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Supplementary Material

Electronically induced steric clash: synthesis of NMe_2-modified β-diketiminate-supported boron difluoride compounds

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Computational details

Atom coordinates for $^{o}L^{Ph}BF_2$ structure optimized at M06-2X/6-31+G(d,p) level.

C	0.252902	0.504872	-0.079710	C	-2.844301	3.037638	0.757949
C	0.109269	0.109862	1.253892	H	-2.283117	-4.079880	3.232329
C	1.246655	-0.163505	2.017460	H	-2.453071	-6.405155	2.375074
C	2.512559	-0.026663	1.454834	H	-3.300038	-6.827711	0.076400
C	2.657945	0.388171	0.131398	H	-3.940514	-4.906756	-1.366307
C	1.521942	0.651230	-0.633223	H	-3.747515	-2.588741	-0.506884
N	-1.180789	-0.048183	1.831770	H	-4.294785	1.166821	1.720077
C	-2.172590	0.840163	1.606317	H	-5.907024	-3.310054	1.525117
N	-1.869461	2.148010	1.356210	H	-6.652164	-2.188401	2.700368
C	-0.706181	2.797162	1.945864	H	-5.023972	-2.827735	2.988882
C	-3.515117	0.423725	1.647668	H	-6.592366	0.242394	1.676594
C	-3.859516	-0.938747	1.698328	H	-6.921007	-1.030240	0.479760
N	-5.160119	-1.322047	1.535794	H	-5.658953	0.171848	0.157610
C	-6.131146	-0.428346	0.937403	H	-3.457342	2.493364	0.037379
N	-2.908115	-1.869697	1.925991	H	-2.310645	3.831384	0.228070
C	-3.025391	-3.195723	1.424908	H	-3.500117	3.503232	1.507714
C	-2.651694	-4.274273	2.230200	H	-0.285684	2.169043	2.730369
C	-2.748349	-5.574288	1.741932	H	-1.026610	3.743968	2.393281
C	-3.222244	-5.812665	0.452240	H	0.071805	2.994701	1.198862
C	-3.585635	-4.735023	-0.354594	H	1.124559	-0.486659	3.046326
C	-3.480141	-3.431887	0.123912	H	3.389814	-0.243940	2.056176
B	-1.568863	-1.374167	2.570294	H	3.646509	0.497632	-0.302635
F	-0.580520	-2.320923	2.385698	H	1.621687	0.959039	-1.669707
F	-1.778650	-1.105206	3.923771	H	-0.634964	0.693819	-0.676604
C	-5.713729	-2.483454	2.219137				

Atom coordinates for $^{p}L^{Ph}BF_2$ structure optimized at M06-2X/6-31+G(d,p) level.

N	-0.005448	0.313624	0.071939	C	4.592768	-1.008986	-2.642064
C	-0.006554	0.117859	1.422861	C	3.869597	-0.125145	-1.847912
C	2.447760	0.126095	1.478603	H	-1.166029	0.903648	-2.235420
N	2.506626	0.321658	0.128891	H	-2.388073	-0.666963	-3.718621
C	1.204741	0.175831	2.142099	H	-2.627756	-3.058369	-3.082155
B	1.261033	1.069276	-0.464769	H	-1.605446	-3.869235	-0.964723
F	1.245701	2.369233	0.027573	H	-0.359812	-2.299486	0.493887
F	1.292385	1.027974	-1.843976	H	3.765947	0.918366	-2.124365
H	1.180047	0.278588	3.213380	H	5.063876	-0.644744	-3.549872
N	-1.184050	-0.004223	2.087679	H	5.290586	-3.034193	-2.901464
N	3.594690	0.011974	2.196165	H	4.179463	-3.850888	-0.831532
C	4.916072	0.088929	1.588065	H	2.859034	-2.288853	0.568333
C	3.537933	-0.196309	3.633258	H	4.881884	0.736012	0.711931
C	-2.476982	0.064205	1.420278	H	5.603231	0.526438	2.315194
C	-1.191200	-0.212770	3.525843	H	5.284912	-0.896893	1.282368
C	-0.708628	-0.592103	-0.767512	H	4.530129	-0.476436	3.986310
C	-0.825882	-1.943008	-0.422243	H	3.223132	0.714988	4.156206
C	-1.521871	-2.824061	-1.247187	H	2.844998	-1.005556	3.884822
C	-2.091166	-2.371826	-2.435475	H	-0.504103	-1.016665	3.808577
C	-1.955871	-1.028757	-2.790699	H	-0.907744	0.700716	4.062725
C	-1.275074	-0.140742	-1.964397	H	-2.196207	-0.500911	3.833284
C	3.252854	-0.579723	-0.677382	H	-2.407543	0.712385	0.547027
C	3.363469	-1.929668	-0.326161	H	-2.824770	-0.923813	1.097492
C	4.101722	-2.806430	-1.118282	H	-3.199420	0.496265	2.115775
C	4.720881	-2.350959	-2.280100				

