Electronic Supplementary Information for Dalton Transactions

Supporting Information for

Synthesis and Reactivity of Copper(I) Complexes Containing a Bis(imidazolin-2-imine) Pincer Ligand

Dejan Petrovic, Thomas Bannenberg, Sören Randoll, Peter G. Jones, and Matthias Tamm*

Contents:

Page 2: Energies of all optimized structures.

Pages 3 – 15: Presentations of the calculated molecular structures together with Cartesian coordinates of their atomic positions.

Electronic Supplementary Information for Dalton Transactions

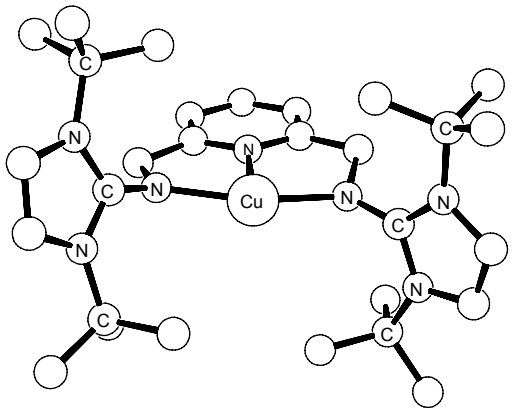
Energies of all optimized structures:

Compound	E(0 K)[a] [Ha]	H(298 K)[b] [Ha]	G(298 K)[b] [Ha]
5	-3156.718361	-3156.677054	-3156.790589
5·NCMe	-3289.481957	-3289.435523	-3289.560758
6a	-3407.360311	-3407.309803	-3407.446620
6b	-3559.797012	-3559.744175	-3559.889070
9a	-5731.090014	-5731.046048	-5731.167891
9b	-3617.164237	-3617.120535	-3617.240765
NCMe	-132.748112	-132.743571	-132.771078
CN*t*Bu	-250.606911	-250.598542	-250.636208
CN*o*Xy	-403.043413	-403.032848	-403.077920

[a]DFT energy incl. ZPE.

[b]standard conditions T = 298.15 K and p = 1 atm.

Electronic Supplementary Information for Dalton Transactions



Structure of 5 (atom, x-, y-, z-positions in Å):

H	4.620985	-1.589771	-3.955627
H	3.182561	-2.519010	-4.328597
H	3.075424	-0.758520	-4.241050
H	5.088684	0.152456	-2.924587
H	-3.686657	-1.753542	-3.211748
H	-5.385079	-1.907361	-2.720575
H	-4.309504	-3.283349	-2.581377
H	5.245294	2.240562	-1.234117
H	-5.540059	0.093731	-2.270072
H	5.059950	-2.728898	-1.777684
H	3.784892	-3.864113	-2.237114
H	-4.781964	2.656700	-1.960127
H	4.469408	3.849132	0.028122
H	1.453011	-2.967445	-2.823730
H	1.095196	-1.241487	-2.681549
H	-3.519128	4.368737	-1.740560
H	-2.705334	-3.555199	-0.977831
H	-5.997938	-1.857393	-0.275557
H	-1.823806	-2.089930	-1.424756
H	-5.148203	-3.402841	-0.161822
H	-1.387534	3.126423	-2.092427
H	1.990017	3.337533	-0.077324
H	3.752113	-3.097279	-0.647145
H	5.555140	2.818126	0.991627
H	1.298446	-2.220750	-1.228296
H	4.403379	3.888994	1.784073
H	-4.391533	4.256461	-0.192971
H	-2.258439	-2.386915	0.258300
H	-2.892026	5.175675	-0.312892
H	-4.777039	-2.106929	0.976959
H	-0.599785	2.237433	-0.775269
H	-0.665731	4.007311	-0.736033
H	1.294783	2.046195	0.924507
H	1.949017	3.504347	1.685395
H	2.280307	-2.550537	0.640658
H	4.569504	0.846340	2.345288
H	-3.237689	-1.084566	1.759910
H	3.583861	2.083974	3.131482
H	2.803523	0.659204	2.438028
H	-3.311882	3.009468	1.783941
H	3.130377	-1.505152	1.765138
H	-1.911904	4.059038	1.540321
H	-1.695712	2.300314	1.601747
H	-2.635933	0.346127	2.561863

