Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Photophysical properties of iminopyrrolyl boron complexes: a DFT interpretation

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Computational studies - Coordinates of optimized ground and singlet excited states

Compound A (S_0)

N	-0.73380	-1.41377	0.13120
N	-2.68435	-0.05814	0.10073
C	-0.41019	-0.06799	0.02894
H	1.54621	1.00387	-0.07011
C	0.41409	-2.11444	0.17802
H	0.41887	-3.19537	0.26735
H	2.55295	-1.50816	0.10284
C	1.50669	-1.22246	0.09530
C	-4.20128	1.64237	-0.81400
C	-6.33262	0.48320	0.55663
H	-7.16160	0.02252	1.09262
C	0.99110	0.07562	0.00504
H	-3.38435	2.06566	-1.39714
C	-1.58928	0.68620	0.00236
C	-5.06260	-0.08253	0.65232
C	-3.98119	0.50249	-0.02155
C	-6.54501	1.63150	-0.20889
H	-7.53998	2.06903	-0.28056
C	-5.47271	2.20531	-0.89649
H	-5.62878	3.08505	-1.51977
H	-4.89314	-0.96189	1.26868
H	-1.63921	1.77022	-0.07790
B	-2.28816	-1.64582	0.22135
C	-2.85934	-2.44001	-1.06667
C	-2.12220	-2.51963	-2.26300
C	-4.12861	-3.04902	-1.06217
C	-2.61821	-3.17475	-3.39355
C	-4.63602	-3.70417	-2.18701
C	-3.88054	-3.77059	-3.35974
H	-1.13165	-2.06408	-2.31517
H	-4.73324	-3.02307	-0.15467
H	-2.01668	-3.22020	-4.30222
H	-5.62262	-4.16679	-2.14617
H	-4.27154	-4.28395	-4.23881
C	-2.65522	-2.25638	1.67733
C	-2.80226	-3.64447	1.85556
C	-2.72027	-1.45646	2.83339
C	-3.01456	-4.20556	3.11865
C	-2.93764	-2.00517	4.09930
C	-3.08725	-3.38644	4.24679
H	-2.75366	-4.30184	0.98614

H	-2.60209	-0.37447	2.74646
H	-3.12629	-5.28561	3.22001
H	-2.98851	-1.35396	4.97256
H	-3.25796	-3.81965	5.23270

Compound A (S_1)

N	-0.761246000	-1.435794000	0.107709000
N	-2.667959000	-0.043491000	0.018078000
C	-0.380400000	-0.119320000	-0.096630000
H	1.643670000	0.840729000	-0.298800000
C	0.356917000	-2.192315000	0.195739000
H	0.310964000	-3.262123000	0.365632000
H	2.527533000	-1.698358000	0.061957000
C	1.498027000	-1.358329000	0.035094000
C	-4.105312000	1.916561000	-0.278780000
C	-6.328027000	0.277818000	0.203566000
H	-7.193633000	-0.355623000	0.392277000
C	1.049330000	-0.053142000	-0.151175000
H	-3.257368000	2.564915000	-0.477080000
C	-1.498923000	0.714433000	-0.170916000
C	-5.064912000	-0.280079000	0.227502000
C	-3.907526000	0.521582000	-0.014404000
C	-6.505475000	1.648049000	-0.060666000
H	-7.504764000	2.080094000	-0.081063000
C	-5.381812000	2.452965000	-0.299337000
H	-5.510053000	3.514893000	-0.507225000
H	-4.934973000	-1.335966000	0.439534000
H	-1.501089000	1.783457000	-0.317522000
B	-2.319682000	-1.619799000	0.204846000
C	-2.879126000	-2.472099000	-1.066895000
C	-2.291965000	-2.304366000	-2.335551000
C	-3.956687000	-3.371372000	-0.983544000
C	-2.746534000	-2.998617000	-3.458843000
C	-4.422181000	-4.072575000	-2.100241000
C	-3.816900000	-3.889340000	-3.344591000
H	-1.451672000	-1.616470000	-2.451295000
H	-4.440498000	-3.543233000	-0.020283000
H	-2.264230000	-2.844872000	-4.424833000
H	-5.256967000	-4.766408000	-1.995535000
H	-4.175213000	-4.435355000	-4.217771000
C	-2.711489000	-2.188353000	1.673280000
C	-2.611576000	-3.567237000	1.943551000
C	-3.049727000	-1.354816000	2.754468000
C	-2.851102000	-4.089184000	3.217595000
C	-3.298401000	-1.865933000	4.031450000
C	-3.201675000	-3.238427000	4.268456000
H	-2.348002000	-4.252716000	1.136186000
H	-3.122492000	-0.276607000	2.601925000
H	-2.767793000	-5.163021000	3.388816000
H	-3.565547000	-1.188998000	4.843647000
H	-3.395211000	-3.641236000	5.263036000

