Supporting Information

Structures, Energies, and Spin-Spin Coupling Constants of Methyl-substituted 1,3-Diborata-2,4-diphosphoniocyclobutanes: Four-member B-P-B-P Rings $B_2P_2(CH_3)_nH_{8-n}$ with n = 0, 1, 2, 4

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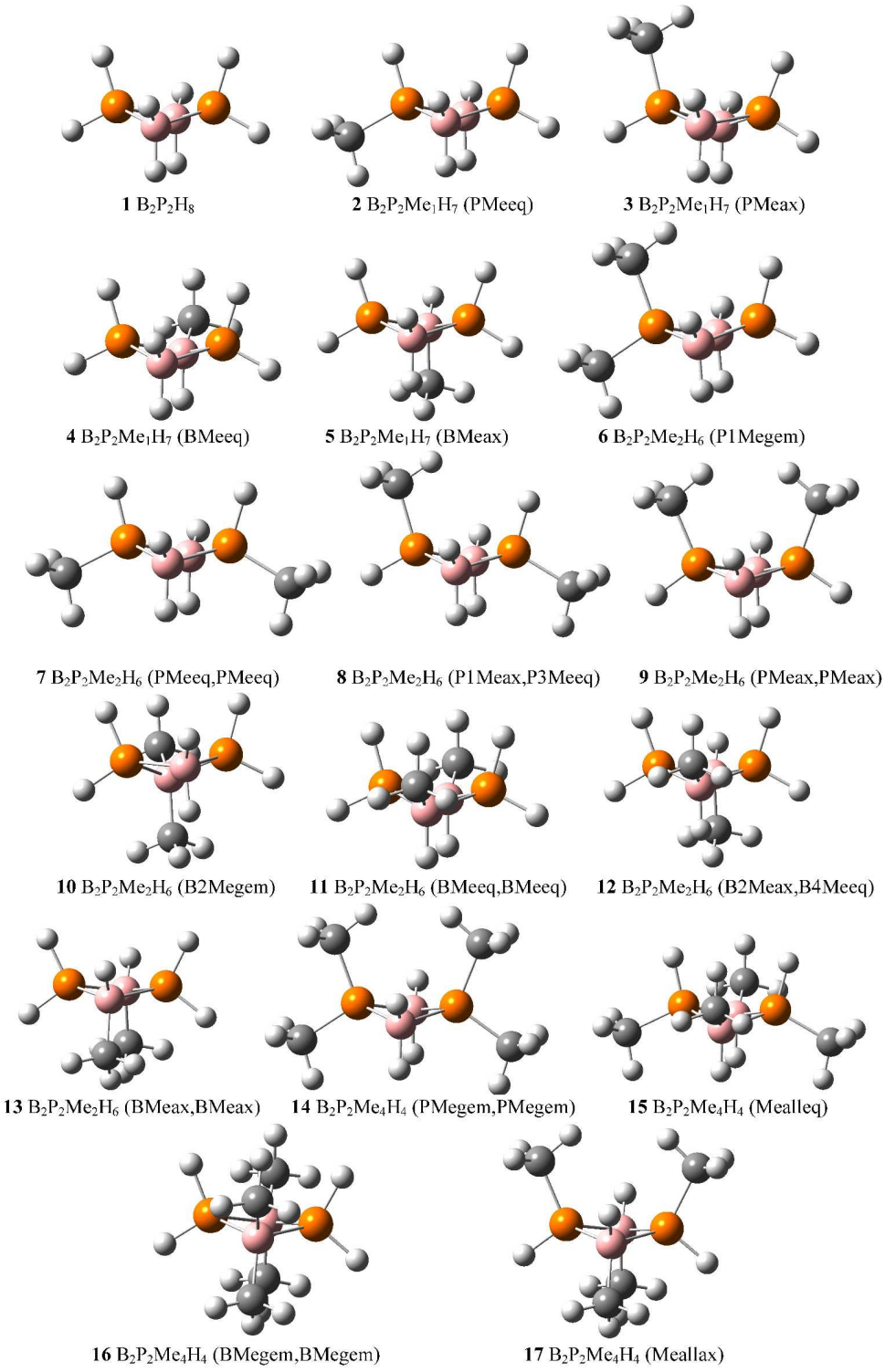

Fig. S1. Equilibrium structures of molecules $B_2P_2(CH_3)_nH_{8-n}$

Table S1. Cartesian coordinates of minima and TS structures calculated at MP2/aug-cc-pVTZ

