

*Electronic Supplementary Information for*

**Copper(II) Complexes of Bis(aryl-imino)acenaphthene  
Ligands: Synthesis, Structure, DFT Studies and Evaluation in  
Reverse ATRP of Styrene**

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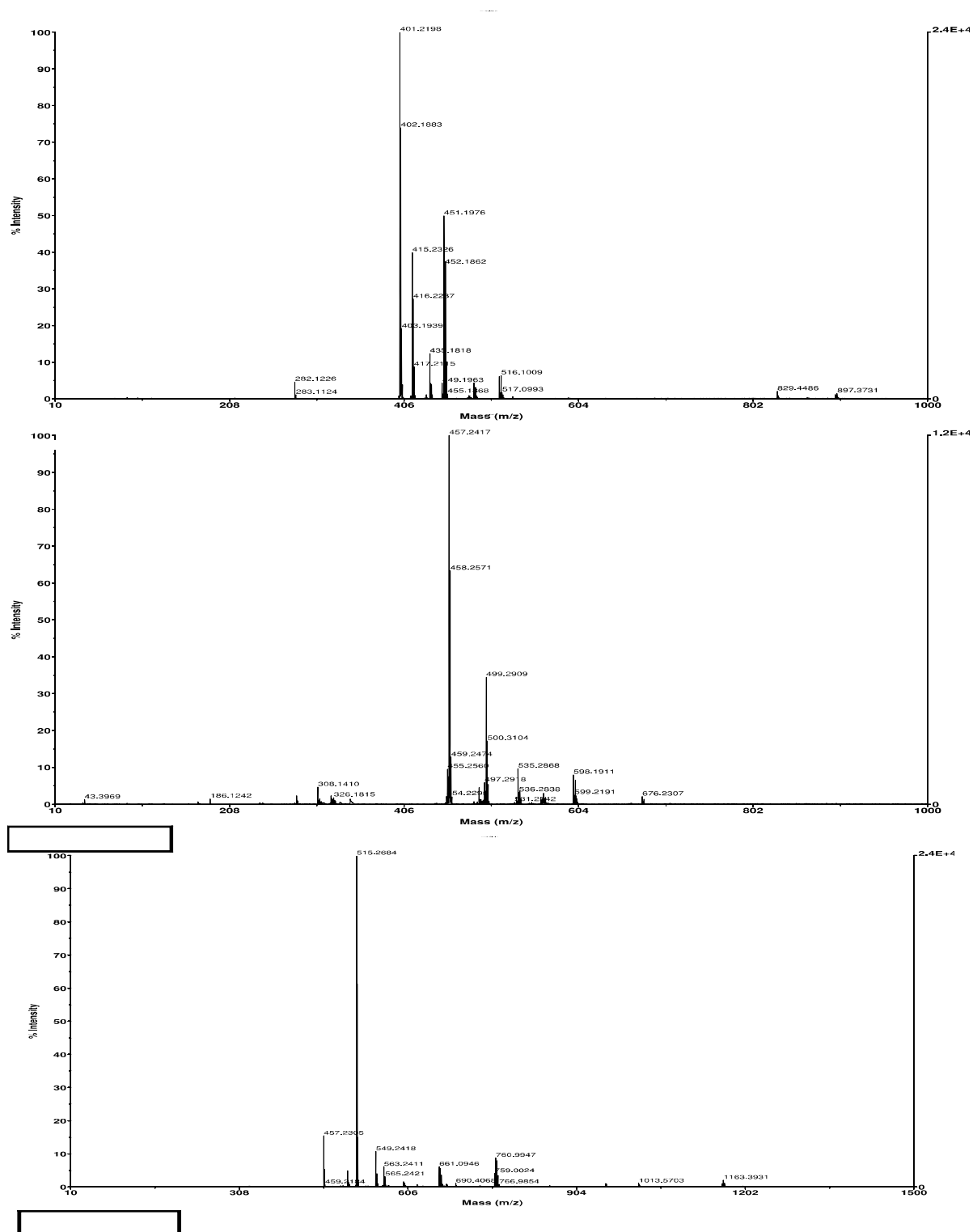
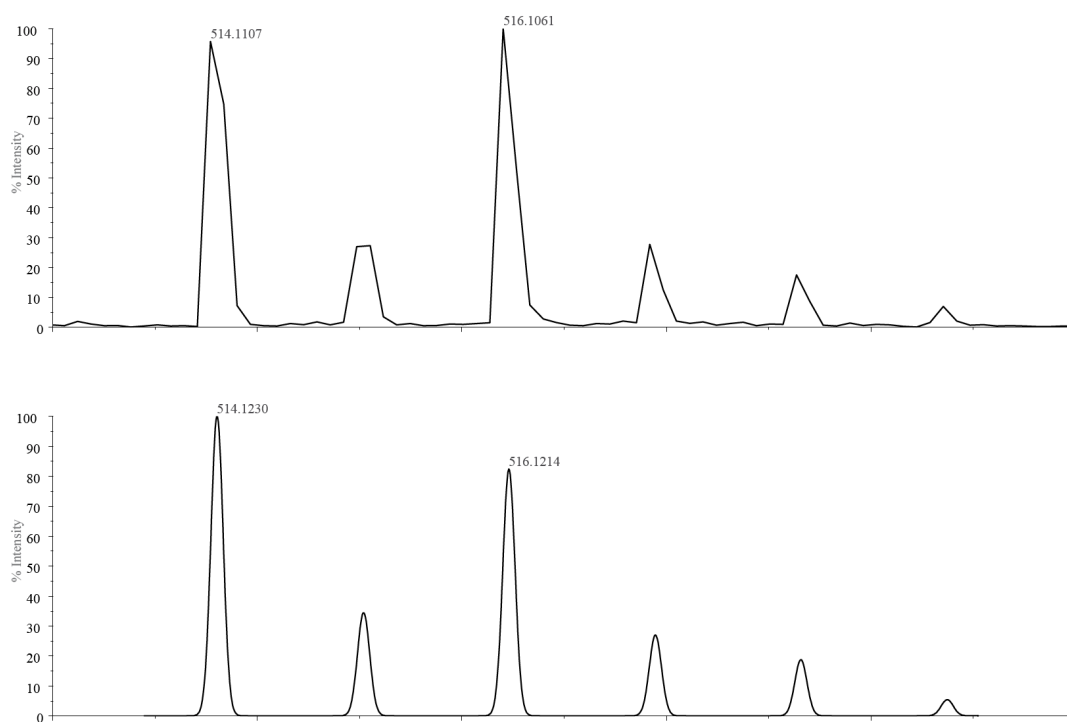
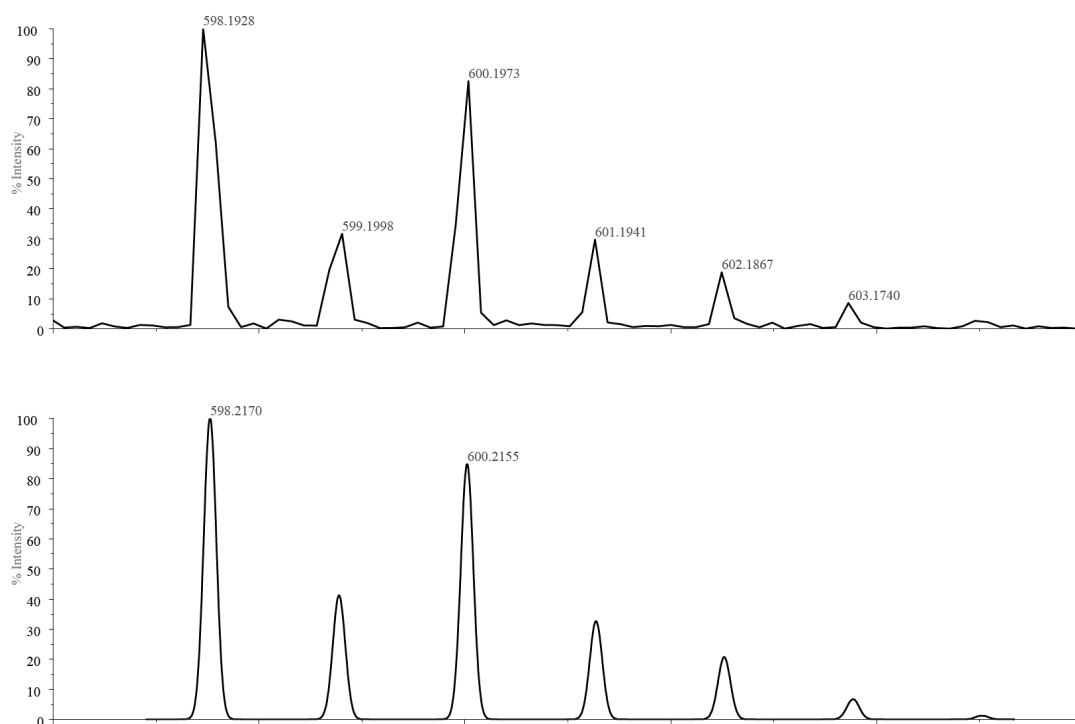