Compound B (S_0)

N	-0.08336	0.51181	18.11648
N	-1.90705	0.43696	16.59691
C	-1.93024	1.59984	17.35529
C	1.89279	-0.60183	13.29323
H	2.49896	-0.62809	12.38735
C	-3.02807	2.39200	16.96419
H	-3.31058	3.35505	17.37382
C	0.32258	-0.53933	15.65903
C	-2.94659	0.47778	15.74384
H	-3.13563	-0.32271	15.03682
C	-3.66889	1.67536	15.94739
H	-4.55903	1.97254	15.40388
C	0.19773	-1.58010	14.71963
H	-0.51458	-2.38518	14.90640
C	2.07998	-0.52106	18.56399
H	2.10081	-0.89170	17.54292
C	2.03258	0.44661	14.20562
H	2.74876	1.24614	14.01398
C	-1.11155	-1.88438	17.58983
C	1.25322	0.47422	15.36469
H	1.37976	1.30777	16.05827
C	0.99047	0.25023	18.99587
C	1.00274	0.75698	20.30672
H	0.14379	1.30531	20.68943
C	-0.84731	1.59284	18.24025
H	-0.61861	2.37728	18.95823
C	0.96747	-1.61464	13.55317
H	0.84578	-2.43727	12.84775
C	-2.37026	-2.04113	18.20004
H	-3.07109	-1.20433	18.20774
C	-0.63080	-4.20961	18.20017
H	0.05700	-5.05581	18.19105
C	-1.88727	-4.33683	18.79609
H	-2.18629	-5.27936	19.25561
C	-2.75802	-3.24517	18.79380
H	-3.74295	-3.33117	19.25404
C	-0.25449	-3.00092	17.60853
H	0.72620	-2.93206	17.13579
B	-0.66717	-0.47072	16.94046
N	4.23990	-0.51136	21.60078
N	6.06294	-0.43677	23.12112
C	6.08646	-1.59955	22.36260
C	2.26224	0.60022	26.42411
H	1.65591	0.62603	27.32989
C	7.18421	-2.39168	22.75406
H	7.46701	-3.35464	22.34441
C	3.83295	0.53880	24.05860
C	7.10208	-0.47762	23.97466
H	7.29075	0.32281	24.68183
C	7.82448	-1.67518	23.77131
H	8.71435	-1.97242	24.31524
C	3.95743	1.57921	24.99843
H	4.66963	2.38447	24.81208
C	2.07685	0.52163	21.15283

H	2.05581	0.89266	22.17376
C	2.12271	-0.44780	25.51120
H	1.40647	-1.24741	25.70231
C	5.26760	1.88476	22.12886
C	2.90237	-0.47491	24.35230
H	2.77604	-1.30817	23.65834
C	3.16622	-0.24980	20.72118
C	3.15405	-0.75647	19.41028
H	4.01309	-1.30466	19.02757
C	5.00386	-1.59244	21.47722
H	4.77538	-2.37686	20.75914
C	3.18753	1.61319	26.16480
H	3.30910	2.43550	26.87060
C	6.52629	2.04176	21.51870
H	7.22699	1.20483	21.51037
C	4.78713	4.21046	21.52021
H	4.09938	5.05669	21.52998
C	6.04364	4.33799	20.92443
H	6.34282	5.28084	20.46567
C	6.91424	3.24621	20.92586
H	7.89919	3.33246	20.46569
C	4.41068	3.00135	22.11089
H	3.42993	2.93223	22.58350
B	4.82313	0.47085	22.77740

