Electronic Supplementary Information

Luminescent Cu^{I} thiocyanate complexes based on tris(2-pyridyl)phosphine and its oxide: from mono-, di- and trinuclear species to coordination polymer

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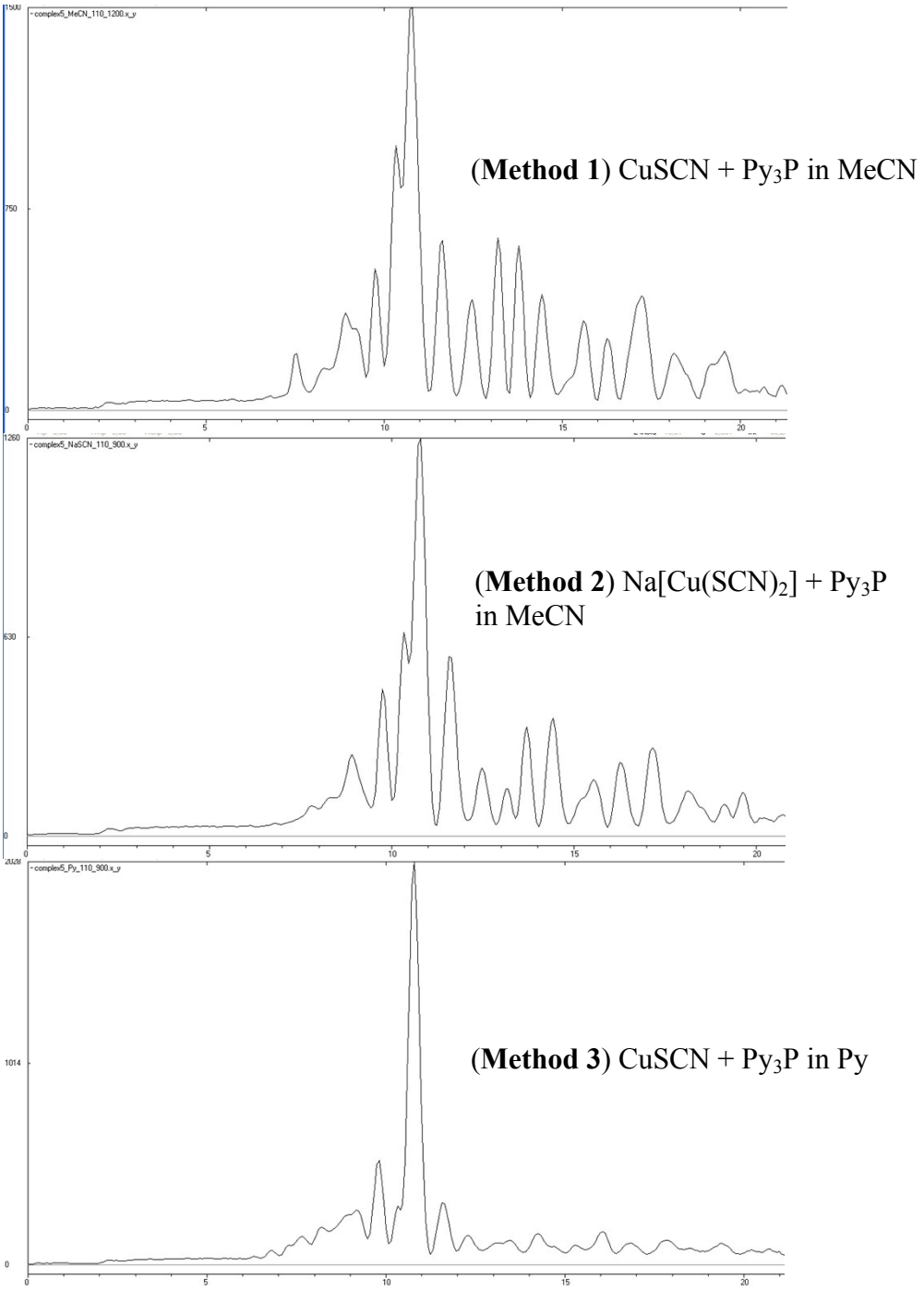


Figure S1. PXRD patterns (298 K) of samples **5** obtained by methods 1, 2 and 3.

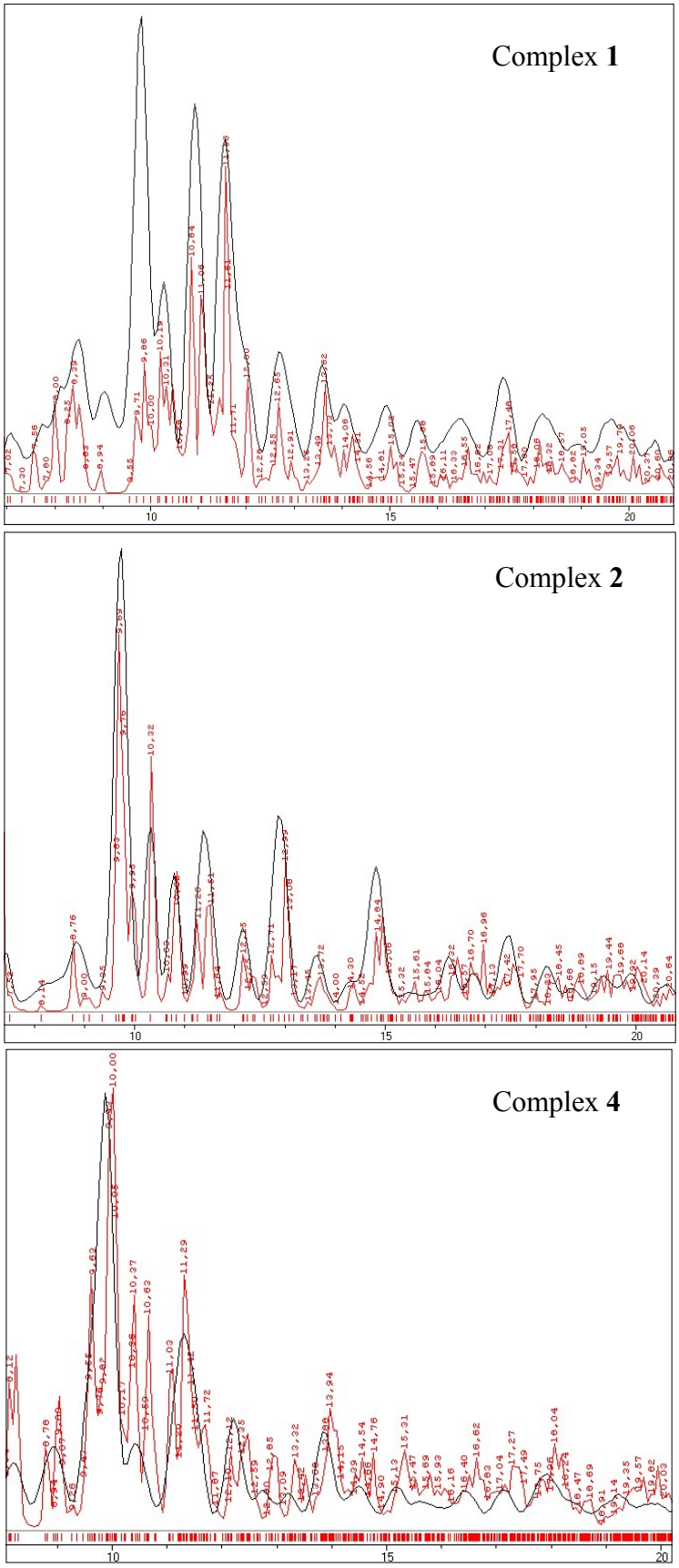


Figure S2. Experimental and simulated PXRD patterns for complexes **1**, **2** and **4**. Simulated patterns calculated from the X-ray structures of **1**, **2** and **4** are represented by red lines.

Table S1. X-Ray crystallographic data for complexes **1-4** and **6**.

Compound	**1**·CH_2Cl_2	**2**	**3**	**4**·$CHCl_3$	**6**·$CHCl_3$
Empirical formula	$C_{16}H_{12}CuN_4OPS{\cdot}CH_2Cl_2$	$C_{32}H_{24}Cu_2N_8O_2P_2S_2$	$C_{32}H_{24}Cu_2N_8O_2P_2S_2{\cdot}$ $2[C_{16}H_{12}CuN_4OPS]$	$C_{34}H_{25}Cl_3Cu_3N_9O_2P_2S_3$	$C_{17}H_{12}CuN_5OPS_2{\cdot}CHCl_3$
Formula mass [g/mol]	487.79	805.73	1611.46	1046.72	580.31
Space group	C2/c	P-1	P2/c	P-1	$P2_1/c$
a [Å]	20.506(3)	8.3784(8)	25.1513(11)	11.8672(7)	11.9247(6)
b [Å]	12.2936(17)	9.0242(8)	8.253(4)	12.4871(7)	10.7519(4)
c [Å]	16.937(2)	13.1937(11)	33.3853(15)	18.2320(11)	18.7122(7)
α [°]	90	71.147(3)	90	84.626(2)	90
β [°]	105.973(4)	78.454(3)	109.3330(10)	89.461(2)	97.860(2)
γ [°]	90	65.128(3)	90	62.746(2)	90
V [Å^3]	4104.9(10)	854.08(13)	6539.2(5)	2389.5(2)	2376.61(17)
Z	8	1	4	2	4
$D_{calcd.}$ [g·cm^{-3}]	1.579	1.567	1.637	1.455	1.622
μ [mm^{-1}]	1.519	1.504	1.572	1.727	1.520
Temperature [K]	296(2)	296(2)	296(2)	200(2)	296(2)
Reflections collected	58293	42492	127884	108400	44040
Independent reflections	4473 [R_{int} = 0.0628]	3717 [R_{int}= 0.0565]	14274 [R_{int} = 0.0665]	11016 [R_{int} = 0.0360]	5451 [R_{int}= 0.0393]
R_1, wR_2 [$I > 2\sigma(I)$]	0.0408, 0.1003	0.0854, 0.2799	0.0375, 0.0751	0.0389, 0.0933	0.0505, 0.1383
R_1, wR_2 (all data)	0.0640, 0.1143	0.0996, 0.2828	0.0548, 0.0806	0.0515, 0.1053	0.0583, 0.1474
Goodness of fit	1.023	1.122	1.061	1.032	1.058

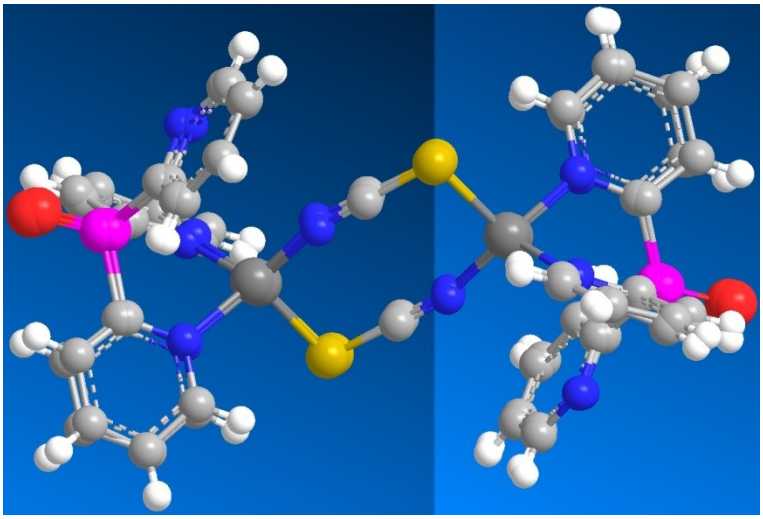


Figure S3. The structure of the dinuclear complexes from co-crystal **3** overlaid on the structure of the individual complex **2**.

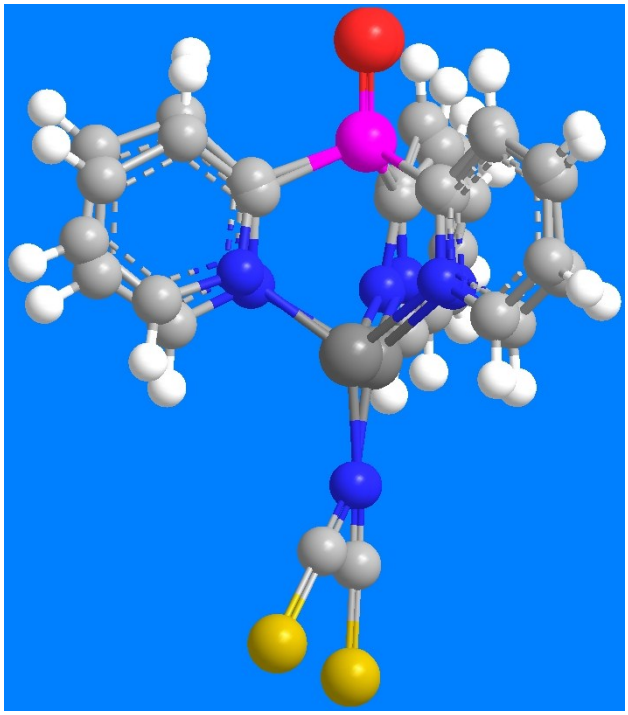


Figure S4. Overlaid structures of the two independent molecules [Cu(Py_3P=O)(*N*CS)] within co-crystal **3**.

Figure S5. FT-IR spectrum of complex **1** (KBr).

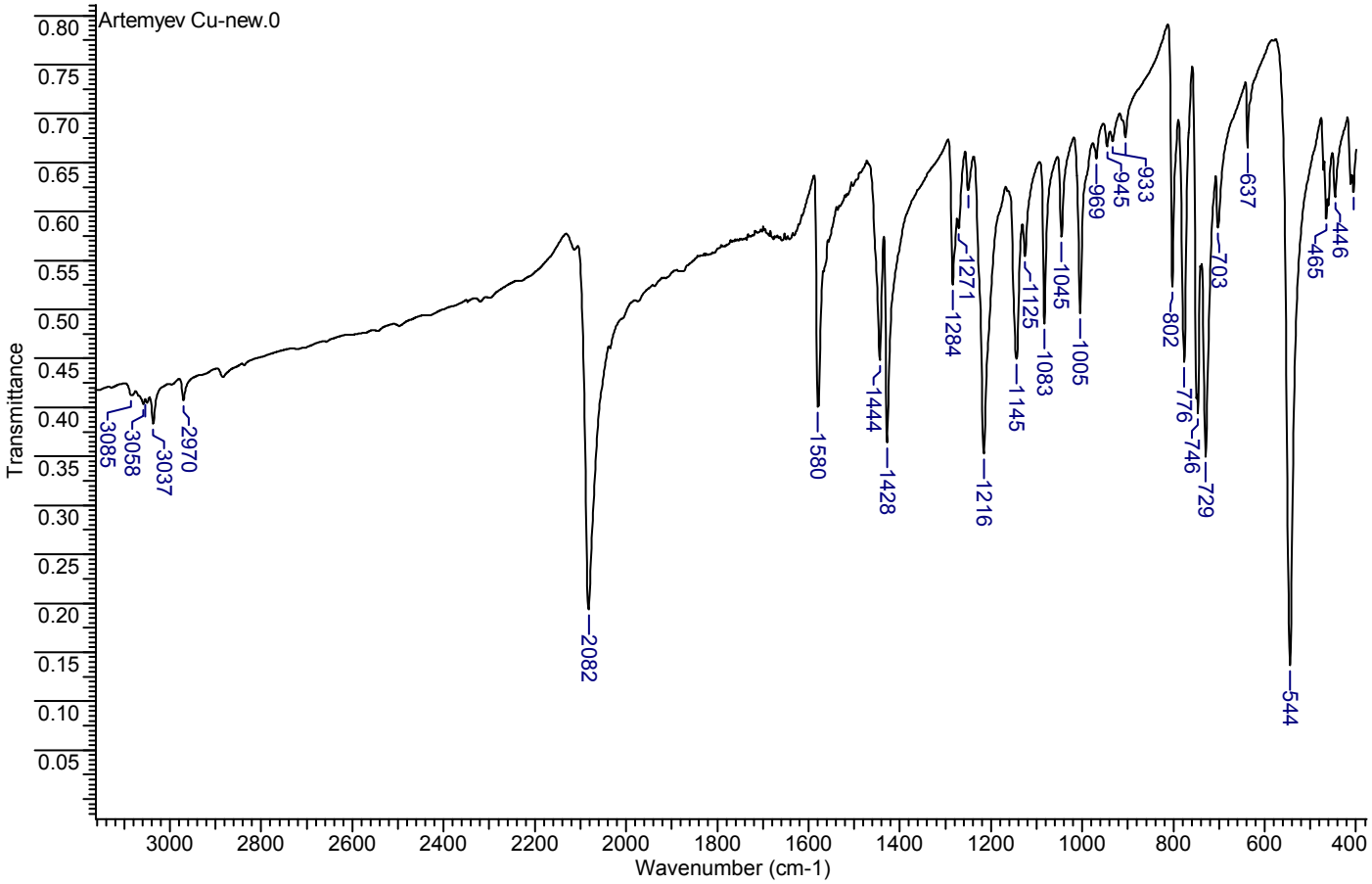


Figure S6. FT-IR spectrum of complex **2** (KBr).

