Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Material for:

Copper hydrotris(3,5-diphenylpyrazolyl)borate dithiocarbamates: mimicking copper green proteins

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Supporting Figures and Tables

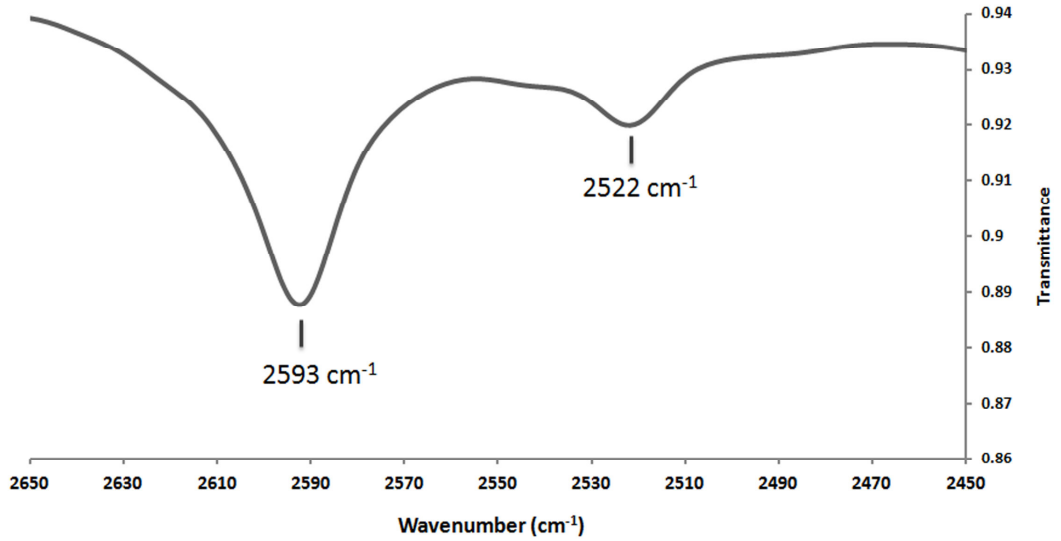

Figure S1 IR spectrum of [$Tp^{Ph2}Cu(S_2CN(CH_2)_4)$] **3** in the B-H region in CH_2Cl_2.

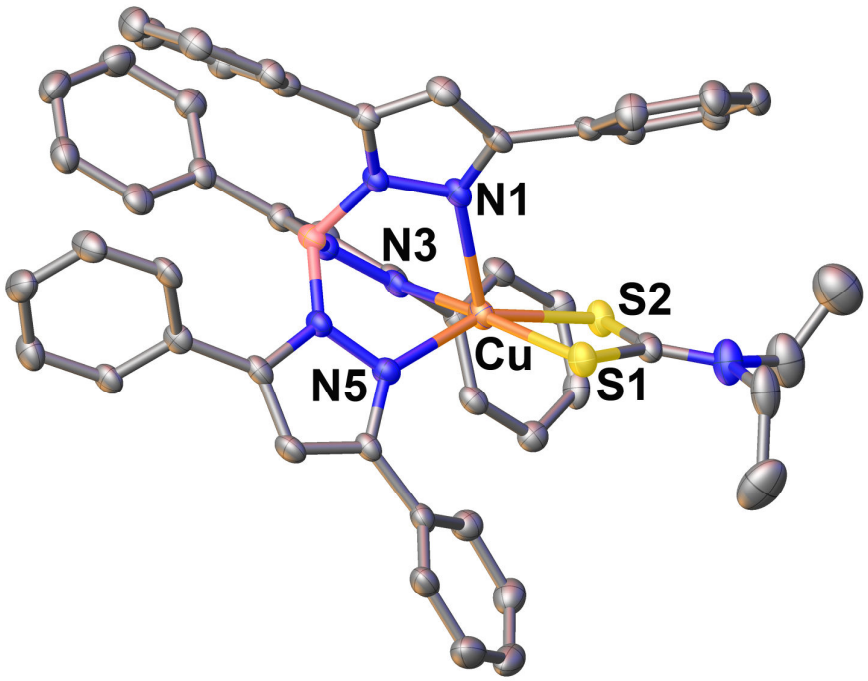

Figure S2 Structure of [$Tp^{Ph2}Cu(S_2CNEt_2)$] **1**. Hydrogen atoms are omitted and only selected atoms labelled in the interests of clarity.