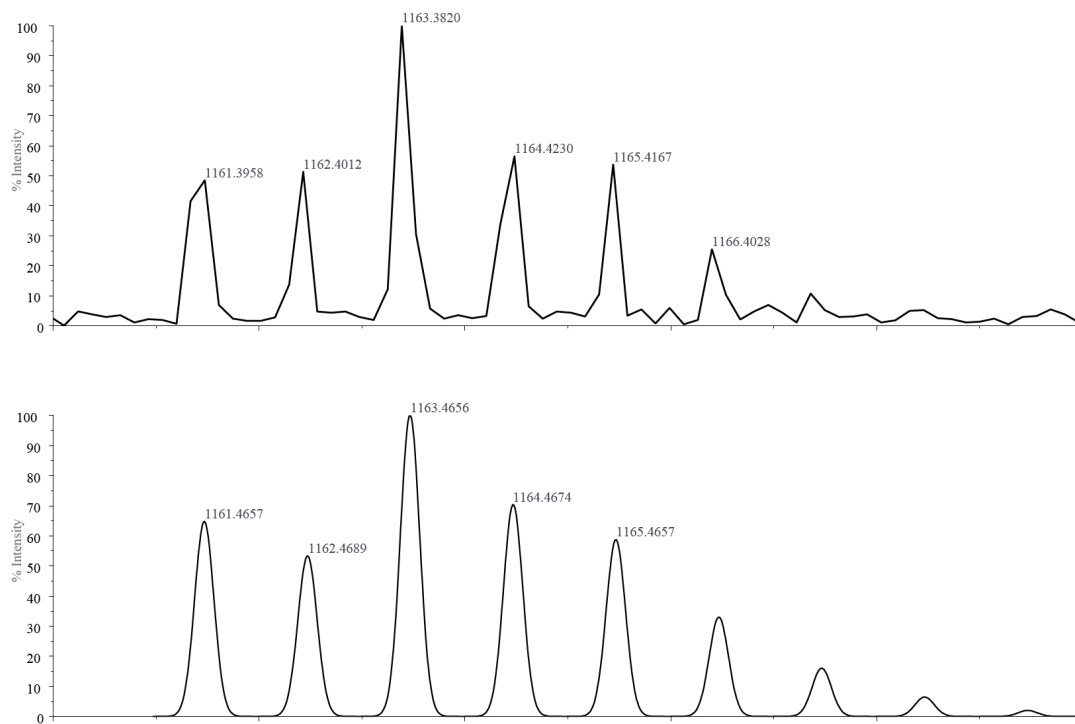
Figure S1. MALDI-TOF-MS spectra of complexes 1 (top), 2 (middle) and 3 (bottom).



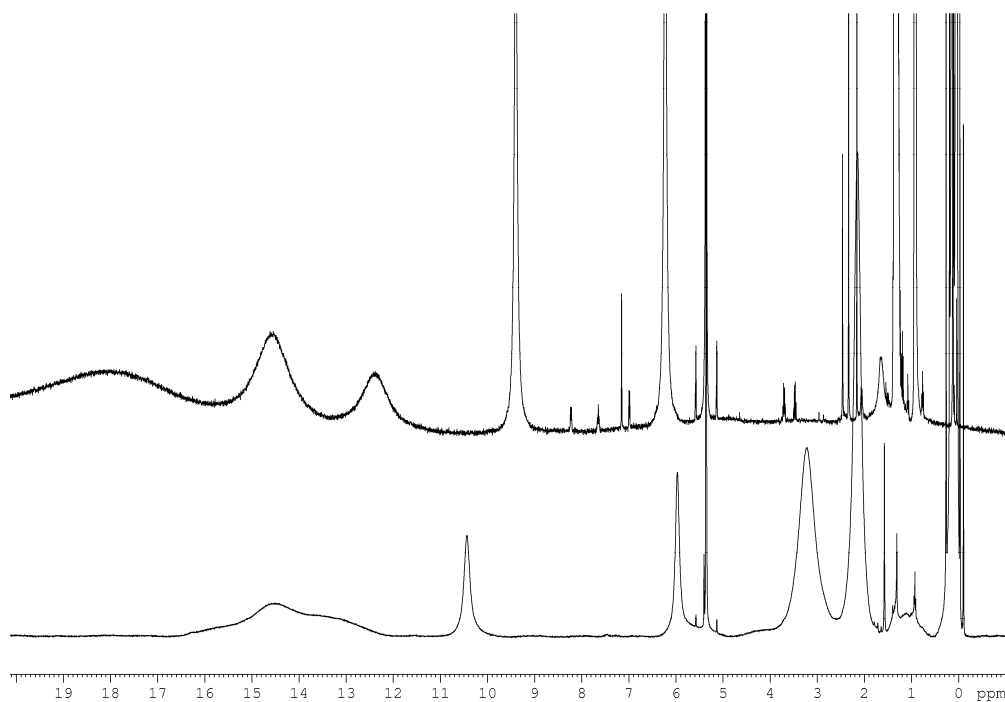
**Figure S2.** Experimental (top) and simulated (bottom) isotopic pattern of a MALDI-TOF-MS peak of complex **1**.



