Supplementary Information (SI) for Dalton Transactions.
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$[Cu_2(\mathbf{NBDA})(\mu\text{-}Cl)]^-$ (**1**) (Electronic Energy: -5429.727040 Hartree)

Atom	X (Å)	Y (Å)	Z (Å)
Cu1	1.609568	-0.54762	0.109026
Cu2	-1.60971	-0.54782	0.109048
Cl3	0	-1.99778	0.450409
O4	-4.65319	2.085957	-0.41639
O5	4.653263	2.085609	-0.4175
N6	-1.15157	1.624848	-0.36866
N7	1.151618	1.624788	-0.3688
N8	3.414362	0.17188	-0.06588
N9	-3.41436	0.171971	-0.06604
C10	0.000049	3.689642	-0.8487
C11	5.181284	-0.66548	1.393316
C12	4.375012	-1.36224	-2.27561
H13	3.329958	-1.09447	-2.10651
C14	5.0309	-1.43825	-0.91205
C15	-3.59321	1.459174	-0.32029
C16	0.000026	2.314644	-0.52932
C17	4.561409	-0.63132	0.135336
C18	6.264456	-1.51372	1.582288
H19	6.750185	-1.55381	2.549733
C20	2.297923	2.243296	-0.51039
C21	3.593259	1.458981	-0.32072
C22	-2.29786	2.243422	-0.51013
C23	4.633207	0.163917	2.537762
H24	4.130864	1.025833	2.100827
C25	-4.56131	-0.63124	0.135557
C26	6.118604	-2.27117	-0.68085
H27	6.490799	-2.90034	-1.47999
C28	-2.39202	3.615966	-0.8285
H29	-3.38001	4.042179	-0.92377
C30	6.736266	-2.313	0.556041
H31	7.583065	-2.9686	0.720915
C32	-1.24722	4.331404	-0.99711
C33	2.392123	3.615849	-0.82876
C34	-4.63172	0.163098	2.538344
H35	-4.12863	1.024579	2.101428
C36	-5.18042	-0.66586	1.393882
C37	1.247344	4.331344	-0.99724
C38	-5.03146	-1.4378	-0.91186
C39	-6.73589	-2.3131	0.556994
H40	-7.58255	-2.96881	0.72214
C41	-6.26346	-1.5142	1.583228
H42	-6.74855	-1.55468	2.550987
C43	3.5869	-0.63825	3.31639
H44	2.785339	-0.98024	2.658589

H45	3.141087	-0.03163	4.108952
H46	4.044345	-1.51898	3.775525
C47	5.006344	-0.24159	-3.10791
H48	4.991141	0.705647	-2.56811
H49	4.474792	-0.1172	-4.05546
H50	6.050211	-0.48081	-3.33183
C51	5.713797	0.705351	3.470514
H52	6.198337	-0.08993	4.042922
H53	5.27088	1.397286	4.190729
H54	6.481738	1.239999	2.909276
C55	-6.11899	-2.2708	-0.68028
H56	-6.49169	-2.89967	-1.47941
C57	4.389057	-2.68208	-3.04231
H58	5.398078	-2.9618	-3.35659
H59	3.782603	-2.59232	-3.94637
H60	3.98198	-3.49568	-2.43948
C61	-4.37637	-1.36123	-2.27575
H62	-3.33121	-1.09358	-2.10713
C63	-5.00819	-0.24024	-3.10723
H64	-6.05219	-0.4794	-3.33059
H65	-4.47723	-0.11552	-4.05507
H66	-4.99266	0.706815	-2.56712
C67	-3.58612	-0.63993	3.317008
H68	-4.04426	-1.52035	3.776043
H69	-3.13989	-0.03372	4.109656
H70	-2.78476	-0.9825	2.659245
C71	-4.39091	-2.68074	-3.04304
H72	-3.98349	-3.49462	-2.44083
H73	-3.78502	-2.59057	-3.94743
H74	-5.40013	-2.96028	-3.35682
C75	-5.71198	0.705433	3.470956
H76	-5.26856	1.396908	4.191308
H77	-6.19737	-0.08944	4.043214
H78	-6.4793	1.240828	2.909592
H79	-1.27475	5.387254	-1.24303
H80	1.274892	5.387193	-1.24317
H81	3.380124	4.042001	-0.92414

$[Cu_2(\mathbf{NBDA})(\mu\text{-}N_3)]^-$ (**3**) (Electronic Energy: -5133.685005 Hartree)

