1)-C(30) 1.811(12)
N(1)-C(4) 1.379(9)	P(1)-C(30) 1.821(5)	P(1)-C(20) 1.828(12)
C(10)-N(2) 1.308(9)	S(1)-C(11) 1.610(5)	N(3)-N(4) 1.121(18)
C(10)-S(2) 1.747(7)	N(1)-C(11) 1.173(6)	N(3)-N(2) 1.217(17)
N(2)-C(13) 1.460(8)	C(1)-Pt(1)-N(1) 169.92(17)	C(1)-Pt(1)-N(2) 169.6(5)
N(2)-C(11) 1.462(8)	C(1)-Pt(1)-N(2) 82.10(15)	C(1)-Pt(1)-N(1) 81.9(4)
N(1)-Pt(1)-C(1) 82.2(2)	N(1)-Pt(1)-N(2) 90.71(14)	N(2)-Pt(1)-N(1) 87.8(4)
N(1)-Pt(1)-S(1) 174.21(17)	C(1)-Pt(1)-P(1) 95.33(12)	C(1)-Pt(1)-P(1) 94.8(3)
C(1)-Pt(1)-S(1) 100.48(17)	N(1)-Pt(1)-P(1) 91.86(11)	N(2)-Pt(1)-P(1) 95.5(3)
N(1)-Pt(1)-S(2) 101.72(18)	N(2)-Pt(1)-P(1) 177.42(10)	N(1)-Pt(1)-P(1) 176.7(3)
C(1)-Pt(1)-S(2) 176.06(17)	C(20)-P(1)-Pt(01) 116.83(15)	C(40)-P(1)-Pt(1) 116.1(4)
S(1)-Pt(1)-S(2) 75.58(6)	C(40)-P(1)-Pt(01) 114.79(15)	C(30)-P(1)-Pt(1) 115.1(4)
C(10)-S(1)-Pt(1) 87.1(3)	C(30)-P(1)-Pt(01) 110.13(15)	C(20)-P(1)-Pt(1) 109.8(4)
N(2)-C(10)-S(1) 124.8(5)	C(11)-N(1)-Pt(1) 160.4(4)	N(3)-N(2)-Pt(1) 128.2(10)
N(2)-C(10)-S(2) 124.9(5)	N(1)-C(11)-S(1) 178.2(4)	N(4)-N(3)-N(2) 175.5(16)
S(1)-C(10)-S(2) 110.2(4)		
C(10)-N(2)-C(11) 122.2(6)		
C(13)-N(2)-C(11) 117.6(6)		
N(2)-C(11)-C(12) 111.8(5)		
N(2)-C(13)-C(14) 112.7(5)		

Table S3. Numerical absorption data for all the complexes in their CH_2Cl_2 solutions (10^{-5} M).

Complex	Absorption / nm (10^5 ε/M^{-1} cm^{-1})
1a	396 (0.250), 372 (0.586), 305 (1.419), 278 (1.636)
1b	386 (0.159), 363 (0.398), 329 (0.452), 297 (1.050)
2a	443 (0.103), 392 (0.419), 372 (0.320), 346 (0.314), 305 (0.873), 283 (1.146)
2b	428 (0.089), 380 (0.294), 360 (0.250), 334 (0.248), 287 (1.431)
3a	407 (0.376), 384 (0.309), 312 (1.230), 277 (1.279)
3b	408 (0.220), 388 (0.195), 299 (0.935), 281 (1.398)

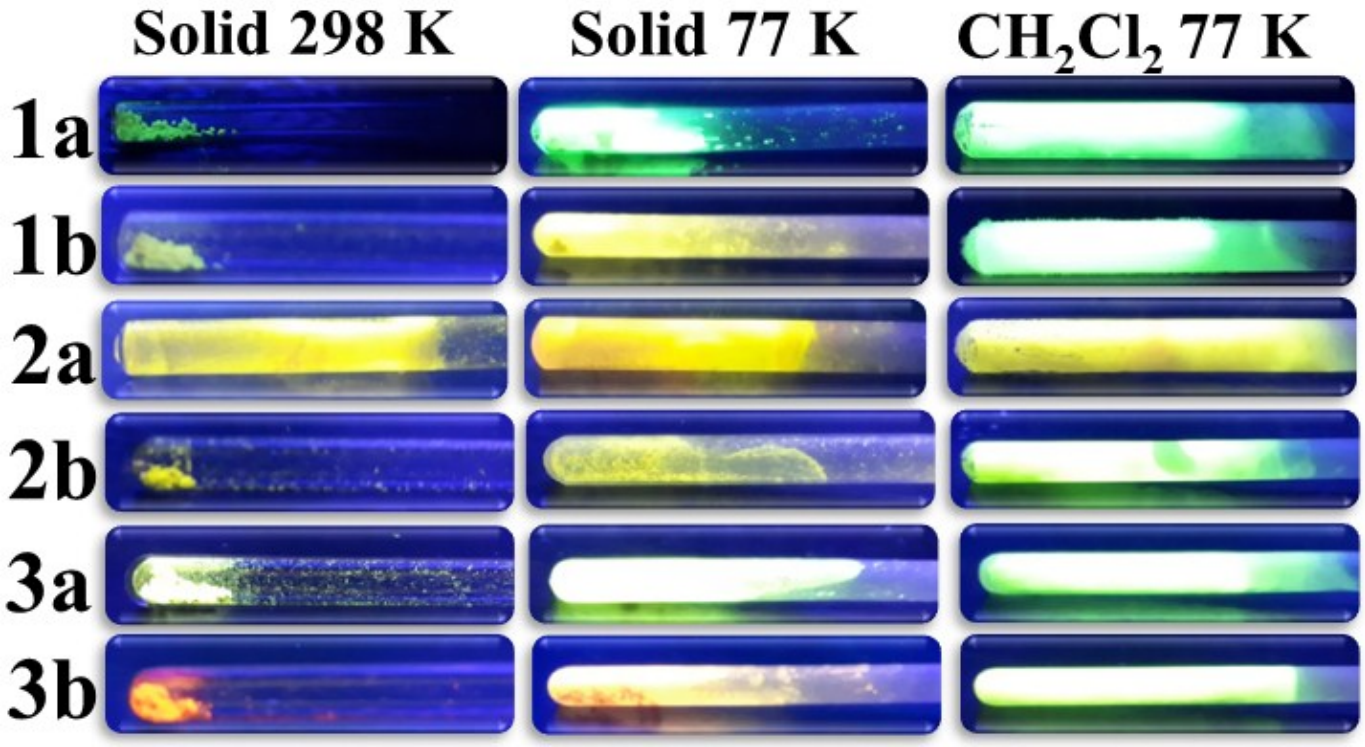

Figure S18. Photographic images of all the samples in different conditions under UV light irradiation (λ = 365 nm).

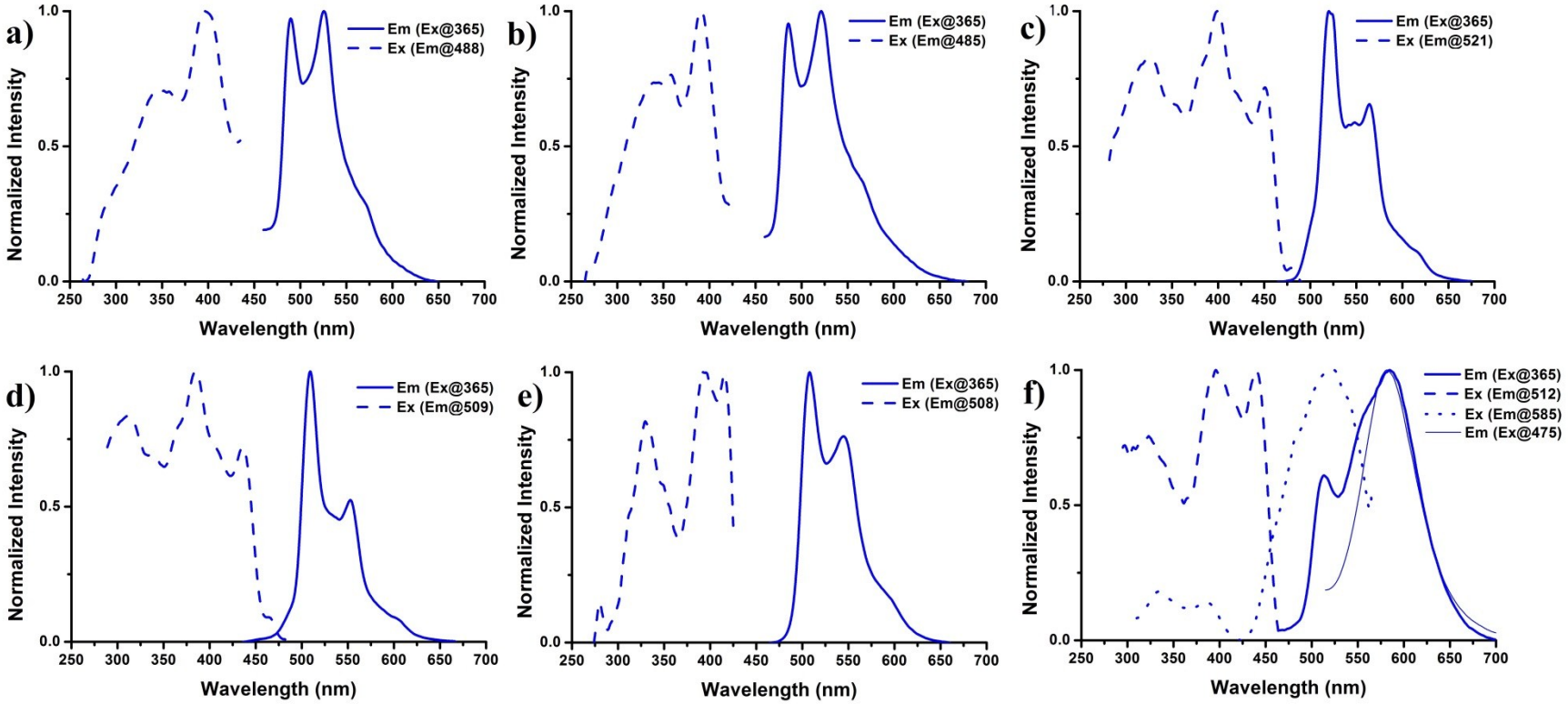

Figure S19. Emission and excitation spectra in polystyrene films (5%) at 298 K for the complexes a) **1a**, b) **1b**, c) **2a**, d) **2b**, e) **3a** and f) **3b**.

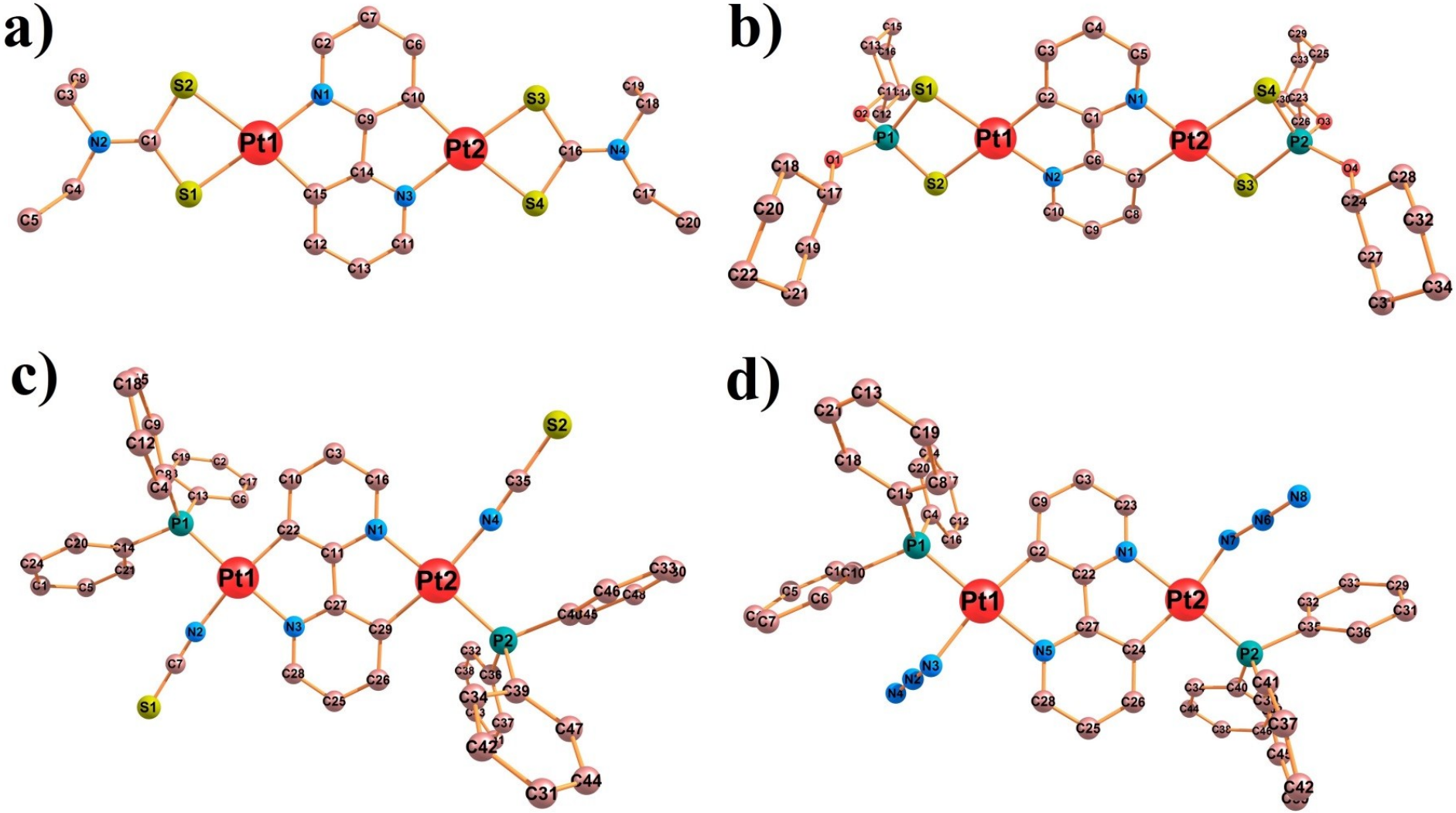

Figure S20. DFT optimized geometries of the ground states (S_0) for the complexes a) **2a**, b) **2b**, c) **3a** and d) **3b** in gas phase.

Table S4. Selected bonds (Å) and angles (°) for the optimized geometries of the complexes **2a**, **2b**, **3a** and **3b** in ground state (gas phase).