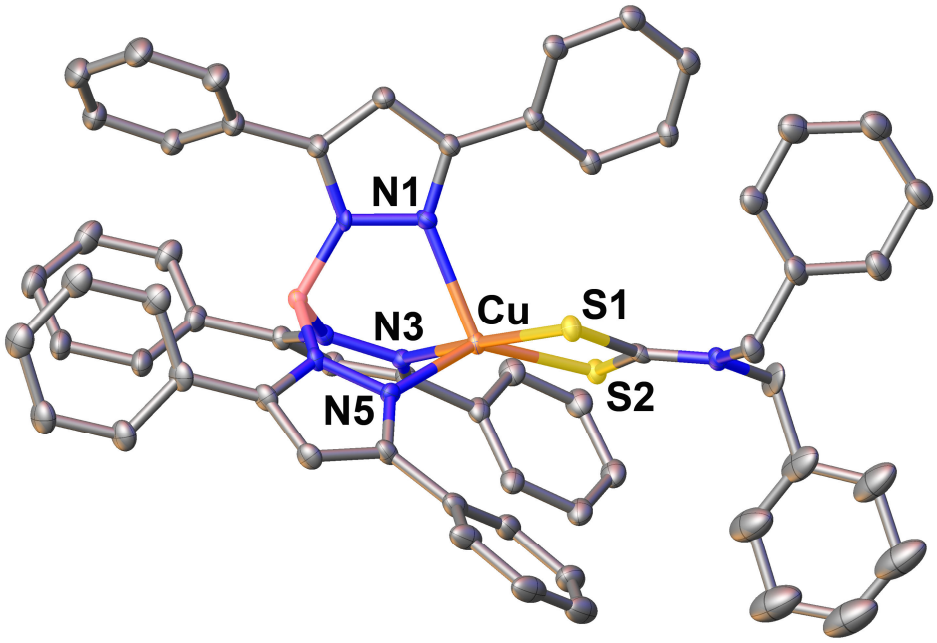

Figure S3 Structure of [$Tp^{Ph2}Cu(S_2CNBz_2)$] **2**. Hydrogen atoms are omitted and only selected atoms labelled in the interests of clarity.

