Electronic Supplementary Information for Dalton Transactions
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SUPPORTING INFORMATION

XYZ coordinates of the BP86 optimized complexes:

1

H	-1.491998	0.702318	-10.568750
H	-1.934265	2.395446	-10.299890
H	-0.226259	1.944582	-10.414847
C	-1.203460	1.616231	-10.040631
H	0.222022	-3.934453	-9.733245
H	0.983333	-5.198932	-8.753779
C	0.233616	-4.396108	-8.741478
H	0.933526	-1.727742	-8.997489
H	-0.744545	-4.860703	-8.562917
C	-1.181863	1.413523	-8.556510
H	-2.278509	-0.455815	-8.558631
H	-0.141004	3.250816	-8.138702
C	-1.778783	0.301111	-7.956117
C	0.896233	-2.079933	-7.968429
H	4.036309	2.507554	-7.841041
C	-0.595898	2.361287	-7.709162
C	0.553979	-3.398977	-7.671777
H	4.032957	5.180330	-7.507855
H	1.434910	-0.163479	-7.164592
H	5.577525	4.749789	-6.765332
C	1.207506	-1.199962	-6.944150
C	3.725267	2.518717	-6.797281
H	3.148214	0.445273	-6.822198
C	4.508755	4.905584	-6.558751
H	0.320666	4.760373	-6.761633
Cl	4.472052	-1.716332	-6.701364
C	-1.739615	0.147949	-6.577091
C	-0.616825	2.188349	-6.326919
C	0.505509	-3.746376	-6.318263
C	3.185590	1.367391	-6.247978
H	-2.164390	-0.709933	-6.055394
H	0.199190	-4.751577	-6.039899
H	1.291648	6.903126	-6.137363
C	3.915668	3.650027	-6.001026
H	4.419669	5.746013	-5.863554
H	3.766624	-4.098253	-5.959601
N	-1.164022	1.063156	-5.787337
C	0.274704	4.474057	-5.714206
N	1.198802	-1.556264	-5.655144
H	3.087038	-6.464696	-5.447658
C	-0.144260	3.192264	-5.359709
C	0.819835	-2.821792	-5.325503
C	0.982657	6.818437	-5.090808
C	3.656068	-4.464543	-4.939114
N	2.799611	1.293217	-4.968156
C	0.589790	5.417887	-4.733212
H	1.796169	7.181913	-4.451954
C	3.275823	-5.762626	-4.636084
C	3.608434	3.520046	-4.646020
Cl	5.819105	0.449631	-4.445825
Pt	4.723396	-1.650486	-4.327726
C	3.078094	2.335580	-4.141453
H	3.825269	4.344973	-3.972751
N	-0.225251	2.833919	-4.049371
N	3.938723	-3.571595	-3.979545
Pt	1.857599	-0.368780	-4.018504
H	-0.043861	-5.107292	-4.061530
C	0.663955	-3.083759	-3.894949
Pt	-1.014687	0.915463	-3.700192
H	2.056600	-7.989042	-3.615372
Cl	-2.102739	-1.186187	-3.578095
H	3.713325	-8.223756	-3.051494
C	0.464250	5.018084	-3.397252
C	0.153784	-4.276330	-3.389703
C	3.175914	-6.173006	-3.301306
C	2.824231	-7.584724	-2.945808
C	0.061312	3.727511	-3.091479
N	0.923559	-2.035518	-3.069245
H	0.656452	5.720973	-2.587197
C	2.916133	2.076285	-2.711187
C	3.872470	-3.936572	-2.670041
N	2.521730	0.815486	-2.380225
C	3.482923	-5.228337	-2.318262
N	4.863635	-1.795929	-2.239631
H	-0.062091	3.367675	-2.070448
H	-0.593212	-6.519408	-2.163177
H	2.474192	-7.671796	-1.912484
C	-0.154675	-4.409070	-2.035015
H	3.550950	4.002190	-1.998894
H	5.847008	-0.013801	-1.969774
C	0.531148	-2.112132	-1.791676
C	4.330106	-2.927480	-1.701377
C	3.233738	3.000635	-1.719393
H	3.456022	-5.521992	-1.272034
C	5.430549	-0.876184	-1.448644
C	-0.721898	-5.676442	-1.477111
Cl	-0.757003	0.978282	-1.327689
H	0.548948	-1.186968	-1.220787
C	0.008964	-3.271527	-1.241819
H	-1.799072	-5.551173	-1.294205
C	2.497891	0.464389	-1.090211
H	2.255803	-0.568321	-0.867613
H	-0.257926	-5.928618	-0.516049
C	4.312431	-3.103043	-0.319193
C	3.175821	2.657048	-0.365262
H	-0.308420	-3.262706	-0.199972
C	5.477084	-1.032926	-0.070649
C	2.814468	1.343658	-0.066652
H	3.867275	-3.998319	0.108818
H	5.974558	-0.274234	0.531523
C	4.894597	-2.153354	0.528779
H	4.493131	4.099583	0.528485
C	3.505673	3.653103	0.702496
H	2.770343	4.469165	0.705831
H	2.766114	0.995034	0.963162
H	3.502410	3.195619	1.696216
C	4.930432	-2.362413	2.011764
H	5.672549	-3.134138	2.261257
H	3.960292	-2.703578	2.392598
H	5.213086	-1.447549	2.541482
H	0.127494	7.492933	-4.938383