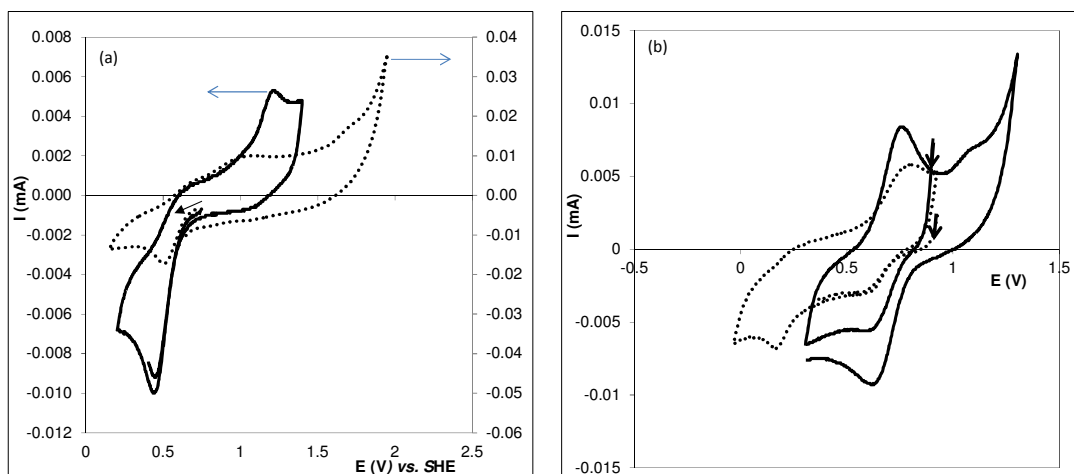
**Figure S3.** Experimental (top) and simulated (bottom) isotopic pattern of a MALDI-TOF-MS peak of complex **2**.



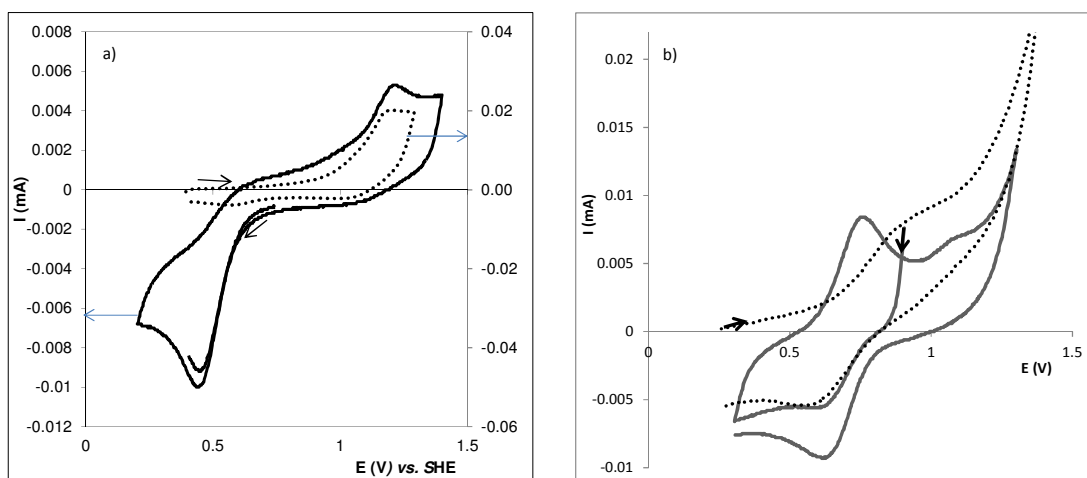
**Figure S4.** Experimental (top) and simulated (bottom) isotopic pattern of a MALDI-TOF-MS peak of complex **3**.



**Fig. S5** <sup>1</sup>H NMR spectra of **1** (top) and **2** (bottom) in CD<sub>2</sub>Cl<sub>2</sub>. Notice the broadened resonances in the region between 10 and 18 ppm. TMS peak resonances of the solution of complex and of the capillary, at *ca.* 0 ppm, were used to determine the molar magnetic susceptibilities (by the Evans method) and the numbers of unpaired electrons.



**Figure S6.** Cyclic voltammograms of **1** (dotted line) and **2** (solid line) in (a)  $\text{CH}_2\text{Cl}_2$  and in (b) MeOH at a Pt working electrode. Potentials measured vs. SHE, at a scan rate of 200 mV/s.



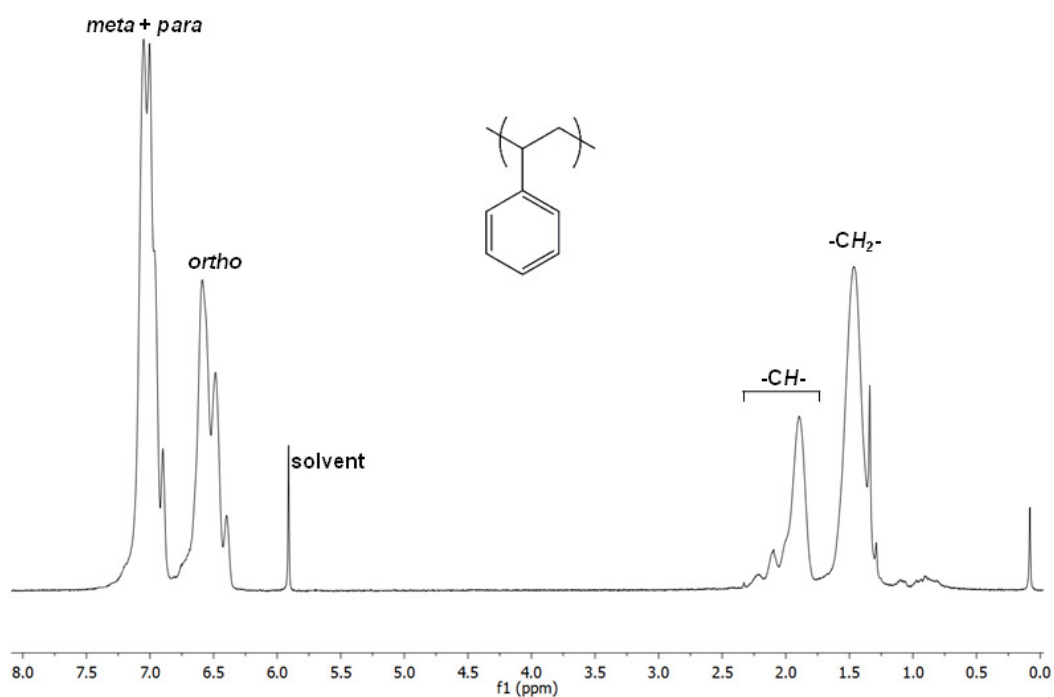
**Figure S7.** Cyclic voltammograms of **2** (solid line) and **3** (dotted line) in (a)  $\text{CH}_2\text{Cl}_2$  and (b) MeOH at a Pt working electrode. Potentials measured vs. SHE, at a scan rate of 200 mV/s.