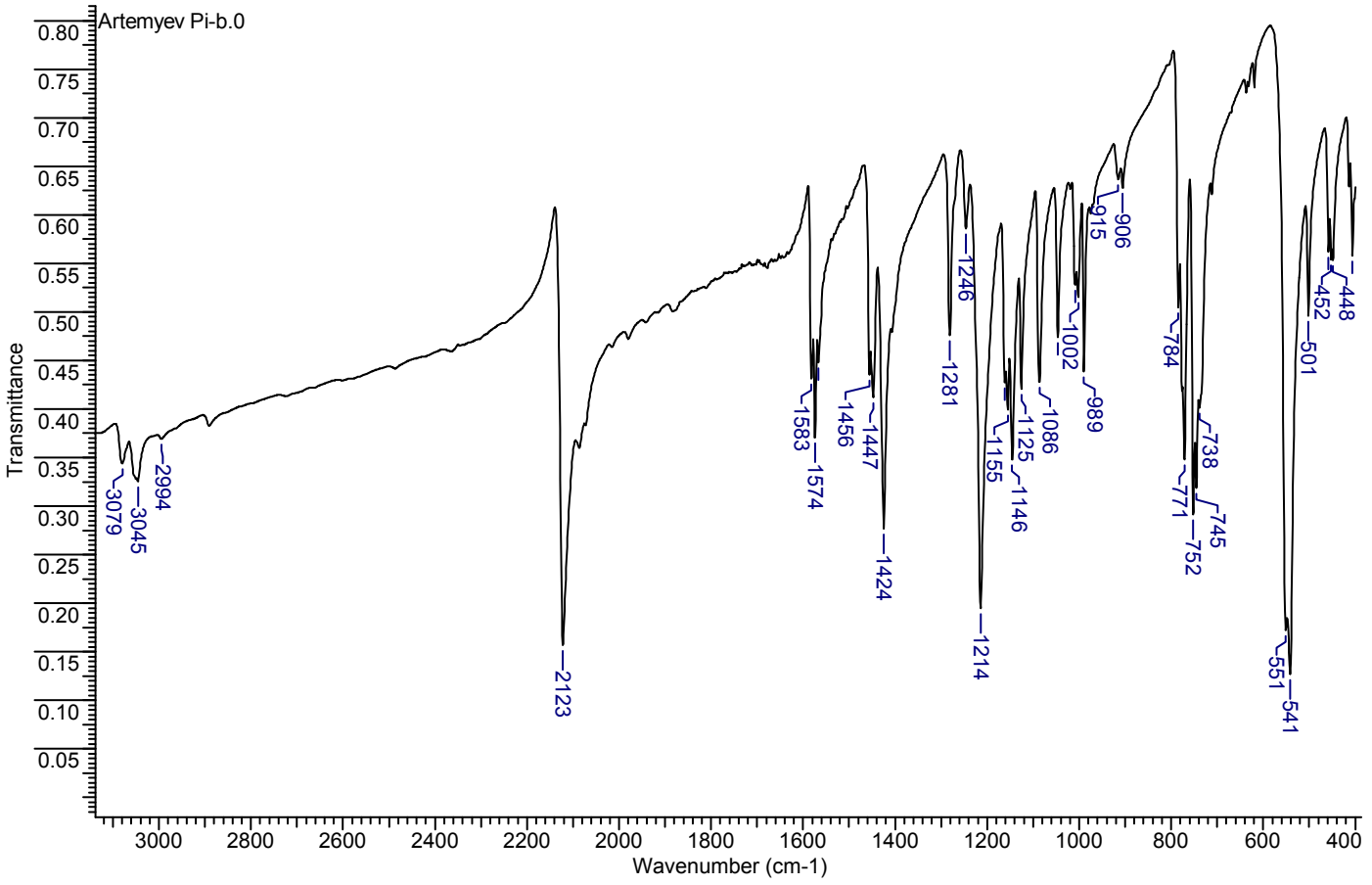


Figure S7. FT-IR spectrum of complex **3** (KBr).

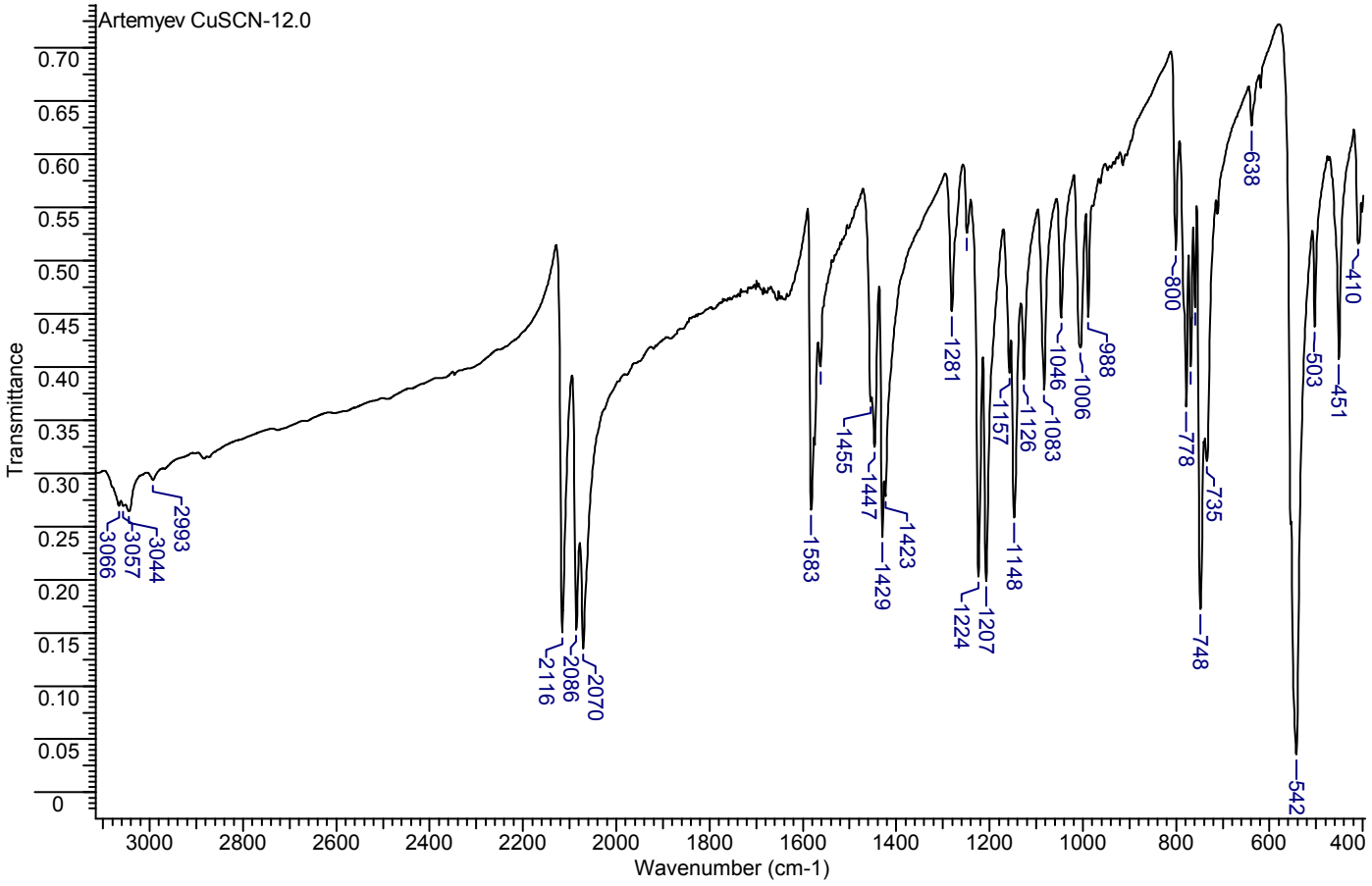


Figure S8. FT-IR spectrum of complex **4** (KBr).

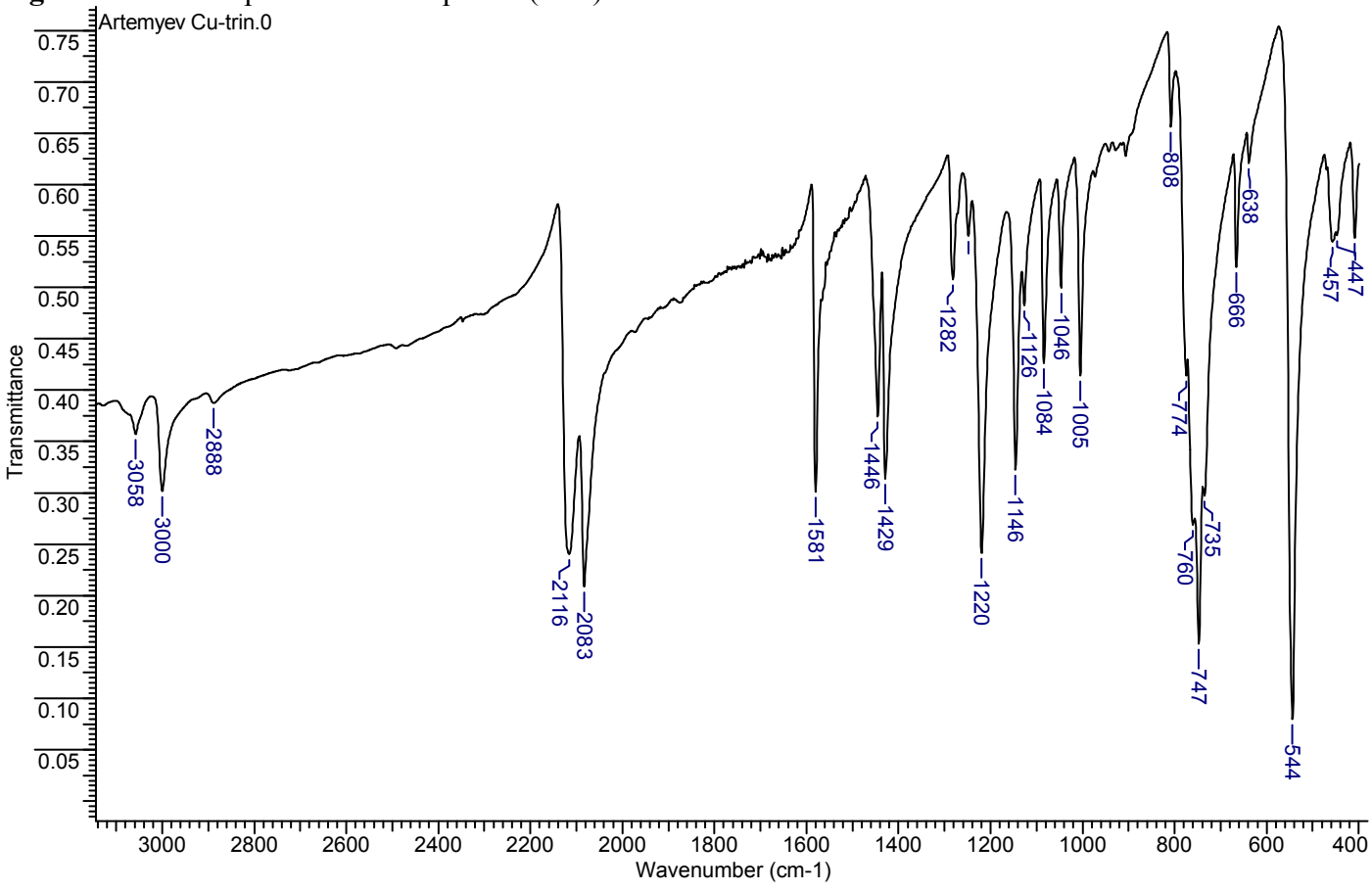


Figure S9. FT-IR spectrum of complex **5** (KBr).

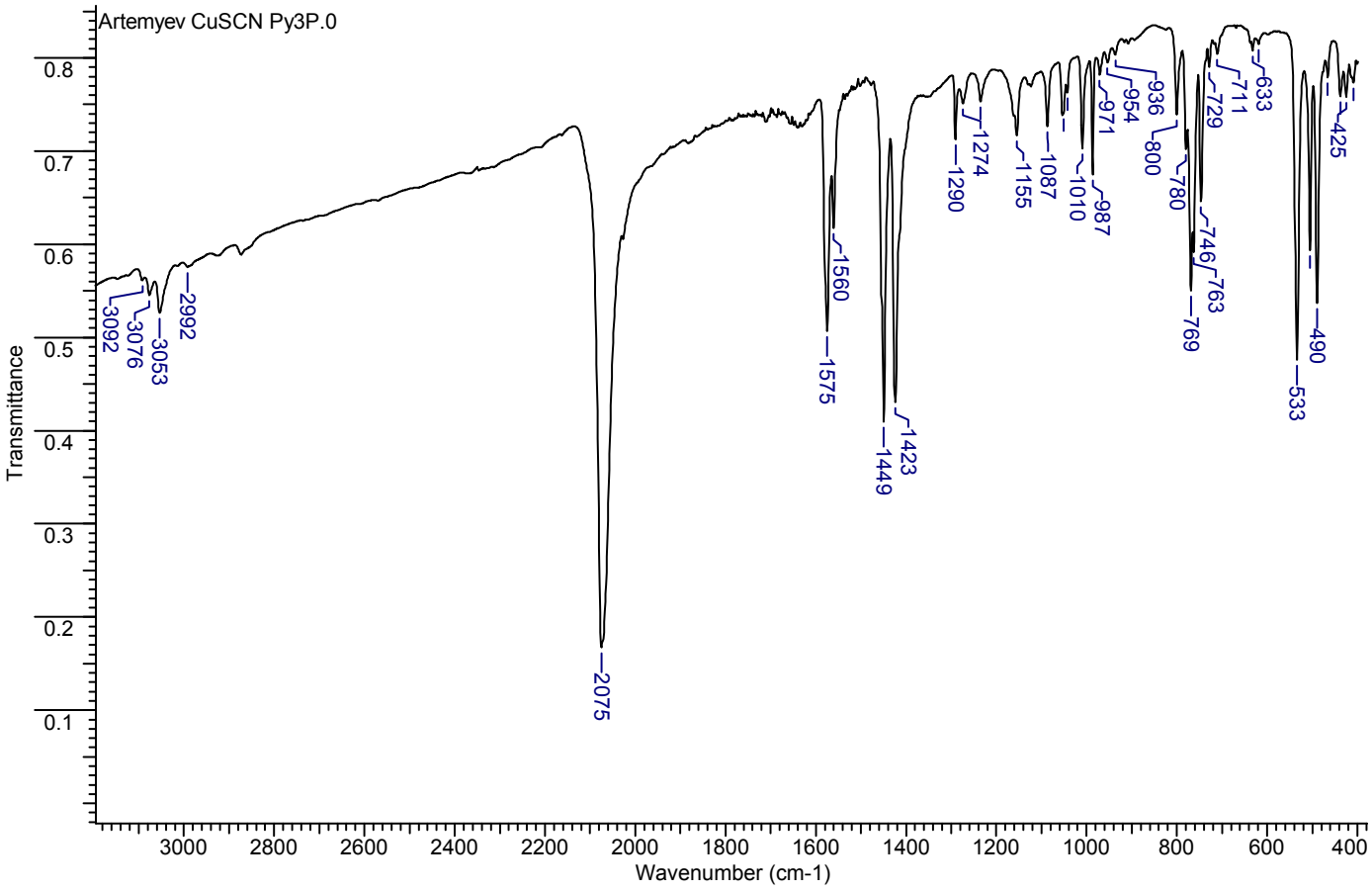


Figure S10. Typical FT-IR spectrum of complex **1** or **2** recorded for $CHCl_3$ solution.

