

Sandwich-like compounds based on bare all-boron cluster B_6^{2-}

Supporting Information

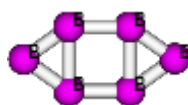
Li-ming Yang, Jian Wang, Yi-hong Ding*, Chia-chung Sun

State Key Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, Jilin

University, Changchun 130023, People's Republic of China

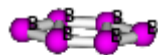
(E-mail: yhdd@mail.jlu.edu.cn; Fax: +86-431-88498026)

The coordinates of designed cluster-assembled compounds are listed as follows:



5	-2.071716	0.000015	0.000853
5	-0.830479	-0.887684	-0.000554
5	2.071718	-0.000015	0.000886
5	-0.830449	0.887678	-0.000275
5	0.830478	0.887684	-0.000595
5	0.830448	-0.887678	-0.000316

|State=1-A|HF=-148.8432897



Li



Charge = -3 Multiplicity = 1

Li,0,0.,0.,0.

B,0,0.,2.0631012169,2.4229219666

B,0,-0.8898591801,0.8286615669,2.4613552587

B,0,-0.8898591801,-0.8286615669,2.4613552587

B,0,0.,-2.0631012169,2.4229219666

B,0,0.8898591801,-0.8286615669,2.4613552587

B,0,0.8898591801,0.8286615669,2.4613552587

B,0,0.8286615669,0.8898591801,-2.4613552587

B,0,2.0631012169,0.,-2.4229219666

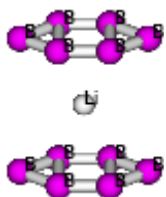
B,0,0.8286615669,-0.8898591801,-2.4613552587

B,0,-0.8286615669,-0.8898591801,-2.4613552587

B,0,-2.0631012169,0.,-2.4229219666

B,0,-0.8286615669,0.8898591801,-2.4613552587

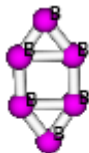
State=1-A1\HF=-305.2405097



Charge = -3 Multiplicity = 1

B,0,-2.5672181325,2.0659643031,0.
 B,0,-2.5932156741,0.830100654,-0.8867597386
 B,0,-2.5932156741,-0.830100654,-0.8867597386
 B,0,-2.5672181325,-2.0659643031,0.
 B,0,-2.5932156741,-0.830100654,0.8867597386
 B,0,-2.5932156741,0.830100654,0.8867597386
 B,0,2.5672181325,2.0659643031,0.
 B,0,2.5932156741,0.830100654,-0.8867597386
 B,0,2.5932156741,-0.830100654,-0.8867597386
 B,0,2.5672181325,-2.0659643031,0.
 B,0,2.5932156741,-0.830100654,0.8867597386
 B,0,2.5932156741,0.830100654,0.8867597386
 Li,0,0.,0.,0.

State=1-AG\HF=-305.2323036



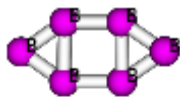
Charge = -3 Multiplicity = 1

B,0,-0.0000001166,1.2448482699,-1.2448484351
 B,0,0.6255895729,2.5729642694,-1.6882340528
 B,0,0.6329710048,3.7514119062,-2.8562426159
 B,0,-0.0000003907,4.1720940397,-4.1720945934
 B,0,-0.5922153849,-2.4732393523,1.6357080564
 B,0,0.5922157697,-1.6357076728,2.4732395139
 B,0,1.4663806323,-1.6400994979,3.7139052514
 B,0,0.5858322678,-2.8830179674,3.7115220418
 B,0,-1.4663801309,-3.7139051711,1.640100128
 B,0,-0.5858316503,-3.7115217141,2.8830185148
 B,0,-0.625589972,1.6882336528,-2.5729644348

B,0,-0.6329716236,2.8562420589,-3.7514122259

Li,0,0.0000000356,-0.3805047024,0.3805047529

State=1-A1\HF=-305.2570786



Charge = -3 Multiplicity = 1

B,0,0.,0.8383813409,2.3341368328

B,0,0.,-0.8383813409,2.3341368328

B,0,0.,-2.0741098631,3.214121037

B,0,0.,-0.8279608194,4.0894462212

B,0,-0.8383813409,0.,-2.3341368328

B,0,0.8383813409,0.,-2.3341368328

B,0,2.0741098631,0.,-3.214121037

B,0,0.8279608194,0.,-4.0894462212

B,0,-2.0741098631,0.,-3.214121037

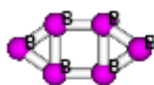
B,0,-0.8279608194,0.,-4.0894462212

B,0,0.,2.0741098631,3.214121037

B,0,0.,0.8279608194,4.0894462212

Li,0,0.,0.,0.

State=1-A1\HF=-305.2389001



Charge = -3 Multiplicity = 1

B,0,0.,0.8378292274,2.0316244774

B,0,0.,-0.8378292274,2.0316244774

B,0,0.,-2.0698375453,2.9226352338

B,0,0.,-0.8262689159,3.8009289799

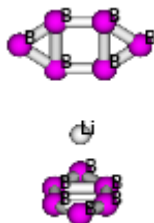
B,0,0.,-2.0633637067,-2.8133345453

B,0,0.,2.0633637067,-2.8133345453

B,0,0.,2.0698375453,2.9226352338

B,0,0.,0.8262689159,3.8009289799
Li,0,0.,0.,-0.557432705
B,0,-0.8861882317,0.8301470296,-2.8873121672
B,0,0.8861882317,-0.8301470296,-2.8873121672
B,0,-0.8861882317,-0.8301470296,-2.8873121672
B,0,0.8861882317,0.8301470296,-2.8873121672

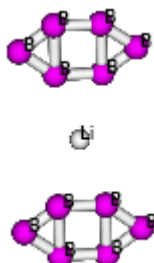
State=1-A1\HF=-305.2379286



Charge = -3 Multiplicity = 1

B,0,0.,0.8368435556,-1.9825734929
B,0,0.,-0.8368435556,-1.9825734929
B,0,0.,-2.0703749492,-2.8701206105
B,0,0.,-0.8267684597,-3.7486642148
B,0,-2.0633850806,0.,2.7650620287
B,0,2.0633850806,0.,2.7650620287
B,0,0.,2.0703749492,-2.8701206105
B,0,0.,0.8267684597,-3.7486642148
Li,0,0.,0.,0.5229284689
B,0,0.8301002548,-0.8871887335,2.8397088744
B,0,-0.8301002548,0.8871887335,2.8397088744
B,0,-0.8301002548,-0.8871887335,2.8397088744
B,0,0.8301002548,0.8871887335,2.8397088744

State=1-A1\HF=-305.2422567

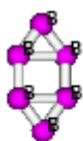


Charge = -3 Multiplicity = 1

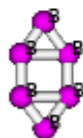
B,0,0.,0.8389585746,2.3573981266
B,0,0.,-0.8389585746,2.3573981266
B,0,0.,-2.0737531842,3.2389853983
B,0,0.,-0.8275843026,4.1140833045

B,0,0.,0.8389585746,-2.3573981266
B,0,0.,-0.8389585746,-2.3573981266
B,0,0.,-2.0737531842,-3.2389853983
B,0,0.,-0.8275843026,-4.1140833045
B,0,0.,2.0737531842,-3.2389853983
B,0,0.,0.8275843026,-4.1140833045
B,0,0.,2.0737531842,3.2389853983
B,0,0.,0.8275843026,4.1140833045
Li,0,0.,0.,0.

State=1-AG\HF=-305.235703



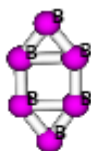
Li



Charge = -3 Multiplicity = 1

B,0,2.3259640752,0.0000122624,0.0000119627
B,0,3.5777008205,0.0000255558,0.8846160775
B,0,5.2370014321,0.0000343735,0.8938664914
B,0,6.4658217666,0.0000340876,0.0000332544
B,0,-2.3259640752,-0.0000122624,-0.0000119627
B,0,-3.5777099197,-0.0000121673,0.8845792765
B,0,-5.2370106264,-0.0000208452,0.8938126225
B,0,-6.4658217666,-0.0000340876,-0.0000332544
B,0,-3.5777008205,-0.0000255558,-0.8846160775
B,0,-5.2370014321,-0.0000343735,-0.8938664914
B,0,3.5777099197,0.0000121673,-0.8845792765
B,0,5.2370106264,0.0000208452,-0.8938126225
Li,0,0.,0.,0.

State=1-AG\HF=-305.2739826



Charge = -3 Multiplicity = 1

B,0,0.,0.,2.3264768618
 B,0,0.,0.8845904156,3.5782025005
 B,0,0.,0.8938150054,5.2375333863
 B,0,0.,0.,6.4663558947
 B,0,0.,0.,-2.3264768618
 B,0,-0.8845904156,0.,-3.5782025005
 B,0,-0.8938150054,0.,-5.2375333863
 B,0,0.,0.,-6.4663558947
 B,0,0.8845904156,0.,-3.5782025005
 B,0,0.8938150054,0.,-5.2375333863
 B,0,0.,-0.8845904156,3.5782025005
 B,0,0.,-0.8938150054,5.2375333863
 Li,0,0.,0.,0.

State=1-A1\HF=-305.27398

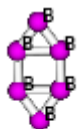


Charge = -3 Multiplicity = 1

Li,0,-1.0365331342,0.0272608409,-0.0252695367
 B,0,4.3017105992,-0.1117448844,-0.7832117803
 B,0,2.6473270001,-0.0682497803,-0.8138237606
 B,0,4.2571326993,-0.1133750589,1.0060513794
 B,0,5.5128213275,-0.1449992554,0.142031144
 B,0,-3.3692317128,-0.7403986294,-0.9768549092
 B,0,-3.3528836653,-1.976227113,-0.0907726776
 B,0,-3.2445275453,2.1497614567,-0.0843139465
 B,0,-3.3256456607,0.9192727658,-0.9742568963

B,0,-3.4132562879,-0.7420346169,0.7956254567
B,0,-3.3696693144,0.9176718603,0.7982235245
B,0,2.6031736277,-0.0698611136,0.9562810341
B,0,1.374968813,-0.0361721356,0.040183154

State=1-A\HF=-305.2597497



Li



Charge = -3 Multiplicity = 1

Li,0,0.0044574625,0.5059296537,-0.8750471649
B,0,-0.4666625607,-1.485819383,4.1167582664
B,0,-0.4544395537,-0.6616721873,2.674404921
B,0,0.428652268,-2.8284141764,3.3450653638
B,0,-0.0244393241,-2.7739052968,4.7976985499
B,0,-1.0188101709,3.2184158749,-1.9951479563
B,0,0.3671272993,2.7052462031,-2.3561482007
B,0,-0.3371805189,0.693764856,-3.5227224471
B,0,-1.1683069923,1.9401041771,-2.8063549973
B,0,1.1982537728,1.458906882,-3.0725156506
B,0,1.0482121023,0.1187538872,-3.7767630556
B,0,0.4310808619,-1.9895794901,1.9111540534
B,0,-0.0061616612,-0.6993591391,1.2095994522

State=1-A1\HF=-305.2594747



Li

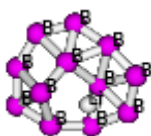


Charge = -3 Multiplicity = 1

B,0,-0.0000001211,1.2429687084,-1.2429689108
B,0,0.883380665,2.1292096102,-2.1292007473
B,0,0.8952646473,3.3025236298,-3.3025148341
B,0,-0.0000004064,4.1706224234,-4.1706231025

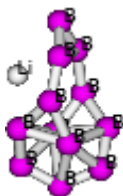
B,0,0.0000063786,-2.6455270425,1.4602221724
 B,0,-0.0000059786,-1.4602217417,2.6455272803
 B,0,-0.0000150291,-1.2092079524,4.1424216453
 B,0,-0.0000057831,-2.7097666835,3.8808070248
 B,0,0.0000155505,-4.1424214484,1.2092086269
 B,0,0.0000064253,-3.8808065836,2.7097673154
 B,0,-0.88338108,2.1292003146,-2.1292098708
 B,0,-0.8952652909,3.3025142092,-3.3025240803
 Li,0,0.0000000372,-0.3818124056,0.3818124678

State=1-A1\HF=-305.2572029



5	0	-1.118509	-0.685952	0.774488
5	0	1.051244	-1.699400	-0.420720
5	0	-2.048389	-1.468325	-0.342085
5	0	-2.310755	0.076532	-0.158524
5	0	-0.362775	0.719931	0.278204
5	0	-0.534892	-1.981131	-0.125158
5	0	1.101227	1.679045	-0.021366
5	0	-0.378729	2.307737	-0.157560
5	0	-1.794205	1.611761	-0.160688
5	0	2.385608	-0.853248	-0.247796
5	0	1.031333	-0.000830	-0.472959
5	0	2.427728	0.711055	0.040881
3	0	0.918521	-0.695294	1.688806

State=1-A\HF=-305.4341441



1	5	0	-0.614960	1.113656	-0.661272
2	5	0	-2.214701	0.818946	-0.482516
3	5	0	-3.323206	-0.034078	0.048531
4	5	0	-2.104149	-0.402609	0.849130
5	5	0	-0.511135	-0.805378	0.942660
6	5	0	1.064396	-0.122295	0.920557

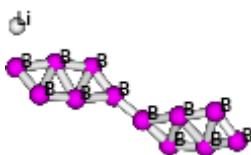
7	5	0	0.617995	1.650969	0.175537
8	5	0	0.783790	0.096248	-0.859893
9	5	0	0.513708	-1.607833	0.016223
10	5	0	1.882883	-1.274690	-0.592973
11	5	0	2.655479	-0.025398	-0.135231
12	5	0	2.063019	1.245490	0.499757
13	3	0	-1.355196	-1.088380	-1.200851

State=1-A\HF=-305.4074433



1	5	0	-2.044158	-0.522665	0.613212
2	5	0	0.655522	-1.646865	0.141796
3	5	0	-1.964964	-1.079448	-1.038285
4	5	0	-1.912138	0.453564	-0.760552
5	5	0	-2.005596	1.059811	0.852502
6	5	0	-0.960590	-1.684285	0.001936
7	5	0	2.184799	1.375252	-0.223289
8	5	0	0.635451	1.632233	-0.311066
9	5	0	-0.954555	1.733795	-0.101654
10	5	0	2.197506	-1.372350	0.228172
11	5	0	1.280473	-0.050440	-0.257600
12	5	0	2.936698	-0.011048	-0.045186
13	3	0	-0.080746	0.187414	1.500024

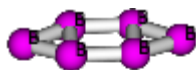
State=1-A\HF=-305.4238527



1	5	0	-1.820733	0.906625	-0.489917
2	5	0	-3.266347	0.453230	-0.002634
3	5	0	-4.694740	-0.331031	0.455168
4	5	0	-3.339509	-1.062792	0.732444
5	5	0	-1.908794	-0.623583	0.187752
6	5	0	-0.476637	0.094779	-0.426717
7	5	0	2.421296	0.298577	0.303284
8	5	0	3.801091	1.017457	0.666534
9	5	0	5.105362	0.209233	0.509043
10	5	0	3.916716	-0.433548	-0.324550

11	5	0	2.456685	-0.935645	-0.797116
12	5	0	1.039050	-0.402528	-0.495154
13	3	0	-5.389066	1.348712	-0.530228

State=1-A\HF=-305.3666704



Charge = -3 Multiplicity = 1

Na,0,0.,0.,0.