**Table S1.** Variation of styrene conversion and  $M_n$  of the isolated polystyrenes (determined by GPC/SEC chromatography) with reaction time in the controlled radical polymerisation of styrene with complex **1**, and the corresponding  $M_n$  theoretical values. Reaction conditions:  $[\text{Styrene}]_0/[\text{Cu}]_0/[\text{AIBN}]_0 = 200/1/0.8$ , toluene (50% v/v), 80 °C.

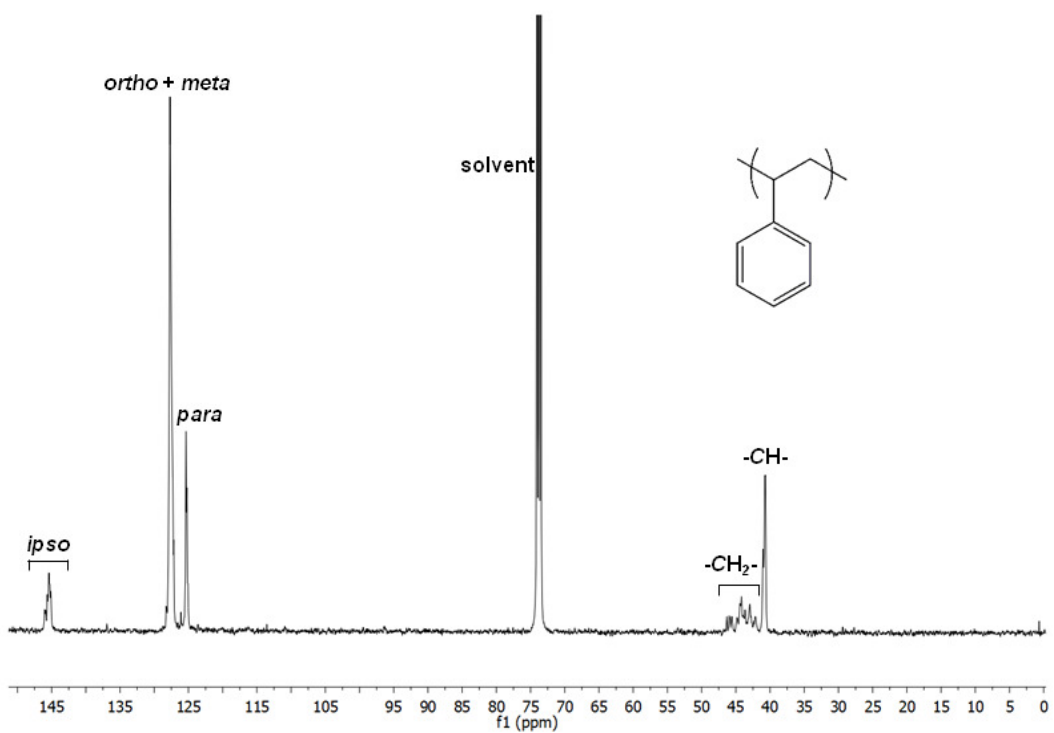
Entry	Time (h)	Conversion (%)	$M_n$ (GPC) (g/mol)	$M_n$ (theo) <sup>a</sup> (g/mol)	PDI
0	0	0	0	0	
1	1.5	0.7	120	182	2.21
2	3.0	5.7	1050	1484	2.30
3	6.0	11.0	2300	2864	2.24
4	15.5	36.3	10500	9452	2.28
5	21.5	51.2	14700	13331	2.33
6	24.0	60.5	17800	15753	2.36
7	45.0	80.7	22900	21012	2.20

<sup>a</sup> calculated using the equation  $M_n(\text{theo}) = M_{\text{RU}} \times ([\text{Sty}]_0/[\text{AIBN}]_0) \times \text{conv.}$ , where  $M_{\text{RU}} = 104.15$  g/mol and  $[\text{Sty}]_0/[\text{AIBN}]_0 = 200/0.8 = 250$ .

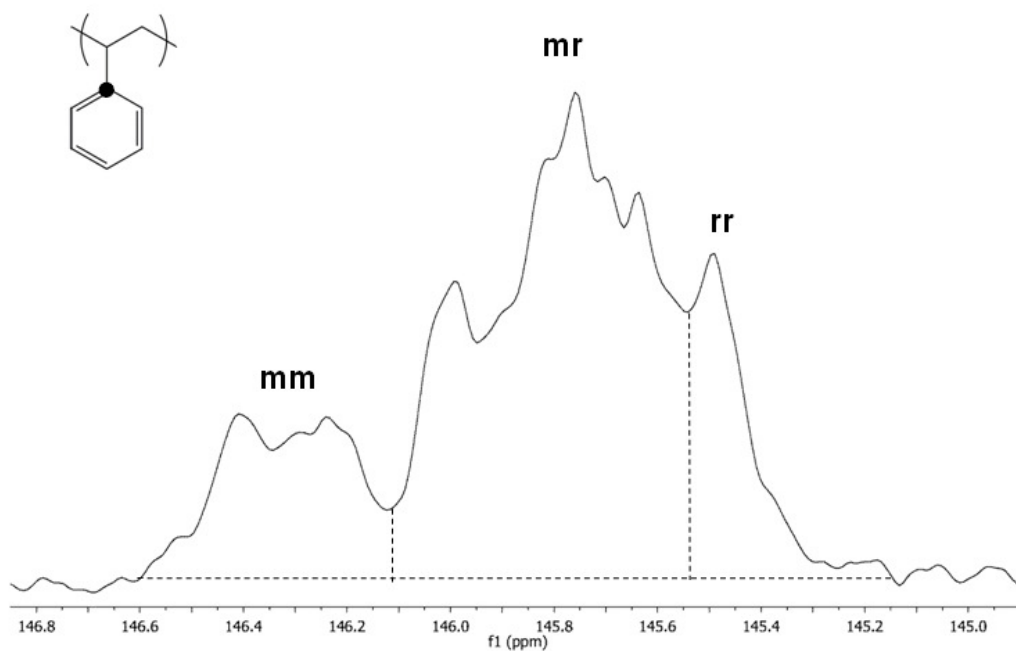




**Figure S8.**  $^1\text{H}$  NMR spectrum of the polystyrene of entry 7 (Table S1) (400 MHz,  $\text{CDCl}_2\text{CDCl}_2$ , 120 °C).



**Figure S9.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of the polystyrene of entry 7 (Table S1) (100 MHz,  $\text{CDCl}_2\text{CDCl}_2$ , 120 °C).



**Figure S10.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of the aromatic *ipso* carbon region of the polystyrene of entry 7 (Table S1) (100 MHz,  $\text{CDCl}_2\text{CDCl}_2$ , 120 °C), and the corresponding assignment of triad sequences. The normalised triad intensities ( $mm = 0.16$ ,  $mr = 0.69$  and  $rr = 0.15$ ) reveal an atactic polymer ( $P_m = 0.50$ ).