2a	**2b**	**3a**	**3b**
Pt(1)-N(1) 2.098	Pt(1)-N(2) 2.092	Pt(1)-N(3) 2.315	Pt(1)-N(5) 2.133
Pt(1)-C(15) 2.020	Pt(1)-C(2) 2.016	Pt(1)-C(22) 2.036	Pt(1)-C(2) 2.053
Pt(1)-S(1) 2.366	Pt(1)-S(1) 2.388	Pt(1)-N(2) 2.066	Pt(1)-N(3) 2.128
Pt(1)-S(2) 2.497	Pt(1)-S(2) 2.519	Pt(1)-P(1) 2.313	Pt(1)-P(1) 2.295
S(1)-C(1) 1.743	P(1)-S(1) 2.052	P(1)-C(13) 1.841	P(1)-C(4) 1.842
S(2)-C(1) 1.733	P(1)-S(2) 2.029	P(1)-C(8) 1.842	P(1)-C(10) 1.840
C(1)-N(2) 1.338	P(1)-O(1) 1.604	P(1)-C(14) 1.839	P(1)-C(15) 1.844
N(2)-C(3) 1.473	P(1)-O(2) 1.604	N(2)-C(7) 1.185	N(3)-N(2) 1.218
N(2)-C(4) 1.473	O(1)-C(17) 1.466	C(7)-S(1) 1.625	N(2)-N(4) 1.156
N(1)-Pt(1)-C(15) 81.75	O(2)-C(11) 1.466	C(22)-Pt(1)-N(3) 81.06	C(2)-Pt(1)-N(5) 80.89
N(1)-Pt(1)-S(1) 177.50	C(2)-Pt(1)-N(2) 81.96	N(3)-Pt(1)-N(2) 90.15	N(5)-Pt(1)-N(3) 87.98
N(1)-Pt(1)-S(2) 104.25	N(2)-Pt(1)-S(2) 99.14	N(2)-Pt(1)-P(1) 91.80	N(3)-Pt(1)-P(1) 93.61
C(15)-Pt(1)-S(1) 100.73	C(2)-Pt(1)-S(1) 96.88	P(1)-Pt(1)-C(22) 96.97	P(1)-Pt(1)-C(2) 97.51
C(15)-Pt(1)-S(2) 173.98	S(1)-Pt(1)-S(2) 82.00	N(3)-Pt(1)-P(1) 177.97	N(5)-Pt(1)-P(1) 177.67
S(1)-Pt(1)-S(2) 73.26	C(2)-Pt(1)-S(2) 178.88	C(22)-Pt(1)-N(2) 171.19	C(2)-Pt(1)-N(3) 168.87
Pt(1)-S(1)-C(1) 88.68	N(2)-Pt(1)-S(1) 178.85	Pt(1)-N(2)-C(7) 170.99	Pt(1)-N(3)-N(2) 120.32
Pt(1)-S(2)-C(1) 84.76	Pt(1)-S(1)-P(1) 88.40	N(2)-C(7)-S(1) 179.80	N(3)-N(2)-N(4) 175.55
S(1)-C(1)-S(2) 113.29	Pt(1)-S(2)-P(1) 85.39		
S(1)-C(1)-N(2) 122.85	S(1)-P(1)-S(2) 104.19		
S(2)-C(1)-N(2) 123.84	S(1)-P(1)-O(1) 113.54		
C(1)-N(2)-C(3) 121.61	S(2)-P(1)-O(2) 114.90		
C(1)-N(2)-C(4) 121.76	O(1)-P(1)-O(2) 96.15		
N(2)-C(3)-C(8) 112.63	P(1)-O(1)-C(17) 121.55		
N(2)-C(4)-C(5) 112.75	P(1)-O(2)-C(11) 121.55		

Table S5. Selected bonds (Å) and angles (°) for the optimized geometries of the complexes **2a**, **2b**, **3a** and **3b** in ground state (CH_2Cl_2 solvent).

2a	**2b**	**3a**	**3b**
Pt(1)-N(1) 2.104	Pt(1)-N(2) 2.097	Pt(1)-N(3) 2.145	Pt(1)-N(5) 2.142
Pt(1)-C(15) 2.023	Pt(1)-C(2) 2.018	Pt(1)-C(22) 2.031	Pt(1)-C(2) 2.044
Pt(1)-S(1) 2.368	Pt(1)-S(1) 2.393	Pt(1)-N(2) 2.091	Pt(1)-N(3) 2.149
Pt(1)-S(2) 2.496	Pt(1)-S(2) 2.522	Pt(1)-P(1) 2.320	Pt(1)-P(1) 2.304
S(1)-C(1) 1.751	P(1)-S(1) 2.056	P(1)-C(13) 1.838	P(1)-C(4) 1.841
S(2)-C(1) 1.742	P(1)-S(2) 2.033	P(1)-C(8) 1.840	P(1)-C(10) 1.842
C(1)-N(2) 1.328	P(1)-O(1) 1.602	P(1)-C(14) 1.841	P(1)-C(15) 1.841
N(2)-C(3) 1.478	P(1)-O(2) 1.602	N(2)-C(7) 1.180	N(3)-N(2) 1.210
N(2)-C(4) 1.478	O(1)-C(17) 1.473	C(7)-S(1) 1.639	N(2)-N(4) 1.161
N(1)-Pt(1)-C(15) 81.64	O(2)-C(11) 1.473	C(22)-Pt(1)-N(3) 81.03	C(2)-Pt(1)-N(5) 80.95
N(1)-Pt(1)-S(1) 177.68	C(2)-Pt(1)-N(2) 81.90	N(3)-Pt(1)-N(2) 90.49	N(5)-Pt(1)-N(3) 88.40
N(1)-Pt(1)-S(2) 104.39	N(2)-Pt(1)-S(2) 99.41	N(2)-Pt(1)-P(1) 92.25	N(3)-Pt(1)-P(1) 93.79
C(15)-Pt(1)-S(1) 100.65	C(2)-Pt(1)-S(1) 96.89	P(1)-Pt(1)-C(22) 96.21	P(1)-Pt(1)-C(2) 96.84
C(15)-Pt(1)-S(2) 173.92	S(1)-Pt(1)-S(2) 81.78	N(3)-Pt(1)-P(1) 177.19	N(5)-Pt(1)-P(1) 177.69
S(1)-Pt(1)-S(2) 73.30	C(2)-Pt(1)-S(2) 178.67	C(22)-Pt(1)-N(2) 171.52	C(2)-Pt(1)-N(3) 169.31
Pt(1)-S(1)-C(1) 88.96	N(2)-Pt(1)-S(1) 178.79	Pt(1)-N(2)-C(7) 174.11	Pt(1)-N(3)-N(2) 121.47
Pt(1)-S(2)-C(1) 85.14	Pt(1)-S(1)-P(1) 88.67	N(2)-C(7)-S(1) 179.73	N(3)-N(2)-N(4) 175.77
S(1)-C(1)-S(2) 112.57	Pt(1)-S(2)-P(1) 85.70		
S(1)-C(1)-N(2) 123.17	S(1)-P(1)-S(2) 103.84		
S(2)-C(1)-N(2) 124.25	S(1)-P(1)-O(1) 113.66		
C(1)-N(2)-C(3) 121.83	S(2)-P(1)-O(2) 114.97		
C(1)-N(2)-C(4) 121.95	O(1)-P(1)-O(2) 96.20		
N(2)-C(3)-C(8) 112.56	P(1)-O(1)-C(17) 122.33		
N(2)-C(4)-C(5) 112.65	P(1)-O(2)-C(11) 122.33		

Table S6. The energies of the selected molecular orbitals of the complex **2a** together with their compositions in CH_2Cl_2.

	Complex 2a			
	Energy	Components(%)		
MO	(eV)	Pt	μ-bpy	dedtc
LUMO+5	-0.591	38	24	38
LUMO+4	-0.871	7	31	62
LUMO+3	-1.038	27	23	50
LUMO+2	-1.108	22	20	58
LUMO+1	-1.341	9	47	44
LUMO	-1.993	5	88	7
HOMO	-5.711	43	23	34
HOMO-1	-5.847	45	7	48
HOMO-2	-6.002	46	12	42
HOMO-3	-6.228	50	5	45
HOMO-4	-6.253	88	8	4
HOMO-5	-6.309	86	8	6

Table S7. The energies of the selected molecular orbitals of the complex **2b** together with their compositions in CH_2Cl_2.

	Complex 2b			
	Energy	Components(%)		
MO	(eV)	Pt	μ-bpy	dcdtp
LUMO+5	-0.347	3	3	94
LUMO+4	-0.685	10	86	4
LUMO+3	-0.844	38	24	38
LUMO+2	-1.272	14	84	2
LUMO+1	-1.324	38	27	35
LUMO	-2.066	5	93	3
HOMO	-5.876	45	29	26
HOMO-1	-6.051	49	8	43
HOMO-2	-6.180	51	12	37
HOMO-3	-6.373	91	7	2
HOMO-4	-6.432	91	6	3
HOMO-5	-6.475	62	7	30

Table S8. The energies of the selected molecular orbitals of the complex **3a** together with their compositions in CH_2Cl_2.

	Complex 3a				
	Energy	Components(%)			
MO	(eV)	Pt	μ-bpy	SCN	PPh_3
LUMO+5	-1.130	26	2	1	71
LUMO+4	-1.168	4	2	1	93
LUMO+3	-1.192	19	9	1	72
LUMO+2	-1.442	35	17	3	45
LUMO+1	-1.545	12	64	3	21
LUMO	-2.145	4	88	1	7
HOMO	-5.791	26	16	58	0
HOMO-1	-5.929	20	4	76	0
HOMO-2	-6.007	8	3	88	1
HOMO-3	-6.021	8	2	88	2
HOMO-4	-6.534	11	53	35	1
HOMO-5	-6.652	84	4	0	12

Table S9. The energies of the selected molecular orbitals of the complex **3b** together with their compositions in CH_2Cl_2.

	Complex 3b				
	Energy	Components(%)			
MO	(eV)	Pt	μ-bpy	N_3	PPh_3
LUMO+5	-1.047	24	8	5	63
LUMO+4	-1.084	4	1	1	94
LUMO+3	-1.088	14	8	1	78
LUMO+2	-1.338	34	18	6	42
LUMO+1	-1.373	12	63	1	24
LUMO	-2.000	4	88	1	7
HOMO	-5.581	21	10	67	2
HOMO-1	-5.641	16	5	76	3
HOMO-2	-5.939	28	27	44	1
HOMO-3	-6.085	25	13	58	4
HOMO-4	-6.378	44	27	24	5
HOMO-5	-6.462	86	3	1	8

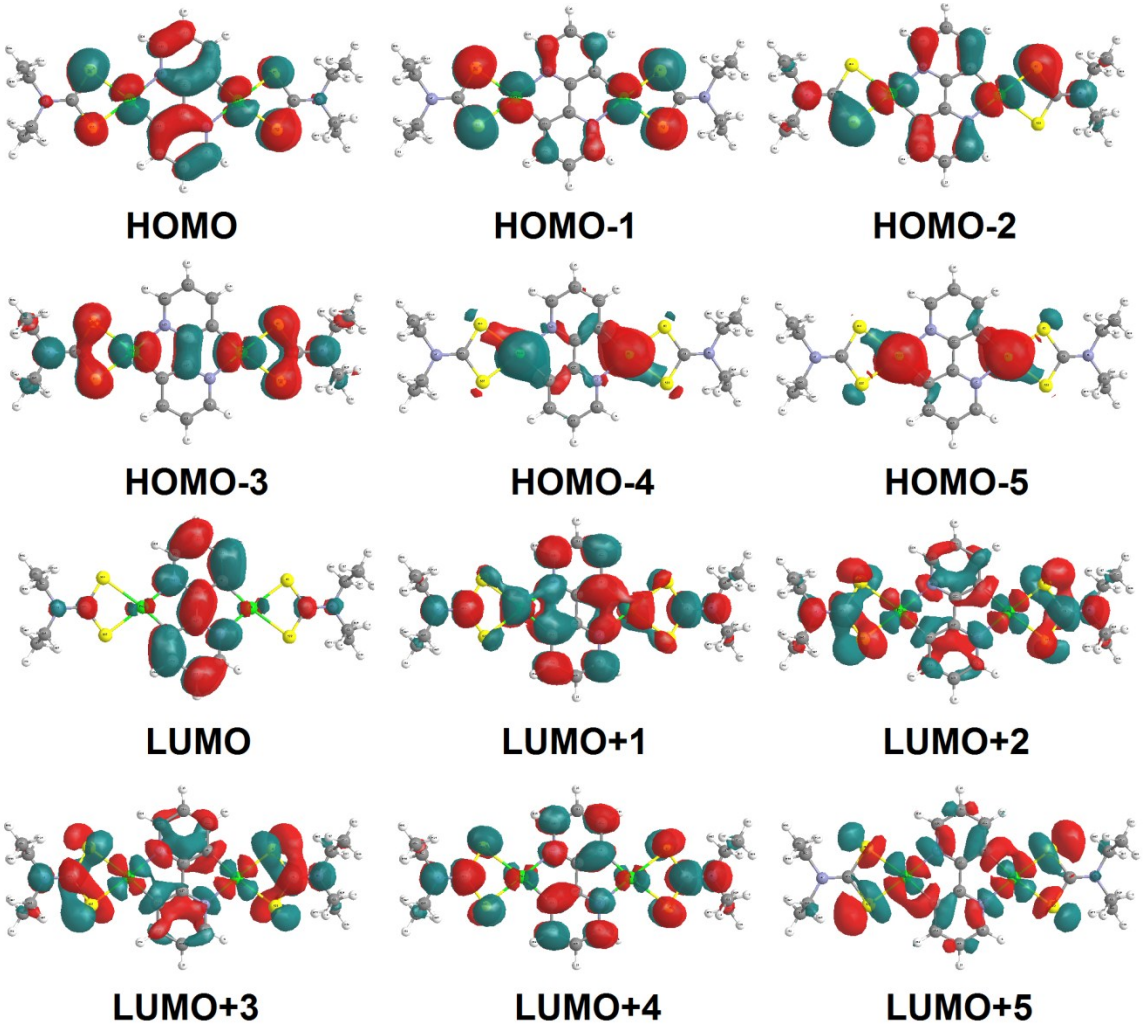

Figure S21. Selected molecular orbital plots of the complex **2a** in CH_2Cl_2 solvent.

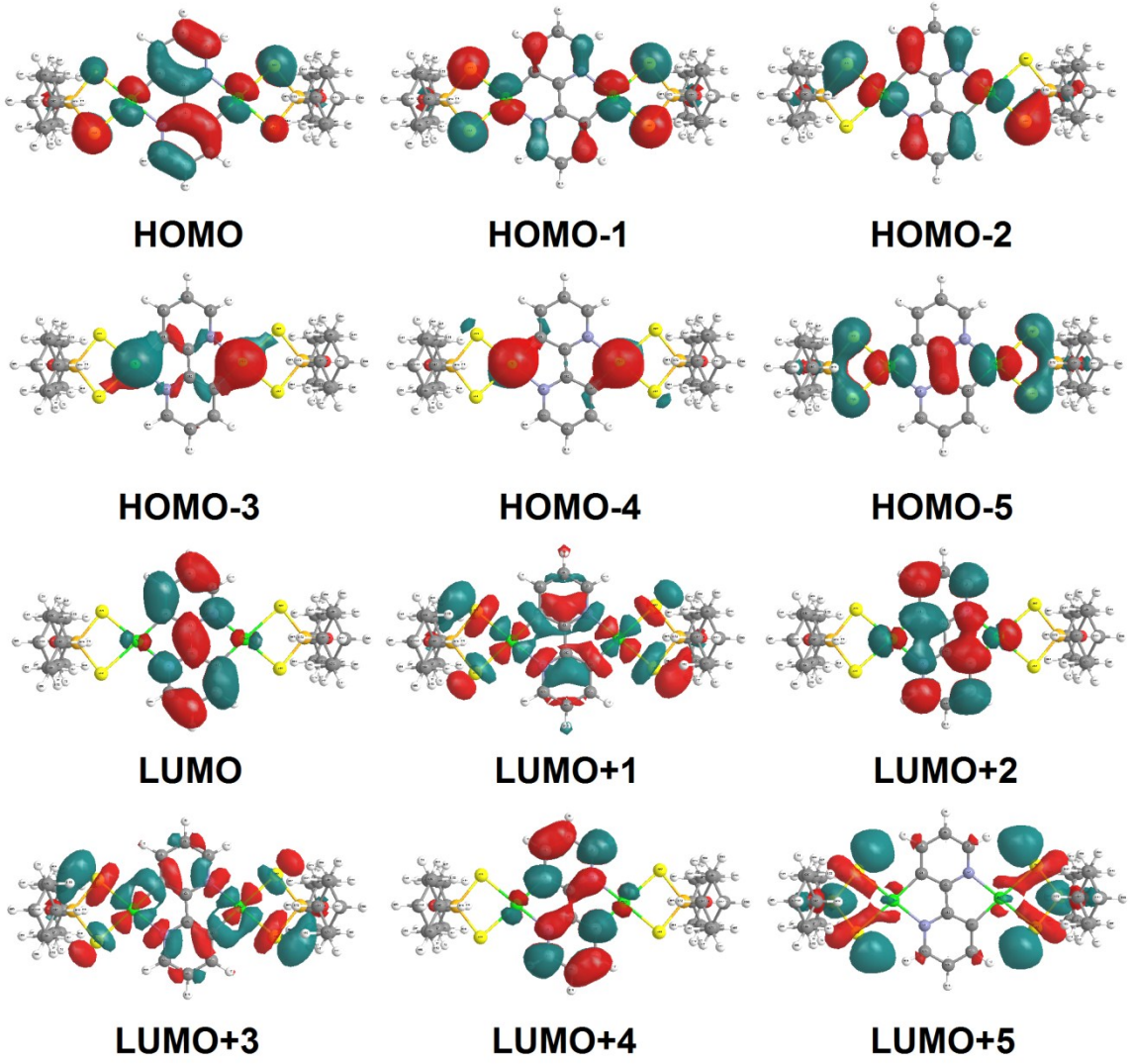

Figure S22. Selected molecular orbital plots of the complex **2b** in CH_2Cl_2 solvent.