B,0,0.,2.0645477987,2.7611571855

B,0,-0.8887261199,0.8294794505,2.8194207669

B,0,-0.8887261199,-0.8294794505,2.8194207669

B,0,0.,-2.0645477987,2.7611571855

B,0,0.8887261199,-0.8294794505,2.8194207669

B,0,0.8887261199,0.8294794505,2.8194207669

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B,0,2.0645477987,0.,-2.7611571855

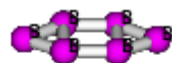
B,0,0.8294794505,-0.8887261199,-2.8194207669

B,0,-0.8294794505,-0.8887261199,-2.8194207669

B,0,-2.0645477987,0.,-2.7611571855

B,0,-0.8294794505,0.8887261199,-2.8194207669

State=1-A1\HF=-460.0255786



Charge = -3 Multiplicity = 1

B,0,0.,2.0658448957,2.8355822003

B,0,-0.8874106946,0.8300838911,2.8793862808

B,0,-0.8874106946,-0.8300838911,2.8793862808

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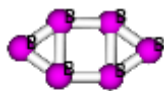
B,0,0.8874106946,-0.8300838911,2.8793862808

B,0,0.8874106946,0.8300838911,2.8793862808

B,0,0.,2.0658448957,-2.8355822003

B,0,-0.8874106946,0.8300838911,-2.8793862808
B,0,-0.8874106946,-0.8300838911,-2.8793862808
B,0,0,-2.0658448957,-2.8355822003
B,0,0.8874106946,-0.8300838911,-2.8793862808
B,0,0.8874106946,0.8300838911,-2.8793862808
Na,0,0,0,0.

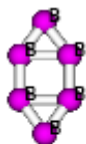
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Charge = -3 Multiplicity = 1

B,0,0,0.835439279,2.4152027489
B,0,0,-0.835439279,2.4152027489
B,0,0,-2.0708740248,3.3010559459
B,0,0,-0.8278313917,4.1815244356
B,0,0,-2.0656387005,-3.0875560566
B,0,0,2.0656387005,-3.0875560566
B,0,0,2.0708740248,3.3010559459
B,0,0,0.8278313917,4.1815244356
Na,0,0,0,-0.4577150359
B,0,-0.8866689699,0.8311803628,-3.1533702672
B,0,0.8866689699,-0.8311803628,-3.1533702672
B,0,-0.8866689699,-0.8311803628,-3.1533702672
B,0,0.8866689699,0.8311803628,-3.1533702672

State=1-A1\HF=-460.02215



Charge = -3 Multiplicity = 1

Na,0,-0.8807737922,0.000004533,-0.0000069537
B,0,4.7465918253,0.4468674725,-0.7729128684
B,0,3.0862856066,0.4437220831,-0.7674708885

B,0,4.7465750203,-0.4469163305,0.7729878173
 B,0,5.9794626991,-0.0000307742,0.0000472081
 B,0,-3.5502572259,1.0341482982,-1.7886734618
 B,0,-3.6114017361,-0.352100552,-1.1635505823
 B,0,-3.6114164838,0.3521377253,1.1634935579
 B,0,-3.611400842,1.1840546222,-0.2754012812
 B,0,-3.6114173778,-1.1840174489,0.2753442568
 B,0,-3.5502961133,-1.0341117541,1.7886174027
 B,0,3.0862689203,-0.4437538511,0.767519621
 B,0,1.8387080501,-0.0000094632,0.0000145167

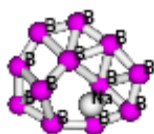
State=1-A1\HF=-460.0400373



Charge = -3 Multiplicity = 1

B,0,0.,0.8348053769,-2.3820759728
 B,0,0.,-0.8348053769,-2.3820759728
 B,0,0.,-2.0710918068,-3.2662439203
 B,0,0.,-0.8282536443,-4.1472907315
 B,0,-2.0654298322,0.,3.0567080431
 B,0,2.0654298322,0.,3.0567080431
 B,0,0.,2.0710918068,-3.2662439203
 B,0,0.,0.8282536443,-4.1472907315
 Na,0,0.,0.,0.4452308717
 B,0,0.8310667738,-0.8872022947,3.1245743113
 B,0,-0.8310667738,0.8872022947,3.1245743113
 B,0,-0.8310667738,-0.8872022947,3.1245743113
 B,0,0.8310667738,0.8872022947,3.1245743113

State=1-A1\HF=-460.025081



Charge = -3 Multiplicity = 1

5	0	-1.005097	-0.938503	0.574436
5	0	1.095355	-1.227730	-1.076252

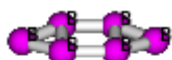
5	0	-1.924210	-1.717777	-0.559807
5	0	-2.471175	-0.343286	-0.026570
5	0	-0.646336	0.668235	0.280876
5	0	-0.323763	-1.904491	-0.622649
5	0	0.498474	1.982957	-0.103383
5	0	-1.066011	2.251734	0.149594
5	0	-2.283658	1.252754	0.202220
5	0	2.215004	-0.088836	-1.029652
5	0	0.706060	0.386873	-0.750852
5	0	1.990546	1.379183	-0.474961
11	0	1.461277	-0.773233	1.562273

State=1-A\HF=-460.2119885



1	5	0	0.079205	-0.655800	1.055696
2	5	0	-1.454601	-0.976317	0.575121
3	5	0	-2.819217	-1.228095	-0.110539
4	5	0	-1.699095	-1.463738	-1.090820
5	5	0	-0.146511	-1.167347	-1.076188
6	5	0	1.296572	-0.637184	-0.625634
7	5	0	1.570408	-1.035885	1.285250
8	5	0	1.222750	0.633788	0.615646
9	5	0	0.099649	1.813245	-0.228609
10	5	0	1.463124	1.409357	-0.922060
11	5	0	2.704386	0.522300	-0.624357
12	5	0	2.782106	-0.590165	0.429001
13	11	0	-2.317625	1.534473	0.326133

State=1-A\HF=-460.1461246



Charge = -3 Multiplicity = 1

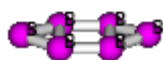
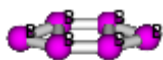
K,0,0.,0.,0.

B,0,0.,2.0612720486,3.103744918

B,0,-0.889918209,0.8250308078,3.1896129208

B,0,-0.889918209,-0.8250308078,3.1896129208
 B,0,0.,-2.0612720486,3.103744918
 B,0,0.889918209,-0.8250308078,3.1896129208
 B,0,0.889918209,0.8250308078,3.1896129208
 B,0,0.8250308078,0.889918209,-3.1896129208
 B,0,2.0612720486,0.,-3.103744918
 B,0,0.8250308078,-0.889918209,-3.1896129208
 B,0,-0.8250308078,-0.889918209,-3.1896129208
 B,0,-2.0612720486,0.,-3.103744918
 B,0,-0.8250308078,0.889918209,-3.1896129208

State=1-A1\HF=-897.6831844



Charge = -3 Multiplicity = 1

B,0,0.,2.0615998923,3.129369713
 B,0,-0.8894718118,0.8247479536,3.2076169791
 B,0,-0.8894718118,-0.8247479536,3.2076169791
 B,0,0.,-2.0615998923,3.129369713
 B,0,0.8894718118,-0.8247479536,3.2076169791
 B,0,0.8894718118,0.8247479536,3.2076169791
 B,0,0.,2.0615998923,-3.129369713
 B,0,-0.8894718118,0.8247479536,-3.2076169791
 B,0,-0.8894718118,-0.8247479536,-3.2076169791
 B,0,0.,-2.0615998923,-3.129369713
 B,0,0.8894718118,-0.8247479536,-3.2076169791
 B,0,0.8894718118,0.8247479536,-3.2076169791
 K,0,0.,0.,0.

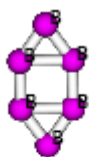
State=1-AG\HF=-897.681385



Charge = -3 Multiplicity = 1

K,0,-0.8691128385,-0.0037805693,0.0037722321
B,0,5.2094736015,0.6372982609,-0.6364988862
B,0,3.5659925305,0.6278864943,-0.6271056441
B,0,5.2171964554,-0.6315382689,0.6307906388
B,0,6.451032439,0.0066504618,-0.0066146837
B,0,-3.8715223249,0.0436728589,-1.2160306549
B,0,-3.7738766916,-1.4550901602,-1.4610251933
B,0,-3.7738892069,1.4592327086,1.4568553221
B,0,-3.8715273596,1.2160664253,-0.0422058944
B,0,-3.8734245453,-1.2118262904,0.0379004418
B,0,-3.8734295802,-0.039395456,1.211762516
B,0,3.5736829017,-0.6324540699,0.6316982739
B,0,2.3229205666,-0.0061368011,0.0061392821

State=1-A\HF=-897.6907525



Charge = -3 Multiplicity = 1

K,0,-0.8838843845,0.0000056698,-0.0000089173
B,0,5.2263030886,0.4488782981,-0.7763913001
B,0,3.5836928012,0.4461462934,-0.7716643347
B,0,5.2262816626,-0.4489453482,0.7764967539
B,0,6.4646285818,-0.0000414686,0.0000652202
B,0,-3.781173951,1.0326253266,-1.7860390787
B,0,-3.8750982858,-0.3523498687,-1.1628444771
B,0,-3.8751172276,0.3523995839,1.1627662869
B,0,-3.8750973923,1.1835673102,-0.2748327764
B,0,-3.8751181211,-1.1835175949,0.2747545861
B,0,-3.7812232358,-1.0325768161,1.7859627834
B,0,3.5836715061,-0.4461922699,0.7717366447
B,0,2.3370112344,-0.0000149912,0.0000235776

State=1-A1\HF=-897.6910129



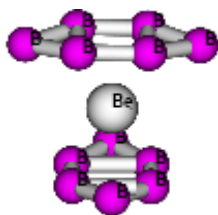
1	5	0	1.129119	-0.893380	-0.482603
2	5	0	-0.461608	-1.041277	1.629656
3	5	0	2.285693	-1.737066	0.313296
4	5	0	2.753612	-0.439789	-0.443980
5	5	0	0.753445	0.694694	-0.243319
6	5	0	0.789686	-1.808523	0.892523
7	5	0	-0.188862	2.042766	0.228372
8	5	0	1.212487	2.212453	-0.578659
9	5	0	2.320141	1.077115	-0.839542
10	5	0	-1.575740	0.098021	1.801576
11	5	0	-0.186441	0.560263	1.154707
12	5	0	-1.522025	1.507394	1.063810
13	19	0	-1.923555	-0.598071	-1.183115

State=1-A\HF=-897.8793117



1	5	0	-0.020514	0.814515	-1.060719
2	5	0	-1.292509	1.683104	-0.427062
3	5	0	-2.019543	2.020087	0.853545
4	5	0	-0.916195	1.031867	1.177378
5	5	0	0.292730	-0.059194	0.872761
6	5	0	1.974551	-0.021849	0.537754
7	5	0	1.556066	1.260790	-0.822898
8	5	0	0.364149	-0.737078	-0.788839
9	5	0	1.041272	-1.545303	0.452024
10	5	0	2.605373	-1.612206	0.322896
11	5	0	3.528249	-0.356397	0.014887
12	5	0	3.024969	1.060736	-0.334586
13	19	0	-2.668052	-0.931335	-0.209774

State=1-A\HF=-897.8346612



Charge = -2 Multiplicity = 1

Be,0,0.,0.,0.

B,0,0.,2.0331134611,1.594916954

B,0,-0.9219055868,0.8155303962,1.7068309103

B,0,-0.9219055868,-0.8155303962,1.7068309103

B,0,0.,-2.0331134611,1.594916954

B,0,0.9219055868,-0.8155303962,1.7068309103

B,0,0.9219055868,0.8155303962,1.7068309103

B,0,0.8155303962,0.9219055868,-1.7068309103

B,0,2.0331134611,0.,-1.594916954

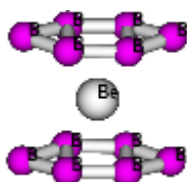
B,0,0.8155303962,-0.9219055868,-1.7068309103

B,0,-0.8155303962,-0.9219055868,-1.7068309103

B,0,-2.0331134611,0.,-1.594916954

B,0,-0.8155303962,0.9219055868,-1.7068309103

State=1-A1\HF=-312.5993792



Charge = -2 Multiplicity = 1

B,0,0.,2.0711832638,1.9432332287

B,0,-0.8793674956,0.8358732319,1.8819153731

B,0,-0.8793674956,-0.8358732319,1.8819153731

B,0,0.,-2.0711832638,1.9432332287

B,0,0.8793674956,-0.8358732319,1.8819153731

B,0,0.8793674956,0.8358732319,1.8819153731

B,0,0.,2.0711832638,-1.9432332287

B,0,-0.8793674956,0.8358732319,-1.8819153731

B,0,-0.8793674956,-0.8358732319,-1.8819153731

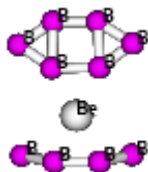
B,0,0.,-2.0711832638,-1.9432332287

B,0,0.8793674956,-0.8358732319,-1.8819153731

B,0,0.8793674956,0.8358732319,-1.8819153731

Be,0,0.,0.,0.

