Electronic Supplementary Material (ESI) for Dalton Transactions

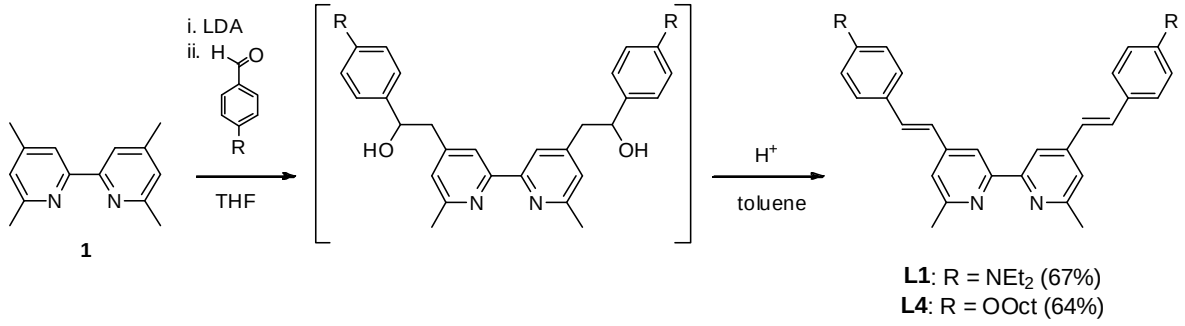
Supplementary Informations for

Heteroleptic diimine copper(I) complexes with large extinction coefficients: synthesis, quantum chemistry calculations and photophysical study

Martina Sandroni,[a] Megumi Kayanuma,[b] Huriye Akdas-Kilig,[c] Yann Pellegrin,[a] Errol Blart,[a] Mateusz Rebarz,[d] Olivier Poizat,[d] Michel Sliwa,[d*] Hubert Le Bozec,[c] Chantal Daniel,[b*] Fabrice Odobel[a]*

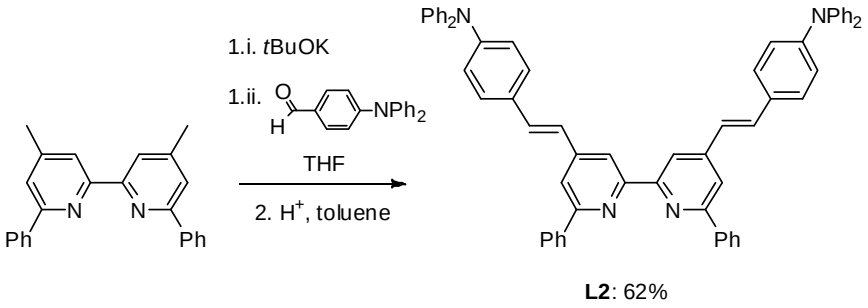
Synthesis of the ligands

Ligands **L1** and **L4** were classically prepared according to a Knoevenagel reaction. The methyl groups on the 4 and 4' positions in tetramethyl-bipyridine **1** were selectively deprotonated with lithium diisopropylamine (LDA), followed by the addition of two equivalents of the corresponding aldehyde. The resulting dialcohol was then dehydrated in presence of an acid (PPTS, pyridinium *p*-toluenesulfonate).[1]



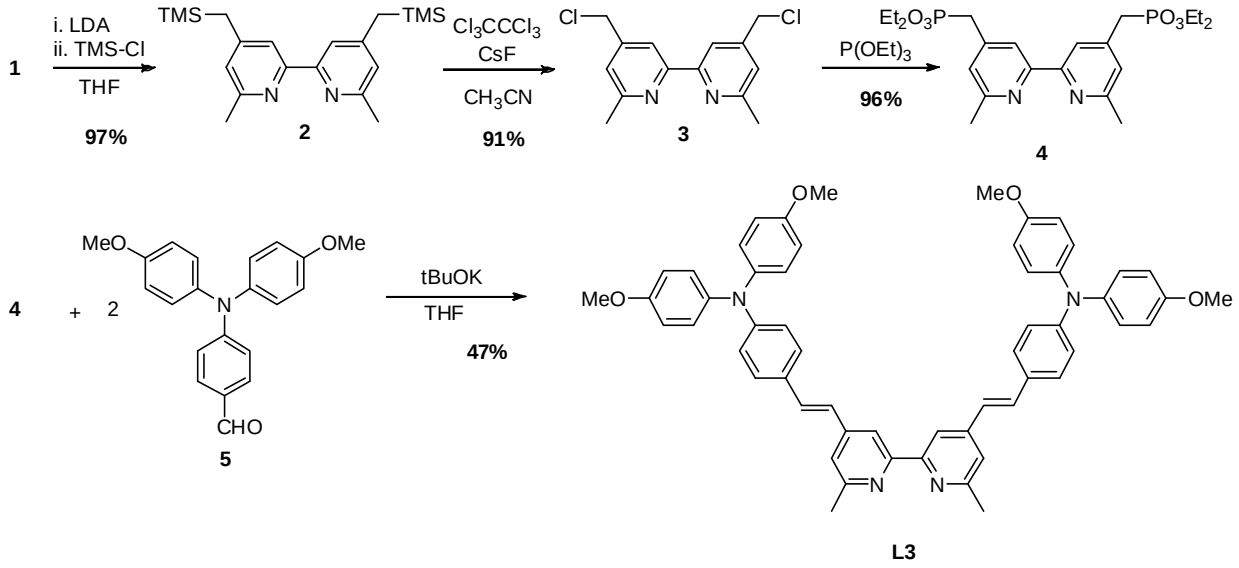
Scheme 1. Synthesis of ligands **L1** and **L4**.

Ligand **L2**[2] was also prepared with Knoevenagel reaction in 62% yield, but tBuOK was used as a base to deprotonate 4,4'-dimethyl-6,6'-diphenyl-2,2'-bipyridine (Scheme 2).



Scheme 2. Synthesis of ligand **L2**.

Ligand **L3** was prepared in 47% according to a Horner-Wadsworth-Emmons reaction between the 4,4'-methylphosphonate ethyl ester-6,6'-dimethyl-2,2'-bipyridine **4** and the aldehyde **5** (Scheme 4).[3] The 4,4'-methylphosphonate ethyl ester-6,6'-dimethyl-2,2'-bipyridine **4** was prepared in three steps from 4,4',6,6'-tetramethyl-2,2'-bipyridine **1** (Scheme 3)[4, 5]: dilithiation of **1** with LDA, followed by reaction with chlorotrimethylsilane and subsequent chlorination with hexachloroethane afforded selectively the resulting bis-chloromethyl derivative **3**, which was finally converted into the phosphonate ester derivative **4** in 85 % overall yield.[6] All these styryl bipyridine ligands display a t*rans* geometry for the vinyl double bond as proved by the high coupling constant measured on the ^{1}H NMR spectra.



Scheme 3. Synthesis of ligand **L3**.

Computational study

Table S1. TD-DFT (CAM-B3LYP) transition energies (in nm) to the low-lying singlet excited states of complexes **C1-C5** and associated oscillator strengths f calculated in dichloromethane. The main character of the state is given in percentage (in parenthesis).