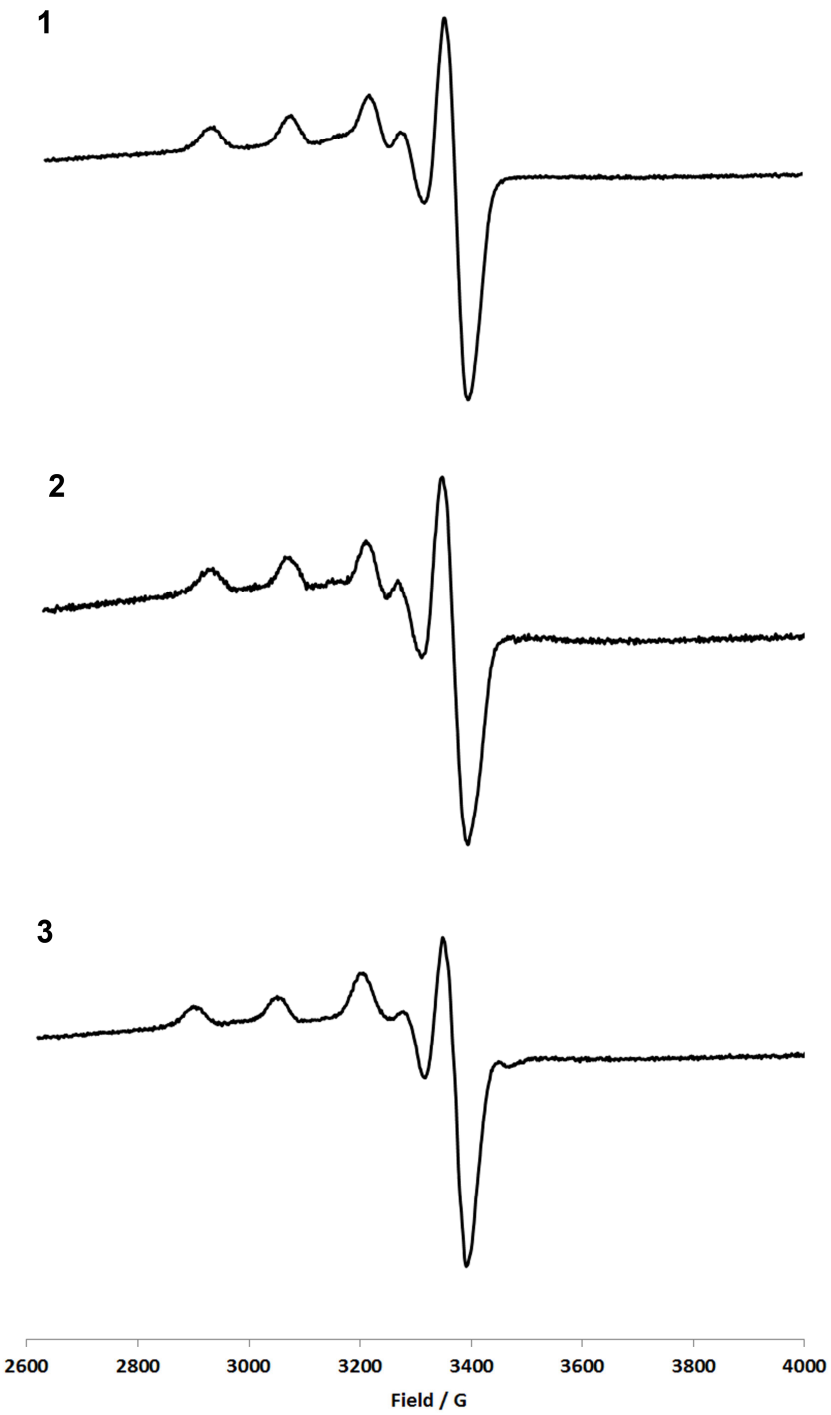

Figure S4 ESR spectra of **1**, **2** and **3** in frozen CH_2Cl_2 at 150 K.

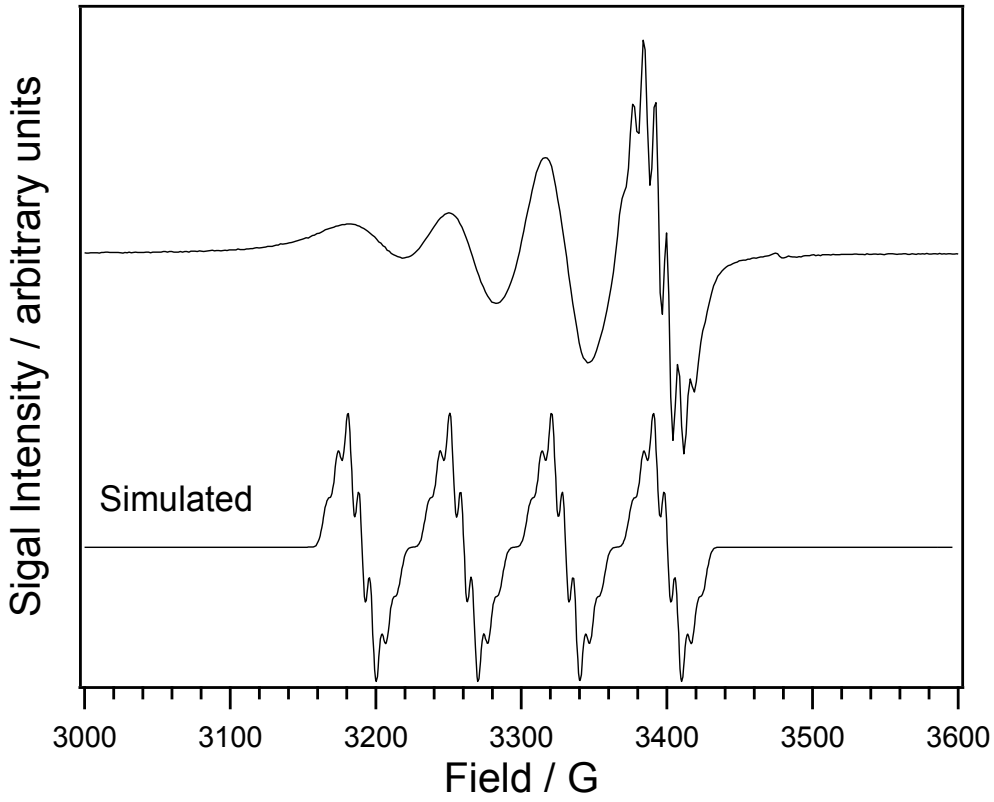

Figure S5 Simulated spectrum of [$Tp^{Ph2}Cu(S_2CN(CH_2)_4$] **3** at 295 K.