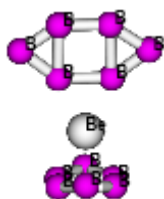
State=1-AG\HF=-312.5399665



Charge = -2 Multiplicity = 1

B,0,0.,0.8742742917,1.3245906373
 B,0,0.,-0.8742742917,1.3245906373
 B,0,0.,-2.0908405388,2.2243073715
 B,0,0.,-0.8236017312,3.0625321123
 B,0,0.,-2.0288636065,-1.9655666698
 B,0,0.,2.0288636065,-1.9655666698
 B,0,0.,2.0908405388,2.2243073715
 B,0,0.,0.8236017312,3.0625321123
 Be,0,0.,0.,-0.4790857588
 B,0,-0.8912810746,0.8276362646,-2.2271145738
 B,0,0.8912810746,-0.8276362646,-2.2271145738
 B,0,-0.8912810746,-0.8276362646,-2.2271145738
 B,0,0.8912810746,0.8276362646,-2.2271145738

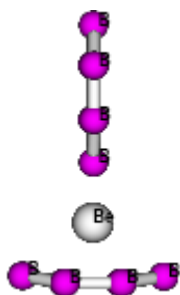
State=1-A1\HF=-312.556129



Charge = -2 Multiplicity = 1

B,0,0.,0.8575689677,-1.2974699262
 B,0,0.,-0.8575689677,-1.2974699262
 B,0,0.,-2.0731419803,-2.1855399405
 B,0,0.,-0.8214643444,-3.0309849614
 B,0,-2.0341792953,0.,1.9650846479
 B,0,2.0341792953,0.,1.9650846479
 B,0,0.,2.0731419803,-2.1855399405
 B,0,0.,0.8214643444,-3.0309849614
 Be,0,0.,0.,0.4828053875
 B,0,0.8282334934,-0.9001696481,2.1778940126
 B,0,-0.8282334934,0.9001696481,2.1778940126
 B,0,-0.8282334934,-0.9001696481,2.1778940126
 B,0,0.8282334934,0.9001696481,2.1778940126

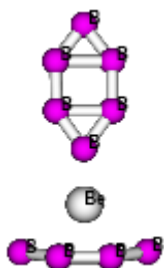
State=1-A1\HF=-312.5712758



Charge = -2 Multiplicity = 1

Be,0,-1.0214197796,0.0001246663,-0.0001289035
 B,0,3.7101788396,0.6423873964,-0.6415882178
 B,0,2.0707636482,0.6251021999,-0.6243311412
 B,0,3.7104670322,-0.6416046979,0.6408383613
 B,0,4.9122997096,0.0005733892,-0.0005515811
 B,0,-2.8086714542,0.0427516222,-1.2157322696
 B,0,-2.6081275776,-1.4441659787,-1.4459201824
 B,0,-2.6081400043,1.4441460158,1.4459177059
 B,0,-2.808676501,1.2157714525,-0.0412804807
 B,0,-2.8091602116,-1.2156270954,0.041188315
 B,0,-2.8091652581,-0.0426834213,1.2155638548
 B,0,2.0709205824,-0.6260304782,0.6252760852
 B,0,0.7944470186,-0.0007201376,0.0007226734

State=1-A\HF=-312.6121276

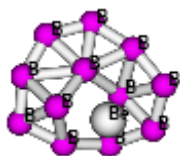


Charge = -2 Multiplicity = 1

Be,0,-1.0320144775,0.0000005629,0.0000000659
 B,0,3.6974319855,0.4552476828,-0.7874063407
 B,0,2.0610071747,0.4500248041,-0.7783711299
 B,0,3.6975191918,-0.4551826923,0.7872864835
 B,0,4.9003521336,0.0000643555,-0.0001162462
 B,0,-2.6052596032,1.0225610446,-1.7686329393
 B,0,-2.7931390858,-0.3585385911,-1.1651901129
 B,0,-2.7932578131,0.3585779632,1.1651253268
 B,0,-2.7931381847,1.1886869997,-0.2706402978
 B,0,-2.7932587141,-1.1886456217,0.2705766714
 B,0,-2.6056763759,-1.0225392574,1.7686005046
 B,0,2.0610832218,-0.4501513754,0.7785858974

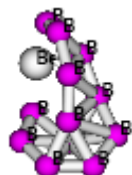
B,0,0.7919476514,-0.0001057624,0.0001821304

State=1-A\HF=-312.6141679



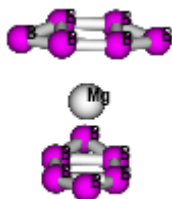
1	5	0	-1.103821	-0.652213	0.859525
2	5	0	1.014198	-1.684354	-0.588808
3	5	0	-2.137796	-1.435373	-0.194381
4	5	0	-2.288806	0.149577	-0.107827
5	5	0	-0.337645	0.715697	0.170178
6	5	0	-0.564243	-1.909501	-0.189301
7	5	0	1.162603	1.689732	0.057622
8	5	0	-0.317096	2.321728	-0.217038
9	5	0	-1.735732	1.651693	-0.215996
10	5	0	2.323820	-0.908690	-0.120294
11	5	0	1.085451	0.052612	-0.594204
12	5	0	2.372753	0.649352	0.290220
13	4	0	0.657892	-0.800326	1.062880

State=1-A\HF=-312.7588999



1	5	0	0.141360	-0.724455	-0.940930
2	5	0	1.685766	-0.544711	-0.534900
3	5	0	3.016013	0.292737	0.005316
4	5	0	2.364314	-0.770265	0.963988
5	5	0	0.789609	-0.929879	0.917910
6	5	0	-0.835907	-0.547430	0.723799
7	5	0	-1.356575	-1.211698	-1.055340
8	5	0	-1.273706	0.494502	-0.711299
9	5	0	-0.027194	1.651886	-0.384577
10	5	0	-1.168998	1.488741	0.717722
11	5	0	-2.295622	0.427799	0.902535
12	5	0	-2.477472	-0.776219	-0.062910
13	4	0	1.798015	1.436240	-0.676643

State=1-A\HF=-312.7475972



Charge = -2 Multiplicity = 1

Mg,0,0.,0.,0.

B,0,0.,2.0438503218,2.0237859816

B,0,-0.8945633166,0.8304026825,2.2149092036

B,0,-0.8945633166,-0.8304026825,2.2149092036

B,0,0.,-2.0438503218,2.0237859816

B,0,0.8945633166,-0.8304026825,2.2149092036

B,0,0.8945633166,0.8304026825,2.2149092036

B,0,0.8304026825,0.8945633166,-2.2149092036

B,0,2.0438503218,0.,-2.0237859816

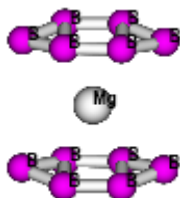
B,0,0.8304026825,-0.8945633166,-2.2149092036

B,0,-0.8304026825,-0.8945633166,-2.2149092036

B,0,-2.0438503218,0.,-2.0237859816

B,0,-0.8304026825,0.8945633166,-2.2149092036

State=1-A1\HF=-497.9745034



Charge = -2 Multiplicity = 1

B,0,0.,2.0532145029,2.115051107

B,0,-0.8868283137,0.8330659968,2.2734015752

B,0,-0.8868283137,-0.8330659968,2.2734015752

B,0,0.,-2.0532145029,2.115051107

B,0,0.8868283137,-0.8330659968,2.2734015752

B,0,0.8868283137,0.8330659968,2.2734015752

B,0,0.,2.0532145029,-2.115051107

B,0,-0.8868283137,0.8330659968,-2.2734015752

B,0,-0.8868283137,-0.8330659968,-2.2734015752

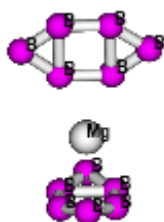
B,0,0.,-2.0532145029,-2.115051107

B,0,0.8868283137,-0.8330659968,-2.2734015752

B,0,0.8868283137,0.8330659968,-2.2734015752

Mg,0,0.,0.,0.

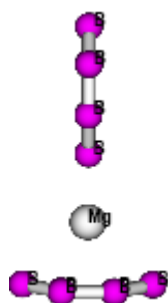
State=1-AG\HF=-497.9570995



Charge = -2 Multiplicity = 1

B,0,0.,0.847268081,-1.8026345204
 B,0,0.,-0.847268081,-1.8026345204
 B,0,0.,-2.0797037597,-2.6686274756
 B,0,0.,-0.8277880307,-3.5306861256
 B,0,-2.0329602324,0.,2.3351862957
 B,0,2.0329602324,0.,2.3351862957
 B,0,0.,2.0797037597,-2.6686274756
 B,0,0.,0.8277880307,-3.5306861256
 Mg,0,0.,0.,0.4097216976
 B,0,0.8320865904,-0.8930917697,2.5875478944
 B,0,-0.8320865904,0.8930917697,2.5875478944
 B,0,-0.8320865904,-0.8930917697,2.5875478944
 B,0,0.8320865904,0.8930917697,2.5875478944

State=1-A1\HF=-497.9501306

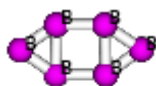


Charge = -2 Multiplicity = 1

Mg,0,-0.878528363,0.0001572806,-0.0001608599
 B,0,4.2227132518,0.6418578543,-0.6410571388
 B,0,2.5819559229,0.6296003415,-0.6288216139
 B,0,4.2225839974,-0.6417445508,0.6409802244
 B,0,5.4254940598,0.0000027706,0.0000205214
 B,0,-3.1182285527,0.0418366609,-1.2171814737
 B,0,-2.8875516668,-1.4410996004,-1.4428088418
 B,0,-2.8875640533,1.4410372312,1.4428463455
 B,0,-3.1182336041,1.2172182238,-0.040365069
 B,0,-3.1177706406,-1.2173838731,0.0405545481
 B,0,-3.1177756918,-0.0420531096,1.2173200914

B,0,2.5818533025,-0.629640071,0.6288834604
B,0,1.3209917459,-0.0000093509,0.0000150098

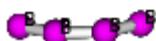
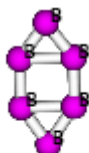
State=1-A\HF=-497.9869664



Charge = -2 Multiplicity = 1

B,0,0.,0.8498624827,1.820384771
B,0,0.,-0.8498624827,1.820384771
B,0,0.,-2.0815349323,2.6902324636
B,0,0.,-0.8277337109,3.5514591663
B,0,0.,-2.0356448359,-2.3590060738
B,0,0.,2.0356448359,-2.3590060738
B,0,0.,2.0815349323,2.6902324636
B,0,0.,0.8277337109,3.5514591663
Mg,0,0.,0.,-0.4123647141
B,0,-0.8905126583,0.8323139691,-2.6041163351
B,0,0.8905126583,-0.8323139691,-2.6041163351
B,0,-0.8905126583,-0.8323139691,-2.6041163351
B,0,0.8905126583,0.8323139691,-2.6041163351

State=1-A1\HF=-497.9433482



Charge = -2 Multiplicity = 1

Mg,0,-0.8784679772,0.000003257,-0.000004749
B,0,4.220024925,0.4542102427,-0.7856124937
B,0,2.5802015916,0.4472479079,-0.7735686937
B,0,4.2200130626,-0.4542415344,0.7856581205
B,0,5.4232079942,-0.0000201067,0.0000293178
B,0,-2.8890634664,1.0210264252,-1.7659783566
B,0,-3.1145395188,-0.35479178,-1.1656239676
B,0,-3.1145494905,0.3548148746,1.1655902932
B,0,-3.1145386214,1.1871938261,-0.2741037219

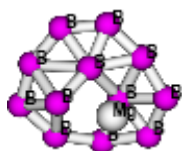
B,0,-3.1145503879,-1.1871707315,0.2740700475

B,0,-2.8890901309,-1.0210050024,1.7659471199

B,0,2.5801899112,-0.4472670402,0.7735965907

B,0,1.3210172767,-0.0000048977,0.0000071414

State=1-A1\HF=-497.9876227



1	5	0	-0.994662	-0.686642	0.634366
2	5	0	0.645511	-1.730543	-0.922255
3	5	0	-2.312711	-1.399673	-0.107972
4	5	0	-2.412119	0.153400	0.075224
5	5	0	-0.476131	0.757659	-0.006449
6	5	0	-0.861498	-2.022274	-0.403992
7	5	0	0.976720	1.658588	-0.544317
8	5	0	-0.490338	2.343980	-0.403272
9	5	0	-1.897083	1.694136	-0.093362
10	5	0	2.047777	-0.940709	-0.992955
11	5	0	0.707861	-0.043026	-0.895715
12	5	0	2.229025	0.603266	-0.666036
13	12	0	1.182354	-0.161734	1.802806

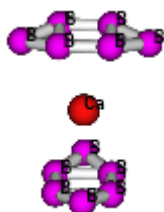
State=1-A\HF=-498.1184171



1	5	0	0.093414	-0.728426	1.004388
2	5	0	-1.428324	-0.941007	0.529535
3	5	0	-2.902627	-0.614257	-0.157632
4	5	0	-1.902770	-1.517822	-0.961360
5	5	0	-0.345901	-1.326228	-0.783601
6	5	0	1.188422	-0.661710	-0.619744
7	5	0	1.629218	-0.919110	1.319864
8	5	0	1.399882	0.651716	0.642944
9	5	0	0.230541	1.701637	-0.022519
10	5	0	1.429369	1.346049	-0.989365
11	5	0	2.604263	0.327147	-0.915250
12	5	0	2.772271	-0.604051	0.312344

13 12 0 -1.986565 1.369192 0.266831

State=1-A\HF=-498.0909108



Charge = -2 Multiplicity = 1

Ca,0,0.,0.,0.