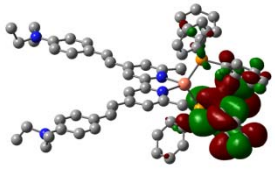
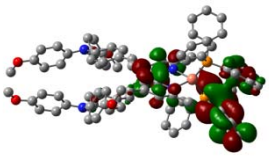
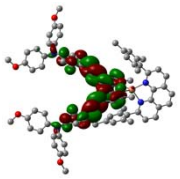
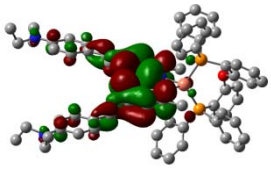
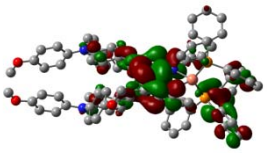
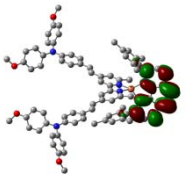
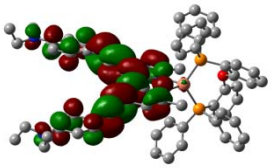
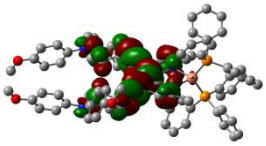
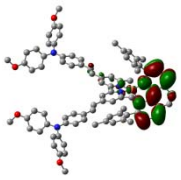
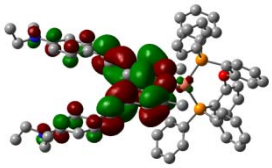
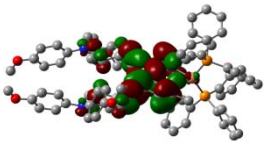
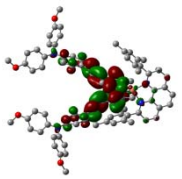
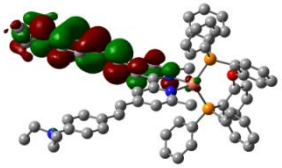
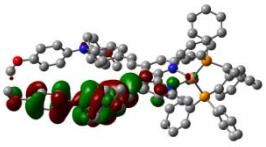
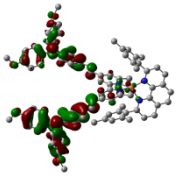
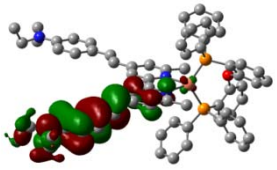
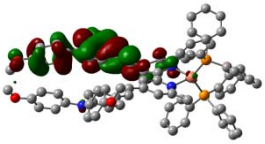
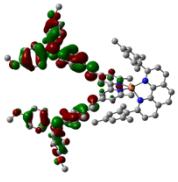
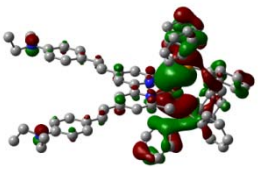
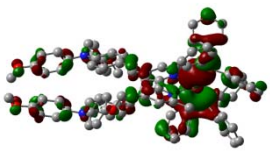
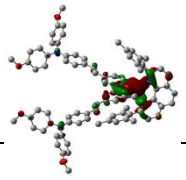
complex	state	ΔE (nm)	f
C1	$ILCT_{L1}$ (94)	410	1.37
	$ILCT_{L1}$ (90)	397	1.95
	$MLCT_{L1}$ (72) / $ILCT_{L1}$ (14)	325	0.07
	$ILCT_{L1}$ (92)	310	0.08
	$ILCT_{L1}$ (67) / $MLCT_{L1}$ (22)	299	0.23
	$ILCT_{L1}$ (83)	291	0.26
	$ILCT_{L1}$ (79)	280	0.06
	$ILCT_{L1}$ (70) / $LLCT_{DPEPhos}$ (16)	280	0.09
	$MLCT_{DPEPhos}$ (65) / $LLCT_{DPEPhos}$ (13)	262	0.09
	$ILCT_{L1}$ (39) / $MLCT_{L1}$ (34)	257	0.11
	$MLCT_{DPEPhos}$ (57)	252	0.07
C2	$ILCT_{L3}$ (90)	410	2.04
	$ILCT_{L3}$ (84)	398	1.64
	$ILCT_{L3}$ (81)	306	0.07
	$ILCT_{L3}$ (50) / $MLCT_{L3}$ (28)	298	0.06
	$ILCT_{L3}$ (64)	294	0.08
	$ILCT_{L3}$ (75)	293	0.12
	$ILCT_{L3}$ (79)	287	0.28
	$ILCT_{L3}$ (59)	275	0.05
	$ILCT_{L3}$ (49) / $LLCT_{DPEPhos}$ (12)	269	0.07
	$ILCT_{L3}$ (41) /$MLCT_{L3}$ (28)	264	0.06
	$ILCT_{L3}$ (63)	260	0.09
	$ILCT_{L3}$ (59)	259	0.11
	$ILCT_{L3}$ (26) / $MLCT_{DPEPhos}$ (25) / $LLCT_{DPEPhos}$ (12)	258	0.18
	$ILCT_{L3}$ (32) /$MLCT_{DPEPhos}$ (21) / $MLCT_{L3}$ (14)	258	0.09
	$ILCT_{L3}$ (78)	257	0.23

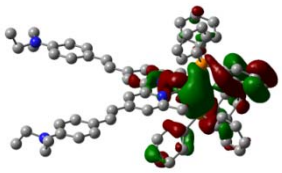
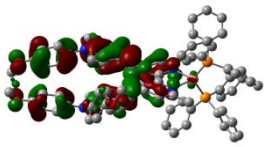
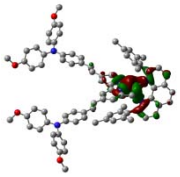
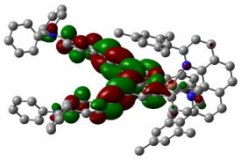
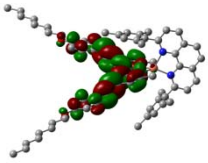
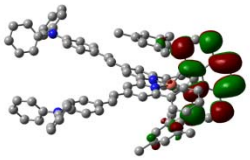
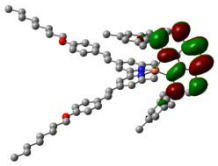
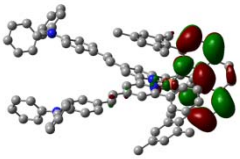
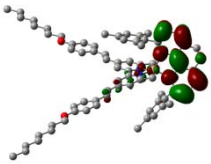
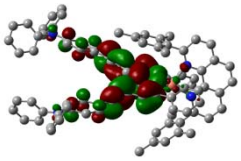
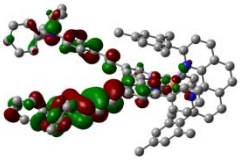
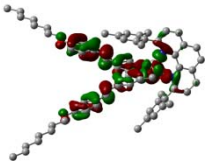
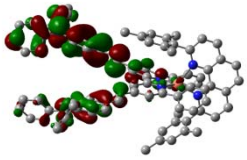
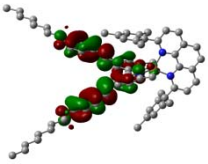
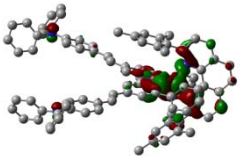
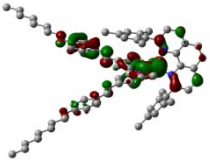
	$ILCT_{L3}$ (78)	256	0.24
C3	$MLCT_{Mes2Phen}$ (43) / $MLCT_{L3}$ (28) / $ILCT_{L3}$ (12)	442	0.35
	$MLCT_{Mes2Phen}$ (37) / $ILCT_{L3}$ (23) / $MLCT_{L3}$ (22)	421	0.73
	$ILCT_{L3}$ (87)	419	1.51
	$MLCT_{L3}$ (61) / $ILCT_{L3}$ (22)	404	0.61
	$MLCT_{Mes2Phen}$ (53) / $ILCT_{L3}$ (26) / $MLCT_{L3}$ (10)	374	0.21
	$MLCT_{L3}$ (47) / $MLCT_{Mes2Phen}$ (28) / $ILCT_{L3}$ (12)	355	0.10
	$ILCT_{L3}$ (63) / $MLCT_{L3}$ (12)	307	0.06
	$ILCT_{L3}$ (64)	303	0.08
	$ILCT_{L3}$ (79)	302	0.10
	$MLCT_{L3}$ (36) / LLC_{L3} (25) / $ILCT_{L3}$ (13)	292	0.14
	$ILCT_{L3}$ (73)	273	0.11
	$ILCT_{L3}$ (55) / $LLCT_{Mes2Phen}$ (21)	271	0.13
	$ILCT_{L3}$ (56)	268	0.16
	$ILCT_{L3}$ (24) / $IL_{Mes2Phen}$ (17) / $MLCT_{Mes2Phen}$ (13)	267	0.06
	$ILCT_{L3}$ (19) / $IL_{Mes2Phen}$ (19) / $MLCT_{Mes2Phen}$ (16)	267	0.37
	$ILCT_{L3}$ (65) / $LLCT_{L3}$ (16)	265	0.18
	$ILCT_{L3}$ (64)	264	0.25
	$ILCT_{L3}$ (71)	264	0.09
	$IL_{Mes2Phen}$ (22) / $LLCT_{L3}$ (16) / $MLCT_{L3}$ (10)	260	0.05
	$IL_{Mes2Phen}$ (33) / $MLCT_{Mes2Phen}$ (17)	255	0.39
	$ILCT_{Mes2Phen}$ (21) / $MLCT_{Mes2Phen}$ (18)	253	0.19
	$MLCT_{Mes2Phen}$ (51) / $ILCT_{L3}$ (12)	252	0.07
	$IL_{Mes2Phen}$ (66) / $LLCT_{L3}$ (11)	250	0.05
C4	$MLCT_{Mes2Phen}$ (51) / $MLCT_{L2}$ (23) / $ILCT_{L2}$ (13)	448	0.28
	$ILCT_{L2}$ (80)	409	1.43
	$ILCT_{L2}$ (41) / $MLCT_{L2}$ (28) / $MLCT_{Mes2Phen}$ (19)	407	1.13
	$ILCT_{L2}$ (34) / $MLCT_{Mes2Phen}$ (31) / $MLCT_{L2}$ (18)	373	0.75
	$MLCT_{Mes2Phen}$ (43) / $MLCT_{L2}$ (37)	363	0.13
	$ILCT_{L2}$ (41) / $MLCT_{L2}$ (13)	317	0.07
	$MLCT_{L2}$ (46) / $ILCT_{L2}$ (14)	309	0.05
	$MLCT_{L2}$ (63) / $ILCT_{L2}$ (12)	302	0.09

