Electronic Supplementary Information for Dalton Transactions

Supporting Information for

Dehydrogenation reactivity of a frustrated carbene-borane Lewis pair

Dirk Holschumacher, Christina Taouss, Thomas Bannenberg, Cristian G. Hrib,

Constantin G. Daniliuc, Peter G. Jones and Matthias Tamm*

* *Institut für Anorganische und Analytische Chemie, Technische Universität Carolo-Wilhelmina, Hagenring 30, D-38106 Braunschweig, Germany.*

Fax: +49 (251) 391-5309; Tel: +49 (251) 391-5387; E-mail: m.tamm@tu-bs.de

Contents:

Electronic Supplementary Information for Dalton Transactions

1. Computational Details

All computations were performed using the hybrid density functional method M05-2X implemented in the Gaussian03 program.[1] For all main-group elements (C, H, N, B, F) the all-electron triple-ζ basis set (6-311G**) was used.[2]

[1] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, T. Ishida, M. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, GAUSSIAN 03, Revision C.02, Gaussian, Inc., Wallingford, CT, 2004.

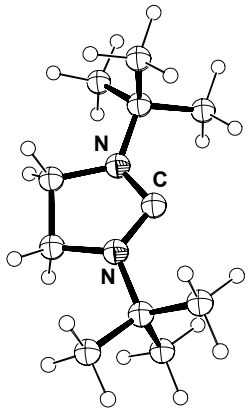
[2] X. Cao and M. Dolg, *J. Chem. Phys.* 2001, **115**, 7348.

Energies for the optimized structure:

Compound	E(0 K)[a] [Ha]	H(298 K)[b] [Ha]	G(298 K)[b] [Ha]
H_4tBu_2ImC: (**1b**)	-541.613456	-541.612512	-541.668949
$B(C_6F_5)_3$	-2208.520061	-2208.519116	-2208.608800
H_4tBu_2ImC-$B(C_6F_5)_3$ (adduct)	-2750.160193	-2750.159249	-2750.275053
$[H_4tBuImCH][HB(C_6F_5)_3]$ (**3b**)	-2751.375203	-2751.374259	-2751.499391

[a]DFT energy incl. ZPE.
[b]standard conditions T = 298.15 K and p = 1 atm.

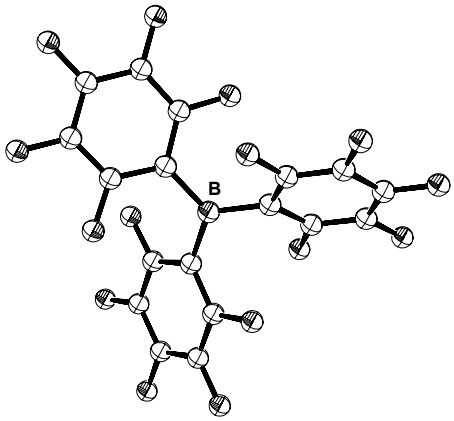
Electronic Supplementary Information for Dalton Transactions



Structure of the carbene 1b (atom, x-, y-, z-positions in Å):

N	-1.06947	-0.23621	-0.14261
N	1.06947	-0.23632	0.14270
C	2.75954	0.49057	-1.48126
C	-2.56661	1.59119	-0.75883
C	-3.41923	-0.74191	-0.60123
C	0.75652	-1.65712	-0.09361
C	-2.44491	0.27179	-0.00135
C	2.44491	0.27178	0.00133
C	0.00000	0.56438	0.00029
C	-0.75653	-1.65711	0.09361
C	3.41932	-0.74212	0.60062
C	2.56682	1.59098	0.75910
C	-2.75984	0.49010	1.48124
H	2.65639	-0.43924	-2.04376
H	2.06808	1.22637	-1.89158
H	-2.33648	1.43898	-1.81366
H	3.78131	0.85196	-1.60717
H	-3.14926	-0.96422	-1.63473
H	1.03312	-1.94763	-1.11212
H	-3.58654	1.96769	-0.66683
H	-4.42541	-0.32341	-0.58915
H	-1.26525	-2.31012	-0.61053
H	-1.86947	2.32269	-0.35974
H	-3.43877	-1.67230	-0.03218
H	3.43886	-1.67233	0.03129
H	4.42550	-0.32363	0.58854
H	1.86958	2.32258	0.36039
H	3.58676	1.96748	0.66699
H	1.26513	-2.31022	0.61055
H	-1.03313	-1.94770	1.11213
H	-3.78171	0.85151	1.60694
H	3.14955	-0.96471	1.63413
H	2.33689	1.43839	1.81403
H	-2.06847	1.22580	1.89185
H	-2.65690	-0.43979	2.04345