Compound B (S_1)

N	-0.11726	0.48235	18.19666
N	-1.89367	0.39484	16.61829
C	-1.97626	1.54316	17.39559
C	2.01505	-0.57811	13.41631
H	2.64665	-0.59275	12.52767
C	-3.09979	2.30592	16.98146
H	-3.42435	3.25236	17.39787
C	0.37578	-0.54543	15.73769
C	-2.91149	0.41210	15.73695
H	-3.05573	-0.38301	15.01383
C	-3.68301	1.58598	15.93775
H	-4.56444	1.86033	15.36859
C	0.13213	-1.43582	14.67301
H	-0.70183	-2.13647	14.74188
C	1.82091	-0.84383	18.77291
H	1.62862	-1.48023	17.91561
C	2.27594	0.31946	14.45307
H	3.11319	1.01384	14.37727
C	-1.12474	-1.92559	17.59611
C	1.46270	0.33449	15.59010
H	1.68735	1.05460	16.37884
C	0.94998	0.25590	19.02111
C	1.25065	1.09112	20.14459
H	0.60719	1.92861	20.39844
C	-0.93493	1.57378	18.32081
H	-0.76127	2.35629	19.04812
C	0.93387	-1.45556	13.52906
H	0.71627	-2.16018	12.72566

C	-2.27647	-2.00371	18.40272
H	-2.85617	-1.09947	18.59947
C	-0.85094	-4.34030	17.92216
H	-0.28711	-5.25212	17.72263
C	-1.99661	-4.38663	18.71808
H	-2.33287	-5.33158	19.14571
C	-2.70990	-3.20944	18.95808
H	-3.60766	-3.23136	19.57677
C	-0.42666	-3.12613	17.37402
H	0.46490	-3.12000	16.74418
B	-0.65057	-0.49625	16.98896
N	4.27586	-0.48137	21.51907
N	6.05479	-0.39007	23.09442
C	6.14017	-1.53675	22.31499
C	2.14654	0.55665	26.30516
H	1.51615	0.56621	27.19473
C	7.26781	-2.29562	22.72515
H	7.59522	-3.24000	22.30631
C	3.78253	0.53744	23.98133
C	7.07484	-0.40462	23.97322
H	7.21759	0.38983	24.69737
C	7.85056	-1.57510	23.76871
H	8.73448	-1.84678	24.33529
C	4.02577	1.42386	25.04943
H	4.85807	2.12666	24.98236
C	2.33493	0.84196	20.94555
H	2.52683	1.47800	21.80320
C	1.88590	-0.33686	25.26485
H	1.05008	-1.03320	25.33876
C	5.27399	1.92990	22.12508
C	2.69760	-0.34534	24.12662
H	2.47306	-1.06229	23.33498
C	3.20671	-0.25696	20.69656
C	2.90532	-1.09291	19.57381
H	3.54810	-1.93110	19.32051
C	5.09723	-1.56971	21.39167
H	4.92572	-2.35126	20.66282
C	3.22572	1.43689	26.19464
H	3.44296	2.13854	27.00074
C	6.42237	2.01534	21.31448
H	7.00434	1.11389	21.11168
C	4.99093	4.34509	21.81059
H	4.42479	5.25415	22.01622
C	6.13335	4.39866	21.01048
H	6.46487	5.34657	20.58566
C	6.84964	3.22490	20.76269
H	7.74494	3.25253	20.14072
C	4.57282	3.12715	22.35511
H	3.68370	3.11523	22.98830
B	4.80712	0.49647	22.72830

Compound C (S_0)