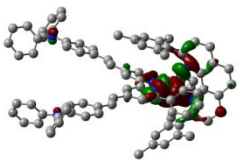
	$MLCT_{L2}$ (22) / $IL_{Mes2Phen}$ (21) / $ILCT_{L2}$ (14) / $MLCT_{Mes2Phen}$ (12) / $LLCT_{Mes2Phen}$ (10)	299	0.06
	$ILCT_{L2}$ (65)	294	0.08
	$MLCT_{L2}$ (38) / $ILCT_{L2}$ (36)	290	0.08
	$ILCT_{Mes2Phen}$ (25) / $MLCT_{Mes2Phen}$ (21) / $LLCT_{Mes2Phen}$ (10)	289	0.21
	$ILCT_{L2}$ (33) / $MLCT_{Mes2Phen}$ (18) / $LLCT_{Mes2Phen}$ (13)	281	0.09
	$LLCT_{Mes2Phen}$ (25) / $ILCT_{L2}$ (25) / $MLCT_{Mes2Phen}$ (10)	276	0.06
	$LLCT_{Mes2Phen}$ (32) / $MLCT_{Mes2Phen}$ (26)	275	0.06
	$ILCT_{L2}$ (58)	271	0.15
	$LLCT_{Mes2Phen}$ (23) / $ILCT_{L2}$ (16) / $MLCT_{L2}$ (11)	269	0.06
	$ILCT_{L2}$ (68)	267	0.18
	$ILCT_{L2}$ (21) / $LLCT_{L2}$ (13)	257	0.05
	$ILCT_{L2}$ (30) / $MLCT_{L2}$ (11) / $LLCT_{L2}$ (10)	250	0.17
C5	$MLCT_{Mes2Phen}$ (53) / $MLCT_{L4}$ (38)	447	0.12
	$MLCT_{L4}$ (56) / $MLCT_{Mes2Phen}$ (32)	421	0.10
	$MLCT_{L4}$ (45) / $MLCT_{Mes2Phen}$ (43)	395	0.42
	$ILCT_{L4}$ (52) / $MLCT_{L4}$ (34)	362	1.48
	$MLCT_{Mes2Phen}$ (52) / $MLCT_{L4}$ (33)	359	0.07
	$MLCT_{L4}$ (26) / $ILCT_{Mes2Phen}$ (24) / $LLCT_{L4}$ (19) / $ILCT_{L4}$ (13)	332	0.45
	$ILCT_{Mes2Phen}$ (40) / $MLCT_{L4}$ (26) / $ILCT_{L4}$ (14)	330	0.43
	$LLCT_{L4}$ (56) / $ILCT_{Mes2Phen}$ (16)	324	0.06
	$LLCT_{L4}$ (40) / $MLCT_{Mes2Phen}$ (13) / $ILCT_{Mes2Phen}$ (11) / $MLCT_{L4}$ (10)	306	0.14
	$MLCT_{Mes2Phen}$ (51) / $LLCT_{L4}$ (16) / $ILCT_{Mes2Phen}$ (15)	303	0.06
	$MLCT_{L4}$ (56)	279	0.05
	$ILCT_{Mes2Phen}$ (70) / $MLCT_{Mes2Phen}$ (16)	275	0.10
	$ILCT_{Mes2Phen}$ (52)	271	0.26
	$LLCT_{L4}$ (51) / $ILCT_{L4}$ (14) / $MLCT_{L4}$ (12)	268	0.09
	$MLCT_{L4}$ (41) / $LLCT_{L4}$ (22) / $ILCT_{L4}$ (20)	267	0.06
	$ILCT_{L4}$ (41) / $LLCT_{L4}$ (21) / $MLCT_{L4}$ (13)	264	0.24
	$ILCT_{Mes2Phen}$ (42) / $LLCT_{L4}$ (16)	262	0.08
	$ILCT_{L4}$ (58)	260	0.05
	$ILCT_{L4}$ (59)	259	0.06
	$MLCT_{Mes2Phen}$ (58) / $ILCT_{Mes2Phen}$ (14)	254	0.05

	$ILCT_{Mes2Phen}$ (44) / $LLCT_{Mes2Phen}$ (33)	253	0.05
	$ILCT_{Mes2Phen}$ (58) / $MLCT_{Mes2Phen}$ (10)	252	0.09
	$ILCT_{Mes2Phen}$ (55)	251	0.20
	$ILCT_{Mes2Phen}$ (33) / $LLCT_{Mes2Phen}$ (13) / $ILCT_{L4}$ (13)	250	0.06

Table S2. Graphical representation of the optimized structure and frontier molecular orbitals (from HOMO-3 to LUMO+3) of the copper (I) complexes **C1** to **C5** calculated using CAM-B3LYP functional considering solvent effect of dichloromethane with their energies in atomic unit.

L+3	 -0.00979	 -0.01001	 -0.03758
L+2	 -0.01152	 -0.01105	 -0.04061
L+1	 -0.03380	 -0.04086	 -0.04642
L	 -0.05723	 -0.05797	 -0.05599
H	 -0.23755	 -0.23574	 -0.23040
H-1	 -0.23817	 -0.23681	 -0.23088
H-2			

	-0.27335	-0.27065	-0.25817
H-3	 -0.29572	 -0.28123	 -0.26584
	C1	**C2**	**C3**
L+3	 -0.04014	 -0.03600	
L+2	 -0.04278	 -0.04174	
L+1	 -0.04698	 -0.04666	
L	 -0.05974	 -0.05588	
H	 -0.24019	 -0.25183	
H-1	 -0.24117	 -0.26121	
H-2			

	-0.25886	-0.26425
H-3	 -0.26957	 -0.27341
	C4	**C5**

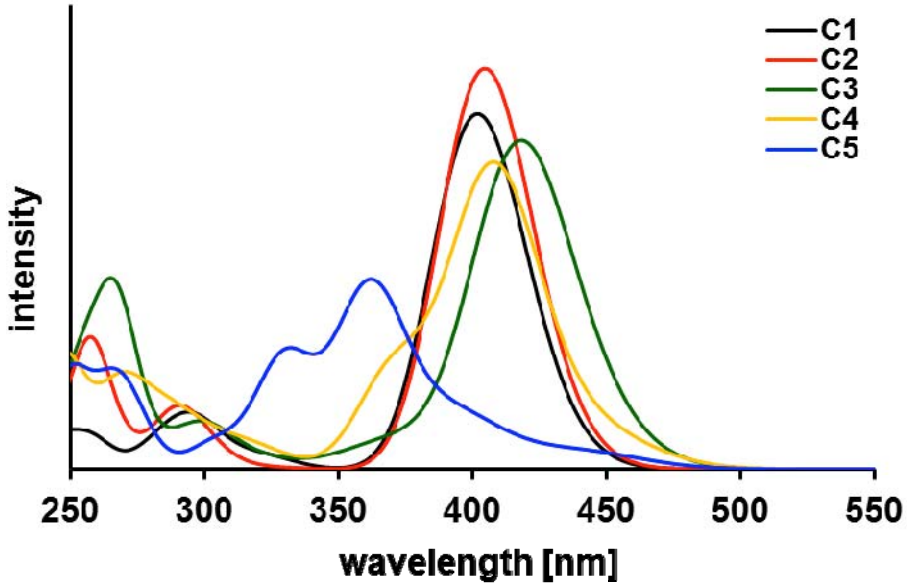


Figure S1. Theoretical UV-Vis absorption spectra of the complexes **C1-C5** in dichloromethane.

