Supplementary material to:

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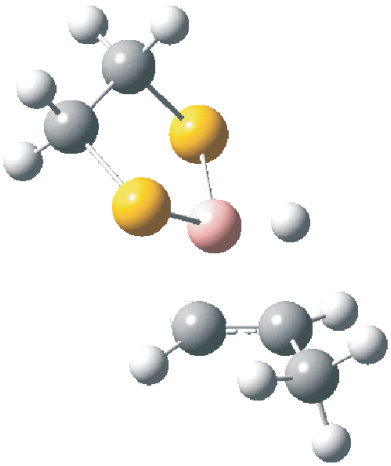
Energies and Cartesian coordinates of geometry optimized TSs and products of hydroboration

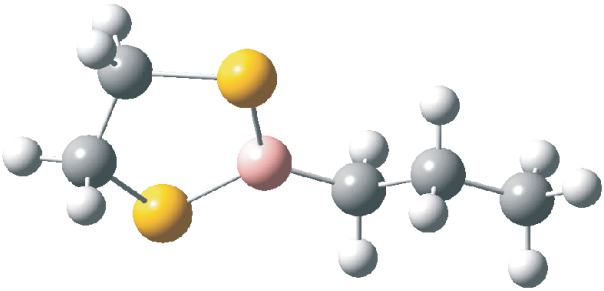
Energy and coordinates for the transition state structure (1,3,2-dithiaborolane + propene)



HF = –1018.3876905 a.u.

C,–0.6738328189,–2.0673878651,0.7950439506
H,–0.5929467711,–2.1470192095,1.8781589557
C,0.5123734895,–1.8937890624,0.0564220938
H,1.4682126073,–1.9863190097,0.5629208766
H,0.5075030897,–2.1331519031,–1.0031061239
C,–1.9639710123,–2.5603217908,0.1958554749
H,–1.960451611,–3.6567948355,0.2659616925
H,–2.8400243272,–2.1862110713,0.7337921997
H,–2.0455472553,–2.2885067475,–0.8601526679
B,–0.1433906354,–0.298061347,0.3073097611
H,–1.1648164037,–0.4050421386,0.9963016296
S,–0.7128013118,0.569391613,–1.3078457779
S,1.1221460792,0.7900792896,1.2646978759
C,0.9157445286,2.2461307126,0.1499388732
H,0.0711678985,2.8547881643,0.4874900271
H,1.8324971457,2.8423960944,0.2247078601
C,0.6900538332,1.7669180674,–1.2833061714
H,0.414297547,2.6012241748,–1.9380171961
H,1.59533686,1.2941084041,–1.6779649525

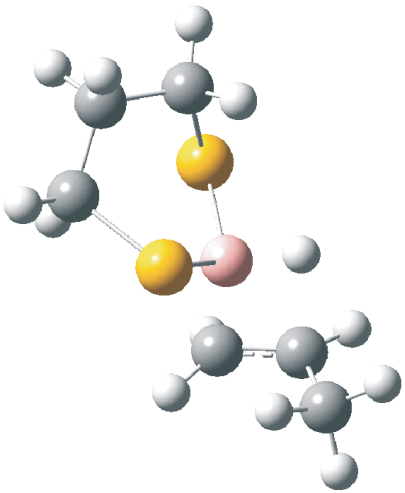
Energy and coordinates for the product compound (2-propyl-1,3,2-dithiaborolane)



HF = –1018.4748188 a.u.

B,0.0375364961,–0.0972358947,–0.2760314339
S,0.0692088851,–0.1101706408,1.541164132
S,1.686360356,–0.0869889052,–1.0394096334
C,2.6266678221,0.1980411763,0.5287798851
H,3.626929164,–0.2313944175,0.4154077414
H,2.7238938101,1.2794795342,0.6688272545
C,1.8837295481,–0.4403803624,1.6969173085
H,2.2266905094,–0.0336905442,2.6534220001
H,2.0268480442,–1.5257510596,1.7069413951
C,–1.2915330944,–0.134620414,–1.125220963
H,–1.1287883622,0.3475016347,–2.1003324118
H,–1.4855806014,–1.195947905,–1.359965796
C,–2.5499097121,0.4611303839,–0.4610109365
H,–2.7320241028,–0.0422595665,0.4983631127
H,–2.3703231493,1.5181332544,–0.2214100529
C,–3.8010577275,0.3457961824,–1.3398127312
H,–4.0304354877,–0.7037095312,–1.5659419324
H,–4.6784059245,0.7808011489,–0.8455184196
H,–3.6629752556,0.8677678641,–2.2956230756

Energy and coordinates for the transition state structure (1,3,2-dithiaborinane + propene)



HF = –1057.7008416 a.u.