H	1.957029	-3.027373	3.695864
H	-2.199495	-2.013106	4.240345
H	-0.143781	-3.171833	5.018431
C	-4.362433	-2.198453	-2.478279
C	3.542926	-1.638669	-3.794296
C	4.515480	0.343349	-2.038312
C	4.595915	1.388092	-1.190795
C	3.167607	-1.787278	-2.306951
C	3.990216	-2.936123	-1.698287
C	-4.730821	0.489470	-1.687460
C	-4.355327	1.771915	-1.529628
C	-3.953286	-1.821429	-1.037802
C	1.658819	-2.067101	-2.240677
C	-2.597426	-2.489013	-0.766716
C	-5.032154	-2.321133	-0.061728
C	4.546105	3.231300	0.925497
C	2.976457	0.015917	-0.417922
C	-3.403604	4.276201	-0.658766
C	-2.964938	0.503732	-0.277326
C	3.467314	2.137761	0.978171
C	-1.218908	3.107013	-1.012827
C	2.085161	2.794627	0.865975
C	-2.555195	3.058291	-0.256992
C	3.612433	1.372151	2.303396
C	2.195076	-1.602594	1.198312
C	-2.352895	3.097684	1.267278
C	-2.356249	-0.438068	1.838287
C	1.038285	-1.792197	2.173229
C	-1.223190	-1.244316	2.464510
C	1.056489	-2.531267	3.353298
C	-1.285870	-1.961529	3.659422
C	-0.127388	-2.608197	4.092585
N	-3.867955	-0.312365	-0.951397
N	3.664442	1.193403	-0.185725
N	-3.278494	1.797068	-0.658066
N	3.515372	-0.504402	-1.587432
N	1.963929	-0.436799	0.329848
N	-1.973797	0.167328	0.550974
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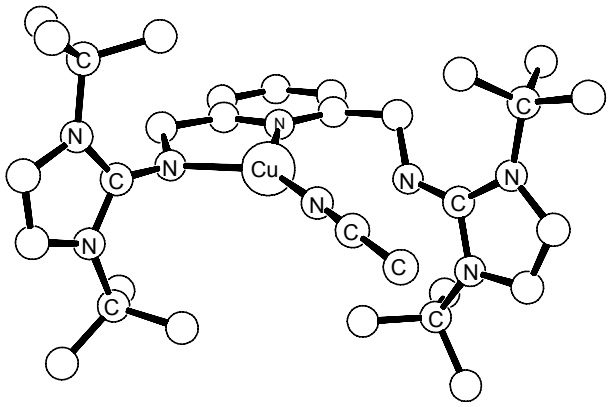
Cu	0.007621	0.061441	0.187204

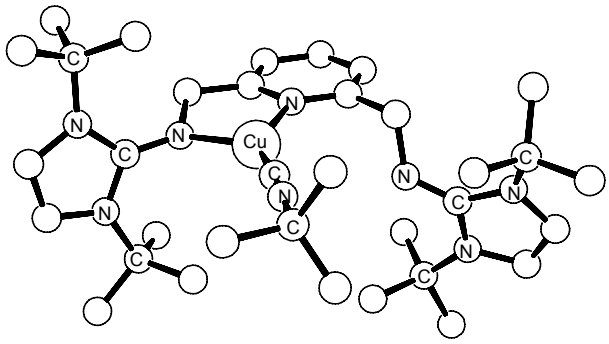
Electronic Supplementary Information for Dalton Transactions



Structure of 5 · NCMe (atom, x-, y-, z-positions in Å):