Table S3
Cartesian coordinates of the optimized structures of comples C1 to C5

C1

Cu	2.312740	-0.263231	0.176108	H	-8.593494	6.679981	-1.888510	C	5.927312	-0.034352	0.758659
C	-0.738512	-3.433819	0.491436	C	-9.309190	7.448539	0.019953	C	5.781052	-1.528017	2.644186
C	-0.021979	3.398489	-0.570288	H	-9.288343	8.295898	-1.976441	C	7.177733	-0.547797	0.417274
C	-1.951614	-2.718009	0.383842	C	-7.167295	10.149395	-2.889539	C	7.036208	-2.049308	2.318875
C	-1.355276	2.952539	-0.430304	H	-6.447213	10.088174	-0.832577	H	5.232683	-1.925538	3.497953
C	-1.823480	-1.324687	0.238377	H	-8.202868	10.101562	-0.982113	C	7.728999	-1.561537	1.205819
C	-1.514047	1.583997	-0.145852	H	-8.699154	6.784367	0.648405	H	7.698371	-0.162716	-0.460845
C	-0.417149	0.740934	-0.014708	H	-9.407180	8.413721	0.538848	H	7.468274	-2.840213	2.933099
C	-0.573364	-0.711871	0.205071	H	-10.313651	7.010910	-0.086825	H	8.705322	-1.971480	0.943812
C	0.481117	-2.771894	0.452103	H	-6.247023	9.756648	-3.344723	C	4.723923	0.634387	-2.235754
C	1.043228	2.512058	-0.429146	H	-8.022563	9.781015	-3.475937	C	5.566079	1.228200	-1.279687
H	-2.730776	-0.732728	0.142665	H	-7.154053	11.247988	-2.953517	C	4.890453	1.008936	-3.578903
H	-2.524002	1.198106	-0.029499	H	-9.763464	-5.403515	-1.068611	C	6.543054	2.156646	-1.634734
N	0.579756	-1.423668	0.310695	H	-10.643049	-6.948783	-1.154854	C	5.86675-	1.937937	-3.948588
N	0.857483	1.193346	-0.153842	H	-11.40512	-5.539452	-0.372663	H	4.234763	0.578002	-4.336973
C	-2.544008	3.763982	-0.551622	H	-7.719256	-9.237376	2.407571	C	6.698186	2.508216	-2.979044
C	-3.268954	-3.310247	0.413224	H	-9.487030	-9.080739	2.550179	H	7.155222	2.604130	-0.850465
H	-0.736485	-4.517949	0.603716	H	-8.786309	-10.502378	1.731800	H	5.973862	2.218828	-4.996979
H	0.195974	4.442245	-0.798976	P	3.502598	-0.640753	-1.696657	H	7.459044	3.236059	-3.264893
C	2.457901	2.957296	-0.627142	P	3.468537	0.045307	2.059777	O	5.315786	0.996480	0.069201
H	2.914733	2.412081	-1.467095	C	2.906565	-0.758139	3.606536				
H	2.510187	4.032795	-0.835180	C	1.757844	-1.559960	3.589106				
H	3.061955	2.731102	0.262675	C	3.569502	-0.523200	4.824746				
C	1.769958	-3.520149	0.555314	C	1.288777	-2.147515	4.770151				
H	1.603869	-4.572458	0.815539	H	1.216055	-1.698909	2.654359				
H	2.308677	-3.472201	-0.401016	C	3.104332	-1.113815	6.000434				
H	2.413602	-3.056848	1.316171	H	4.444121	0.129975	4.848170				
H	-3.476326	3.212771	-0.407675	C	1.965424	-1.931648	5.974169				
H	-4.096278	-2.602878	0.316430	H	0.388836	-2.764969	4.746973				
C	-2.619176	5.097102	-0.820231	H	3.623116	-0.927160	6.942299				
H	-1.688718	5.655350	-0.966337	H	1.599491	-2.387034	6.896651				
C	-3.546700	-4.637297	0.547769	C	3.540938	1.796174	2.591768				
H	-2.705886	-5.331596	0.643447	C	4.735512	2.505959	2.768397				
C	-4.845745	-5.259275	0.580796	C	2.308649	2.435234	2.815044				
C	-4.945709	-6.661672	0.727954	C	4.697029	3.848645	3.160914				
C	-6.062167	-4.544120	0.473187	H	5.69291	2.010678	2.597572				
C	-6.164301	-7.317100	0.766619	C	2.274409	3.772674	3.212219				
H	-4.026880	-7.244676	0.825579	H	1.376629	1.884540	2.669894				
C	-7.288868	-5.178343	0.509380	C	3.469919	4.483783	3.381806				
H	-6.043273	-3.461177	0.344621	H	5.629897	4.398702	3.296862				
C	-7.383888	-6.593214	0.657997	H	1.313693	4.260193	3.387396				
H	-6.181354	-8.397122	0.907280	H	3.444165	5.531203	3.688998				
H	-8.193839	-4.583139	0.395536	C	4.577820	-2.124949	-1.766732				
C	-3.830343	5.873598	-0.933607	C	5.264767	-2.476623	-2.942625				
C	-3.764100	7.256381	-1.217544	C	4.782580	-2.872487	-0.600404				
C	-5.125409	5.324014	-0.773938	C	6.111791	-3.585777	-2.953297				
C	-4.897115	8.045558	-1.336386	H	5.137528	-1.878295	-3.846848				
H	-2.783379	7.715984	-1.358850	C	5.631658	-3.983917	-0.610377				
C	-6.267559	6.091477	-0.888022	H	4.290235	-2.565721	0.321368				
H	-5.241983	4.265304	-0.541371	C	6.292086	-4.345474	-1.788061				
C	-6.195527	7.486725	-1.174710	H	6.637175	-3.855691	-3.870892				
H	-4.781704	9.099599	-1.583231	H	5.781878	-4.556577	0.306271				
H	-7.235555	5.619159	-0.726583	H	6.957016	-5.211388	-1.800207				
N	-7.332924	8.245058	-1.287111	C	2.405856	-0.751070	-3.158822				
N	-8.599797	-7.225743	0.694286	C	1.612999	0.375416	-3.446042				
C	-8.662319	7.638318	-1.353659	C	2.262715	-1.905370	-3.941773				
C	-7.282120	9.698442	-1.431802	C	0.718447	0.358149	-4.516623				
C	-9.852936	-6.484602	0.819977	H	1.693853	1.270178	-2.827668				
C	-8.714728	-8.676749	0.555650	C	1.360009	-1.922502	-5.011738				
C	-8.672666	-9.41944	1.892154	H	2.856687	-2.792468	-3.721136				
H	-7.917659	-9.032254	-0.113598	C	0.592465	-0.792052	-5.306858				
H	-9.667289	-8.879329	0.041274	H	0.114731	1.241910	-4.730017				
C	-10.451171	-6.066914	-0.525387	H	1.260516	-2.824758	-5.617240				
H	-9.683198	-5.607751	1.461201	H	-0.106673	-0.807790	-6.145343				
H	-10.559634	-7.133570	1.360517	C	5.203362	-0.508418	1.871242				