**Table S2.** Coordinates for optimised geometries.**(a) [CuCl<sub>2</sub>(Ph-BIAN)]: tetracoordinated Cu(II)****[CuCl<sub>2</sub>(Ph-BIAN)]**

C	-14.880814	23.854837	41.222350
C	-15.221879	24.457039	39.919211
C	-13.983044	24.733045	39.277721
C	-12.843673	24.379575	40.051467
C	-13.365284	23.840985	41.321407
C	-16.397862	24.806393	39.277586
C	-16.324645	25.410241	37.996614
C	-15.118855	25.646523	37.358749
C	-13.892412	25.306542	37.991420
C	-12.584111	25.484057	37.465070
C	-11.474967	25.108927	38.203961
C	-11.583697	24.560919	39.507267
C	-16.961432	23.282769	42.266212
C	-17.641358	23.797893	43.378223
C	-19.024864	23.662935	43.464571
C	-19.730553	22.976415	42.473178
C	-19.044386	22.421494	41.390022
C	-17.663084	22.573944	41.280249
H	-17.079687	24.295446	44.162343
H	-20.806719	22.854681	42.555613
H	-17.121335	22.119848	40.456241
C	-11.443796	23.341629	42.662164
C	-10.674606	24.513330	42.646728
C	-9.321119	24.454612	42.975863
C	-8.730205	23.234867	43.314559
C	-9.505664	22.073124	43.348108
C	-10.864227	22.124901	43.044951
H	-11.145905	25.462832	42.412413
H	-7.675906	23.193793	43.572365
H	-11.482509	21.234447	43.102096
Cl	-15.500596	21.036568	44.590903
Cl	-13.248013	23.525866	45.680470
Cu	-14.285358	22.759541	43.847241
H	-17.365732	24.620548	39.726972
H	-17.250916	25.683089	37.499651
H	-15.105091	26.095255	36.368903
H	-12.458487	25.917291	36.476183
H	-10.483901	25.247586	37.782095
H	-10.686600	24.303625	40.057034
H	-19.548849	24.074815	44.321965
H	-19.582528	21.857200	40.633509
H	-8.731476	25.367071	42.979915
H	-9.057842	21.125554	43.632757
N	-15.552213	23.412057	42.227423
N	-12.835233	23.364294	42.392982

**[CuCl<sub>2</sub>(Mes-BIAN)]**

C	-14.880814	23.854837	41.222350
C	-15.221879	24.457039	39.919211
C	-13.983044	24.733045	39.277721
C	-12.843673	24.379575	40.051467
C	-13.365284	23.840985	41.321407
C	-16.397862	24.806393	39.277586
C	-16.324645	25.410241	37.996614
C	-15.118855	25.646523	37.358749
C	-13.892412	25.306542	37.991420

C	-12.584111	25.484057	37.465070
C	-11.474967	25.108927	38.203961
C	-11.583697	24.560919	39.507267
C	-16.961432	23.282769	42.266212
C	-17.641358	23.797893	43.378223
C	-19.024864	23.662935	43.464571
C	-19.730553	22.976415	42.473178
C	-19.044386	22.421494	41.390022
C	-17.663084	22.573944	41.280249
H	-17.079687	24.295446	44.162343
H	-20.806719	22.854681	42.555613
H	-17.121335	22.119848	40.456241
C	-11.443796	23.341629	42.662164
C	-10.674606	24.513330	42.646728
C	-9.321119	24.454612	42.975863
C	-8.730205	23.234867	43.314559
C	-9.505664	22.073124	43.348108
C	-10.864227	22.124901	43.044951
H	-11.145905	25.462832	42.412413
H	-7.675906	23.193793	43.572365
H	-11.482509	21.234447	43.102096
Cl	-15.500596	21.036568	44.590903
Cl	-13.248013	23.525866	45.680470
Cu	-14.285358	22.759541	43.847241
H	-17.365732	24.620548	39.726972
H	-17.250916	25.683089	37.499651
H	-15.105091	26.095255	36.368903
H	-12.458487	25.917291	36.476183
H	-10.483901	25.247586	37.782095
H	-10.686600	24.303625	40.057034
H	-19.548849	24.074815	44.321965
H	-19.582528	21.857200	40.633509
H	-8.731476	25.367071	42.979915
H	-9.057842	21.125554	43.632757
N	-15.552213	23.412057	42.227423
N	-12.835233	23.364294	42.392982

[CuCl<sub>2</sub>(Dipp-BIAN)]

C	16.207561	8.420557	17.140307
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C	14.603421	9.008392	15.130422
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C	17.050150	9.170068	13.645330
C	18.335132	9.205164	13.037063
C	19.474579	8.954383	13.783859
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C	13.426384	7.044560	17.798344
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C	11.364435	8.198467	18.398241
C	12.095806	9.271262	18.900177
C	13.494280	9.273553	18.867926
C	14.104317	5.778039	17.277266
C	13.645094	5.404635	15.853883
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C	19.734207	8.118208	18.395260

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C	20.374435	6.863151	18.466287
C	19.768524	10.701021	18.555230
C	19.980595	11.341656	19.942449
C	20.234455	11.650126	17.433642
C	19.594409	5.551573	18.470753
C	19.855186	4.753375	19.762754
C	19.886541	4.708740	17.213951
Cl	18.385969	8.196698	21.522392
Cl	15.342614	6.713954	21.106573
Cu	16.898265	7.790110	19.881873
H	13.660905	8.945841	15.661334
H	13.674173	9.522430	13.250356
H	15.762246	9.649574	11.960345
H	18.420017	9.429784	11.976983
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H	11.452215	6.246493	17.512614
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H	18.525889	5.792358	18.458336
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H	12.577319	5.158395	15.826462
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H	19.285346	3.791997	17.219470
H	19.656098	5.261777	16.295436
N	15.573917	8.177146	18.229227
N	18.303880	8.137496	18.285395

(b)  $[\text{CuCl}_2(\text{Ar-BIAN})]^-$ : tetracoordinated Cu(I)

$[\text{CuCl}_2(\text{Ph-BIAN})]^-$

C	-14.868805	23.860799	41.258958
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C	-16.381436	24.954262	39.374617
C	-16.310909	25.561639	38.092485
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C	-13.895277	25.297871	38.004382
C	-12.594156	25.389733	37.436524
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C	-16.955552	23.281567	42.268137
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C	-9.294079	24.443453	42.899668
C	-8.718713	23.241365	43.319630
C	-9.519966	22.102027	43.440925
C	-10.880081	22.148640	43.140762
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H	-7.661713	23.199209	43.571298
H	-11.530086	21.287963	43.280082
Cl	-13.914868	20.373050	44.057456
Cl	-14.809974	24.124325	45.666938
Cu	-14.299859	22.671765	43.911398
H	-17.343824	24.828973	39.856389
H	-17.235158	25.898464	37.629420
H	-15.106323	26.176135	36.423413
H	-12.469089	25.818645	36.444726
H	-10.508273	25.004266	37.692030
H	-10.708116	24.068000	39.972023
H	-19.523649	24.053983	44.359010
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H	-8.689321	25.345124	42.832115
H	-9.088420	21.168567	43.794088
N	-15.550926	23.367437	42.237195
N	-12.832334	23.378367	42.428089