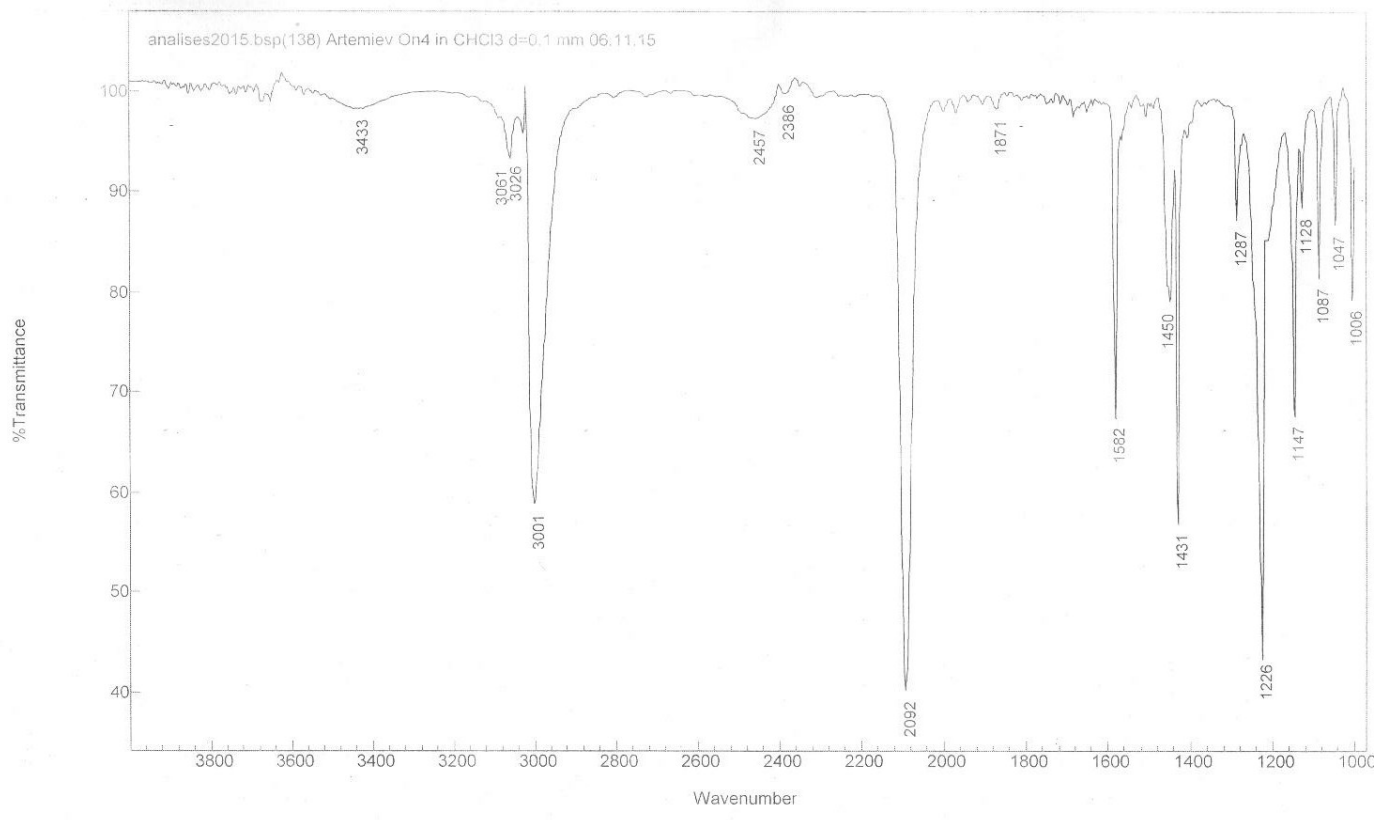


Figure S11. FT-IR spectrum of complex **6** (KBr).

Figure S12. ^{1}H NMR spectrum of complex **1** ($CDCl_3$).

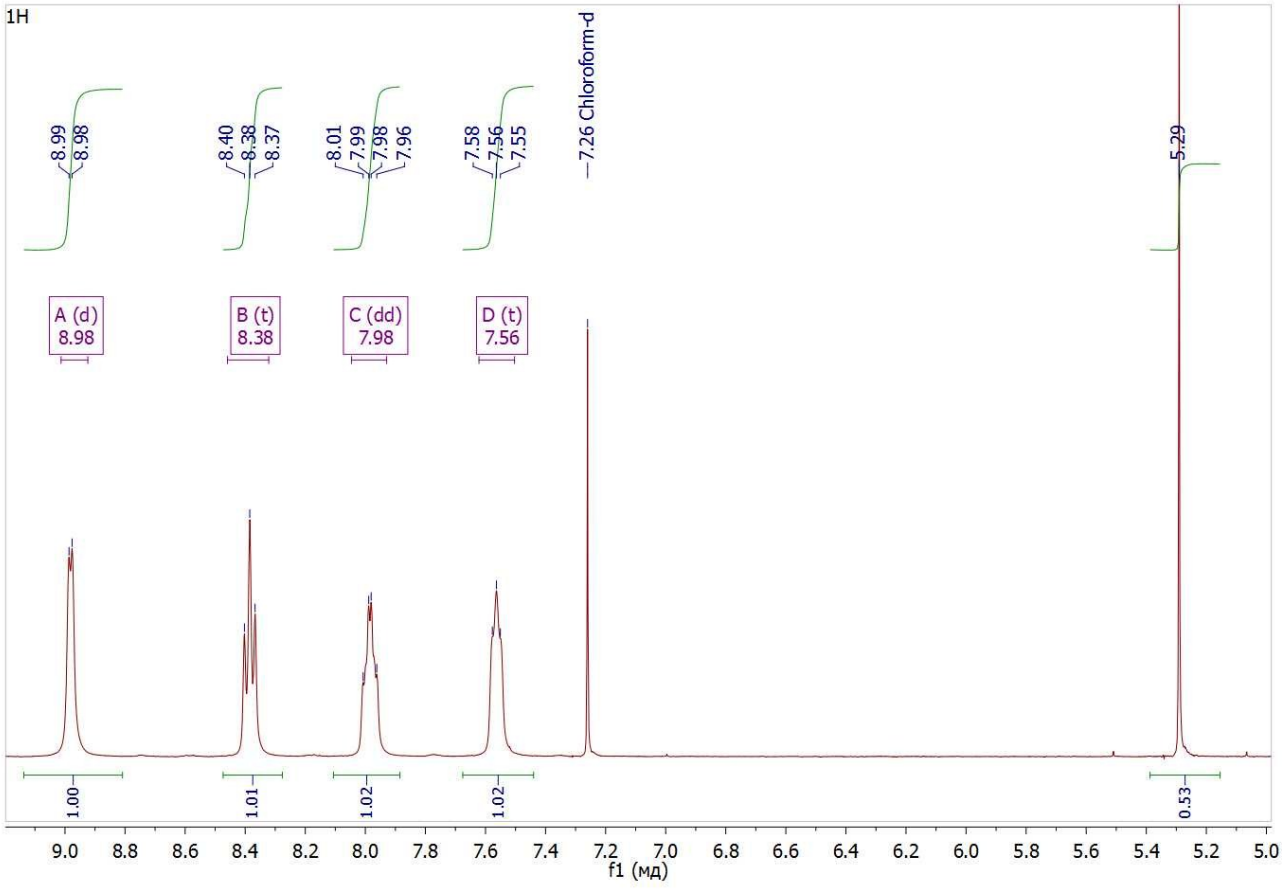


Figure S13. ^{13}C NMR spectrum of complex **1** ($CDCl_3$).

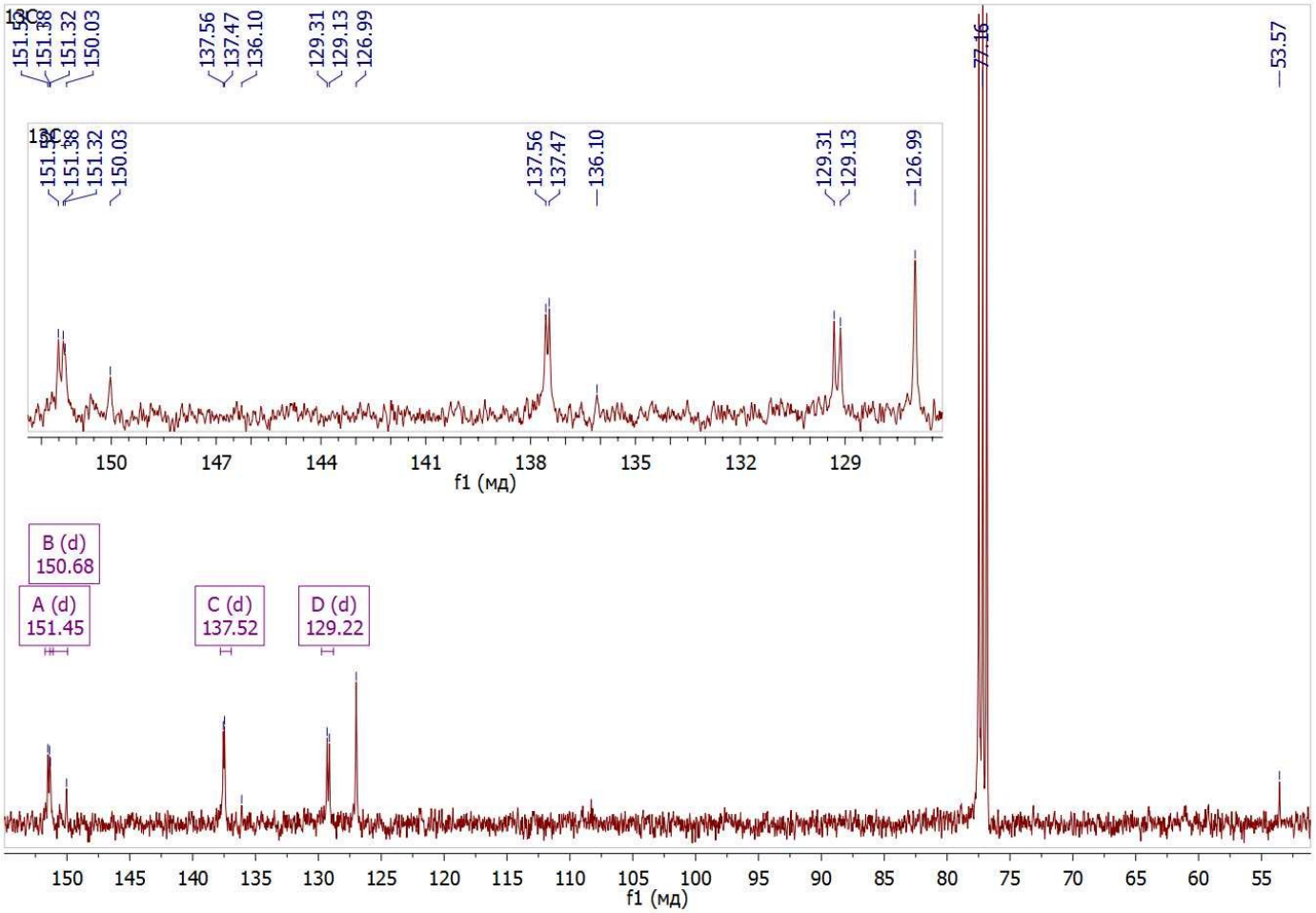


Figure S14. ^{31}P NMR spectrum of complex **1** ($CDCl_3$).

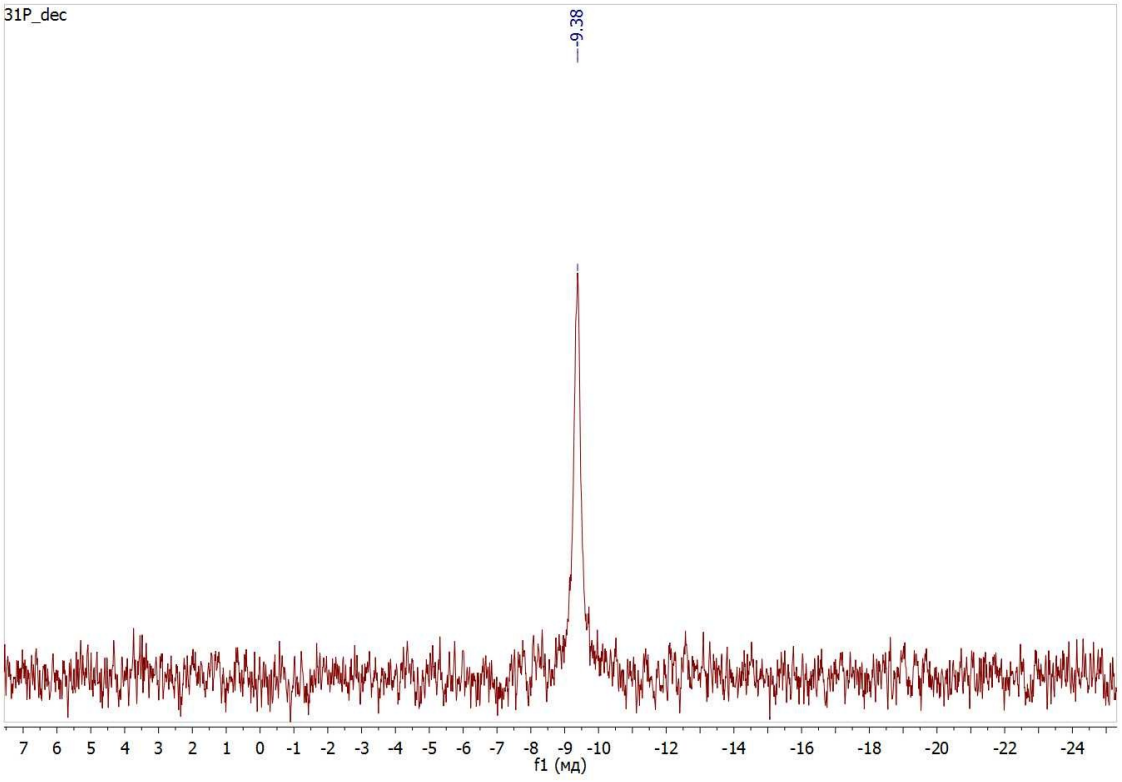


Figure S15. ^{1}H NMR spectrum of complex **2** ($CDCl_3$).

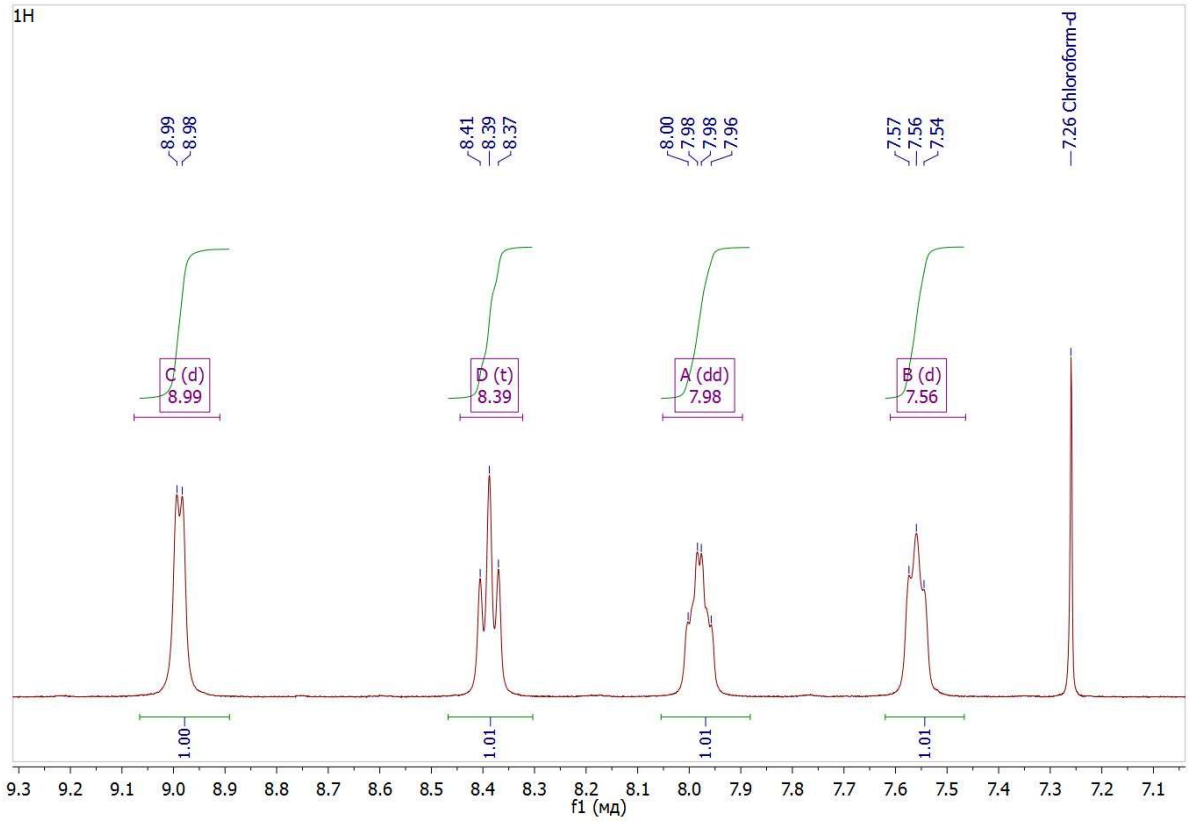


Figure S16. ^{13}C NMR spectrum of complex **2** ($CDCl_3$).