C2

Cu	1.409031	-3.513809	0.140474	C	5.633030	9.540169	-0.795557	C	2.241442	-3.094696	3.746312
C	-2.738563	-2.333215	-0.373912	C	6.001863	10.279632	-1.926296	C	4.097100	-4.839700	4.899510
C	3.623319	0.220166	0.516871	C	4.618408	10.035931	0.040089	H	3.405679	-6.295686	3.452136
C	-2.722006	-0.959650	-0.032152	C	5.399106	11.501508	-2.218070	C	3.028886	-2.664890	4.815328
C	2.663581	1.190727	0.148483	H	6.791469	9.909709	-2.579070	H	1.527202	-2.411202	3.281616
C	-1.443176	-0.394604	0.141789	C	4.001866	11.249800	-0.250327	C	3.959890	-3.537584	5.393464
C	1.349246	0.714747	-0.018668	H	4.333664	9.476475	0.932127	H	4.821561	-5.521053	5.349229
C	1.058403	-0.630489	0.176059	C	4.399114	11.998449	-1.374554	H	2.916737	-1.648438	5.196612
C	-0.298567	-1.171562	-0.021272	H	5.722168	12.058796	-3.095882	H	4.576532	-3.201784	6.229474
C	-1.565052	-3.053056	-0.522022	H	3.226425	11.652729	0.401971	C	1.928204	-5.669676	-2.585790
C	3.272806	-1.111094	0.697360	C	-11.396570	0.185170	0.780965	C	2.488505	-6.033419	-3.823067
H	-1.348659	0.651754	0.431922	C	-12.524575	-0.197680	0.048840	C	0.923577	-6.462885	-2.019977
H	0.561031	1.399113	-0.331297	C	-11.121672	-0.423023	2.006771	C	2.028634	-7.168773	-4.490847
N	-0.344157	-2.488130	-0.349629	C	-13.358066	-1.200870	0.535174	H	3.283137	-5.425823	-4.260516
N	1.998300	-1.545720	0.530242	H	-12.739444	0.290319	-0.903281	C	0.460043	-7.599704	-2.691603
C	2.963383	2.592045	-0.054980	C	-11.941755	-1.433753	2.502206	H	0.523802	-6.200326	-1.041471
C	-3.920911	-0.163273	0.134310	H	-10.243111	-0.103507	2.568709	C	1.011139	-7.952754	-3.926591
H	-3.675506	-2.865211	-0.527193	C	-13.063653	-1.831080	1.758869	H	2.467405	-7.446744	-5.450420
H	4.665666	0.493959	0.675200	H	-14.237494	-1.521129	-0.024100	H	-0.321593	-8.212661	-2.239560
C	4.297678	-2.143501	1.046830	H	-11.706482	-1.899339	3.457218	H	0.656565	-8.842685	-4.450017
H	4.509996	-2.778530	0.173164	C	-10.967969	2.549334	0.480499	C	2.696350	-2.898004	-2.899326
H	5.235951	-1.676146	1.369822	C	-11.927017	2.818846	1.466027	C	3.525108	-1.792054	-2.637048
H	3.926307	-2.806982	1.838847	C	-10.557811	3.590274	-0.371022	C	1.868013	-2.879171	-4.032307
C	-1.577457	-4.509635	-0.854608	C	-12.494905	4.084624	1.593448	C	3.538607	-0.697134	-3.502878
H	-2.599397	-4.881503	-0.995255	H	-12.257585	2.021500	2.130178	H	4.168734	-1.787791	-1.756959
H	-0.994001	-4.695922	-1.765910	C	-11.109350	4.860959	-0.240164	C	1.885312	-1.781575	-4.899445
H	-1.101814	-5.074295	-0.038048	H	-9.824410	3.390994	-1.152988	H	1.212999	-3.725601	-4.242063
H	2.124074	3.231560	-0.339540	C	-12.094779	5.113252	0.733428	C	2.719470	-0.689599	-4.638935
H	-3.781894	0.887624	0.400002	H	-13.250336	4.254141	2.358370	H	4.186261	0.154776	-3.286962
C	4.206806	3.124474	0.087805	H	-10.812285	5.669765	-0.908703	H	1.243607	-1.784167	-5.782300
H	5.010790	2.440853	0.374326	O	11.646810	8.415042	-2.291891	H	2.730393	0.166608	-5.315943
C	-5.169968	-0.680563	-0.026983	O	3.772068	13.198887	-1.564103	C	1.646691	-6.582426	1.399916
H	-5.225291	-1.738972	-0.293263	O	-12.616609	6.376895	0.764539	C	2.862977	-6.790192	0.717137
C	-6.475178	-0.089506	0.085671	O	-13.918602	-2.821373	2.150238	C	0.730523	-7.645647	1.442537
C	-7.573182	-0.949677	-0.156867	C	-13.622808	-3.486348	3.380296	C	3.174144	-8.010083	0.118271
C	-6.769181	1.255763	0.412257	H	-13.655090	-2.782575	4.227901	C	1.027636	-8.874005	0.846024
C	-8.874438	-0.512652	-0.082385	H	-14.400505	-4.248139	3.500410	H	-0.230496	-7.501488	1.934547
H	-7.376681	-1.989539	-0.425454	H	-12.631944	-3.967846	3.339827	C	2.248622	-9.054670	0.188506
C	-8.080046	1.713373	0.491602	C	11.996251	7.708425	-3.483597	H	4.123427	-8.126560	-0.407146
H	-5.955179	1.952265	0.621798	H	11.433824	8.092668	-4.350216	H	0.303120	-9.687395	0.894442
C	-9.163405	0.834966	0.244916	H	13.067307	7.884780	-3.630048	H	2.485140	-10.011089	-0.279901
H	-9.693366	-1.200320	-0.288954	H	11.807345	6.628146	-3.372009	C	4.320331	-4.754945	-1.417518
H	-8.285481	2.751831	0.752075	C	4.210123	13.992793	-2.669723	C	4.664994	-5.517461	-0.286625
C	4.657932	4.480020	-0.077618	H	5.281507	14.237028	-2.580752	C	5.338013	-4.453096	-2.337499
C	6.031989	4.733270	0.142795	H	4.030069	13.475791	-3.626534	C	5.968567	-5.960332	-0.067489
C	3.848966	5.581925	-0.441173	H	3.616429	14.912663	-2.629492	C	6.647949	-4.891221	-2.129938
C	6.572328	5.992905	0.012680	C	-13.664489	6.622708	1.705891	H	5.100124	-3.849075	-3.213912
H	6.678526	3.904578	0.438621	H	-13.308744	6.489476	2.740793	C	6.965036	-5.647165	-0.996309
C	4.378184	6.859045	-0.576723	H	-13.966647	7.664153	1.549957	H	6.186778	-6.525161	0.839734
H	2.784385	5.432682	-0.627547	H	-14.522860	5.954948	1.524295	H	7.422848	-4.636628	-2.853766
C	5.756493	7.092083	-0.351705	P	2.567450	-4.228599	-1.651077	H	7.988952	-5.983569	-0.826328
H	7.632347	6.153886	0.203495	P	1.236788	-4.870920	1.896279	O	3.719858	-5.705244	0.717745
H	3.737642	7.692411	-0.865858	C	-0.325603	-5.017841	2.847059				
N	6.355760	8.346822	-0.469423	C	-1.342305	-4.080217	2.621613				
N	-10.506085	1.210738	0.303091	C	-0.471839	-5.958502	3.883529				
C	7.721830	8.338936	-0.923847	C	-2.510834	-4.102603	3.391664				
C	8.708830	9.059505	-0.244546	H	-1.211436	-3.315352	1.857410				
C	8.046552	7.641392	-2.088686	C	-1.639305	-5.983782	4.647454				
C	10.014807	9.069887	-0.725407	H	0.334805	-6.662016	4.097012				
H	8.443836	9.611869	0.658229	C	-2.663933	-5.059174	4.398758				
C	9.350414	7.637263	-2.578735	H	-3.293210	-3.363872	3.207692				
H	7.262634	7.092174	-2.611463	H	-1.744702	-6.714550	5.451126				
C	10.341890	8.355939	-1.893382	H	-3.572358	-5.075902	5.004185				
H	10.800265	9.621880	-0.208327	C	2.373931	-4.405349	3.254898				
H	9.582393	7.087287	-3.488610	C	3.303594	-5.277737	3.833217				