[CuCl<sub>2</sub>(Mes-BIAN)]<sup>-</sup>

C	-14.878190	23.780202	41.352988
C	-15.224051	24.353879	40.032239
C	-13.992037	24.673475	39.399112
C	-12.858254	24.355451	40.195554
C	-13.381694	23.778153	41.455155
C	-16.405051	24.614017	39.361823
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C	-15.136642	25.502738	37.450906
C	-13.904107	25.247144	38.115070
C	-12.592591	25.506663	37.626967
C	-11.486842	25.198532	38.400727
C	-11.596907	24.619316	39.694076
C	-16.994057	23.311982	42.302459
C	-17.706881	24.404642	42.835354
C	-19.103938	24.337490	42.844751
C	-19.800712	23.225678	42.361273
C	-19.056870	22.149699	41.866292

C	-17.658715	22.161657	41.831863
C	-16.975450	25.600688	43.394987
C	-21.312788	23.191118	42.364072
C	-16.877529	20.973365	41.325214
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C	-10.770821	24.391447	43.286997
C	-9.385739	24.321414	43.470017
C	-8.638078	23.203491	43.087340
C	-9.316454	22.128519	42.504195
C	-10.699599	22.142746	42.297655
C	-11.560915	25.595888	43.738376
C	-7.148171	23.139019	43.338762
C	-11.414130	20.956891	41.696025
Cl	-14.338152	20.271921	44.075861
Cl	-14.414149	24.109575	45.799314
Cu	-14.312487	22.606722	44.012552
H	-17.367524	24.386179	39.805731
H	-17.268227	25.394941	37.540937
H	-15.130103	25.944114	36.456693
H	-12.463420	25.949295	36.641715
H	-10.493478	25.404764	38.010126
H	-10.703785	24.394131	40.265951
H	-19.659426	25.177586	43.259210
H	-19.575449	21.261586	41.507881
H	-8.882300	25.165728	43.938867
H	-8.758434	21.240772	42.209642
H	-16.424559	26.140967	42.612834
H	-17.680915	26.303939	43.850647
H	-16.243261	25.294153	44.154223
H	-21.689421	22.169206	42.488762
H	-21.725421	23.801469	43.175652
H	-21.733048	23.577125	41.423746
H	-16.150292	20.631897	42.074207
H	-17.552065	20.143896	41.086679
H	-16.314130	21.216950	40.413978
H	-12.379163	25.299422	44.408362
H	-10.913458	26.304305	44.266504
H	-12.013230	26.126860	42.889609
H	-6.922124	22.683149	44.313035
H	-6.637046	22.538413	42.576772
H	-6.696760	24.138246	43.338512
H	-10.718330	20.124039	41.547377
H	-12.233122	20.620234	42.345850
H	-11.855409	21.200814	40.719932
N	-15.573273	23.329702	42.337264
N	-12.827380	23.319473	42.521684

[CuCl<sub>2</sub>(Dipp-BIAN)]<sup>-</sup>

C	16.212234	8.409307	17.231793
C	17.713177	8.384508	17.263165
C	18.182002	8.675982	15.887699
C	17.015614	8.865426	15.097664
C	15.811420	8.718346	15.838332
C	14.603825	8.877660	15.182002
C	14.617422	9.182031	13.793658
C	15.791779	9.324301	13.075365
C	17.049900	9.165897	13.720795
C	18.338730	9.277191	13.128320
C	19.476261	9.092259	13.894552
C	19.420939	8.789459	15.282143
C	14.132196	8.175593	18.327897
C	13.441662	6.962547	18.094243
C	12.042174	7.000482	18.077002

C	11.341797	8.180909	18.314096
C	12.044064	9.346091	18.613262
C	13.443564	9.370026	18.646314
C	14.176077	5.641326	17.872727
C	14.060539	5.163726	16.410929
C	13.694447	4.550568	18.846999
C	14.182541	10.653689	19.019581
C	14.086496	11.709509	17.900042
C	13.692079	11.226695	20.361586
C	19.736884	8.089703	18.446841
C	20.447391	9.263193	18.794161
C	21.845581	9.196107	18.822405
C	22.523936	8.009255	18.554922
C	21.798660	6.850704	18.286764
C	20.399217	6.855929	18.242182
C	19.732409	10.570007	19.132232
C	20.183724	11.134671	20.491371
C	19.907227	11.617549	18.014385
C	19.635705	5.557795	17.985714
C	20.040352	4.451907	18.977766
C	19.801977	5.078116	16.529451
Cl	16.893183	9.627575	21.486059
Cl	16.848786	5.537482	20.605053
Cu	16.901845	7.795278	20.050688
H	13.659064	8.774711	15.702991
H	13.665588	9.306220	13.283599
H	15.758086	9.557839	12.013546
H	18.425059	9.508057	12.068891
H	20.452311	9.180436	13.424318
H	20.338658	8.651403	15.841897
H	11.493815	6.082104	17.883246
H	10.254356	8.186819	18.291957
H	11.497092	10.258643	18.836087
H	15.233112	5.799402	18.103073
H	15.236197	10.404175	19.170983
H	22.410345	10.091798	19.068198
H	23.610970	7.981644	18.580391
H	22.326729	5.915861	18.116471
H	18.666339	10.352717	19.240285
H	18.574720	5.747583	18.168792
H	14.445717	5.910503	15.707407
H	14.629990	4.237034	16.266542
H	13.016044	4.958901	16.139524
H	12.631934	4.310560	18.707034
H	14.271128	3.631958	18.688049
H	13.859442	4.863841	19.881110
H	13.045387	12.014578	17.727498
H	14.656642	12.606805	18.171433
H	14.482785	11.330595	16.951147
H	13.838423	10.498028	21.163204
H	14.277120	12.117056	20.619258
H	12.633323	11.516760	20.327024
H	19.613523	12.041772	20.722539
H	19.985290	10.413663	21.288690
H	21.250561	11.395655	20.498590
H	19.543294	11.245723	17.049874
H	19.350750	12.531500	18.257083
H	20.963135	11.892827	17.887910
H	19.843296	4.770300	20.004654
H	19.440787	3.552799	18.793925
H	21.099234	4.176824	18.881469
H	20.851131	4.843127	16.304458
H	19.212819	4.168512	16.357986



H	19.470373	5.836212	15.810919
N	15.556842	8.177317	18.315510
N	18.314451	8.135779	18.374436

(c) [CuCl(Ar-BIAN)]: tricoordinated Cu(I)

[CuCl(Ph-BIAN)]