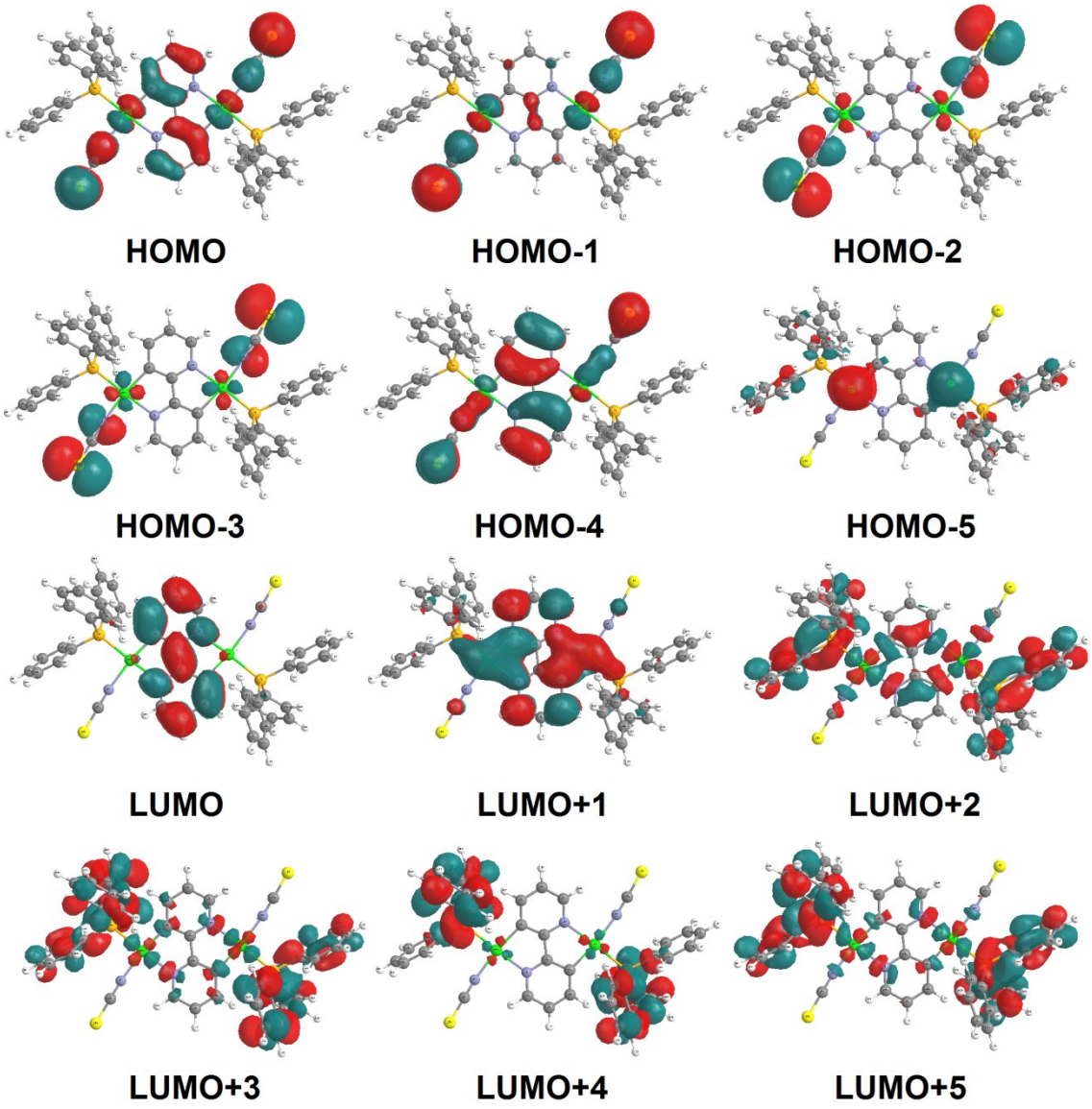

Figure S23. Selected molecular orbital plots of the complex **3a** in CH_2Cl_2 solvent.

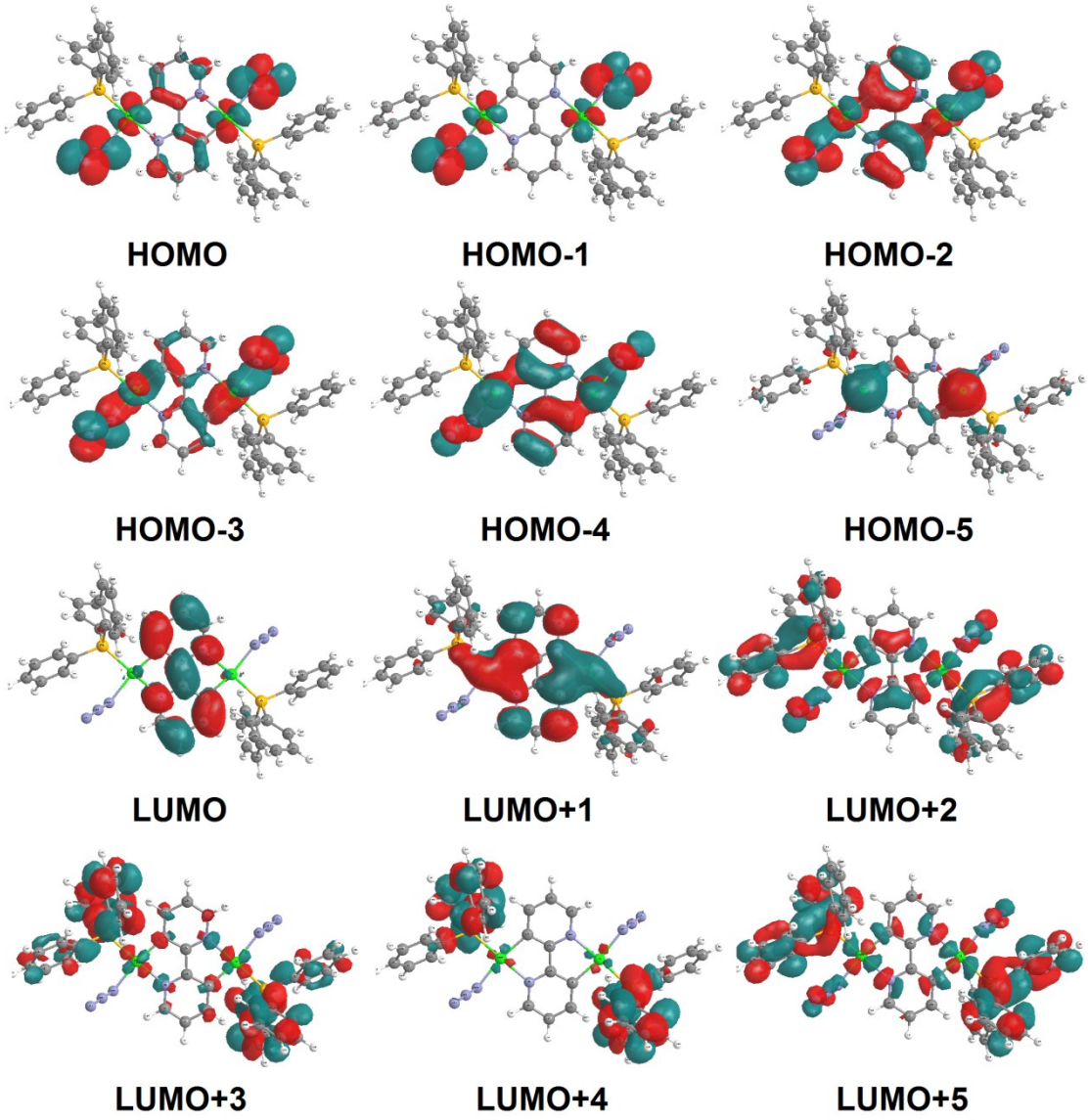

Figure S24. Selected molecular orbital plots of the complex **3b** in CH_2Cl_2 solvent.

Table S10. Wavelengths and nature of transitions for the complex **2a** where M = Pt, L = μ-bpy, L′ = dedtc.

Excited state	Oscillator strength	Calculated λ (nm)	Transitions (Major Contribution)	Assignment
$S_0 \rightarrow S_1$	0.041	413	HOMO→LUMO (95%)	ILCT/MLCT/L′LCT
$S_0 \rightarrow S_3$	0.298	367	H-2→LUMO (96%)	MLCT/L′LCT/ILCT
$S_0 \rightarrow S_{17}$	0.157	305	H-7→LUMO (12%)	L′LCT/ILCT/MLCT
			H-1→L+1 (14%)	IL′CT/MLCT
			H-1→L+4 (12%)	MLCT/ML′CT/IL′CT
			HOMO→L+2 (25%)	ILCT/ML′CT/IL′CT
			HOMO→L+3 (25%)	IL′CT /ILCT/ML′CT
$S_0 \rightarrow S_{18}$	0.063	302	H-7→LUMO (19%)	L′LCT/ILCT/MLCT
			H-6→LUMO (57%)	ILCT/L′LCT
$S_0 \rightarrow S_{20}$	0.030	300	H-4→L+1 (86%)	MLCT/ML′CT
$S_0 \rightarrow S_{23}$	0.461	293	H-3→L+1 (76%)	MLCT/IL′CT
$S_0 \rightarrow S_{25}$	0.145	282	H-2→L+2 (10%)	IL′CT/ML′CT/MLCT
			H-2→L+3 (11%)	IL′CT/ML′CT/MLCT
			H-1→L+4 (42%)	MLCT/ML′CT/IL′CT

Table S11. Wavelengths and nature of transitions for the complex **2b** where M = Pt, L = μ-bpy, L′ = dcdtp.

Excited state	Oscillator strength	Calculated λ (nm)	Transitions (Major Contribution)	Assignment
$S_0 \rightarrow S_1$	0.041	401	HOMO→LUMO (95%)	ILCT/MLCT/L′LCT
$S_0 \rightarrow S_5$	0.209	358	H-2→LUMO (96%)	MLCT/L′LCT/ILCT
$S_0 \rightarrow S_{14}$	0.037	302	H-6→LUMO (12%)	ILCT/L′LCT/MLCT
			H-1→L+2 (83%)	MLCT/L′LCT
$S_0 \rightarrow S_{15}$	0.018	292	H-3→L+2 (92%)	MLCT
$S_0 \rightarrow S_{16}$	0.121	291	H-6→LUMO (80%)	ILCT/L′LCT/MLCT
			H-1→L+2 (11%)	MLCT/L′LCT

Table S12. Wavelengths and nature of transitions for the complex **3a** where M = Pt, L = μ-bpy, L′ = SCN and L″ = PPh_3.

Excited state	Oscillator strength	Calculated λ (nm)	Transitions (Major Contribution)	Assignment
$S_0 \rightarrow S_1$	0.107	404	HOMO→LUMO (96%)	L′LCT/MLCT/ILCT
$S_0 \rightarrow S_9$	0.016	332	H-6→LUMO (83%)	MLCT/L″LCT
$S_0 \rightarrow S_{10}$	0.044	325	H-4→LUMO (70%)	L′LCT/MLCT
			H-1→L+1 (18%)	L′LCT/MLCT/ML″CT
$S_0 \rightarrow S_{11}$	0.238	319	H-4→LUMO (17%)	L′LCT/MLCT
			H-1→L+1 (78%)	L′LCT/MLCT/ML″CT
$S_0 \rightarrow S_{17}$	0.040	304	H-6→L+2 (56%)	ML″CT/MLCT
			H-5→L+5 (13%)	ML″CT
$S_0 \rightarrow S_{23}$	0.090	288	H-12→LUMO (34%)	L″LCT/MLCT/ILCT
			H-10→LUMO (13%)	L″LCT/MLCT
			H-8→LUMO (10%)	L″LCT/MLCT
			HOMO→L+6 (17%)	L′L″CT/L′LCT/MLCT/ML″CT
$S_0 \rightarrow S_{24}$	0.044	286	H-8→LUMO (26%)	L″LCT/MLCT
			H-5→L+1 (34%)	MLCT/ML″CT
			HOMO→L+6 (10%)	L′L″CT/L′LCT/MLCT/ML″CT
$S_0 \rightarrow S_{26}$	0.040	284	H-8→LUMO (37%)	L″LCT/MLCT
			H-5→L+1 (46%)	MLCT/ML″CT
$S_0 \rightarrow S_{28}$	0.197	283	H-12→LUMO (12%)	L″LCT/MLCT/ILCT
			H-3→L+3 (11%)	L′L″CT/L′MCT
			H-2→L+4 (26%)	L′L″CT
			HOMO→L+6 (19%)	L′L″CT/L′LCT/MLCT/ML″CT
$S_0 \rightarrow S_{30}$	0.199	283	H-12→LUMO (10%)	L″LCT/MLCT/ILCT
			H-3→L+3 (14%)	L′L″CT/L′MCT
			H-2→L+4 (25%)	L′L″CT
			HOMO→L+6 (31%)	L′L″CT/L′LCT/MLCT/ML″CT

Table S13. Wavelengths and nature of transitions for the complex **3b** where M = Pt, L = μ-bpy, L′ = N_3 and L″ = PPh_3.