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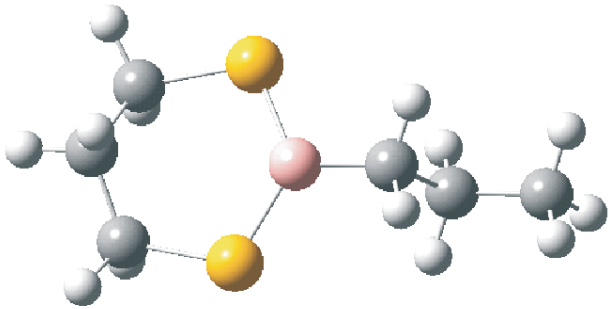
C,–1.738252145,0.5226469323,1.1666725311
H,–1.500272037,1.4417461126,1.6951771014
H,–1.8174206299,–0.3714915671,1.7783371102
C,–3.3655086285,–0.5112472715,–0.526413242
H,–4.3606525477,–0.3576912264,–0.0861691325
H,–3.468786238,–0.4991100135,–1.6154952982
H,–3.0017368166,–1.4918866481,–0.207548427
B,–0.5788523893,0.2512788548,–0.1204457265
H,–1.1647110162,0.3695738,–1.2026516454
S,0.0932254398,–1.5447758239,–0.1509149614
S,0.7230587921,1.6516616199,–0.0005039289
C,2.095849834,0.7548093784,–0.8495615177
H,1.7201996956,0.3824687556,–1.806565405
H,2.8675927686,1.5006574244,–1.0639085971
C,1.6516233963,–1.2221315128,0.7847495926
H,1.3964858,–0.7165696842,1.7201918826
H,2.0665430802,–2.2019301198,1.0405506541
C,2.6810074475,–0.3964410069,–0.0104020645
H,3.4091813986,0.0072386866,0.7071606719
H,3.2326295991,–1.0591746309,–0.6917364378

Energy and coordinates for the product compound (2-propyl-1,3,2-dithiaborinane)



HF = -1057.7870344 a.u

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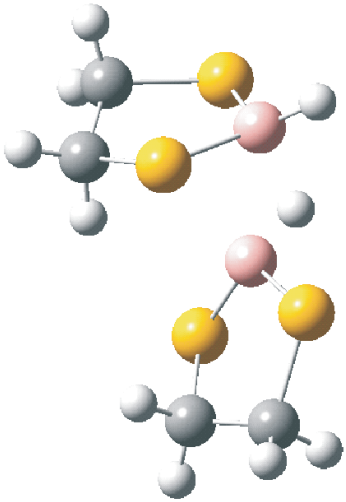
C,–1.282528645,2.2150115036,0.6363163882
C,1.2827805588,2.214823051,0.6364158098
H,–1.2825583398,2.4470515252,1.7070420159
H,–2.1532894043,2.7065795304,0.1925428852
H,0.0002121484,2.4733847019,–1.0903381876
H,0.0002662731,3.8190487097,0.0520754502
H,1.2827580266,2.4468562691,1.7071428964
H,2.1536474779,2.7062683497,0.1927148421
B,–0.0000520724,–0.4090619285,0.3389536674
S,–1.6102555048,0.4049898852,0.4418446339
S,1.6102633007,0.4047559201,0.4419580362
C,–0.0001616617,–1.9746606518,0.0760796762
H,–0.8796414234,–2.4363684182,0.5494846369
H,0.8791559039,–2.4365175259,0.5496411038
C,–0.0000588429,–2.3406779948,–1.4293351436
H,0.8788930869,–1.8926963248,–1.9122210186
H,–0.8788330452,–1.8925214926,–1.9123833751
C,–0.0001882792,–3.8547063116,–1.6745401849
H,–0.0001079925,–4.0841758004,–2.7475159308
H,0.8855119196,–4.3276674813,–1.2310319739
H,–0.8860700112,–4.3274876993,–1.2312030038