Atom	X (Å)	Y (Å)	Z (Å)
Cu1	1.564145	0.511927	-0.00812
Cu2	-1.60784	0.478809	-0.06378
N3	3.362965	-0.20755	0.082049
N4	-3.40266	-0.26072	-0.04652
N5	1.136897	-1.73057	0.115679
C6	-2.30187	-2.38193	0.119979
N7	-1.1577	-1.74766	0.09153
C8	-4.99348	1.059509	-1.33206
C9	0.003803	-3.85666	0.23794
C10	3.567191	-1.51696	0.12739
C11	-3.59117	-1.56913	0.06119
C12	-2.39076	-3.78906	0.207776
H13	-3.37638	-4.23095	0.226978
C14	-0.00551	-2.44894	0.148349
C15	-1.2425	-4.51843	0.265874
H16	-1.26793	-5.60046	0.333848
C17	6.010507	2.159474	1.106493
H18	6.346741	2.679769	1.994766
C19	6.677288	2.363983	-0.08962
H20	7.526611	3.035346	-0.1325
C21	4.499379	0.634655	0.02194
N22	-0.04325	2.780966	-0.1873
C23	6.247136	1.709921	-1.2283
H24	6.768033	1.873019	-2.16528
N25	-0.03142	1.57449	-0.10662
C26	2.289272	-2.34803	0.16856
C27	1.258802	-4.49986	0.293324
H28	1.298824	-5.58135	0.362654
C29	2.39718	-3.75367	0.258698
H30	3.388475	-4.18143	0.295775
C31	-5.19063	0.947678	1.093518
C32	4.923029	1.300198	1.184393
C33	5.1587	0.846171	-1.1961
C34	-6.07965	1.925489	-1.35852
H35	-6.43278	2.312338	-2.30643
C36	-6.71938	2.304826	-0.19258
H37	-7.5646	2.981729	-0.2297
C38	-4.54813	0.570053	-0.09505
C39	-6.27168	1.816364	1.022141
H40	-6.77523	2.120049	1.931762
C41	4.220273	1.03865	2.500902
H42	3.180027	0.80675	2.261592
N43	-0.05468	3.909372	-0.26249
C44	-4.31535	0.612412	-2.61099

H45	-3.27518	0.397584	-2.35689
C46	4.410819	1.138986	-3.58936
H47	5.308656	1.677785	-3.9029
H48	3.670289	1.875308	-3.27236
H49	4.01835	0.613568	-4.4636
C50	4.71226	0.148003	-2.46448
H51	3.782139	-0.37221	-2.23663
C52	-4.66901	0.461896	2.431611
H53	-4.18024	-0.49618	2.259951
C54	5.735731	-0.90249	-2.89969
H55	5.378446	-1.44743	-3.77786
H56	5.909071	-1.61395	-2.09187
H57	6.688735	-0.43275	-3.16036
C58	-4.94149	-0.69089	-3.11736
H59	-4.94191	-1.45538	-2.33991
H60	-4.39591	-1.07007	-3.98591
H61	-5.97987	-0.51884	-3.41589
C62	4.817302	-0.19486	3.185864
H63	4.818675	-1.05574	2.516864
H64	4.251893	-0.44867	4.086755
H65	5.853373	0.001029	3.477421
C66	-4.30684	1.673452	-3.70841
H67	-3.90325	2.619511	-3.34343
H68	-5.30863	1.860413	-4.10398
H69	-3.68735	1.338699	-4.54344
C70	-5.76709	0.220732	3.464485
H71	-6.23874	1.152358	3.787613
H72	-5.34336	-0.25159	4.353837
H73	-6.54221	-0.43498	3.0647
C74	4.214783	2.235392	3.448201
H75	5.21379	2.456491	3.833141
H76	3.576793	2.023719	4.309138
H77	3.833933	3.13145	2.955088
C78	-3.61427	1.432491	2.970102
H79	-2.79995	1.560945	2.254039
H80	-3.18836	1.065139	3.907386
H81	-4.05737	2.414532	3.156424
O82	-4.6565	-2.19021	0.122273
O83	4.640839	-2.12753	0.143049

$[Cu_2(\mathbf{NBDA})(XylNC)_2]^-$ (**4**) (Electronic Energy: -5775.650169 Hartree)

