SUPPORTING INFORMATIONS of COMPUTATIONS

Planar, Twisted and Trans-Bent: Conformational Flexibility of Neutral Diborenes

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Supporting information:

All the computational methods employed Gaussian03 suite of program.
Gaussian-03 reference:

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

The Optimized geometry of **3c**:

1	5	0	0.118898	-0.429964	0.667322
2	1	0	1.107355	-0.384262	1.345722
3	7	0	-0.643222	-2.182308	2.444355
4	7	0	-2.109038	-1.901315	0.858114
5	6	0	-0.862902	-1.449977	1.277079
6	6	0	-1.710338	-3.026084	2.715732
7	1	0	-1.723651	-3.667042	3.579995
8	6	0	-2.618783	-2.851285	1.731037
9	1	0	-3.580264	-3.306971	1.570000
10	6	0	-2.852145	-1.493497	-0.302906
11	6	0	-2.684240	-2.195060	-1.503619
12	6	0	-3.506588	-1.858588	-2.582739
13	1	0	-3.389304	-2.400936	-3.516373
14	6	0	-4.467368	-0.853849	-2.493464
15	6	0	-4.589231	-0.162217	-1.287027
16	1	0	-5.323051	0.634694	-1.202973
17	6	0	-3.792267	-0.457933	-0.181742
18	6	0	-3.959298	0.342194	1.088446
19	1	0	-3.262211	0.032832	1.864152
20	1	0	-4.977066	0.246333	1.479992

21	1	0	-3.778371	1.402054	0.890006
22	6	0	-5.356506	-0.512620	-3.665467
23	1	0	-5.139722	-1.148235	-4.526530
24	1	0	-5.218080	0.528390	-3.971220
25	1	0	-6.413334	-0.641877	-3.411176
26	6	0	-1.655828	-3.287118	-1.672038
27	1	0	-1.064953	-3.438586	-0.771525
28	1	0	-0.964942	-3.026294	-2.478291
29	1	0	-2.132987	-4.236542	-1.936457
30	6	0	0.502275	-2.127714	3.312450
31	6	0	1.585239	-2.986312	3.079052
32	6	0	2.623461	-3.009539	4.015210
33	1	0	3.462817	-3.677610	3.845029
34	6	0	2.607726	-2.210864	5.157137
35	6	0	1.524462	-1.350092	5.343834
36	1	0	1.499872	-0.708191	6.220117
37	6	0	0.465159	-1.287109	4.437909
38	6	0	-0.676716	-0.332139	4.697156
39	1	0	-1.358779	-0.268882	3.852091
40	1	0	-0.292664	0.672858	4.890864
41	1	0	-1.249734	-0.639154	5.578200
42	6	0	3.723993	-2.273461	6.173434
43	1	0	4.517705	-2.950369	5.850750
44	1	0	3.356003	-2.628350	7.141434
45	1	0	4.167671	-1.287101	6.337672
46	6	0	1.663058	-3.882561	1.866871
47	1	0	0.845450	-3.705637	1.171791
48	1	0	1.645213	-4.937360	2.159945
49	1	0	2.598548	-3.707277	1.328746
50	5	0	-0.118898	0.429964	-0.667322
51	1	0	-1.107355	0.384262	-1.345722
52	7	0	0.643222	2.182308	-2.444355
53	7	0	2.109038	1.901315	-0.858114
54	6	0	0.862902	1.449977	-1.277079
55	6	0	1.710338	3.026084	-2.715732
56	1	0	1.723651	3.667042	-3.579995
57	6	0	2.618783	2.851285	-1.731037
58	1	0	3.580264	3.306971	-1.570000
59	6	0	2.852145	1.493497	0.302906
60	6	0	2.684240	2.195060	1.503619
61	6	0	3.506588	1.858588	2.582739

62	1	0	3.389304	2.400936	3.516373
63	6	0	4.467368	0.853849	2.493464
64	6	0	4.589231	0.162217	1.287027
65	1	0	5.323051	-0.634694	1.202973
66	6	0	3.792267	0.457933	0.181742
67	6	0	3.959298	-0.342194	-1.088446
68	1	0	3.262211	-0.032832	-1.864152
69	1	0	4.977066	-0.246333	-1.479992
70	1	0	3.778371	-1.402054	-0.890006
71	6	0	5.356506	0.512620	3.665467
72	1	0	5.139722	1.148235	4.526530
73	1	0	5.218080	-0.528390	3.971220
74	1	0	6.413334	0.641877	3.411176
75	6	0	1.655828	3.287118	1.672038
76	1	0	1.064953	3.438586	0.771525
77	1	0	0.964942	3.026294	2.478291
78	1	0	2.132987	4.236542	1.936457
79	6	0	-0.502275	2.127714	-3.312450
80	6	0	-1.585239	2.986312	-3.079052
81	6	0	-2.623461	3.009539	-4.015210
82	1	0	-3.462817	3.677610	-3.845029
83	6	0	-2.607726	2.210864	-5.157137
84	6	0	-1.524462	1.350092	-5.343834
85	1	0	-1.499872	0.708191	-6.220117
86	6	0	-0.465159	1.287109	-4.437909
87	6	0	0.676716	0.332139	-4.697156
88	1	0	1.358779	0.268882	-3.852091
89	1	0	0.292664	-0.672858	-4.890864
90	1	0	1.249734	0.639154	-5.578200
91	6	0	-3.723993	2.273461	-6.173434
92	1	0	-4.517705	2.950369	-5.850750
93	1	0	-3.356003	2.628350	-7.141434
94	1	0	-4.167671	1.287101	-6.337672
95	6	0	-1.663058	3.882561	-1.866871
96	1	0	-0.845450	3.705637	-1.171791
97	1	0	-1.645213	4.937360	-2.159945
98	1	0	-2.598548	3.707277	-1.328746

The Cartesian coordinates of the simplified model of trans-bent **3c**, R”(H)B=B(H)R” (R” = :C(NRCH)$_2$), used for MO model, which is based on X-ray coordinates of **3c** and optimized with constraint.

1	5	.000000	.000000	-.798528
2	5	.000000	.000000	.798528
3	6	1.382359	.000000	-1.487896
4	7	2.573404	.485132	-1.011858
5	7	1.724739	-.481713	-2.725440
6	6	3.080205	-.334956	-2.985958
7	6	3.613021	.276159	-1.898873
8	1	2.637364	.867407	-.081168
9	1	1.044980	-.915227	-3.328133
10	1	3.541379	-.668173	-3.899062
11	1	4.626686	.573244	-1.693027
12	6	-1.382359	.000000	1.487896
13	7	-2.573404	-.485132	1.011858
14	7	-1.724739	.481713	2.725440
15	6	-3.080205	.334956	2.985958
16	6	-3.613021	-.276159	1.898873
17	1	-2.637364	-.867407	.081168
18	1	-1.044980	.915227	3.328133
19	1	-3.541379	.668173	3.899062
20	1	-4.626686	-.573244	1.693027
21	1	-.690951	-.735788	-1.490872
22	1	.690951	.735788	1.490872