Atom coordinates for $^{o}L^{Ph}BCl_2$ structure optimized at M06-2X/6-31+G(d,p) level.

C	0.432876	0.612150	-0.158077	C	2.795710	0.829463	0.297040
C	0.217760	0.193251	1.154656	C	1.719209	0.937806	-0.582249
C	1.293318	0.075724	2.035358	N	-1.107942	-0.129200	1.590259
C	2.578365	0.390350	1.603093	C	-2.109625	0.769005	1.444372

N	-1.815109	2.094575	1.292997
C	-0.735281	2.728499	2.044849
C	-3.447165	0.350383	1.470857
C	-3.794242	-1.006359	1.532071
N	-5.107963	-1.375629	1.464497
C	-6.095678	-0.472487	0.906838
N	-2.837512	-1.951943	1.680293
C	-3.109493	-3.313213	1.327892
C	-2.891404	-4.334152	2.253307
C	-3.157615	-5.654298	1.901833
C	-3.648096	-5.961338	0.632585
C	-3.857015	-4.938917	-0.291941
C	-3.580278	-3.617346	0.050829
B	-1.447488	-1.511733	2.186393
Cl	-0.163313	-2.753399	1.716567
Cl	-1.519029	-1.349920	4.087837
C	-5.645218	-2.445914	2.300573
C	-2.796286	3.004573	0.734943
H	-2.508364	-4.081536	3.238011
H	-2.981095	-6.445402	2.623678
H	-3.857641	-6.991469	0.362895
H	-4.223476	-5.169729	-1.287412
H	-3.725417	-2.814859	-0.666534
H	-4.222826	1.091965	1.583554
H	-5.879970	-3.343159	1.716658
H	-6.556810	-2.077827	2.782276
H	-4.930340	-2.707785	3.080237
H	-6.481467	0.238256	1.652349
H	-6.933749	-1.066753	0.533124
H	-5.667217	0.083206	0.071250
H	-3.368701	2.505449	-0.048509
H	-2.266945	3.851328	0.289990
H	-3.489096	3.391809	1.496415
H	-0.397365	2.069419	2.844179
H	-1.127533	3.643920	2.499461
H	0.118226	2.978076	1.404263
H	1.110459	-0.268202	3.049485
H	3.412432	0.292019	2.290647
H	3.798581	1.077020	-0.035793
H	1.880678	1.263513	-1.605173
H	-0.410640	0.678822	-0.839029

Atom coordinates for $^{p}L^{Ph}BCl_2$ structure optimized at M06-2X/6-31+G(d,p) level.