Energies and Cartesian coordinates of geometry optimized TSs and products of disproportionation

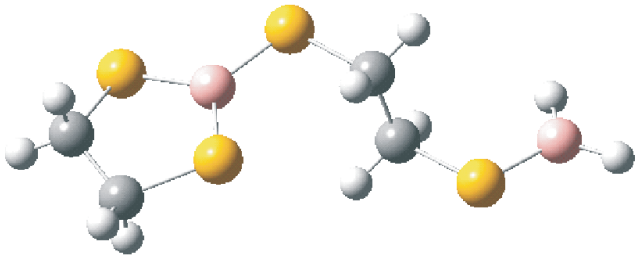
Energy and coordinates for the transition state structure (2 × (1,3,2-dithiaborolane))



HF = –1801.0048887 a.u.

C,3.1442986099,0.6483659513,0.4109210023
C,1.8500308614,0.9473406207,1.1629885242
H,3.8600512658,0.123545685,1.0504167288
H,3.6055718803,1.5806025603,0.0698990753
H,2.0490312042,1.2649778352,2.1916710955
H,1.2568390905,1.7206856282,0.6645391335
B,1.2998853656,–1.2276326014,–0.4311501613
H,1.0453584069,–2.3589947691,–0.6904168044
C,–3.3802740882,–0.0479470682,–0.1210172693
C,–2.7372654316,1.2660485177,0.3117671938
H,–4.1770830897,–0.3402814825,0.5707539093
H,–3.8012843892,0.039643966,–1.1271315824
H,–2.5192216201,1.2623966796,1.3846509851
H,–3.3876123166,2.1180977976,0.0879633385
B,–0.6740030767,–0.2684810459,–0.4157539346
H,0.1404458246,–0.6331065996,–1.2777670546
S,–2.1156843312,–1.4045218989,–0.1380953821
S,–1.1598893071,1.5021797474,–0.6252113313
S,2.8198573234,–0.4110139802,–1.0758396042
S,0.8018258518,–0.5728843179,1.259270377

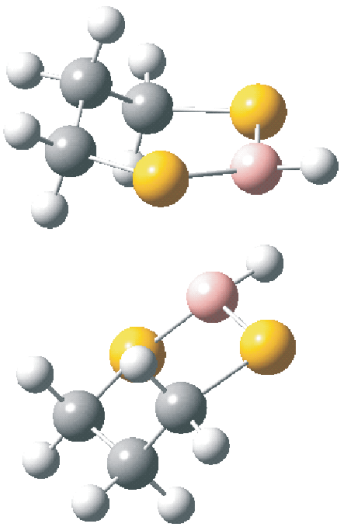
Energy and coordinates for the product compound (2-(ethylenedithioborane)-1,3,2-dithiaborolane)



HF = –1801.0287237 a.u.

C,–2.8228006532,–1.7266859125,–0.186781876
C,–3.7751692403,–0.5539240796,0.0128543804
H,–3.1829941963,–2.6234771663,0.3269751268
H,–2.6950140135,–1.9554527036,–1.2492841515
H,–4.0916732763,–0.4774666182,1.0577043871
H,–4.6638560327,–0.6557057387,–0.617896918
B,–1.2822824082,0.4768877995,0.1260031032
S,–1.1628513505,–1.2991123892,0.512786032
S,–2.9211262226,1.0202752256,–0.4534465518
S,0.0498152685,1.6890665982,0.3015065357
C,1.5631129917,0.6801374471,0.6535061208
H,2.2572236064,1.3745000048,1.1355538549
H,1.3203900983,–0.1028689853,1.3769328486
C,2.1832572598,0.09858176,–0.6146605786
H,2.4545627606,0.8896300408,–1.3174107454
H,1.4854946635,–0.5821068067,–1.108864718
S,3.6963767161,–0.9030604393,–0.2358449508
B,5.0221506748,0.2740770489,–0.2064370301
H,4.823887667,1.4299995134,–0.4288499079
H,6.1068046585,–0.1552349948,0.0377845361

