Supporting Information

Synthesis, photophysical properties and cation-binding studies of bipyridine-functionalized gold(I) complexes

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Table S1. Crystal data of compounds **1**, **2**, **5** and **2·Pb**.

	1	**2**	**5**	**2·Pb**
Empirical formula	$C_{36}H_{44}AuN_2P$	$C_{27}H_{20}AuN_3$	$C_{34}H_{21}AuF_5N_2$	$C_{27}H_{20}AuCl_2N_3O_8Pb$
Formula weight	732.67	583.43	780.46	989.52
Temperature, K	120(2)	150(2)	150(2)	100(2)
Wavelength, Å	0.71073	0.71073	1.54184	1.54184
Crystal system	Monoclinic	Orthorhombic	Monoclinic	Triclinic
Space group	$P2_1/c$	$Pca2_1$	$P2_1/c$	$P\bar{1}$
Unit cell dimensions				
a, Å	16.065(2)	15.9964(17)	12.5244(8)	10.2908(4)
b, Å	16.647(2)	7.9167(9)	16.1150(11)	12.7994(3)
c, Å	12.6489(16)	34.774(4)	14.6106(10)	13.1593(4)
α, °	90	90	90	105.118(2)
β, °	95.039(3)	90	102.486(1)	91.445(3)
γ, °	90	90	90	101.445(2)
Volume, Å^3	3369.6(8)	4403.7(9)	2879.1(3)	1634.59(9)
Z	4	8	4	2
ρ (calc.), Mg/m^3	1.444	1.760	1.801	2.010
μ, mm^{-1}	4.439 mm^{-1}	6.700	5.225	20.136
F(000)	1472	2256	1512	924
Crystal size, mm^3	0.216 × 0.191 × 0.062	0.841 × 0.550 × 0.066	0.356 × 0.281 × 0.028	0.214 × 0.187 × 0.031
θ range, °	1.272 to 28.000	2.547 to 31.102	1.665 to 33.044	3.491 to 66.990
Index ranges	−21 ≤ h ≤ 21, −21 ≤ k ≤ 21, −16 ≤ l ≤ 16	−22 ≤ h ≤ 22, −11 ≤ k ≤ 10, −50 ≤ l ≤ 50	−17 ≤ h ≤ 19, −24 ≤ k ≤ 24, −22 ≤ l ≤ 22	−12 ≤ h ≤ 12, −15 ≤ k ≤ 13, −15 ≤ l ≤ 15
Reflections collected	60845	35585	80124	20703
Unique reflections	8134 [R(int) = 0.0391]	12251 [R(int) = 0.0416]	10888 [R(int) = 0.0483]	5841 [R(int) = 0.0731]
Completeness to	θ = 25.242° 100.0 %	θ = 25.242° 99.9 %	θ = 25.242° 99.9 %	θ = 66.990° 100.0 %
Absorption correction	Multi-scan	Numerical		Multi-scan
Max. and min. transmission	0.759 and 0.399	0.643 and 0.017	0.864 and 0.187	0.574 and 0.099
Refinement method		Full-matrix least-squares on F^2		
Data / restraints / parameters	8134 / 0 / 361	12251 / 1 / 562	10888 / 0 / 388	5841 / 24 / 380
Goodness-of-fit	1.040	1.017	1.064	1.017
Final R indices [I>2sigma(I)][a]	$R1$ = 0.0174, w$R2$ = 0.0399	$R1$ = 0.0381, w$R2$ = 0.0833	$R1$ = 0.0353, w$R2$ = 0.0703	$R1$ = 0.0567, w$R2$ = 0.1452
R indices (all data)	$R1$ = 0.0227, w$R2$ = 0.0420	$R1$ = 0.0656, w$R2$ = 0.0930	$R1$ = 0.0592, w$R2$ = 0.0774	$R1$ = 0.0613, w$R2$ = 0.1510
Largest diff. peak and hole, e. Å^{-3}	1.205 and −0.713	1.181 and −1.687	1.564 and −1.178	5.710 and −4.338
CCDC number	1570478	1570479	1570481	1570480

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$.

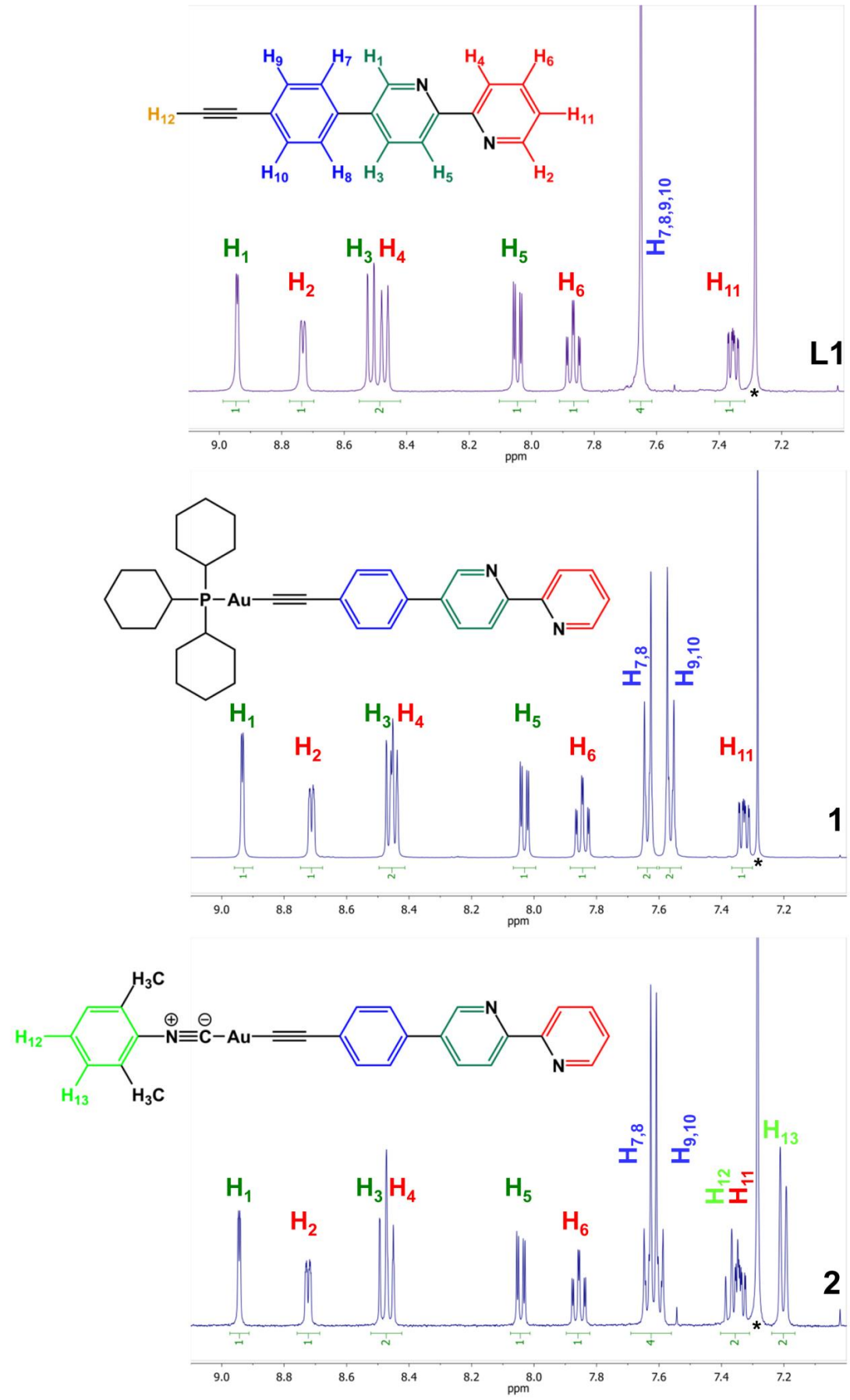

Figure S1. ^{1}H NMR spectrum of **L1**, **1**, and **2**; $CDCl_3$, ambient temperature; signal of $CDCl_3$ residual protons is marked by asterisks.

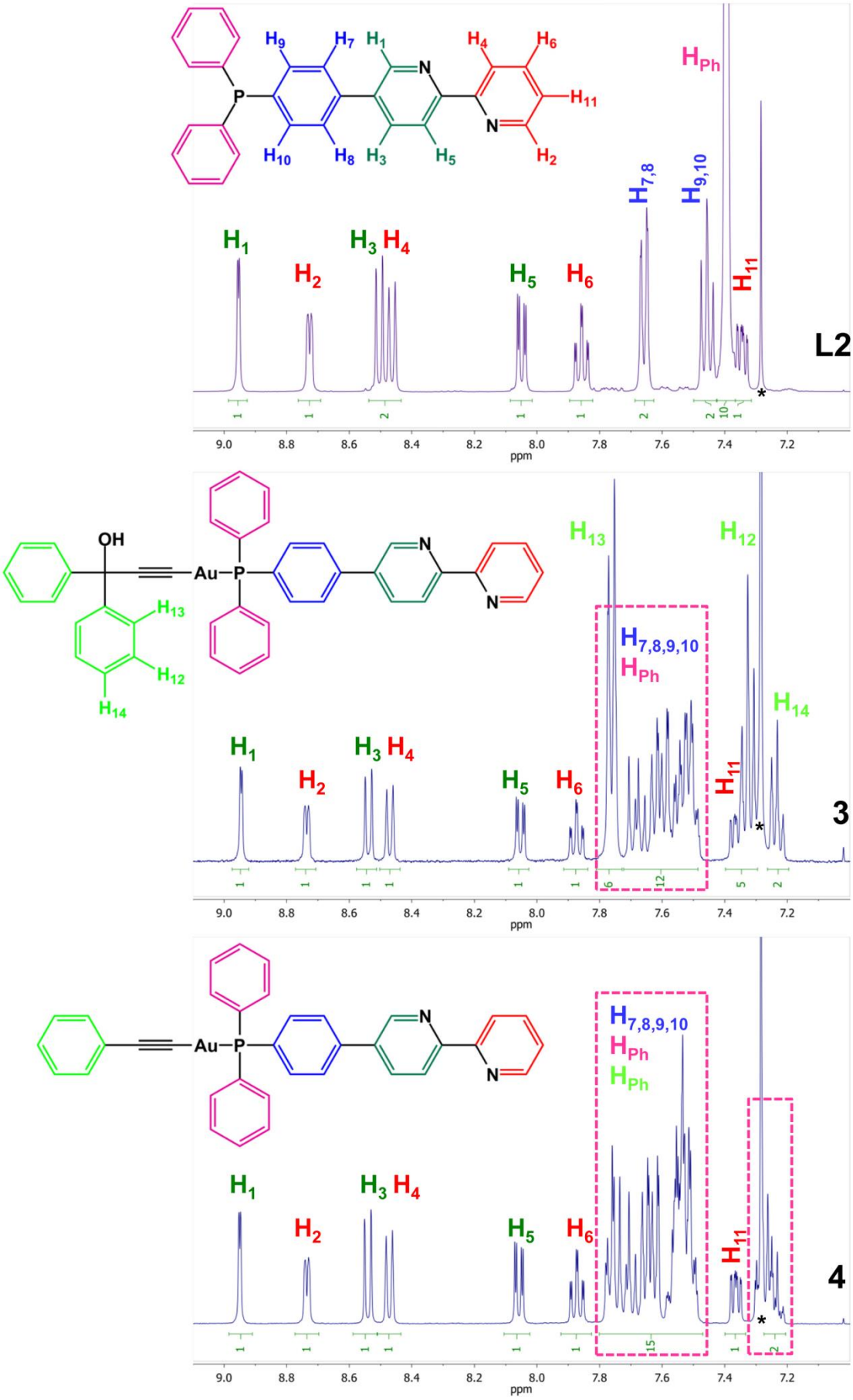

Figure S2. ^{1}H NMR spectrum of **L2**, **3**, and **4**; $CDCl_3$, ambient temperature; signal of $CDCl_3$ residual protons is marked by asterisks.