Atom	X (Å)	Y (Å)	Z (Å)
Cu1	1.27382	-0.44342	-0.99628
Cu2	-1.32854	-0.88861	0.631094
O3	4.606381	-2.65534	-1.47643
N4	3.203953	-0.88375	-0.96895
N5	1.137162	-2.52579	-0.91823
N6	0.567466	0.724343	2.319584
N7	-1.09125	-2.68794	-0.42231
N8	-3.22032	-1.28807	0.238091
O9	-4.54435	-3.1778	0.040657
C10	3.512191	-2.14467	-1.25128
C11	4.216447	0.074076	-0.73628
N12	-0.64698	1.820536	-1.48392
C13	4.402951	1.112051	-1.66758
C14	2.287692	-3.05898	-1.25725
C15	1.50286	1.196608	4.458694
C16	1.465448	1.449544	3.08517
C17	2.309139	2.359975	2.444031
C18	4.932866	0.066037	0.472005
C19	-0.16743	0.084889	1.689774
C20	-4.27929	-0.38163	0.480432
C21	0.058304	-4.66287	-1.17778
C22	2.439875	1.895355	5.204412
C23	-2.22308	-3.3512	-0.38938
C24	5.808336	1.114552	0.733225
C25	-4.70167	-0.12681	1.790182
C26	0.579875	0.191969	5.078965
C27	3.230005	3.030217	3.236299
C28	-3.47678	-2.57213	0.007312
C29	5.981582	2.149893	-0.16455
C30	0.034941	-3.29847	-0.8394
C31	-2.30317	-4.71434	-0.73633
C32	3.684224	1.068628	-3.00076
C33	0.077618	0.929489	-1.32023
C34	4.799374	-1.06219	1.47719
C35	2.243208	2.570658	0.964669
C36	-1.16539	-5.36693	-1.11227
C37	-4.80625	0.355256	-0.59725
C38	-5.64132	0.874142	2.010485
C39	5.283142	2.139956	-1.35993
C40	-4.13596	-0.89858	2.964308
C41	-6.15934	1.610545	0.96297
C42	3.296986	2.800536	4.599686
C43	-1.47278	3.454435	-3.00389
C44	-1.49557	2.887539	-1.72698

C45	3.460808	2.437106	-3.63692
C46	-4.36072	0.061789	-2.01731
C47	1.302961	-5.21466	-1.55636
C48	4.41899	0.130966	-3.96399
C49	2.414795	-4.42429	-1.58047
C50	-0.55717	2.920089	-4.06295
C51	-5.22733	-1.65364	3.722402
C52	-5.74197	1.345495	-0.33088
C53	-2.33809	3.325531	-0.70239
C54	-3.33462	0.017413	3.89178
C55	-3.19306	4.965828	-2.25189
C56	-2.34151	4.50787	-3.24425
C57	-3.19014	4.380558	-0.99725
C58	-2.33448	2.671349	0.643161
C59	6.015285	-1.99041	1.399878
C60	4.591617	-0.57068	2.909995
C61	-4.46959	1.256359	-2.96307
C62	-5.14132	-1.12315	-2.59889
H63	-1.1863	-6.41932	-1.37019
H64	1.360232	-6.26463	-1.81865
H65	3.395937	-4.79193	-1.84456
H66	2.501241	1.719743	6.271
H67	6.368258	1.117679	1.660702
H68	0.724612	0.150108	6.156969
H69	0.758936	-0.8055	4.671003
H70	-0.46555	0.436549	4.880383
H71	3.911775	3.728002	2.76751
H72	6.668233	2.95724	0.058445
H73	-3.26976	-5.19442	-0.68313
H74	2.69757	0.634377	-2.82104
H75	3.916594	-1.6417	1.20408
H76	2.457328	1.642256	0.43251
H77	2.98175	3.302533	0.643721
H78	1.252194	2.908773	0.653412
H79	-5.97262	1.079707	3.022049
H80	5.4341	2.947206	-2.06481
H81	-3.44752	-1.64288	2.565406
H82	-6.89153	2.386342	1.150267
H83	4.027977	3.329095	5.197916
H84	4.396721	2.895577	-3.96375
H85	2.972087	3.12644	-2.94415
H86	2.829716	2.334941	-4.52252
H87	-3.30768	-0.22926	-1.96047
H88	5.406942	0.533698	-4.20138
H89	3.862574	0.021219	-4.89822
H90	4.560397	-0.85602	-3.52271

H91	0.48597	2.954675	-3.74177
H92	-0.65225	3.496416	-4.9814
H93	-0.78967	1.876664	-4.28811
H94	-5.94908	-0.96779	4.172551
H95	-4.79124	-2.25207	4.525728
H96	-5.76569	-2.32072	3.048498
H97	-6.15083	1.927722	-1.14651
H98	-3.97357	0.77669	4.349077
H99	-2.5459	0.533517	3.339053
H100	-2.87099	-0.55892	4.696423
H101	-3.87007	5.784032	-2.46108
H102	-2.35402	4.967484	-4.22441
H103	-3.86799	4.73387	-0.23095
H104	-2.56619	1.608365	0.560098
H105	-3.08644	3.116606	1.291626
H106	-1.35804	2.760611	1.124817
H107	6.921956	-1.45397	1.692801
H108	6.144608	-2.36922	0.387178
H109	5.892636	-2.8386	2.078022
H110	5.471832	-0.04923	3.292059
H111	4.405943	-1.41946	3.572034
H112	3.745478	0.1115	2.983791
H113	-5.5109	1.48137	-3.2057
H114	-3.96515	1.029085	-3.90471
H115	-4.02171	2.157202	-2.54513
H116	-6.19435	-0.85185	-2.71189
H117	-5.09513	-1.99951	-1.95494
H118	-4.75395	-1.38825	-3.586