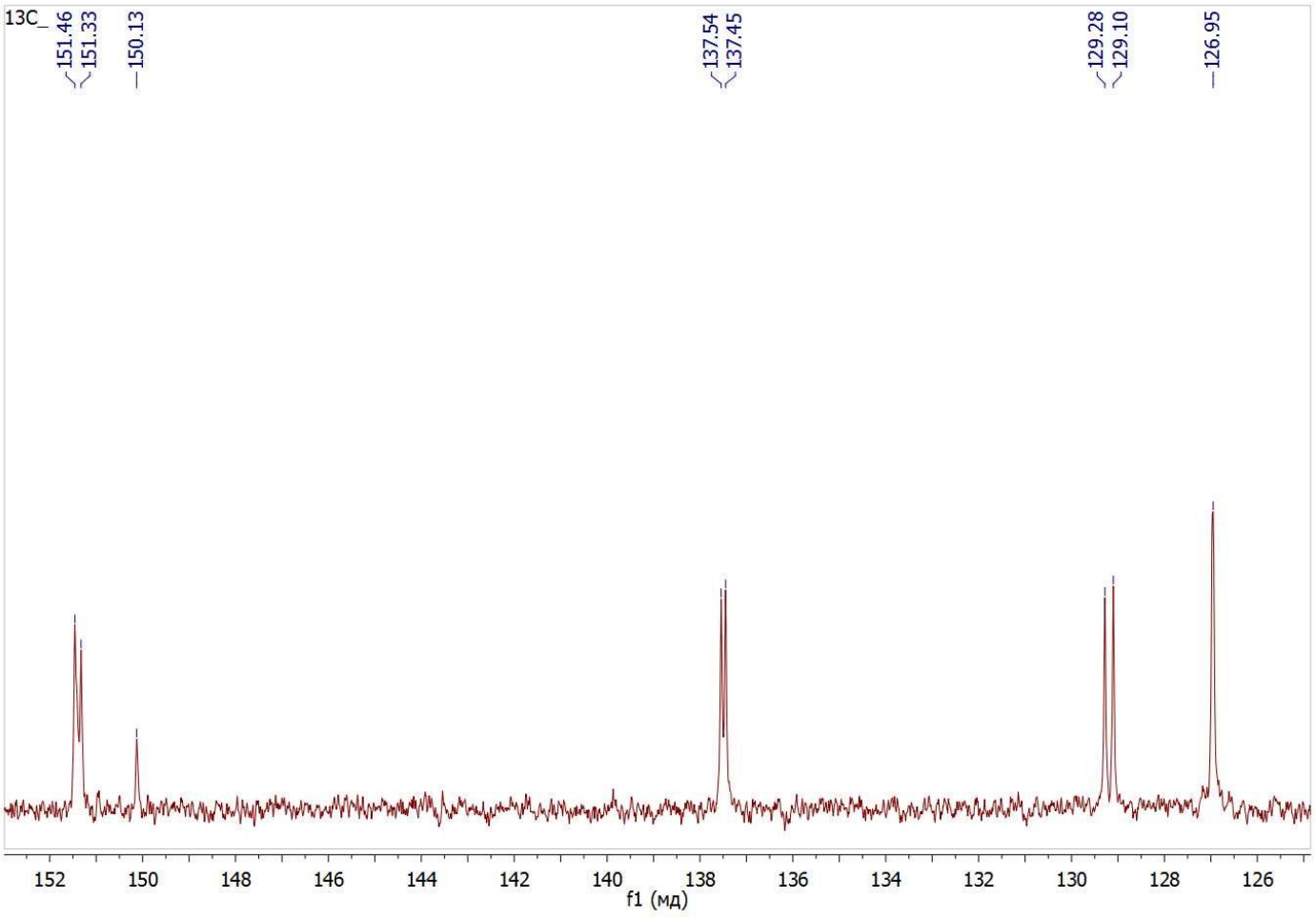


Figure S17. ^{31}P NMR spectrum of complex **2** ($CDCl_3$).

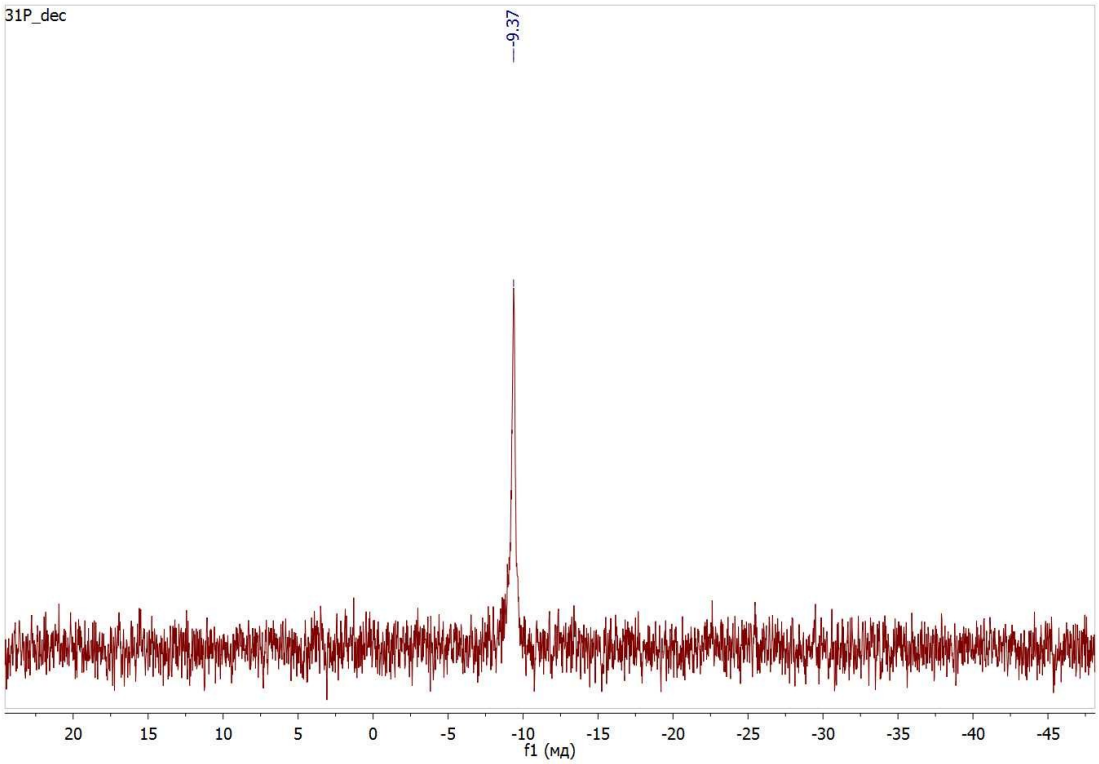


Figure S18. ^{1}H NMR spectrum of complex **3** ($CDCl_3$).

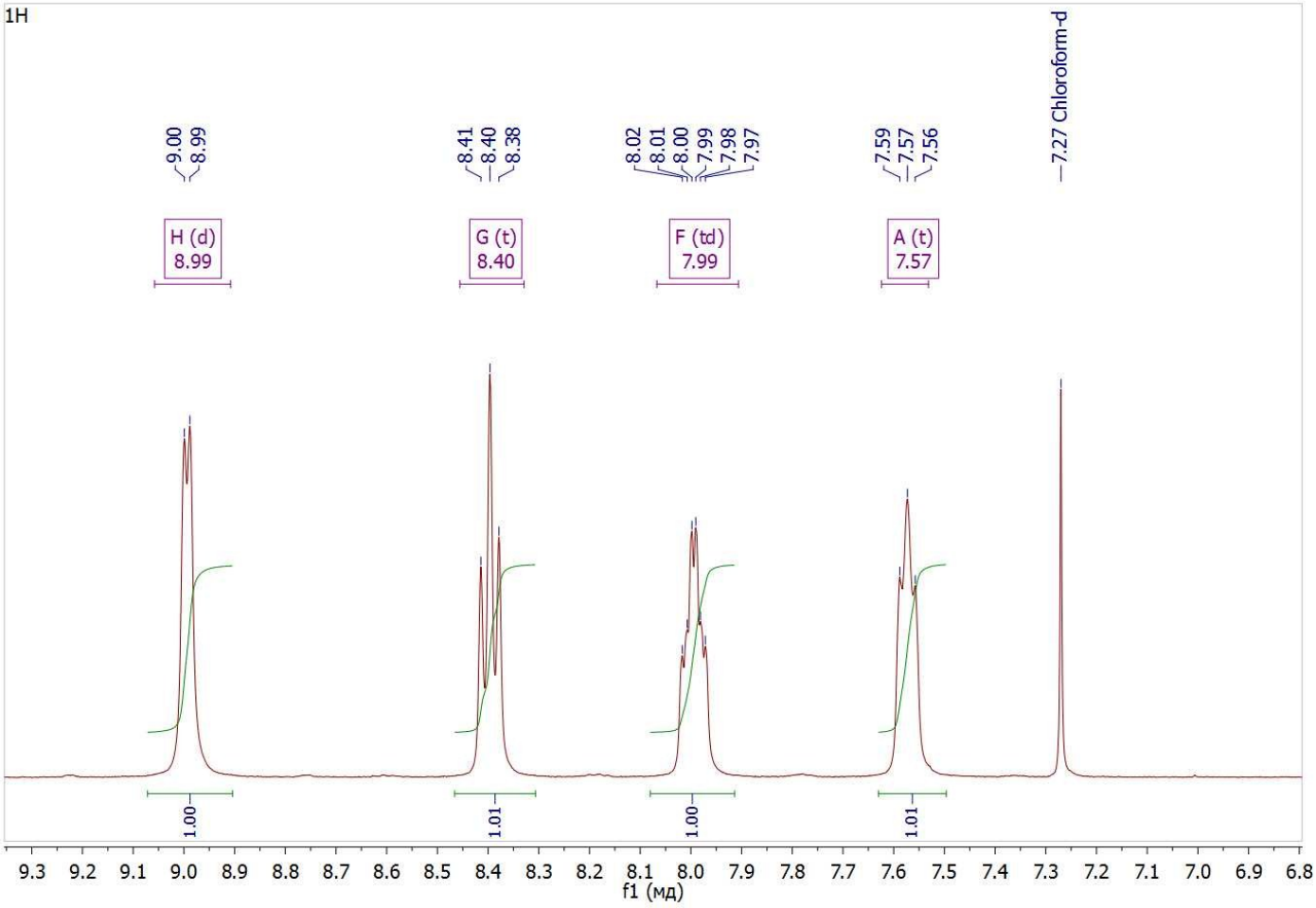


Figure S19. ^{31}P NMR spectrum of complex **3** ($CDCl_3$).

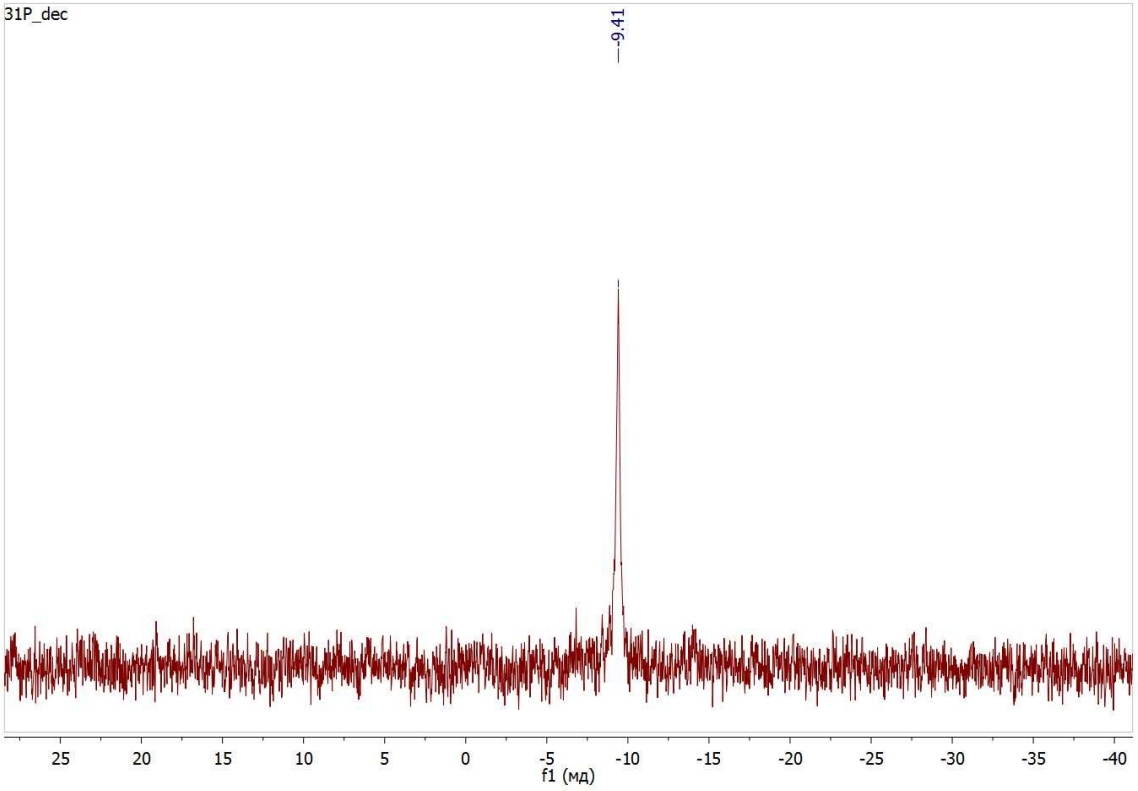


Figure S20. ^{1}H NMR spectrum of complex **4** ($CDCl_3$).

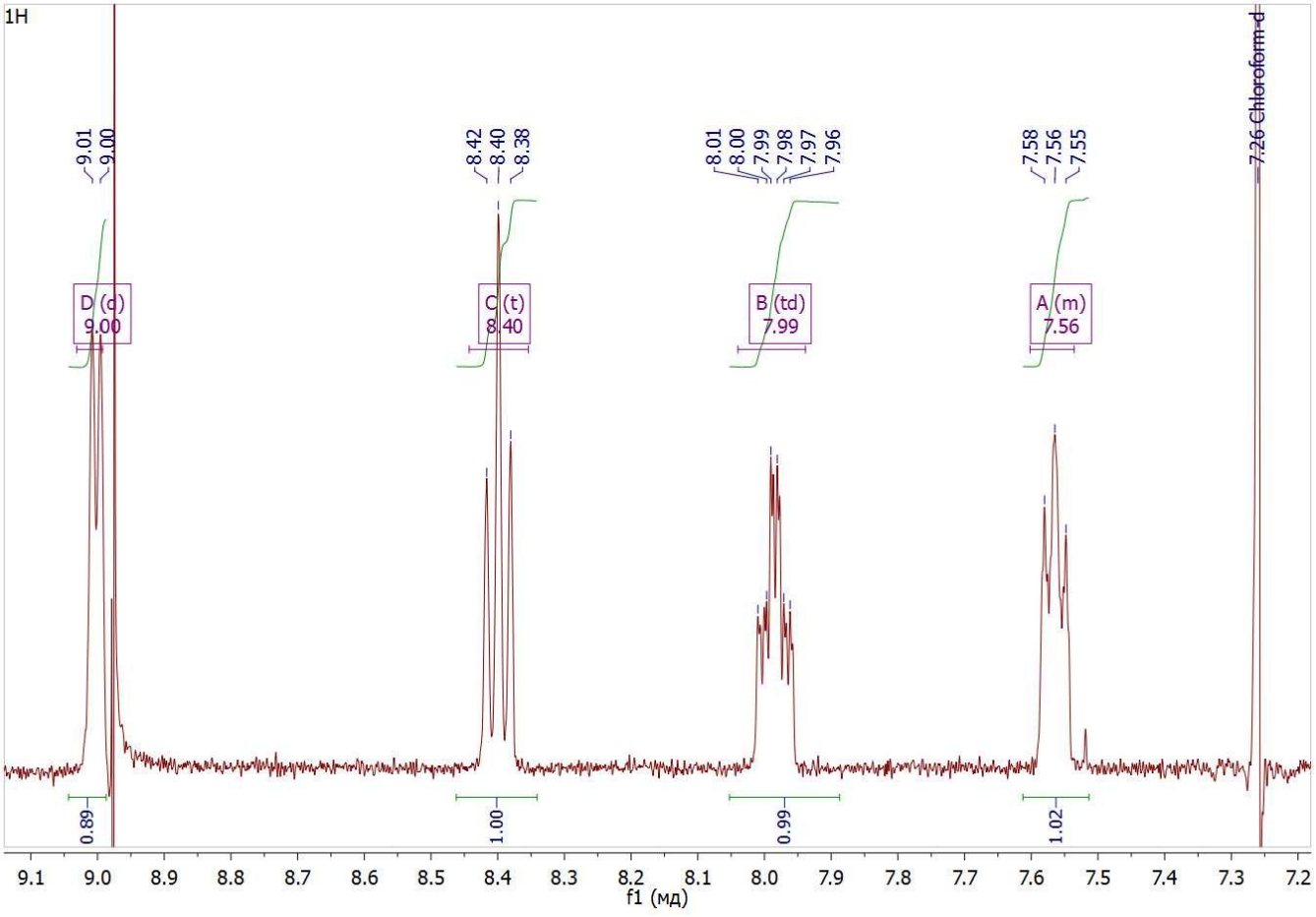


Figure S21. ^{31}P NMR spectrum of complex **4** ($CDCl_3$).