B,0,0.,2.040134903,2.3456050919

B,0,-0.8883067965,0.8293191065,2.5664621535

B,0,-0.8883067965,-0.8293191065,2.5664621535

B,0,0.,-2.040134903,2.3456050919

B,0,0.8883067965,-0.8293191065,2.5664621535

B,0,0.8883067965,0.8293191065,2.5664621535

B,0,0.8293191065,0.8883067965,-2.5664621535

B,0,2.040134903,0.,-2.3456050919

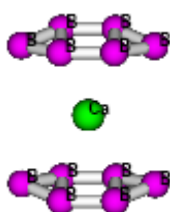
B,0,0.8293191065,-0.8883067965,-2.5664621535

B,0,-0.8293191065,-0.8883067965,-2.5664621535

B,0,-2.040134903,0.,-2.3456050919

B,0,-0.8293191065,0.8883067965,-2.5664621535

State=1-A1\HF=-975.5193788



Charge = -2 Multiplicity = 1

B,0,0.,2.0452121255,2.3830990524

B,0,-0.8860055191,0.829909776,2.582103316

B,0,-0.8860055191,-0.829909776,2.582103316

B,0,0.,-2.0452121255,2.3830990524

B,0,0.8860055191,-0.829909776,2.582103316

B,0,0.8860055191,0.829909776,2.582103316

B,0,0.,2.0452121255,-2.3830990524

B,0,-0.8860055191,0.829909776,-2.582103316

B,0,-0.8860055191,-0.829909776,-2.582103316

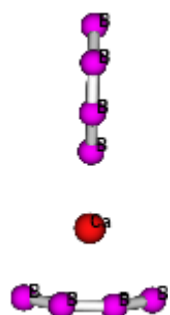
B,0,0.,-2.0452121255,-2.3830990524

B,0,0.8860055191,-0.829909776,-2.582103316

B,0,0.8860055191,0.829909776,-2.582103316

Ca,0,0.,0.,0.

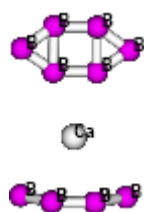
State=1-AG\HF=-975.5129579



Charge = -2 Multiplicity = 1

Ca,0,-0.7934862843,-0.0004467908,0.000442843
B,0,4.6189931036,0.638568186,-0.6377697976
B,0,2.9739839393,0.6263793446,-0.6256028725
B,0,4.6196941261,-0.6375702267,0.6368126774
B,0,5.8304721569,0.0008495299,-0.0008234887
B,0,-3.3396581188,0.0418458343,-1.2149678118
B,0,-3.1000748797,-1.4392640385,-1.4412612914
B,0,-3.100087241,1.4394910206,1.4410079951
B,0,-3.3396631564,1.2150036367,-0.0403778823
B,0,-3.3408458101,-1.2145502026,0.0399241378
B,0,-3.3408508475,-0.0414201879,1.2144862457
B,0,2.9746718345,-0.6268918982,0.6261403133
B,0,1.7173100302,-0.0006538349,0.0006604028

State=1-A\HF=-975.5085683

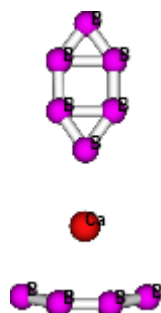


Charge = -2 Multiplicity = 1

B,0,0.,0.8362666445,2.1830979177
B,0,0.,-0.8362666445,2.1830979177
B,0,0.,-2.0769486677,3.040585843
B,0,0.,-0.8308212466,3.915086808
B,0,0.,-2.0352732645,-2.640353965
B,0,0.,2.0352732645,-2.640353965
B,0,0.,2.0769486677,3.040585843
B,0,0.,0.8308212466,3.915086808
Ca,0,0.,0.,-0.3642540154

B,0,-0.8874917381,0.8297630889,-2.8849542864
B,0,0.8874917381,-0.8297630889,-2.8849542864
B,0,-0.8874917381,-0.8297630889,-2.8849542864
B,0,0.8874917381,0.8297630889,-2.8849542864

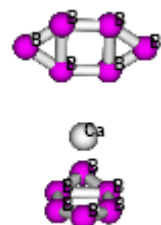
State=1-A1\HF=-975.4863102



Charge = -2 Multiplicity = 1

Ca,0,-0.7940891768,0.0000056453,-0.0000089652
B,0,4.6179507599,0.451442221,-0.7808252838
B,0,2.9733688988,0.4440626254,-0.7680597798
B,0,4.6179267085,-0.4515078802,0.7809295566
B,0,5.8292784062,-0.0000414412,0.0000658124
B,0,-3.0977967595,1.0193107201,-1.7630106411
B,0,-3.339228891,-0.3533811148,-1.1631201143
B,0,-3.3392501286,0.353428593,1.1630447144
B,0,-3.3392279966,1.1843202527,-0.2740768603
B,0,-3.339251023,-1.1842727744,0.2740014604
B,0,-3.0978510599,-1.0192666743,1.7629406924
B,0,2.9733452412,-0.4441049015,0.768126918
B,0,1.717092551,-0.0000122071,0.0000193859

State=1-A1\HF=-975.5087713

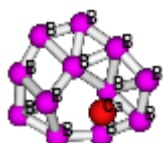


Charge = -2 Multiplicity = 1

B,0,0.,0.8354561903,-2.1756067183
B,0,0.,-0.8354561903,-2.1756067183
B,0,0.,-2.0771710868,-3.0313267883
B,0,0.,-0.8311098055,-3.9059228298
B,0,-2.0331224497,0.,2.6259831565

B,0,2.0331224497,0.,2.6259831565
 B,0,0.,2.0771710868,-3.0313267883
 B,0,0.,0.8311098055,-3.9059228298
 Ca,0,0.,0.,0.3638418476
 B,0,0.8298517071,-0.8886516405,2.8795947424
 B,0,-0.8298517071,0.8886516405,2.8795947424
 B,0,-0.8298517071,-0.8886516405,2.8795947424
 B,0,0.8298517071,0.8886516405,2.8795947424

State=1-A1\HF=-975.4898458



1	5	0	0.988753	-0.948786	-0.538346
2	5	0	-0.623175	-1.143216	1.528871
3	5	0	2.178341	-1.744242	0.312588
4	5	0	2.591587	-0.358270	-0.312365
5	5	0	0.792022	0.672826	-0.174844
6	5	0	0.658763	-1.870303	0.845701
7	5	0	-0.301161	1.997772	0.258041
8	5	0	1.228880	2.258926	-0.212744
9	5	0	2.399321	1.235137	-0.489334
10	5	0	-1.773077	-0.045334	1.578165
11	5	0	-0.319331	0.467206	1.118250
12	5	0	-1.689065	1.382553	0.874286
13	20	0	-1.532965	-0.476067	-1.197067

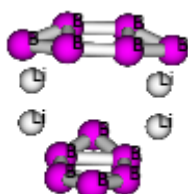
State=1-A\HF=-975.6383119



1	5	0	-0.214304	0.769462	1.042219
2	5	0	1.221124	1.247262	0.494285
3	5	0	2.683975	1.230353	-0.289357
4	5	0	1.478621	1.955364	-0.995111
5	5	0	-0.022691	1.558291	-0.702017
6	5	0	-1.476268	0.750174	-0.484595
7	5	0	-1.699939	0.627783	1.511829
8	5	0	-1.318123	-0.772195	0.556212

9	5	0	-0.463204	-1.800485	-0.514904
10	5	0	-1.759858	-1.194863	-1.153132
11	5	0	-2.911326	-0.199294	-0.823698
12	5	0	-2.924712	0.450455	0.573936
13	20	0	1.851676	-1.155577	0.196083

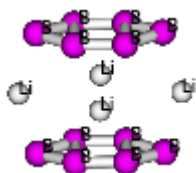
State=1-A\HF=-975.5913537



Charge = 0 Multiplicity = 1

B,0,1.195675688,0.0364999318,-1.9419546978
 B,0,-0.0365162326,-1.1956751903,-1.9419546978
 B,0,-1.195675688,-0.0364999318,-1.9419546978
 B,0,0.0365162326,1.1956751903,-1.9419546978
 B,0,-0.0364999318,1.195675688,1.9419546978
 B,0,-1.1956751903,0.0365162326,1.9419546978
 B,0,0.0364999318,-1.195675688,1.9419546978
 B,0,1.1956751903,-0.0365162326,1.9419546978
 Li,0,2.4417702937,-0.0000166446,0.
 Li,0,-2.4417702937,0.0000166446,0.
 Li,0,0.0000166446,2.4417702937,0.
 Li,0,-0.0000166446,-2.4417702937,0.
 B,0,1.4360475829,1.4360280051,1.684900712
 B,0,-1.4360475829,-1.4360280051,1.684900712
 B,0,-1.4360280051,1.4360475829,-1.684900712
 B,0,1.4360280051,-1.4360475829,-1.684900712

State=1-A1\HF=-328.104283

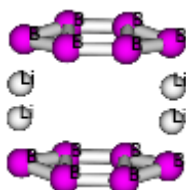


Charge = 0 Multiplicity = 1

B,0,2.1310024631,2.0661882578,0.
 B,0,2.0790011246,0.8333409858,0.8791697907
 B,0,2.0790011246,-0.8333409858,0.8791697907
 B,0,2.1310024631,-2.0661882578,0.
 B,0,2.0790011246,-0.8333409858,-0.8791697907
 B,0,2.0790011246,0.8333409858,-0.8791697907

B,0,-2.1310024631,2.0661882578,0.
 B,0,-2.0790011246,0.8333409858,0.8791697907
 B,0,-2.0790011246,-0.8333409858,0.8791697907
 B,0,-2.1310024631,-2.0661882578,0.
 B,0,-2.0790011246,-0.8333409858,-0.8791697907
 B,0,-2.0790011246,0.8333409858,-0.8791697907
 Li,0,0.,0.,-1.5200471845
 Li,0,0.,0.,1.5200471845
 Li,0,0.,2.6668343602,0.
 Li,0,0.,-2.6668343602,0.

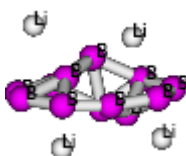
State=1-AG\HF=-328.0603195



Charge = 0 Multiplicity = 1

B,0,1.203628033,0.0377526412,-2.0071706661
 B,0,-0.0377391903,-1.2036259933,-2.0071721422
 B,0,-1.2036308836,-0.0377450173,-2.0071691001
 B,0,0.0377363398,1.2036336172,-2.007167624
 B,0,0.0377391903,1.2036259933,2.0071721422
 B,0,-1.203628033,-0.0377526412,2.0071706661
 B,0,-0.0377363398,-1.2036336172,2.007167624
 B,0,1.2036308836,0.0377450173,2.0071691001
 Li,0,2.4644483081,-0.5544612422,-0.000002803
 Li,0,-2.4644483081,0.5544612422,0.000002803
 Li,0,-0.5544838963,2.4644432112,0.0000050742
 Li,0,0.5544838963,-2.4644432112,-0.0000050742
 B,0,1.4511050284,-1.451093942,1.8944215093
 B,0,-1.451102338,1.4510867463,1.8944290819
 B,0,-1.4511050284,1.451093942,-1.8944215093
 B,0,1.451102338,-1.4510867463,-1.8944290819

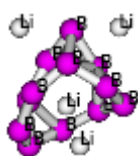
State=1-AG\HF=-328.1033325



5	0	-0.001980	-1.197062	0.900237
5	0	-0.521220	-1.357217	-0.784870

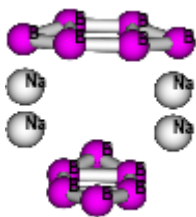
5	0	-2.519240	0.226299	0.352297
5	0	-1.833642	1.589359	0.248819
5	0	1.023798	0.282171	0.431758
5	0	-1.670498	-1.132954	0.330510
5	0	2.481587	0.908657	-0.243365
5	0	1.289064	1.892014	-0.180213
5	0	-0.284343	1.816709	-0.077495
5	0	1.123637	-1.536991	-0.208432
5	0	-1.067085	0.327508	-0.554514
5	0	2.388319	-0.606986	-0.361158
3	0	1.993553	-1.364409	1.768054
3	0	-0.987564	0.456830	1.977538
3	0	-2.553214	-1.180741	-1.580668
3	0	0.866561	0.069143	-1.920883

State=1-A\HF=-328.274168



1	5	0	1.904446	0.996159	-0.844585
2	5	0	-0.476686	2.024844	0.557078
3	5	0	-0.289571	-0.600946	-1.359763
4	5	0	1.783635	-1.230722	0.735788
5	5	0	-0.993601	0.906610	-0.599206
6	5	0	-1.824496	-0.409367	-1.187276
7	5	0	0.249018	-1.465730	0.649874
8	3	0	-0.539681	-0.914182	2.523421
9	5	0	-1.249366	-0.721196	0.480802
10	5	0	2.599979	-0.176108	-0.130157
11	5	0	1.180242	-0.796146	-0.750761
12	5	0	0.557710	1.830392	-0.593543
13	5	0	-1.186899	0.774894	1.180984
14	3	0	1.300955	0.931673	1.360560
15	3	0	-1.387687	-2.484788	-0.872748
16	3	0	-3.130938	0.579489	0.090041