1

P,-1.3276503219,0.,0.1508844589
B,0.,1.4036606694,-0.2618018261
P,1.3276503219,0.,0.1508844589
B,0.,-1.4036606694,-0.2618018261
H,-1.7341779799,0.,1.4930627214
H,-2.5652665972,0.,-0.5083392123
H,0.,2.4271242021,0.3479428868
H,0.,1.4684292919,-1.4617490286
H,1.7341779799,0.,1.4930627214
H,2.5652665972,0.,-0.5083392123
H,0.,-2.4271242021,0.3479428868
H,0.,-1.4684292919,-1.4617490286

TS 1

P,0.,-1.3668335557,0.
B,1.4420560887,0.,0.
P,0.,1.3668335557,0.
B,-1.4420560887,0.,0.
H,0.,-2.2598812606,-1.0805607891
H,0.,-2.2598812606,1.0805607891
H,2.0753567962,0.,-1.0149628674
H,2.0753567962,0.,1.0149628674
H,0.,2.2598812606,-1.0805607891
H,0.,2.2598812606,1.0805607891
H,-2.0753567962,0.,-1.0149628674
H,-2.0753567962,0.,1.0149628674

2

P,-0.3682802115,0.8437056236,-0.0000000054
B,0.2232870429,-0.4068359258,1.3990191228
P,0.0018756858,-1.7816967021,0.0000000113
B,0.223287043,-0.4068359436,-1.3990191176
H,-1.7627531721,1.0153159992,-0.0000000065
H,-0.3654253477,-0.4970751302,2.4322370554
H,1.4138393728,-0.2331109446,1.4537532179
H,-1.2730159894,-2.3662724286,0.000000015
H,0.8190909478,-2.9221004427,0.0000000186
H,-0.3654253476,-0.4970751611,-2.4322370491
H,1.4138393729,-0.2331109631,-1.4537532149
C,0.283388525,2.5463153613,-0.0000000162
H,-0.0458132228,3.0779430817,-0.8904997192
H,-0.0458132228,3.077943093,0.8904996801
H,1.3697887643,2.4824121068,-0.0000000158

TS 2→3

P,0.4837957485,0.872873826,-0.0000000083

B,0.1842021042,-0.4516372493,1.4388045761
P,-0.165492463,-1.7772650884,0.0000000181
B,0.1842021005,-0.4516372771,-1.4388045663
H,1.7497740894,1.4800730746,-0.0000000158
H,-0.7944032047,-0.2000679983,2.0846649893
H,1.1711434886,-0.7122259872,2.0643410187
H,-1.4350018811,-2.3731729367,0.0000000255
H,0.6538640876,-2.9148727474,0.000000028
H,-0.7944032101,-0.2000680385,-2.0846649819
H,1.1711434833,-0.712226027,-2.0643410064
C,-0.6714391727,2.2847731211,-0.0000000204
H,-0.5290042455,2.892189383,-0.8914926817
H,-1.6836365746,1.8843905538,-0.0000000152
H,-0.5290042432,2.8921894002,0.8914926288

3

P,0.5463831309,0.9322066921,-0.0000000097
B,0.4516243856,-0.4437039811,1.4033808015
P,-0.4071048533,-1.5427709938,0.000000016
B,0.4516243855,-0.4437040102,-1.4033807924
H,1.6428544558,1.810077281,-0.0000000188
H,-0.1367511626,-0.2100209688,2.4158170435
H,1.5610154309,-0.8965092884,1.4986473254
H,-1.8081020865,-1.4654971973,0.0000000152
H,-0.2213007949,-2.9328598588,0.0000000304
H,-0.1367511628,-0.2100210189,-2.4158170392
H,1.5610154308,-0.8965093195,-1.498647307
C,-0.9013149955,2.0450465419,-0.0000000212
H,-0.9035987578,2.6689263215,-0.891388341
H,-1.8002545288,1.4297294481,-0.0000000147
H,-0.9035987577,2.6689263399,0.8913882858

4

P,-0.114490521,-0.4287354145,-1.3276531306
B,0.4858404876,0.9260216105,0.
P,-0.114490521,-0.4287354145,1.3276531306
B,0.1188776335,-1.8722673128,0.
H,-1.4529052194,-0.2611520457,-1.7168199284
H,0.521307118,-0.5170092539,-2.5751255732
H,1.6808394869,0.7522564104,0.
H,-1.4529052194,-0.2611520457,1.7168199284
H,0.521307118,-0.5170092539,2.5751255732
H,-0.6329088939,-2.7966578459,0.
H,1.2961264426,-2.1080634536,0.
C,-0.0714711578,2.4214631616,0.
H,0.2792095133,2.9692952614,0.8770802252
H,0.2792095133,2.9692952614,-0.8770802252
H,-1.1620528104,2.4717705044,0.