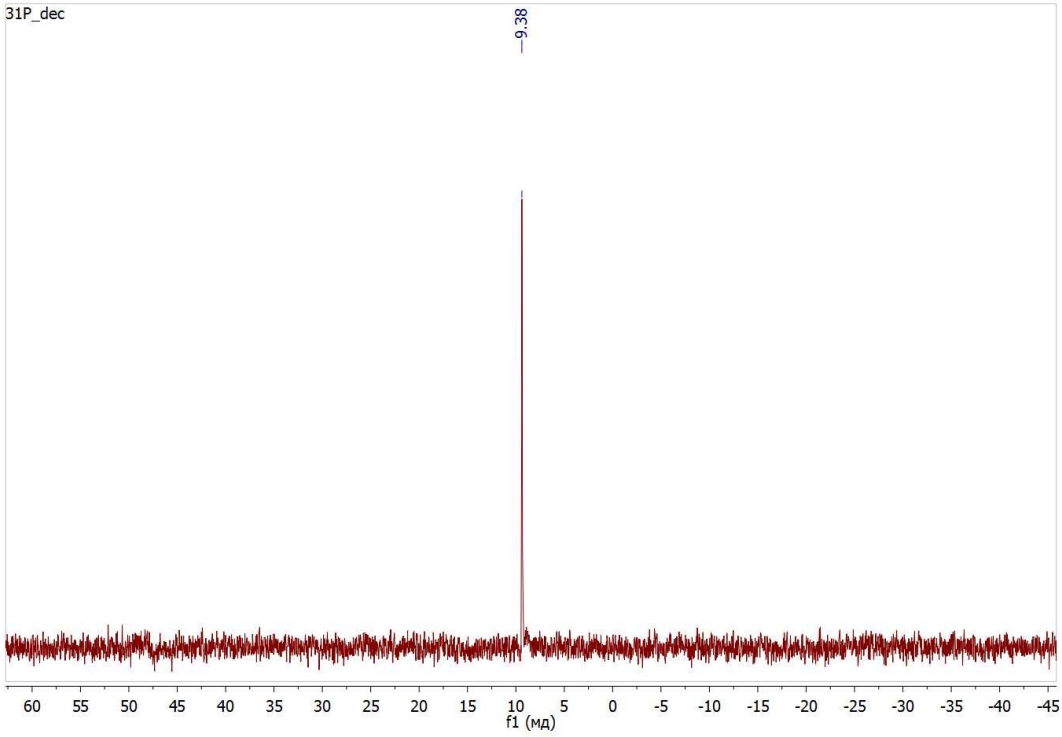


Figure S22. UV-Vis spectrum of complex **6** recorded for $CHCl_3$ solution.

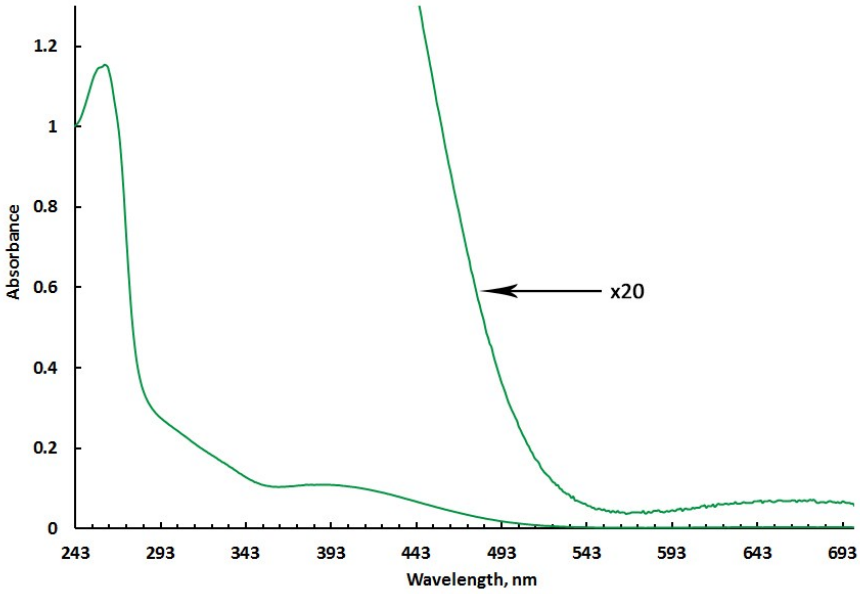
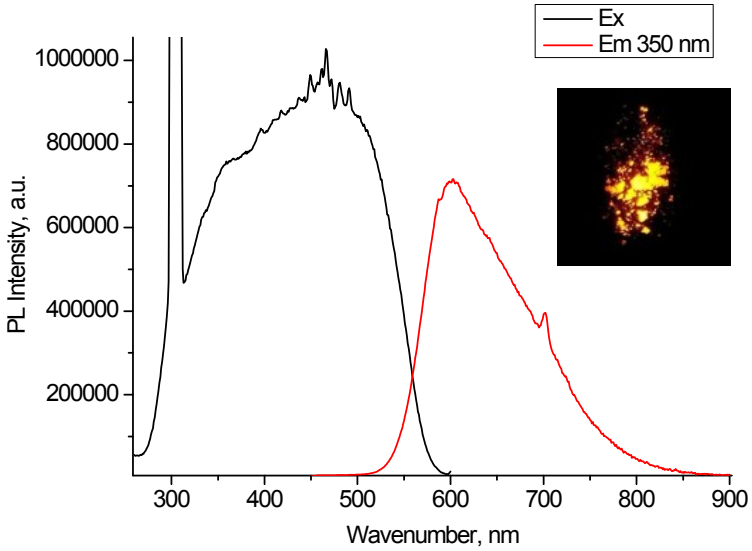
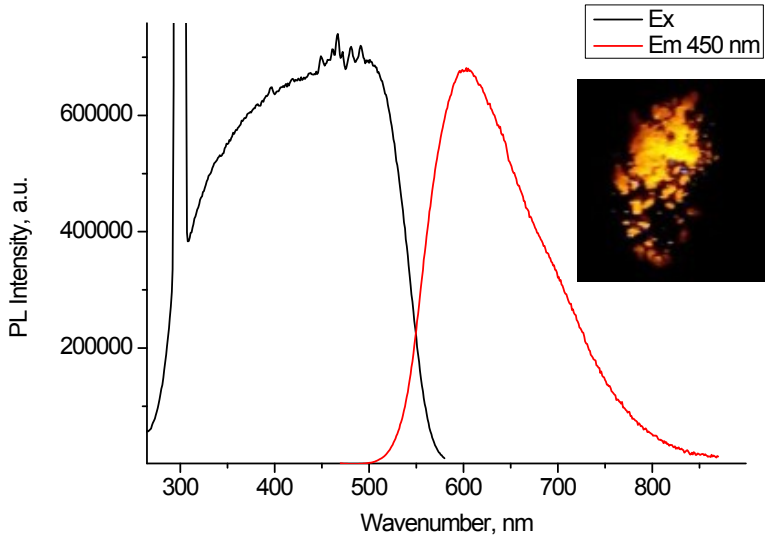


Figure S23. The excitation and emission spectra of complex **1**·CH_2Cl_2.



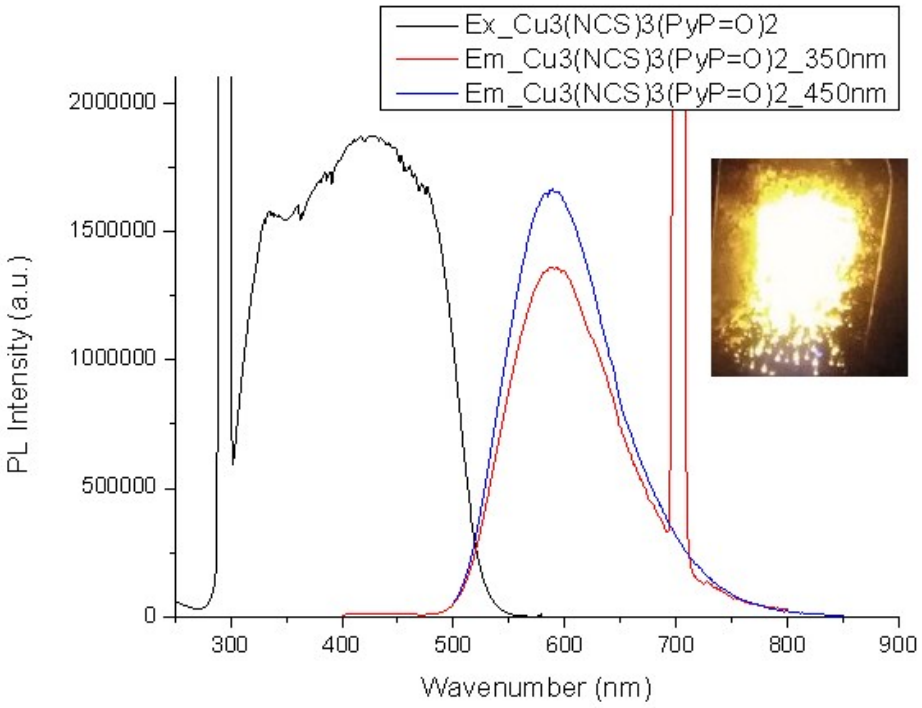
The complex [Cu(*N*,*N*′,*N*″-Py_3P=O)(*N*CS)]·CH_2Cl_2 (**1**·CH_2Cl_2) manifest red luminescence in the solid state at room temperature. The excitation maximum for this compound is about 450 nm. The powder of compounds exhibit photoluminescence with a broad emission with two maxima at *ca.* 610 nm (λ_{exc} = 350 nm). A peak at 700 nm is second harmonic. Quantum yield, ϕ_{PL} = 2%.

Figure S24. The excitation and emission spectra of complex **2**.



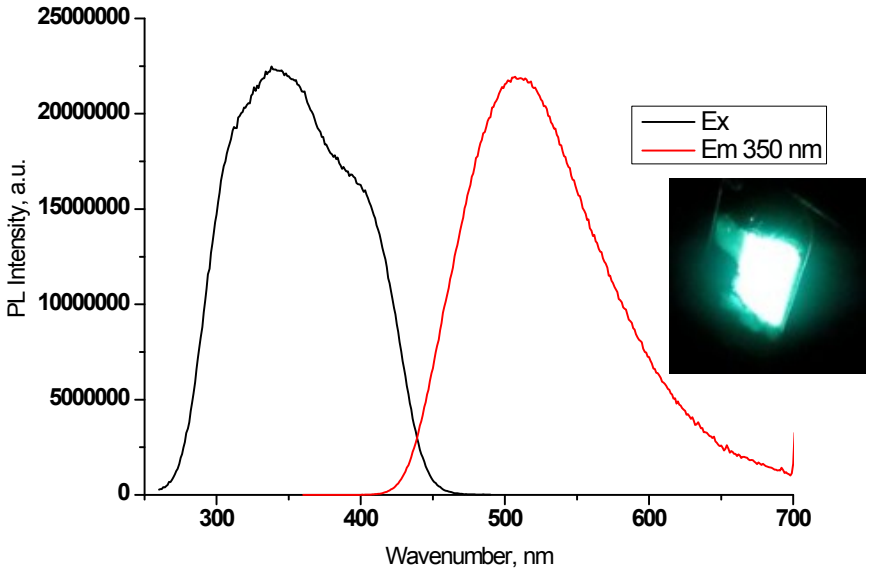
The complex [(*N*,*N*′-Py_3P=O)Cu$\binom{SCN}{NCS}$Cu[(*N*,*N*′-Py_3P=O)] (**2**) manifest orange-red luminescence in the solid state at room temperature. The excitation maximum for compound is about 450 nm. Taking into account these data, were used as the excitation wavelengths 450 nm for recording of emission spectra. The powder of the complex exhibit orange-red photoluminescence with a broad emission with maxima at *ca.* 600 nm. Quantum yield, ϕ_{PL} = 0.5%.

Figure S25. The excitation and emission spectra of complex **4**·2CHCl$_3$.



The compounds {Cu(*N*CS)[(*S*CNCu(*N*,*N*′,*N*″-Py$_3$P=O)]$_2$}·2CHCl$_3$ (**4**·2CHCl$_3$) manifest orange luminescence in the solid state at room temperature. The excitation maximum for compounds is about 350 and 450 nm. Taking into account these data, were used as the excitation wavelengths 350 and 450 nm for recording of emission spectra. The powder of compounds exhibit orange photoluminescence with a broad emission with maxima at *ca.* 590 nm. Quantum yield = 3%.

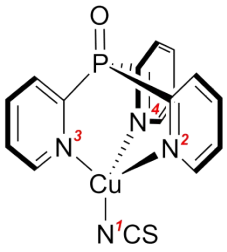
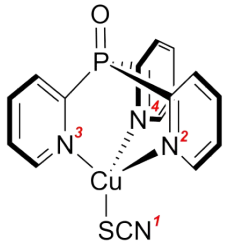
Figure S26. The excitation and emission spectra of complex **5**.



The compounds [Cu(Py$_3$P)NCS]$_n$ (**5**) manifest green luminescence in the solid state at room temperature. The excitation maximum for compounds is about 350 nm. Taking into account these data, were used as the

excitation wavelengths 350 nm for recording of emission spectra. The powder of compounds exhibit green photoluminescence with a broad emission with maxima at *ca.* 510 nm. Quantum yield = 10%.

Table S2. B3LYP/def2-TZVPP selected structural parameters (bond lengths are given in Å and bond angles in degrees) of the isomers **1** and **1′** and the relative stabilities[a] in gas phase (isolated molecule) and in $CHCl_3$ solution (in parentheses).

Isomer **1**		
	Cu–N^1	1.898 (1.919)
	Cu–N^{2,3,4} (mean)	2.143 (2.140)
	N^1–C	1.177 (1.173)
	S–C	1.620 (1.633)
	C–N^1–Cu	179.9 (179.9)
	N^1–C–S	180.0 (180.0)
	τ_4[b]	0.81 (0.81)
	ΔE	0.00 (0.00)
	ΔG	0.00 (0.00)
Isomer **1′**		
	Cu–S	2.273 (2.287)
	Cu–N^{2,3,4} (mean)	2.146 (2.137)
	S–C	1.677 (1.671)
	N^1–C	1.165 (1.166)
	C–S–Cu	96.1 (101.2)
	N^1–C–S	179.2 (179.4)
	τ_4[b]	0.80 (0.81)
	ΔE	1.74 (3.28)
	ΔG	3.00 (5.14)

[a] The difference in internal energies of the isomers **1**, **1′** corrected for the zero-point vibrational energies (ΔE, kcal mol^{-1}) and in Gibbs free energies (ΔG, kcal·mol^{-1}) calculated under the normal conditions (298.15 K, 1 atm). [b] τ_4 is the four-coordinate geometry index of coordination Cu center.