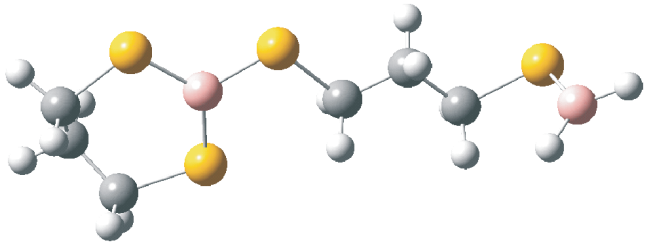
Energy and coordinates for the transition state structure TS4 (2 × (1,3,2-dithiaborinane))



HF = –1879.6344576 a.u.

B,–1.5612408072,0.1417394908,1.1370290244
H,–1.5479979701,–0.0593844959,2.309191305
B,0.5733155428,0.3091268676,0.652596196
H,–0.2880830576,1.0657762916,1.1343073781
S,1.6502512697,–0.3299504744,2.0222071613
S,1.2740625426,1.1365513011,–0.8534826117
S,–2.9193590996,1.2098158367,0.546661251
S,–0.8378239929,–1.2884977418,0.1469498383
C,–1.3801313513,–1.019138252,–1.6027011652
H,–1.3428556934,–2.019287137,–2.0447766777
H,–0.6116181731,–0.3986562711,–2.0773756557
C,–2.8876851959,1.0380460858,–1.2918991452
H,–3.8375098694,1.469815742,–1.6206912459
H,–2.0823346286,1.6588960853,–1.698992505
C,–2.7675012798,–0.402609333,–1.7903493244
H,–3.5370797601,–1.0276473901,–1.3213614969
H,–2.9679055689,–0.4071011825,–2.8718876753
C,2.9957605011,–1.1361643199,1.0481952979
H,3.7441163567,–1.4237651416,1.7928235912
H,2.60508376,–2.0598098271,0.6028251617
C,2.7298377168,0.0525815394,–1.2207276735
H,3.2886157306,0.5955280549,–1.9890339849
H,2.3703862306,–0.8798888888,–1.673268828
C,3.6364875799,–0.2519830134,–0.0255469248
H,3.992110064,0.6830985706,0.4229930915
H,4.5199995605,–0.7830051894,–0.4120751714

Energy and coordinates for the product compound 6C (2-(propylenedithioborane)-1,3,2-dithiaborinane)



HF = –1879.6540132 a.u.

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C,4.4207235661,0.9263901883,–0.7529465391
H,4.7883241681,–1.2054643118,–0.9088757955
H,4.8757717069,–0.3410123399,–2.4473204721
H,4.04459202,1.8172138643,1.1842036683
H,4.3205763473,0.0724069185,1.2381383159
H,3.93564045,1.7210630426,–1.3324489073
H,5.4848018358,1.1922516876,–0.6690860135
B,1.5347399521,–0.3278962533,–0.6656518986
S,2.0154162987,0.6606917786,0.7776590566
S,2.6289850411,–0.9323797098,–1.9844476018
C,–1.112859128,–0.0052473552,0.5101953305
H,–0.6981899053,–0.4042375816,1.4414809356
H,–0.94784115,1.0768178614,0.4977269108
C,–2.6079578867,–0.326809347,0.4023893373
H,–2.7541833187,–1.4138024602,0.3822454851
H,–3.0070335339,0.0661594569,–0.5404371316
C,–3.3845379628,0.2765600922,1.5779718429
H,–3.3041605328,1.3674583717,1.5903888746
H,–2.9995619868,–0.1021697609,2.5308318965
B,–5.9690301096,1.1626389801,0.6796823821
H,–7.1476937723,1.0701427395,0.5276358618
H,–5.3411110713,2.0974106035,0.2832513707
S,–0.2177033601,–0.7655017983,–0.9181990834
S,–5.1810316586,–0.1661608663,1.5469357408