H	-5.466099	2.330195	-1.752332
H	-5.995613	-0.251521	-2.294242
H	-5.236806	3.817556	0.060657
H	-4.279612	4.108595	-1.411868
H	-3.810772	4.851321	0.109645
H	-1.503259	3.932443	-0.219442
H	-2.000728	3.057057	-1.676874
H	-1.244478	2.186028	-0.328654
H	-2.903302	3.654095	1.962251
H	-2.501979	1.933231	1.883556
H	-4.198082	2.452782	2.001829
H	-6.228419	-2.335846	-0.109573
H	-4.849536	-2.492400	0.982878
H	-5.253201	-3.810354	-0.120531
H	-5.941982	-2.292326	-2.586690
H	-4.765542	-3.590025	-2.626995
H	-4.339146	-2.014323	-3.302160
H	-2.398497	-2.545756	-0.083161
H	-2.248782	-2.252925	-1.817265
H	-2.932647	-3.773466	-1.230220
H	-3.275118	-0.159243	2.457503
H	-3.153227	-1.734770	1.704810
H	-2.281603	-1.319710	4.426307
H	-0.128572	-1.883603	5.560534
H	1.965038	-1.932207	4.201140
H	5.221538	2.483155	-1.348265
H	5.825359	0.028204	-2.229071
H	2.036364	-2.339032	0.858769
H	3.028343	-1.770273	2.192324
H	2.883516	-3.621497	-1.744455
H	2.108596	-2.210640	-1.009403
H	2.719325	-2.116520	-2.654831
H	4.140310	-2.844401	0.897473
H	4.914783	-3.940979	-0.238230
H	5.786300	-2.520815	0.353416
H	5.038761	-1.792948	-3.222714
H	6.325548	-2.098414	-2.032768
H	5.268186	-3.405015	-2.552898
H	3.209279	1.353107	2.582277
H	3.410044	3.090341	2.873428

H	4.788255	2.125086	2.325403
H	3.660607	4.669074	0.982453
H	5.106784	3.808076	0.467376
H	3.793198	4.130682	-0.688834
H	1.476586	3.568546	1.278638
H	1.277730	1.842713	0.901487
H	1.551620	3.018573	-0.402032
H	1.495565	1.998477	-4.051967
H	1.794373	0.320275	-4.547552
H	2.883617	1.108849	-3.376261
C	-4.965989	1.451582	-1.394379
C	-5.228882	0.159353	-1.666904
C	-3.467489	0.204088	-0.250970
C	-3.308729	2.768343	0.037659
C	-4.225979	3.944948	-0.333308
C	-3.221045	2.685136	1.570675
C	-1.925469	2.994699	-0.588140
C	-2.642251	-0.760920	1.787576
C	-4.304804	-2.131639	-1.112835
C	-5.210935	-2.723348	-0.019207
C	-2.878684	-2.698719	-1.044410
C	-4.877727	-2.512978	-2.493415
C	-1.340257	-1.045457	2.511940
C	-1.349068	-1.342918	3.875093
C	-0.153960	-1.659520	4.500389
C	1.015245	-1.684002	3.744392
C	0.961638	-1.380257	2.388822
C	2.206032	-1.478168	1.524230
C	3.432136	0.084870	0.056711
C	4.782427	1.545337	-1.067295
C	5.082457	0.314506	-1.511109
C	4.302125	-2.079702	-1.168027
C	2.914923	-2.532392	-1.662799
C	4.806522	-2.890378	0.042409
C	5.298783	-2.340438	-2.314509
C	3.323801	2.559928	0.773739
C	3.706848	2.255367	2.233740
C	1.805302	2.753690	0.628298
C	4.022571	3.860398	0.345358
C	1.021957	0.550527	-2.614297
C	1.845385	1.021407	-3.711874
N	0.398166	0.177493	-1.720767
N	-3.894114	1.492621	-0.518239
N	-4.305165	-0.625059	-0.990073
N	-2.419284	-0.103081	0.514566
N	-0.205698	-1.051210	1.793401
N	2.475155	-0.232731	0.867777
N	3.782273	1.436450	-0.109890
N	4.272829	-0.615217	-0.844858
Cu	-0.484933	-0.259805	-0.094952



Structure of 6a (atom, x-, y-, z-positions in Å):