N	-0.005682	0.265445	-0.005377
C	-0.004573	0.081694	1.352176
C	2.449257	0.086923	1.408958
N	2.512415	0.271306	0.053011
C	1.206354	0.117161	2.067212
B	1.265238	0.966774	-0.560158
Cl	1.247586	2.764195	0.023163
Cl	1.308017	0.923095	-2.400883
H	1.181361	0.238794	3.135847
N	-1.180557	0.016257	2.024608
N	3.593109	0.026309	2.135173
C	4.917381	0.149488	1.538093
C	3.528337	-0.169382	3.574757
C	-2.476216	0.133475	1.366647
C	-1.181536	-0.178767	3.465738
C	-0.796875	-0.627265	-0.795372
C	-0.795485	-1.993714	-0.508387
C	-1.586143	-2.870033	-1.251029
C	-2.368813	-2.388419	-2.297301
C	-2.358267	-1.023753	-2.593143
C	-1.583162	-0.144726	-1.844734
C	3.343605	-0.617244	-0.699776
C	3.335090	-1.983895	-0.413965
C	4.163434	-2.856037	-1.119541
C	4.991720	-2.370050	-2.127976
C	4.988688	-1.005210	-2.423235
C	4.175586	-0.130320	-1.711199
H	-1.576833	0.918782	-2.060312
H	-2.962844	-0.640173	-3.409051
H	-2.979792	-3.069055	-2.881315
H	-1.578500	-3.930189	-1.017082
H	-0.169314	-2.364353	0.300034
H	4.174346	0.933316	-1.926261
H	5.628780	-0.618266	-3.209942
H	5.632312	-3.047441	-2.683329
H	4.149743	-3.916399	-0.886811
H	2.673670	-2.358025	0.364209
H	4.883347	0.861234	0.713225
H	5.596800	0.537658	2.298491
H	5.294391	-0.809281	1.164741
H	4.523682	-0.420208	3.939822
H	3.185005	0.739297	4.083839
H	2.854859	-0.993990	3.827908
H	-0.518097	-1.001399	3.750036
H	-0.864486	0.731035	3.989626
H	-2.191917	-0.432191	3.784755
H	-2.407041	0.845218	0.543980
H	-2.831225	-0.827022	0.976534
H	-3.191943	0.518741	2.094512

Atom coordinates for $^{o}L^{Ph}BBr_2$ structure optimized at M06-2X/6-31+G(d,p) level.

C	0.457728	0.595361	-0.187633
C	0.233171	0.177979	1.121735
C	1.285691	0.130452	2.035336
C	2.568370	0.481787	1.628126
C	2.799128	0.906888	0.319086
C	1.741612	0.960701	-0.587726
N	-1.096131	-0.150403	1.540069
C	-2.095418	0.754744	1.407203
N	-1.794037	2.080398	1.291923
C	-0.728718	2.686684	2.087787
C	-3.433193	0.336940	1.414051
C	-3.781971	-1.018245	1.492025
N	-5.094487	-1.389206	1.457900
C	-6.094590	-0.495186	0.907703
N	-2.821655	-1.964357	1.626857
C	-3.101293	-3.327381	1.289438
C	-2.956490	-4.329181	2.248683
C	-3.260877	-5.646255	1.921290
C	-3.735644	-5.962813	0.647739
C	-3.886645	-4.955994	-0.304658
C	-3.568690	-3.637394	0.014875
B	-1.441905	-1.523977	2.109911
Br	-0.050637	-2.871075	1.615723
Br	-1.560336	-1.311906	4.187841

C	-5.606895	-2.441524	2.333088
C	-2.763214	3.006932	0.740176
H	-2.591252	-4.062092	3.236770
H	-3.133863	-6.426587	2.664853
H	-3.978681	-6.990307	0.396556
H	-4.245234	-5.195680	-1.300822
H	-3.668207	-2.842516	-0.718714
H	-4.207316	1.079139	1.535579
H	-5.834852	-3.360277	1.780925
H	-6.518067	-2.070502	2.812767
H	-4.878290	-2.665212	3.112393
H	-6.464499	0.226985	1.650119
H	-6.939879	-1.095588	0.561403
H	-5.683906	0.046956	0.054526
H	-3.323760	2.528065	-0.064166
H	-2.223986	3.862016	0.324262
H	-3.467092	3.378014	1.499386
H	-0.431164	2.009832	2.888756
H	-1.122503	3.601612	2.541468
H	0.149793	2.931138	1.479991
H	1.085064	-0.197302	3.051888
H	3.388762	0.430395	2.336823
H	3.799705	1.186749	0.005360
H	1.914856	1.280087	-1.610642
H	-0.375294	0.619117	-0.884337

Atom coordinates for $^{p}L^{Ph}BBr_2$ structure optimized at M06-2X/6-31+G(d,p) level.