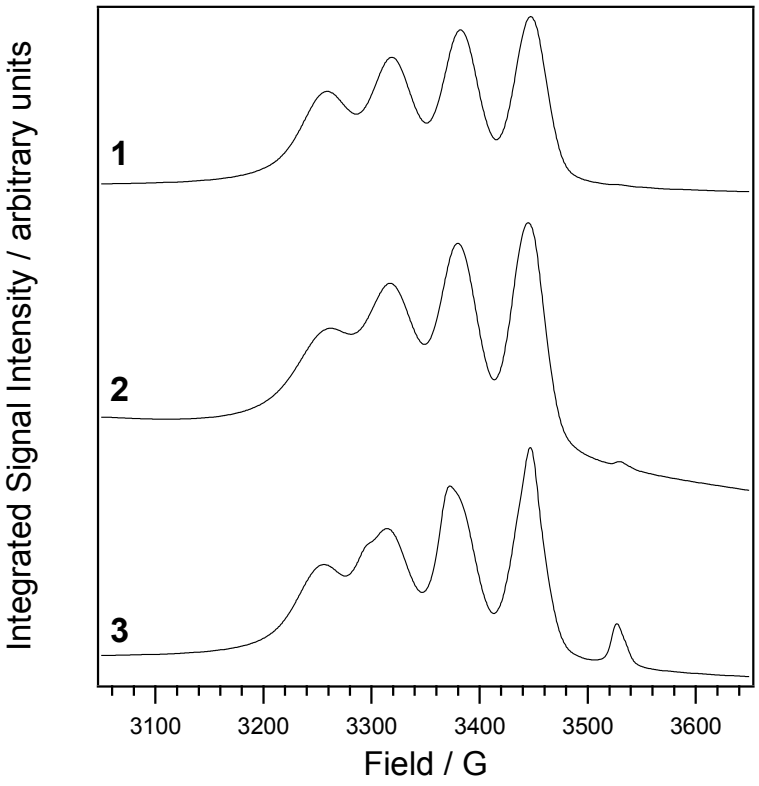

Figure S6 Integrated ESR spectrum of [$Tp^{Ph2}Cu(dtc)$] **1**-**3** at 295 K.

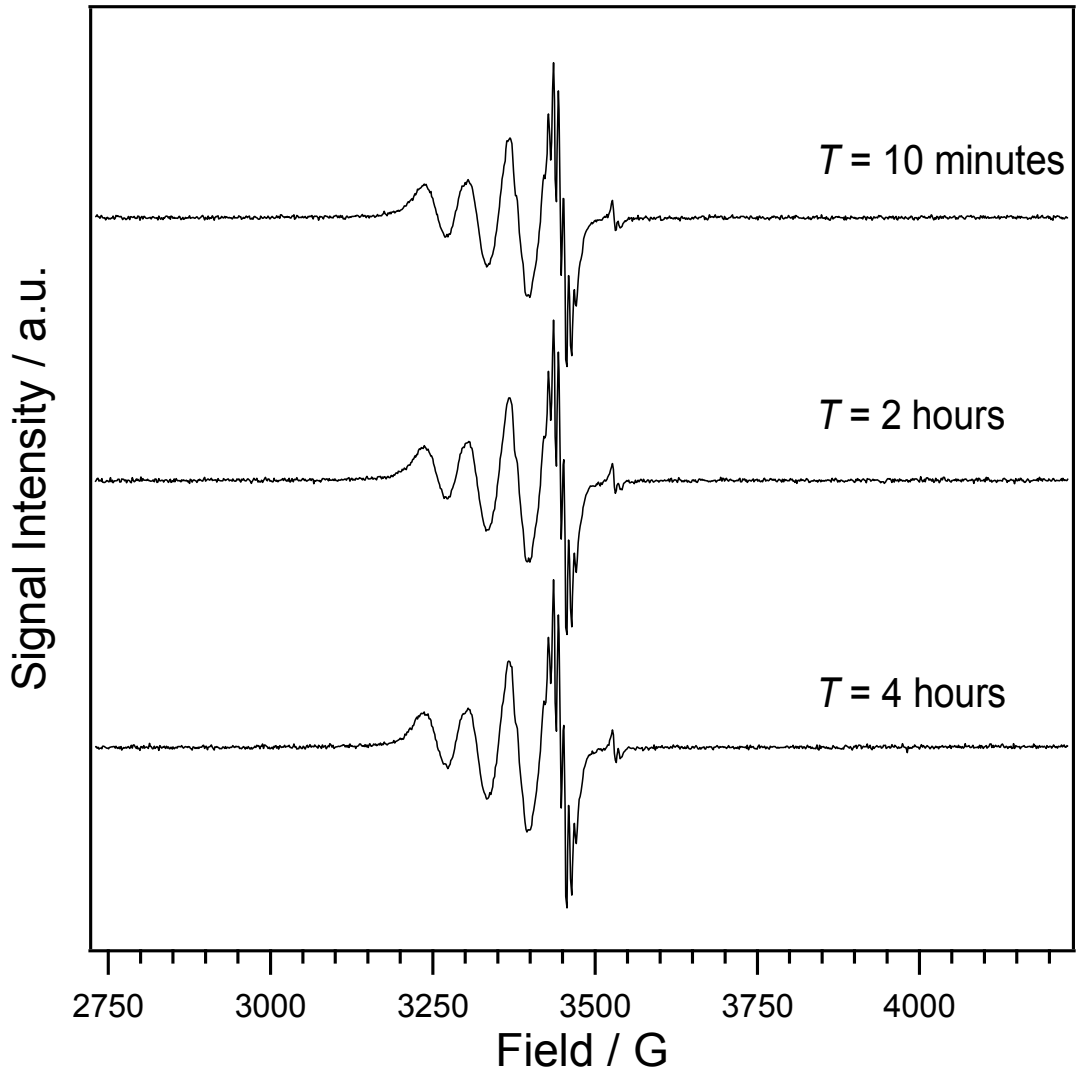

Figure S7 X-band EPR spectra of 1 mM of **3** dissolved in CH_2Cl_2 at different times after dissolution at room temperature. The modulation amplitude = 1.0 G, sweep time = 60 s and microwave power = 0.63 mW.