H	-5.506357	-0.294376	2.951803
H	-6.663621	0.692672	0.731601
H	-4.584703	-2.213610	3.827352
H	-3.879030	-0.676123	4.382405
H	-2.992302	-2.181326	4.578363
H	-1.047180	-1.125325	3.512504
H	-1.922589	0.360569	3.113182
H	-1.106049	-0.565785	1.839113
H	-2.031868	-3.418380	2.743784
H	-2.053072	-2.811633	1.084268
H	-3.541550	-3.442180	1.825101
H	-6.634290	-0.989249	-1.932642
H	-5.033865	-1.432076	-2.534892
H	-6.013331	-0.260361	-3.418667
H	-7.166477	1.320238	-1.189288
H	-6.333009	2.099849	-2.520047
H	-5.866281	2.488620	-0.862130
H	-3.088317	0.444749	-2.411153
H	-3.515230	2.003148	-1.705417
H	-4.182064	1.529960	-3.273209
H	-2.989752	-2.820202	-1.082382
H	-3.057327	-1.600747	-2.340568
H	-1.583411	-4.108372	-2.701743
H	0.757060	-4.510663	-3.476971
H	2.488737	-2.770595	-3.017333
H	6.447391	-1.466775	1.808931
H	7.074863	0.392709	-0.011933
H	1.669129	0.574414	-1.844707
H	2.927240	-0.495454	-2.477469
H	3.554450	3.375836	-1.212123
H	2.715711	1.893507	-0.727662
H	3.825268	2.678352	0.394881
H	3.802025	1.075729	-3.074942
H	4.905169	2.432834	-3.234483
H	5.547920	0.792633	-3.090414
H	6.288957	2.609341	0.134655
H	7.007955	2.039127	-1.387084
H	5.980827	3.464700	-1.379785
H	2.519923	-3.036977	0.170586
H	2.734438	-4.178768	1.513079

H	4.070407	-3.871855	0.393109
H	4.100603	-3.565362	3.488569
H	5.496818	-3.394416	2.430964
H	5.053058	-2.083418	3.548795
H	1.991685	-2.333819	3.137216
H	1.851048	-1.146668	1.818533
H	2.894934	-0.812424	3.217181
H	1.902908	3.982214	1.766357
H	0.634358	3.703748	2.974015
H	1.126095	5.357351	2.570744
H	-1.797467	4.273812	2.429293
H	-2.217208	4.946140	0.840939
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H	-0.391415	5.346661	-0.901562
H	1.296311	4.949884	-0.525762
H	0.516072	6.337311	0.252846
C	-5.121053	-0.258737	1.951638
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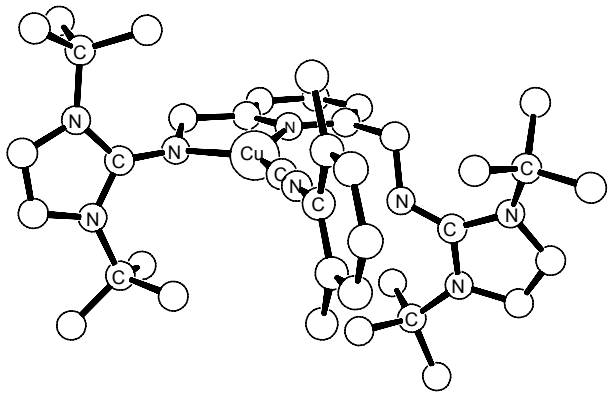
C	-3.668488	-0.555834	0.247514
C	-2.952966	-1.475590	2.555185
C	-3.660959	-1.636775	3.910211
C	-2.625486	-2.874096	2.005857
C	-1.678297	-0.644768	2.761589
C	-2.520946	-1.884477	-1.419134
C	-5.138520	0.560380	-1.612717
C	-5.734873	-0.606172	-2.420402
C	-3.895006	1.160040	-2.286796
C	-6.192140	1.681747	-1.522088
C	-1.100606	-2.194616	-1.851952
C	-0.803700	-3.377659	-2.522909
C	0.498030	-3.597660	-2.953307
C	1.462930	-2.629776	-2.700927
C	1.108464	-1.465935	-2.023866
C	2.149987	-0.407858	-1.710274
C	3.894322	-0.491985	-0.030095
C	5.802126	-0.966658	1.112738
C	6.114925	-0.034120	0.202602
C	4.847540	1.644956	-1.216140
C	3.653093	2.438849	-0.657876
C	4.760980	1.466443	-2.744421
C	6.115863	2.477214	-0.934651
C	3.711361	-2.269189	1.822050
C	3.224863	-3.410025	0.909886
C	2.531264	-1.592117	2.541960
C	4.660668	-2.853213	2.879928
C	-0.475864	2.010201	0.139833
C	-0.108805	4.433405	1.058770
C	0.958688	4.358430	2.163062
C	-1.454213	4.922711	1.621347
C	0.358091	5.319200	-0.108319
N	-3.878325	-0.758861	1.598883
N	-4.814202	0.079787	-0.217177
N	-2.535982	-0.864312	-0.386381
N	-0.159753	-1.262912	-1.608831
N	2.650527	-0.629903	-0.377643
N	4.444112	-1.247376	1.010018
N	4.951439	0.319875	-0.501875