TS 4→5

P,0.0272288845,-0.4238302893,-1.3700795307
B,-0.5902426986,0.9038428683,-0.0000000011
P,0.0272288812,-0.4238302881,1.370079531
B,0.6989722933,-1.6950219227,0.0000000015
H,-0.9505778262,-0.9181092023,-2.2451331849
H,0.9844519018,0.04876328,-2.2809970485
H,-1.7889810287,0.9701446937,-0.0000000026
H,-0.9505778316,-0.9181092004,2.2451331833
H,0.9844518963,0.0487632819,2.2809970507
H,0.1286407936,-2.7455813529,0.0000000012
H,1.8952239406,-1.7410939189,0.0000000029
C,0.2309658853,2.2843587784,-0.0000000007
H,-0.0198899662,2.8817579742,-0.8789846688
H,-0.0198899683,2.8817579749,0.8789846662
H,1.3152423134,2.1476089126,0.0000000006

5

P,-0.186451761,-0.4522219595,-1.3373770619
B,-0.6578296452,0.9567861102,0.
P,-0.186451761,-0.4522219595,1.3373770619
B,0.9117759697,-1.4068593215,0.
H,-1.2864126072,-1.1915874763,-1.7960934659
H,0.4094892306,-0.0675554598,-2.5488337732
H,-1.8003619962,1.3116064895,0.
H,-1.2864126072,-1.1915874763,1.7960934659
H,0.4094892306,-0.0675554598,2.5488337732
H,0.9458271121,-2.5980261709,0.
H,1.964312735,-0.827050194,0.
C,0.4815207893,2.0988823205,0.
H,0.3755519251,2.739013963,-0.8783008991
H,0.3755519251,2.739013963,0.8783008991
H,1.5026489307,1.7107842217,0.

6

P,0.0629018342,-0.7196001165,0.
B,0.3943771816,0.6145666189,-1.400967744
P,-0.0809325075,1.9254745579,0.
B,0.3943771816,0.6145666189,1.400967744
H,-0.2278187378,0.5817853176,-2.4207648912
H,1.5926884147,0.695679625,-1.4892671979
H,-1.4401697026,2.2745478841,0.
H,0.5137363392,3.1963935293,0.
H,-0.2278187378,0.5817853176,2.4207648912
H,1.5926884147,0.695679625,1.4892671979
C,-1.6655048967,-1.3042969601,0.
H,-1.8626991799,-1.8987201517,0.8912667691
H,-2.3297562423,-0.4408703336,0.
H,-1.8626991799,-1.8987201517,-0.8912667691
C,1.0717651612,-2.2357058375,0.

H,0.8594401428,-2.8266703509,0.8902577305
H,0.8594401428,-2.8266703509,-0.8902577305
H,2.1217150119,-1.9495390592,0.

TS 6
P,0.,0.,-0.7272474727
B,0.,-1.4376082597,0.6244642311
P,0.,0.,1.9967471028
B,0.,1.4376082597,0.6244642311
H,1.0162141738,-2.075290123,0.6306710649
H,-1.0162141738,-2.075290123,0.6306710649
H,1.0782816243,0.,2.8938021522
H,-1.0782816243,0.,2.8938021522
H,1.0162141738,2.075290123,0.6306710649
H,-1.0162141738,2.075290123,0.6306710649
C,-1.4448867232,0.,-1.8378010711
H,-1.4366834072,0.8914260732,-2.4640148173
H,-1.4366834072,-0.8914260732,-2.4640148173
H,-2.3477684958,0.,-1.229883663
C,1.4448867232,0.,-1.8378010711
H,1.4366834072,-0.8914260732,-2.4640148173
H,1.4366834072,0.8914260732,-2.4640148173
H,2.3477684958,0.,-1.229883663

7
P,0.,1.3244797216,-0.3340344051
B,-1.3945289682,0.,0.073158015
P,0.,-1.3244797216,-0.3340344051
B,1.3945289682,0.,0.073158015
H,0.,1.6898887189,-1.6908257564
H,-2.4361982093,0.,-0.5100482625
H,-1.4416643163,0.,1.2793477209
H,0.,-1.6898887189,-1.6908257564
H,2.4361982093,0.,-0.5100482625
H,1.4416643163,0.,1.2793477209
C,0.,2.9231686159,0.5452567115
H,0.8906173515,3.4950673711,0.2925988998
H,-0.8906173515,3.4950673711,0.2925988998
H,0.,2.7107162977,1.6126219571
C,0.,-2.9231686159,0.5452567115
H,-0.8906173515,-3.4950673711,0.2925988998
H,0.8906173515,-3.4950673711,0.2925988998
H,0.,-2.7107162977,1.6126219571

TS 7→9
P,1.361683684,0.0000000002,-0.4004190431
B,0.0000000002,-1.4349936223,-0.4462249339
P,-1.3616836839,0.,-0.4004190431
B,-0.0000000001,1.4349936225,-0.4462249339
H,2.2717500894,0.0000000003,-1.4699858105