$[Cu_2(DPFN)(\mu\text{-}N_3)]^+$ (**2**) (Electronic Energy: -5128.807354 Hartree)

Atom	X (Å)	Y (Å)	Z (Å)
Cu1	-1.36748	0.642934	0.656284
C2	0.015302	-1.53031	-1.16934
C3	0.01922	-2.64913	-2.02164
C4	-1.2189	-3.17338	-2.43618
C5	-2.36868	-2.58701	-2.01232
C6	-2.27881	-1.46214	-1.16373
C7	-3.57819	-0.79267	-0.6997
C8	-3.80544	-0.95247	0.810603
C9	-4.95226	-1.56696	1.285867
C10	-5.11496	-1.67943	2.656137
C11	-4.14311	-1.1744	3.500209
C12	-3.03526	-0.56633	2.939327
C13	-3.66876	0.67708	-1.13821
C14	-4.63337	1.087043	-2.04284
C15	-4.67997	2.427508	-2.38651
C16	-3.77642	3.309185	-1.8174
C17	-2.84651	2.809594	-0.92397
F18	-4.61446	-1.44999	-1.33255
N19	-1.13738	-0.95862	-0.75534
N20	-2.8695	-0.46296	1.621975
N21	-2.79273	1.519545	-0.59909
N22	-0.01365	1.700331	1.628755
N23	-0.04873	2.850796	1.96062
N24	-0.09537	3.932821	2.303475
C25	1.261082	-3.18213	-2.4139
C26	2.407057	-2.60573	-1.96842
C27	2.310453	-1.48216	-1.11851
C28	3.603805	-0.83657	-0.61426
C29	3.758904	0.616225	-1.08495
C30	4.822913	0.977901	-1.89438
C31	4.929874	2.302087	-2.28243
C32	3.987547	3.216356	-1.8492
C33	2.963972	2.770596	-1.03405
C34	3.757498	-0.95931	0.905408
C35	4.828556	-1.64057	1.455928
C36	4.919436	-1.70526	2.835374
C37	3.950353	-1.09039	3.610626
C38	2.918686	-0.42734	2.971282
F39	4.648511	-1.54772	-1.1762
N40	1.167413	-0.96708	-0.73284
N41	2.850495	1.494034	-0.66551
N42	2.824382	-0.36795	1.645018
Cu43	1.303652	0.748877	0.546756
H44	-5.42245	2.775903	-3.09182

H45	-3.78957	4.362742	-2.05696
H46	-2.12459	3.45224	-0.43723
H47	-5.33917	0.388517	-2.4632
H48	-5.70494	-1.94202	0.611651
H49	-5.99772	-2.15953	3.056304
H50	-4.23884	-1.24453	4.574109
H51	-2.24991	-0.14067	3.550037
H52	-3.33127	-2.96457	-2.3141
H53	-1.24367	-4.03248	-3.09438
H54	1.291422	-4.04608	-3.06544
H55	3.37238	-2.98792	-2.25529
H56	5.556397	0.250742	-2.20403
H57	5.747485	2.612573	-2.91903
H58	4.043885	4.257897	-2.131
H59	2.213894	3.448063	-0.64821
H60	5.573837	-2.10118	0.826452
H61	5.742787	-2.23248	3.298312
H62	3.991199	-1.12288	4.689893
H63	2.134698	0.076793	3.522045

[Cu_2(py-np)(μ-Cl)$_2$] (Electronic Energy: -5113.938203 Hartree)