N	-0.306739	3.088965	0.543689
Cu	-0.870332	0.294202	-0.470433

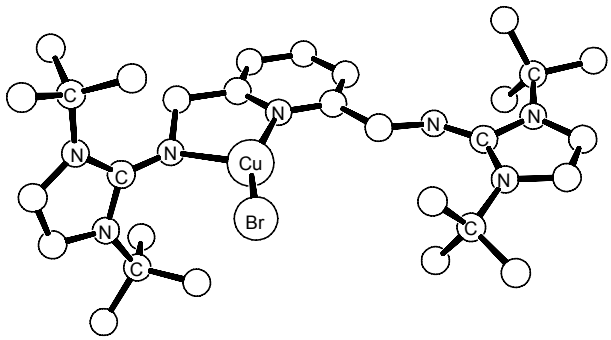


Structure of 6b (atom, x-, y-, z-positions in Å):

H	-5.638237	0.473180	2.930809
H	-6.624253	1.312216	0.571745
H	-4.979073	-1.476225	4.054346
H	-4.147956	0.047931	4.449283
H	-3.412331	-1.494020	4.859045
H	-1.334883	-0.733238	3.719838
H	-2.095075	0.755979	3.133964
H	-1.333583	-0.368815	1.990922
H	-2.509911	-3.018165	3.254176
H	-2.406595	-2.637890	1.530976
H	-3.973744	-3.045806	2.265412
H	-6.889079	-0.620295	-1.799165
H	-5.408868	-1.430837	-2.322397
H	-6.174760	-0.234138	-3.369584
H	-6.963828	1.840800	-1.405987
H	-6.011939	2.259653	-2.816320
H	-5.458768	2.767842	-1.217787
H	-3.163354	0.028809	-2.486418
H	-3.247574	1.715542	-1.975387
H	-4.047186	1.200021	-3.465210
H	-3.445064	-2.949180	-0.526968
H	-3.516857	-1.968495	-1.977936
H	-2.350936	-4.597768	-2.103105
H	-0.132472	-5.386800	-2.936559
H	1.823505	-3.841337	-2.790243
H	6.068869	-2.210198	1.885545
H	6.862639	-0.768884	-0.226867
H	1.508448	-0.314285	-2.090567
H	2.603849	-1.635964	-2.509447
H	3.668438	2.339301	-1.914132
H	2.684013	1.060013	-1.188343
H	3.893492	1.896038	-0.216299
H	3.621235	-0.257418	-3.362151
H	4.861326	0.922284	-3.753412
H	5.325363	-0.731539	-3.337322
H	6.333282	1.507187	-0.469419
H	6.950617	0.609396	-1.873724
H	6.087096	2.122530	-2.105438
H	1.979566	-3.600339	0.519726
H	2.071079	-4.507247	2.043008
H	3.426148	-4.554502	0.905654