C	-14.886614	23.870098	41.197212
C	-15.215171	24.321909	39.828347
C	-13.972194	24.567907	39.183396
C	-12.840090	24.301453	40.002869
C	-13.374004	23.880668	41.312579
C	-16.385493	24.602515	39.144344
C	-16.303408	25.106986	37.821030
C	-15.092626	25.332416	37.190117
C	-13.871180	25.074521	37.870039
C	-12.558978	25.300145	37.372761
C	-11.456249	25.046841	38.170087
C	-11.576661	24.550491	39.492989
C	-16.952351	23.359891	42.319199
C	-17.622090	23.857326	43.450531
C	-18.992825	23.650620	43.589119
C	-19.699644	22.912196	42.636260
C	-19.023972	22.372887	41.537866
C	-17.658433	22.596157	41.372408
H	-17.054504	24.386954	44.210252
H	-20.764955	22.738691	42.759171
H	-17.127579	22.153050	40.535301
C	-11.466715	23.461956	42.705376
C	-10.903500	24.115733	43.812454
C	-9.553345	23.940776	44.108191
C	-8.764176	23.084694	43.335287
C	-9.335508	22.399996	42.259579
C	-10.679581	22.586900	41.939190
H	-11.534150	24.749630	44.428715
H	-7.716604	22.936642	43.581186
H	-11.131633	22.037575	41.118657
Cl	-14.728416	24.190165	46.053308
Cu	-14.230301	23.645021	44.001977
H	-17.357487	24.447035	39.596753
H	-17.226906	25.322154	37.291218
H	-15.070039	25.719020	36.174486
H	-12.426276	25.683975	36.364479
H	-10.461468	25.235487	37.776885
H	-10.683334	24.374655	40.079836
H	-19.505101	24.050714	44.459406
H	-19.559438	21.768222	40.810762
H	-9.122446	24.461547	44.958445
H	-8.736522	21.709823	41.671645
N	-15.559537	23.547765	42.246906
N	-12.851914	23.619331	42.465639

[CuCl(Mes-BIAN)]

C	-14.867602	23.796255	41.331167
C	-15.242418	24.453409	40.068219
C	-14.022638	24.829963	39.440854
C	-12.867352	24.489998	40.192981
C	-13.350960	23.815790	41.416735
C	-16.439550	24.726043	39.428096
C	-16.401209	25.373709	38.166087

C	-15.212357	25.737465	37.555369
C	-13.965892	25.469106	38.185117
C	-12.668334	25.768864	37.685407
C	-11.541093	25.434411	38.416619
C	-11.618916	24.790975	39.680087
C	-16.982203	23.238574	42.255196
C	-17.686186	24.347051	42.760314
C	-19.083630	24.287703	42.771609
C	-19.785742	23.170845	42.307864
C	-19.047181	22.079746	41.837429
C	-17.649658	22.082753	41.808658
C	-16.958904	25.557837	43.295815
C	-21.296833	23.144023	42.307585
C	-16.879668	20.876230	41.329203
C	-11.383791	23.261362	42.634961
C	-10.715935	24.434974	43.040862
C	-9.343754	24.353898	43.304691
C	-8.629362	23.159144	43.185579
C	-9.332537	22.010001	42.805950
C	-10.704381	22.027355	42.549970
C	-11.451342	25.741264	43.237107
C	-7.152826	23.095410	43.500403
C	-11.445991	20.763108	42.191655
Cl	-14.087896	20.981944	45.382006
Cu	-14.539433	22.305605	43.724526
H	-17.392275	24.455861	39.868133
H	-17.340978	25.587474	37.665262
H	-15.228444	26.229935	36.586385
H	-12.565199	26.262210	36.722306
H	-10.559811	25.670683	38.015336
H	-10.711826	24.548873	40.222463
H	-19.635681	25.137777	43.167393
H	-19.570651	21.190039	41.493364
H	-8.824204	25.254444	43.626401
H	-8.802187	21.063388	42.722911
H	-16.432702	26.105970	42.503780
H	-17.660546	26.251631	43.767909
H	-16.208214	25.272249	44.042721
H	-21.679020	22.139308	42.518247
H	-21.709132	23.826089	43.058414
H	-21.703117	23.447151	41.332965
H	-16.207157	20.501802	42.112012
H	-17.561230	20.066540	41.052795
H	-16.257782	21.104819	40.454633
H	-12.356758	25.602603	43.839426
H	-10.812780	26.464406	43.753142
H	-11.759560	26.195337	42.286851
H	-6.975908	22.653006	44.489704
H	-6.612600	22.479586	42.772005
H	-6.699650	24.092284	43.502163
H	-10.764800	19.907032	42.174919
H	-12.234802	20.558080	42.926504
H	-11.924811	20.830892	41.206429
N	-15.548119	23.249180	42.278179
N	-12.786759	23.263400	42.422894

[CuCl(Dipp-BIAN)]

C	16.222308	8.419163	17.121132
C	17.741800	8.401562	17.130819
C	18.178281	8.661134	15.743444
C	16.993955	8.815749	14.975716
C	15.798737	8.678576	15.735620
C	14.577417	8.805623	15.094843

C	14.567639	9.069107	13.700391
C	15.732498	9.206424	12.963250
C	17.002474	9.082980	13.591003
C	18.280327	9.201277	12.977311
C	19.435403	9.057467	13.727402
C	19.406718	8.784830	15.120981
C	14.147299	8.221832	18.266107
C	13.464456	6.992798	18.139191
C	12.066575	7.014199	18.215220
C	11.370103	8.201105	18.427013
C	12.070869	9.394279	18.583865
C	13.468798	9.434971	18.514581
C	14.197123	5.665375	17.960137
C	13.790725	4.949444	16.657602
C	13.993229	4.754193	19.187281
C	14.205821	10.750794	18.753619
C	13.740173	11.866102	17.798499
C	14.077352	11.186250	20.227937
C	19.761370	8.124630	18.353979
C	20.444003	9.242526	18.882824
C	21.831855	9.150936	19.035134
C	22.521906	7.986739	18.708316
C	21.820586	6.880496	18.235525
C	20.432946	6.916579	18.051746
C	19.709842	10.514811	19.296937
C	19.841150	10.764031	20.812242
C	20.172670	11.736295	18.479164
C	19.691631	5.653124	17.618590
C	19.663310	4.626062	18.769657
C	20.270179	5.032838	16.333120
Cl	17.210795	7.662157	21.967491
Cu	16.650355	7.950082	19.893787
H	13.641726	8.710219	15.632943
H	13.609058	9.167626	13.199363
H	15.678932	9.410986	11.896981
H	18.346307	9.407349	11.912078
H	20.400274	9.154117	13.238165
H	20.333510	8.675495	15.672478
H	11.517673	6.081774	18.114864
H	10.285060	8.194475	18.483549
H	11.524328	10.314058	18.772020
H	15.269271	5.873586	17.894455
H	15.270657	10.586564	18.562960
H	22.377542	10.004495	19.428323
H	23.599376	7.934860	18.838814
H	22.359098	5.963189	18.013950
H	18.644286	10.370157	19.091813
H	18.652060	5.919754	17.405816
H	13.970404	5.581641	15.780520
H	14.368579	4.025866	16.535281
H	12.728953	4.676268	16.661500
H	12.936749	4.493037	19.320489
H	14.557055	3.821605	19.066748
H	14.339096	5.244323	20.103574
H	12.687010	12.124465	17.958858
H	14.329810	12.775610	17.962416
H	13.856927	11.570255	16.749677
H	14.466613	10.415970	20.902319
H	14.642411	12.109404	20.403678
H	13.031362	11.375477	20.497067
H	19.289736	11.668750	21.096174
H	19.432149	9.923300	21.381939
H	20.888213	10.905318	21.106155