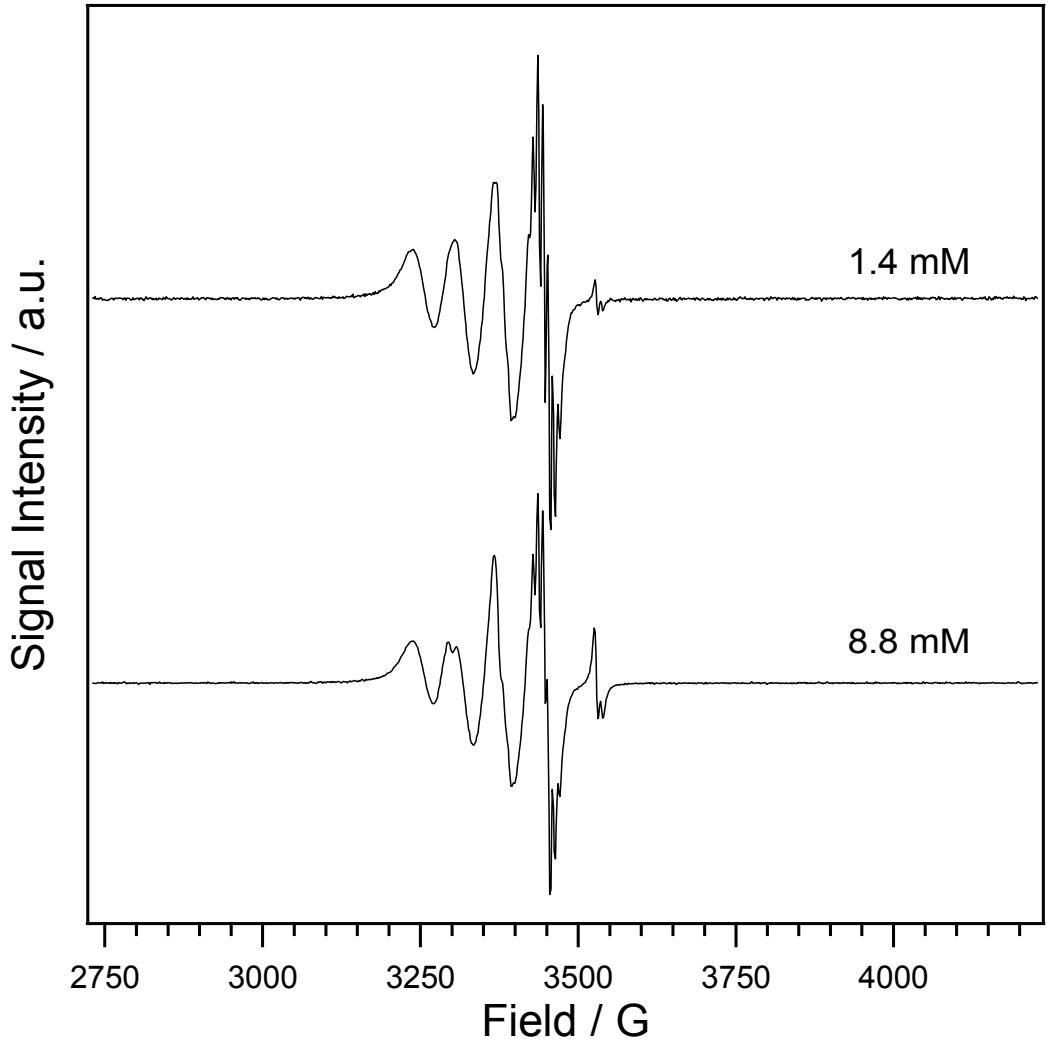

Figure S8 X-band EPR spectra of **3** dissolved in CH_2Cl_2 at different concentrations at room temperature. The modulation amplitude = 1.0 G, sweep time = 60 s and microwave power = 0.63 mW. The signal intensity has been normalised so they are the same size.

Table S1 Coordinates for [$Tp^{Ph2}Cu(S_2CNEt_2)$] **1**.