Excited state	Oscillator strength	Calculated λ (nm)	Transitions (Major Contribution)	Assignment
$S_0 \rightarrow S_1$	0.040	417	HOMO→LUMO (97%)	L′LCT/MLCT/ILCT
$S_0 \rightarrow S_3$	0.060	378	H-2→LUMO (95%)	L′LCT/MLCT/ILCT
$S_0 \rightarrow S_4$	0.020	369	H-1→L+5 (15%)	L′L″CT/L′MCT
			HOMO→L+2 (71%)	L′L″CT/L′MCT/L′LCT
$S_0 \rightarrow S_9$	0.033	340	H-6→LUMO (24%)	MLCT/ILCT/L′LCT
			H-4→LUMO (70%)	MLCT/ILCT/L′LCT
$S_0 \rightarrow S_{11}$	0.075	327	H-2→L+2 (68%)	L′L″CT/L′MCT/ILCT
$S_0 \rightarrow S_{12}$	0.046	325	H-6→LUMO (66%)	MLCT/ILCT/L′LCT
			H-4→LUMO (24%)	MLCT/ILCT/L′LCT
$S_0 \rightarrow S_{17}$	0.021	312	H-6→L+2 (21%)	ILCT/MLCT/ML″CT
			H-5→L+5 (14%)	ML″CT
			H-4→L+2 (33%)	ML″CT/LL″CT/L′L″CT
$S_0 \rightarrow S_{20}$	0.032	303	H-3→L+1 (94%)	L′LCT/L′L″CT/MLCT/ILCT
$S_0 \rightarrow S_{27}$	0.135	290	H-10→LUMO (57%)	MLCT/ILCT/L″LCT
			HOMO→L+8 (13%)	L′LCT/L′L″CT/MLCT/ILCT
$S_0 \rightarrow S_{30}$	0.112	286	H-10→LUMO (15%)	MLCT/ILCT/L″LCT
			HOMO→L+8 (51%)	L′LCT/L′L″CT/MLCT/ILCT
$S_0 \rightarrow S_{37}$	0.156	280	H-6→L+2 (15%)	ILCT/MLCT/ML″CT
			H-4→L+2 (14%)	ML″CT/LL″CT/L′L″CT
			H-3→L+5 (17%)	L′L″CT/LL″CT
			HOMO→L+10 (16%)	L′L″CT/ML″CT/ILCT
$S_0 \rightarrow S_{40}$	0.029	277	H-1→L+9 (14%)	L′L″CT/ML″CT
			HOMO→L+10 (31%)	L′L″CT/ML″CT/ILCT

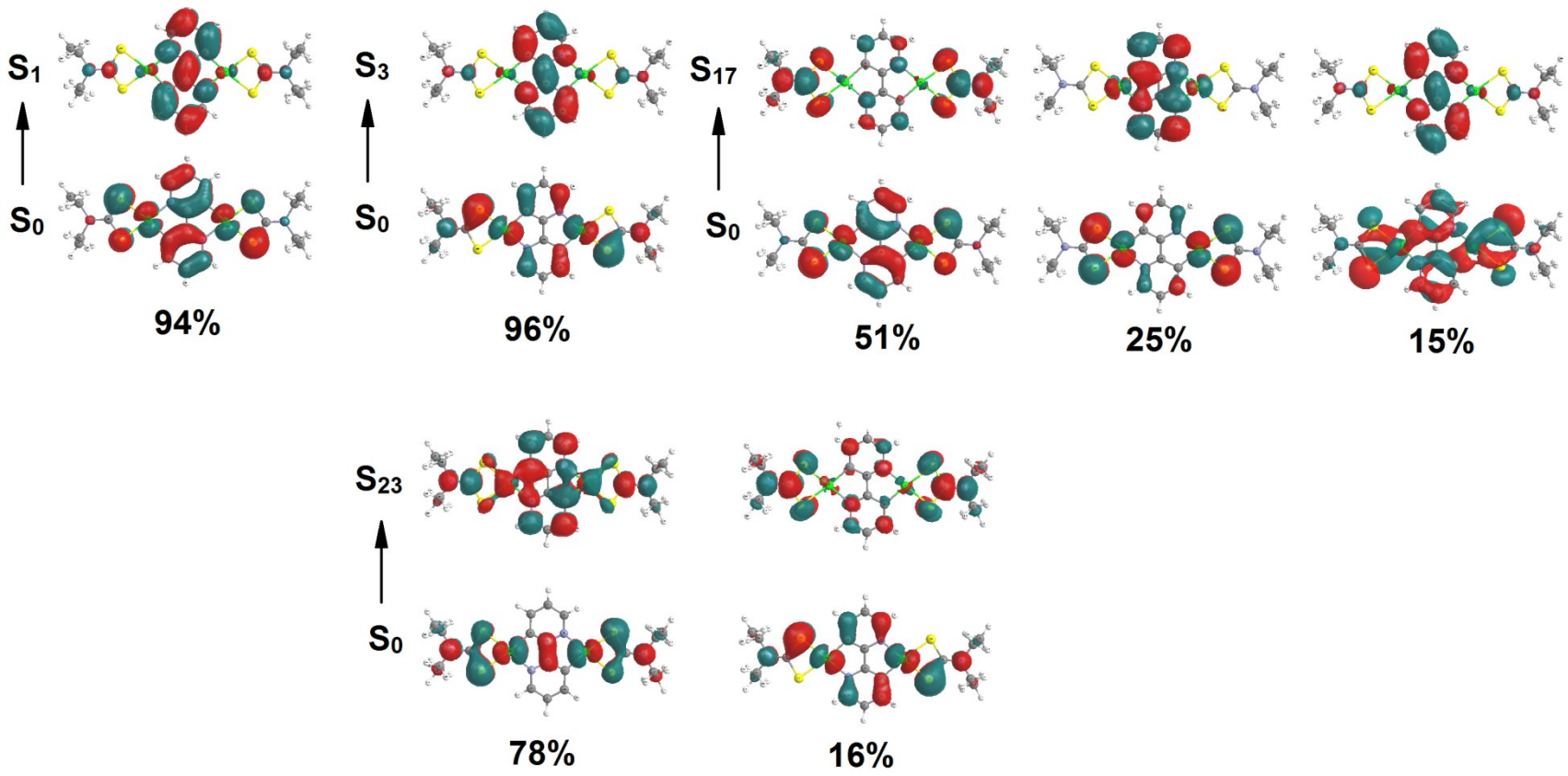

Figure S25. NTO pairs of the various electronic transitions for the complex **2a** in CH_2Cl_2.

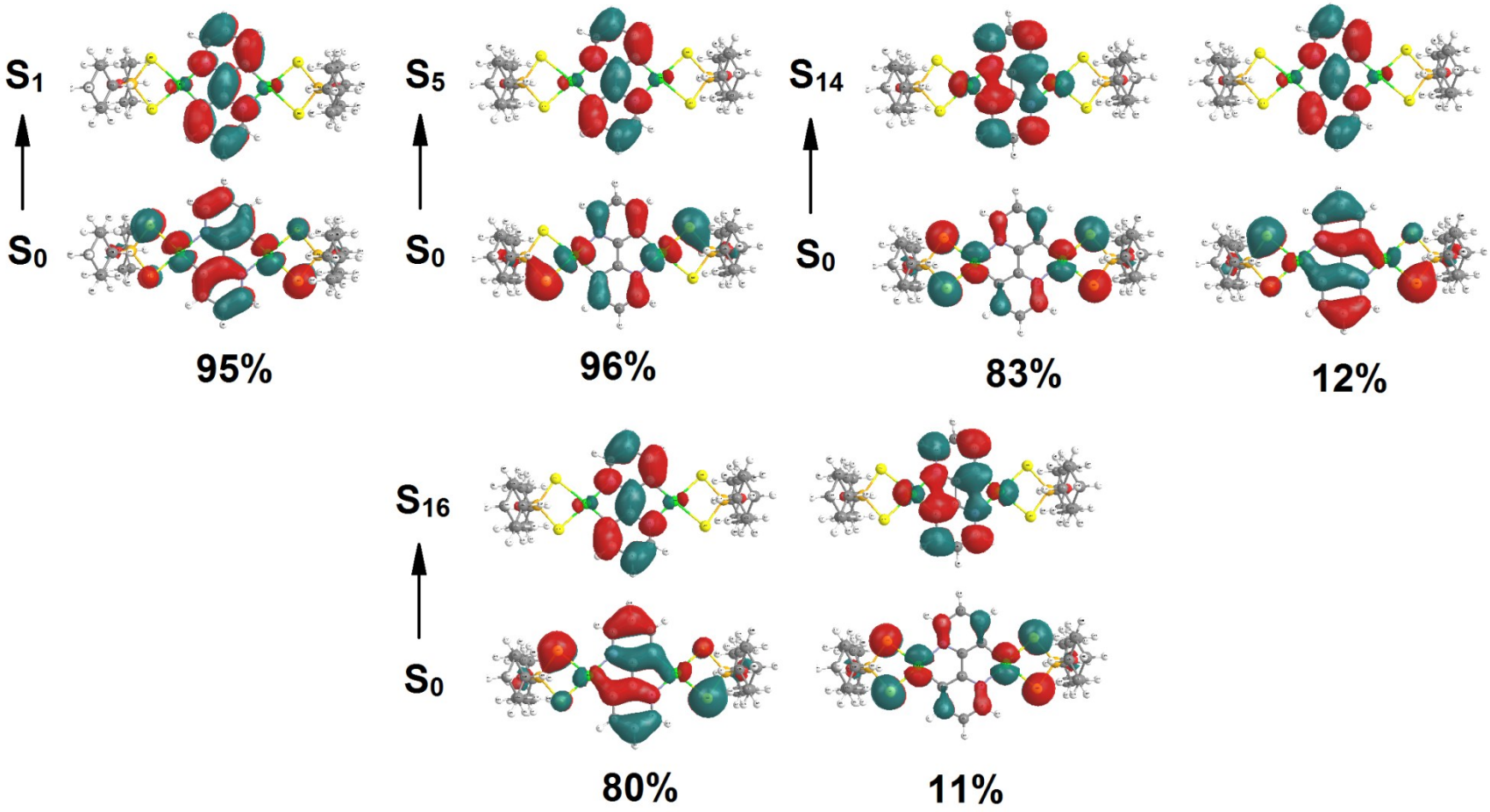

Figure S26. NTO pairs of the various electronic transitions for the complex **2b** in CH_2Cl_2.

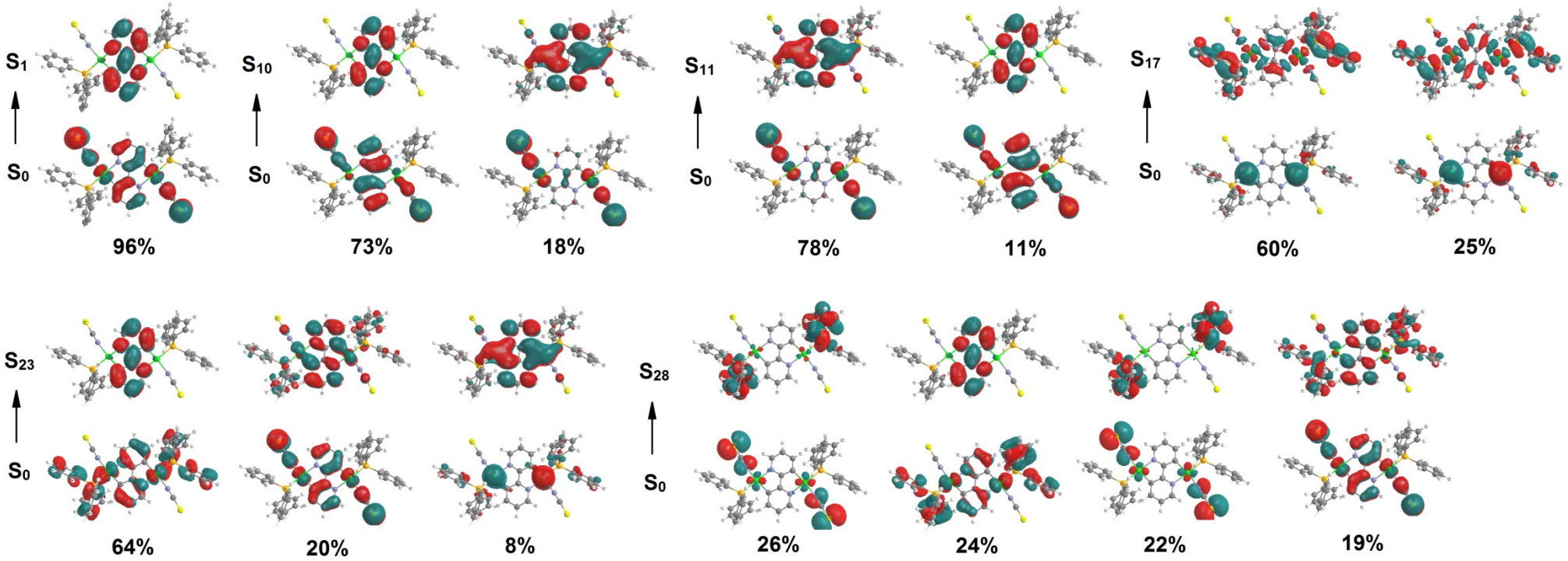

Figure S27. NTO pairs of the various electronic transitions for the complex **3a** in CH_2Cl_2.

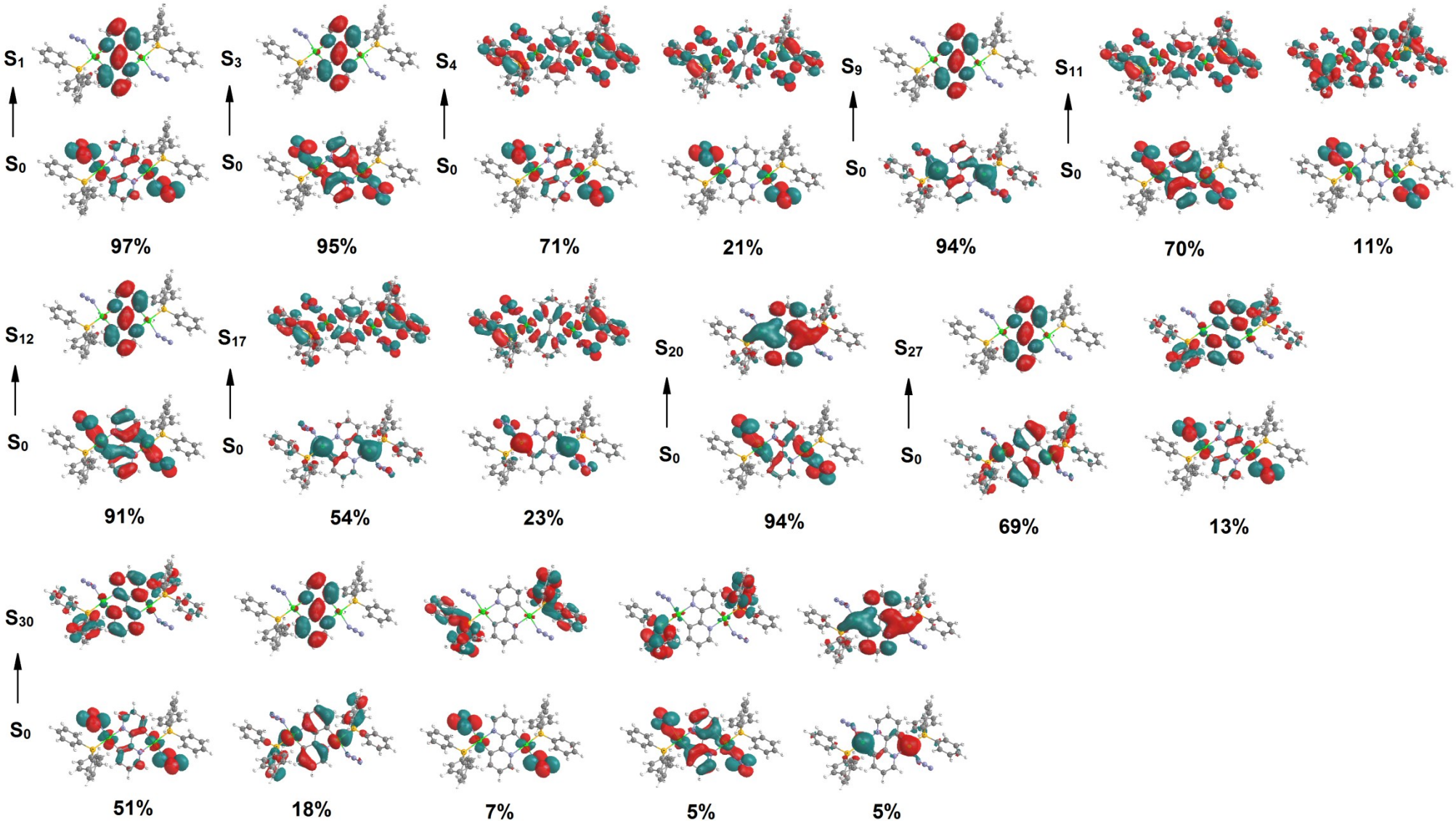

Figure S28. NTO pairs of the various electronic transitions for the complex **3b** in CH_2Cl_2.