N	-1.52068	1.00931	16.53253
N	-3.39316	0.95141	15.07253

C	-3.19211	2.22640	15.58363
C	0.02512	-1.39498	12.03249
H	0.57795	-1.71161	11.14767
C	-4.15759	3.10262	15.04937
H	-4.25896	4.16124	15.25975
C	-1.40746	-0.57544	14.34378
C	-4.44513	1.00147	14.23519
H	-4.79282	0.12233	13.70359
C	-4.94926	2.32118	14.20011
H	-5.79852	2.65427	13.61365
C	-1.72267	-1.76823	13.66682
H	-2.53284	-2.39580	14.04105
C	0.47928	-0.24856	17.14678
H	0.38142	-0.82731	16.23225
C	0.35483	-0.20243	12.68138
H	1.16680	0.41906	12.30255
C	-2.96700	-1.22022	16.52382
C	-0.35717	0.19740	13.81464
H	-0.08191	1.13602	14.29976
C	-0.46139	0.75084	17.43315
C	-0.32550	1.48214	18.62560
H	-1.07460	2.22282	18.90077
C	-2.08930	2.20717	16.44403
H	-1.70377	3.06604	16.98907
C	-1.02092	-2.17547	12.52815
H	-1.29119	-3.10682	12.02944
C	-4.22209	-1.03740	17.13406
H	-4.78132	-0.11855	16.94835
C	-2.84796	-3.40113	17.63711
H	-2.30138	-4.32541	17.82668
C	-4.09690	-3.19387	18.22635
H	-4.53164	-3.95276	18.87759
C	-4.78385	-2.00535	17.97100
H	-5.76056	-1.83072	18.42370
C	-2.29718	-2.42708	16.80048
H	-1.32642	-2.61990	16.34199
B	-2.31435	-0.07247	15.58900
N	6.11825	-0.70326	22.71308
N	7.84388	-0.66275	24.34457
C	8.11806	-1.58548	23.34419
C	3.80663	-1.10936	27.49901
H	3.17525	-1.40173	28.33852
C	9.33662	-2.23423	23.62695
H	9.81476	-3.00338	23.03112
C	5.43974	-0.34152	25.30591
C	8.84365	-0.71605	25.24330
H	8.84949	-0.08764	26.12732
C	9.79240	-1.67728	24.82715
H	10.70565	-1.92863	25.35527
C	5.30339	0.47535	26.44371
H	5.83286	1.42848	26.48276
C	0.74358	1.24705	19.47959
H	0.83692	1.84435	20.38514
C	3.92989	-1.94316	26.38483
H	3.39586	-2.89328	26.35187
C	6.65702	1.64645	23.83448
C	4.73892	-1.56195	25.31188

H	4.82036	-2.23390	24.45520
C	1.70868	0.26570	19.19181
C	1.54171	-0.47926	18.01168
H	2.24883	-1.27217	17.77263
C	7.08221	-1.56458	22.40439
H	7.03359	-2.18271	21.51053
C	4.50136	0.10129	27.52616
H	4.41701	0.75999	28.39114
C	7.89161	2.16604	23.40224
H	8.74587	1.49637	23.28674
C	5.75491	3.92122	23.68788
H	4.91117	4.60186	23.80595
C	6.99262	4.40919	23.26353
H	7.12201	5.47016	23.04757
C	8.06326	3.52425	23.12142
H	9.03584	3.89177	22.79214
C	5.59556	2.56154	23.96716
H	4.62233	2.20856	24.31072
B	6.46611	0.06534	24.11984
C	2.84773	0.02228	20.09928
C	2.73277	0.20308	21.48838
C	4.09905	-0.38285	19.60071
C	3.80305	-0.02243	22.34488
C	5.17735	-0.60394	20.44665
C	5.03924	-0.44568	21.83653
H	1.77363	0.49229	21.91505
H	4.24371	-0.47796	18.52565
H	3.67813	0.08928	23.41865
H	6.14744	-0.85274	20.01935

Compound C (S_1)