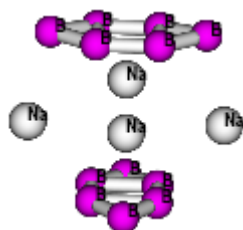
State=1-A\HF=-328.2410901



Charge = 0 Multiplicity = 1

B,0,1.1987565668,0.0357145946,-2.1310104753
 B,0,-0.0357309375,-1.1987560798,-2.1310104753
 B,0,-1.1987565668,-0.0357145946,-2.1310104753
 B,0,0.0357309375,1.1987560798,-2.1310104753
 B,0,-0.0357145946,1.1987565668,2.1310104753
 B,0,-1.1987560798,0.0357309375,2.1310104753
 B,0,0.0357145946,-1.1987565668,2.1310104753
 B,0,1.1987560798,-0.0357309375,2.1310104753
 Na,0,2.7505216263,-0.0000187492,0.
 Na,0,-2.7505216263,0.0000187492,0.
 Na,0,0.0000187492,2.7505216263,0.
 Na,0,-0.0000187492,-2.7505216263,0.
 B,0,1.4496341829,1.4496144199,1.9636253998
 B,0,-1.4496341829,-1.4496144199,1.9636253998
 B,0,-1.4496144199,1.4496341829,-1.9636253998
 B,0,1.4496144199,-1.4496341829,-1.9636253998

State=1-A1\HF=-947.1883299

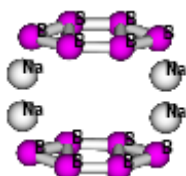


Charge = 0 Multiplicity = 1

B,0,-2.1549674538,0.8332011263,0.8755152116
 B,0,-2.2386873132,2.0642309392,-0.0057354821
 B,0,-2.1566475754,0.8264661695,-0.8775977195
 B,0,-2.1549666926,-0.8332030906,-0.8755152159
 B,0,-2.2386854315,-2.0642329799,0.0057354777
 B,0,-2.1566468238,-0.8264681354,0.8775977152
 B,0,2.2386853843,0.0058621107,2.0642315845
 B,0,2.1566546265,0.8776340631,0.8264008184
 B,0,2.1549600315,0.8754802879,-0.833268163
 B,0,2.2386853938,-0.00586007,-2.0642315801
 B,0,2.1566554281,-0.8776320972,-0.8264008141

B,0,2.1549608279,-0.8754783235,0.8332681672
 Na,0,-0.2316191096,-0.0207224307,2.5944029152
 Na,0,-0.2316191233,0.0207222196,-2.5944029157
 Na,0,0.2316178426,2.5944015755,0.0207497098
 Na,0,0.2316202076,-2.5944013643,-0.0207497093

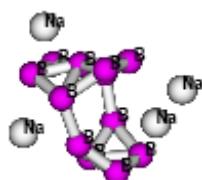
State=1-A\HF=-947.1594536



Charge = 0 Multiplicity = 1

B,0,-0.7074369247,-2.40968577,-0.0364124043
 B,0,-1.5842934027,-1.5328411379,1.2036572751
 B,0,-2.4096804135,-0.7074558198,0.0363997759
 B,0,-1.5328239355,-1.5843004519,-1.2036699035
 B,0,1.5842934027,1.5328411379,-1.2036572751
 B,0,0.7074369247,2.40968577,0.0364124043
 B,0,1.5328239355,1.5843004519,1.2036699035
 B,0,2.4096804135,0.7074558198,-0.0363997759
 Na,0,1.9635483256,-1.9635350554,0.4952251341
 Na,0,-1.9635483256,1.9635350554,-0.4952251341
 Na,0,-0.3501976987,0.350206224,-2.7768610061
 Na,0,0.3501976987,-0.350206224,2.7768610061
 B,0,2.5337957922,0.4748067262,1.4559210301
 B,0,0.4747929114,2.5338053845,-1.4559088413
 B,0,-2.5337957922,-0.4748067262,-1.4559210301
 B,0,-0.4747929114,-2.5338053845,1.4559088413

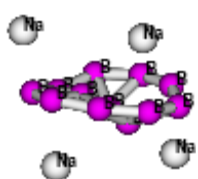
State=1-AG\HF=-947.1833105



1	5	0	1.253170	1.159071	0.628634
2	5	0	0.267069	-1.287702	1.087068
3	5	0	-1.417382	1.000643	1.484869
4	5	0	1.611726	0.560566	-1.955032
5	5	0	-1.034236	-0.370294	0.734566
6	5	0	-2.205993	0.626426	0.190089

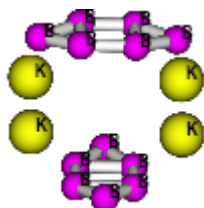
7	5	0	0.017565	0.504238	-1.760631
8	11	0	1.544871	-1.885917	-1.429642
9	5	0	-1.291394	-0.258955	-0.995302
10	5	0	2.337208	0.709981	-0.562771
11	5	0	0.978261	1.645119	-0.911716
12	5	0	0.187066	0.378462	1.678255
13	5	0	-0.615845	-1.657050	-0.175520
14	11	0	2.651094	-0.608956	1.826385
15	11	0	-1.059095	2.905620	-0.194842
16	11	0	-3.176513	-1.779158	0.051506

State=1-A\HF=-947.2585558



1	5	0	-0.168625	0.028048	-0.914757
2	5	0	0.818725	-1.068700	-1.672827
3	5	0	2.194748	0.902764	0.428419
4	5	0	1.329931	1.230338	1.757353
5	5	0	-1.109658	0.567139	0.325656
6	5	0	1.588227	0.196032	-0.869962
7	5	0	-2.455133	-0.510025	0.740794
8	5	0	-1.778950	0.362182	1.835889
9	5	0	-0.233292	0.931456	1.932493
10	5	0	-0.631041	-1.587097	-1.428321
11	5	0	0.645755	0.380713	0.568286
12	5	0	-1.810181	-1.393594	-0.396574
13	11	0	-2.728613	0.408958	-1.805427
14	11	0	0.504624	2.780552	-0.330754
15	11	0	3.480837	-1.238882	-0.678889
16	11	0	-0.525260	-1.968472	1.766684

State=1-A\HF=-947.3271679

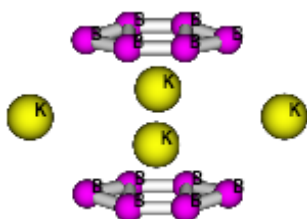


Charge = 0 Multiplicity = 1

B,0,1.2009153376,0.034738964,-2.2872212325

B,0,-0.0347553019,-1.2009148649,-2.2872212325
 B,0,-1.2009153376,-0.034738964,-2.2872212325
 B,0,0.0347553019,1.2009148649,-2.2872212325
 B,0,-0.034738964,1.2009153376,2.2872212325
 B,0,-1.2009148649,0.0347553019,2.2872212325
 B,0,0.034738964,-1.2009153376,2.2872212325
 B,0,1.2009148649,-0.0347553019,2.2872212325
 K,0,3.2037368839,-0.0000217927,0.
 K,0,-3.2037368839,0.0000217927,0.
 K,0,0.0000217927,3.2037368839,0.
 K,0,-0.0000217927,-3.2037368839,0.
 B,0,1.4561843515,1.456164541,2.1773180893
 B,0,-1.4561843515,-1.456164541,2.1773180893
 B,0,-1.456164541,1.4561843515,-2.1773180893
 B,0,1.456164541,-1.4561843515,-2.1773180893

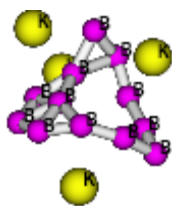
State=1-A1\HF=-2697.7440601



Charge = 0 Multiplicity = 1

B,0,-2.4542801481,0.,2.0591609663
 B,0,-2.5580013296,0.8781818363,0.8290317936
 B,0,-2.5580013296,0.8781818363,-0.8290317936
 B,0,-2.4542801481,0.,-2.0591609663
 B,0,-2.5580013296,-0.8781818363,-0.8290317936
 B,0,-2.5580013296,-0.8781818363,0.8290317936
 B,0,2.4542801481,0.,2.0591609663
 B,0,2.5580013296,0.8781818363,0.8290317936
 B,0,2.5580013296,0.8781818363,-0.8290317936
 B,0,2.4542801481,0.,-2.0591609663
 B,0,2.5580013296,-0.8781818363,-0.8290317936
 B,0,2.5580013296,-0.8781818363,0.8290317936
 K,0,0.,-2.1774133848,0.
 K,0,0.,2.1774133848,0.
 K,0,0.,0.,3.7163490455
 K,0,0.,0.,-3.7163490455

State=1-AG\HF=-2697.7246534



1	5	0	-0.154951	-0.149836	1.170946
2	5	0	-0.352224	0.942911	2.405435
3	5	0	-1.407491	-1.341099	1.301844
4	5	0	-2.927998	-1.189984	-1.343321
5	5	0	-2.202313	-1.568713	-0.066531
6	5	0	-1.116431	-0.414333	2.524885
7	5	0	1.217210	0.340298	-1.884693
8	5	0	-0.316786	0.366135	-1.873938
9	5	0	-1.751791	-0.309891	-1.709409
10	5	0	0.505789	1.405469	1.155376
11	5	0	0.938004	0.458947	-0.063480
12	5	0	2.165640	-0.407195	-0.920272
13	19	0	1.636628	3.052441	-1.122988
14	19	0	-3.048826	1.263670	0.658912
15	19	0	0.302485	-2.640881	-1.616341
16	19	0	2.531646	-1.183837	1.897038

State=1-A\HF=-2697.8664437



1	5	0	-1.043939	1.557150	-0.480407
2	5	0	-0.604783	-0.980332	-1.174566
3	5	0	1.503520	0.926348	-1.483622
4	5	0	-1.385368	0.896488	2.089637
5	5	0	0.889715	-0.408895	-0.832178
6	5	0	2.251987	0.289007	-0.272069
7	5	0	0.160099	0.500490	1.779579
8	19	0	-1.755595	-1.937403	1.952953
9	5	0	1.217484	-0.485017	0.895545
10	5	0	-2.126413	1.353750	0.776066
11	5	0	-0.548869	1.846354	1.055256
12	5	0	-0.205620	0.660513	-1.638371
13	5	0	0.213278	-1.633454	0.011162
14	19	0	-3.185574	0.197780	-1.909267
15	19	0	1.952127	3.070993	0.472659

16 19 0 2.904545 -2.521475 -0.707407

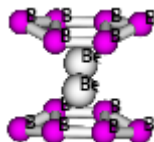
State=1-A\HF=-2697.8131821



Charge = 0 Multiplicity = 1

B,0,-1.0025972577,1.3724172719,0.809031615
B,0,-0.9169918547,1.4964576762,-0.8483064399
B,0,-1.0396454198,0.081208106,-1.5307953851
B,0,-1.0025958338,-1.3724183663,-0.8090316218
B,0,-0.9169903137,-1.4964586822,0.8483064336
B,0,-1.0396453461,-0.0812092388,1.530795378
B,0,0.572914246,-0.7228075415,1.1352106213
B,0,0.4246408677,0.896067787,1.5283058722
B,0,1.6627845122,0.5989550074,0.4647989151
B,0,0.5729135065,0.7228080753,-1.1352106177
B,0,0.424641804,-0.8960674064,-1.5283058695
B,0,1.6627851343,-0.5989533472,-0.4647989043
Be,0,0.530510535,2.0776079856,0.1308215368
Be,0,0.5305126832,-2.0776074955,-0.1308215334

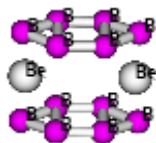
State=1-A\HF=-327.5183294



Charge = 0 Multiplicity = 1

B,0,2.0540526743,2.0791982548,0.
B,0,1.7194524804,0.8681254476,0.859121356
B,0,1.7194524804,-0.8681254476,0.859121356
B,0,2.0540526743,-2.0791982548,0.
B,0,1.7194524804,-0.8681254476,-0.859121356
B,0,1.7194524804,0.8681254476,-0.859121356
B,0,-2.0540526743,2.0791982548,0.
B,0,-1.7194524804,0.8681254476,0.859121356
B,0,-1.7194524804,-0.8681254476,0.859121356
B,0,-2.0540526743,-2.0791982548,0.
B,0,-1.7194524804,-0.8681254476,-0.859121356
B,0,-1.7194524804,0.8681254476,-0.859121356
Be,0,0.,0.,-1.1756927735
Be,0,0.,0.,1.1756927735

State=1-AG\HF=-327.1658417



Charge = 0 Multiplicity = 1

B,0,-1.8234914024,0.,2.0489341675
B,0,-1.7670349245,0.9008071362,0.8250062009
B,0,-1.7670349245,0.9008071362,-0.8250062009
B,0,-1.8234914024,0.,-2.0489341675
B,0,-1.7670349245,-0.9008071362,-0.8250062009
B,0,-1.7670349245,-0.9008071362,0.8250062009
B,0,1.8234914024,0.,2.0489341675
B,0,1.7670349245,0.9008071362,0.8250062009
B,0,1.7670349245,0.9008071362,-0.8250062009
B,0,1.8234914024,0.,-2.0489341675
B,0,1.7670349245,-0.9008071362,-0.8250062009
B,0,1.7670349245,-0.9008071362,0.8250062009
Be,0,0.,0.,-1.9257016508
Be,0,0.,0.,1.9257016508

State=1-AG\HF=-327.3574606



1	5	0	1.524615	1.746834	0.209795
2	5	0	-1.976303	-0.720661	0.567069
3	5	0	-1.369150	1.522907	-0.034740
4	5	0	0.065197	2.155856	0.460119
5	5	0	0.303543	0.970443	-0.658678
6	5	0	-1.070368	-0.015493	-0.802266
7	5	0	-2.595866	0.527624	-0.072885
8	5	0	-0.568289	-1.420435	1.021459
9	5	0	0.793441	-1.884188	0.265074
10	5	0	2.106848	-1.103378	-0.097804
11	5	0	2.345293	0.422803	-0.144150
12	5	0	0.472348	-0.677598	-0.954018
13	4	0	0.852473	-0.073846	1.042900
14	4	0	-0.891609	-1.832047	-0.741619