N	-0.006076	0.035167	-0.073801
C	-0.009042	-0.055324	1.288597
C	2.457915	-0.048585	1.344960
N	2.516745	0.042261	-0.016173
C	1.208921	-0.003711	1.990938
B	1.268843	0.615585	-0.707433
Br	1.255041	2.654508	-0.359504
Br	1.314780	0.259246	-2.675121
H	1.184291	0.203487	3.044882
N	-1.173120	-0.009804	1.988445
N	3.588593	0.003015	2.097177
C	4.929887	0.155353	1.542220
C	3.491857	-0.096679	3.546021
C	-2.488542	0.135294	1.372898
C	-1.142014	-0.108951	3.440224
C	-0.949852	-0.732239	-0.826969
C	-1.096246	-2.092942	-0.570741
C	-2.061321	-2.830401	-1.258627
C	-2.873428	-2.208010	-2.202737
C	-2.718010	-0.842591	-2.458736
C	-1.768084	-0.102739	-1.767164
C	3.497740	-0.720458	-0.725300
C	3.639143	-2.080401	-0.462319
C	4.638304	-2.812992	-1.105273
C	5.489512	-2.186530	-2.011488
C	5.339070	-0.821916	-2.274645
C	4.354865	-0.086860	-1.627309
H	-1.641487	0.961861	-1.941428
H	-3.348378	-0.352933	-3.194355
H	-3.621610	-2.781126	-2.740776
H	-2.171716	-3.891594	-1.057946
H	-0.447391	-2.566652	0.161900
H	4.230987	0.977082	-1.807438
H	5.999880	-0.329094	-2.980846
H	6.264339	-2.755883	-2.514682
H	4.744772	-3.873612	-0.899502
H	2.959936	-2.557370	0.240077
H	4.914558	0.858795	0.710318
H	5.566266	0.574520	2.322684
H	5.352359	-0.794954	1.199191
H	4.483895	-0.294289	3.950275
H	3.112824	0.834819	3.984044
H	2.835672	-0.920885	3.840291
H	-0.495644	-0.929710	3.764341
H	-0.788225	0.824531	3.894821
H	-2.150405	-0.311732	3.798882
H	-2.439150	0.838919	0.542480
H	-2.889772	-0.817253	1.011106
H	-3.162091	0.550900	2.123500

Atom coordinates for $^{o}L^{Ph}BI_2$ structure optimized at M06-2X/LANL2DZ level.

C	0.483508	0.633612	-0.189401
C	0.247490	0.220197	1.120373
C	1.294999	0.156666	2.037841
C	2.579418	0.518141	1.640729
C	2.819993	0.947102	0.335712
C	1.768824	1.003365	-0.578677
N	-1.086108	-0.156729	1.503348
C	-2.091494	0.748619	1.383255
N	-1.797199	2.076790	1.279887
C	-0.751787	2.693318	2.096123
C	-3.426969	0.330089	1.393792
C	-3.776809	-1.023007	1.468021
N	-5.091625	-1.386436	1.445500
C	-6.087176	-0.480476	0.904460
N	-2.816623	-1.975855	1.590408
C	-3.142798	-3.343750	1.290920
C	-2.981812	-4.339614	2.252895
C	-3.295715	-5.658418	1.936170
C	-3.773907	-5.984723	0.667387
C	-3.927667	-4.984700	-0.292061
C	-3.605909	-3.664993	0.016379
B	-1.420790	-1.548883	2.009852
I	0.136405	-3.059524	1.402118
I	-1.464185	-1.392660	4.412193
C	-5.614284	-2.418455	2.340484
C	-2.777618	2.998652	0.738081
H	-2.605226	-4.074581	3.236990
H	-3.162082	-6.433002	2.684365
H	-4.017349	-7.014084	0.424596
H	-4.284721	-5.232264	-1.286721
H	-3.703759	-2.879116	-0.726804
H	-4.200809	1.071996	1.514263
H	-5.862850	-3.339583	1.802054
H	-6.514985	-2.023998	2.821078
H	-4.887182	-2.643786	3.120591
H	-6.435946	0.250452	1.648522
H	-6.945448	-1.071550	0.574876
H	-5.682847	0.050850	0.041481
H	-3.328107	2.526175	-0.076935
H	-2.247570	3.867107	0.338757

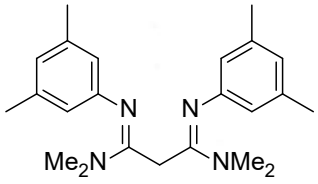
H	-3.489123	3.348243	1.500361
H	-0.452675	2.018084	2.897751
H	-1.168435	3.596685	2.552372
H	0.128736	2.959175	1.501002
H	1.096783	-0.182285	3.050918
H	3.394598	0.460329	2.354712
H	3.822807	1.227898	0.030240
H	1.950108	1.321480	-1.600471
H	-0.340871	0.655461	-0.896097

Atom coordinates for $^{p}L^{Ph}BI_2$ structure optimized at M06-2X/ LANL2DZ level.