H,0.0000000002,-2.0893141948,0.562314143
H,0.0000000002,-2.056782736,-1.4702308388
H,-2.2717500893,-0.0000000001,-1.4699858105
H,-0.0000000001,2.089314195,0.562314143
H,-0.0000000001,2.0567827362,-1.4702308388
C,2.4379495637,0.0000000003,1.0743669359
H,3.0616808103,0.8915681651,1.0910592913
H,1.7954214592,0.0000000002,1.9531957354
H,3.0616808104,-0.8915681644,1.0910592913
C,-2.4379495636,-0.0000000001,1.0743669359
H,-3.0616808101,-0.8915681648,1.0910592913
H,-1.7954214591,0.,1.9531957354
H,-3.0616808103,0.8915681646,1.0910592913

8
P,0.5541738587,1.3808481986,0.
B,0.4643934626,0.0024646026,1.3987919718
P,-0.3804592627,-1.0983426742,0.
B,0.4643934626,0.0024646026,-1.3987919718
H,1.6392712058,2.2740012888,0.
H,-0.110392802,0.2345847068,2.420750949
H,1.5774581828,-0.450417225,1.4853868026
H,-1.7823108659,-0.994306181,0.
H,-0.110392802,0.2345847068,-2.420750949
H,1.5774581828,-0.450417225,-1.4853868026
C,-0.9056923244,2.4790126589,0.
H,-0.9154071549,3.1029000924,-0.8913986059
H,-1.7970423977,1.852820702,0.
H,-0.9154071549,3.1029000924,0.8913986059
C,-0.0856943871,-2.8983421897,0.
H,-0.5145586499,-3.3531796361,0.890679098
H,-0.5145586499,-3.3531796361,-0.890679098
H,0.9914678061,-3.0534975354,0.

TS 8
P,0.5157845339,-1.2604893405,0.
B,0.,0.,1.4354190883
P,-0.5157845339,1.2604893405,0.
B,0.,0.,-1.4354190883
H,1.8606496352,-1.6665384176,0.
H,0.928089957,0.4141089637,2.073709562
H,-0.928089957,-0.4141089637,2.073709562
H,-1.8606496352,1.6665384176,0.
H,0.928089957,0.4141089637,-2.073709562
H,-0.928089957,-0.4141089637,-2.073709562
C,-0.405461185,-2.8360323771,0.
H,-0.1714081578,-3.4141740054,-0.8916810291
H,-0.1714081578,-3.4141740054,0.8916810291
H,-1.4673030532,-2.5962175182,0.
C,0.405461185,2.8360323771,0.

H,0.1714081578,3.4141740054,-0.8916810291
H,0.1714081578,3.4141740054,0.8916810291
H,1.4673030532,2.5962175182,0.

9
P,1.3365403255,0.,-0.3899020063
B,0.,-1.4062775005,-0.740488783
P,-1.3365403255,0.,-0.3899020063
B,0.,1.4062775005,-0.740488783
H,2.4942632647,0.,-1.1854942777
H,0.,-2.3845940578,-0.0505051134
H,0.,-1.5800017877,-1.9303578717
H,-2.4942632647,0.,-1.1854942777
H,0.,2.3845940578,-0.0505051134
H,0.,1.5800017877,-1.9303578717
C,2.0083073458,0.,1.3100420255
H,2.6093277216,0.8911247197,1.4802672127
H,1.1759438392,0.,2.0113063714
H,2.6093277216,-0.8911247197,1.4802672127
C,-2.0083073458,0.,1.3100420255
H,-2.6093277216,-0.8911247197,1.4802672127
H,-1.1759438392,0.,2.0113063714
H,-2.6093277216,0.8911247197,1.4802672127

10
P,-0.2395486355,-0.6128190143,-1.3408283069
B,0.0695831522,0.8579864887,0.
P,-0.2395486355,-0.6128190143,1.3408283069
B,0.2083652478,-1.9930070753,0.
H,-1.5656901893,-0.6867797075,-1.7953881952
H,0.4652588825,-0.5983240576,-2.5553676284
H,-1.5656901893,-0.6867797075,1.7953881952
H,0.4652588825,-0.5983240576,2.5553676284
H,-0.3928084873,-3.022135985,0.
H,1.4077780559,-2.0557968342,0.
C,-0.9399889365,2.0980530748,0.
H,-0.7708458168,2.7274312724,0.8781145294
H,-0.7708458168,2.7274312724,-0.8781145294
H,-1.9946630527,1.8153503667,0.
C,1.6477426641,1.1979974832,0.
H,1.8965421102,1.7984903099,-0.8791971797
H,1.8965421102,1.7984903099,0.8791971797
H,2.3089916049,0.3285655844,0.