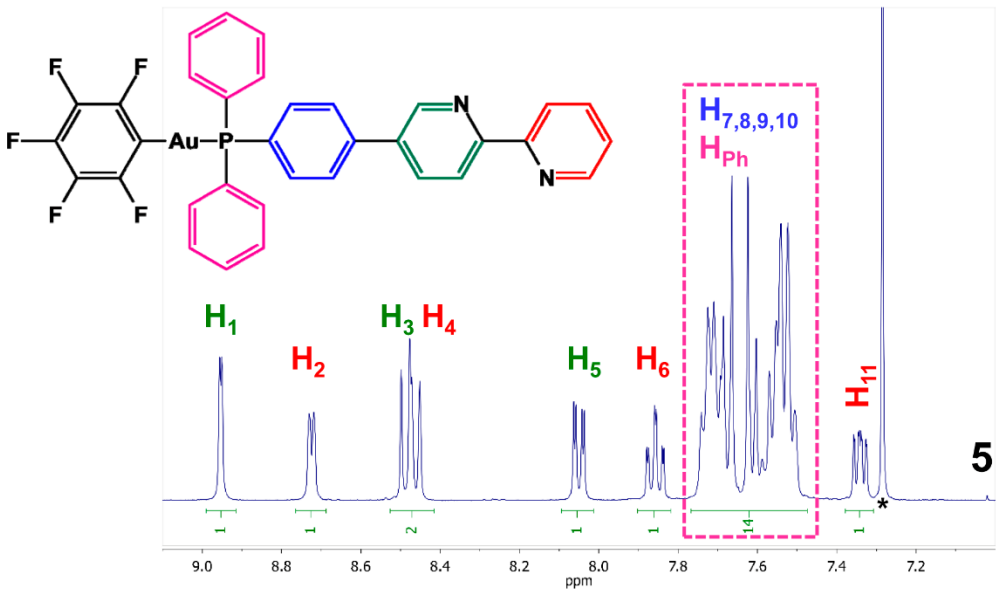

Figure S3. ^{1}H NMR spectrum of **5**; $CDCl_3$, ambient temperature; signal of $CDCl_3$ residual protons is marked by asterisks. For proton numeration see Figs. S1 and S2.

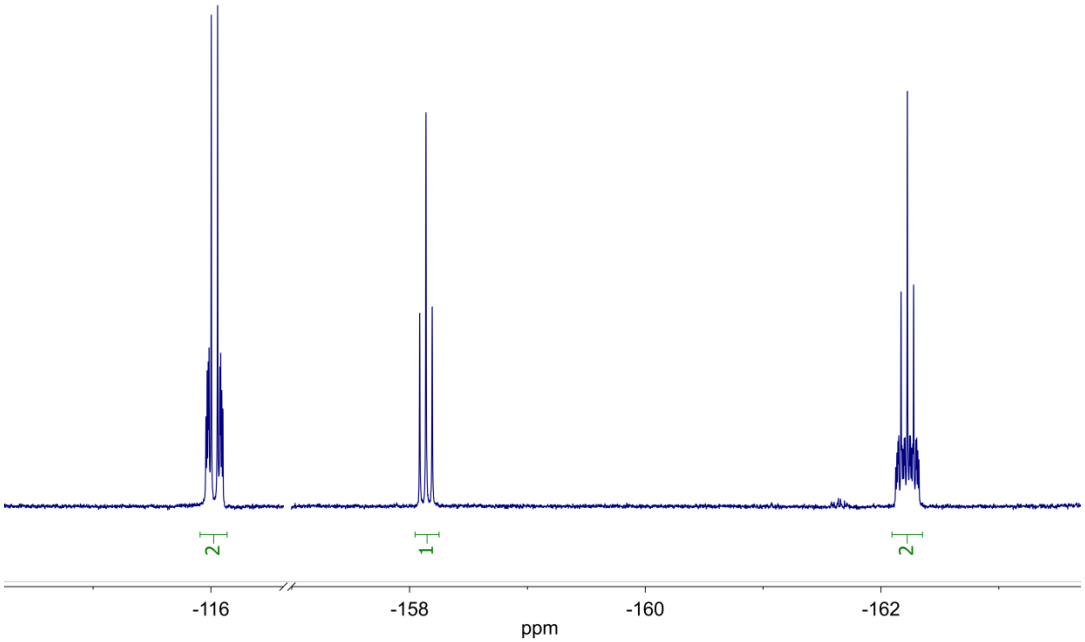

Figure S4. ^{19}F NMR spectrum of **5**; $CDCl_3$, ambient temperature.

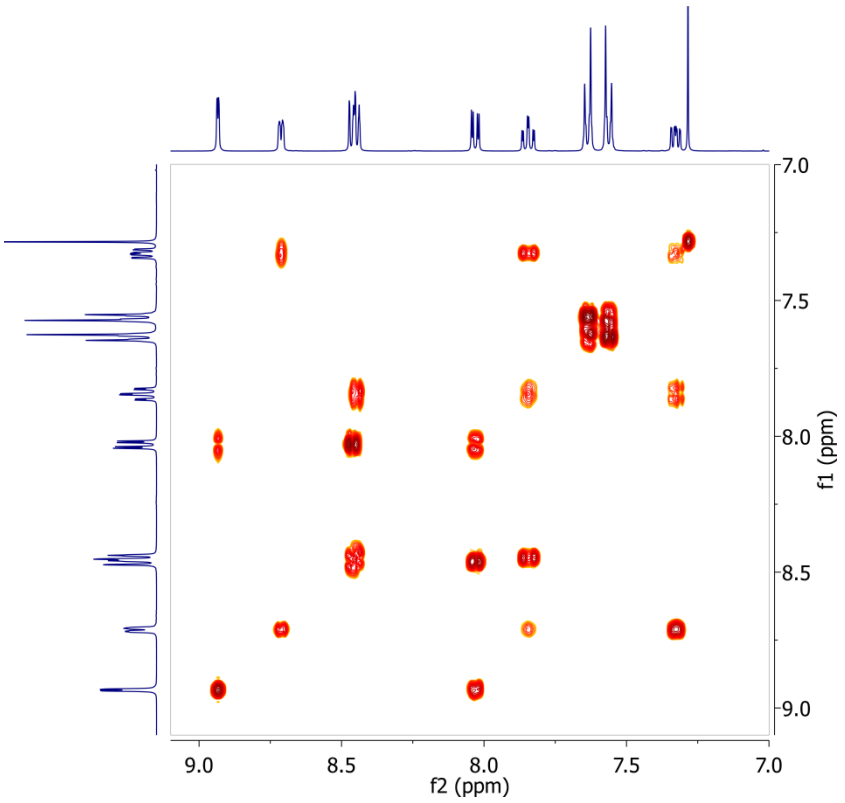

Figure S5. $^{1}H^{1}H$ COSY NMR spectrum of **1**, $CDCl_3$, ambient temperature, aromatic range.

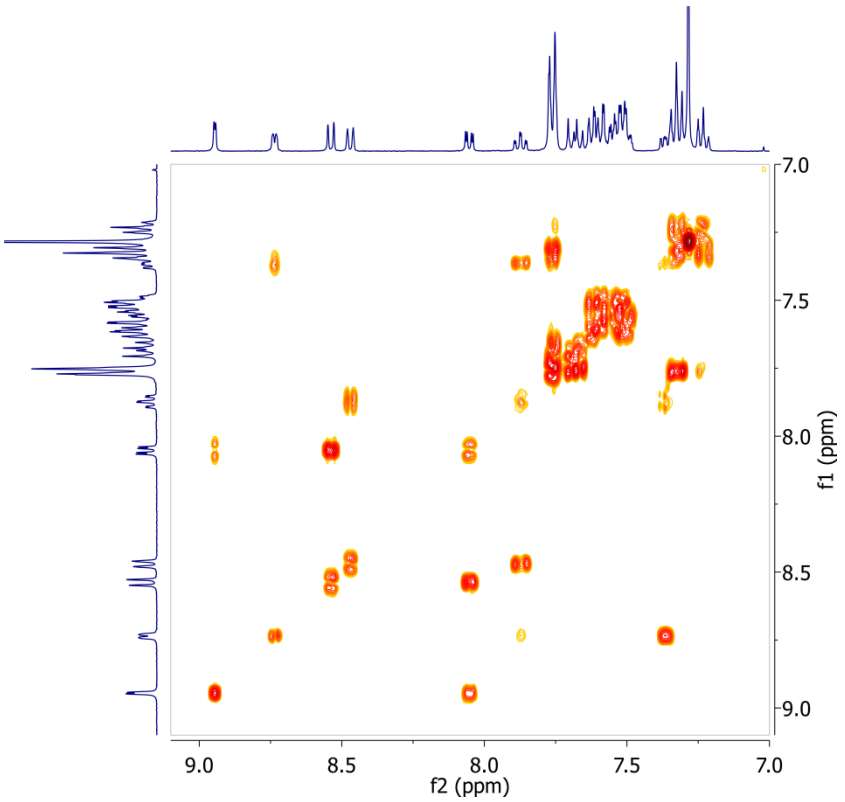

Figure S6. $^{1}H^{1}H$ COSY NMR spectrum of **3**, $CDCl_3$, ambient temperature, aromatic range.