Atom	X (Å)	Y (Å)	Z (Å)
Cu1	1.292681	-1.27099	-0.00155
Cl2	-0.00055	-1.99532	-1.82939
N3	1.143478	0.961448	-0.00021
N4	3.248675	-0.63487	0.000339
C5	0	1.673905	-4E-06
C6	0	3.081101	0.000021
C7	1.251979	3.730517	-6.8E-05
H8	1.294945	4.81309	-6E-06
C9	2.393977	2.988581	-0.0002
H10	3.354492	3.481485	-0.00018
C11	2.299317	1.573754	-0.00028
C12	3.495546	0.683532	-0.00024
C13	4.794486	1.175944	-0.0006
H14	4.984621	2.238977	-0.00135
C15	5.856904	0.290832	-6.9E-05
H16	6.874388	0.659245	-0.00036
C17	5.594383	-1.06694	0.000853
H18	6.39104	-1.79771	0.001437
C19	4.274929	-1.48189	0.000962
H20	4.018999	-2.5337	0.001517
N21	-1.14348	0.961448	0.000178
N22	-3.24867	-0.63487	-0.00034
C23	-1.25198	3.730517	0.000138
H24	-1.29495	4.813091	0.000121
C25	-2.39398	2.988581	0.000243
H26	-3.35449	3.481485	0.000249
C27	-2.29932	1.573755	0.000266
C28	-3.49555	0.683532	0.000187
C29	-4.79449	1.175945	0.000461
H30	-4.98462	2.238978	0.001154
C31	-5.8569	0.290833	-0.0001
H32	-6.87439	0.659247	0.000114
C33	-5.59438	-1.06694	-0.00097
H34	-6.39104	-1.79771	-0.00157
C35	-4.27493	-1.48189	-0.00099
H36	-4.019	-2.5337	-0.0015
Cu37	-1.29268	-1.27099	0.0016
Cl38	0.000552	-1.99524	1.829464

$[Cu_2(DPFN)(\mu\text{-}Cl)]^+$ (Electronic Energy: -5424.860625 Hartree)

Atom	X (Å)	Y (Å)	Z (Å)
C1	-2.29891	-0.00091	1.796516
C2	-2.39105	-0.00265	3.204795
H3	-3.35624	-0.00328	3.684348
C4	-1.24158	-0.00346	3.932285
H5	-1.26926	-0.00479	5.01504
C6	-6.1E-05	-0.00252	3.268113
C7	1.241452	-0.0031	3.932299
H8	1.269127	-0.00442	5.015055
C9	2.390921	-0.00198	3.204817
H10	3.356107	-0.00231	3.684384
C11	2.298792	-0.00034	1.796539
C12	-4.9E-05	-0.00085	1.861058
C13	-3.59495	-2.7E-05	0.97188
C14	-3.73673	1.272692	0.126124
C15	-4.79937	2.139201	0.324285
H16	-5.54054	1.941333	1.082721
C17	-4.88661	3.262862	-0.48153
H18	-5.70573	3.958304	-0.35283
C19	-3.92289	3.48116	-1.45
H20	-3.96197	4.343626	-2.10035
C21	-2.89794	2.562006	-1.57509
H22	-2.11826	2.673232	-2.31892
C23	-3.73754	-1.27194	0.125052
C24	-4.80123	-2.13751	0.321664
H25	-5.54277	-1.93958	1.079718
C26	-4.88897	-3.26036	-0.48523
H27	-5.70889	-3.9551	-0.35778
C28	-3.92473	-3.47879	-1.45317
H29	-3.96423	-4.34064	-2.10431
C30	-2.89874	-2.56058	-1.57668
H31	-2.11856	-2.67188	-2.31998
C32	3.594849	0.00072	0.971953
C33	3.736343	1.273155	0.12574
C34	4.798765	2.14001	0.323545
H35	5.539967	1.942668	1.082084
C36	4.885734	3.263332	-0.48277
H37	5.704679	3.959031	-0.35437
C38	3.921965	3.480967	-1.45136
H39	3.960863	4.343154	-2.10209
C40	2.897233	2.561516	-1.57605
H41	2.117504	2.672222	-2.31991
C42	3.737871	-1.27146	0.125578
C43	4.801805	-2.13663	0.32261
H44	5.543227	-1.93817	1.080642

C45	4.889969	-3.25978	-0.48382
H46	5.710086	-3.95421	-0.35602
C47	3.92587	-3.47888	-1.45176
H48	3.965675	-4.34098	-2.10254
C49	2.899607	-2.56104	-1.57571
H50	2.119531	-2.6729	-2.31903
N51	-1.15594	-9.5E-05	1.152694
N52	1.155834	0.000124	1.152699
N53	-2.8082	1.484594	-0.79958
N54	-2.80854	-1.48398	-0.80011
N55	2.807778	1.484424	-0.80006
N56	2.809	-1.48415	-0.79958
F57	-4.63938	-6.4E-05	1.872921
F58	4.639227	0.001323	1.873062
Cl59	-0.00016	-0.00272	-2.83738
Cu60	-1.29953	0.000262	-0.99963
Cu61	1.299717	-0.00046	-0.99992