TS 10
P,0.,-1.3751533919,-0.620558359
B,0.,0.,0.8619485837
P,0.,1.3751533919,-0.620558359
B,0.,0.,-2.0521530746
H,1.0831181561,-2.2677144359,-0.6326453346

H,-1.0831181561,-2.2677144359,-0.6326453346
H,1.0831181561,2.2677144359,-0.6326453346
H,-1.0831181561,2.2677144359,-0.6326453346
H,1.0166015677,0.,-2.682660575
H,-1.0166015677,0.,-2.682660575
C,-1.3703142657,0.,1.7001034522
H,-1.4159953882,-0.8801280212,2.3474177966
H,-1.4159953882,0.8801280212,2.3474177966
H,-2.2762039915,0.,1.088797046
C,1.3703142657,0.,1.7001034522
H,1.4159953882,0.8801280212,2.3474177966
H,1.4159953882,-0.8801280212,2.3474177966
H,2.2762039915,0.,1.088797046

11
P,-1.3275040112,0.,0.0113854519
B,0.,1.4196536626,-0.4115411486
P,1.3275040112,0.,0.0113854519
B,0.,-1.4196536626,-0.4115411486
H,-1.7004679759,0.,1.3664483789
H,-2.5841235642,0.,-0.6139835639
H,0.,1.4213025904,-1.6178882358
H,1.7004679759,0.,1.3664483789
H,2.5841235642,0.,-0.6139835639
H,0.,-1.4213025904,-1.6178882358
C,0.,2.8192684223,0.3577570101
H,0.8772180588,3.4120131732,0.090282967
H,-0.8772180588,3.4120131732,0.090282967
H,0.,2.7107803301,1.4441501037
C,0.,-2.8192684223,0.3577570101
H,-0.8772180588,-3.4120131732,0.090282967
H,0.8772180588,-3.4120131732,0.090282967
H,0.,-2.7107803301,1.4441501037

TS 11→13
P,0.,-1.3728963496,0.3309978056
B,-1.4581368543,0.,0.2693525558
P,0.,1.3728963496,0.3309978056
B,1.4581368543,0.,0.2693525558
H,0.0000000001,-2.2462353327,1.4286139424
H,0.0000000001,-2.2845158929,-0.7382144614
H,-2.0907636416,-0.0000000001,1.2888899418
H,-0.0000000001,2.2462353327,1.4286139424
H,-0.0000000001,2.2845158929,-0.7382144614
H,2.0907636416,0.0000000001,1.2888899418
C,-2.2739257361,-0.0000000001,-1.1163711422
H,-2.9176126818,-0.8795277328,-1.1843470066
H,-2.9176126819,0.8795277326,-1.1843470066
H,-1.6319746102,0.,-2.0011708784
C,2.2739257361,0.0000000001,-1.1163711422

H,1.6319746102,0.,-2.0011708784
H,2.9176126818,0.8795277328,-1.1843470066
H,2.9176126819,-0.8795277326,-1.1843470066

12
P,-0.3340394206,-0.0164883999,-1.3371706023
B,0.5596919651,1.1541875016,-0.0000000144
P,-0.3340394206,-0.0164883664,1.3371706027
B,-0.4988776658,-1.4926141065,0.0000000187
H,-1.574112482,0.4740725424,-1.7763917114
H,0.3094517435,-0.2641443741,-2.5607728421
H,1.6831015462,0.7104277658,-0.0000000089
H,-1.574112482,0.4740725868,1.7763916995
H,0.3094517435,-0.2641443101,2.5607728487
H,-1.5550099317,-2.0553412705,0.0000000257
C,0.3724237215,2.7396149934,-0.0000000342
H,0.8425078955,3.1887358492,0.8773450023
H,0.8425078955,3.1887358272,-0.877345082
H,-0.6754578363,3.0460403495,-0.0000000381
C,0.8344794661,-2.398737482,0.00000003
H,0.8512378988,-3.0476204273,0.8781821305
H,0.8512378988,-3.0476204492,-0.8781820543
H,1.763166086,-1.8242422528,0.0000000228

TS 12
P,0.,0.,-1.3735428445
B,-0.5878215088,-1.3341825142,0.
P,0.,0.,1.3735428445
B,0.5878215088,1.3341825142,0.
H,0.9949763266,-0.4267803206,-2.267106517
H,-0.9949763266,0.4267803206,-2.267106517
H,-1.7900667645,-1.3585380893,0.
H,0.9949763266,-0.4267803206,2.267106517
H,-0.9949763266,0.4267803206,2.267106517
H,1.7900667645,1.3585380893,0.
C,0.1841156058,-2.7405485141,0.
H,-0.0860758458,-3.3297946964,0.8787262638
H,-0.0860758458,-3.3297946964,-0.8787262638
H,1.2718245125,-2.6385064929,0.
C,-0.1841156058,2.7405485141,0.
H,0.0860758458,3.3297946964,0.8787262638
H,0.0860758458,3.3297946964,-0.8787262638
H,-1.2718245125,2.6385064929,0.