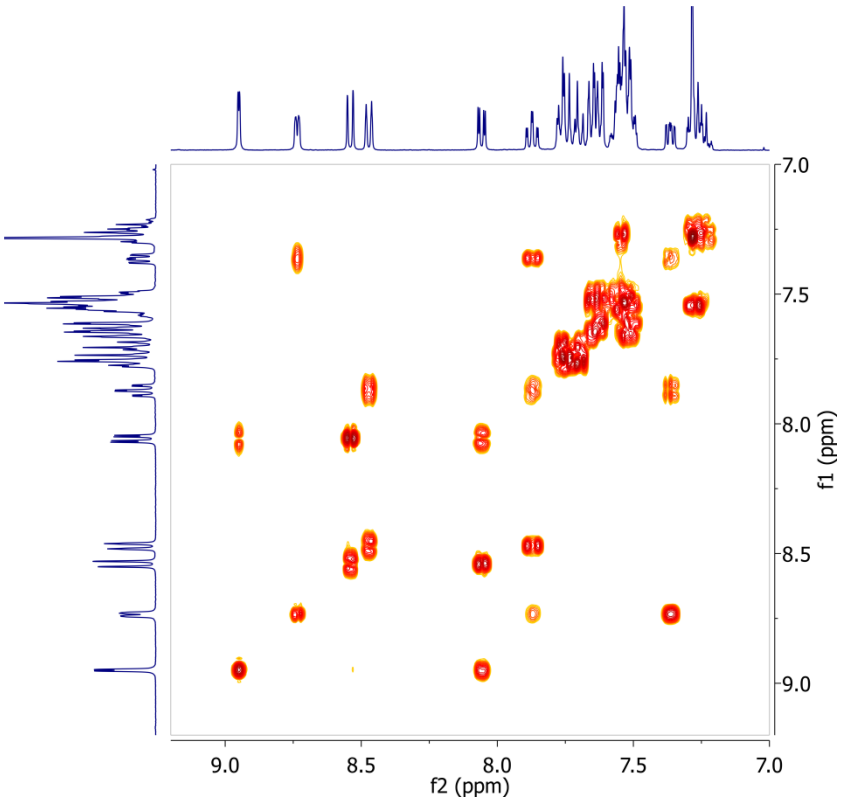

Figure S7. $^{1}H^{1}H$ COSY NMR spectrum of **4**, $CDCl_3$, ambient temperature, aromatic range.

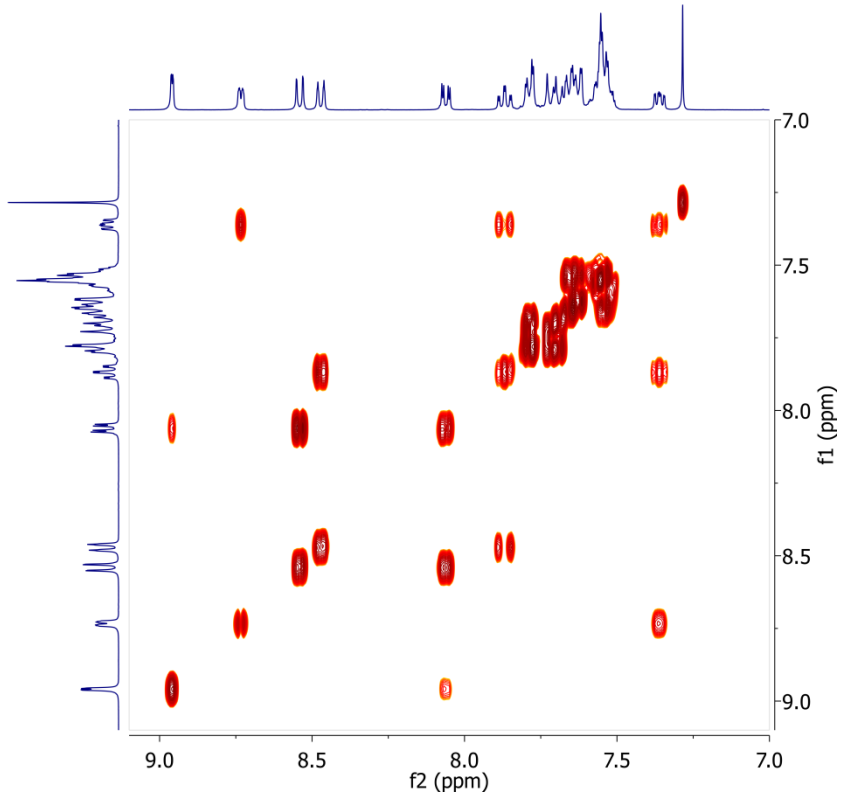

Figure S8. $^{1}H^{1}H$ COSY NMR spectrum of **5**, $CDCl_3$, ambient temperature, aromatic range.

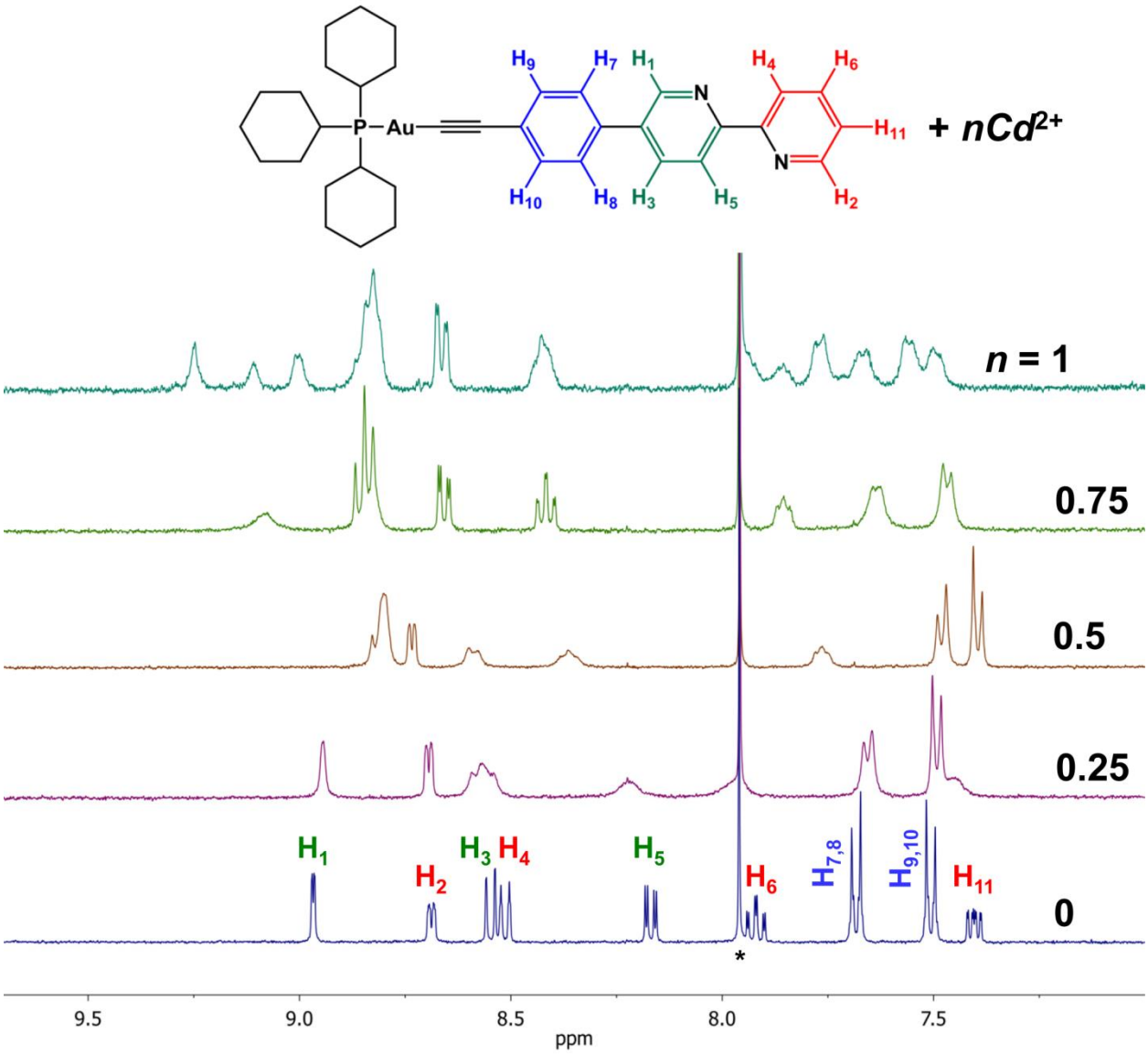

Figure S9. ^{1}H NMR spectrum of **1 + Cd(ClO$_4$)$_2$**; $CDCl_3$ + CD_3CN, ambient temperature; signal of $CDCl_3$ residual protons is marked by asterisks.

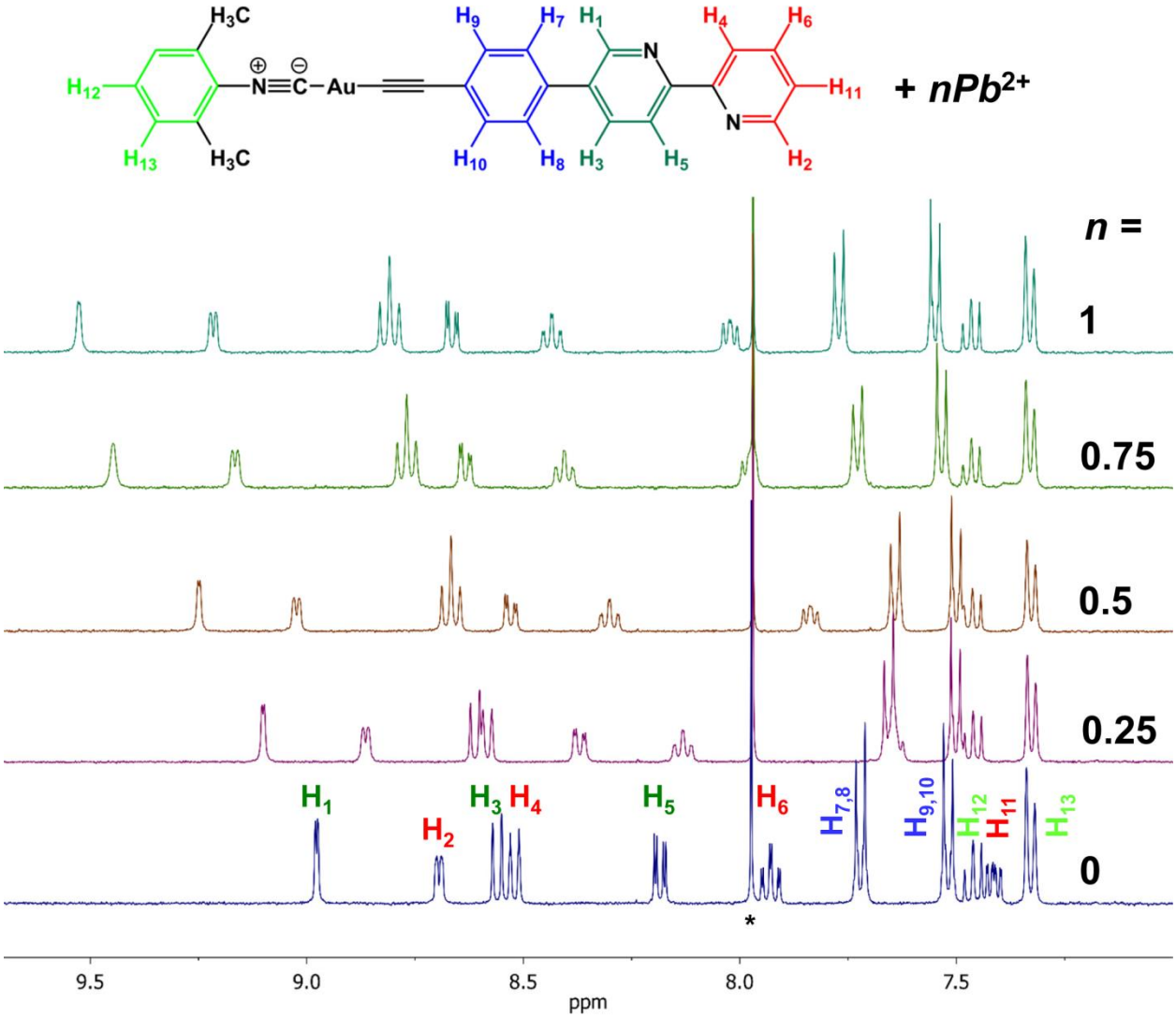

Figure S10. ^{1}H NMR spectrum of **2 + Pb(ClO$_4$)$_2$**; $CDCl_3$ + CD_3CN, ambient temperature; signal of $CDCl_3$ residual protons is marked by asterisks.