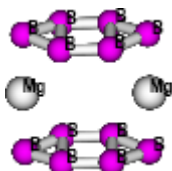
State=1-A\HF=-327.489281



Charge = 0 Multiplicity = 1

B,0,-1.037188091,1.4565865107,0.7870656372
 B,0,-1.0367628081,1.4569184281,-0.7857308661
 B,0,-1.1017533363,0.0003950044,-1.5598815144
 B,0,-1.0371865801,-1.4565876409,-0.7870656446
 B,0,-1.0367613077,-1.4569195579,0.7857308587
 B,0,-1.1017533468,-0.0003962013,1.5598815066
 B,0,0.343577503,-0.8152271406,1.5543492268
 B,0,0.3442154884,0.8142385601,1.5559850642
 B,0,1.6198820719,-0.0001494324,0.7828686755
 B,0,0.3435766712,0.8152274374,-1.5543492246
 B,0,0.3442163408,-0.8142382626,-1.555985062
 B,0,1.6198820772,0.0001510484,-0.7828686645
 Mg,0,1.0996451468,2.2134325129,0.0009356386
 Mg,0,1.0996474345,-2.2134314346,-0.0009356312

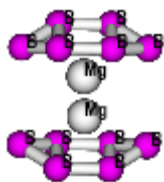
State=1-A\HF=-698.2076604



Charge = 0 Multiplicity = 1

B,0,-2.2236279658,0.,2.0527396928
 B,0,-2.1465273323,0.8984410567,0.8259281113
 B,0,-2.1465273323,0.8984410567,-0.8259281113
 B,0,-2.2236279658,0.,-2.0527396928
 B,0,-2.1465273323,-0.8984410567,-0.8259281113
 B,0,-2.1465273323,-0.8984410567,0.8259281113
 B,0,2.2236279658,0.,2.0527396928
 B,0,2.1465273323,0.8984410567,0.8259281113
 B,0,2.1465273323,0.8984410567,-0.8259281113
 B,0,2.2236279658,0.,-2.0527396928
 B,0,2.1465273323,-0.8984410567,-0.8259281113
 B,0,2.1465273323,-0.8984410567,0.8259281113
 Mg,0,0.,0.,-2.1133539874
 Mg,0,0.,0.,2.1133539874

State=1-AG\HF=-698.0870114



Charge = 0 Multiplicity = 1

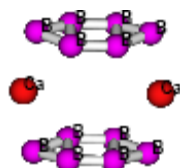
B,0,1.7225559483,2.0044927242,0.
B,0,2.1315009154,0.8351287373,0.8668351831
B,0,2.1315009154,-0.8351287373,0.8668351831
B,0,1.7225559483,-2.0044927242,0.
B,0,2.1315009154,-0.8351287373,-0.8668351831
B,0,2.1315009154,0.8351287373,-0.8668351831
B,0,-1.7225559483,2.0044927242,0.
B,0,-2.1315009154,0.8351287373,0.8668351831
B,0,-2.1315009154,-0.8351287373,0.8668351831
B,0,-1.7225559483,-2.0044927242,0.
B,0,-2.1315009154,-0.8351287373,-0.8668351831
B,0,-2.1315009154,0.8351287373,-0.8668351831
Mg,0,0.,0.,-1.4203928154
Mg,0,0.,0.,1.4203928154

State=1-AG\HF=-697.9462859



1	5	0	-3.222026	1.300806	-0.016903
2	5	0	2.511446	1.788466	-0.133116
3	5	0	-0.518958	2.297932	-0.140167
4	5	0	-2.063882	2.297774	-0.184886
5	5	0	-1.648487	0.658827	0.131345
6	5	0	1.516584	0.765965	0.577510
7	5	0	1.093435	2.293108	-0.095831
8	5	0	1.775903	-2.035264	-0.086309
9	5	0	1.096217	-0.757903	0.765555
10	5	0	0.191073	-1.924269	0.063318
11	5	0	-3.262891	-0.238162	-0.006556
12	5	0	-0.430077	-0.426933	0.351672
13	12	0	-2.080815	-2.074217	-0.213566
14	12	0	3.314842	-0.434261	-0.297114

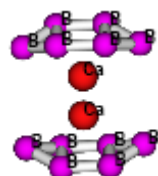
State=1-A\HF=-698.1872302



Charge = 0 Multiplicity = 1

B,0,-2.3424530919,0.2065397172,1.1968283575
B,0,-2.4439721051,1.7206428577,1.1178123865
B,0,-2.3421983972,1.1774528456,-0.2977386751
B,0,-2.3424505781,-0.2065656841,-1.1968289247
B,0,-2.4439532316,-1.7206699227,-1.1178129775
B,0,-2.3421857301,-1.1774788097,0.2977381079
B,0,2.5098878836,1.7135918585,1.1287554646
B,0,2.408997809,1.1801373383,-0.2904071895
B,0,2.4085324672,-0.1987625517,-1.1973125303
B,0,2.5099066831,-1.7135653375,-1.1287548983
B,0,2.4090105066,-1.1801119086,0.2904077321
B,0,2.4085300374,0.1987879763,1.1973130729
Ca,0,0.032823539,2.0606442129,1.3470782794
Ca,0,0.0328461437,-2.0606444863,-1.3470782918

State=1-A\HF=-1653.1219055

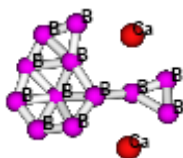


Charge = 0 Multiplicity = 1

B,0,1.9246602254,2.0061340331,0.
B,0,2.3226891541,0.8318079869,0.8663162338
B,0,2.3226891541,-0.8318079869,0.8663162338
B,0,1.9246602254,-2.0061340331,0.
B,0,2.3226891541,-0.8318079869,-0.8663162338
B,0,2.3226891541,0.8318079869,-0.8663162338
B,0,-1.9246602254,2.0061340331,0.
B,0,-2.3226891541,0.8318079869,0.8663162338
B,0,-2.3226891541,-0.8318079869,0.8663162338
B,0,-1.9246602254,-2.0061340331,0.
B,0,-2.3226891541,-0.8318079869,-0.8663162338
B,0,-2.3226891541,0.8318079869,-0.8663162338
Ca,0,0.,0.,-1.7005008697

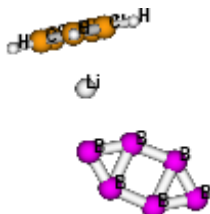
Ca,0,0.,0.,1.7005008697

State=1-AG\HF=-1653.0678261



1	5	0	0.841156	-3.140536	0.128558
2	5	0	2.602897	1.466512	-0.217194
3	5	0	2.983951	-1.346676	0.143781
4	5	0	2.342155	-2.793252	0.151348
5	5	0	1.219027	-1.530729	0.370055
6	5	0	1.680545	0.076173	-0.066394
7	5	0	3.378055	0.173273	0.017441
8	5	0	-2.832231	1.034858	0.624995
9	5	0	-1.061828	0.714629	0.700188
10	5	0	-1.767858	2.039782	1.012135
11	5	0	-0.256953	-2.054404	-0.139856
12	5	0	-0.048705	-0.430258	0.066758
13	20	0	-2.701751	-1.179609	-0.379030
14	20	0	0.431698	2.627267	-0.318924

State=1-A\HF=-1653.2294343



Charge = -2 Multiplicity = 1^M

B,0,-1.3756480317,-1.416524244,-0.0108469494
B,0,-1.8885256931,0.0299328617,-0.0030864885
B,0,-4.7120777916,1.0283841968,0.0066281215
B,0,-2.8959575698,-1.4041108264,-0.0082609674
B,0,-4.2205454239,-0.4100479781,-0.0011702824
B,0,-3.1953865079,1.0492298316,0.0041910859
Li,0,0.6474316343,-0.3760471995,-0.0046192523
C,0,2.5882061875,0.122139481,-1.2002513773
C,0,2.2353613421,1.2656700761,-0.4424179739
C,0,2.9033903722,-0.9224215654,-0.2965986051
H,0,2.5768515568,0.046724236,-2.2820496311
C,0,2.33512167,0.9285326389,0.9300926648

H,0,1.9089336118,2.2195264438,-0.84119979
 C,0,2.7480106013,-0.4231319077,1.0201602774
 H,0,3.175107357,-1.9373559024,-0.5653415201
 H,0,2.0971511689,1.5797742513,1.7637501504
 H,0,2.879825454,-0.9895789754,1.9355160343

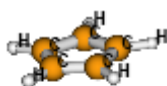
|State=1-A|HF=-350.0463939



Charge = -2 Multiplicity = 1

B,0,0.0864834009,-2.067119785,-2.7612489933
 B,0,0.0372487246,-0.8320353383,-1.8824213163
 B,0,-0.0939461311,2.0782338561,-2.7559031278
 B,0,0.0271163521,-0.8213913983,-3.6365793439
 B,0,-0.0448979659,0.8338717335,-3.6339560296
 B,0,-0.0352993538,0.8418274339,-1.8796537377
 Li,0,0.0071221804,-0.0000003835,0.3915728782
 C,0,1.2075314666,-0.0161448815,2.3373617419
 C,0,0.3856536618,1.1385805038,2.3400123137
 C,0,0.3642492511,-1.1550815367,2.3332538173
 H,0,2.2914732304,-0.0263712808,2.3059858141
 C,0,-0.9653400458,0.7131617068,2.3374270073
 H,0,0.7287231655,2.1658946187,2.299974081
 C,0,-0.9785420994,-0.7044359539,2.3332507113
 H,0,0.6884446027,-2.188154628,2.2861611738
 H,0,-1.8348100831,1.3597042621,2.3002183205
 H,0,-1.8600359973,-1.3344833629,2.2939211701

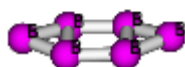
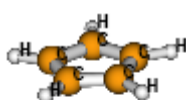
State=1-A|HF=-350.0300568



5	0	4.451740	1.469924	0.004500
5	0	3.655044	0.534073	-0.888612
5	0	1.922724	-1.799131	-0.007133

5	0	3.671028	0.515680	0.892122
5	0	2.677054	-0.810253	0.882241
5	0	2.661517	-0.792244	-0.889201
11	0	-0.251086	-0.453747	-0.001831
6	0	-3.011451	-0.856717	-0.219796
6	0	-2.822725	-0.278800	1.059577
6	0	-2.690711	0.120991	-1.193543
1	0	-3.326805	-1.876104	-0.419121
6	0	-2.384997	1.056449	0.876889
1	0	-2.972170	-0.776372	2.012739
6	0	-2.303351	1.303734	-0.515921
1	0	-2.723207	-0.015780	-2.269946
1	0	-2.143874	1.763082	1.664560
1	0	-1.988119	2.232210	-0.980908

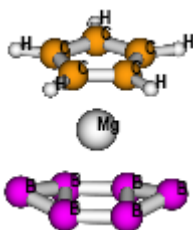
State=1-A\HF=-504.810682



Charge = -2 Multiplicity = 1^M

B,0,-3.0478458877,2.0637100434,-0.0060858064
 B,0,-3.1434569305,0.8331807187,0.8838925518
 B,0,-3.0486952701,-2.0635878824,0.0050638807
 B,0,-3.1427198531,0.8282638921,-0.889356313
 B,0,-3.1434945399,-0.8330372777,-0.884996798
 B,0,-3.1437865955,-0.8281066717,0.8882868792
 C,0,2.7549560622,-1.1601263514,0.3204460895
 C,0,2.7555168661,-0.6622839931,-1.0049968918
 C,0,2.7529978566,-0.0529188546,1.2034632529
 H,0,2.7463043245,-2.206938611,0.6088481556
 C,0,2.7540722625,0.7527671603,-0.9411380246
 H,0,2.751794523,-1.2610960593,-1.9110737639
 C,0,2.7525480654,1.1293208914,0.4236393722
 H,0,2.7486913817,-0.1019586233,2.2885432283
 H,0,2.747842426,1.4307162226,-1.7895615668
 H,0,2.7417072861,2.1460125188,0.8047958247
 K,0,-0.1582574333,-0.0026001408,0.0003128085

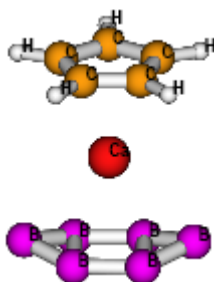
|State=1-A\HF=-942.4525441



Charge = -1 Multiplicity = 1^M

B,0,-2.0342730798,2.0195008766,-0.0026068285
 B,0,-2.2946875735,0.8218654272,0.8908827016
 B,0,-2.0127880493,-2.0427423907,0.0013434825
 B,0,-2.2924791563,0.8202514674,-0.8944931137
 B,0,-2.2833450321,-0.8478478078,-0.8926861525
 B,0,-2.2854642712,-0.8462831968,0.8926429333
 C,0,1.9467577276,-1.1553287662,0.317803639
 C,0,1.9400189133,-0.654783992,-1.0079768134
 C,0,1.9349519904,-0.0461294123,1.205770346
 H,0,1.9213922084,-2.1985298771,0.6031022717
 C,0,1.9349489275,0.767461853,-0.9412855708
 H,0,1.9329804195,-1.2503560269,-1.9117756257
 C,0,1.9369080167,1.1419445475,0.4250055959
 H,0,1.9344197769,-0.0969966336,2.2872598719
 H,0,1.9191725911,1.444774597,-1.7853175603
 H,0,1.9042032914,2.1539058901,0.8061748648
 Mg,0,-0.1465413274,0.0003745659,0.0024364904

|State=1-A|HF=-542.671122

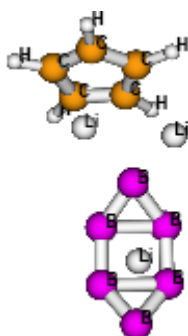


Charge = -1 Multiplicity = 1^M

B,0,-2.3447864134,2.0262872651,0.0089780778
 B,0,-2.6262003724,0.8262327872,0.8934862699
 B,0,-2.3467174242,-2.027153069,-0.0088101597
 B,0,-2.6282677578,0.8338281057,-0.885122239
 B,0,-2.6295750725,-0.8268490958,-0.8925796243
 B,0,-2.6274825116,-0.8345275113,0.8860207207
 C,0,2.2642507073,-1.1615430514,0.317065756
 C,0,2.2628827089,-0.6588666806,-1.0074527558