2

C	-1.509928	2.767867	-6.248716
N	-2.183977	1.536607	-5.751875
C	-1.561993	3.829358	-5.163344
N	-0.952188	3.296998	-3.906523
Pt	-1.439383	1.205783	-3.774855
Cl	-2.287548	-1.018842	-3.779157
Cl	-0.671433	1.080087	-1.515928
Cl	4.383293	-1.823715	-6.514737
Cl	6.001536	0.280940	-4.259694
C	5.281789	-4.562787	-2.860179
N	5.901412	-2.267712	-2.279089
C	5.230479	-3.498675	-1.777366
Pt	5.153724	-1.943888	-4.256583
N	4.667591	-4.034808	-4.116777
C	3.263608	2.001388	-2.831184
N	2.334144	0.922956	-2.377353
N	1.378812	-1.660336	-5.652711
C	0.450794	-2.739741	-5.197709
N	3.073147	1.037871	-5.067555
C	3.029645	2.311411	-4.297171
Pt	1.856671	-0.367788	-4.015723
C	0.685436	-3.047966	-3.731498
N	0.640481	-1.773470	-2.962787
H	4.778727	-5.479569	-2.522514
H	6.324283	-4.822307	-3.087536
H	4.190650	-3.225955	-1.547480
H	5.698167	-3.870353	-0.853554
H	0.566470	-3.641686	-5.814818
H	-0.576194	-2.367842	-5.310659
H	1.669261	-3.510831	-3.570517
H	-0.079990	-3.750351	-3.367819
H	3.149238	2.902829	-2.213131
H	4.290041	1.627895	-2.718468
H	3.796275	3.012994	-4.659796
H	2.046654	2.775855	-4.457990
H	-2.604486	4.090557	-4.937965
H	-1.056141	4.745953	-5.497289
H	-1.974798	3.142638	-7.172683
H	-0.469950	2.493989	-6.476607
H	2.735091	0.435003	-1.569205
H	1.393233	1.265134	-2.066837
H	0.833063	-1.923438	-1.966279
H	-0.330917	-1.380607	-3.023375
H	0.976783	-1.173755	-6.461299
H	2.319844	-2.002307	-5.963261
H	4.044332	0.644146	-5.008078
H	2.879997	1.189154	-6.063688
H	-2.031608	0.727003	-6.362115
H	-3.201557	1.660364	-5.670054
H	0.067598	3.389591	-3.907626
H	-1.297411	3.785983	-3.071757
H	5.748613	-1.456694	-1.670835
H	6.919146	-2.389856	-2.361786
H	3.647875	-4.127898	-4.111790
H	5.010374	-4.526291	-4.950957