C3

Cu	-0.364449	-5.083066	0.047029	C	-10.775157	4.708711	-1.654531	H	-1.883699	-10.653979	-2.442553
C	-3.529600	-2.266991	0.801975	C	-11.315769	6.194034	0.195396	H	0.984586	-8.818100	3.419373
C	3.256723	-2.780768	-0.532604	C	-11.714423	5.471149	-0.944516	H	-2.650126	-6.338878	-4.517163
C	-2.899594	-1.048259	0.471606	H	-8.703850	4.107353	-1.779872	C	1.047823	-6.186639	2.884154
C	2.818202	-1.475556	-0.220452	H	-11.066303	4.149846	-2.542110	C	-1.902267	-4.328676	-2.895885
C	-1.519334	-1.117463	0.213488	H	-9.674833	6.716496	1.495352	H	0.121208	-10.662583	1.949693
C	1.444073	-1.336947	0.051139	H	-12.060387	6.778091	0.737090	H	-2.517492	-8.805127	-4.060795
C	0.596833	-2.434959	0.006971	O	-13.033610	5.574207	-1.285712	C	2.446275	-6.001323	2.871203
C	-0.844881	-2.327232	0.287272	C	7.175885	5.936061	-1.404686	C	0.234035	-5.427148	3.745182
C	-2.803720	-3.451577	0.861422	C	8.355672	6.520421	0.626116	C	0.833075	-4.453995	4.553523
C	2.362650	-3.846551	-0.562597	C	7.902756	7.837193	0.520290	C	3.001866	-5.012852	3.688599
H	-0.986950	-0.213543	-0.079002	C	6.712773	7.240557	-1.513939	C	2.212003	-4.223717	4.533078
H	1.053071	-0.358019	0.324710	C	7.071022	8.199914	-0.547958	C	-1.242742	-5.701203	3.870556
N	-1.470458	-3.493316	0.607824	H	9.005186	6.233234	1.453794	H	0.201335	-3.866216	5.225252
N	1.041437	-3.685490	-0.296496	H	8.196980	8.569384	1.270490	C	3.345291	-6.877935	2.033121
H	-4.597228	-2.299067	1.022760	H	6.909145	5.190204	-2.154745	H	4.084443	-4.859307	3.668774
H	4.304651	-2.973816	-0.765687	H	6.082761	7.544612	-2.350519	C	2.832994	-3.144916	5.383570
C	-3.464680	-4.734772	1.277057	O	6.566856	9.456840	-0.738226	C	-3.160990	-3.738696	-2.642312
C	2.817908	-5.215661	-0.980139	C	10.867251	4.619647	-0.595221	C	-0.850819	-3.567618	-3.434720
C	3.662440	-0.305273	-0.162822	C	10.153688	3.323681	1.320415	C	-1.071567	-2.205443	-3.691088
C	-3.561526	0.231375	0.383497	C	11.481803	3.167496	1.722080	C	-3.332313	-2.378417	-2.900614
C	5.002251	-0.264905	-0.396245	C	12.191209	4.478787	-0.200975	C	-2.298019	-1.592485	-3.426765
H	3.144435	0.621782	0.093276	C	12.506303	3.751066	0.961946	C	0.497134	-4.168511	-3.744682
H	5.513713	-1.197917	-0.651900	H	9.347934	2.884220	1.909385	H	-0.257815	-1.612826	-4.118723
C	5.852332	0.898094	-0.340967	H	11.708878	2.609666	2.629165	C	-4.312075	-4.560674	-2.117016
C	-4.882704	0.468527	0.601512	H	10.614776	5.186484	-1.492698	H	-4.301827	-1.918602	-2.687945
H	-2.912034	1.068214	0.114982	H	13.000820	4.922249	-0.781558	C	-2.527656	-0.130015	-3.712414
H	-5.523831	-0.376017	0.872210	O	13.834395	3.669172	1.273013	H	-1.679835	-6.013077	2.914522
C	-5.556193	1.739431	0.517147	H	3.034685	-5.227929	-2.059498	H	-1.421955	-6.509884	4.598795
C	-4.902297	2.949642	0.183555	H	3.734724	-5.504553	-0.450316	H	-1.774961	-4.809154	4.227717
C	-6.944568	1.806876	0.777151	H	2.032700	-5.955980	-0.779094	H	2.928737	-2.209620	4.809151
C	-7.644712	2.998204	0.711526	H	-3.490930	-4.803268	2.375012	H	2.218422	-2.931553	6.268948
C	-5.587362	4.148793	0.113652	H	-4.497738	-4.784121	0.910360	H	3.840164	-3.431770	5.717240
C	-6.978078	4.199705	0.376924	H	-2.898982	-5.597142	0.898364	H	3.502173	-7.855192	2.518111
H	-7.472893	0.891987	1.053954	C	14.186062	2.995066	2.481911	H	2.916888	-7.074826	1.041644
H	-8.714131	3.024438	0.920738	C	6.854265	10.440484	0.256844	H	4.330553	-6.409948	1.903524
H	-3.835205	2.947734	-0.041399	C	-13.456895	4.909672	-2.476624	H	-4.713462	-5.228634	-2.896473
H	-5.064410	5.067589	-0.152718	C	-5.257881	11.327229	-0.337331	H	-3.999739	-5.199215	-1.278949
N	-7.680722	5.397809	0.310636	H	13.732663	3.491093	3.355877	H	-5.128596	-3.909156	-1.777489
C	5.381301	2.194969	-0.024466	H	13.873344	1.938366	2.453688	H	-2.950434	0.378064	-2.831477
C	7.233854	0.764248	-0.613034	H	15.278222	3.055833	2.546541	H	-1.594394	0.374231	-3.998387
C	8.097075	1.845593	-0.574716	H	6.470607	10.128510	1.242016	H	-3.248735	-0.001130	-4.535193
C	6.229784	3.285752	0.018186	H	7.937151	10.633184	0.325990	H	1.201305	-3.962256	-2.924798
C	7.611548	3.135422	-0.256872	H	6.337959	11.350246	-0.070175	H	0.444855	-5.258452	-3.873587
H	7.625720	-0.221346	-0.873826	H	-12.914147	5.294111	-3.355818	H	0.912951	-3.728259	-4.662003
H	9.157897	1.715194	-0.790166	H	-13.308592	3.820137	-2.398433				
H	4.328025	2.348203	0.213652	H	-14.525464	5.131206	-2.574541				
H	5.844778	4.273035	0.274370	H	-4.893123	10.940996	-1.303346				
N	8.475583	4.224840	-0.217258	H	-6.308833	11.642964	-0.439025				
C	9.838354	4.042083	0.164606	H	-4.644786	12.180061	-0.024480				
C	7.994963	5.561855	-0.326267	C	0.538297	-8.603174	2.448108				
C	-9.048580	5.398854	-0.095177	C	-2.224450	-6.719521	-3.588199				
C	-7.018122	6.657572	0.379507	C	0.063798	-9.618332	1.638186				
C	-6.177186	6.960835	1.462962	C	-2.152622	-8.076682	-3.334821				
C	-7.227781	7.615427	-0.617268	C	-0.495970	-9.290716	0.384724				
C	-6.609632	8.865134	-0.546890	C	-1.606328	-8.522075	-2.111715				
C	-5.550521	8.197883	1.537849	C	-0.560910	-7.916387	0.040980				
C	-5.763393	9.158821	0.531310	C	-1.133076	-7.528669	-1.216688				
H	-7.891735	7.381935	-1.450508	C	-1.747720	-5.787804	-2.638795				
H	-6.789447	9.599352	-1.330393	C	0.463342	-7.256988	2.031144				
H	-6.025897	6.216155	2.245847	C	-0.987216	-10.271702	-0.537142				
H	-4.902973	8.449590	2.378465	C	-1.516558	-9.902867	-1.742033				
O	-5.110102	10.34905	0.693096	N	-0.092490	-6.913808	0.851608				
C	-9.993346	6.154279	0.616089	N	-1.197966	-6.190096	-1.481157				
C	-9.445993	4.685571	-1.228568	H	-0.925311	-11.323416	-0.254942				