1	Cu1	1.12	0.06	0.08
2	S2	3.31	-0.15	1.04
3	S3	2.62	0.03	-1.79
4	B4	-1.91	0.04	0.04
5	H5	-3.09	0.05	0.03
6	N6	-1.41	-1.28	-0.63
7	N7	-0.08	-1.57	-0.61
8	N8	-0.06	1.59	-0.68
9	N9	-1.39	1.30	-0.71
10	N10	-0.04	0.16	1.76
11	N11	-1.38	0.08	1.50
12	N12	5.16	-0.24	-0.93
13	C13	-2.09	-2.22	-1.34
14	C14	-1.15	-3.14	-1.80
15	H15	-1.36	-4.05	-2.34
16	C16	0.09	-2.71	-1.30
17	C17	0.10	2.81	-1.22
18	C18	-1.15	3.32	-1.61
19	H19	-1.36	4.27	-2.06
20	C20	-2.08	2.34	-1.26
21	C21	0.11	0.03	3.09
22	C22	-1.14	-0.17	3.70
23	H23	-1.35	-0.24	4.75
24	C24	-2.07	-0.11	2.66
25	C25	-3.55	-2.28	-1.55
26	C26	-4.46	-2.21	-0.48
27	H27	-4.10	-2.06	0.53
28	C28	-5.83	-2.33	-0.71
29	H29	-6.52	-2.27	0.13
30	C30	-6.31	-2.55	-2.00
31	H31	-7.38	-2.65	-2.18
32	C32	-5.42	-2.64	-3.07
33	H33	-5.78	-2.81	-4.08
34	C34	-4.05	-2.51	-2.84
35	H35	-3.35	-2.57	-3.67
36	C36	1.40	3.50	-1.33
37	C37	2.38	3.39	-0.34
38	H38	2.20	2.77	0.53
39	C39	3.58	4.09	-0.45
40	H40	4.33	4.00	0.33
41	C41	3.82	4.91	-1.55
42	H42	4.76	5.45	-1.64
43	C43	2.85	5.03	-2.55
44	H44	3.03	5.66	-3.42
45	C45	1.65	4.33	-2.44
46	H46	0.91	4.41	-3.23
47	C47	1.39	0.17	3.82
48	C48	1.78	-0.81	4.74
49	H49	1.19	-1.72	4.84
50	C50	2.93	-0.64	5.51
51	H51	3.23	-1.42	6.21
52	C52	3.70	0.52	5.38
53	H53	4.59	0.65	5.98
54	C54	3.31	1.51	4.48
55	H55	3.90	2.41	4.38
56	C56	2.16	1.34	3.71
57	H57	1.85	2.11	3.02
58	C58	1.37	-3.41	-1.43
59	C59	1.69	-4.09	-2.62
60	H60	1.00	-4.02	-3.46
61	C61	2.87	-4.81	-2.74
62	H62	3.10	-5.32	-3.68
63	C63	3.76	-4.89	-1.67
64	H64	4.68	-5.46	-1.76
65	C65	3.45	-4.23	-0.48
66	H66	4.13	-4.29	0.37
67	C67	2.27	-3.50	-0.36
68	H68	2.04	-3.00	0.58
69	C69	-3.54	2.41	-1.44
70	C70	-4.22	3.57	-1.04
71	H71	-3.66	4.37	-0.57
72	C72	-5.60	3.69	-1.23
73	H73	-6.11	4.60	-0.91
74	C74	-6.32	2.65	-1.82
75	H75	-7.39	2.75	-1.97
76	C76	-5.65	1.50	-2.23
77	H77	-6.20	0.68	-2.69
78	C78	-4.28	1.38	-2.05
79	H79	-3.77	0.48	-2.38
80	C80	-3.54	-0.19	2.79
81	C81	-4.40	0.77	2.23
82	H82	-3.98	1.59	1.65
83	C83	-5.77	0.69	2.42
84	H84	-6.42	1.44	1.97
85	C85	-6.32	-0.35	3.17
86	H86	-7.40	-0.41	3.32
87	C87	-5.48	-1.31	3.74
88	H88	-5.90	-2.12	4.33
89	C89	-4.10	-1.23	3.55
90	H90	-3.45	-1.98	3.99
91	C91	3.86	-0.14	-0.61
92	C92	5.61	-0.25	-2.33
93	H93	4.82	-0.70	-2.94
94	H94	6.48	-0.91	-2.39
95	C95	5.95	1.15	-2.85
96	H96	5.08	1.81	-2.80
97	H97	6.29	1.09	-3.89
98	H98	6.75	1.61	-2.26
99	C99	6.21	-0.34	0.09
100	H100	7.09	0.19	-0.30
101	H101	5.87	0.19	0.98
102	C102	6.57	-1.79	0.45
103	H103	5.70	-2.30	0.87
104	H104	7.38	-1.80	1.18
105	H105	6.90	-2.35	-0.44

Table S2 Coordinates for [$Tp^{Ph2}Cu(S_2CNBz_2)$] **2**.