N	-0.006344	0.147593	-0.060628
C	-0.006201	0.003937	1.304080
C	2.453275	0.009159	1.361545
N	2.516501	0.152706	-0.001732
C	1.207637	0.030570	2.011141
B	1.268262	0.766866	-0.648946
I	1.249596	3.043597	-0.048534
I	1.320976	0.666734	-2.896686
H	1.182462	0.196764	3.072844
N	-1.173822	0.019185	1.992711
N	3.587397	0.029607	2.103920
C	4.918623	0.199859	1.532802
C	3.505939	-0.123783	3.549028
C	-2.477677	0.183738	1.360141
C	-1.159275	-0.134255	3.440024
C	-0.899548	-0.686840	-0.812755
C	-0.911650	-2.060506	-0.573943
C	-1.790905	-2.886264	-1.274808
C	-2.649433	-2.341608	-2.226315
C	-2.626948	-0.966868	-2.471922
C	-1.760542	-0.139856	-1.766029
C	3.447526	-0.677716	-0.711154
C	3.454419	-2.051354	-0.471890
C	4.369140	-2.873194	-1.130683
C	5.268931	-2.324701	-2.040982
C	5.251962	-0.950061	-2.287545
C	4.349825	-0.126896	-1.623115
H	-1.740887	0.931672	-1.940526
H	-3.290486	-0.536180	-3.214968
H	-3.329860	-2.982529	-2.777545
H	-1.794123	-3.954684	-1.083075
H	-0.225717	-2.476115	0.160329
H	4.333723	0.944553	-1.798455
H	5.947703	-0.516405	-2.998726
H	5.977241	-2.962600	-2.559631
H	4.368059	-3.941608	-0.938891
H	2.736656	-2.469994	0.229498
H	4.881235	0.924958	0.719856
H	5.568268	0.599802	2.312312
H	5.334863	-0.741134	1.157273
H	4.502216	-0.334334	3.935926
H	3.129479	0.790693	4.023059
H	2.853468	-0.959620	3.818071
H	-0.516396	-0.967285	3.739184
H	-0.809432	0.781738	3.931214
H	-2.171607	-0.349296	3.779937
H	-2.405467	0.908750	0.549488
H	-2.872046	-0.759102	0.966075
H	-3.164569	0.581254	2.108344

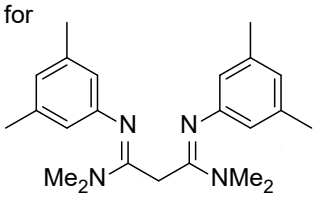
Selected NMR spectra:

^{1}H NMR for



*unidentified impurities

^{13}C NMR for



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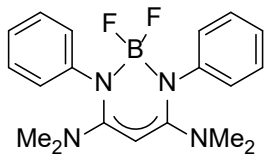

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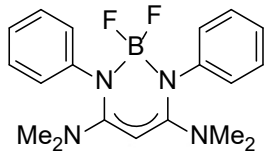

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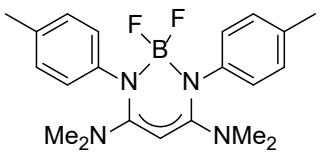

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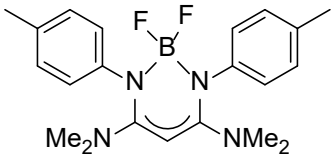

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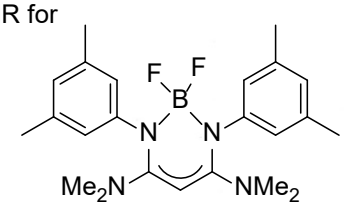

^{13}C NMR for