H	20.043838	11.570792	17.402882
H	19.594496	12.625014	18.758942
H	21.230976	11.961430	18.657026
H	19.200211	5.051468	19.666219
H	19.093465	3.735809	18.476119
H	20.677156	4.304274	19.035551
H	21.299378	4.684103	16.476155
H	19.671536	4.166078	16.028832
H	20.270983	5.751409	15.505650
N	15.585282	8.220665	18.222656
N	18.342946	8.193411	18.238414

(d) [Cu<sub>2</sub>Cl<sub>2</sub> (Ar-BIAN)<sub>2</sub>]: binuclear Cu(I)

[Cu<sub>2</sub>Cl<sub>2</sub>(Ph-BIAN)<sub>2</sub>]

C	-14.976083	23.112158	41.334645
C	-15.135323	23.484164	39.911682
C	-13.846950	23.881810	39.460605
C	-12.837994	23.774995	40.456754
C	-13.504272	23.231103	41.660771
C	-16.186646	23.495785	39.011806
C	-15.944734	23.922675	37.680229
C	-14.697692	24.344929	37.253750
C	-13.593911	24.338600	38.149694
C	-12.261938	24.744386	37.863046
C	-11.286510	24.677884	38.842539
C	-11.553505	24.186454	40.146791
C	-17.176770	22.628113	42.144296
C	-17.960191	23.724716	41.750120
C	-19.349581	23.608548	41.714099
C	-19.967195	22.404741	42.062484
C	-19.186064	21.322093	42.475974
C	-17.798161	21.432950	42.539765
H	-17.478378	24.664819	41.498478
H	-21.049720	22.317648	42.030512
H	-17.182882	20.615779	42.904055
C	-11.775406	22.851430	43.276348
C	-11.469836	23.447775	44.510375
C	-10.166407	23.392384	45.000664
C	-9.170062	22.712008	44.295156
C	-9.486452	22.079653	43.090099
C	-10.781329	22.148105	42.576612
H	-12.264193	23.931237	45.071263
H	-8.159305	22.658882	44.690204
H	-11.034809	21.639594	41.651244
H	-17.185923	23.196364	39.304194
H	-16.775183	23.927354	36.979791
H	-14.556184	24.682278	36.230025
H	-12.014023	25.109481	36.869526
H	-10.275689	24.999723	38.608166
H	-10.750695	24.132603	40.872320
H	-19.950018	24.465131	41.418760
H	-19.659067	20.389745	42.771689
H	-9.935256	23.865987	45.950689
H	-8.725424	21.523713	42.548541
N	-15.772156	22.718384	42.268376
N	-13.118231	22.884256	42.840288
Cu	-14.752276	22.277798	44.102515
Cl	-14.985513	23.601603	46.093509
Cl	-15.045048	20.038534	44.912036
Cu	-15.229348	21.359678	46.910147

N	-16.787356	21.068246	48.352201
N	-14.125450	20.551738	48.571846
C	-16.136115	19.169519	52.858903
C	-17.446151	19.305661	53.393978
C	-18.449832	19.889851	52.641214
C	-18.234542	20.348816	51.315793
C	-16.972461	20.224446	50.761477
C	-15.933706	19.659680	51.551328
C	-14.671835	19.634258	50.896838
C	-13.596793	19.056876	51.549662
C	-13.788361	18.530924	52.853728
C	-15.008945	18.590391	53.503278
C	-16.357490	20.573825	49.462020
C	-14.882167	20.261561	49.573562
C	-18.142335	21.343870	48.062311
C	-19.777112	22.901627	47.193434
C	-20.779754	21.937698	47.330678
C	-18.458547	22.605989	47.534750
C	-20.454282	20.666434	47.810264
C	-19.143208	20.365852	48.178834
C	-12.721338	20.396810	48.553139
C	-11.897042	20.981899	49.527962
C	-10.510914	20.864870	49.427298
C	-9.936550	20.163174	48.364395
C	-10.758543	19.601087	47.383722
C	-12.144139	19.731652	47.459743
H	-19.058589	20.777472	50.758127
H	-19.443204	19.992418	53.068966
H	-17.655051	18.949335	54.399587
H	-15.111818	18.192319	54.509665
H	-12.939605	18.078033	53.358473
H	-12.616255	19.006882	51.091616
H	-17.661856	23.328936	47.387519
H	-20.016206	23.884995	46.798158
H	-21.802976	22.168541	47.047500
H	-21.221440	19.900826	47.892611
H	-18.883961	19.372660	48.533182
H	-12.345362	21.542234	50.343057
H	-9.879314	21.329549	50.180083
H	-8.856395	20.071276	48.291452
H	-10.319980	19.074274	46.540831
H	-12.791613	19.339797	46.681105

[Cu<sub>2</sub>Cl<sub>2</sub>(Mes-BIAN)<sub>2</sub>]

C	-14.950337	23.259690	41.454469
C	-15.160278	23.754676	40.079817
C	-13.865590	23.937171	39.522129
C	-12.811299	23.605390	40.416023
C	-13.456743	23.167368	41.669422
C	-16.271170	24.042828	39.308147
C	-16.071975	24.511546	37.982379
C	-14.810145	24.688347	37.439864
C	-13.648301	24.400897	38.208880
C	-12.291544	24.528532	37.800390
C	-11.263574	24.205987	38.670459
C	-11.502253	23.739661	39.990523
C	-17.154365	22.987195	42.283557
C	-17.825293	24.162180	42.671931
C	-19.220826	24.181479	42.582897
C	-19.954935	23.075376	42.143304
C	-19.251866	21.920612	41.785476
C	-17.857343	21.844968	41.855950
C	-17.059832	25.359472	43.183134

C	-21.465551	23.110819	42.100267
C	-17.126144	20.573501	41.496237
C	-11.624023	22.650714	43.081130
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[Cu<sub>2</sub>Cl<sub>2</sub>(Dipp-BIAN)<sub>2</sub>]

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C	14.748844	9.442465	13.784398
C	15.931092	9.404190	13.064987
C	17.156043	9.080259	13.710955
C	18.445457	9.004231	13.115635
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C	19.457788	8.388195	15.268120
C	14.164080	8.677491	18.385547
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C	11.889580	7.884038	18.490990
C	11.431538	9.197971	18.560391
C	12.346749	10.246280	18.580675
C	13.726999	10.018437	18.500898

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C	14.686525	11.205285	18.586276
C	14.479248	12.207659	17.433042
C	14.570547	11.914752	19.950408
C	19.665239	7.626596	18.460566
C	20.535180	8.603455	19.000984
C	21.894612	8.288270	19.096670
C	22.378024	7.040580	18.708164
C	21.494507	6.077116	18.230480
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H	19.652828	10.688043	17.383420
H	19.739308	11.973152	18.603096
H	21.220134	11.166509	18.052363
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