N	-1.683137000	0.954248000	16.749343000
N	-3.495618000	0.834273000	15.213597000
C	-3.510070000	2.037836000	15.906756000
C	0.292877000	-0.527775000	12.015286000
H	0.901811000	-0.630307000	11.116701000
C	-4.608030000	2.818009000	15.462906000
H	-4.882333000	3.805119000	15.816468000
C	-1.288562000	-0.264709000	14.361901000
C	-4.532985000	0.833923000	14.355082000
H	-4.729281000	-0.004074000	13.695420000
C	-5.248696000	2.050644000	14.487751000
H	-6.132589000	2.322145000	13.920999000
C	-1.594980000	-1.213666000	13.366470000
H	-2.456538000	-1.870019000	13.500780000
C	0.213921000	-0.408741000	17.396249000
H	-0.008520000	-1.090878000	16.582431000
C	0.617248000	0.424522000	12.983023000
H	1.482070000	1.073606000	12.842384000
C	-2.805738000	-1.442065000	16.342189000
C	-0.167772000	0.552733000	14.132694000
H	0.106171000	1.312509000	14.866879000
C	-0.614408000	0.731035000	17.583601000
C	-0.282494000	1.608132000	18.658780000

H	-0.881704000	2.493516000	18.854111000
C	-2.447237000	2.083068000	16.806734000
H	-2.226287000	2.907010000	17.473756000
C	-0.822351000	-1.346213000	12.210118000
H	-1.089588000	-2.092620000	11.461289000
C	-3.944898000	-1.412434000	17.169686000
H	-4.482620000	-0.472285000	17.309118000
C	-2.626590000	-3.836264000	16.838948000
H	-2.104093000	-4.783084000	16.698802000
C	-3.758131000	-3.775969000	17.653873000
H	-4.124702000	-4.672094000	18.155321000
C	-4.417578000	-2.555213000	17.818257000
H	-5.303498000	-2.493979000	18.451309000
C	-2.162393000	-2.684168000	16.197243000
H	-1.282632000	-2.761277000	15.555723000
B	-2.283689000	-0.082103000	15.625498000
N	6.013373000	-0.822750000	22.775596000
N	7.735357000	-0.751609000	24.414299000
C	7.920017000	-1.819279000	23.545065000
C	3.679343000	-0.369297000	27.556207000
H	3.024804000	-0.483837000	28.420651000
C	9.083289000	-2.534960000	23.926738000
H	9.485951000	-3.416697000	23.441913000
C	5.378012000	-0.065631000	25.298064000
C	8.730211000	-0.774341000	25.321405000
H	8.799122000	-0.036607000	26.113211000
C	9.589355000	-1.867643000	25.044260000
H	10.475562000	-2.127421000	25.612881000
C	5.517082000	0.744971000	26.442127000
H	6.290950000	1.514308000	26.461307000
C	0.784621000	1.346807000	19.483933000
H	0.997453000	2.052308000	20.283307000
C	3.522380000	-1.190494000	26.438269000
H	2.743769000	-1.953804000	26.426195000
C	6.817390000	1.586622000	23.623493000
C	4.364508000	-1.039732000	25.332667000
H	4.222241000	-1.702319000	24.477110000
C	1.622027000	0.206550000	19.309084000
C	1.286530000	-0.651878000	18.219824000
H	1.873894000	-1.548308000	18.037522000
C	6.906306000	-1.837124000	22.589023000
H	6.807772000	-2.565213000	21.793372000
C	4.685849000	0.599378000	27.555566000
H	4.822104000	1.246119000	28.423020000
C	7.988454000	1.826809000	22.879092000
H	8.646968000	0.991907000	22.630672000
C	6.360283000	3.992124000	23.497766000
H	5.716578000	4.835352000	23.750374000
C	7.527491000	4.199455000	22.760982000
H	7.801250000	5.202508000	22.432691000
C	8.342817000	3.107966000	22.451085000
H	9.258255000	3.255648000	21.877073000
C	6.015841000	2.703993000	23.917953000
H	5.104423000	2.571345000	24.503710000
B	6.438373000	0.076526000	24.082581000
C	2.735496000	-0.057911000	20.186470000
C	2.927346000	0.649803000	21.410694000

C	3.716638000	-1.045099000	19.877704000
C	3.989169000	0.399629000	22.245607000
C	4.785545000	-1.301201000	20.702392000
C	4.960729000	-0.586878000	21.924906000
H	2.199768000	1.394243000	21.723917000
H	3.649246000	-1.595388000	18.942293000
H	4.081181000	0.941813000	23.180852000
H	5.518580000	-2.038550000	20.385505000