1	Cu1	0.16	-0.19	-0.15
2	S2	1.83	0.95	1.14
3	S3	2.25	-0.69	-1.24
4	N4	-1.01	1.55	-0.64
5	N5	-2.33	1.39	-0.31
6	N6	-1.12	-1.32	-1.27
7	N7	-2.44	-1.03	-1.05
8	N8	-0.92	-0.80	1.49
9	N9	-2.25	-0.53	1.41
10	N10	4.29	0.39	0.17
11	B11	-2.85	-0.02	0.07
12	H12	-4.03	0.01	0.17
13	C13	-0.83	2.86	-0.88
14	C14	-2.03	3.55	-0.68
15	H15	-2.22	4.60	-0.86
16	C16	-2.97	2.59	-0.33
17	C17	-1.07	-2.10	-2.37
18	C18	-2.37	-2.28	-2.88
19	H19	-2.65	-2.90	-3.72
20	C20	-3.21	-1.60	-2.02
21	C21	-0.70	-1.41	2.67
22	C22	-1.91	-1.52	3.37
23	H23	-2.07	-1.97	4.34
24	C24	-2.88	-0.96	2.54
25	C25	0.43	3.43	-1.39
26	C26	1.25	2.73	-2.29
27	H27	0.97	1.72	-2.58
28	C28	2.39	3.32	-2.82
29	H29	3.01	2.76	-3.52
30	C30	2.74	4.63	-2.47
31	H31	3.62	5.09	-2.90
32	C32	1.93	5.34	-1.57
33	H33	2.19	6.36	-1.30
34	C34	0.79	4.74	-1.04
35	H35	0.18	5.29	-0.33
36	C36	-4.41	2.82	-0.09
37	C37	-4.79	3.82	0.82
38	H38	-4.03	4.37	1.36
39	C39	-6.14	4.12	1.03
40	H40	-6.42	4.90	1.73
41	C41	-7.13	3.41	0.34
42	H42	-8.18	3.64	0.50
43	C43	-6.76	2.41	-0.57
44	H44	-7.51	1.86	-1.11
45	C45	-5.41	2.12	-0.78
46	H46	-5.13	1.36	-1.50
47	C47	0.15	-2.76	-2.88
48	C48	0.91	-3.60	-2.06
49	H49	0.64	-3.71	-1.02
50	C50	2.00	-4.30	-2.58
51	H51	2.58	-4.95	-1.93
52	C52	2.34	-4.17	-3.93
53	H53	3.19	-4.71	-4.33
54	C54	1.59	-3.33	-4.76
55	H55	1.85	-3.23	-5.80
56	C56	0.49	-2.64	-4.24
57	H57	-0.10	-1.99	-4.88
58	C58	-4.69	-1.54	-2.08
59	C59	-5.30	-1.21	-3.30
60	H60	-4.68	-0.95	-4.15
61	C61	-6.69	-1.19	-3.42
62	H62	-7.14	-0.92	-4.37
63	C63	-7.49	-1.51	-2.33
64	H64	-8.57	-1.50	-2.42
65	C65	-6.89	-1.85	-1.11
66	H66	-7.51	-2.11	-0.25
67	C67	-5.50	-1.87	-0.99
68	H68	-5.05	-2.16	-0.05
69	C69	0.62	-1.90	3.12
70	C70	0.94	-1.85	4.49
71	H71	0.24	-1.40	5.19
72	C72	2.16	-2.35	4.95
73	H73	2.39	-2.29	6.01
74	C74	3.08	-2.90	4.06
75	H75	4.03	-3.28	4.41
76	C76	2.76	-2.96	2.70
77	H77	3.47	-3.38	1.99
78	C78	1.54	-2.47	2.23
79	H79	1.30	-2.53	1.18
80	C80	-4.33	-0.87	2.82
81	C81	-5.04	0.33	2.68
82	H82	-4.54	1.23	2.34
83	C83	-6.40	0.39	2.99
84	H84	-6.94	1.32	2.87
85	C85	-7.06	-0.75	3.46
86	H86	-8.12	-0.70	3.70
87	C87	-6.36	-1.95	3.61
88	H88	-6.87	-2.84	3.97
89	C89	-5.00	-2.00	3.29
90	H90	-4.46	-2.94	3.40
91	C91	2.96	0.24	0.04
92	C92	5.24	-0.11	-0.84
93	H93	5.94	0.71	-1.05
94	H94	4.68	-0.31	-1.75
95	C95	6.02	-1.34	-0.41
96	C96	5.40	-2.60	-0.38
97	H97	4.36	-2.69	-0.68
98	C98	6.12	-3.73	0.00
99	H99	5.63	-4.70	0.01
100	C100	7.46	-3.62	0.37
101	H101	8.02	-4.50	0.67
102	C102	8.08	-2.37	0.35
103	H103	9.13	-2.28	0.62
104	C104	7.36	-1.24	-0.04
105	H105	7.86	-0.27	-0.07
106	C106	4.90	1.01	1.36
107	H107	5.62	0.30	1.77
108	H108	4.11	1.14	2.10
109	C109	5.59	2.33	1.08
110	C110	6.91	2.53	1.49
111	H111	7.45	1.73	1.98
112	C112	7.54	3.76	1.27
113	H113	8.57	3.90	1.60
114	C114	6.86	4.80	0.64
115	H115	7.35	5.75	0.47
116	C116	5.54	4.60	0.22
117	H117	5.00	5.40	-0.27
118	C118	4.91	3.38	0.44
119	H119	3.88	3.24	0.12

Table S3 Coordinates for [$Tp^{Ph2}Cu(S_2CN(CH_2)_4)$] **3**.