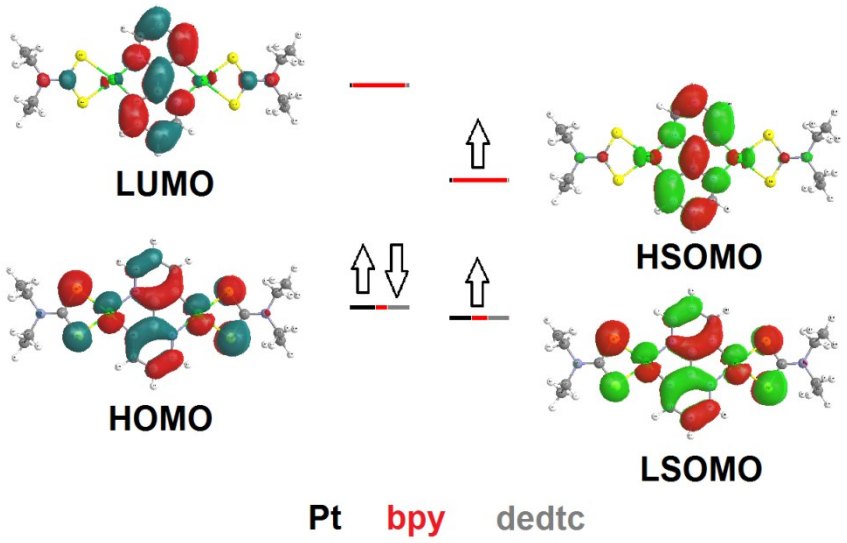

Figure S29. Molecular orbital plots of the calculated S_0 (left) and T_1 (right) states of the complex **2a** (HOMO [Pt 43%, 20 %, dedtc 37%], LUMO [Pt 4%, bpy 88%, dedtc 8%], LSOMO [Pt 38%, bpy 26%, dedtc 36%], HSOMO [Pt 6%, bpy 90%, dedtc 3%]).

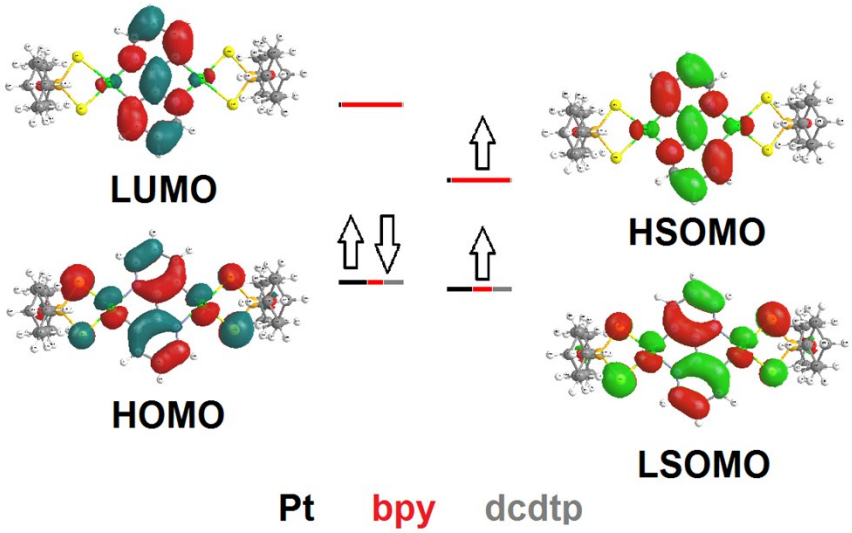

Figure S30. Molecular orbital plots of the calculated S_0 (left) and T_1 (right) states of the complex **2b** (HOMO [Pt 44%, bpy 25%, dcdtp 31%], LUMO [Pt 5%, bpy 93%, dcdtp 2%], LSOMO [Pt 39%, bpy 30%, dcdtp 31%], HSOMO [Pt 7%, bpy 90%, dcdtp 3%]).

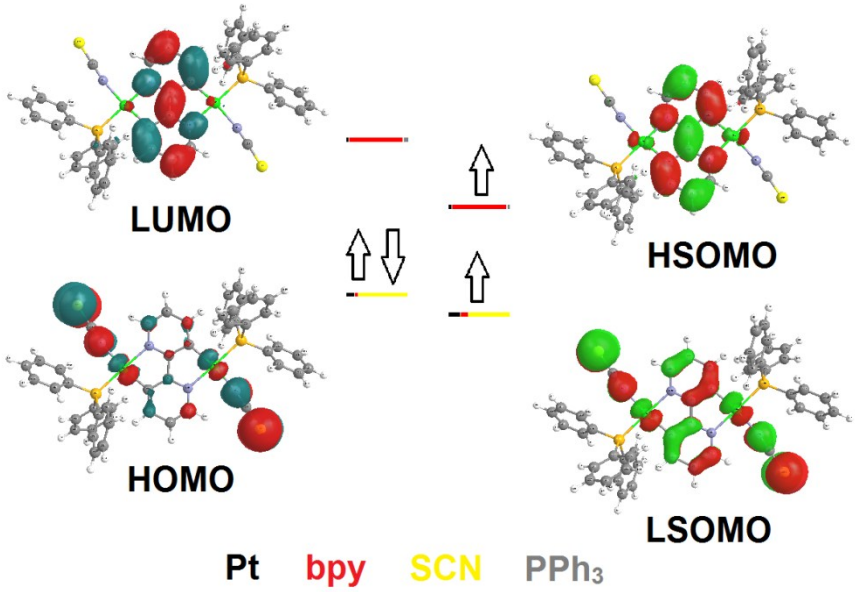

Figure S31. Molecular orbital plots of the calculated S_0 (left) and T_1 (right) states of the complex **3a** (HOMO [Pt 14%, bpy 5%, SCN 80%, PPh_3 1%], LUMO [Pt 4%, bpy 87%, SCN 1%, PPh_3 8%], LSOMO [Pt 20%, bpy 12%, SCN 67%, PPh_3 1%], HSOMO [Pt 5%, bpy 88%, SCN 2%, PPh_3 5%]).

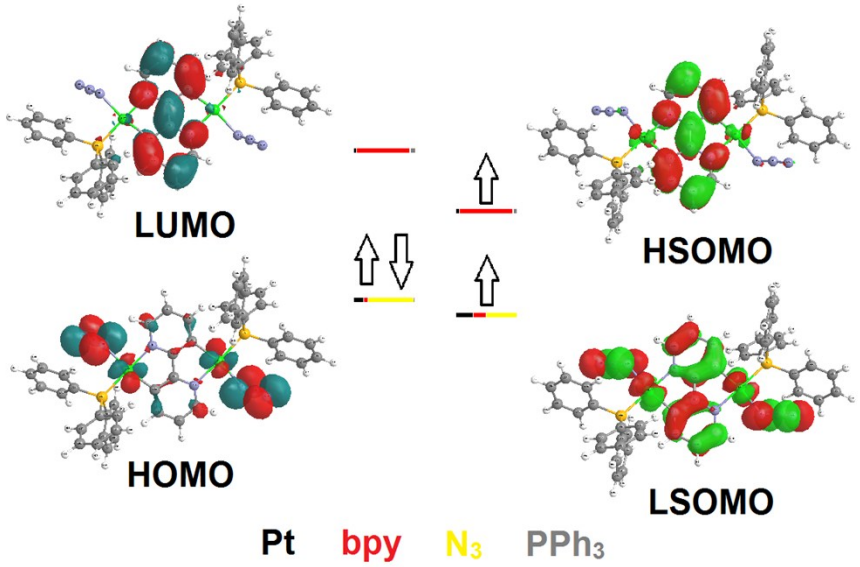

Figure S32. Molecular orbital plots of the calculated S_0 and T_1 states of the complex **3b** (HOMO [Pt 17%, bpy 7%, N_3 73%, PPh_3 3%], LUMO [Pt 5%, bpy 86%, N_3 1%, PPh_3 8%], LSOMO [Pt 28%, bpy 20%, N_3 50%, PPh_3 2%], HSOMO [Pt 6%, bpy 87%, N_3 2%, PPh_3 5%]).

XYZ Cartesian coordinates

Complex **2a**, S_0 in gas phase

Pt	2.11207200	-0.43660400	1.76064500
S	4.36020600	-1.16852800	1.85843900
N	0.12299600	0.23210600	1.76308500
C	4.32676400	-0.91116600	3.58202500
C	-0.63462200	0.64637500	2.79278400
H	-0.16976500	0.64218900	3.77205700
N	5.37839100	-1.15519500	4.37312600
C	5.32370900	-0.91654200	5.82597900
H	4.64779800	-0.07802200	6.00791200
H	6.32682800	-0.60413000	6.13555100
C	6.64887500	-1.67283300	3.83647900
H	6.42416200	-2.30851600	2.97648800
H	7.08385900	-2.31501000	4.60969700
C	7.62397200	-0.55938000	3.44527300
H	8.55800700	-0.99646300	3.07496200
H	7.86553200	0.08037700	4.30137000
H	7.19804100	0.06512300	2.65470400
C	-2.51122700	1.04650800	1.30696300
H	-3.53992500	1.37070500	1.16869900
C	-1.95209400	1.05786400	2.59180600
H	-2.53440700	1.38642100	3.44756700
S	2.80503100	-0.31364800	4.15636000
C	4.87301400	-2.15137400	6.61013300
H	4.87362300	-1.93053800	7.68338700
H	5.54219200	-3.00213000	6.43929600
H	3.85981600	-2.44166300	6.31791900
C	-0.43244700	0.22769300	0.53087500
C	-1.74257200	0.61918600	0.21673000
N	-0.12299600	-0.23210600	-1.76308500
C	0.63462200	-0.64637500	-2.79278400
H	0.16976500	-0.64218900	-3.77205700
C	2.51122700	-1.04650800	-1.30696300
H	3.53992500	-1.37070500	-1.16869900
C	1.95209400	-1.05786400	-2.59180600
H	2.53440700	-1.38642100	-3.44756700
C	0.43244700	-0.22769300	-0.53087500
C	1.74257200	-0.61918600	-0.21673000
Pt	-2.11207200	0.43660400	-1.76064500
S	-4.36020600	1.16852800	-1.85843900
C	-4.32676400	0.91116600	-3.58202500
N	-5.37839100	1.15519500	-4.37312600
C	-5.32370900	0.91654200	-5.82597900
H	-4.64779800	0.07802200	-6.00791200
H	-6.32682800	0.60413000	-6.13555100
C	-6.64887500	1.67283300	-3.83647900
H	-6.42416200	2.30851600	-2.97648800
H	-7.08385900	2.31501000	-4.60969700
C	-7.62397200	0.55938000	-3.44527300
H	-8.55800700	0.99646300	-3.07496200
H	-7.86553200	-0.08037700	-4.30137000
H	-7.19804100	-0.06512300	-2.65470400
S	-2.80503100	0.31364800	-4.15636000
C	-4.87301400	2.15137400	-6.61013300
H	-4.87362300	1.93053800	-7.68338700
H	-5.54219200	3.00213000	-6.43929600
H	-3.85981600	2.44166300	-6.31791900

Complex **2a**, T_1 in gas phase

Pt	2.11868900	-0.43783500	1.75888200
S	4.37366200	-1.17138700	1.85509300
N	0.15006900	0.22647000	1.78989800
C	4.33622500	-0.91338800	3.57616800
C	-0.63302600	0.64223500	2.78141700
H	-0.19487100	0.64906200	3.77503300
N	5.38471900	-1.15677100	4.37175600
C	5.32680600	-0.91673100	5.82440800
H	4.65139500	-0.07754700	6.00478700
H	6.32947700	-0.60451900	6.13552100
C	6.65603900	-1.67652400	3.83884600
H	6.43243100	-2.31586100	2.98118800
H	7.08984600	-2.31542100	4.61534600
C	7.63148500	-0.56452800	3.44442700
H	8.56571300	-1.00318100	3.07657900
H	7.87232700	0.07815500	4.29850700
H	7.20682900	0.05736300	2.65112500
C	-2.53090700	1.04497900	1.27367900
H	-3.55943300	1.36922100	1.13935500
C	-1.96125800	1.05465200	2.57154800
H	-2.54058200	1.38108800	3.42916000
S	2.81064000	-0.31400400	4.14868000
C	4.87420500	-2.15056600	6.60897600
H	4.87350800	-1.92862800	7.68198100
H	5.54307500	-3.00188100	6.43992900
H	3.86121700	-2.44090000	6.31599000
C	-0.40958800	0.21534600	0.50486700
C	-1.76637300	0.62245300	0.19863700
N	-0.15006900	-0.22647000	-1.78989800
C	0.63302600	-0.64223500	-2.78141700
H	0.19487100	-0.64906200	-3.77503300
C	2.53090700	-1.04497900	-1.27367900
H	3.55943300	-1.36922100	-1.13935500
C	1.96125800	-1.05465200	-2.57154800
H	2.54058200	-1.38108800	-3.42916000
C	0.40958800	-0.21534600	-0.50486700
C	1.76637300	-0.62245300	-0.19863700
Pt	-2.11868900	0.43783500	-1.75888200
S	-4.37366200	1.17138700	-1.85509300
C	-4.33622500	0.91338800	-3.57616800
N	-5.38471900	1.15677100	-4.37175600
C	-5.32680600	0.91673100	-5.82440800
H	-4.65139500	0.07754700	-6.00478700
H	-6.32947700	0.60451900	-6.13552100
C	-6.65603900	1.67652400	-3.83884600
H	-6.43243100	2.31586100	-2.98118800
H	-7.08984600	2.31542100	-4.61534600
C	-7.63148500	0.56452800	-3.44442700
H	-8.56571300	1.00318100	-3.07657900
H	-7.87232700	-0.07815500	-4.29850700
H	-7.20682900	-0.05736300	-2.65112500
S	-2.81064000	0.31400400	-4.14868000
C	-4.87420500	2.15056600	-6.60897600
H	-4.87350800	1.92862800	-7.68198100
H	-5.54307500	3.00188100	-6.43992900
H	-3.86121700	2.44090000	-6.31599000