Table S3. Selected structural parameters of the complex SC*N*Cu(*N*,*N*′,*N*″-Py_3P=O), **1**, in gas phase (isolated molecule), in $CHCl_3$ solution and in crystal.

Medium	Gas	$CHCl_3$ solution (ε = 4.71)	Crystal
Method	B3LYP/ def2-TZVPP	C-PCM B3LYP/ def2-TZVPP	X-Ray
Cu(1)–N(1)	1.898	1.919	1.889(2)
Cu(1)–N(2)	2.140	2.138	2.094(2)
Cu(1)–N(3)	2.146	2.142	2.068(2)
Cu(1)–N(4)	2.143	2.140	2.081(2)

P(1)–O(1)	1.482	1.486	1.4805(19)
N(1)–C(1)	1.177	1.173	1.150(3)
S(1)–C(1)	1.620	1.633	1.627(3)
N(1)–Cu(1)–N(3)	123.4	122.8	126.20(9)
N(1)–Cu(1)–N(4)	122.9	122.4	126.34(9)
N(1)–Cu(1)–N(2)	122.8	122.4	112.35(10)
C(1)–N(1)–Cu(1)	179.9	179.9	166.2(2)
N(1)–C(1)–S(1)	180.0	180.0	179.3(3)
$\tau_4{}^a$	0.81	0.81	0.76

[a] τ_4 is the four-coordinate geometry index.

Table S4. Selected structural parameters of the complex NC*S*Cu(*N*,*N*′,*N*″-Py_3P=O), **1**′, in gas phase (isolated molecule), in $CHCl_3$ solution.

Medium	Gas	$CHCl_3$ solution (ε = 4.71)
Method	B3LYP/ def2-TZVPP	C-PCM B3LYP/ def2-TZVPP
Cu(1)–S(1)	2.273	2.287
Cu(1)–N(2)	2.125	2.117
Cu(1)–N(3)	2.158	2.147
Cu(1)–N(4)	2.155	2.147
P(1)–O(1)	1.483	1.486
N(1)–C(1)	1.165	1.166
S(2)–C(1)	1.677	1.671
S(1)–Cu(1)–N(3)	127.3	126.8
S(1)–Cu(1)–N(4)	120.3	119.7
S(1)–Cu(1)–N(2)	120.4	119.8
C(1)–S(1)–Cu(1)	96.1	101.2
N(1)–C(1)–S(1)	179.2	179.4
$\tau_4{}^a$	0.80	0.80

[a] τ_4 is the four-coordinate geometry index.

Table S5. Selected structural parameters of the complex (*N*,*N*′-Py_3P=O)Cu$^{(SCN}_{NCS)}$Cu(*N*,*N*′-Py_3P=O), **2**, in gas phase (isolated molecule), in $CHCl_3$ solution and in crystal.

Medium	Gas	$CHCl_3$ solution (ε = 4.71)	Crystal
Method	B3LYP/ def2-TZVPP	C-PCM B3LYP/ def2-TZVPP	X-Ray
Cu(1)–N(1)	1.957	1.961	1.925(9)
Cu(1)–N(2)	2.126	2.122	2.075(9)
Cu(1)–N(4)	2.146	2.131	2.074(9)
Cu(1)–S(1′)	2.463	2.508	2.400(3)
P(1)–O(1)	1.484	1.489	1.472(8)
N(1)–C(1)	1.166	1.167	1.181(14)
S(1)–C(1)	1.651	1.649	1.623(11)
N(1)–Cu(1)–S(1′)	107.1	104.4	102.1(3)
N(1)–Cu(1)–N(4)	120.1	123.1	125.4(4)
N(1)–Cu(1)–N(2)	123.2	122.7	118.1(4)

C(1)–N(1)–Cu(1)	158.0	159.4	161.9(9)
N(1)–C(1)–S(1)	179.2	179.1	178.3(11)
τ_4[a]	0.83	0.81	0.83

[a] τ_4 is the four-coordinate geometry index.

Table S6. Selected structural parameters of the complex SC*N*Cu(*N*,*N*′,*N*″-Py_3P=O), **1**, in its S_0 and T_1 states calculated at the C-PCM (ε = 4.71) B3LYP/def2-TZVPP level of theory.

	S_0	T_1	Δ[a]
Cu(1)–N(1)	1.919	1.889	0.030
Cu(1)–N(2)	2.138	2.124	0.014
Cu(1)–N(3)	2.142	1.930	0.212
Cu(1)–N(4)	2.140	2.124	0.016
P(1)–O(1)	1.486	1.487	-0.001
N(1)–C(1)	1.173	1.179	-0.006
S(1)–C(1)	1.633	1.609	0.024
N(1)–Cu(1)–N(3)	122.8	151.2	-28.4
N(1)–Cu(1)–N(4)	122.4	105.2	17.2
N(1)–Cu(1)–N(2)	122.4	105.2	17.2
C(1)–N(1)–Cu(1)	179.9	165.9	14.0
N(1)–C(1)–S(1)	180.0	178.8	1.2
τ_4[b]	0.81	0.73	

[a] Differences between structural parameters of S_0 and T_1 states of complex **1**. [b] τ_4 is the four-coordinate geometry index.

Table S7. Selected structural parameters of the complex Cu*N*CS[*S*CNCu(*N*,*N*′,*N*″-Py_3P=O)]$_2$, **4**, in gas phase (isolated molecule), in $CHCl_3$ solution and in crystals.

Medium	Gas	$CHCl_3$ solution (ε = 4.71)	Crystal
Method	B3LYP/ def2-TZVPP	C-PCM B3LYP/ def2-TZVPP	X-Ray
Cu(1)–N(7)	1.926	1.928	1.912(3)
Cu(1)–S(2)	2.334	2.324	2.2266(10)
Cu(1)–S(3)	2.334	2.324	2.2412(11)
Cu(2)–N(8)	1.909	1.922	1.895(3)
Cu(2)–N(5)	2.149	2.140	2.034(3)
Cu(2)–N(4)	2.144	2.140	2.086(3)
Cu(2)–N(6)	2.119	2.126	2.095(3)
Cu(3)–N(9)	1.909	1.922	1.896(3)
Cu(3)–N(1)	2.144	2.140	2.063(3)
Cu(3)–N(3)	2.149	2.140	2.066(3)
Cu(3)–N(2)	2.120	2.126	2.079(3)
N(7)–C(2)	1.170	1.171	1.137(5)
N(8)–C(3)	1.168	1.166	1.147(4)
N(9)–C(19)	1.168	1.166	1.135(4)
S(1)–C(2)	1.639	1.636	1.634(4)
S(2)–C(3)	1.643	1.652	1.657(4)
S(3)–C(19)	1.644	1.652	1.658(4)
P(1)–O(1)	1.483	1.486	1.485(2)
P(2)–O(2)	1.483	1.486	1.481(3)
N(7)–Cu(1)–S(2)	128.0	126.5	126.09(10)

N(7)–Cu(1)–S(3)	128.1	126.5	121.03(10)
S(2)–Cu(1)–S(3)	103.9	107.0	112.88(4)
N(8)–Cu(2)–N(4)	122.6	122.1	118.21(13)
N(8)–Cu(2)–N(5)	121.7	122.0	131.56(13)
N(8)–Cu(2)–N(6)	123.3	122.6	113.32(12)
N(9)–Cu(3)–N(1)	122.6	122.1	122.38(12)
N(9)–Cu(3)–N(2)	123.2	122.6	120.27(12)
N(9)–Cu(3)–N(3)	121.8	122.0	120.38(12)
C(2)–N(7)–Cu(1)	179.1	179.5	176.3(3)
N(7)–C(2)–S(1)	179.9	180.0	179.5(4)
C(3)–S(2)–Cu(1)	103.5	103.6	104.7(1)
C(19)–S(3)–Cu(1)	103.5	103.6	103.6(1)
C(3)–N(8)–Cu(2)	173.4	178.0	167.6(3)
N(8)–C(3)–S(2)	178.3	178.4	178.2(3)
C(19)–N(9)–Cu(3)	173.4	178.0	173.6(3)
N(9)–C(19)–S(3)	178.3	178.4	177.8(4)
τ_4 [Cu(2) / Cu(3)][a]	0.81 / 0.81	0.82 / 0.82	0.82 / 0.83
$\Delta_{Cu(1)}$[b]	0.003	0.000	0.002
$\Delta_{S(1)}$[c]	0.007	0.308	0.184
$\Delta_{S(2)}$[c]	0.018	0.083	0.502
$\Delta_{S(3)}$[c]	0.017	0.082	0.469
$\Delta_{N(7)}$[d]	0.017	0.115	0.055
$\Delta_{N(8)}$[d]	0.014	0.029	0.451
$\Delta_{N(9)}$[d]	0.013	0.028	0.326

[a] τ_4 is the four-coordinate geometry index. [b] $\Delta_{Cu(1)}$ is the displacement of the Cu(1) atom out of the plane of N(7), S(2) and S(3) atoms. [c] $\Delta_{S(n)}$ is the displacement of the S(n) atom out of the plane of three Cu atoms, n = 1-3. [d] $\Delta_{N(n)}$ is the displacement of the N(n) atom out of the plane of three Cu atoms, n = 7-9.

Table S8. Singlet-singlet electronic transitions (oscillator strength, *f*, is equal to or greater than 0.01) in the absorption spectra of the complex **1** in $CHCl_3$ solution.

Transitions	Character	*E* (eV)	λ (nm)	*f*
HOMO−4 → LUMO (2%) HOMO−3 → LUMO+1 (2%) HOMO−1 → LUMO+1 (38%) HOMO → LUMO (55%)	(M+L^{SCN})LCT	2.4457	506.95	0.0099
HOMO−4 → LUMO+1 (2%) HOMO−3 → LUMO (2%) HOMO−1 → LUMO (49%) HOMO → LUMO+1 (44%)	(M+L^{SCN})LCT	2.4463	506.82	0.0100
HOMO−6 → LUMO+1 (2%) HOMO−5 → LUMO (3%) HOMO−4 → LUMO (18%) HOMO−3 → LUMO+1 (16%)	(M+L^{SCN})LCT	3.1807	389.80	0.0095

HOMO−1 → LUMO+2 (2%) HOMO−1 → LUMO+4 (22%) HOMO → LUMO+2 (2%) HOMO → LUMO+3 (27%)				
HOMO−5 → LUMO+1 (4%) HOMO−4 → LUMO+1 (23%) HOMO−3 → LUMO (11%) HOMO−1 → LUMO+2 (2%) HOMO−1 → LUMO+3 (29%) HOMO → LUMO+4 (20%)	$(M+L^{SCN})LCT$	3.1813	389.73	0.0095
HOMO−6 → LUMO+1 (3%) HOMO−5 → LUMO (4%) HOMO−4 → LUMO (20%) HOMO−4 → LUMO+1 (5%) HOMO−3 → LUMO (3%) HOMO−3 → LUMO+1 (20%) HOMO−1 → LUMO+4 (17%) HOMO → LUMO+3 (24%)	$(M+L^{SCN})LCT$	3.1919	388.43	0.0143
HOMO−6 → LUMO (3%) HOMO−5 → LUMO+1 (4%) HOMO−4 → LUMO (3%) HOMO−4 → LUMO+1 (22%) HOMO−3 → LUMO (17%) HOMO−3 → LUMO+1 (5%) HOMO−1 → LUMO+3 (20%) HOMO → LUMO+4 (21%)	$(M+L^{SCN})LCT$	3.1924	388.37	0.0145
HOMO−4 → LUMO (38%) HOMO−4 → LUMO+1 (9%) HOMO−3 → LUMO (9%) HOMO−3 → LUMO+1 (38%)	$(M+L^{SCN})LCT$	3.4239	362.12	0.0453
HOMO−6 → LUMO (6%) HOMO−6 → LUMO+1 (42%) HOMO−5 → LUMO (38%) HOMO−5 → LUMO+1 (6%)	$(M+L^{SCN})LCT$	3.7668	329.15	0.0374
HOMO−6 → LUMO+2 (7%)	$(M+L^{SCN})LCT$	3.8543	321.67	0.0195

HOMO−3 → LUMO+2 (89%) HOMO−1 → LUMO+2 (3%)				
HOMO−5 → LUMO+2 (8%) HOMO−4 → LUMO+2 (89%) HOMO → LUMO+2 (3%)	(M+L^{SCN})LCT	3.8589	321.29	0.0195
HOMO−4 → LUMO+3 (34%) HOMO−4 → LUMO+4 (19%) HOMO−3 → LUMO+3 (12%) HOMO−3 → LUMO+4 (25%)	(M+L^{SCN})LCT	3.9651	312.69	0.0075
HOMO−5 → LUMO+2 (91%) HOMO−4 → LUMO+2 (7%)	(M+L^{SCN})LCT	4.3099	287.67	0.0056
HOMO−6 → LUMO+2 (91%) HOMO−3 → LUMO+2 (6%)	(M+L^{SCN})LCT	4.3125	287.50	0.0056
HOMO−6 → LUMO+3 (13%) HOMO−6 → LUMO+4 (37%) HOMO−5 → LUMO+3 (31%) HOMO−5 → LUMO+4 (12%)	(M+L^{SCN})LCT	4.4350	279.56	0.0112
HOMO−7 → LUMO (5%) HOMO−5 → LUMO+5 (85%) HOMO−4 → LUMO+5 (5%)	ILT (M+L^{SCN})LCT	4.9596	249.99	0.0141
HOMO−7 → LUMO+1 (5%) HOMO−6 → LUMO+5 (85%) HOMO−3 → LUMO+5 (5%)	ILT (M+L^{SCN})LCT	4.9622	249.86	0.0144
HOMO−7 → LUMO (78%) HOMO−5 → LUMO+5 (6%) HOMO−1 → LUMO+7 (3%)	ILT (M+L^{SCN})LCT	5.0823	243.95	0.2055
HOMO−7 → LUMO+1 (79%) HOMO−6 → LUMO+5 (6%) HOMO → LUMO+7 (3%)	ILT (M+L^{SCN})LCT	5.0846	243.84	0.2065
HOMO−11 → LUMO (7%) HOMO−11 → LUMO+1 (3%) HOMO−10 → LUMO (2%) HOMO−10 → LUMO+1 (7%) HOMO−9 → LUMO (21%) HOMO−9 → LUMO+1 (15%)	ILT	5.1780	239.45	0.0502

HOMO−8 → LUMO (14%) HOMO−8 → LUMO+1 (21%) HOMO−7 → LUMO (2%) HOMO−7 → LUMO+1 (4%)				
HOMO−11 → LUMO (3%) HOMO−11 → LUMO+1 (7%) HOMO−10 → LUMO (7%) HOMO−10 → LUMO+1 (3%) HOMO−9 → LUMO (14%) HOMO−9 → LUMO+1 (21%) HOMO−8 → LUMO (20%) HOMO−8 → LUMO+1 (14%) HOMO−7 → LUMO (4%) HOMO−7 → LUMO+1 (3%)	ILT	5.1782	239.43	0.0482