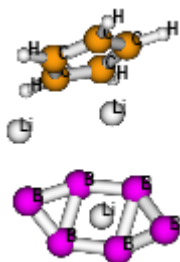
C,0,2.2579143537,-0.0558645613,1.2045822797
 H,0,2.2771149623,-2.2068135632,0.6010874684
 C,0,2.2590213323,0.758217584,-0.9387900611
 H,0,2.2831504441,-1.2536362478,-1.9130476834
 C,0,2.2568662764,1.1305117656,0.4279136605
 H,0,2.2777700837,-0.1083918829,2.2869326482
 H,0,2.2737077023,1.4378916336,-1.7825595417
 H,0,2.263187417,2.1436175782,0.8113414663
 Ca,0,-0.1582697561,-0.0038245132,-0.001676643

State=1-A\HF=-1020.2166393



5	0	1.055234	0.434100	0.656047
5	0	2.006785	-0.727422	0.349454
5	0	4.836945	-0.453545	-0.390572
5	0	2.274262	0.947216	-0.119598
5	0	3.788350	0.602050	-0.639675
5	0	3.513034	-1.134199	-0.148826
3	0	-0.957225	-0.582158	0.578079
6	0	-2.528295	-0.905049	-0.973406
6	0	-3.020085	-1.137075	0.334840
6	0	-2.278619	0.482145	-1.108524
1	0	-2.400367	-1.648018	-1.749848
6	0	-3.048927	0.098656	1.022272
1	0	-3.334218	-2.093429	0.734389
6	0	-2.601657	1.106497	0.130283
1	0	-2.009301	0.977008	-2.038217
1	0	-3.391292	0.259680	2.036258
1	0	-2.645020	2.175167	0.329765
3	0	-0.403674	1.682793	-0.314383
3	0	3.785114	0.271882	1.643210

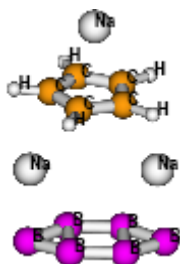
State=1-A\HF=-365.1769888



Charge = 0 Multiplicity = 1^M

B,0,-1.9406115019,1.9358890805,0.0587206318^M
 B,0,-1.5707218883,0.4330201673,0.048714349^M
 B,0,-3.161091932,-1.9271629361,-0.0424817687^M
 B,0,-3.0832274289,1.0823763784,-0.4467695663^M
 B,0,-3.4388163419,-0.5218611633,-0.561532699^M
 B,0,-1.8539849986,-1.1914371055,-0.0351954496^M
 Li,0,0.5743085993,-0.6661491386,-0.0376775574^M
 C,0,2.1180248505,0.8482501909,0.7387200766^M
 C,0,2.4322500849,-0.4776088349,1.1290510733^M
 C,0,2.1191235393,0.8952298812,-0.6874535268^M
 H,0,2.0397950506,1.6894720122,1.42493052^M
 C,0,2.6398549605,-1.2412176987,-0.0434177314^M
 H,0,2.5302648831,-0.8289850536,2.1478071786^M
 C,0,2.4343215253,-0.4013090414,-1.1635206701^M
 H,0,2.0293886218,1.777414106,-1.317745111^M
 H,0,2.9105148931,-2.2887458077,-0.0780052587^M
 H,0,2.5277488391,-0.6853341461,-2.203290948^M
 Li,0,0.245193747,2.033401666,0.0936020618^M
 Li,0,-3.2384662104,-0.1865892609,1.6369924304^M

|State=1-A|HF=-365.1683717

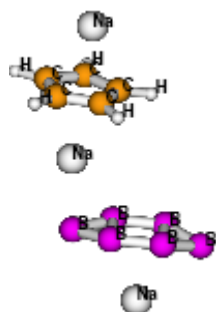


Charge = 0 Multiplicity = 1

B,0,3.0500145024,2.0988749721,-0.0000040889
 B,0,3.0630386614,0.8636979065,0.8903904516
 B,0,3.3020854459,-2.014249392,0.0001289418
 B,0,3.0636479819,0.8628467165,-0.889478343
 B,0,3.1856918693,-0.788411709,-0.8920905109
 B,0,3.1851215221,-0.7875311065,0.8913170846

Na,0,0.8431131634,-1.8936140794,-0.0003215768
 Na,0,0.6189020667,1.9237386727,-0.0011057091
 C,0,-1.7607348902,-0.9488114956,-0.7131850605
 C,0,-1.7644031822,-0.9524843089,0.7128960457
 C,0,-1.8879746741,0.3940469899,-1.1492242056
 H,0,-1.6903940663,-1.8154409645,-1.3626128765
 C,0,-1.8936788001,0.3881060807,1.1550910542
 H,0,-1.6967515754,-1.8223898148,1.3581724884
 C,0,-1.983746873,1.2205515411,0.00489626
 H,0,-1.8939426066,0.7284370663,-2.1793084191
 H,0,-1.904193188,0.7173823604,2.1867556924
 H,0,-2.1299746789,2.2965228089,0.0074408101
 Na,0,-4.1156073465,-0.2018610693,-0.0053554354

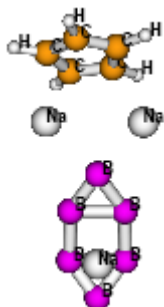
State=1-A\HF=-829.4477739



Charge = 0 Multiplicity = 1

B,0,3.7375104462,2.1078231117,-0.1405099109
 B,0,3.076663303,1.0293318645,-0.9713245911
 B,0,2.1775771482,-1.6585212262,0.0976903635
 B,0,3.06988757,1.1457055759,0.8179402206
 B,0,2.483887803,-0.4017537978,0.9052337299
 B,0,2.4900019082,-0.5164972949,-0.86305976
 C,0,-2.9857945995,-1.135485475,-0.3451294178
 C,0,-2.8230864873,-0.702876873,1.0001258719
 C,0,-2.5131189916,-0.1004540061,-1.199433935
 H,0,-3.3668092602,-2.0988248091,-0.6624221141
 C,0,-2.2501053025,0.5991764788,0.9767464569
 H,0,-3.0561771745,-1.2798976851,1.8869797239
 C,0,-2.0585618341,0.9712673819,-0.3823956449
 H,0,-2.4648630861,-0.1394647931,-2.2809480997
 H,0,-1.9601622724,1.1840134103,1.8410966762
 H,0,-1.5916436345,1.8842694861,-0.7306269152
 Na,0,-0.2303939665,-1.0061713535,0.0572955748
 Na,0,-4.5717813679,0.8558457636,-0.0298215489
 Na,0,5.06576559,-0.340200596,0.0249285674

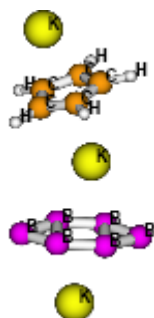
State=1-A\HF=-829.4640095



Charge = 0 Multiplicity = 1

B,0,-1.1071140836,0.0548451552,-0.6700189014
B,0,-2.0449538647,-0.8313068805,0.1559067343
B,0,-4.5984143569,-0.0296450606,1.4239011573
B,0,-2.1499383505,0.9171155986,0.0446439419
B,0,-3.5167992749,0.9155684928,0.9576233841
B,0,-3.4098475148,-0.8905388126,1.0696118278
Na,0,0.9089018998,-1.4477517203,-0.233492603
C,0,3.0825836543,-0.4518094951,1.2506327858
C,0,3.3634321777,-1.2396152417,0.1041404391
C,0,3.0303567058,0.9014841404,0.846662705
H,0,3.0142947595,-0.8104103024,2.2710034281
C,0,3.447646253,-0.3740870751,-1.015942895
H,0,3.5878833507,-2.30235691,0.1033194828
C,0,3.2582754533,0.9498137904,-0.5587001204
H,0,2.9734906678,1.7532655892,1.5188921895
H,0,3.7025760482,-0.6635974579,-2.0286063882
H,0,3.4090209037,1.8457759879,-1.1550757728
Na,0,0.7680074364,1.6971833076,-0.2377597475
Na,0,-4.369695753,-0.1814593842,-1.2839651391

State=1-A\HF=-829.4786442

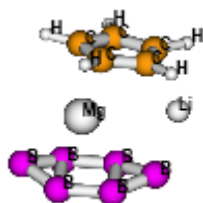


Charge = 0 Multiplicity = 1

B,0,2.7214953134,-1.9964615056,0.0434669772

B,0,2.820715523,-0.7580141338,0.9114346022
 B,0,3.2571830058,2.0870481595,-0.021024914
 B,0,2.8031340967,-0.7837321816,-0.8617257659
 B,0,3.0497516068,0.8613141,-0.8880108782
 B,0,3.0671608412,0.8871335999,0.8851360725
 C,0,-3.0117946417,1.2953453044,0.0517522899
 C,0,-2.8229026572,0.5315018949,-1.1292945293
 C,0,-2.8213262973,0.434895705,1.1644232324
 H,0,-3.2284592116,2.3569789486,0.0964089956
 C,0,-2.5153468792,-0.7998304073,-0.7462621386
 H,0,-2.8672178724,0.9080482535,-2.1452786436
 C,0,-2.5142726197,-0.8594427818,0.67074891
 H,0,-2.8641334948,0.7250636886,2.2084464495
 H,0,-2.2702602829,-1.6161730941,-1.4159048834
 H,0,-2.2673830759,-1.7287781308,1.2691928007
 K,0,0.0994361654,0.6828683916,0.0273998632
 K,0,-5.2991630865,-0.5056640985,-0.0195123263
 K,0,5.649178489,-0.4196563606,-0.0126433255

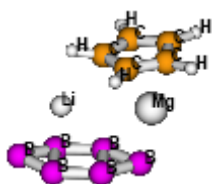
State=1-A\HF=-2142.3982832



Charge = 0 Multiplicity = 1

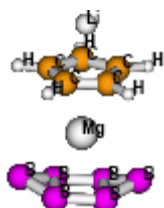
B,0,-2.2807349626,-1.984324997,0.4117846097
 B,0,-2.267005475,-0.6372938943,1.0960578463
 B,0,-1.7176901904,1.9155343373,-0.4809626474
 B,0,-2.5513512661,-0.9702361598,-0.6752707583
 B,0,-2.2639832844,0.6173781612,-1.0481591976
 B,0,-1.9729530522,0.9422229031,0.6728788016
 Li,0,0.103838412,2.3970267925,0.5440543007
 C,0,1.9926281959,-0.5826084157,-0.7835534228
 C,0,2.0802931071,0.8309860375,-0.7792976489
 C,0,1.9106391566,-1.0184400828,0.5855268075
 H,0,2.1205425233,-1.2221857508,-1.6486656847
 C,0,2.045139225,1.2702317843,0.5643937367
 H,0,2.1899919428,1.4538073067,-1.6572882349
 C,0,1.9167410433,0.1307821,1.4048386964
 H,0,1.9338043525,-2.0449041405,0.9312951142
 H,0,2.2679182023,2.2802253952,0.9080163865
 H,0,1.8948754924,0.1318054981,2.4866479008

Mg,0,-0.2206064224,-0.6110008748,-0.1160536059
State=1-A\HF=-550.1584496



Charge = 0 Multiplicity = 1

B,0,2.0409280787,-1.2552061979,-0.0085894692
B,0,2.2422356082,-0.0184237529,0.8869620596
B,0,2.6691053621,2.7859090211,0.0107242092
B,0,2.2581320153,-0.0141077116,-0.893134457
B,0,2.5944906964,1.5939213283,-0.90552545
B,0,2.5769891974,1.5895114031,0.9198508521
C,0,-1.7281834079,0.7592787169,0.0022627967
C,0,-1.9554490895,-0.0413134009,-1.1516433815
C,0,-1.9523253945,-0.0460965435,1.1537439894
H,0,-1.6508493131,1.8459673406,0.0049541232
C,0,-2.3064142663,-1.3407726552,-0.7173085637
H,0,-1.9020503927,0.2895405724,-2.1802097994
C,0,-2.3047941043,-1.3436558678,0.7148856904
H,0,-1.8956480957,0.2805008793,2.1834677161
H,0,-2.5828846963,-2.1698908305,-1.3556468225
H,0,-2.5798544556,-2.1753636639,1.350496405
Li,0,0.4714762557,1.7749065835,-0.0134180991
Mg,0,-0.1024624191,-1.2273446664,-0.0021574364
HF=-550.1673512

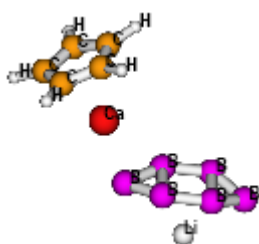


Charge = 0 Multiplicity = 1

B,0,-1.9380262163,1.9821403719,-0.0003693698
B,0,-2.3207463604,0.819125833,0.8962477584
B,0,-1.9072903206,-2.0078010308,-0.0016804337
B,0,-2.3071677196,0.8206936988,-0.9045178221
B,0,-2.2930981771,-0.8502061215,-0.9037117784
B,0,-2.3063972696,-0.851723336,0.8962598433
C,0,1.951750643,-1.1581735216,0.3212032371