Complex **2a**, S_0 in CH_2Cl_2

Pt	2.11985900	-0.41672800	1.76375000
S	4.37641000	-1.13164500	1.85620600
N	0.11994400	0.23934000	1.76379700
C	4.34756700	-0.89328700	3.59115900
C	-0.63946800	0.65664800	2.79213900
H	-0.17780000	0.66123200	3.77268600
N	5.38729100	-1.14853700	4.37712900
C	5.33709700	-0.91726500	5.83633000
H	4.66417700	-0.07867500	6.02537500
H	6.34148600	-0.60815200	6.13943900
C	6.65949800	-1.67993600	3.84367800
H	6.43313900	-2.30489700	2.97699000
H	7.07503200	-2.33339800	4.61589700
C	7.65206300	-0.57507100	3.47710800
H	8.58072700	-1.02749000	3.11359000
H	7.89483700	0.04805600	4.34415100
H	7.24915900	0.06683200	2.68802400
C	-2.51786000	1.04042600	1.30465500
H	-3.54806400	1.36027100	1.16824900
C	-1.95884600	1.06256500	2.58944700
H	-2.54150500	1.39466300	3.44279200
S	2.81358300	-0.29292400	4.15825300
C	4.89300400	-2.15847200	6.61243900
H	4.90064700	-1.93812200	7.68515500
H	5.56559000	-3.00431700	6.43530000
H	3.87867500	-2.45334400	6.32773900
C	-0.43438200	0.22669300	0.53013300
C	-1.74718600	0.60944700	0.21587900
N	-0.11994400	-0.23934000	-1.76379700
C	0.63946800	-0.65664800	-2.79213900
H	0.17780000	-0.66123200	-3.77268600
C	2.51786000	-1.04042600	-1.30465500
H	3.54806400	-1.36027100	-1.16824900
C	1.95884600	-1.06256500	-2.58944700
H	2.54150500	-1.39466300	-3.44279200
C	0.43438200	-0.22669300	-0.53013300
C	1.74718600	-0.60944700	-0.21587900
Pt	-2.11985900	0.41672800	-1.76375000
S	-4.37641000	1.13164500	-1.85620600
C	-4.34756700	0.89328700	-3.59115900
N	-5.38729100	1.14853700	-4.37712900
C	-5.33709700	0.91726500	-5.83633000
H	-4.66417700	0.07867500	-6.02537500
H	-6.34148600	0.60815200	-6.13943900
C	-6.65949800	1.67993600	-3.84367800
H	-6.43313900	2.30489700	-2.97699000
H	-7.07503200	2.33339800	-4.61589700
C	-7.65206300	0.57507100	-3.47710800
H	-8.58072700	1.02749000	-3.11359000
H	-7.89483700	-0.04805600	-4.34415100
H	-7.24915900	-0.06683200	-2.68802400
S	-2.81358300	0.29292400	-4.15825300
C	-4.89300400	2.15847200	-6.61243900
H	-4.90064700	1.93812200	-7.68515500
H	-5.56559000	3.00431700	-6.43530000
H	-3.87867500	2.45334400	-6.32773900

Complex **2b**, S_0 in gas phase

Pt	2.77796800	0.00008500	0.00180400
N	-1.17395600	0.00058800	1.34187000
C	0.02693900	0.00034800	0.72014300
C	1.27986300	0.00061900	1.35134700
C	1.24087800	0.00118000	2.75134100
C	0.00526500	0.00143600	3.41143900
C	-1.18584500	0.00113400	2.68601900
H	2.15852300	0.00140500	3.33397100
H	-0.04330900	0.00188700	4.49622500
H	-2.15740600	0.00132500	3.16593900
N	1.17392900	-0.00052200	-1.34181500
C	-0.02696800	-0.00025300	-0.72009200
C	-1.27988700	-0.00051300	-1.35130500
C	-1.24089300	-0.00112000	-2.75129900
C	-0.00527800	-0.00142100	-3.41139200
C	1.18582800	-0.00110900	-2.68596400
H	-2.15853800	-0.00133900	-3.33393100
H	0.04330300	-0.00191200	-4.49617800
H	2.15739400	-0.00132200	-3.16587400
Pt	-2.77799500	0.00009600	-0.00176500
S	4.57742800	0.00067900	1.57162600
P	5.88322100	0.00013100	-0.01183600
S	4.68196100	-0.00038900	-1.64743200
O	6.95387200	1.19399700	0.03977500
O	6.95378800	-1.19378900	0.04070800
C	6.53739300	-2.59925100	0.01536500
C	7.10411200	-3.24092500	-1.24912600
C	7.05326500	-3.26634800	1.28833000
H	5.44168400	-2.64199700	-0.00653000
C	6.80815000	-4.75095000	-1.26954200
H	8.18908200	-3.07001400	-1.26654400
H	6.68202700	-2.74578600	-2.13072200
C	6.75736100	-4.77635300	1.26654900
H	8.13654100	-3.09614700	1.35310800
H	6.59589900	-2.78955900	2.16258600
C	7.32164900	-5.44387600	0.00247300
H	7.25879200	-5.20172600	-2.16200400
H	5.72308500	-4.90772700	-1.35617400
H	7.17204200	-5.24509700	2.16715400
H	5.66975500	-4.93425200	1.30648800
H	7.05742200	-6.50862500	-0.01334800
H	8.42010200	-5.39252600	0.02499800
C	6.53756100	2.59949000	0.01474400
C	7.05331400	3.26633900	1.28789000
C	7.10447800	3.24135500	-1.24956200
H	5.44185800	2.64230500	-0.00729800
C	6.75749200	4.77636500	1.26632800
H	8.13657300	3.09606600	1.35276800
H	6.59581200	2.78943900	2.16201300
C	6.80859500	4.75139700	-1.26975900
H	8.18944300	3.07039700	-1.26687400
H	6.68249200	2.74638800	-2.13130300
C	7.32197200	5.44407700	0.00243900
H	7.17208400	5.24493100	2.16706700
H	5.66988900	4.93431200	1.30616000
H	7.25937300	5.20230100	-2.16208800
H	5.72354800	4.90824700	-1.35650000
H	7.05780700	6.50884400	-0.01323100
H	8.42041900	5.39266200	0.02509000
S	-4.57747600	-0.00054300	-1.57152900
P	-5.88323900	-0.00008000	0.01196700

S	-4.68192100	0.00099500	1.64753700	N	1.21080600	-0.00021600	1.34605700	H	-8.42654700	5.39291500	0.01540000
O	-6.95354600	-1.19427000	-0.03939800	C	-0.02512700	-0.00010900	0.68352000	C	-6.54299300	-2.60043500	0.00897000
O	-6.95414300	1.19351900	-0.04071800	C	-1.31205300	-0.00023100	1.35261000	C	-7.07027600	-3.26107300	1.28052900
C	-6.53681300	-2.59964000	-0.01441900	C	-1.27804600	-0.00046600	2.73707400	C	-7.09870800	-3.24764400	-1.25747500
C	-6.53812200	2.59910100	-0.01581000	C	-0.02606400	-0.00057200	3.40099700	H	-5.44713800	-2.64326700	-0.00279900
C	-7.10378900	-3.24174700	1.24973700	C	1.17940200	-0.00044200	2.67559500	C	-6.77459900	-4.77127100	1.26845900
C	-7.05211300	-3.26657300	-1.28770500	H	-2.19285500	-0.00057000	3.32284200	H	-8.15400900	-3.09021800	1.33485300
H	-5.44110300	-2.64212700	0.00784800	H	0.02618800	-0.00075500	4.48482100	H	-6.62040000	-2.78031400	2.15648000
C	-7.05493900	3.26584900	-1.28857400	H	2.13813200	-0.00052100	3.18483900	C	-6.80286800	-4.75783100	-1.26807300
C	-7.10425400	3.24082600	1.24891700	N	-1.21080600	0.00023200	-1.34605500	H	-8.18342400	-3.07662600	-1.28518100
H	-5.44241100	2.64215200	0.00540200	C	0.02512700	0.00012800	-0.68351700	H	-6.66898600	-2.75691300	-2.13788400
C	-6.80744300	-4.75169800	1.26991400	C	1.31205400	0.00025100	-1.35260700	C	-7.32784100	-5.44458800	0.00259300
H	-8.18881000	-3.07112600	1.26684000	C	1.27804600	0.00048400	-2.73707100	H	-7.19749400	-5.23545300	2.16756600
H	-6.68213500	-2.74669700	2.13159100	C	0.02606500	0.00058700	-3.40099400	H	-5.68747200	-4.92925800	1.31897400
C	-6.75582900	-4.77650900	-1.26616600	C	-1.17940200	0.00045800	-2.67559200	H	-7.24572400	-5.21255800	-2.16239300
H	-8.13541200	-3.09663200	-1.35278200	H	2.19285600	0.00058800	-3.32284000	H	-5.71713400	-4.91522800	-1.34439700
H	-6.59458600	-2.78948400	-2.16171100	H	-0.02618700	0.00076900	-4.48481800	H	-7.06365800	-6.50940100	-0.00590100
C	-6.75943300	4.77593800	-1.26721600	H	-2.13813200	0.00053800	-3.18483600	H	-8.42643400	-5.39298400	0.01508400
H	-8.13820700	3.09533800	-1.35268000	Pt	2.78360100	0.00002700	-0.00586300	S	4.59732500	0.00016500	-1.57552000
H	-6.59796500	2.78904100	-2.16302500	S	-4.59732400	-0.00019200	1.57552300	P	5.88981600	-0.00000600	0.01560400
C	-6.80868000	4.75093100	1.26891100	P	-5.88981600	-0.00000500	-0.01560100	S	4.67724900	-0.00016900	1.64743100
H	-8.18916900	3.06963200	1.26700600	S	-4.67724900	0.00020400	-1.64742800	O	6.95943200	1.19415400	-0.02341700
H	-6.68151200	2.74593700	2.13033700	O	-6.95941800	-1.19417700	0.02340000	O	6.95942000	-1.19416600	-0.02369500
C	-7.32035000	-5.44446800	-0.00242500	O	-6.95943400	1.19414200	0.02372100	C	6.54302200	2.60041700	-0.00904000
H	-7.25825900	-5.20279000	2.16212900	C	-6.54304200	2.60041000	0.00930700	C	6.54301300	-2.60042800	-0.00923800
H	-5.72236500	-4.90821500	1.35686100	C	-7.09871900	3.24763300	-1.25714900	C	7.09874100	3.24766500	1.25738400
H	-7.17009900	-5.24515500	-2.16701200	C	-7.07039400	3.26100900	1.28085600	C	7.07031500	3.26100400	-1.28062100
H	-5.66816900	-4.93411800	-1.30579400	H	-5.44718700	2.64326600	-0.00241100	H	5.44716700	2.64326000	0.00272600
C	-7.32313200	5.44351500	-0.00290600	C	-6.80291200	4.75782700	-1.26770200	C	7.07035000	-3.26107000	-1.28077200
H	-7.17478600	5.24442400	-2.16764600	H	-8.18342900	3.07658900	-1.28490200	C	7.09869000	-3.24762100	1.25723300
H	-5.67189400	4.93412400	-1.30783900	H	-6.66894800	2.75693100	-2.13755000	H	5.44715700	-2.64327200	0.00248800
H	-7.25890400	5.20173200	2.16157100	C	-6.77475100	4.77121400	1.26883200	C	6.80291600	4.75785500	1.26792800
H	-5.72360400	4.90801200	1.35486400	H	-8.15412600	3.09012900	1.33513200	H	8.18345400	3.07663600	1.28509900
H	-7.05585400	-6.50915200	0.01323800	H	-6.62054600	2.78024000	2.15681700	H	6.66901100	2.75696900	2.13780900
H	-8.41881000	-5.39339600	-0.02529100	C	-7.32795400	5.44454500	0.00295600	C	6.77465400	4.77120600	-1.26860500
H	-7.05917700	6.50833600	0.01258000	H	-7.24574100	5.21256200	-2.16203100	H	8.15404600	3.09013500	-1.33493700
H	-8.42158500	5.39187100	-0.02475600	H	-5.71717900	4.91524900	-1.34397700	H	6.62043600	2.78022000	-2.15655600
				H	-7.19769400	5.23536700	2.16793000	C	6.77469100	-4.77127100	-1.26870200
Complex **2b**, T_1 in gas phase				H	-5.68763000	4.92922400	1.31939500	H	8.15408300	-3.09020300	-1.33505900
Pt	-2.78360000	-0.00000400	0.00586600	H	-7.06379500	6.50936400	-0.00550400	H	6.62050200	-2.78032100	-2.15674300

C	6.80286600	-4.75781100	1.26783100
H	8.18340200	-3.07658900	1.28497500
H	6.66892900	-2.75688900	2.13762300
C	7.32790000	5.44456100	-0.00276100
H	7.24577500	5.21260900	2.16223300
H	5.71718400	4.91526600	1.34424300
H	7.19755500	5.23535200	-2.16772700
H	5.68752900	4.92920200	-1.31912700
C	7.32789400	-5.44457200	-0.00281000
H	7.19762300	-5.23545500	-2.16779000
H	5.68756700	-4.92927100	-1.31925400
H	7.24569600	-5.21252600	2.16217100
H	5.71713200	-4.91522000	1.34411700
H	7.06372800	6.50937700	0.00569500
H	8.42649200	5.39294500	-0.01524800
H	7.06372300	-6.50938800	0.00568200
H	8.42648700	-5.39295500	-0.01526200

Complex **2b**, S_0 in CH_2Cl_2

Pt	2.78053200	-0.00030400	-0.01143600
N	-1.16621500	-0.00029200	1.34954000
C	0.03115700	-0.00028100	0.71988600
C	1.28697100	-0.00028300	1.34520400
C	1.25598800	-0.00029300	2.74622600
C	0.02435400	-0.00030000	3.41377800
C	-1.17085900	-0.00030000	2.69454900
H	2.17448200	-0.00029500	3.32720800
H	-0.01812100	-0.00030500	4.49816100
H	-2.13748700	-0.00030200	3.18368100
N	1.16621800	-0.00023400	-1.34956200
C	-0.03115300	-0.00025300	-0.71990700
C	-1.28696700	-0.00023600	-1.34522500
C	-1.25598600	-0.00018300	-2.74624700
C	-0.02435200	-0.00015400	-3.41379900
C	1.17086100	-0.00018400	-2.69457100
H	-2.17448100	-0.00015900	-3.32722700
H	0.01812100	-0.00011300	-4.49818200
H	2.13748900	-0.00016800	-3.18370400
Pt	-2.78052700	-0.00029900	0.01141500
S	4.59058000	-0.00037700	1.55405600
P	5.89903600	0.00010100	-0.03171100
S	4.68594000	-0.00034700	-1.66348700
O	6.96726800	1.19292500	0.01655100
O	6.96822500	-1.19186300	0.01653000
C	6.56861700	-2.60968000	0.00619900
C	7.15967200	-3.25780000	-1.24279000
C	7.07859000	-3.25209200	1.29340400
H	5.47410800	-2.66199700	-0.02862900
C	6.88141900	-4.77171100	-1.24780400
H	8.24288600	-3.07644500	-1.24767100
H	6.74402000	-2.78047200	-2.13741900
C	6.80020200	-4.76596400	1.28752000
H	8.15929500	-3.07063700	1.36673800
H	6.60679200	-2.77128200	2.15790200
C	7.38772100	-5.44198800	0.03891800
H	7.35057700	-5.22535500	-2.12879500
H	5.79971900	-4.94238000	-1.34627300
H	7.21187100	-5.21552000	2.19883100
H	5.71436100	-4.93612200	1.31738700
H	7.13406100	-6.50915800	0.03325100
H	8.48486000	-5.37764900	0.07398400
C	6.56656800	2.61044300	0.00655200
C	7.07646100	3.25303100	1.29370000
C	7.15674400	3.25921100	-1.24251900
H	5.47200800	2.66193800	-0.02790800
C	6.79693000	4.76669300	1.28814700
H	8.15732500	3.07238300	1.36666600
H	6.60529700	2.77172400	2.15826700
C	6.87736200	4.77291600	-1.24719800
H	8.24009100	3.07866800	-1.24776900
H	6.74117000	2.78172900	-2.13710100
C	7.38356400	5.44335800	0.03947600
H	7.20853500	5.21641100	2.19940700
H	5.71096900	4.93602700	1.31836800
H	7.34590800	5.22705500	-2.12826000
H	5.79550500	4.94279400	-1.34530200
H	7.12911500	6.51034100	0.03406200
H	8.48076100	5.37982100	0.07419600
S	-4.59058000	-0.00031400	-1.55407400
P	-5.89902500	-0.00002000	0.03170100
S	-4.68593400	-0.00031000	1.66347600
O	-6.96804000	-1.19213500	-0.01663900
O	-6.96743500	1.19265200	-0.01645900
C	-6.56825500	-2.60991200	-0.00638000
C	-6.56692800	2.61021500	-0.00627900
C	-7.15875300	-3.25808000	1.24284800
C	-7.07865100	-3.25239700	-1.29337800
H	-5.47372600	-2.66209800	0.02800200
C	-7.07615000	3.25277000	-1.29371000
C	-7.15792000	3.25887800	1.24246100
H	-5.47239600	2.66185000	0.02885500
C	-6.88033600	-4.77196300	1.24777100
H	-8.24198500	-3.07684400	1.24814500
H	-6.74280900	-2.78070600	2.13731600
C	-6.80009100	-4.76623800	-1.28758100
H	-8.15940400	-3.07106700	-1.36630100
H	-6.60723900	-2.77154100	-2.15806000
C	-6.79681700	4.76646900	-1.28795200
H	-8.15694900	3.07198600	-1.36730700
H	-6.60442300	2.77155200	-2.15801800
C	-6.87873400	4.77261600	1.24734700
H	-8.24124700	3.07819300	1.24707400
H	-6.74280500	2.78141300	2.13726700
C	-7.38706100	-5.44230900	-0.03874600
H	-7.34910500	-5.22564700	2.12894900
H	-5.79858000	-4.94251300	1.34582600
H	-7.21205500	-5.21585100	-2.19873000
H	-5.71424200	-4.93627500	-1.31785600
C	-7.38426600	5.44302800	-0.03960700
H	-7.20794800	5.21615800	-2.19944000
H	-5.71086100	4.93594600	-1.31753500
H	-7.34785400	5.22667200	2.12814600
H	-5.79695600	4.94263000	1.34608900
H	-7.13328900	-6.50945300	-0.03316400
H	-8.48422000	-5.37808300	-0.07339400
H	-7.12995300	6.51004300	-0.03401600
H	-8.48143500	5.37935700	-0.07497100