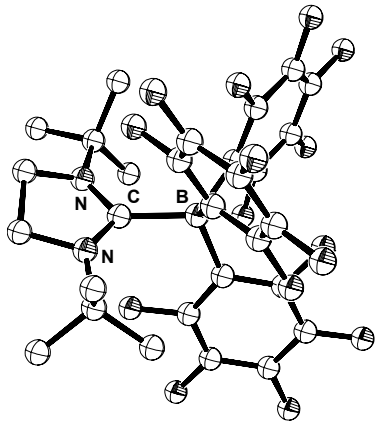
Electronic Supplementary Information for Dalton Transactions



Structure of the borane $B(C_6F_5)_3$ (atom, x-, y-, z-positions in Å):

B	0.00041	0.00233	-0.00154
C	-0.50286	-3.77681	-0.69516
C	-3.02535	2.32614	-0.68379
C	3.53271	1.44522	-0.67926
C	-0.66708	-2.40634	-0.67775
C	-1.75446	1.78741	-0.66647
C	2.42732	0.61853	-0.66270
C	0.55483	-4.33818	-0.00085
C	3.48426	2.65037	-0.00013
C	-4.04004	1.68298	0.00337
C	0.20001	-1.55056	-0.00274
C	1.24655	0.95041	-0.00240
C	-1.44443	0.60482	0.00142
C	2.33547	3.01953	0.67796
C	-3.77877	0.51030	0.69066
C	1.43862	-3.52880	0.69147
C	1.24285	2.17633	0.65903
C	-2.50024	-0.00992	0.67158
C	1.25450	-2.16055	0.67218
F	-1.34473	-4.55831	-1.36288
F	-3.28318	3.44875	-1.34578
F	4.63612	1.09805	-1.33286
F	-1.70230	-1.91510	-1.36335
F	-0.81356	2.44507	-1.34814
F	2.52532	-0.52992	-1.33642
F	4.53769	3.45098	0.00040
F	0.72070	-5.65097	0.00104
F	-5.26191	2.19087	0.00425
F	2.29572	4.17561	1.33159
F	-4.75528	-0.09853	1.35452
F	2.44904	-4.07320	1.36067
F	0.16092	2.57890	1.33003
F	-2.30185	-1.14020	1.35396
F	2.13299	-1.42521	1.35810

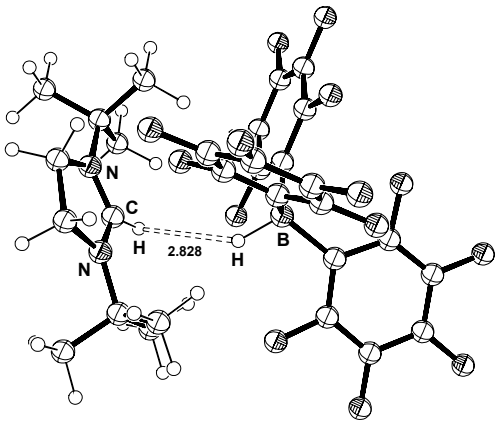
Electronic Supplementary Information for Dalton Transactions



Structure of the carbene-borane adduct 1b-B(C_6F_5)$_3$ (atom, x-, y-, z-positions in Å):

B	-0.12851	0.14048	-0.07875
N	-2.02049	0.99395	-1.92277
N	-0.16923	2.17665	-1.85808
C	-1.92445	1.59076	-3.25723
C	-0.94007	2.69301	-3.00326
C	2.42874	-0.94820	-2.89989
C	2.17757	2.59325	-2.55515
C	-4.42838	0.69449	-2.37843
C	3.66425	-0.96439	-2.28181
C	-2.99315	-1.28454	-2.12126
C	1.32023	-0.56591	-2.17473
C	0.70270	4.48291	-1.83582
C	-3.20769	0.14573	-1.62231
C	1.06634	3.00606	-1.58149
C	-0.85356	1.17071	-1.26022
C	3.74759	-0.58227	-0.95943
C	1.32768	-0.20117	-0.83040
C	2.60080	-0.21012	-0.27057
C	-0.50209	-2.58032	-0.25094
C	1.61051	2.98911	-0.15785
C	-3.54288	0.28534	-0.13844
C	-0.90205	-3.82411	0.21009
C	-0.83440	-1.35510	0.33524
C	-1.68915	-3.92220	1.33490
C	-0.01925	0.90588	1.37040
C	-1.62628	-1.53541	1.47870
C	-0.66850	2.09107	1.67468
C	-2.05784	-2.75599	1.96851
C	0.58590	0.29132	2.46197
C	-0.67396	2.67139	2.92962
C	0.61187	0.83510	3.73149
C	-0.01900	2.04192	3.96825
H	-1.54043	0.84150	-3.95345
H	-0.29244	2.88449	-3.85324
H	-2.87319	1.97262	-3.60828
H	-4.38567	0.50599	-3.45031
H	1.79562	2.41103	-3.55939
H	-2.84234	-1.27935	-3.20189
H	0.52622	4.71489	-2.88403
H	-1.45063	3.61331	-2.71937