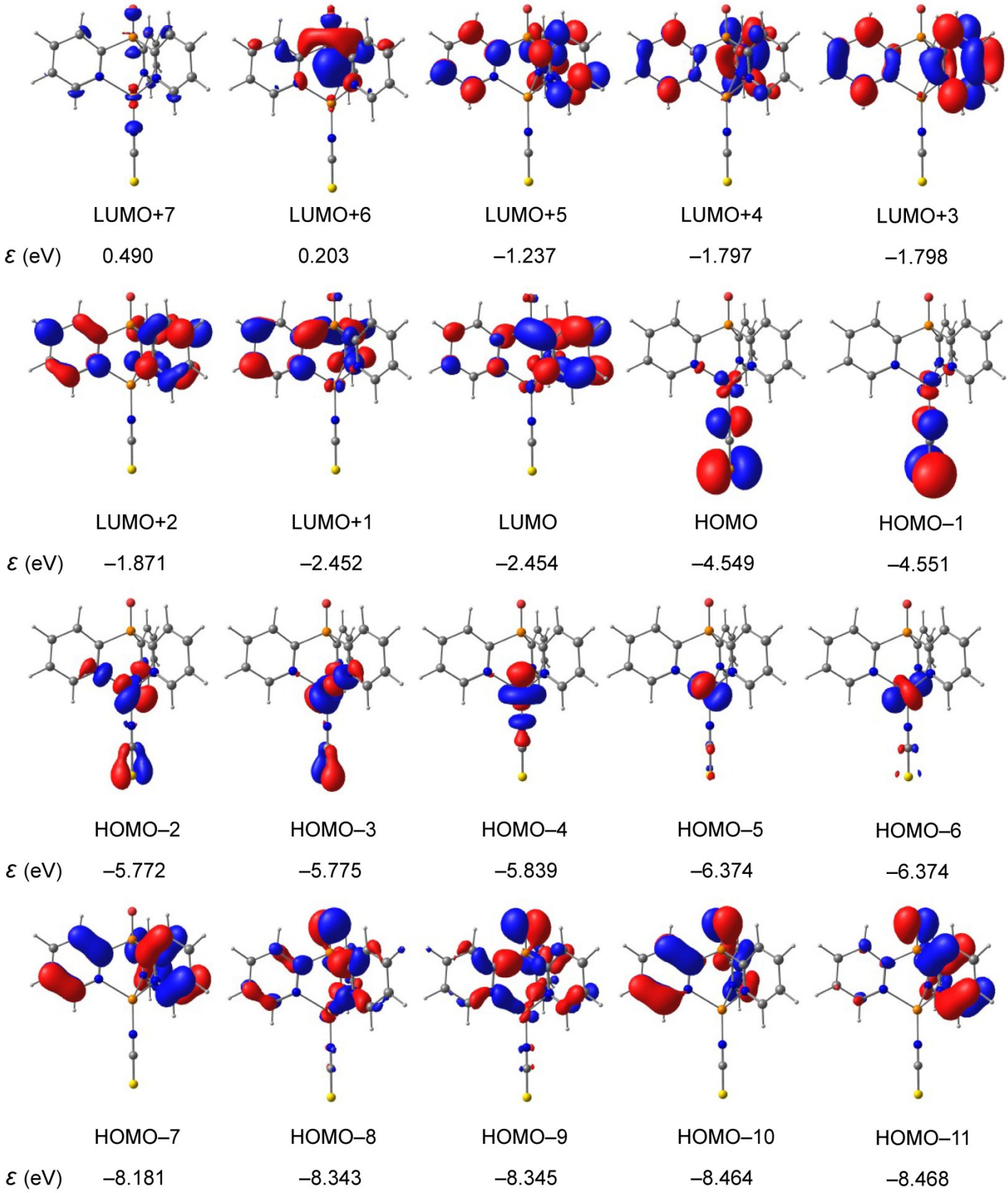
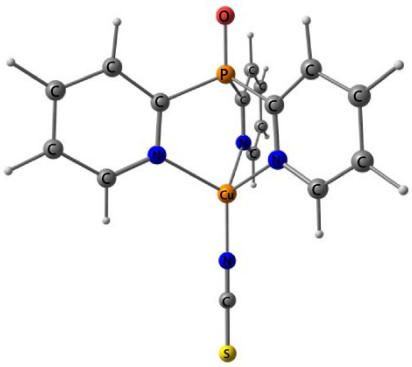


Figure S27. Molecular orbitals involved in the electronic transitions of the complex **1**.

Structural and thermochemical data for the computed structures

Complex 1, SC*N*Cu(*N*,*N*′,*N*″-Py_3P=O), B3LYP/def2-TZVPP

Cu	-1.084222	-0.011872	-0.001326
P	2.142947	0.006446	-0.005992
O	3.625350	0.012357	-0.010217
N	0.089374	-1.709161	-0.568125
N	0.085756	0.356727	1.759124
N	0.074204	1.342471	-1.192024
C	-4.159247	-0.008301	0.004284
C	1.425127	-1.592360	-0.539040
C	1.421937	0.337419	1.645630
C	-0.449108	0.597281	2.958530
H	-1.530525	0.603545	3.002655
C	0.329070	0.826401	4.086928
H	-0.148397	1.016701	5.037812
C	1.711606	0.805501	3.966860
H	2.342718	0.980200	4.827856
C	2.275161	0.556213	2.721016
H	3.344699	0.528415	2.567987
C	1.410990	1.267392	-1.115394
C	-0.467939	2.260923	-1.995157
H	-1.549593	2.285169	-2.025093
C	0.303309	3.136894	-2.749651
H	-0.179965	3.864696	-3.386131
C	1.686577	3.057252	-2.668368
H	2.312440	3.726118	-3.243748
C	2.257665	2.102997	-1.834591
H	3.328052	1.994810	-1.731407
C	2.282553	-2.627433	-0.893563
H	3.351331	-2.472799	-0.850319
C	1.724188	-3.835332	-1.294744
H	2.358758	-4.664216	-1.578319
C	0.342115	-3.959175	-1.325081
H	-0.131594	-4.881396	-1.630794
C	-0.440513	-2.872343	-0.954249
H	-1.521684	-2.921168	-0.961975
N	-2.982246	-0.010116	0.003598
S	-5.779460	-0.005671	0.005194



Electronic Energy = -3291.787633 a.u.

- Thermochemistry -
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and zero-point Energies=-3291.532888 a.u.
Sum of electronic and thermal Energies=-3291.510595 a.u.
Sum of electronic and thermal Enthalpies=-3291.509651 a.u.
Sum of electronic and thermal Free Energies=-3291.588535 a.u.

Complex 1, SC*N*Cu(*N*,*N*′,*N*″-Py_3P=O), B3LYP/def2-TZVPP, C-PCM ($CHCl_3$)

Cu	-1.072483	0.009590	-0.002896
P	2.132458	-0.004076	-0.005265
O	3.618268	-0.008488	-0.008919
N	0.083017	1.710403	-0.586359
N	0.071709	-1.358386	-1.185671
N	0.080414	-0.342413	1.768234
C	-4.164306	0.005897	0.002960
C	1.419913	1.590930	-0.552807
C	1.409406	-1.277260	-1.104715
C	-0.459411	-2.288576	-1.983721
H	-1.539732	-2.324545	-2.023897
C	0.317705	-3.168771	-2.726639

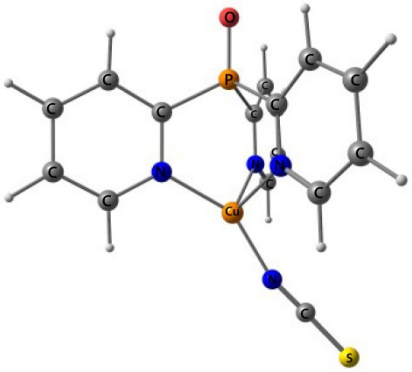
Electronic Energy = -3291.81302819 a.u.

- Thermochemistry -
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and zero-point Energies=-3291.558227 a.u.
Sum of electronic and thermal Energies=-3291.536001 a.u.
Sum of electronic and thermal Enthalpies=-3291.535057 a.u.
Sum of electronic and thermal Free Energies=-3291.613067 a.u.

H	-0.160236	-3.904181	-3.357652
C	1.699406	-3.082348	-2.639892
H	2.331606	-3.753303	-3.204905
C	2.260678	-2.116650	-1.812288
H	3.330346	-2.007788	-1.709245
C	1.417719	-0.321819	1.650365
C	-0.446005	-0.573924	2.973827
H	-1.526134	-0.583368	3.030668
C	0.335591	-0.792146	4.101694
H	-0.138532	-0.974900	5.055242
C	1.716802	-0.769877	3.976060
H	2.352440	-0.935901	4.834818
C	2.273220	-0.529984	2.724898
H	3.342383	-0.502705	2.573777
C	2.279048	2.621200	-0.913683
H	3.347537	2.469981	-0.868236
C	1.727187	3.828246	-1.327041
H	2.365826	4.651726	-1.615325
C	0.346388	3.955722	-1.362488
H	-0.124542	4.875845	-1.677165
C	-0.439089	2.873751	-0.984496
H	-1.518946	2.933904	-0.998361
N	-2.991478	0.007293	0.001658
S	-5.797759	0.003847	0.004835

Complex 1, SC*N*Cu(*N*,*N*′,*N*″-Py_3P=O), B3LYP/def2-TZVPP, C-PCM ($CHCl_3$), T_1

Cu	-0.776787	-0.000125	0.854075
P	1.888600	-0.000072	-0.883441
O	3.109095	-0.000173	-1.732733
N	-0.313169	1.589102	-0.476472
N	-0.313214	-1.589260	-0.476177
N	0.975634	-0.000093	1.661859
C	-3.821031	0.000150	0.781446
C	0.825178	1.463881	-1.191319
C	0.824991	-1.463927	-1.191235
C	-1.059363	-2.688771	-0.624988
H	-1.963275	-2.739231	-0.033490
C	-0.708453	-3.710855	-1.492979
H	-1.344980	-4.578705	-1.584535
C	0.462991	-3.588711	-2.233159
H	0.761154	-4.365728	-2.923556
C	1.242749	-2.451103	-2.077781
H	2.160269	-2.312042	-2.630644
C	2.121488	-0.000061	0.869567
C	1.130286	-0.000055	3.014459
H	0.217657	-0.000125	3.596737
C	2.354062	0.000046	3.622745
H	2.408683	0.000049	4.701562
C	3.535105	0.000123	2.820316
H	4.513967	0.000215	3.277272
C	3.395658	0.000075	1.450754
H	4.258172	0.000115	0.797971
C	1.243145	2.451184	-2.077622
H	2.160773	2.312195	-2.630324
C	0.463430	3.588824	-2.232987



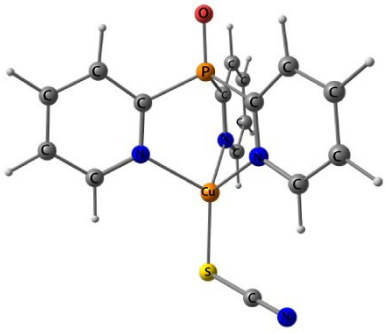
Electronic Energy = -3291.73969381 a.u.

- Thermochemistry -
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and zero-point Energies=-3291.487085 a.u.
Sum of electronic and thermal Energies=-3291.465118 a.u.
Sum of electronic and thermal Enthalpies=-3291.464174 a.u.
Sum of electronic and thermal Free Energies=-3291.541803 a.u.

H	0.761752	4.365950	-2.923194
C	-0.708178	3.710856	-1.493047
H	-1.344683	4.578721	-1.584614
C	-1.059279	2.688636	-0.625289
H	-1.963328	2.739008	-0.033988
N	-2.660608	0.000014	0.987193
S	-5.411142	0.000347	0.532999

Complex 1′, NC*S*Cu(*N*,*N*′,*N*″-Py_3P=O), B3LYP/def2-TZVPP

Cu	-1.059988	0.185984	0.661315
P	1.791195	-0.213560	-0.775076
O	3.101819	-0.397969	-1.442986
N	-0.877846	-0.374126	-1.380598
N	0.394912	-1.261052	1.330342
N	0.402932	1.761110	0.509412
C	-4.022335	0.161543	0.569275
C	0.361604	-0.511338	-1.880098
C	1.548576	-1.338403	0.651320
C	0.202494	-2.090585	2.357907
H	-0.746277	-1.996307	2.870825
C	1.155263	-3.023627	2.748919
H	0.955345	-3.675632	3.587556
C	2.350663	-3.098773	2.047588
H	3.111066	-3.814944	2.328748
C	2.555800	-2.240583	0.973784
H	3.464124	-2.256952	0.388344
C	1.556231	1.478859	-0.113460
C	0.217114	2.996462	0.979276
H	-0.731689	3.179203	1.467610
C	1.176499	3.993345	0.849549
H	0.981997	4.980138	1.245553
C	2.371358	3.697859	0.208021
H	3.136644	4.453562	0.092073
C	2.569618	2.414532	-0.287184
H	3.477388	2.127902	-0.798865
C	0.611014	-0.871139	-3.198214
H	1.631416	-0.965561	-3.541425
C	-0.476525	-1.098862	-4.034435
H	-0.322138	-1.380993	-5.067382
C	-1.756627	-0.958663	-3.521362
H	-2.630058	-1.126466	-4.135501
C	-1.921286	-0.594432	-2.188634
H	-2.906299	-0.474601	-1.751803
S	-2.979166	0.508953	1.834947
N	-4.733492	-0.082526	-0.320083



Electronic Energy = -3291.78480281 a.u.

- Thermochemistry -
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Sum of electronic and zero-point Energies=-3291.530109 a.u.
Sum of electronic and thermal Energies=-3291.507917 a.u.
Sum of electronic and thermal Enthalpies=-3291.506972 a.u.
Sum of electronic and thermal Free Energies=-3291.583753 a.u.

Complex 1′, NC*S*Cu(*N*,*N*′,*N*″-Py_3P=O), B3LYP/def2-TZVPP, C-PCM ($CHCl_3$)

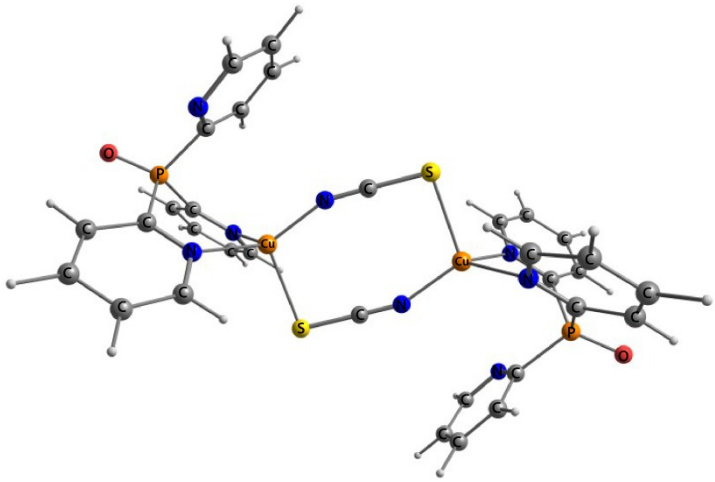
Cu	1.051517	-0.641757	-0.038905
P	-1.809887	0.769014	0.046260
O	-3.135982	1.437850	0.086266
N	0.841879	1.461254	0.083529
N	-0.381494	-1.046487	1.507870
N	-0.384458	-0.864252	-1.619393
C	4.133248	-0.587868	-0.037177
C	-0.409985	1.949052	0.112836

Electronic Energy = -3291.80757397 a.u.

- Thermochemistry -
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and zero-point Energies=-3291.552974 a.u.
Sum of electronic and thermal Energies=-3291.530670 a.u.
Sum of electronic and thermal Enthalpies=-3291.529725 a.u.

C	-1.548987	-0.387237	1.441849	Sum of electronic and thermal Free Energies=-3291.607558 a.u.
C	-0.183416	-1.886379	2.527058	
H	0.770487	-2.396394	2.547535	
C	-1.137494	-2.101463	3.513873	
H	-0.930077	-2.791235	4.319255	
C	-2.343401	-1.419616	3.442074	
H	-3.105829	-1.565298	4.194811	
C	-2.557095	-0.542408	2.385139	
H	-3.477404	0.013964	2.284428	
C	-1.552360	-0.218829	-1.473858	
C	-0.189015	-1.580369	-2.729497	
H	0.765285	-2.083355	-2.812043	
C	-1.146244	-1.681846	-3.731406	
H	-0.940724	-2.274060	-4.611476	
C	-2.352741	-1.014842	-3.577326	
H	-3.117986	-1.073871	-4.338945	
C	-2.563583	-0.265724	-2.425450	
H	-3.484395	0.273583	-2.258436	
C	-0.687866	3.307434	0.191378	
H	-1.713692	3.644837	0.211490	
C	0.377754	4.199039	0.241994	
H	0.197774	5.263449	0.303339	
C	1.670560	3.698686	0.212306	
H	2.527742	4.355395	0.249611	
C	1.862012	2.324316	0.132816	
H	2.855467	1.896191	0.107491	
S	3.009031	-1.821808	-0.105779	
N	4.927314	0.264773	0.010849	

Complex 2, (*N*,*N*′-Py$_3$P=O)Cu $^{(SCN}_{NCS)}$ Cu(*N*,*N*′-Py$_3$P=O), B3LYP/def2-TZVPP

Cu	2.508675	0.545734	0.153670	
S	-1.013307	-2.448148	-0.611515	
P	5.790549	-0.285495	-0.155561	
O	7.265929	-0.416697	-0.251153	
N	1.372789	-1.002897	-0.224561	
N	3.958422	0.573347	1.708629	
N	4.750639	-2.609916	0.624977	
N	3.857522	1.282423	-1.344504	
C	0.390212	-1.608823	-0.386000	
C	3.592617	0.983134	2.927781	
H	2.544573	1.223215	3.049861	
C	4.492760	1.113596	3.976584	
H	4.141894	1.442553	4.944763	
C	5.830927	0.821934	3.754811	
H	6.557636	0.915906	4.550715	
C	6.221144	0.404908	2.489300	
H	7.247434	0.163836	2.252058	
C	5.252629	0.284767	1.500055	
C	4.861404	-1.830080	-0.454229	
C	4.417356	-2.208565	-1.717453	
H	4.523857	-1.545669	-2.564470	
C	3.817436	-3.451963	-1.859133	
H	3.445781	-3.775249	-2.822076	
C	3.689568	-4.262456	-0.741716	

Electronic Energy = -6583.58667797 a.u.