Complex **3a**, S_0 in gas phase

Pt	-2.74559400	0.60973900	-0.03351500

P	-4.77563100	-0.49725600	0.00371600
S	-4.56476600	5.11764000	-0.03270400
C	-8.47010400	2.15483700	-0.91970400
H	-9.32601000	2.79010800	-1.13023100
C	-5.79883300	-2.34367400	4.14401400
H	-6.03661500	-2.77418500	5.11291300
N	0.83758400	-1.56613100	0.08493500
C	-0.73798700	-3.33465800	0.18956700
H	-0.92537900	-4.40202900	0.25272300
C	-4.19725400	-1.67606500	-2.45851800
H	-3.65178400	-0.75436600	-2.64168300
C	-7.70728500	2.36907400	0.23170300
H	-7.95872000	3.17538700	0.91375100
C	-4.18026700	-1.41377500	2.60357300
H	-3.16261000	-1.11049100	2.38157100
N	-3.67745700	2.45244200	-0.10577800
C	-4.05305600	3.57606200	-0.07681800
C	-4.83888300	-1.86882700	-1.22358100
C	-5.51751000	-3.07309500	-0.98560700
H	-6.00935100	-3.24524400	-0.03377600
C	-1.79939400	-2.42500600	0.13538900
H	-2.81105100	-2.81530700	0.15413300
C	-0.19443700	-0.69631200	0.03654600
C	-4.24496600	-2.66622100	-3.43981100
H	-3.74486500	-2.50550200	-4.39070300
C	-5.18587400	-1.22594900	1.64342900
C	-6.24948500	0.53076700	-0.38530000
C	-5.55379900	-4.06590600	-1.96721100
H	-6.07568300	-4.99804600	-1.76886800
C	0.57769800	-2.88082800	0.16006200
H	1.43153500	-3.54491600	0.19598100
C	-4.48724800	-1.97231200	3.84601200
H	-3.70007900	-2.10814600	4.58228800
C	-4.92113500	-3.86384500	-3.19489100
H	-4.94951100	-4.63860100	-3.95611100
C	-6.80915200	-2.14827400	3.19893600
H	-7.83461700	-2.42242600	3.43080400
C	-7.01771700	0.32051800	-1.53839700
H	-6.75955700	-0.47086700	-2.23361800
C	-6.60406700	1.56262200	0.49968100
H	-6.00951700	1.74873900	1.38792000
C	-1.56077000	-1.04344600	0.05216200
C	-6.50789600	-1.58761900	1.95798300
H	-7.30405700	-1.41505400	1.23999700
C	-8.12503400	1.13134300	-1.80111500
H	-8.71287400	0.96022300	-2.69879200
N	-0.83754700	1.56610600	-0.08410400
C	0.73800700	3.33466700	-0.18839800
H	0.92539200	4.40205300	-0.25133300
C	1.79942200	2.42501300	-0.13438100
H	2.81107500	2.81532900	-0.15302200
C	0.19448000	0.69628900	-0.03583200
C	-0.57767400	2.88081900	-0.15902000
H	-1.43152400	3.54489400	-0.19486700
C	1.56080900	1.04343700	-0.05143400
Pt	2.74563600	-0.60976400	0.03398000
P	4.77562500	0.49726600	-0.00390800
S	4.56428600	-5.11782800	0.03258200
C	8.47084900	-2.15476100	0.91667400
H	9.32695500	-2.78999200	1.12651100
C	5.79714700	2.34481100	-4.14412800
H	6.03455500	2.77556600	-5.11301000
C	4.19840900	1.67514400	2.45901500
H	3.65320800	0.75328200	2.64216000
C	7.70704100	-2.36911100	-0.23405800
H	7.95791100	-3.17547000	-0.91625900
C	4.17922200	1.41429400	-2.60338600
H	3.16168700	1.11078600	-2.38113900
N	3.67752100	-2.45246300	0.10613500
C	4.05287700	-3.57615800	0.07696200
C	4.83934800	1.86844200	1.22380300
C	5.51762100	3.07291800	0.98587500
H	6.00892700	3.24547900	0.03384300
C	4.24645700	2.66497700	3.44061700
H	3.74689200	2.50384200	4.39172000
C	5.18515000	1.22646600	-1.64358400
C	6.24972600	-0.53079700	0.38406200
C	5.55424700	4.06540500	1.96779600
H	6.07585000	4.99770900	1.76949100
C	4.48572500	1.97313800	-3.84580700
H	3.69830600	2.10897200	-4.58181700
C	4.92227200	3.86281100	3.19574300
H	4.95090900	4.63731500	3.95721000
C	6.80778900	2.14940700	-3.19939400
H	7.83313300	2.42379600	-3.43151600
C	7.01895100	-0.32042900	1.53647300
H	6.76136000	0.47099800	2.23186000
C	6.60357200	-1.56270800	-0.50114800
H	6.00825500	-1.74890800	-1.38885500
C	6.50701300	1.58843600	-1.95847000
H	7.30342800	1.41585300	-1.24076800
C	8.12651800	-1.13120400	1.79829900
H	8.71512800	-0.95999900	2.69545500

Complex **3a**, T_1 in gas phase

Pt	2.74649200	-0.60961300	-0.02519100
P	4.78906400	0.50402800	0.00535400
S	4.58869900	-5.11303900	-0.04977500
C	8.44963500	-2.22371300	-0.84425000
H	9.29727500	-2.87555800	-1.03674400
C	5.83451600	2.42239700	4.10917400
H	6.07732700	2.86984300	5.06916400
N	-0.86797500	1.57551700	0.05947200
C	0.75888300	3.32281400	0.13353500
H	0.94479000	4.39069000	0.17547100
C	4.24225000	1.64837100	-2.48183300
H	3.67074000	0.73945600	-2.64760300
C	7.70295700	-2.37544900	0.32750600
H	7.96066200	-3.14885000	1.04465300
C	4.20101300	1.50241700	2.57796900
H	3.17541600	1.23046200	2.35262800
N	3.67517300	-2.45683200	-0.07089400
C	4.06176900	-3.57708800	-0.06558300
C	4.88569300	1.84874400	-1.24927800
C	5.59552800	3.03896000	-1.03323000
H	6.08822000	3.21743800	-0.08305700
C	1.83173600	2.40317900	0.09118700
H	2.84201400	2.79618100	0.09812400
C	0.18380900	0.66279100	0.02346300
C	4.32004600	2.61648500	-3.48303500

H	3.81787700	2.45013300	-4.43187300
C	5.20807300	1.26045800	1.63171900
C	6.25147700	-0.55384400	-0.35353800
C	5.66098000	4.01046500	-2.03425700
H	6.20611600	4.93263900	-1.85246200
C	-0.56854700	2.87109300	0.11471900
H	-1.40340200	3.56148400	0.14311800
C	4.51503100	2.08270800	3.80870800
H	3.72594700	2.26118800	4.53377600
C	5.02715400	3.80031100	-3.25997800
H	5.07822600	4.55862300	-4.03647600
C	6.84575300	2.17484600	3.17740900
H	7.87691600	2.42599100	3.41027700
C	7.00355300	-0.40689500	-1.52668900
H	6.74216100	0.35404200	-2.25396900
C	6.61080300	-1.54689100	0.57304000
H	6.03041800	-1.68237800	1.48005900
C	1.58901900	1.03519400	0.03340800
C	6.53756300	1.59264000	1.94814800
H	7.33395100	1.38147200	1.24093500
C	8.09901300	-1.24028400	-1.76794800
H	8.67418600	-1.11725300	-2.68156800
N	0.86796000	-1.57551000	-0.05934100
C	-0.75890200	-3.32281300	-0.13322700
H	-0.94482300	-4.39069000	-0.17506500
C	-1.83174500	-2.40316600	-0.09096400
H	-2.84202700	-2.79615900	-0.09787700
C	-0.18381400	-0.66278000	-0.02334900
C	0.56852900	-2.87109200	-0.11447400
H	1.40339600	-3.56146900	-0.14283700
C	-1.58901700	-1.03517500	-0.03330500
Pt	-2.74650300	0.60961700	0.02522700
P	-4.78905200	-0.50406000	-0.00545500
S	-4.58866000	5.11305500	0.05064100
C	-8.44977500	2.22372900	0.84333900
H	-9.29745600	2.87557900	1.03563300
C	-5.83416500	-2.42268000	-4.10923600
H	-6.07691200	-2.87017100	-5.06922100
C	-4.24254200	-1.64806800	2.48191800
H	-3.67113900	-0.73908300	2.64767200
C	-7.70280200	2.37547900	-0.32822800
H	-7.96032300	3.14889500	-1.04542500
C	-4.20078000	-1.50252400	-2.57800800
H	-3.17521200	-1.23048300	-2.35264100
N	-3.67522400	2.45681000	0.07093900
C	-4.06172900	3.57710000	0.06595800
C	-4.88578700	-1.84864200	1.24929100
C	-5.59548100	-3.03894200	1.03326100
H	-6.08801000	-3.21756600	0.08303000
C	-4.32040900	-2.61607600	3.48321700
H	-3.81840200	-2.44957200	4.43211400
C	-5.20789000	-1.26062900	-1.63179500
C	-6.25151000	0.55384800	0.35314700
C	-5.66100200	-4.01033900	2.03439000
H	-6.20602700	-4.93258200	1.85261600
C	-4.51471700	-2.08286800	-3.80874300
H	-3.72559800	-2.26129500	-4.53378400
C	-5.02738200	-3.79998900	3.26018400
H	-5.07851100	-4.55821700	4.03676000
C	-6.84544900	-2.17519800	-3.17750300
H	-7.87658400	-2.42643800	-3.41039000
C	-7.00389900	0.40686400	1.52609200
H	-6.74270500	-0.35409700	2.25341700
C	-6.61059700	1.54691300	-0.57350500
H	-6.02998200	1.68240400	-1.48037600
C	-6.53734100	-1.59293200	-1.94825000
H	-7.33377000	-1.38180300	-1.24106800
C	-8.09940700	1.24026600	1.76709600
H	-8.67481400	1.11722000	2.68056800

Complex **3a**, S_0 in CH_2Cl_2

Pt	-2.74720500	0.61027300	-0.00692000
P	-4.76806400	-0.52934800	0.00346900
S	-4.71862700	5.09982600	-0.07098000
C	-8.49351000	2.16166100	-0.67702300
H	-9.36266800	2.79601300	-0.82589800
C	-5.69824200	-2.60906600	4.05095800
H	-5.91472600	-3.09482600	4.99813200
N	0.83065800	-1.57269700	0.04197400
C	-0.75613100	-3.33775800	0.09600900
H	-0.94989200	-4.40487600	0.12834700
C	-4.22003300	-1.50798900	-2.55112100
H	-3.69898500	-0.56346200	-2.68068600
C	-7.81456800	2.17970700	0.54545800
H	-8.15225800	2.82813200	1.34865300
C	-4.13657300	-1.49673000	2.57364200
H	-3.14209900	-1.10828900	2.38130100
N	-3.70215300	2.47059700	-0.03817000
C	-4.13057000	3.57023000	-0.05265400
C	-4.83142400	-1.80571200	-1.32073000
C	-5.48006300	-3.03930100	-1.15915200
H	-5.94700100	-3.29641100	-0.21467700
C	-1.81250000	-2.42118600	0.07069900
H	-2.82499000	-2.80812200	0.08012300
C	-0.19727400	-0.69645800	0.02035300
C	-4.27035800	-2.42269000	-3.60351500
H	-3.79663200	-2.17959300	-4.55016800
C	-5.14006500	-1.35384700	1.60299000
C	-6.25213300	0.51987500	-0.28949400
C	-5.51808100	-3.95634200	-2.21215000
H	-6.01663400	-4.91119600	-2.07272600
C	0.56077200	-2.88715000	0.07891000
H	1.40873600	-3.55924400	0.09520700
C	-4.41593600	-2.12331000	3.79041600
H	-3.63118700	-2.22456300	4.53441900
C	-4.91771700	-3.64958900	-3.43481800
H	-4.94907000	-4.36516200	-4.25143500
C	-6.70773200	-2.45878400	3.09570000
H	-7.71045000	-2.82387100	3.29787700
C	-6.93522600	0.50746200	-1.51333900
H	-6.60844500	-0.14177500	-2.31834000
C	-6.69867600	1.36728700	0.73867800
H	-6.17844200	1.39269800	1.69138500
C	-1.56395900	-1.03972300	0.02958100
C	-6.43488900	-1.82948600	1.88131000
H	-7.23449000	-1.69713200	1.15901400
C	-8.05115700	1.32737100	-1.70387800
H	-8.57440800	1.30621800	-2.65557400
N	-0.83052500	1.57263400	-0.03578600
C	0.75621500	3.33776000	-0.08839800

H	0.94997000	4.40490100	-0.12003200
C	1.81259500	2.42118800	-0.06345100
H	2.82507200	2.80816100	-0.07243400
C	0.19740500	0.69640800	-0.01417100
C	-0.56067600	2.88711800	-0.07199900
H	-1.40865700	3.55918200	-0.08835100
C	1.56408100	1.03969500	-0.02316800
Pt	2.74733700	-0.61035300	0.01074200
P	4.76814000	0.52937900	-0.00133100
S	4.71699100	-5.10083200	0.02958200
C	8.49432100	-2.16245600	0.67187400
H	9.36363100	-2.79699400	0.81906100
C	5.69313300	2.61457700	-4.04720400
H	5.90838800	3.10165300	-4.99398200
C	4.22319700	1.50528000	2.55507800
H	3.70209500	0.56072800	2.68422200
C	7.81477600	-2.17816100	-0.55029800
H	8.15210300	-2.82498800	-1.35492900
C	4.13327300	1.50050900	-2.56927400
H	3.13891700	1.11218800	-2.37609900
N	3.70237600	-2.47067700	0.03565500
C	4.12992400	-3.57075400	0.03302800
C	4.83318200	1.80423300	1.32428600
C	5.48190400	3.03785700	1.16331700
H	5.94777500	3.29591400	0.21857200
C	4.27497800	2.41880400	3.60842500
H	3.80233500	2.17475700	4.55537500
C	5.13812000	1.35591500	-1.60027300
C	6.25258200	-0.52013400	0.28867200
C	5.52137600	3.95372600	2.21728100
H	6.01997500	4.90862400	2.07831600
C	4.41107000	2.12878400	-3.78553000
H	3.62527900	2.23134100	-4.52825300
C	4.92240700	3.64574900	3.44032400
H	4.95489600	4.36040400	4.25770000
C	6.70393000	2.46267900	-3.09358900
H	7.70644600	2.82783800	-3.29663600
C	6.93628900	-0.51005300	1.51220600
H	6.60985500	0.13757000	2.31864400
C	6.69869200	-1.36549400	-0.74136700
H	6.17796700	-1.38914200	-1.69384300
C	6.43264900	1.83169300	-1.87972400
H	7.23322600	1.69816400	-1.15872900
C	8.05238000	-1.33023700	1.70059100
H	8.57610000	-1.31089000	2.65206700