1	Cu1	1.11	-0.23	0.01
2	S2	2.64	0.50	-1.70
3	S3	3.28	-0.37	1.02
4	N4	-1.40	-0.65	1.34
5	N5	-0.08	-0.92	1.52
6	N6	-1.33	1.44	-0.08
7	N7	0.02	1.63	0.06
8	N8	-1.44	-0.89	-1.17
9	N9	-0.13	-1.24	-1.28
10	N10	5.09	0.70	-0.66
11	C11	-2.09	-0.90	2.49
12	C12	-1.18	-1.33	3.44
13	H13	-1.40	-1.67	4.44
14	C14	0.07	-1.35	2.79
15	C15	-1.94	2.63	-0.37
16	C16	-0.95	3.60	-0.44
17	H17	-1.10	4.66	-0.59
18	C18	0.25	2.94	-0.15
19	C19	-2.19	-1.61	-2.06
20	C20	-1.31	-2.44	-2.76
21	H21	-1.57	-3.14	-3.53
22	C22	-0.03	-2.18	-2.23
23	C23	-3.56	-0.77	2.66
24	C24	-4.05	-0.08	3.78
25	H25	-3.36	0.39	4.47
26	C26	-5.43	0.02	4.00
27	H27	-5.80	0.55	4.87
28	C28	-6.32	-0.58	3.11
29	H29	-7.39	-0.50	3.28
30	C30	-5.84	-1.27	2.00
31	H31	-6.53	-1.74	1.30
32	C32	-4.47	-1.37	1.77
33	H33	-4.10	-1.92	0.92
34	C34	-3.39	2.84	-0.54
35	C35	-3.85	3.56	-1.65
36	H36	-3.14	3.90	-2.40
37	C37	-5.21	3.84	-1.81
38	H38	-5.55	4.40	-2.68
39	C39	-6.13	3.40	-0.86
40	H40	-7.19	3.62	-0.98
41	C41	-5.69	2.69	0.25
42	H42	-6.39	2.34	1.00
43	C43	-4.33	2.41	0.42
44	H44	-3.99	1.87	1.30
45	C45	-3.65	-1.53	-2.23
46	C46	-4.39	-2.72	-2.29
47	H47	-3.88	-3.67	-2.17
48	C48	-5.77	-2.69	-2.49
49	H49	-6.33	-3.62	-2.53
50	C50	-6.43	-1.47	-2.63
51	H51	-7.51	-1.45	-2.79
52	C52	-5.70	-0.28	-2.59
53	H53	-6.20	0.67	-2.70
54	C54	-4.32	-0.31	-2.39
55	H55	-3.77	0.62	-2.37
56	C56	1.32	-1.87	3.37
57	C57	2.05	-2.89	2.74
58	H58	1.71	-3.27	1.78
59	C59	3.17	-3.44	3.35
60	H60	3.72	-4.23	2.85
61	C61	3.59	-2.98	4.60
62	H62	4.47	-3.40	5.07
63	C63	2.88	-1.96	5.24
64	H64	3.20	-1.60	6.21
65	C65	1.75	-1.42	4.63
66	H66	1.19	-0.63	5.13
67	C67	1.58	3.57	0.01
68	C68	2.44	3.21	1.05
69	H69	2.15	2.42	1.74
70	C70	3.67	3.85	1.21
71	H71	4.32	3.56	2.03
72	C72	4.05	4.87	0.33
73	H73	5.00	5.38	0.47
74	C74	3.19	5.24	-0.70
75	H75	3.48	6.04	-1.39
76	C76	1.97	4.60	-0.86
77	H77	1.31	4.88	-1.68
78	C78	1.22	-2.85	-2.62
79	C79	2.23	-3.12	-1.68
80	H80	2.11	-2.80	-0.65
81	C81	3.39	-3.80	-2.06
82	H82	4.16	-4.00	-1.32
83	C83	3.56	-4.22	-3.38
84	H84	4.46	-4.75	-3.67
85	C85	2.56	-3.96	-4.32
86	H86	2.68	-4.28	-5.35
87	C87	1.40	-3.28	-3.94
88	H88	0.64	-3.06	-4.68
89	C89	3.82	0.32	-0.47
90	C90	5.59	1.31	-1.90
91	H91	5.14	2.31	-2.02
92	H92	5.29	0.71	-2.76
93	C93	7.10	1.38	-1.69
94	H94	7.57	0.44	-2.02
95	H95	7.56	2.20	-2.25
96	C96	7.25	1.53	-0.17
97	H97	7.05	2.57	0.13
98	H98	8.23	1.25	0.21
99	C99	6.14	0.62	0.38
100	H100	6.47	-0.42	0.49
101	H101	5.73	0.95	1.34
102	B102	-1.90	0.00	0.02
103	H103	-3.08	0.06	0.02