H	3.532965	-3.718824	3.895777
H	4.921691	-3.892445	2.827724
H	4.645892	-2.366391	3.699379
H	1.562829	-2.346975	3.325194
H	1.539145	-1.389746	1.824294
H	2.632596	-0.946045	3.154318
H	1.275004	6.914715	-0.961680
H	2.414892	5.454357	2.904296
H	2.339740	7.277239	1.238206
H	-0.975302	4.393873	-1.790253
H	0.554907	3.818036	-2.439546
H	0.152893	5.537227	-2.526269
H	1.948127	2.038590	2.273717
H	0.422945	2.595940	2.946522
H	1.945368	3.233079	3.578837
C	-5.244694	0.320477	1.945009
C	-5.735978	0.742629	0.764006
C	-3.838612	-0.401513	0.334232
C	-3.250826	-1.052489	2.767849
C	-4.007758	-0.978759	4.104097
C	-3.021510	-2.532390	2.420299
C	-1.920058	-0.298986	2.906056
C	-2.925927	-2.140474	-1.062945
C	-5.124823	0.653603	-1.693929
C	-5.944674	-0.481896	-2.330706
C	-3.806574	0.901966	-2.442631
C	-5.941997	1.958859	-1.769862
C	-1.584686	-2.673038	-1.528560
C	-1.478086	-3.957395	-2.057780
C	-0.244477	-4.392025	-2.520914
C	0.846048	-3.532355	-2.441869
C	0.680694	-2.261191	-1.900553
C	1.857459	-1.311283	-1.776013
C	3.606394	-1.293031	-0.100850
C	5.470146	-1.768626	1.112357
C	5.866097	-1.045927	0.055559
C	4.764027	0.496537	-1.631325
C	3.677042	1.501604	-1.212383
C	4.624402	0.073683	-3.106515
C	6.122709	1.215364	-1.499566
C	3.262470	-2.696296	2.027547
C	2.642345	-3.916250	1.322047
C	2.174175	-1.781194	2.616862
C	4.158688	-3.191269	3.173687
C	-0.191761	1.610067	-0.132788
C	0.798384	3.866184	0.404339
C	1.395193	4.037677	1.666456
C	0.736896	4.881947	-0.567081
C	1.304058	6.109261	-0.237493
C	1.946993	5.286062	1.941586
C	1.904208	6.312876	1.002500
C	0.083201	4.645978	-1.903200
C	1.431732	2.916783	2.671220
N	-4.084617	-0.392333	1.693258
N	-4.874641	0.323108	-0.239679
N	-2.763912	-0.957321	-0.236045
N	-0.524902	-1.848910	-1.452650

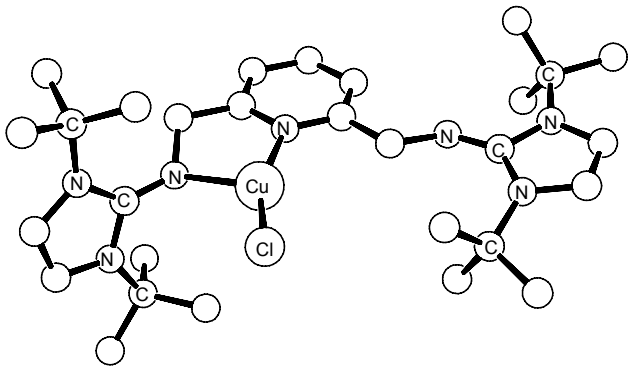
N	2.349087	-1.353887	-0.422431
N	4.088180	-1.912857	1.056137
N	4.736455	-0.693721	-0.702356
N	0.228382	2.593857	0.094215
Cu	-0.966807	-0.080555	-0.491900



Structure of 9a (atom, x-, y-, z-positions in Å):

H	6.284096	-1.378725	1.761398
H	6.908219	-0.578734	-0.724378
H	5.687648	-0.648584	3.829266
H	4.925328	-2.184580	3.348089
H	4.249827	-1.232771	4.665927
H	2.061343	-1.344308	3.628170
H	2.638768	-2.163975	2.160828
H	1.751338	-0.648873	2.027241
H	3.120171	0.922685	4.311926
H	2.862098	1.559887	2.679986
H	4.493050	1.555530	3.388701
H	6.199618	2.536512	-1.725205
H	4.485672	2.927733	-1.561614
H	5.184048	2.699116	-3.166043
H	6.992539	0.373654	-2.601345
H	5.874063	0.408489	-3.956564
H	5.861791	-0.976924	-2.863200
H	2.700724	0.961838	-2.237911
H	3.366605	-0.593406	-2.694772
H	3.552561	0.803202	-3.775225
H	2.936779	3.008379	0.578512
H	2.596465	2.569928	-1.087259
H	1.097805	4.594980	0.643582
H	-1.372866	4.915791	0.858163
H	-2.878094	2.942722	0.456009
H	-7.752104	-0.604652	-0.345885
H	-6.358185	-2.890413	-0.445749
H	-1.601791	-0.428432	0.271845
H	-1.953316	0.189173	-1.319629
H	-2.057151	-3.049361	1.559556
H	-2.597776	-1.368391	1.556793
H	-3.626802	-2.605828	2.260805
H	-2.023909	-1.867814	-1.232706
H	-1.914149	-3.577203	-0.923356