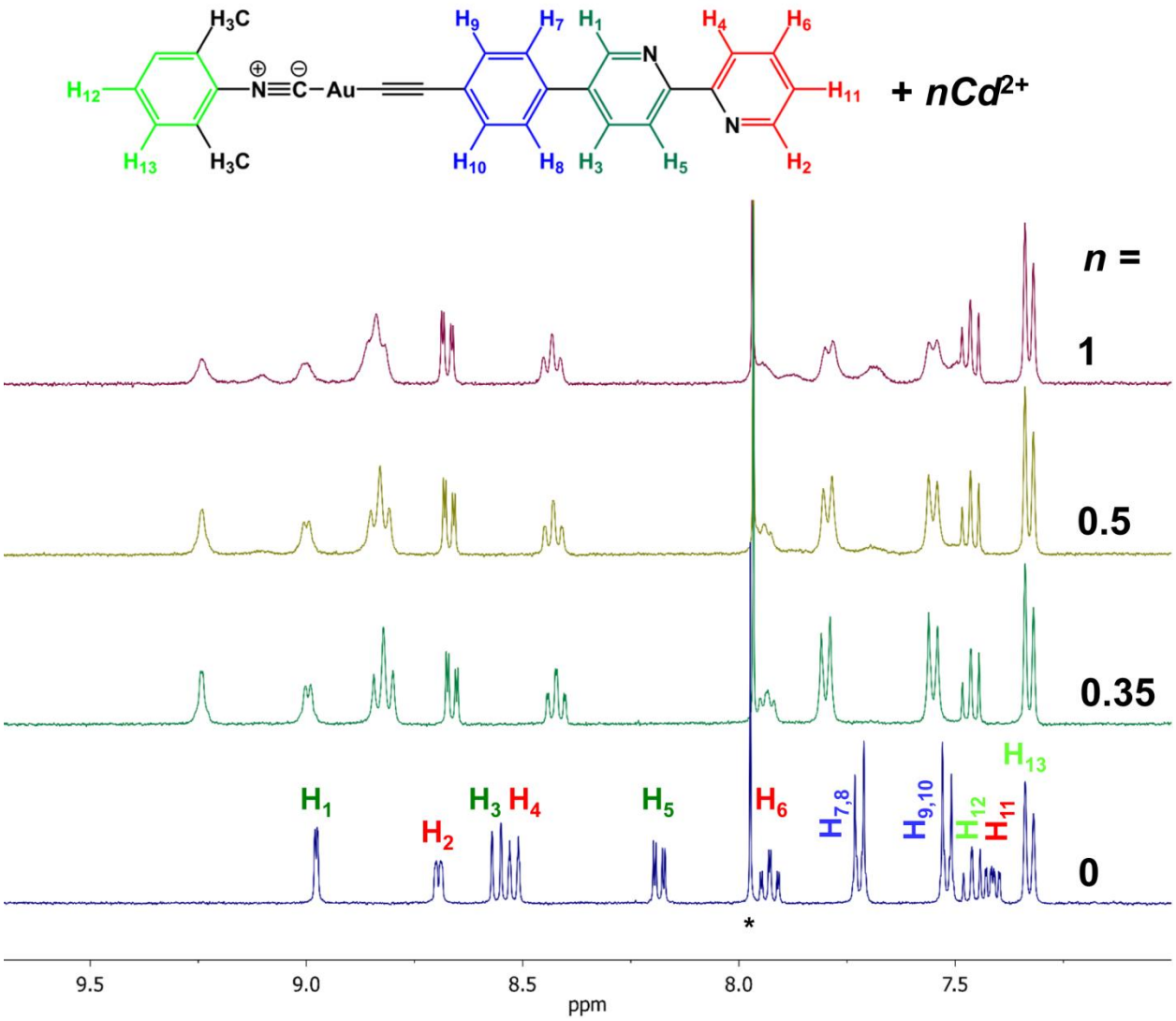

Figure S11. ^{1}H NMR spectrum of **2 + Cd(ClO$_4$)$_2$**; $CDCl_3$ + CD_3CN, ambient temperature; signal of $CDCl_3$ residual protons is marked by asterisks.

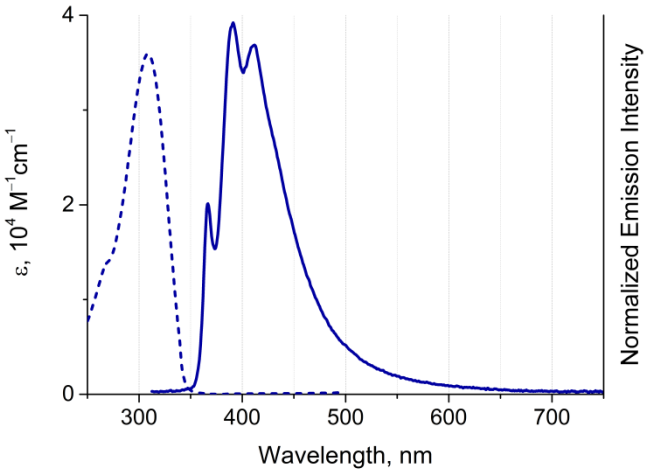

Figure S12. Absorbance (dash line) and emission (solid line) spectra of **L1** (dichloroethane solution, r.t.), λ_{excit} = 310 nm.

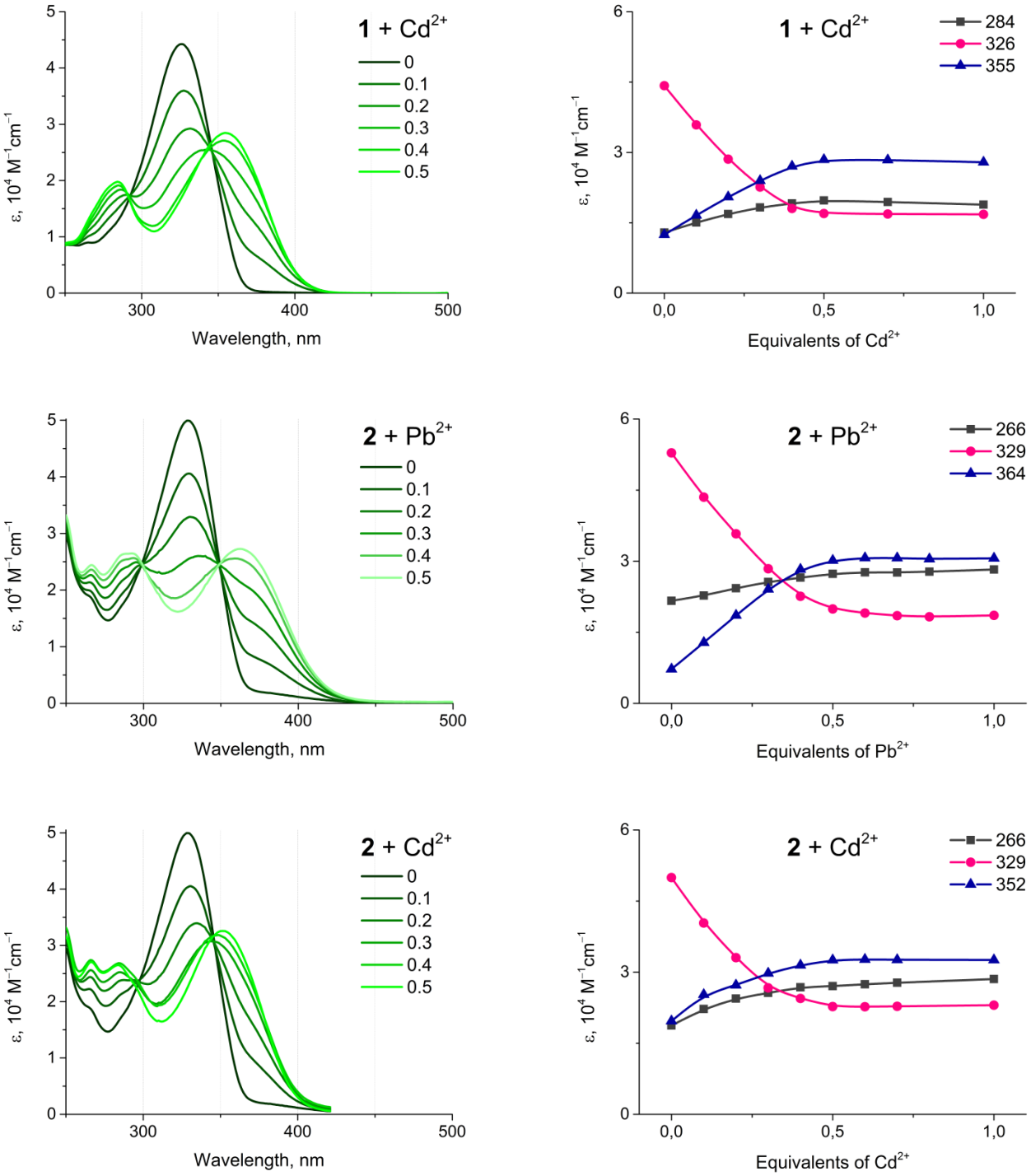

Figure S13. Left: Absorbance spectra of **1** (10^{-5} M) and **2** (10^{-5} M) under **M(ClO$_4$)$_2$** titration; molar equivalents of M(II) are indicated; measured in dichloroethane at r.t. Right: Dependence of extinction coefficient on molar equivalents of M(II); wavelengths are indicated on diagrams.

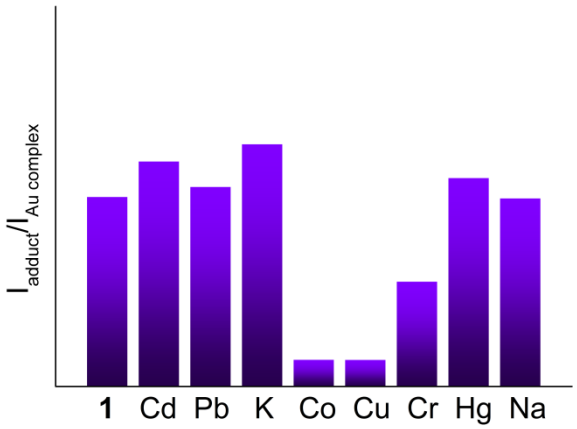

Figure S14. Relation of integral emission intensity I_{adduct}/I_1, dichloroethane solution, r.t.