C4

Cu	-0.340452	-3.923780	0.071870	H	9.073657	2.962956	-1.192195	H	-2.647570	-5.093335	-4.573460
C	-3.467005	-1.008370	0.906410	H	4.196720	3.628362	-0.505668	C	1.175575	-5.060805	2.789017
C	3.283422	-1.581070	-0.577224	H	5.668034	5.569671	-0.633287	C	-1.780333	-3.098607	-2.947612
C	-2.836977	0.180420	0.496388	N	8.323728	5.533693	-0.991557	H	0.277826	-9.524851	1.751762
C	2.784688	-0.271799	-0.453756	C	9.639350	5.451226	-1.547060	H	-2.512210	-7.562462	-4.146725
C	-1.498883	0.052316	0.093195	C	7.870461	6.832540	-0.600008	C	2.581874	-5.025476	2.940693
C	1.398960	-0.160744	-0.255169	C	-8.839466	6.852728	1.049188	C	0.367640	-4.131795	3.477574
C	0.591767	-1.292253	-0.188490	C	-6.721262	8.020004	0.796401	C	0.982874	-3.121823	4.225317
C	-0.856376	-1.180618	0.106085	C	-5.644999	8.238863	1.668288	C	3.151688	-3.991184	3.690816
C	-2.784673	-2.223791	0.903542	C	-7.145330	9.045525	-0.060615	C	2.372379	-3.017028	4.326062
C	2.438386	-2.687974	-0.504238	C	-6.491725	10.279193	-0.048328	C	-1.126149	-4.277270	3.540857
H	-0.975310	0.940803	-0.252722	C	-4.990063	9.472394	1.668802	H	0.349078	-2.406154	4.756333
H	0.973114	0.830929	-0.122456	C	-5.410279	10.497191	0.812858	C	3.476903	-6.080198	2.339591
N	-1.481924	-2.323754	0.506635	H	-7.991752	8.866814	-0.726274	H	4.240809	-3.950359	3.783049
N	1.094326	-2.550342	-0.310397	H	-6.825565	11.071405	-0.719953	C	3.008595	-1.886040	5.093083
H	-4.506035	-1.005502	1.230638	H	-5.331687	7.438983	2.340860	C	-3.026312	-2.453450	-2.756068
H	4.338617	-1.747510	-0.779755	H	-4.156498	9.637672	2.353230	C	-0.654787	-2.366477	-3.366727
C	-3.482323	-3.418333	1.435170	H	-4.901707	11.462340	0.820592	C	-0.772948	-0.975512	-3.515517
C	3.020025	-4.034299	-0.723338	C	-9.300376	7.572539	2.159960	C	-3.093863	-1.068217	-2.911925
C	3.593012	0.925440	-0.517900	C	-9.750399	6.216462	0.197519	C	-1.972766	-0.307086	-3.271687
C	-3.464438	1.482659	0.466493	C	-11.119444	6.291550	0.466486	C	0.661045	-3.023465	-3.698338
C	-4.258531	-3.291043	2.601349	C	-10.669831	7.648422	2.420256	H	0.103593	-0.406158	-3.839167
C	-3.382897	-4.679077	0.832285	C	-11.583693	7.005744	1.577379	C	-4.269109	-3.221785	-2.380278
C	-4.024943	-5.789027	1.384443	H	-9.376435	5.664840	-0.666150	H	-4.051676	-0.567558	-2.743351
C	-4.894030	-4.399800	3.160676	H	-11.826996	5.798995	-0.201754	C	-2.082315	1.191064	-3.400211
C	-4.776146	-5.656084	2.555645	H	-8.577932	8.069408	2.810379	H	-1.547015	-4.703661	2.623895
H	-2.804760	-4.782462	-0.080872	H	-11.021570	8.206477	3.289392	H	-1.397077	-4.948675	4.373374
H	-3.939821	-6.760317	0.894225	H	-12.653346	7.064237	1.783338	H	-1.606193	-3.307892	3.727155
H	-4.324186	-2.320229	3.095658	C	7.340292	7.050305	0.679038	H	3.162100	-1.014276	4.436435
H	-5.473611	-4.285235	4.077539	C	7.970132	7.896710	-1.507503	H	2.369120	-1.563033	5.926714
H	-5.270816	-6.524414	2.993485	C	7.532716	9.170105	-1.138767	H	3.989271	-2.175834	5.495293
C	4.350658	-4.299692	-0.347141	C	6.898065	8.325680	1.039056	H	3.435192	-7.012319	2.926491
C	2.305539	-5.038520	-1.393904	C	6.991203	9.389086	0.133124	H	3.189672	-6.326963	1.307523
C	2.900830	-6.266542	-1.688052	H	8.392749	7.713723	-2.497337	H	4.520235	-5.738905	2.334410
C	4.949865	-5.522476	-0.647424	H	7.609267	9.991708	-1.852403	H	-4.450369	-4.062014	-3.067685
C	4.227550	-6.512796	-1.321847	H	7.277660	6.215966	1.379450	H	-4.193942	-3.646938	-1.368168
H	1.288836	-4.835362	-1.721146	H	6.490479	8.491874	2.037305	H	-5.147789	-2.564067	-2.405880
H	2.330601	-7.027088	-2.224702	H	6.648130	10.384617	0.418734	H	-2.520454	1.626014	-2.487508
H	4.912184	-3.548014	0.209136	C	10.719573	5.986442	-0.831696	H	-1.099630	1.650064	-3.575198
H	5.979709	-5.710181	-0.339863	C	9.851289	4.870968	-2.805028	H	-2.742166	1.470575	-4.236134
H	4.695417	-7.469308	-1.559769	C	11.141453	4.818415	-3.337277	H	1.408260	-2.827855	-2.916215
C	4.939452	0.970468	-0.704593	C	12.006547	5.933205	-1.370712	H	0.569263	-4.111455	-3.808790
H	3.042536	1.861970	-0.399452	C	12.223105	5.348197	-2.623364	H	1.059033	-2.617218	-4.639309
H	5.478777	0.025370	-0.821025	H	9.001002	4.464634	-3.354810				
C	5.767423	2.149564	-0.772231	H	11.299658	4.371781	-4.319806				
C	-4.746282	1.761132	0.825282	H	10.538698	6.444534	0.142493				
H	-2.821941	2.297775	0.124371	H	12.843914	6.346187	-0.805853				
H	-5.380376	0.935759	1.164098	H	13.229572	5.309020	-3.042211				
C	-5.393746	3.049832	0.804139	C	0.688699	-7.477288	2.292573				
C	-4.754616	4.242432	0.390548	C	-2.203365	-5.484016	-3.657830				
C	-6.740775	3.156990	1.213867	C	0.203282	-8.473170	1.470053				
C	-7.417864	4.366041	1.216191	C	-2.128669	-6.843789	-3.420333				
C	-5.413939	5.457288	0.386195	C	-0.390298	-8.118410	0.239517				
C	-6.768358	5.552228	0.800429	C	-1.552500	-7.310489	-2.218284				
H	-7.262563	2.258490	1.550301	C	-0.482567	-6.736071	-0.063543				
H	-8.452856	4.406328	1.552747	C	-1.061718	-6.331769	-1.315650				
H	-3.717745	4.215219	0.053430	C	-1.686378	-4.567330	-2.715199				
H	-4.895805	6.353392	0.046990	C	0.576934	-6.116360	1.927886				
N	-7.430734	6.777470	0.795217	C	-0.889093	-9.083787	-0.693070				
C	5.265163	3.465459	-0.647999	C	-1.450516	-8.697352	-1.878524				
C	7.159269	2.013765	-0.972689	N	-0.029113	-5.752681	0.776926				
C	8.004323	3.109224	-1.046145	N	-1.116569	-4.992767	-1.575530				
C	6.092619	4.570239	-0.718609	H	-0.811176	-10.140337	-0.433427				
C	7.489304	4.421105	-0.920291	H	-1.831866	-9.437253	-2.583448				
H	7.582281	1.011021	-1.065073	H	1.164391	-7.716935	3.242770				