H	-3.172150	-2.960400	-2.010979
H	-5.054509	-4.055676	0.988052
H	-4.758233	-4.344853	-0.744186
H	-3.536887	-4.774965	0.447008
H	-4.475963	2.426147	-1.185791
H	-5.829013	3.578041	-1.120790
H	-5.938685	2.131930	-2.138567
H	-7.965545	2.935487	-0.020818
H	-8.097034	1.518375	-1.060932
H	-8.216757	1.349585	0.706388
H	-5.947555	3.374265	1.404735
H	-4.661980	2.145964	1.493370
H	-6.265300	1.802836	2.158585
C	5.706965	-0.780041	1.084258
C	6.018206	-0.380359	-0.160727
C	3.947977	0.423247	0.307964
C	4.734395	-1.164760	3.690474
C	3.792942	-0.405884	2.740623
C	3.551907	1.003788	3.310885
C	2.477577	-1.191021	2.628336
C	2.392696	2.278588	-0.041244
C	4.896534	0.833419	-2.091744
C	5.203986	2.342452	-2.132890
C	3.542069	0.483425	-2.730176
C	5.980105	0.107148	-2.912956
C	0.903648	2.512365	0.154458
C	0.410357	3.773791	0.477845
C	-0.962426	3.947089	0.594272
C	-1.805245	2.863468	0.375384
C	-1.254190	1.628999	0.047882
C	-2.100351	0.400899	-0.246686
C	-4.482155	-0.195898	-0.063604
C	-6.692424	-0.748330	-0.261977
C	-5.994512	-1.891408	-0.309182
C	-3.606666	-2.663607	0.088526
C	-2.926506	-2.398116	1.446861
C	-2.620057	-2.761260	-1.088404
C	-4.300416	-4.035671	0.198419
C	-6.179829	1.743122	-0.013206
C	-5.558982	2.520420	-1.189628
C	-5.728412	2.304204	1.348513
C	-7.708964	1.877409	-0.104557
N	4.447886	-0.287990	1.392813
N	4.947331	0.350809	-0.669701
N	2.730423	0.920413	0.295807
N	0.084297	1.464470	-0.045696
N	-3.481574	0.614843	0.067957
N	-5.798078	0.304006	-0.103524
N	-4.632679	-1.597075	-0.170797
Cu	1.034236	-0.295465	-0.342820
Br	1.266278	-2.523889	-0.987274



Structure of 9b (atom, x-, y-, z-positions in Å):

H	-6.358005	1.800271	1.402143
H	-6.911076	0.769447	-1.014419
H	-5.849079	1.273897	3.556785
H	-5.027352	2.733482	2.951348
H	-4.424212	1.903837	4.382139
H	-2.194022	1.852071	3.410546
H	-2.711609	2.540220	1.855804
H	-1.862210	0.997169	1.892602
H	-3.338921	-0.299919	4.289327
H	-3.048342	-1.108536	2.740367
H	-4.699353	-0.991783	3.389940
H	-6.259439	-2.441040	-1.682639
H	-4.566846	-2.861205	-1.408505
H	-5.192577	-2.771218	-3.056255
H	-6.946957	-0.346372	-2.793577
H	-5.779775	-0.553559	-4.090901
H	-5.759769	0.934517	-3.141737
H	-2.695633	-1.034887	-2.202087
H	-3.285382	0.499123	-2.813974
H	-3.483856	-0.978042	-3.779226
H	-3.058149	-2.765913	0.811201
H	-2.695635	-2.504799	-0.886593
H	-1.237540	-4.366676	1.043159
H	1.224994	-4.688704	1.329632
H	2.759467	-2.775533	0.769167
H	7.652900	0.615936	-0.586869
H	6.262094	2.878202	-0.935869
H	1.535198	0.567634	0.284193
H	1.855047	-0.163737	-1.265738
H	2.098351	3.327544	1.296286
H	2.590164	1.636155	1.424973
H	3.692987	2.900360	1.946949
H	1.846008	1.888910	-1.341017
H	1.834648	3.624428	-1.233611
H	2.991364	2.821015	-2.308956
H	5.064569	4.199297	0.455071
H	4.670604	4.320701	-1.277400
H	3.528202	4.892560	-0.068002
H	4.358360	-2.478952	-0.905992
H	5.711834	-3.617362	-0.719893
H	5.798828	-2.319530	-1.922866
H	7.873799	-2.842231	0.245212