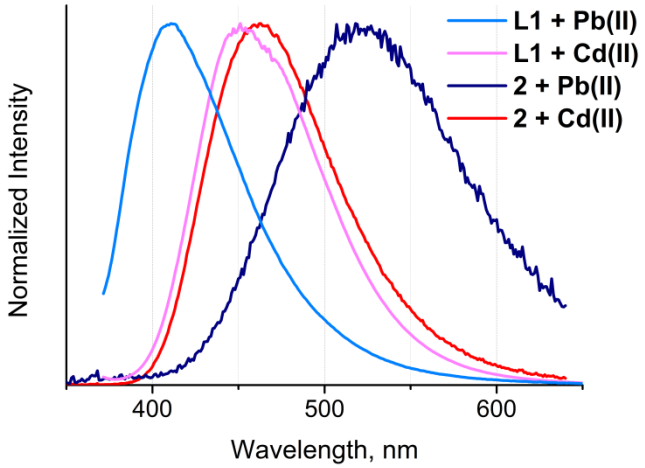

Figure S15. Normalized emission spectra of **L1** and **2** (10^{-5} M) upon treatment with $M(ClO_4)_2$ (dichloroethane solution, r.t.).

Table S2. Photophysical properties of adducts **1-2** with Pb(II) and Cd(II) in dichloroethane solution at r.t.

Adduct	λ_{abs}/nm (ε $10^4/M^{-1}cm^{-1}$)	λ_{em}/nm (λ_{excit}/нм)	QY, %	τ / ns
1:Pb^{2+} 2:1	288 (2.13), 363 (2.19)	450 (350)	2.2	0.42
1:Cd^{2+} 2:1	284 (1.98), 355 (2.85)	393 (310)	4.2	1.84
2:Pb^{2+} 2:1	268 (2.72), 284 (2.87), 363 (3.02)	520 (330)	11	1.64
2:Cd^{2+} 2:1	266 (2.86), 283 (2.77), 351 (3.26)	463 (350)	44	1.59

Computational details

Geometric properties

The optimized geometries of native complexes **1-5** are shown in Fig. SC1. Important bonding parameters of these complexes are listed in Table SC1.

Table SC1. Characteristic bond distances and bond angles obtained for the DFT-optimized (BP86/ZORA-scalar/TZP/COSMO) structures of **1-5** and the corresponding experimental values as determined by XRD. The numbering of atoms follows Fig. SC1.

	Bond type	**XRD, Å**	**Calculated**	**Angle type**	**XRD, °**	**Calculated, °**
1	P−Au	2.2990(6)	2.353	P1−Au1−C1	175.42(6)	178.8
	Au−C1	2.008(2)	2.001	Au1−C1−C2	177.5(2)	178.3
	C1−C2	1.208(3)	1.234	C1−C2−C3	178.2(2)	178.9
2	N3−C19	1.13(2)	1.173	N3−C19−Au1	180(1)	179.7
	C19−Au	1.97(1)	1.967	C19−Au1−C1	177.8(5)	179.5
	Au−C1	1.95(1)	1.978	Au1−C1−C2	174(1)	178.8
	C1−C2	1.22(2)	1.232	C1−C2−C3	177(1)	179.5
3	P−Au	-	2.333	P1−Au1−C1	-	176.8
	Au−C1	-	1.998	Au1−P1−C2	-	115.1
	P−C2	-	1.833			
4	P−Au	-	2.327	P1−Au1−C1	-	179.5
	Au−C1	-	1.995	Au1−P1−C2	-	112.9
	P−C2	-	1.835			
5	P−Au1	2.2642(8)	2.328	P1−Au1−C1	176.63(8)	178.7
	Au−C1	2.047(2)	2.070	Au1−P1−C2	113.07(9)	112.1
	P−C2	1.814(3)	1.834			

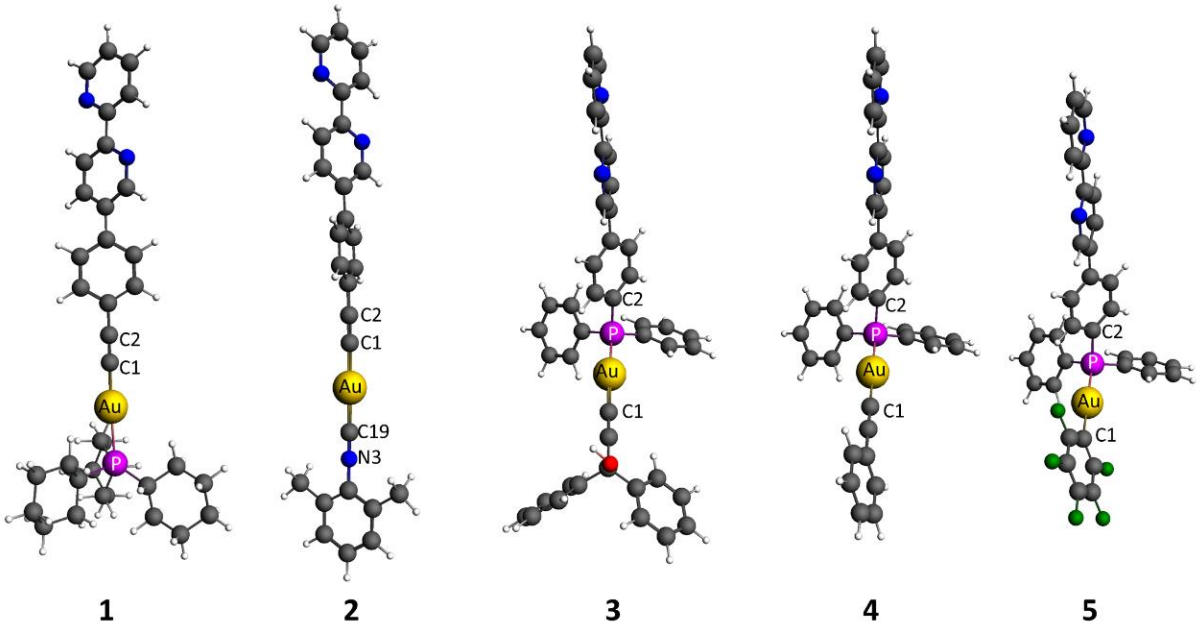

Figure SC1. Ball and stick representation of **1-5** optimized at the BP86/ZORA-scalar/TZP/COSMO level of theory.

Electronic properties

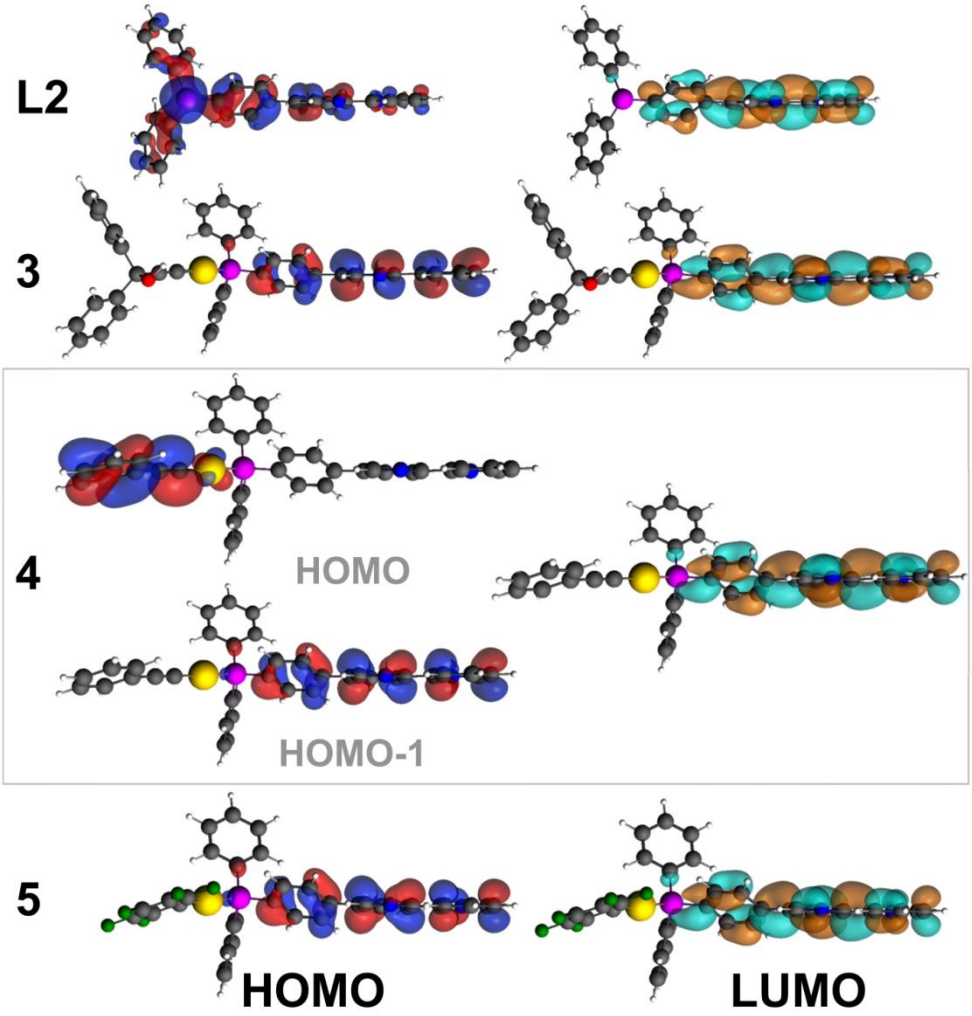

Figure SC2. Frontier molecular orbitals involved in the first excitation of **L2**, **3, 4** and **5**. Color code: Au = yellow, P = pink, C = gray, N = blue, F = green and H = white.