13
P,0.,-1.3573943755,0.5228144234
B,-1.445562362,0.,0.2503270219
P,0.,1.3573943755,0.5228144234
B,1.445562362,0.,0.2503270219
H,0.,-1.9749177192,1.7822038488

H,0.,-2.4748522795,-0.3293910792
H,-2.2823643574,0.,1.1071233216
H,0.,1.9749177192,1.7822038488
H,0.,2.4748522795,-0.3293910792
H,2.2823643574,0.,1.1071233216
C,-1.9573726704,0.,-1.2783576036
H,-2.576154141,-0.8791697601,-1.4702008393
H,-2.576154141,0.8791697601,-1.4702008393
H,-1.1564704062,0.,-2.0209145037
C,1.9573726704,0.,-1.2783576036
H,1.1564704062,0.,-2.0209145037
H,2.576154141,0.8791697601,-1.4702008393
H,2.576154141,-0.8791697601,-1.4702008393

14
P,1.3342545339,0.,-0.0718734258
B,0.,-1.4019391234,-0.4111406688
P,-1.3342545339,0.,-0.0718734258
B,0.,1.4019391234,-0.4111406688
H,0.,-2.3943742566,0.2614201569
H,0.,-1.5643364224,-1.6074690565
H,0.,2.3943742566,0.2614201569
H,0.,1.5643364224,-1.6074690565
C,1.983698427,0.,1.6354192119
H,2.5869370016,0.8911290479,1.8062613498
H,1.1524715075,0.,2.3379559098
H,2.5869370016,-0.8911290479,1.8062613498
C,2.8311750841,0.,-1.112983112
H,3.4267449399,0.8906103508,-0.9145086848
H,3.4267449399,-0.8906103508,-0.9145086848
H,2.5218019795,0.,-2.1563439164
C,-1.983698427,0.,1.6354192119
H,-2.5869370016,-0.8911290479,1.8062613498
H,-1.1524715075,0.,2.3379559098
H,-2.5869370016,0.8911290479,1.8062613498
C,-2.8311750841,0.,-1.112983112
H,-3.4267449399,-0.8906103508,-0.9145086848
H,-3.4267449399,0.8906103508,-0.9145086848
H,-2.5218019795,0.,-2.1563439164

TS 14
P,0.,-1.3565705766,0.
B,1.4321027263,0.,0.
P,0.,1.3565705766,0.
B,-1.4321027263,0.,0.
H,2.0748055908,0.,-1.0172563843
H,2.0748055908,0.,1.0172563843
H,-2.0748055908,0.,-1.0172563843
H,-2.0748055908,0.,1.0172563843
C,0.,-2.4711211565,-1.4439099688

H,0.8917253467,-3.0971347873,-1.4358844966
H,-0.8917253467,-3.0971347873,-1.4358844966
H,0.,-1.8640947555,-2.3475445243
C,0.,-2.4711211565,1.4439099688
H,-0.8917253467,-3.0971347873,1.4358844966
H,0.8917253467,-3.0971347873,1.4358844966
H,0.,-1.8640947555,2.3475445243
C,0.,2.4711211565,-1.4439099688
H,-0.8917253467,3.0971347873,-1.4358844966
H,0.8917253467,3.0971347873,-1.4358844966
H,0.,1.8640947555,-2.3475445243
C,0.,2.4711211565,1.4439099688
H,0.8917253467,3.0971347873,1.4358844966
H,-0.8917253467,3.0971347873,1.4358844966
H,0.,1.8640947555,2.3475445243

15
P,0.,1.3236598975,-0.2014545498
B,-1.4091043772,0.,0.2123199814
P,0.,-1.3236598975,-0.2014545498
B,1.4091043772,0.,0.2123199814
H,0.,1.6633695998,-1.5682118884
H,-1.4012689265,0.,1.4242095314
H,0.,-1.6633695998,-1.5682118884
H,1.4012689265,0.,1.4242095314
C,0.,2.9425806607,0.645541812
H,0.8901202478,3.510955077,0.382588263
H,-0.8901202478,3.510955077,0.382588263
H,0.,2.7507944415,1.7169745817
C,-2.8274658709,0.,-0.5299388452
H,-3.4185529386,-0.8764935198,-0.2544510545
H,-3.4185529386,0.8764935198,-0.2544510545
H,-2.7365954238,0.,-1.6182859203
C,2.8274658709,0.,-0.5299388452
H,3.4185529386,0.8764935198,-0.2544510545
H,3.4185529386,-0.8764935198,-0.2544510545
H,2.7365954238,0.,-1.6182859203
C,0.,-2.9425806607,0.645541812
H,-0.8901202478,-3.510955077,0.382588263
H,0.8901202478,-3.510955077,0.382588263
H,0.,-2.7507944415,1.7169745817