H	2.91254	3.39689	-2.61212
H	-4.56261	1.76066	-2.19290
H	2.68635	1.69824	-2.21167
H	-5.30313	0.17464	-1.98826
H	-3.88091	-1.88052	-1.90605
H	1.54657	5.08717	-1.50706
H	-2.13526	-1.75610	-1.66733
H	-0.16722	4.76897	-1.24426
H	2.56749	3.51196	-0.18836
H	-4.16670	1.16638	0.01379
H	-4.08487	-0.59092	0.21723
H	1.79300	2.00577	0.24086
H	0.95674	3.53684	0.51557
H	-2.66353	0.41973	0.46789
F	2.31791	-1.29069	-4.18395
F	4.75337	-1.32152	-2.95420
F	0.16029	-0.57915	-2.86344
F	0.19441	-2.65639	-1.39632
F	-0.54759	-4.92650	-0.44919
F	4.93326	-0.55413	-0.35280
F	-1.34777	2.77149	0.72347
F	2.83106	0.22056	0.97850
F	-2.09220	-5.10347	1.78781
F	-2.05410	-0.50282	2.23160
F	1.12040	-0.93221	2.33982
F	-2.82282	-2.80725	3.05851
F	-1.29477	3.83461	3.13810
F	1.21150	0.19525	4.73408
F	-0.00620	2.58284	5.18298



Structure of the ion pair (3b) (atom, x-, y-, z-positions in Å):

B	-0.77018	0.01306	-0.03990
N	2.71877	1.66224	-1.91913
N	3.86977	0.05681	-0.93025
C	2.53083	3.28055	-3.73565
C	1.03820	1.28113	-3.66776
C	1.74824	2.33346	-2.82361
C	-3.96547	0.42865	-2.30262
C	0.74520	3.11505	-1.97534

C	-4.91452	-0.31666	-1.63149
C	2.90951	0.37472	-1.76882
C	-2.68872	0.52973	-1.77619
C	3.82413	-2.32019	-1.54123
C	3.59702	2.40147	-0.99506
C	5.77678	-1.33755	-0.34637
C	4.25512	-1.30640	-0.48632
C	-4.57412	-0.94081	-0.44464
C	-2.29495	-0.08399	-0.60042
C	0.26465	-2.33298	-0.54688
C	4.40758	1.28137	-0.31065
C	0.73963	-3.60121	-0.26328
C	-3.28667	-0.81075	0.04089
C	-0.23126	-1.46193	0.40935
C	3.58903	-1.60727	0.85647
C	0.74202	-4.04147	1.04633
C	-0.54204	1.14195	1.11822
C	0.75463	1.53752	1.39111
C	-0.22033	-1.95259	1.70690
C	-1.50743	1.83123	1.83642
C	0.25493	-3.21137	2.03923
C	1.10557	2.54984	2.25951
C	-1.20636	2.84693	2.73269
C	0.10874	3.21685	2.94460
H	1.84284	3.72475	-4.45395
H	3.30289	2.73959	-4.28440
H	0.32865	1.78958	-4.31785
H	1.74727	0.74021	-4.29811
H	2.99222	4.09377	-3.17536
H	0.46935	0.58531	-3.05390
H	0.00743	3.57359	-2.63283
H	4.28316	-2.09697	-2.50583
H	2.32367	-0.36383	-2.29109
H	4.23126	3.08738	-1.55103
H	2.74423	-2.36748	-1.65883
H	6.26019	-1.05666	-1.28297
H	1.23826	3.91102	-1.41554
H	4.15284	-3.30923	-1.22602
H	0.22262	2.45265	-1.28903
H	-0.06473	0.35286	-0.95758
H	5.47294	1.36189	-0.51112
H	6.08467	-2.34977	-0.08844
H	2.99726	2.95618	-0.27857
H	6.12072	-0.67556	0.44830
H	4.23276	1.26164	0.76233
H	2.50643	-1.54387	0.76926
H	3.86274	-2.61321	1.17634
H	3.91470	-0.90672	1.62546
F	-4.28626	1.03915	-3.44829
F	-1.81895	1.28282	-2.48509
F	-6.14946	-0.42995	-2.12047
F	0.34748	-1.95077	-1.84490
F	1.23585	-4.38327	-1.23104
F	-5.49111	-1.65318	0.21358
F	1.78957	0.92368	0.76074
F	1.21864	-5.24954	1.34860
F	-3.01933	-1.41406	1.20888

F	-2.80681	1.54456	1.69421
F	2.39594	2.89385	2.41909
F	-0.67921	-1.20690	2.71891
F	0.25223	-3.63400	3.30437
F	-2.17661	3.48074	3.39241
F	0.40973	4.19950	3.79287