- Thermochemistry -
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and zero-point Energies=-6583.077259 a.u.
Sum of electronic and thermal Energies=-6583.030593 a.u.
Sum of electronic and thermal Enthalpies=-6583.029648 a.u.
Sum of electronic and thermal Free Energies=-6583.166609 a.u.

H	3.216818	-5.232687	-0.804919	
C	4.173363	-3.798179	0.477241	
H	4.089236	-4.405494	1.371128	
C	5.161004	0.956659	-1.352056	
C	3.429703	2.200685	-2.216884	
H	2.377810	2.449106	-2.161645	
C	4.274848	2.819485	-3.129056	
H	3.875513	3.552220	-3.816348	
C	5.621554	2.485847	-3.132128	
H	6.306475	2.953843	-3.826627	
C	6.076249	1.539765	-2.222092	
H	7.113868	1.242382	-2.167332	
Cu	-2.508683	-0.545709	-0.153803	
S	1.013299	2.448199	0.611275	
P	-5.790542	0.285468	0.155712	
O	-7.265916	0.416651	0.251432	
N	-1.372798	1.002944	0.224340	
N	-3.958565	-0.573363	-1.708631	
N	-4.750723	2.609893	-0.624938	
N	-3.857388	-1.282410	1.344499	
C	-0.390220	1.608878	0.385748	
C	-3.592861	-0.983154	-2.927811	
H	-2.544824	-1.223221	-3.049981	
C	-4.493094	-1.113638	-3.976534	
H	-4.142308	-1.442597	-4.944741	
C	-5.831246	-0.821993	-3.754647	
H	-6.558023	-0.915983	-4.550486	
C	-6.221359	-0.404964	-2.489104	
H	-7.247631	-0.163905	-2.251775	
C	-5.252758	-0.284801	-1.499946	
C	-4.861391	1.830068	0.454286	
C	-4.417243	2.208570	1.717469	
H	-4.523666	1.545681	2.564501	
C	-3.817324	3.451976	1.859087	
H	-3.445593	3.775277	2.821996	
C	-3.689557	4.262459	0.741651	
H	-3.216813	5.232696	0.804805	
C	-4.173447	3.798164	-0.477261	
H	-4.089402	4.405471	-1.371162	
C	-5.160874	-0.956667	1.352164	
C	-3.429477	-2.200658	2.216849	
H	-2.377586	-2.449062	2.161519	
C	-4.274532	-2.819463	3.129101	
H	-3.875125	-3.552186	3.816364	
C	-5.621243	-2.485845	3.132289	
H	-6.306095	-2.953845	3.826853	
C	-6.076034	-1.539778	2.222286	
H	-7.113661	-1.242412	2.167615	

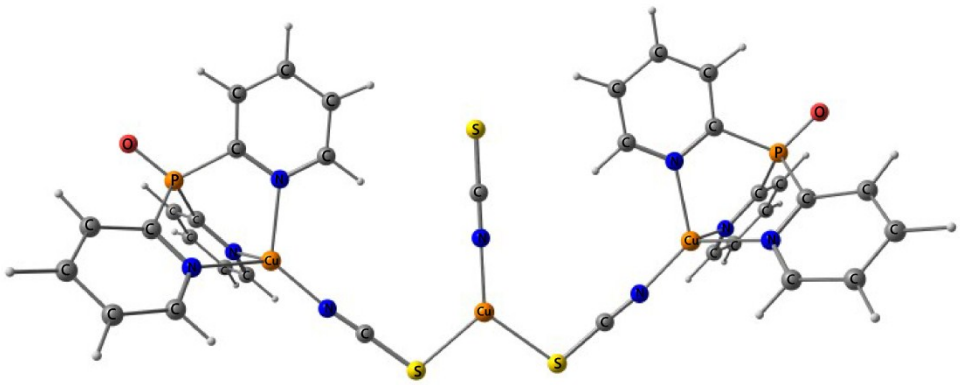
Complex 2, (*N*,*N*′-Py$_3$P=O)Cu $^{(SCN}_{NCS)}$ Cu(*N*,*N*′-Py$_3$P=O), B3LYP/def2-TZVPP, C-PCM ($CHCl_3$)

Cu	2.571014	0.525092	0.102115	
S	-1.015084	-2.457245	-0.470169	Electronic Energy = -6583.61836162 a.u.
P	5.868103	-0.197635	-0.086742	
O	7.353732	-0.289387	-0.130350	- Thermochemistry -

N	1.382890	-1.009933	-0.178159	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
N	3.957561	0.639988	1.703876	Sum of electronic and zero-point Energies=-6583.108885 a.u.
N	4.925359	-2.558217	0.732551	Sum of electronic and thermal Energies=-6583.062068 a.u.
N	3.913069	1.230112	-1.395340	Sum of electronic and thermal Enthalpies=-6583.061123 a.u.
C	0.394907	-1.618867	-0.300417	Sum of electronic and thermal Free Energies=-6583.199568 a.u.
C	3.545166	1.070183	2.901347	
H	2.484996	1.259908	2.998800	
C	4.412158	1.279446	3.965674	
H	4.022494	1.622084	4.913501	
C	5.766768	1.046278	3.783619	
H	6.469725	1.202829	4.590168	
C	6.205381	0.604443	2.541524	
H	7.248521	0.407018	2.343405	
C	5.269752	0.405498	1.534573	
C	5.030122	-1.798236	-0.363702	
C	4.663817	-2.236728	-1.632783	
H	4.767380	-1.593368	-2.494839	
C	4.155644	-3.522777	-1.764937	
H	3.855585	-3.896032	-2.734484	
C	4.035685	-4.313194	-0.631781	
H	3.640206	-5.317518	-0.688228	
C	4.434529	-3.787741	0.593786	
H	4.355449	-4.379763	1.497864	
C	5.230859	0.963426	-1.352962	
C	3.472430	2.078318	-2.330576	
H	2.409991	2.279884	-2.326193	
C	4.314579	2.685700	-3.253251	
H	3.902380	3.358980	-3.991092	
C	5.673247	2.414964	-3.202297	
H	6.356904	2.874148	-3.902960	
C	6.141823	1.539239	-2.230143	
H	7.189979	1.294083	-2.142311	
Cu	-2.571022	-0.525102	-0.102089	
S	1.015077	2.457225	0.470243	
P	-5.868106	0.197649	0.086711	
O	-7.353734	0.289419	0.130297	
N	-1.382897	1.009923	0.178190	
N	-3.957546	-0.640018	-1.703866	
N	-4.925326	2.558211	-0.732601	
N	-3.913104	-1.230094	1.395358	
C	-0.394915	1.618852	0.300473	
C	-3.545136	-1.070233	-2.901324	
H	-2.484967	-1.259969	-2.998757	
C	-4.412114	-1.279501	-3.965662	
H	-4.022438	-1.622155	-4.913479	
C	-5.766724	-1.046317	-3.783632	
H	-6.469670	-1.202872	-4.590190	
C	-6.205353	-0.604461	-2.541550	
H	-7.248494	-0.407023	-2.343450	
C	-5.269738	-0.405512	-1.534587	
C	-5.030106	1.798244	0.363660	
C	-4.663805	2.236745	1.632738	
H	-4.767381	1.593396	2.494801	
C	-4.155604	3.522785	1.764879	
H	-3.855537	3.896042	2.734422	

C	-4.035622	4.313185	0.631715
H	-3.640107	5.317497	0.688149
C	-4.434491	3.787734	-0.593845
H	-4.355363	4.379732	-1.497935
C	-5.230891	-0.963399	1.352957
C	-3.472484	-2.078288	2.330614
H	-2.410047	-2.279863	2.326249
C	-4.314651	-2.685648	3.253287
H	-3.902468	-3.358919	3.991145
C	-5.673317	-2.414902	3.202310
H	-6.356986	-2.874068	3.902971
C	-6.141872	-1.539189	2.230135
H	-7.190025	-1.294026	2.142284

Complex 4, Cu*N*CS[*S*CNCu(*N*,*N*′,*N*″-Py_3P=O)]$_2$, B3LYP/def2-TZVPP



Cu	5.447443	-0.678417	0.017393
P	7.808392	1.493993	-0.025461
O	8.905467	2.491279	-0.044103
N	6.869607	-0.490461	1.610470
N	5.079552	1.405365	-0.098630
N	6.964656	-0.650457	-1.504090
C	3.123416	-2.687875	0.026036
C	7.809251	0.459183	1.487748
C	6.138892	2.231538	-0.114405
C	3.856192	1.939014	-0.158953
H	3.020431	1.252634	-0.140245
C	3.645937	3.311784	-0.239771
H	2.627944	3.672451	-0.281720
C	4.742512	4.159250	-0.258425
H	4.610351	5.231297	-0.320495
C	6.020502	3.612329	-0.193492
H	6.911130	4.224502	-0.202242
C	7.898948	0.308411	-1.420696
C	7.022351	-1.508191	-2.525812
H	6.247779	-2.263366	-2.556592
C	8.012478	-1.442701	-3.498465
H	8.017417	-2.159060	-4.307875
C	8.979028	-0.450695	-3.408423
H	9.762004	-0.374491	-4.150962
C	8.924602	0.446292	-2.348686
H	9.647557	1.240374	-2.227148
C	8.774650	0.695577	2.459588
H	9.506051	1.475752	2.303394
C	8.760029	-0.087769	3.607140

Electronic Energy = -8715.37348432 a.u.

- Thermochemistry -
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and zero-point Energies=-8714.851915 a.u.
Sum of electronic and thermal Energies=-8714.799054 a.u.
Sum of electronic and thermal Enthalpies=-8714.798110 a.u.
Sum of electronic and thermal Free Energies=-8714.955931 a.u.

H	9.494707	0.067853	4.385764
C	7.787733	-1.069547	3.737540
H	7.740105	-1.699142	4.614856
C	6.860893	-1.238651	2.716415
H	6.084598	-1.990304	2.775472
N	4.058917	-1.988567	0.026779
S	1.837126	-3.710869	0.025333
O	-8.902090	2.495228	-0.043011
P	-7.806615	1.496177	-0.024866
C	-7.898714	0.311859	-1.421076
C	-6.135895	2.231054	-0.112722
C	-8.774881	0.697321	2.459250
H	-9.504891	1.478889	2.303509
C	-8.761920	-0.087003	3.606152
C	-7.791333	-1.070547	3.736000
N	-6.871637	-0.491266	1.609655
C	-7.809626	0.460088	1.487468
Cu	-5.449613	-0.680531	0.016747
N	-6.966067	-0.648587	-1.504905
C	-7.024888	-1.505400	-2.527352
H	-6.251621	-2.261892	-2.558478
C	-8.014546	-1.437409	-3.500297
H	-8.020438	-2.153108	-4.310285
C	-8.979394	-0.443791	-3.409808
H	-9.761966	-0.365624	-4.152569
C	-8.923783	0.452254	-2.349341
H	-9.645383	1.247509	-2.227431
C	-6.015108	3.611706	-0.190603
H	-6.904670	4.225433	-0.199089
C	-4.736153	4.156467	-0.254711
H	-4.602128	5.228337	-0.315842
C	-3.641017	3.307122	-0.236479
H	-2.622351	3.666021	-0.277824
C	-3.853706	1.934641	-0.156890
H	-3.019233	1.246670	-0.138568
N	-5.077991	1.403065	-0.097353
C	-6.864506	-1.240380	2.714990
H	-6.089503	-1.993394	2.773656
H	-7.745010	-1.700943	4.612810
N	-4.061409	-1.991029	0.026000
C	-3.125421	-2.689689	0.025217
S	-1.838405	-3.711780	0.024466
H	-9.496541	0.069229	4.384707
Cu	-0.001165	-2.272269	0.011901
N	-0.000478	-0.346154	0.000841
C	0.000928	0.823555	0.013277
S	0.002902	2.462829	0.034325

Complex 4, Cu*N*CS[*S*CNCu(*N*,*N'*,*N''*-$Py_3P{=}O$)]$_2$, B3LYP/def2-TZVPP, C-PCM ($CHCl_3$)

Cu	5.518252	-0.625053	-0.002875
P	7.968348	1.422917	-0.032582
O	9.109530	2.374350	-0.045073
N	7.044042	-0.649162	1.496905
N	5.238947	1.480625	0.086133
N	6.909688	-0.532642	-1.625560

Electronic Energy = -8715.41354164 a.u.

- Thermochemistry -
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Sum of electronic and zero-point Energies=-8714.892134 a.u.

C	3.135533	-2.589160	0.015805	Sum of electronic and thermal Energies=-8714.839195 a.u.
C	8.021746	0.264295	1.384474	Sum of electronic and thermal Enthalpies=-8714.838251 a.u.
C	6.339879	2.250484	0.065945	Sum of electronic and thermal Free Energies=-8714.996568 a.u.
C	4.047529	2.081522	0.157126	
H	3.178498	1.438220	0.171250	
C	3.909293	3.463208	0.210281	
H	2.918837	3.890942	0.265781	
C	5.048094	4.253829	0.189530	
H	4.973739	5.331848	0.229443	
C	6.292477	3.637286	0.115805	
H	7.209824	4.207211	0.096336	
C	7.899139	0.370001	-1.529299	
C	6.854557	-1.297751	-2.719217	
H	6.043963	-2.012503	-2.763616	
C	7.778199	-1.193940	-3.751987	
H	7.689934	-1.836087	-4.616452	
C	8.799462	-0.261060	-3.648314	
H	9.533762	-0.155774	-4.434982	
C	8.864045	0.539643	-2.513963	
H	9.638466	1.281361	-2.384246	
C	9.065613	0.368402	2.294763	
H	9.825307	1.123319	2.154916	
C	9.097395	-0.513545	3.368537	
H	9.895150	-0.461070	4.096509	
C	8.089419	-1.458896	3.488259	
H	8.074904	-2.163322	4.307412	
C	7.081962	-1.493008	2.531960	
H	6.278260	-2.214394	2.591799	
N	4.051296	-1.866936	0.011698	
S	1.868279	-3.648709	0.019515	
O	-9.109583	2.374276	-0.045585	
P	-7.968378	1.422874	-0.032862	
C	-7.898913	0.369854	-1.529496	
C	-6.339944	2.250491	0.065839	
C	-9.065953	0.368507	2.294405	
H	-9.825649	1.123392	2.154390	
C	-9.097864	-0.513358	3.368243	
C	-8.089881	-1.458675	3.488180	
N	-7.044241	-0.649064	1.496914	
C	-8.021954	0.264359	1.384273	
Cu	-5.518227	-0.625025	-0.002629	
N	-6.909419	-0.532764	-1.625540	
C	-6.854084	-1.297938	-2.719140	
H	-6.043461	-2.012669	-2.763362	
C	-7.777558	-1.194218	-3.752069	
H	-7.689129	-1.836415	-4.616480	
C	-8.798869	-0.261365	-3.648620	
H	-9.533044	-0.156152	-4.435414	
C	-8.863665	0.539404	-2.514327	
H	-9.638133	1.281104	-2.384784	
C	-6.292586	3.637298	0.115607	
H	-7.209944	4.207199	0.095969	
C	-5.048229	4.253880	0.189456	
H	-4.973909	5.331904	0.229294	
C	-3.909410	3.463291	0.210409	

H	-2.918973	3.891059	0.265993
C	-4.047602	2.081598	0.157338
H	-3.178554	1.438321	0.171607
N	-5.238993	1.480663	0.086235
C	-7.082288	-1.492834	2.532027
H	-6.278576	-2.214195	2.592035
H	-8.075466	-2.163036	4.307389
N	-4.051268	-1.866901	0.012204
C	-3.135519	-2.589143	0.016394
S	-1.868275	-3.648702	0.020210
H	-9.895724	-0.460849	4.096097
Cu	0.000017	-2.266266	0.054394
N	0.000002	-0.338529	0.102768
C	-0.000026	0.831858	0.142475
S	-0.000055	2.467145	0.198133