3

Cl	4.125763	-1.846383	-6.458232
N	-2.458180	1.384103	-5.633033
N	1.070411	-1.544817	-5.635726
N	2.792540	0.910873	-5.447300
Cl	5.537773	0.382226	-4.009520
Pt	5.080386	-1.964574	-4.248611
N	-1.088711	3.342136	-3.465456
N	4.838839	-4.085015	-4.563922
Pt	1.849622	-0.380124	-4.021576
Pt	-1.359710	1.223631	-3.779999
Cl	-1.844332	-1.116531	-4.018797
N	0.905092	-1.664959	-2.593743
N	2.628848	0.782108	-2.403630
N	6.201516	-2.105462	-2.408112
Cl	-0.419013	1.087460	-1.566275
H	5.542217	-4.370605	-5.254706
H	-0.040256	-1.851958	-2.985654
H	3.743868	1.081102	-5.061260
H	-2.810654	0.428825	-5.785994
H	-1.794457	3.642275	-2.783179
H	6.362937	-1.123521	-2.145653
H	1.910128	-1.943112	-6.100496
H	1.791823	1.191761	-1.944067
H	-1.130119	3.966062	-4.275994
H	-3.268515	2.003113	-5.527588
H	2.325439	1.795543	-5.663117
H	3.291161	1.508708	-2.695257
H	1.379478	-2.539467	-2.354370
H	0.423189	-2.283356	-5.340801
H	7.118601	-2.524554	-2.600630
H	4.900396	-4.710261	-3.755830
H	-0.174989	3.439050	-3.012158
H	-1.934966	1.674849	-6.463703
H	0.719173	-1.118030	-1.740333
H	0.558687	-0.965308	-6.307236
H	3.125302	0.195326	-1.726772
H	2.961125	0.381635	-6.314525
H	5.781094	-2.597709	-1.615377
H	3.921836	-4.194738	-5.007641

2 (with restrained angles)

Pt	3.760248	0.014197	-0.007461
Pt	0.659036	0.977137	-1.062203
Pt	-2.435384	1.947269	-2.121645
Cl	2.872944	-0.505666	2.120110
Cl	-1.997785	4.147853	-1.380531
Cl	-1.544194	2.458507	-4.249909
Cl	3.329106	-2.185789	-0.752320
N	-3.287576	1.319894	-0.221036
N	-0.012518	1.023586	0.970099
N	0.164017	-1.074486	-1.462254
N	-2.901368	-0.106342	-2.653970
N	4.220244	2.069240	0.529095
N	1.153416	3.029852	-0.659733
N	1.330394	0.930800	-3.093650
N	4.608129	0.648256	-1.907666
C	-3.360122	-0.167245	-0.214964
C	-3.799135	-0.651311	-1.590135
C	0.678296	2.184647	1.625318
C	0.704813	-1.428897	-2.824146
C	0.617265	3.380729	0.704732
C	0.648148	-0.235642	-3.748899
C	5.122375	2.612821	-0.531455
C	4.682012	2.135519	-1.908331
H	6.132508	2.238235	-0.317542
H	5.172443	3.710825	-0.506577
H	5.382684	2.510720	-2.669627
H	3.685679	2.527688	-2.166334
H	4.186329	0.251614	-2.752900
H	5.557184	0.246765	-1.884164
H	3.382207	2.637276	0.665237
H	4.698182	2.050199	1.439574
H	0.278488	0.153693	1.452557
H	-1.027439	1.123149	1.033892
H	1.697170	1.830239	1.840869
H	0.207465	2.419329	2.591771
H	1.149988	4.243955	1.127421
H	-0.427693	3.684947	0.531291
H	2.145283	3.254396	-0.768799
H	0.634010	3.596510	-1.360042
H	-0.828846	-1.297173	-1.356833
H	0.679398	-1.640719	-0.758894
H	2.346027	0.839425	-3.156368
H	1.032742	1.798569	-3.576277
H	-0.369848	0.114458	-3.974760
H	1.127584	-0.473270	-4.710471
H	1.748646	-1.733563	-2.646214
H	0.172171	-2.292458	-3.246184
H	-4.061115	-0.540255	0.547172
H	-2.363677	-0.557693	0.045286
H	-3.841908	-1.750122	-1.610919
H	-4.812206	-0.285398	-1.804740
H	-3.382777	-0.088408	-3.562668
H	-2.062556	-0.672384	-2.793836
H	-4.236858	1.720396	-0.248539
H	-2.867906	1.720246	0.623464