TS 15→17
P,0.0000000001,1.3654408167,-0.0216777093
B,1.4485331582,0.0000000001,-0.1150651089
P,0.0000000001,-1.3654408165,-0.0216777093
B,-1.448533158,0.0000000001,-0.1150651089
H,0.0000000001,2.2883745004,-1.0849953785
H,2.0860068336,0.0000000001,0.909470436
H,0.0000000001,-2.2883745002,-1.0849953785

H,-2.0860068334,0.0000000001,0.909470436
C,0.0000000001,2.4179928684,1.4719930658
H,-0.8916825811,3.0411756505,1.5015533315
H,0.0000000001,1.759192081,2.3388286811
H,0.8916825813,3.0411756505,1.5015533315
C,2.2747798369,0.0000000001,-1.4973055544
H,2.9190359397,0.8794079809,-1.5662552946
H,2.9190359397,-0.8794079806,-1.5662552946
H,1.6340923608,0.0000000001,-2.3831100778
C,0.0000000001,-2.4179928682,1.4719930658
H,0.8916825813,-3.0411756502,1.5015533315
H,0.0000000001,-1.7591920808,2.3388286811
H,-0.8916825811,-3.0411756502,1.5015533315
C,-2.2747798367,0.0000000001,-1.4973055544
H,-1.6340923606,0.0000000001,-2.3831100778
H,-2.9190359395,-0.8794079806,-1.5662552946
H,-2.9190359395,0.8794079809,-1.5662552946

16
P,0.,-1.3638071827,0.1998692413
B,-1.4606620006,0.,-0.0603204772
P,0.,1.3638071827,0.1998692413
B,1.4606620006,0.,-0.0603204772
H,0.,-1.9612844327,1.4718952806
H,0.,-2.4956800722,-0.6342598546
H,0.,1.9612844327,1.4718952806
H,0.,2.4956800722,-0.6342598546
C,-1.9337581328,0.,-1.6018670121
H,-2.5524573145,-0.8800551131,-1.7982299913
H,-2.5524573145,0.8800551131,-1.7982299913
H,-1.1279031281,0.,-2.3386434922
C,-2.6221405878,0.,1.0439166474
H,-3.2612884798,0.8791360697,0.9230925693
H,-3.2612884798,-0.8791360697,0.9230925693
H,-2.2605366115,0.,2.0745725327
C,1.9337581328,0.,-1.6018670121
H,1.1279031281,0.,-2.3386434922
H,2.5524573145,0.8800551131,-1.7982299913
H,2.5524573145,-0.8800551131,-1.7982299913
C,2.6221405878,0.,1.0439166474
H,3.2612884798,-0.8791360697,0.9230925693
H,3.2612884798,0.8791360697,0.9230925693
H,2.2605366115,0.,2.0745725327

TS 16
P,0.,-1.3823013353,0.
B,1.4707928952,0.,0.
P,0.,1.3823013353,0.
B,-1.4707928952,0.,0.
H,0.,-2.2740947827,-1.0861977465

H,0.,-2.2740947827,1.0861977465
H,0.,2.2740947827,-1.0861977465
H,0.,2.2740947827,1.0861977465
C,2.308243496,0.,-1.3718974229
H,2.9549213649,0.8805299505,-1.4191224076
H,2.9549213649,-0.8805299505,-1.4191224076
H,1.6947592763,0.,-2.2764993067
C,2.308243496,0.,1.3718974229
H,2.9549213649,-0.8805299505,1.4191224076
H,2.9549213649,0.8805299505,1.4191224076
H,1.6947592763,0.,2.2764993067
C,-2.308243496,0.,-1.3718974229
H,-2.9549213649,-0.8805299505,-1.4191224076
H,-2.9549213649,0.8805299505,-1.4191224076
H,-1.6947592763,0.,-2.2764993067
C,-2.308243496,0.,1.3718974229
H,-2.9549213649,0.8805299505,1.4191224076
H,-2.9549213649,-0.8805299505,1.4191224076
H,-1.6947592763,0.,2.2764993067