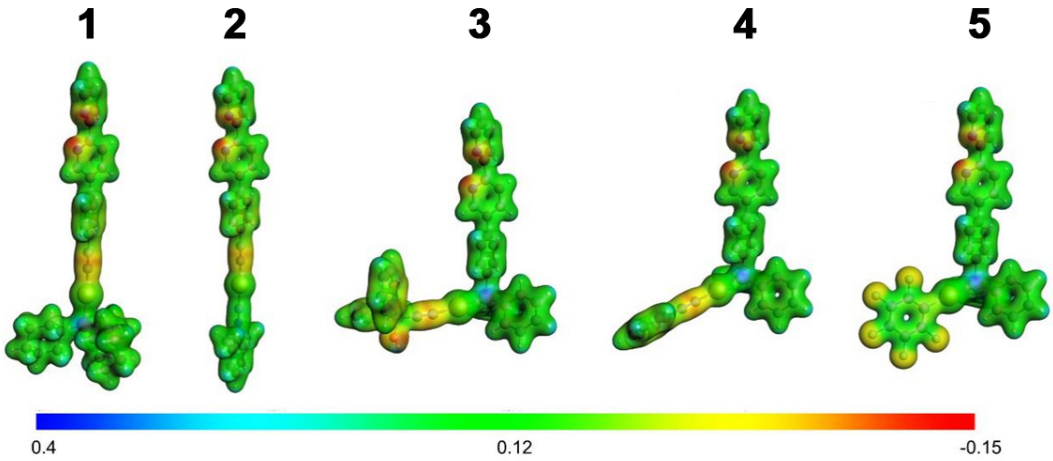

Figure SC3. Molecular electrostatic potential (MEP) isosurfaces of complexes **1-5** (most negative potentials = red). The MEPs are obtained from single point calculations at the B3LYP/ZORA-scalar/TZP/COSMO level of theory.

Table SC2. Important energy values calculated for **L1**, **L2** and **1-5**. E_{HOMO} is the energy of the highest occupied molecular orbital and E_{LUMO} is the energy of the lowest unoccupied molecular orbital. $E_{HOMO\text{-}LUMO}$ is the HOMO-LUMO energy gap. Data obtained at BP86/ZORA-scalar/TZP/COSMO.

BP86/ZORA-scalar/TZP/COSMO							
	1	**2**	**3**	**4**	**5**	**L1**	**L2**
E_{HOMO} [eV]	−5.7	−5.8	−6.3	−5.9	−6.3	−6.0	−5.8
E_{LUMO} [eV]	−3.1	−3.1	−3.3	−3.3	−3.3	−3.1	−3.1
$E_{HOMO\text{-}LUMO}$ [eV]	2.6	2.7	3.0	2.7	3.0	2.9	2.7

Table SC3. Important energy values calculated for **L1**, **L2** and **1-5**. The electron densities at Au atoms contributing to the HOMOs and LUMOs are indicated. Data obtained at B3LYP/ZORA-scalar/TZP/COSMO.

B3LYP/ZORA-scalar/TZP/COSMO							
	1	**2**	**3**	**4**	**5**	**L1**	**L2**
E_{HOMO} [eV]	−6.1	−6.2	−6.7	−6.4	−6.7	−6.5	−6.3
E_{LUMO} [eV]	−2.3	−2.4	−2.5	−2.5	−2.5	−2.4	−2.3
$E_{HOMO\text{-}LUMO}$ [eV]	3.8	3.8	4.3	4.0	4.3	4.1	4.0
Au % HOMO	3.1	1.6	0	3.1	0	-	-
Au % LUMO	0	3.1	0	0	0	-	-

Calculated UV-Vis spectra

The calculated spectra exhibit absorptions that can be assigned to those observed in the experimental spectra between 250-500 nm. These excitations correspond to intraligand transitions. Description of selected transitions is provided in Table SC4. Systematic calculations are typically used for prediction of the excitation spectra and they are typically dependent on the theoretical level and the type of molecules studied. In the current scenario, we deal with molecules that differ by their composition. These calculations were performed using the B3LYP functional.

The calculated UV-Vis spectra of **L1**, **L2** and **1-5** show qualitative similarities to the experimentally measured spectra in the region 250-400 nm (Fig. SC4). The first absorption in all spectra is predominantly defined by the first excitation. A comparison between the theoretically calculated excitations and the experimentally determined ones is provided in Table SC4.

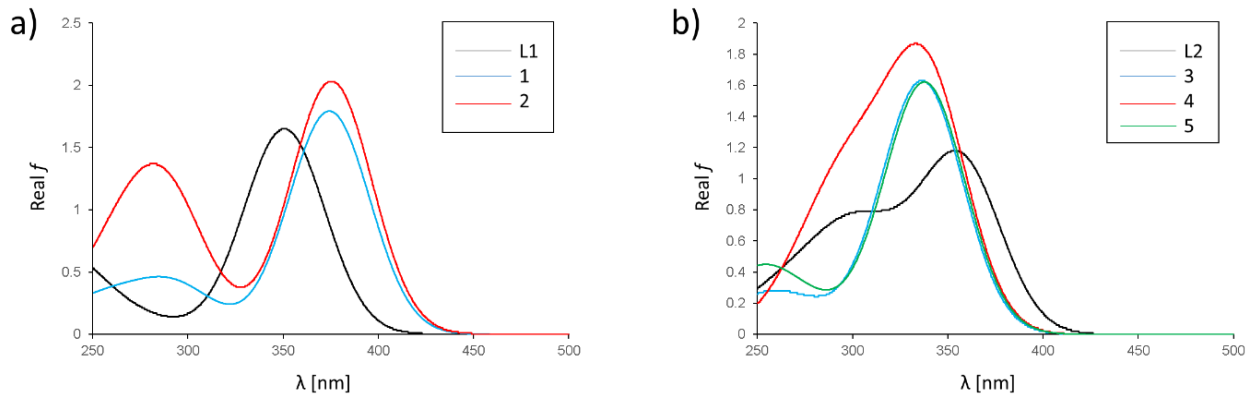

Figure SC4. TDDFT simulated UV-Vis spectra of **L1**, **L2** and **1-5**, as obtained at the B3LYP/ZORA-scalar/TZP/COSMO level of theory and convoluted using 20 allowed excitations.

Table SC4. Energies of the first excitation and description of the most pronounced transitions contributing to the lowest-energy excitation, as calculated at B3LYP/ZORA-scalar/TZP/COSMO. The used structures were optimized at BP86/ZORA-scalar/TZP/COSMO.

	Calculated [eV]	**Calculated [nm]**	**Real (*f*)**	**Experimental [nm]**	**Characterization**
L1	3.54	351	1.65	308	99 % HOMO→LUMO
L2	3.48	356	1.13	313	96 % HOMO→LUMO
1	3.31	374	1.83	326	98 % HOMO→LUMO
2	3.30	375	2.04	329	97 % HOMO→LUMO
3	3.68	337	1.63	307	98 % HOMO→LUMO
4	3.65	339	1.44	307	42 % * HOMO→LUMO
5	3.67	338	1.62	308	98 % HOMO→LUMO
2·Cd$(ClO_4)_2$	3.99	414	1.28	ca. 375	97 % HOMO→LUMO

* Major HOMO−1→LUMO

Cartesian coordinates (Å) of L1, L2, 1-5 and 2·Cd$(ClO_4)_2$

L1

C	14.33988122	5.00602370	-7.31906642
C	12.54635689	6.53822981	-6.92307269
C	12.37987554	6.62209317	-8.30003778
H	14.74862272	3.28218706	-2.58685654
H	14.69517604	4.56076159	-11.02041739
C	13.78137271	6.55718028	-2.69960923
C	13.21634663	5.87178537	-9.14335546
H	11.60581652	7.25085476	-8.73682941
C	13.74637334	5.25881556	-12.84351555
C	14.20807585	4.36034499	-4.37228632
H	12.55952561	6.16504089	-14.42631286
H	15.15504662	4.36903361	-6.96498782
H	13.62312966	7.41709859	-2.04839300
H	14.35387852	3.48909289	-5.01182088
N	12.08268854	6.71197488	-11.11511211
C	13.06732374	5.92281768	-10.62468750
C	11.93200276	6.77454225	-12.44778813
C	13.77560541	5.57869152	-4.93462341
C	14.61850751	5.10510473	0.45798697
C	13.54777183	5.70843457	-6.38855378
C	13.91771736	5.18135692	-11.46288440
N	14.19071428	5.07457209	-8.64659380
C	14.43271146	5.21092827	-0.73853717
C	13.56732487	6.67188891	-4.06936088
H	11.88575176	7.09999369	-6.26111177
H	11.12765287	7.42103721	-12.80947548
C	14.21367606	5.33431374	-2.14245896
C	12.73222153	6.07232617	-13.35380201
H	14.39562193	4.69172291	-13.51214285
H	13.25490711	7.63400079	-4.47735134
C	14.42375986	4.23584059	-3.00344456
H	14.78347771	5.01171487	1.51365607

L2

H	-3.68634720	2.16390890	2.76444000
N	-0.19626605	-0.88007697	-5.50848631
N	-2.62628848	-0.29392054	-8.15011024
C	-1.40353149	-0.74371002	-6.10656823
C	-0.16547023	-1.08779378	-4.18583407
C	-1.41544811	-0.48755206	-7.57423808
C	-2.66001183	-0.05153684	-9.47089525
C	-2.60099503	-0.83305245	-5.37721764
C	-1.30616107	-1.17060479	-3.36221206
H	0.82867188	-1.21468710	-3.74827507
C	-0.21989114	-0.44629668	-8.31204408
H	-3.65188083	0.10274098	-9.90441600
C	-1.52132537	0.01047087	-10.27976525
H	-3.55172567	-0.72048456	-5.89567019
C	-2.55024262	-1.04578756	-4.00537421
C	-1.19319601	-1.37471880	-1.90150782
H	0.72857148	-0.61103052	-7.80304468
C	-0.27583491	-0.19330733	-9.68132634
H	-1.61594524	0.21324888	-11.34682830
H	-3.47482008	-1.08895470	-3.42782920
C	-2.14703976	-2.13822036	-1.20114924
C	-0.13201505	-0.80674688	-1.16740137
H	0.63975877	-0.15639597	-10.27314875
H	-2.96396411	-2.61515537	-1.74556564
C	-2.05522299	-2.31703688	0.18075872
H	0.61589032	-0.19665196	-1.67609581
C	-0.03429872	-0.99660428	0.21008345
C	-1.00194332	-1.74200827	0.91111396
H	-2.80862061	-2.91830590	0.69175478
H	0.80502507	-0.55298029	0.75125461
H	-2.02002551	-6.68603483	3.19485786
H	-0.53066655	-4.79339944	2.60944480
H	-2.78227904	0.10144590	1.72701181
H	-2.94554025	2.85081652	5.04445340
H	-1.28644438	1.45587453	6.28190950
H	-0.36002244	-0.59534227	5.23609487
C	-1.95814904	-3.26214186	3.17844503
C	-3.23295503	-3.02668895	3.72000821
C	-4.06393178	-4.09784975	4.07034677
C	-3.63548659	-5.41550700	3.87770548
C	-2.36549668	-5.66112113	3.34081776
C	-1.52906650	-4.59302670	3.00593753
H	-3.57980650	-2.00372719	3.87292988
H	-5.05034994	-3.89968835	4.49364049
H	-4.28467895	-6.24882916	4.15176878
P	-0.74496284	-1.93830749	2.73328069
C	-1.51930529	-0.40193422	3.41515101
C	-2.45348283	0.39114034	2.72654980
C	-2.96296836	1.55594412	3.31096343
C	-2.54961725	1.94016564	4.59159854
C	-1.61933194	1.15818583	5.28589790
C	-1.10169371	-0.00005027	4.69808433