C5

Cu	-0.307822	-4.178322	0.040786	C	-10.961328	7.881662	0.737370	C	3.116329	-4.057157	3.698184
C	-3.489632	-1.393106	0.775633	H	-11.534154	7.232669	0.051371	C	2.304855	-3.236115	4.489899
C	3.306780	-1.891012	-0.512121	H	-11.194850	7.538205	1.760743	C	-1.141863	-4.672435	3.713498
C	-2.859305	-0.170951	0.468916	C	-11.438770	9.323254	0.572706	H	0.271055	-2.830537	5.082023
C	2.869621	-0.586721	-0.203014	H	-10.874965	9.978309	1.259738	C	3.508617	-5.957837	2.098812
C	-1.478097	-0.226760	0.224701	H	-11.208030	9.670830	-0.449891	H	4.200664	-3.916559	3.716950
C	1.497511	-0.439727	0.069426	C	-12.936187	9.468322	0.837049	C	2.903059	-2.145257	5.341524
C	0.647430	-1.538556	0.027852	H	-13.489886	8.800709	0.152264	C	-3.072656	-2.801629	-2.639904
C	-0.799654	-1.436173	0.289740	H	-13.158091	9.114556	1.860002	C	-0.743938	-2.652706	-3.377673
C	-2.763499	-2.576434	0.827856	C	-13.454079	10.895846	0.674033	C	-0.930243	-1.278113	-3.591328
C	2.413067	-2.955559	-0.539797	H	-12.901646	11.566519	1.356758	C	-3.210125	-1.430089	-2.857757
H	-0.946769	0.683218	-0.050190	H	-13.238416	11.249646	-0.350388	C	-2.147432	-0.647165	-3.328569
H	1.109813	0.541068	0.341372	C	-14.953508	11.017415	0.947566	C	0.596231	-3.267267	-3.692988
N	-1.427403	-2.606959	0.587946	H	-15.498337	10.344477	0.262733	H	-0.095095	-0.689039	-3.981090
N	1.093774	-2.787174	-0.273062	H	-15.160869	10.654067	1.969245	C	-4.256990	-3.608998	-2.167027
H	-4.559292	-1.431544	0.982530	C	-15.467974	12.449831	0.789627	H	-4.174564	-0.956920	-2.651054
H	4.354300	-2.086365	-0.743297	H	-14.950119	13.127973	1.486890	C	-2.336374	0.831292	-3.555824
C	-3.436580	-3.869510	1.188543	H	-15.284789	12.818579	-0.232490	H	-1.541045	-4.977493	2.739540
C	2.864500	-4.329705	-0.942373	H	-16.547769	12.519178	0.987662	H	-1.370735	-5.473657	4.435841
C	3.732292	0.575430	-0.152507	H	10.089702	6.914818	-1.107573	H	-1.668161	-3.766300	4.043034
C	-3.537986	1.103805	0.393693	H	10.405132	6.613874	0.611212	H	2.994848	-1.211782	4.763539
C	5.068143	0.580861	-0.391487	C	12.089679	6.185760	-0.687382	H	2.274103	-1.933242	6.217220
H	3.232598	1.512946	0.101679	H	12.575356	5.477536	0.007333	H	3.908562	-2.417995	5.690815
H	5.554363	-0.366083	-0.643875	H	12.262448	5.794128	-1.705374	H	3.681524	-6.908375	2.629013
C	5.956643	1.721190	-0.349477	C	12.764758	7.550860	-0.557418	H	3.099253	-6.207456	1.110718
C	-4.862001	1.307624	0.604268	H	12.290588	8.263272	-1.255289	H	4.485480	-5.474453	1.961427
H	-2.900921	1.954860	0.141325	H	12.595005	7.948611	0.458594	H	-4.693678	-4.195609	-2.991493
H	-5.487677	0.446400	0.856530	C	14.265702	7.482466	-0.835359	H	-3.974123	-4.321842	-1.380286
C	-5.565534	2.567719	0.535891	H	14.728661	6.761983	-0.136995	H	-5.041382	-2.946990	-1.775226
C	-4.928549	3.794007	0.227308	H	14.427755	7.077160	-1.850468	H	-2.778842	1.308965	-2.667268
C	-6.950620	2.591736	0.785792	C	14.977904	8.828633	-0.712662	H	-1.383624	1.327014	-3.787623
C	-7.688125	3.771442	0.736218	H	14.522079	9.550459	-1.414304	H	-3.026223	1.013812	-4.394818
C	-5.642827	4.973958	0.173442	H	14.817788	9.237820	0.301355	H	1.307026	-3.063014	-2.879305
C	-7.031709	4.973618	0.427850	C	16.479225	8.732234	-0.987879	H	0.534915	-4.356489	-3.820629
H	-7.456276	1.655566	1.031802	H	16.926208	8.008210	-0.284307	H	1.010348	-2.830690	-4.612915
H	-8.756953	3.758811	0.940257	H	16.631955	8.316630	-1.999275				
H	-3.857326	3.817923	0.025322	C	17.190532	10.081918	-0.867119				
H	-5.159189	5.922027	-0.065333	H	16.770045	10.808902	-1.580523				
O	-7.636358	6.182190	0.349428	H	17.067211	10.498218	0.145646				
C	5.521977	3.032820	-0.039520	H	18.268337	9.993273	-1.068668				
C	7.324523	1.534323	-0.628206	C	0.719746	-7.664649	2.413778				
C	8.234025	2.589036	-0.605104	C	-2.186778	-5.807248	-3.563803				
C	6.408383	4.090972	-0.011662	C	0.229762	-8.685707	1.620071				
C	7.775811	3.879334	-0.294690	C	-2.117611	-7.164268	-3.304249				
H	7.678856	0.530569	-0.872368	C	-0.371861	-8.368435	0.382608				
H	9.284415	2.412199	-0.827608	C	-1.547878	-7.609474	-2.090974				
H	4.472394	3.220534	0.189441	C	-0.457612	-6.996291	0.038568				
H	6.079572	5.102140	0.231547	C	-1.055678	-6.614569	-1.209288				
O	8.557642	4.983769	-0.239866	C	-1.685390	-4.873238	-2.629885				
C	9.963070	4.852088	-0.529488	C	0.610311	-6.318364	2.003157				
C	-9.048027	6.261271	0.623438	C	-0.885661	-9.352596	-0.523926				
H	2.977285	-4.382989	-2.036497	C	-1.448105	-8.988719	-1.716090				
H	3.834730	-4.573780	-0.491349	N	0.014581	-5.988631	0.839363				
H	2.120116	-5.078190	-0.642264	N	-1.121367	-5.277847	-1.479483				
H	-3.428290	-4.009989	2.279209	H	-0.813992	-10.403688	-0.241777				
H	-4.481651	-3.872115	0.855236	H	-1.831303	-9.743883	-2.403365				
H	-2.905635	-4.718156	0.735745	H	1.195931	-7.874814	3.371531				
H	10.418352	4.144542	0.184546	H	-2.626910	-5.430215	-4.486952				
H	10.087105	4.450208	-1.549682	C	1.180962	-5.232344	2.846660				
C	10.588348	6.227809	-0.404810	C	-1.819395	-3.409934	-2.880789				
H	-9.593836	5.614655	-0.084972	H	0.304957	-9.727812	1.934699				
H	-9.239043	5.898594	1.648128	H	-2.500359	-7.892951	-4.020659				
C	-9.467299	7.709091	0.470213	C	2.581320	-5.061838	2.885203				
H	-8.882382	8.330160	1.167756	C	0.343676	-4.430821	3.647970				
H	-9.222771	8.047664	-0.549806	C	0.922609	-3.445149	4.454624				

References:

1. T. Renouard, H. Le Bozec, S. Brasselet, I. Ledoux and J. Zyss, *Chem. Commun.*, 1999, 871-872.
2. H. Akdas-Kilig, J.-P. Malval, F. Morlet-Savary, A. Singh, L. Toupet, I. Ledoux-Rak, J. Zyss and H. Le Bozec, *Dyes and Pigments*, 2012, **92**, 681-688.
3. S. Karlsson, J. Boixel, Y. Pellegrin, E. Blart, H.-C. Becker, F. Odobel and L. Hammarström, *J. Am. Chem. Soc.*, 2010, **132**, 17977-17979.
4. O. Maury, L. Viau, K. Sénéchal, B. Corre, J.-P. Guégan, T. Renouard, I. Ledoux, J. Zyss and H. Le Bozec, *Chem. Eur. J.*, 2004, **10**, 4454-4466.
5. T. Bessho, E. C. Constable, M. Graetzel, A. Hernandez Redondo, C. E. Housecroft, W. Kylberg, M. K. Nazeeruddin, M. Neuburger and S. Schaffner, *Chem. Commun.*, 2008, 3717-3719.
6. T. Stoll, M. Gennari, I. Serrano, J. Fortage, J. Chauvin, F. Odobel, M. Rebarz, O. Poizat, M. Sliwa, A. Deronzier and M.-N. Collomb, *Chem.-Eur.* , 2013, **19**, 782-792.