17
P,0.,1.3488856332,0.0604439757
B,1.4376643375,0.,-0.2227882677
P,0.,-1.3488856332,0.0604439757
B,-1.4376643375,0.,-0.2227882677
H,0.,2.4517425295,-0.8151888103
H,2.2641883997,0.,0.653026744
H,0.,-2.4517425295,-0.8151888103
H,-2.2641883997,0.,0.653026744
C,0.,2.110642347,1.7220776831
H,-0.8920447297,2.7172310241,1.8654797827
H,0.,1.307823224,2.4578197607
H,0.8920447297,2.7172310241,1.8654797827
C,1.9783387823,0.,-1.7430907754
H,2.5988026611,0.8793100812,-1.9301270754
H,2.5988026611,-0.8793100812,-1.9301270754
H,1.1850360839,0.,-2.4942713157
C,0.,-2.110642347,1.7220776831
H,0.8920447297,-2.7172310241,1.8654797827
H,0.,-1.307823224,2.4578197607
H,-0.8920447297,-2.7172310241,1.8654797827
C,-1.9783387823,0.,-1.7430907754
H,-1.1850360839,0.,-2.4942713157
H,-2.5988026611,-0.8793100812,-1.9301270754
H,-2.5988026611,0.8793100812,-1.9301270754

Table S2. Total energies (hartree) at the MP2/aug-cc-pVTZ computational level

	Minima		TS	
1	C_{2v}	-736.11277	D_{2h}	-736.10956
2	C_s	-775.35177	C_s	-775.34798
3	C_s	-775.35076		
4	C_s	-775.34892	C_s	-775.34491
5	C_s	-775.34719		
6	C_s	-814.59157	C_{2v}	-814.58835
7	C_{2v}	-814.59034	C_{2v}	-814.58605
8	C_s	-814.58946	C_{2h}	-814.58621
9	C_{2v}	-814.58787		
10	C_s	-814.58550	C_{2v}	-814.58286
11	C_{2v}	-814.58481	C_{2v}	-814.58027
12	C_s	-814.58327	C_{2h}	-814.58026
13	C_{2v}	-814.58100		
14	C_{2v}	-893.06878	D_{2h}	-893.06630
15	C_{2v}	-893.06157	C_{2v}	-893.05608
16	C_{2v}	-893.05731	D_{2h}	-893.05609
17	C_{2v}	-893.05675		

Table S3. PSO, DSO, FC, and SD components of coupling constants ^{1}J(B-P), ^{2}J(P-P), ^{1}J(B-C), ^{1}J(P-C), and ^{3}J(P-C) (Hz) for selected molecules

Molecule	PSO	DSO	FC	SD	1J(B-P)
1	-0.9	0.2	55.8	2.2	57.3
2	-1.0	0.3	62.0	2.3	63.6
2	-1.0	0.2	54.6	2.1	55.9
3	-1.0	0.3	63.4	2.4	65.0
3	-0.8	0.2	51.3	2.2	52.9
4	-1.2	0.3	51.9	2.1	53.2
4	-1.1	0.2	55.7	2.2	57.1
5	-0.5	0.3	51.8	2.5	54.1
5	-0.5	0.3	51.8	2.5	54.1
7	-1.1	0.3	60.9	2.2	62.2
9	-0.7	0.3	59.6	2.4	61.5
11	-1.3	0.3	51.9	2.1	52.9
13	-0.1	0.3	51.4	2.7	54.3

Molecule	PSO	DSO	FC	SD	2J(P-P)
1	0.9	0.1	138.6	-0.3	139.3
2	1.3	0.1	116.8	-0.1	118.2
3	0.6	0.1	119.7	-0.3	120.1
4	1.6	0.1	172.7	0.0	174.3
5	0.5	0.1	203.5	-0.4	203.7
7	1.7	0.1	97.7	0.1	99.6
9	-0.5	0.1	120.1	-0.7	119.0
11	2.3	0.1	206.0	0.2	208.6
13	-1.0	0.1	276.4	-0.8	274.6

Molecule	PSO	DSO	FC	SD	1J(B-C)
4	-0.7	0.2	55.5	0.4	55.5
5	-0.6	0.2	46.8	0.4	46.8
11	-0.7	0.2	55.5	0.4	55.5
13	-0.6	0.2	47.2	0.4	47.3

Molecule	PSO	DSO	FC	SD	1J(P-C)
2	-1.1	0.2	28.2	5.0	32.2
3	-0.6	0.2	35.7	5.2	40.5
7	-1.0	0.2	26.7	5.0	30.9
9	-0.5	0.2	32.3	5.2	37.2

Molecule	PSO	DSO	FC	SD	3J(P-C)
2	-0.2	-0.1	48.6	0.0	48.2
3	0.0	0.0	-3.9	0.0	-3.9
7	-0.3	-0.1	46.5	0.0	46.2
9	0.0	0.0	-2.0	0.0	-2.0