1

Au	0.41949088	-2.01298719	4.54010040
C	-2.51446054	-0.64790606	-4.69189735
C	-2.76273275	-0.54519506	-6.05469067
H	0.50402374	-3.55601896	-0.59900471
H	-0.30489769	-2.12297873	-8.96705314
C	-1.14726018	-0.56797307	-0.52019843
C	-1.84477908	-1.09196663	-6.96675180
H	-3.66263202	-0.05961506	-6.42834286
C	-1.44866799	-1.51816726	-10.70945963
C	-0.32713280	-2.54715063	-2.31008274
H	-2.84211021	-0.74658807	-12.19231913
H	0.45195241	-2.27518931	-4.94506825
H	-1.46179470	0.21082444	0.17554168
H	-0.02358244	-3.34134297	-2.99368049
N	-3.19515258	-0.35989224	-8.84169615
C	-2.08190587	-1.01656424	-8.43506476
C	-3.43014762	-0.28395086	-10.16228874
C	-1.03409845	-1.43018135	-2.80129229
C	0.07958762	-1.90912129	2.57129486
C	-1.34887733	-1.29148384	-4.23792783
C	-1.18624952	-1.60649484	-9.34382039
N	-0.71273391	-1.70830394	-6.55081015
C	-0.15454333	-1.81730945	1.36338559
C	-1.43603364	-0.44543336	-1.87492067
H	-3.23697170	-0.24968388	-3.97800069
H	-4.33558361	0.25311198	-10.45753858
C	-0.44084757	-1.69041186	-0.02808212
C	-2.59517704	-0.84269409	-11.13464706
H	-0.76773910	-1.97051681	-11.43187141
H	-1.96385636	0.44314544	-2.22372909
C	-0.03459650	-2.67762163	-0.95574963
C	-0.48593284	-1.79333687	-5.23397590
C	-1.98972968	-3.37867682	9.84127149
C	3.98430547	-5.50210097	7.88379229
H	1.21258848	0.46149507	5.49893413
H	1.68672284	-4.28662984	8.92520895
H	-3.58370849	-2.03777864	9.25131568
H	-0.01681753	0.01879805	7.61528458
C	1.73439458	0.53928390	6.46512428
H	-1.00009056	-1.51330034	9.37203325
H	2.44801150	-2.76394524	9.40488106
C	2.46700607	-4.27440067	6.24991779
C	3.79438007	-5.02814074	6.43655505
C	-3.30183400	-3.09406264	9.09907737
H	1.21769498	-0.79447531	9.65621061
H	0.78113414	2.41899689	6.95820622
H	-4.11702130	-3.70249645	9.51901009
H	-4.07864034	-3.10313014	7.06242020
H	1.62619734	-4.97151777	6.41082296
C	3.84772525	-4.33254586	8.86663572
H	0.75024247	1.64315418	9.49522239
C	-0.81119895	-2.59143330	9.23917442
H	-2.99282513	-4.44795591	7.43565993
C	1.80499765	2.00894193	6.91175877
H	-1.86558877	-2.83976963	5.92116024
H	-1.76603979	-4.45831656	9.79012845
C	2.50950662	-3.59202677	8.68766180
H	4.96572543	-5.98639375	8.00051118
C	1.02439800	-0.34231962	7.51876546
H	2.75706746	0.15771560	6.30096946
H	3.82986425	-5.88220288	5.74332156
H	-0.44020662	-3.97395075	7.61462763
C	-0.65323136	-2.89498605	7.73422733
H	4.67771059	-3.62225550	8.71001658
C	2.34378604	-3.09034528	7.23701676
C	1.72340120	-0.19747506	8.88660614
H	2.75431770	-0.57975682	8.80551369
H	-2.08777305	-3.12718707	10.90823290
H	-2.18153930	-1.50929087	7.04119589
C	-1.97324114	-2.59225030	6.98832000
H	4.62743004	-4.35980413	6.15849588
H	2.37912058	-3.91062837	5.21468694
C	2.47297018	2.15802558	8.28455166
C	-3.15340024	-3.36784813	7.59640145
H	3.22381591	-6.26665176	8.12005089
H	3.53432036	1.86475978	8.20834242
P	0.80121196	-2.08844552	6.86061002
H	2.29639411	1.34455639	10.29831900
C	1.77787296	1.27654958	9.32985697
H	2.45850663	3.21162667	8.60253066
H	3.16136361	-2.37896931	7.01495347
H	3.92985854	-4.68878889	9.90467722
H	0.10798420	-2.82809518	9.79041201
H	2.34574021	2.59529468	6.15343246

2

H	1.90792594	-2.72691575	12.66911104
C	-2.57534135	-0.62109457	-4.73047587
C	-2.84795973	-0.56689300	-6.09162470
H	0.50936255	-3.40207800	-0.60368145
H	-0.38504099	-2.15213858	-8.99517593
C	-1.14869173	-0.41540404	-0.58162950
C	-1.94060879	-1.13576723	-7.00104979
H	-3.75892066	-0.10235772	-6.46548851
C	-1.58117675	-1.65280501	-10.73622332
C	-0.34308646	-2.43833568	-2.33065250
H	-3.03009764	-0.99015795	-12.21818632
H	0.40381003	-2.22571151	-4.98179330
H	-1.45697173	0.37992686	0.09792106
H	-0.04556910	-3.24878314	-2.99753348
N	-3.35261235	-0.52311175	-8.87478207
C	-2.20411545	-1.11527092	-8.46709001
C	-3.61009330	-0.49662769	-10.19301337
C	-1.05996490	-1.33615766	-2.84073209
C	0.11128805	-1.71622469	2.52258876
C	-1.39677157	-1.24003657	-4.27612832
C	-1.29540572	-1.68925806	-9.37288942
N	-0.79412139	-1.72455288	-6.58454658
C	-0.13642032	-1.62552555	1.31893089
C	-1.45315088	-0.32827817	-1.93591797
H	-3.28784630	-0.20337837	-4.01771732
H	-4.54439312	-0.01195818	-10.48894743
C	-0.43484354	-1.52454006	-0.07140643
C	-2.76383997	-1.04393619	-11.16217288
H	-0.89024878	-2.09370947	-11.45623382
H	-1.98874640	0.54887967	-2.30129151
C	-0.03516274	-2.53436380	-0.97715318
C	-0.54466635	-1.76436791	-5.26988066
Au	0.47270421	-1.87931839	4.46091906
C	0.81834934	-2.05359474	6.38963763
N	1.02086763	-2.16259177	7.53999055
C	1.25319259	-2.30788707	8.89724342
C	2.25550374	-1.50855372	9.49476961
C	0.47596499	-3.25104409	9.61009494
C	2.46897761	-1.68223143	10.86666002
C	3.05245098	-0.52154770	8.68654461
C	0.73840437	-3.38106141	10.97828127
C	-0.58027667	-4.07205378	8.92248398
H	3.23340053	-1.08097857	11.36114447
C	1.72216212	-2.60779153	11.60075796
H	2.39894975	0.21977516	8.20373990
H	3.76535586	0.01135753	9.32565167
H	3.61636772	-1.02530208	7.88726694
H	0.15931543	-4.10026289	11.55961780
H	-0.14566386	-4.69443484	8.12618601
H	-1.08135525	-4.73164481	9.63976494
H	-1.34070948	-3.43095614	8.45262325

3

H	-0.47262390	-0.23422978	4.52521181
N	-0.44979029	-1.82715847	-6.16968372
N	-3.01683881	-1.39942963	-8.71087605
C	-1.68497489	-1.68793160	-6.70699169
C	-0.34487467	-1.90849611	-4.83692060
C	-1.77879599	-1.57493566	-8.18978608
C	-3.12479045	-1.29037789	-10.04560046
C	-2.83788941	-1.64804134	-5.90526279
C	-1.43565444	-1.85688734	-3.94672397
H	0.66806656	-2.04078836	-4.44692066
C	-0.62953660	-1.64469839	-8.99496848
H	-4.13673648	-1.14909674	-10.43470253
C	-2.03582710	-1.34850741	-10.92078154
H	-3.81271885	-1.53725818	-6.37703659
C	-2.71100539	-1.73132080	-4.52482910
C	-1.24701727	-1.92294024	-2.48094615
H	0.34319794	-1.78726441	-8.52691077
C	-0.76212956	-1.53005984	-10.37752108
H	-2.18970830	-1.25284674	-11.99586442
H	-3.59894368	-1.67362084	-3.89357250
C	-2.19201773	-2.57246711	-1.66366624
C	-0.13074155	-1.32438471	-1.86215246
H	0.11677657	-1.58069985	-11.02168239
H	-3.04672194	-3.07685682	-2.11655581
C	-2.04650123	-2.59855647	-0.27695843
H	0.61334636	-0.80539006	-2.46734053
C	0.02195368	-1.35373669	-0.47700337
C	-0.94482653	-1.97643983	0.33220601
H	-2.79539966	-3.10951985	0.32884317
H	0.89152232	-0.87430491	-0.02247637
H	-5.04016921	-3.76835561	3.94267122
H	-3.62504044	-1.94076924	3.04864906
Au	1.41359435	-2.13109908	2.94494193
C	3.23818367	-2.37895960	3.72040390
C	4.32795483	-2.55331050	4.26163808
C	-1.86367524	-3.18932449	2.83404749
C	-1.33111221	-4.47878545	3.01316842
C	-2.13374883	-5.50613675	3.51448129
C	-3.46889788	-5.25233064	3.84909195
C	-4.00109463	-3.97029798	3.67862612
C	-3.20337425	-2.93883370	3.17240308
H	-0.28579844	-4.67561648	2.76518636
H	-1.71332757	-6.50327844	3.65181767
H	-1.52209372	1.88937803	5.26627651
H	-4.09248027	-6.05345407	4.24844663
P	-0.76434979	-1.88592723	2.15445689
C	-1.52975990	-0.28642191	2.63233225
C	-2.44619512	0.37850932	1.80089040
C	-3.02917983	1.57853495	2.22007612
C	-2.70248704	2.12118234	3.46692047
C	-1.78541508	1.46513231	4.29649467
C	-1.19659302	0.26861607	3.88068215
H	-2.70323727	-0.03428663	0.82491389
H	-3.73934772	2.08909091	1.56816644
H	-3.15780317	3.05840059	3.79025725
C	5.64220626	-2.73037786	4.90155636
O	6.64681617	-3.03063591	3.88382234
H	6.57092276	-2.32877950	3.20478734
C	5.68554191	-3.94155150	5.85577153
C	6.91698719	-4.30398316	6.42599039
C	7.00227949	-5.40260735	7.28347011
C	5.85560489	-6.14623009	7.59179443
C	4.62715166	-5.78371012	7.03296196
C	4.54315665	-4.68636263	6.16634917
H	7.81289164	-3.72683483	6.19340594
H	7.96623050	-5.67793721	7.71467334
H	5.92231054	-7.00355617	8.26371036
H	3.72872978	-6.35800304	7.26626510
H	3.58763951	-4.40736995	5.71961785
C	6.01159180	-1.44519604	5.68838114
C	5.08518197	-0.88800826	6.58474165
C	5.41172254	0.24818347	7.32828632
C	6.67013403	0.84720331	7.18336781
C	7.59417195	0.29832693	6.29048609
C	7.26831459	-0.84439032	5.54713012
H	4.10051366	-1.34584425	6.69654591
H	4.68160961	0.66974814	8.02166653
H	6.92539716	1.73609441	7.76275441
H	8.57657792	0.75790573	6.16762270
H	7.99555864	-1.27042201	4.85613485