Complex **3b**, S_0 in gas phase

Pt	2.71834200	-0.73266300	-0.13388600
P	4.79135200	0.24612300	-0.03069700
C	8.39997200	-2.66657500	-0.21937900
H	9.23874300	-3.35491000	-0.27796600
C	1.60496700	0.96579800	0.15839800
N	-0.76588100	1.57926200	0.28311000
C	0.88045200	3.25176000	0.60889600
H	1.11538400	4.29200600	0.81368100
C	5.01980500	1.23279500	1.50801200
N	4.07525200	-3.27141800	0.45043600
C	8.23812600	-1.85595100	0.90259300
H	8.94873000	-1.90771600	1.72284900
C	6.39516400	-1.72431300	-1.19264100
H	5.67016700	-1.69396900	-1.99915300
C	7.47573000	-2.59953500	-1.26608400
H	7.59203900	-3.23652200	-2.13845000
N	3.50687700	-2.68363100	-0.45168700
C	4.11508500	1.83232400	-2.27032200
H	3.09670400	1.51182600	-2.07946200
C	1.90202000	2.31281700	0.42203300
H	2.93125600	2.65088900	0.49032700
C	6.22801000	-0.90275200	-0.06438400
C	7.15454600	-0.97739200	0.98358100
H	7.03658100	-0.35512900	1.86418400
C	4.64752600	1.39637100	3.90308400
H	4.23115500	0.98197300	4.81691900
C	5.70141900	3.08561000	-3.60170100
H	5.91417100	3.74672500	-4.43748200
C	5.85659700	3.14283400	2.75084600
H	6.38384000	4.09290500	2.76526200
C	5.15200600	1.37413300	-1.44422200
C	4.48528000	0.71201000	2.69871300
H	3.93560500	-0.22504600	2.67562500
N	4.62643200	-3.89821100	1.25046100
C	5.33122600	2.61436900	3.93090700
H	5.44914600	3.15145700	4.86811500
C	6.47252600	1.76828200	-1.72483600
H	7.29175200	1.39319900	-1.11852100
C	4.39053800	2.68510300	-3.34161600
H	3.57796100	3.02899800	-3.97553300
C	5.70623200	2.45525800	1.54425200
H	6.11625100	2.87922500	0.63343800
C	6.74272400	2.62382600	-2.79248100
H	7.76753400	2.92078800	-2.99818900
C	0.22595400	0.67917100	0.11687000
C	-0.45342600	2.85956700	0.53080400
H	-1.29446900	3.53126900	0.66307500
C	-1.60497300	-0.96578100	-0.15833600
N	0.76587400	-1.57924100	-0.28306500
C	-0.88045800	-3.25174000	-0.60885400
H	-1.11539100	-4.29198400	-0.81364500
C	-1.90202700	-2.31279800	-0.42197800
H	-2.93126300	-2.65087200	-0.49026600
C	-0.22596000	-0.67915400	-0.11681200
C	0.45341900	-2.85954400	-0.53076700
H	1.29446200	-3.53124400	-0.66305200
Pt	-2.71834600	0.73268700	0.13391800
P	-4.79135800	-0.24610800	0.03071500
C	-8.40010200	2.66642500	0.21964200
H	-9.23891000	3.35471000	0.27829000
C	-5.01980300	-1.23269500	-1.50805200
N	-4.07513500	3.27137900	-0.45069400
C	-8.23837300	1.85570300	-0.90227700
H	-8.94910800	1.90734200	-1.72242900
C	-6.39507900	1.72439200	1.19268900
H	-5.66995400	1.69417700	1.99909000
C	-7.47569700	2.59954700	1.26621200
H	-7.59191500	3.23661100	2.13853500
N	-3.50688600	2.68368900	0.45157800
C	-4.11505200	-1.83241500	2.27025300
H	-3.09667800	-1.51188900	2.07940500
C	-6.22804100	0.90273700	0.06448400
C	-7.15474600	0.97720900	-0.98334400

H	-7.03687000	0.35486900	-1.86390500
C	-4.64759200	-1.39609200	-3.90314500
H	-4.23127900	-0.98160800	-4.81696700
C	-5.70135800	-3.08579500	3.60157800
H	-5.91409500	-3.74695400	4.43732700
C	-5.85652000	-3.14270500	-2.75098300
H	-6.38370600	-4.09280600	-2.76544300
C	-5.15198500	-1.37420400	1.44417800
C	-4.48535000	-0.71179800	-2.69873600
H	-3.93574300	0.22529700	-2.67560700
N	-4.62622200	3.89803500	-1.25088900
C	-5.33121800	-2.61413100	-3.93102500
H	-5.44913300	-3.15116600	-4.86826400
C	-6.47249600	-1.76838900	1.72478000
H	-7.29173200	-1.39329000	1.11848800
C	-4.39048500	-2.68525100	3.34150700
H	-3.57790000	-3.02916100	3.97540600
C	-5.70615700	-2.45519700	-1.54434900
H	-6.11611900	-2.87924800	-0.63354800
C	-6.74267400	-2.62399000	2.79238400
H	-7.76747700	-2.92098100	2.99808200

Complex **3b**, T_1 in gas phase

Pt	2.71315800	0.74413800	0.07803900
P	4.79356900	-0.26500600	0.03306000
C	8.36077900	2.66428800	0.53313000
H	9.18912700	3.35489100	0.66562700
C	1.63237200	-0.93974900	-0.21421500
N	-0.78895000	-1.59368000	-0.26448900
C	0.90601800	-3.20946800	-0.72302300
H	1.14179400	-4.23907100	-0.97138800
C	5.11061600	-1.19217400	-1.52593600
N	4.22325700	3.25825400	-0.51007800
C	8.27029400	1.89517700	-0.62530900
H	9.02601400	1.98288400	-1.40092700
C	6.31196600	1.67311100	1.35238400
H	5.54560300	1.60231000	2.11825800
C	7.37822200	2.55241200	1.52145700
H	7.43957800	3.15555100	2.42303700
N	3.44729300	2.72476400	0.25550200
C	4.04597300	-1.93784800	2.19333000
H	3.02989000	-1.63427700	1.96846600
C	1.93631300	-2.25426000	-0.55060900
H	2.96394800	-2.57891500	-0.67608800
C	6.21611900	0.89340100	0.18685200
C	7.20062500	1.01338900	-0.80192000
H	7.13805100	0.42432000	-1.71064200
C	4.86589200	-1.27070600	-3.94132400
H	4.49300600	-0.82694600	-4.86011400
C	5.59984400	-3.20743700	3.54842100
H	5.79058900	-3.89128300	4.37116400
C	6.02973200	-3.04875600	-2.79066200
H	6.56511800	-3.99412500	-2.81144800
C	5.10646800	-1.43675300	1.42461700
C	4.63326400	-0.63269700	-2.72317700
H	4.07111900	0.29666500	-2.69529700
N	4.94468200	3.84148300	-1.20094200
C	5.56228200	-2.48119800	-3.97693500
H	5.73418300	-2.98284800	-4.92537800
C	6.42163300	-1.81946400	1.74573700
H	7.25838300	-1.41372900	1.18494400
C	4.29408100	-2.81961100	3.24795200
H	3.46246400	-3.19683600	3.83659500
C	5.80959700	-2.40725100	-1.56965800
H	6.17384400	-2.86162700	-0.65415700
C	6.66421000	-2.70425400	2.79579000
H	7.68509900	-2.99198700	3.03196600
C	0.21557700	-0.64502400	-0.11331600
C	-0.43746900	-2.84131900	-0.56611100
H	-1.25550300	-3.54474000	-0.68511900
C	-1.63238100	0.93965500	0.21439400
N	0.78893600	1.59361300	0.26461100
C	-0.90605000	3.20935100	0.72331600
H	-1.14182400	4.23893400	0.97176400
C	-1.93633700	2.25415500	0.55084100
H	-2.96396900	2.57880100	0.67632500
C	-0.21558400	0.64494700	0.11345700
C	0.43744200	2.84122200	0.56634800
H	1.25547300	3.54463700	0.68538700
Pt	-2.71316700	-0.74419800	-0.07794000
P	-4.79355600	0.26500800	-0.03310900
C	-8.36097300	-2.66392400	-0.53367300
H	-9.18937300	-3.35444200	-0.66628300
C	-5.11067300	1.19208900	1.52592000
N	-4.22329800	-3.25849700	0.51002700
C	-8.27044800	-1.89499100	0.62487800
H	-9.02618500	-1.98275600	1.40047300
C	-6.31207200	-1.67278900	-1.35275800
H	-5.54570300	-1.60192300	-2.11862000
C	-7.37839900	-2.55197400	-1.52197500
H	-7.43979900	-3.15496900	-2.42364800
N	-3.44717100	-2.72484800	-0.25526100
C	-4.04569900	1.93788500	-2.19325200
H	-3.02965100	1.63422700	-1.96834000
C	-6.21615900	-0.89329500	-0.18708700
C	-7.20070500	-1.01332200	0.80163900
H	-7.13809400	-0.42439100	1.71045000
C	-4.86611100	1.27045200	3.94133200
H	-4.49331100	0.82661200	4.86011800
C	-5.59939500	3.20766000	-3.54836800
H	-5.79004200	3.89155300	-4.37109400
C	-6.02976700	3.04864100	2.79070300
H	-6.56510200	3.99403800	2.81151400
C	-5.10627700	1.43685100	-1.42461400
C	-4.63343900	0.63250500	2.72316000
H	-4.07134100	-0.29688400	2.69526400
N	-4.94511200	-3.84147000	1.20070500
C	-5.56243000	2.48098200	3.97697200
H	-5.73436900	2.98258400	4.92543400
C	-6.42139600	1.81967700	-1.74578600
H	-7.25820800	1.41398700	-1.18505400
C	-4.29368000	2.81971300	-3.24785200
H	-3.46200300	3.19688900	-3.83644200
C	-5.80958700	2.40720200	1.56967300
H	-6.17375400	2.86165300	0.65417600
C	-6.66384200	2.70453600	-2.79581000
H	-7.68469400	2.99236900	-3.03202500

Complex **3b**, S_0 in CH_2Cl_2

Pt	2.71627300	-0.73634500	-0.15054300

P	4.78916800	0.26213400	-0.02441200	H	6.09062900	2.89975400	0.65856200	C	-4.42935900	-0.72817600	-2.70008800
C	8.40254300	-2.65844500	-0.11332100	C	6.76315500	2.64575000	-2.76047300	H	-3.88571900	0.21234900	-2.67209000
H	9.24584700	-3.34240100	-0.14914300	H	7.78467300	2.97070700	-2.93569800	N	-4.57361800	4.01269900	-1.14306200
C	1.61170100	0.95764300	0.14312800	C	0.23082600	0.67835600	0.11208500	C	-5.24615500	-2.63686800	-3.94260600
N	-0.75423600	1.58697900	0.27982000	C	-0.42675200	2.86814700	0.50700000	H	-5.34592400	-3.17625800	-4.88021100
C	0.90970400	3.25500700	0.56268800	H	-1.25427500	3.55433200	0.64328800	C	-6.48162300	-1.80354600	1.68497600
H	1.15328200	4.29652600	0.74691800	C	-1.61176100	-0.95748200	-0.14325900	H	-7.29194200	-1.46997600	1.04384300
C	4.98257800	1.24975000	1.51674100	N	0.75417400	-1.58679400	-0.28000600	C	-4.42794300	-2.63065000	3.38796600
N	4.05358400	-3.33429500	0.35792800	C	-0.90975200	-3.25482500	-0.56292200	H	-3.62779400	-2.94067100	4.05391900
C	8.14833300	-1.92032200	1.04231300	H	-1.15332300	-4.29633400	-0.74721700	C	-5.66392600	-2.47439600	-1.56217300
H	8.79206000	-2.02423100	1.91113700	C	-1.92274300	-2.30621700	-0.38108100	H	-6.08893200	-2.90043300	-0.65974500
C	6.48671900	-1.63893500	-1.18516400	H	-2.95336900	-2.64039600	-0.43246900	C	-6.76238000	-2.64784400	2.75920600
H	5.84436200	-1.53832700	-2.05429900	C	-0.23088600	-0.67817900	-0.11224700	H	-7.78376100	-2.97340800	2.93410100
C	7.56844100	-2.51619400	-1.22744300	C	0.42670400	-2.86795600	-0.50721900				
H	7.76131900	-3.08873300	-2.13027300	H	1.25422500	-3.55414200	-0.64352800				
N	3.52345100	-2.69333000	-0.52050000	Pt	-2.71632400	0.73648700	0.15053000				
C	4.14183700	1.78882300	-2.31049700	P	-4.78909600	-0.26221200	0.02443000				
H	3.12537100	1.44707800	-2.14745400	C	-8.40296300	2.65767700	0.11576200				
C	1.92269400	2.30638600	0.38089500	H	-9.24638300	3.34145800	0.15217800				
H	2.95332100	2.64056800	0.43225300	C	-4.98249700	-1.24900200	-1.51725600				
C	6.22560500	-0.89087000	-0.02375400	N	-4.05447700	3.33439100	-0.35732500				
C	7.06294900	-1.04010800	1.09006400	C	-8.14923800	1.91983300	-1.04015400				
H	6.87917600	-0.47035200	1.99444400	H	-8.79346400	2.02378000	-1.90860400				
C	4.56692600	1.41811700	3.90545500	C	-6.48635200	1.63833900	1.18636000				
H	4.13684000	1.00476200	4.81316500	H	-5.84349500	1.53768600	2.05511800				
C	5.73652000	3.06228900	-3.61286500	C	-7.56822200	2.51537500	1.22940100				
H	5.95844400	3.71458600	-4.45271600	H	-7.76072300	3.08770000	2.13244800				
C	5.79137700	3.16574500	2.76876800	N	-3.52338500	2.69342800	0.52051400				
H	6.31537900	4.11700700	2.78923500	C	-4.14141500	-1.78937200	2.31010100				
C	5.16396400	1.37427200	-1.44282500	H	-3.12509400	-1.44704600	2.14736200				
C	4.42861800	0.73011500	2.69969900	C	-6.22571500	0.89057100	0.02465000				
H	3.88424100	-0.20999200	2.67209500	C	-7.06369700	1.03984900	-1.08867700				
N	4.57194600	-4.01273100	1.14406600	H	-6.88029700	0.47031800	-1.99327400				
C	5.24648900	2.63894700	3.94129400	C	-4.56755100	-1.41551600	-3.90623000				
H	5.34635600	3.17885300	4.87859200	H	-4.13812700	-1.00123800	-4.81383200				
C	6.48219100	1.80192500	-1.68592000	C	-5.73571500	-3.06407600	3.61171900				
H	7.29247100	1.46814500	-1.04485300	H	-5.95748600	-3.71674300	4.45132300				
C	4.42856400	2.62963800	-3.38866800	C	-5.79020200	-3.16484500	-2.77022500				
H	3.62842400	2.93989600	-4.05452100	H	-6.31344800	-4.11651400	-2.79111200				
C	5.66497600	2.47463100	1.56111400	C	-5.16356200	-1.37512300	1.44231500				