H	7.984297	-1.582745	-0.982381
H	8.141013	-1.171695	0.741742
H	5.891242	-3.078641	1.754661
H	4.600849	-1.853080	1.701295
H	6.214698	-1.419192	2.284541
C	-5.773242	1.121841	0.812231
C	-6.049106	0.606708	-0.398146
C	-4.021322	-0.197357	0.230694
C	-3.926850	0.874413	2.567597
C	-4.877335	1.749329	3.401405
C	-3.741486	-0.473809	3.287985
C	-2.588081	1.613103	2.418484
C	-2.497975	-2.110123	0.125899
C	-4.889286	-0.817855	-2.154395
C	-5.242725	-2.314668	-2.064034
C	-3.499575	-0.570244	-2.765358
C	-5.914580	-0.144741	-3.087917
C	-1.014439	-2.341233	0.364231
C	-0.538867	-3.571059	0.812422
C	0.829919	-3.745407	0.968264
C	1.688737	-2.695340	0.662608
C	1.156077	-1.493520	0.209891
C	2.014586	-0.303024	-0.183229
C	4.397153	0.272498	-0.129212
C	6.598045	0.778147	-0.478699
C	5.901600	1.910067	-0.650192
C	3.545317	2.754439	-0.216466
C	2.940710	2.639372	1.197238
C	2.491854	2.758984	-1.338435
C	4.264712	4.116591	-0.283745
C	6.089421	-1.653341	0.126467
C	5.441045	-2.577118	-0.922239
C	5.665456	-2.026496	1.559629
C	7.616141	-1.804871	0.022244
N	3.396982	-0.507401	0.130802
N	-0.179399	-1.325810	0.079384
N	-2.820063	-0.721808	0.319904
N	-4.981215	-0.198428	-0.789068
N	-4.540821	0.632597	1.217985
N	5.708657	-0.237263	-0.146264
N	4.544434	1.647783	-0.421603
Cu	-1.065832	0.397182	-0.413998
Cl	-1.304831	2.432993	-1.226115

Electronic Supplementary Information for Dalton Transactions

Structure of MeCN (atom, x-, y-, z-positions in Å):

H	-1.55395455	1.02204545	-0.06904545
H	-1.55395455	-0.57195455	-0.85004545
H	-1.55395455	-0.45095455	0.91995455
C	0.28104545	0.00004545	-0.00004545
C	-1.17595455	0.00004545	-0.00004545
N	1.43304545	0.00004545	-0.00004545

Structure of *t*BuNC (atom, x-, y-, z-positions in Å):

H	0.000000	1.496837	-1.826343
H	1.296299	-0.748419	-1.826343
H	-1.296299	-0.748419	-1.826343
H	0.885635	1.986503	-0.369122
H	1.277545	-1.760234	-0.369122
H	-2.163180	-0.226269	-0.369122
H	-0.885635	1.986503	-0.369122
H	2.163180	-0.226269	-0.369122
H	-1.277545	-1.760234	-0.369122
C	0.000000	0.000000	2.357934
C	0.000000	0.000000	-0.258267
C	-1.266843	-0.731412	-0.734229
C	1.266843	-0.731412	-0.734229
C	0.000000	1.462824	-0.734229
N	0.000000	0.000000	1.187412

Structure of XyNC (atom, x-, y-, z-positions in Å):

H	2.182706	2.138256	-0.000086
H	3.408785	-0.009761	-0.000323
H	2.170400	-2.150749	-0.000173
H	-1.168464	2.612687	0.877877
H	-1.167982	2.612966	-0.877808
H	0.163720	3.381921	0.000505
H	0.144286	-3.382806	0.000212
H	-1.183188	-2.606062	-0.877673
H	-1.183220	-2.606038	0.878006
C	-0.435874	0.001247	0.000218
C	0.241177	1.233920	0.000168
C	1.635615	1.202188	-0.000039
C	2.324674	-0.006667	-0.000161
C	1.628706	-1.211549	-0.000077
C	0.234102	-1.235271	0.000151
C	-0.520500	2.532564	0.000204
C	-0.535025	-2.529518	0.000176
C	-2.998576	0.008734	-0.000637
N	-1.824384	0.005232	0.000318