4

H	-3.51364389	2.20971524	2.84525565
N	-0.26328037	-0.90616276	-5.55869786
N	-2.72675871	-0.25336665	-8.15285189
C	-1.47647031	-0.71431709	-6.12856981
C	-0.21103141	-1.11231177	-4.23692520
C	-1.50981382	-0.46604410	-7.59740313
C	-2.77892940	-0.01779334	-9.47414124
C	-2.65959968	-0.74140180	-5.37106123
C	-1.33519524	-1.13975319	-3.38782318
H	0.78589621	-1.28578908	-3.82286605
C	-0.32654569	-0.45109436	-8.35540271
H	-3.77513641	0.15137577	-9.89169966
C	-1.65312811	0.01967019	-10.30263982
H	-3.61540558	-0.58211934	-5.86742006
C	-2.58693338	-0.95353560	-4.00023466
C	-1.19657251	-1.35515239	-1.93088146
H	0.62722253	-0.63096361	-7.86177647
C	-0.40139535	-0.20372913	-9.72483187
H	-1.76246568	0.21897291	-11.36893934
H	-3.49862033	-0.94861770	-3.40123775
C	-2.17666856	-2.06368489	-1.20952618
C	-0.08164315	-0.85761381	-1.22589467
H	0.50445037	-0.18570965	-10.33222900
H	-3.03480970	-2.48785790	-1.73250304
C	-2.05773585	-2.25940240	0.16688774
H	0.68702516	-0.29087441	-1.75246741
C	0.04534077	-1.05905384	0.14676391
C	-0.94717258	-1.75375803	0.86093499
H	-2.82907884	-2.82025828	0.69579878
H	0.92139515	-0.66763889	0.66780155
H	-2.01079808	-6.69811072	3.18826466
H	-0.48990485	-4.82965482	2.60014047
Au	1.44949988	-2.40898167	3.29597872
H	-2.71153050	2.84198200	5.11919729
H	-1.05597076	1.39808226	6.30061148
H	-0.19924179	-0.66096863	5.21033827
C	-1.90653530	-3.28363778	3.15973625
C	-3.18184796	-3.01826077	3.68310453
C	-4.03081964	-4.07673285	4.02481014
C	-3.61473238	-5.39939792	3.84365804
C	-2.34242227	-5.66791779	3.32453690
C	-1.48717997	-4.61594213	2.99022199
H	-3.51362931	-1.99003256	3.83029384
H	-5.01896394	-3.86391574	4.43498786
H	-4.27860257	-6.22238033	4.11281974
P	-0.74513253	-1.94923371	2.67398181
C	-1.39115289	-0.40249030	3.41760678
C	-2.32133802	0.41392065	2.75298234
C	-2.79410802	1.57766316	3.36760182

C	-2.34431395	1.93101798	4.64420720
C	-1.41570874	1.12171542	5.30850648
C	-0.93576627	-0.03908381	4.69734778
H	-2.67216525	0.14976197	1.75449777
H	9.48829390	-3.99843508	5.79703425
C	6.07475732	-3.95595189	5.84894253
C	8.22910506	-3.15302169	4.25182727
H	7.56115849	-4.71307190	7.21207701
C	7.38397432	-4.20407436	6.26290727
C	8.46608264	-3.80383029	5.46904109
H	9.06751424	-2.83843148	3.62802780
H	5.23291046	-4.26830819	6.46791077
H	6.74032792	-2.39201845	2.88131156
C	3.32568062	-2.80608377	3.84489180
C	4.48358694	-3.03383112	4.20033535
C	5.82270400	-3.29717685	4.62306822
C	6.92349609	-2.90013265	3.82899658

5

H	-3.69609360	2.15546433	2.79807746
N	-0.19591515	-0.88276393	-5.51285780
N	-2.62597802	-0.29757664	-8.15404862
C	-1.40306937	-0.74010820	-6.10945454
C	-0.16478144	-1.08931270	-4.19045783
C	-1.41476096	-0.48570985	-7.57756835
C	-2.65980484	-0.05861912	-9.47531374
C	-2.60073996	-0.82222331	-5.37931321
C	-1.30546595	-1.16552130	-3.36704345
H	0.82906935	-1.22213996	-3.75417644
C	-0.21876045	-0.44190684	-8.31403267
H	-3.65181277	0.09107269	-9.91001096
C	-1.52052039	0.00531467	-10.28349762
H	-3.55102595	-0.70496569	-5.89739297
C	-2.55005805	-1.03483836	-4.00759794
C	-1.19131750	-1.37210248	-1.90677347
H	0.72987599	-0.60235761	-7.80405910
C	-0.27471721	-0.19232852	-9.68405563
H	-1.61516443	0.20494698	-11.35114612
H	-3.47429638	-1.07219711	-3.42925698
C	-2.14931557	-2.13121486	-1.20786578
C	-0.12477641	-0.81048572	-1.17526681
H	0.64103519	-0.15375542	-10.27548377
H	-2.96907401	-2.60300151	-1.75121520
C	-2.05593057	-2.31632521	0.17226800
H	0.62225785	-0.20013659	-1.68412710
C	-0.02380081	-0.99962154	0.20112206
C	-0.99416696	-1.74726691	0.89257130
H	-2.80967058	-2.91595274	0.68355093
H	0.81248748	-0.55466098	0.74427532
H	-2.00322305	-6.69718016	3.22276228
H	-0.51529233	-4.80280764	2.63158573
Au	1.38135115	-2.35543839	3.33849801
H	-2.92153181	2.85106231	5.06305391
H	-1.23456040	1.47408080	6.27868926
H	-0.31741198	-0.58149240	5.23064845
C	-1.95802099	-3.28109293	3.19210635
C	-3.23723402	-3.03761798	3.71677487
C	-4.06685278	-4.11043305	4.06119614
C	-3.62805642	-5.42582628	3.88055588
C	-2.35205123	-5.67272997	3.35947648
C	-1.51555671	-4.60634854	3.02328104
H	-3.58723455	-2.01531533	3.86250470
H	-5.05811360	-3.91442977	4.47217005
H	-4.27701077	-6.25995961	4.15151610
P	-0.81905942	-1.92738612	2.70978264
C	-1.50586173	-0.38696386	3.42728323
C	-2.45463060	0.39197606	2.74377500
C	-2.96168448	1.55319417	3.33475032
C	-2.52737024	1.94185132	4.60650075
C	-1.58084495	1.17008642	5.28985723
C	-1.06712370	0.01133681	4.70237868
H	-2.79397929	0.09955286	1.74916700
F	7.31197250	-3.68018609	4.87309039
C	3.33958606	-2.77106517	3.86535176
C	3.67410537	-3.46069597	5.02860036
C	4.41601112	-2.40025404	3.06225859
C	4.98460766	-3.77526384	5.38522295
F	6.76207486	-2.30890196	2.55421572
C	5.74376396	-2.68982801	3.37300439
C	6.02937385	-3.38569548	4.54762911
F	5.26161231	-4.45355588	6.53215098
F	4.19808285	-1.71336024	1.89059546
F	2.68918644	-3.87219027	5.89519338

2·Cd$(ClO_4)_2$

H	2.70171084	-3.34303260	12.24387783
Au	0.43295248	-1.72499790	4.34668466
C	0.93735068	-2.06099630	6.21867434
H	-2.76135318	-0.87903257	0.16327488
N	1.25815692	-2.28157215	7.32504842
C	0.39091778	-1.26787114	-1.09831171
C	1.63727455	-2.56023043	8.62694217
C	2.29820480	-1.54916218	9.36300903
C	1.34632282	-3.84357944	9.14634595
C	-2.24853880	-0.87892017	-1.92769968
C	2.67171750	-1.86353185	10.67406910
C	2.58358880	-0.20237879	8.75699508
H	1.42206289	-1.41042425	-0.77500147
H	-3.28626300	-0.75316089	-2.23848353
C	1.74486256	-4.09770358	10.46320731
C	0.64236104	-4.88151456	8.31602785
H	3.18357931	-1.10797263	11.27201054
C	-1.23238947	-1.00238808	-2.89759091
C	-0.04821538	-1.42821913	2.45097331
C	2.40008181	-3.12153974	11.21907974
H	1.65657329	0.29646331	8.43797735
H	3.09117344	0.44466603	9.48115473
C	-0.32850833	-1.29063525	1.25932699
C	0.09297448	-1.18793198	-2.45366847
H	3.22444977	-0.29338742	7.86742899
H	1.53712280	-5.07708566	10.89661423
C	-0.63191133	-1.16638851	-0.12674688
H	1.21083166	-5.11588903	7.40368591
H	0.51324205	-5.80766825	8.88744435
H	0.90836654	-1.24875664	-3.17544457
C	-1.95867355	-0.95899131	-0.57008147
H	-0.35058954	-4.53082994	7.99708310
H	-3.79872283	0.26032129	-6.58839725
N	-1.71724146	-2.10260249	-9.22947080
N	-1.08702637	-1.74522799	-6.57589825
O	0.75200313	-5.33505576	-4.76707439
H	-4.01966979	0.28792721	-8.59843655
H	-4.47817062	-0.06220653	-11.00651387
Cd	0.01407780	-3.05867928	-8.08992947
O	-0.25233039	-5.22989278	-7.02285143
Cl	1.05513816	-5.21816373	-6.21310108
O	1.67786514	-3.84249400	-6.50432827
O	1.95459819	-6.29445382	-6.67921742
H	-3.12873540	-1.77632786	-12.27707698
H	-1.34821966	-3.03441576	-11.04464607
C	-2.15026216	-1.06446266	-7.07126821
C	-2.44612660	-1.20197060	-8.52296806
C	-2.94422502	-0.29515234	-6.20963449
C	-3.44664762	-0.45016928	-9.15468919
C	-2.95680715	-1.58797949	-11.21853695
C	-2.64863171	-0.24723707	-4.85356739
C	-3.70259025	-0.64517401	-10.51000228
C	-1.96661154	-2.29267716	-10.53895196
C	-0.80278349	-1.70283940	-5.26697293
C	-1.55873355	-0.96937073	-4.33612690
H	0.05012643	-2.30286515	-4.94830357
O	0.90557969	-4.31860666	-9.95689678
H	-3.26612619	0.36267254	-4.19419596
O	1.92876516	-2.87565941	-11.68216936
O	1.92607328	-2.20915622	-9.30245737
O	3.36232119	-4.06611688	-10.08525755
Cl	2.07285712	-3.37502480	-10.2951176