C,0,1.9446551216,-0.6554385923,-1.0115102743
C,0,1.9458616336,-0.0436753208,1.2118480979
H,0,1.9101709048,-2.2000322169,0.6060175382
C,0,1.9432953777,0.7712542951,-0.9454704438
H,0,1.9144309022,-1.2520221358,-1.913003209
C,0,1.9483253928,1.1487474025,0.4277447892
H,0,1.9273573189,-0.0940590329,2.2922719737
H,0,1.9094900905,1.4482488087,-1.7879937037
H,0,1.9053564641,2.1599590726,0.8073063572
Mg,0,-0.26965584,0.0060715624,0.0132106671
Li,0,3.7141915944,0.0150028333,0.0006843329

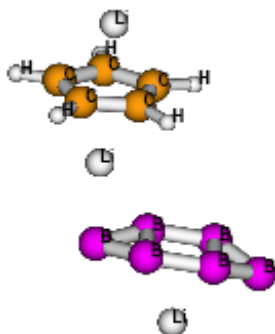
State=1-A\HF=-550.1385031



Charge = 0 Multiplicity = 1

B,0,4.7989434055,1.2032447766,0.0565364341
B,0,3.7429739313,0.6061637045,0.9525865765
B,0,1.7559083875,-1.4260429269,-0.0769834671
B,0,3.6761252752,0.7800144571,-0.8565455994
B,0,2.4730881864,-0.3386321628,-0.8878446796
B,0,2.5348990029,-0.5049072548,0.8700807715
C,0,-2.8164679702,0.2165429396,-1.1950221339
C,0,-3.1458155991,-0.8139862156,-0.2772829099
C,0,-2.4422040348,1.3642198205,-0.4498025519
H,0,-2.8897929062,0.1547614846,-2.2740122208
C,0,-2.975394856,-0.3029639554,1.035257008
H,0,-3.513574136,-1.8001766317,-0.5333042119
C,0,-2.5404435723,1.043150383,0.9285368022
H,0,-2.1796103131,2.331617629,-0.8603502269
H,0,-3.1917780493,-0.8304183056,1.9563399666
H,0,-2.366692436,1.7230518705,1.7537400922
Ca,0,-0.5483004639,-0.4268795117,-0.00294
Li,0,4.5732407896,-1.2274088713,-0.1742936222

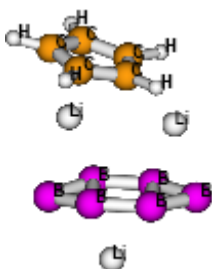
State=1-A\HF=-1027.7053653



Charge = 0 Multiplicity = 1^M

B,0,3.8611154867,-1.4344184073,0.0118309285
 B,0,2.9357701896,-0.6445767322,0.9078130827
 B,0,1.4917340759,1.8421093567,-0.0148719528
 B,0,2.9182043495,-0.6745044715,-0.8915833336
 B,0,1.9964741685,0.6976525183,-0.887092435
 B,0,2.0127971616,0.7263694951,0.8840681504
 C,0,-2.7736019465,0.8765011238,0.2614168371
 C,0,-2.4940410194,0.3798270622,-1.0426523332
 C,0,-2.2337627529,-0.0423195232,1.2059259395
 H,0,-3.2819303088,1.8027434188,0.4938736926
 C,0,-1.7815828126,-0.8447195275,-0.904393315
 H,0,-2.7504909617,0.8640027962,-1.9755246173
 C,0,-1.6214353175,-1.1056764803,0.4850960007
 H,0,-2.2563283223,0.0652606708,2.2820879017
 H,0,-1.3945424878,-1.4519191037,-1.7114229289
 H,0,-1.0873898719,-1.9420939225,0.9152335441
 Li,0,-0.4342322839,0.8403570611,-0.0066690567
 Li,0,-3.6947113309,-1.0327082675,0.0118211002
 Li,0,4.1678595771,1.0314083446,-0.0342948997

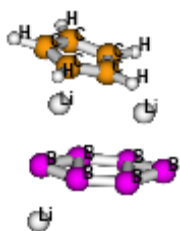
[State=1-A]HF=-365.1687584



Charge = 0 Multiplicity = 1^M

B,0,-2.6713477053,-1.8013336549,0.0002362166^M
 B,0,-2.3030772174,-0.6323577951,-0.8923366301^M
 B,0,-1.6288983565,2.1508426327,-0.0008019439^M
 B,0,-2.3028744503,-0.6320743303,0.8920540189^M
 B,0,-1.8083059319,0.9474754835,0.8985814442^M

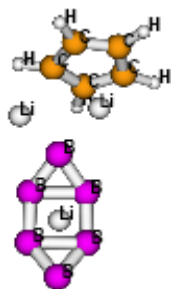
B,0,-1.8089219992,0.947399666,-0.8996193808^M
 C,0,2.6971765764,0.8972176153,-0.0065748395^M
 C,0,2.2803800577,0.1891715973,1.1443735363^M
 C,0,2.2793978557,0.1742441679,-1.1474534663^M
 H,0,3.2401191348,1.8336844205,-0.0129036105^M
 C,0,1.6250818026,-0.9938333705,0.7191360887^M
 H,0,2.4553467835,0.4763175705,2.1726700807^M
 C,0,1.6243177553,-1.0031085188,-0.7057768523^M
 H,0,2.4540385983,0.4470886844,-2.1796983757^M
 H,0,1.3199548324,-1.7958487071,1.3897301884^M
 H,0,1.3214539974,-1.8155458549,-1.3650068631^M
 Li,0,0.5460768362,0.9765801392,-0.0052595581^M
 Li,0,-0.3860988317,-1.8034020457,0.0014990891^M
 Li,0,-3.8972811144,0.9509535501,-0.0021018128^M
[State=1-A]HF=-365.1741199



Charge = 0 Multiplicity = 1

B,0,2.5492961368,-2.0493878986,-0.0009690216
 B,0,2.3814119453,-0.8478820811,0.898840117
 B,0,1.6271054968,1.9395485113,0.0010803834
 B,0,2.3815967814,-0.847297648,-0.899986178
 B,0,1.9615111744,0.7428746432,-0.8881903448
 B,0,1.9621494568,0.7424750548,0.8896649124
 C,0,-2.6754470804,0.9837288137,0.004093657
 C,0,-2.2921356627,0.2537261802,-1.1446733929
 C,0,-2.2890191659,0.247400971,1.1475499807
 H,0,-3.176447266,1.9433996347,0.0074157235
 C,0,-1.6846714268,-0.9520427427,-0.7159882409
 H,0,-2.4547384835,0.5452408798,-2.1738694208
 C,0,-1.6824579257,-0.9559315579,0.7103945824
 H,0,-2.4489690989,0.5331498946,2.1787774103
 H,0,-1.409646626,-1.7686195278,-1.3815577737
 H,0,-1.4066052794,-1.7765365429,1.3707817969
 Li,0,-0.516231185,0.9316478447,0.0001974425
 Li,0,3.6443652516,2.4264780293,-0.0023256038
 Li,0,0.3130123884,-1.8046516179,-0.0018740372

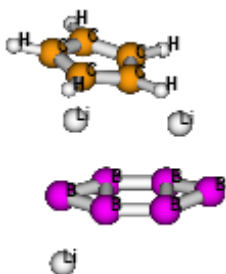
HF=-365.1749816



Charge = 0 Multiplicity = 1

B,0,-4.8400886167,-0.4602147935,-0.389819479
B,0,-3.8152069907,0.6270854672,-0.5978413141
B,0,-1.067149067,0.457312839,0.660263888
B,0,-3.5010514269,-1.125345583,-0.1942815173
B,0,-1.9979842368,-0.7075419369,0.3039951864
B,0,-2.3032042301,0.9826225858,-0.0782501137
C,0,2.4245534685,1.008454793,-0.5312960505
C,0,2.8893091237,0.6968400428,0.7807182569
C,0,2.3553167163,-0.2080640671,-1.2696114536
H,0,2.4062951283,2.0082060755,-0.968746729
C,0,3.0960775221,-0.6948065049,0.8471532881
H,0,3.0915611001,1.4074444583,1.5721858871
C,0,2.7664253225,-1.2541359194,-0.4199339766
H,0,2.0735106937,-0.3085190291,-2.3100219377
H,0,3.466075654,-1.2394095979,1.7068224249
H,0,2.8389319752,-2.2993829014,-0.6932100037
Li,0,0.9538204892,-0.5412468567,0.5309043036
Li,0,-3.7784615514,0.1953904462,1.6654379866
Li,0,0.3436261857,1.769969089,-0.2861900498

State=1-A\HF=-365.1768197

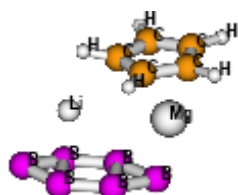


Charge = 0 Multiplicity = 1

B,0,2.5532364965,-2.0510462568,0.0002348981
B,0,2.383755696,-0.8488003637,0.8987426336
B,0,1.6285127978,1.9381362327,0.0008206638

B,0,2.3842880886,-0.8488338837,-0.8982869015
B,0,1.9628707341,0.7409178408,-0.8870212746
B,0,1.9628229343,0.7411654417,0.888817376
C,0,-2.6783163989,0.9842703613,0.0041217551
C,0,-2.2946607234,0.2548882266,-1.1451122058
C,0,-2.2907213009,0.2480345769,1.1476867113
H,0,-3.1801052759,1.943488689,0.0079105582
C,0,-1.6853876214,-0.9505232271,-0.7166776617
H,0,-2.4577334262,0.5462178193,-2.1742169932
C,0,-1.6831784843,-0.9547696049,0.7097467431
H,0,-2.4492310704,0.5336761511,2.1790938256
H,0,-1.4093131498,-1.7662756046,-1.382834612
H,0,-1.4056036143,-1.7748158603,1.3701586415
Li,0,-0.517908661,0.9315368524,0.0000956163
Li,0,3.6440107131,2.4299662259,-0.0034423565
Li,0,0.3132779391,-1.8052991605,-0.0017334097

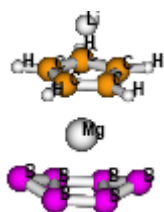
State=1-A\HF=-365.1749899



Charge = 0 Multiplicity = 1

B,0,1.9004467184,-1.4708335972,0.0003754231
B,0,2.1089104172,-0.2324662784,0.8906499926
B,0,2.4942832232,2.5792126729,-0.000060558
B,0,2.0756211738,-0.2255341356,-0.8891309694
B,0,2.3952542616,1.3860823136,-0.9136420171
B,0,2.4317620937,1.378968739,0.9077727609
C,0,-1.8799063248,0.5768634369,-0.0021885953
C,0,-2.1002600155,-0.2270773795,-1.1556603559
C,0,-2.1032790413,-0.2280870733,1.1501372876
H,0,-1.8149058758,1.6644939746,-0.0034094568
C,0,-2.4467063389,-1.5271613878,-0.7197445443
H,0,-2.045378107,0.1027742221,-2.184388459
C,0,-2.4478007377,-1.5280368368,0.7121675263
H,0,-2.0522011896,0.1003319175,2.1796178302
H,0,-2.7162480058,-2.3595289713,-1.3567223373
H,0,-2.7181645314,-2.3610444574,1.3478434097
Li,0,0.299537302,1.6340533491,0.0434338878
Mg,0,-0.2443600521,-1.4010422684,-0.0055044449

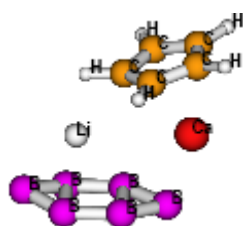
State=1-A\HF=-550.1673702



Charge = 0 Multiplicity = 1

B,0,-2.0694405747,1.9806747105,-0.001611679
 B,0,-2.452161011,0.8176598129,0.8950058296
 B,0,-2.0387063662,-2.009268226,-0.0029210119
 B,0,-2.4385812121,0.8192265292,-0.9057598285
 B,0,-2.4245130452,-0.8516741077,-0.9049540289
 B,0,-2.4378129767,-0.8531896176,0.8950184127
 C,0,1.8203363068,-1.1596406025,0.3199646661
 C,0,1.8132380376,-0.6569056511,-1.0127493716
 C,0,1.8144484872,-0.0451425568,1.2106094371
 H,0,1.7787571504,-2.2014994005,0.6047785482
 C,0,1.8118779411,0.7697875625,-0.946709134
 H,0,1.7830114616,-1.2534890263,-1.9142424577
 C,0,1.8169103478,1.1472801231,0.426506558
 H,0,1.7959460624,-0.0955266921,2.2910331591
 H,0,1.7780695537,1.4467823644,-1.7892322482
 H,0,1.7739411642,2.1584919294,0.8060678577
 Mg,0,-0.4010704957,0.0046011802,0.0119711684
 Li,0,3.5827765875,0.0135359684,-0.0005600944

HF=-550.1385031



Charge = 0 Multiplicity = 1

B,0,-1.7108961764,-1.9187629823,0.0010431745
 B,0,-2.3036677533,-0.8052169301,-0.8822786601
 B,0,-3.6161216048,1.6998844007,-0.0020272803
 B,0,-2.3110751945,-0.8082828719,0.8827437326
 B,0,-3.203534224,0.5723105522,0.9079791621
 B,0,-3.1946482024,0.576106495,-0.9127269023
 C,0,1.1662128863,1.4501624267,0.0173133566
 C,0,1.8226106219,0.9064879985,1.1580883551

C,0,1.7997729414,0.92548642,-1.1451714021
 H,0,0.5424327028,2.3440323412,0.0318879042
 C,0,2.835519684,0.0380601395,0.7014335182
 H,0,1.6159967195,1.1586587198,2.1905185135
 C,0,2.8212400454,0.0496225348,-0.7231467307
 H,0,1.5726636096,1.1940062245,-2.169108131
 H,0,3.5401222771,-0.4970594505,1.3267625278
 H,0,3.5127049901,-0.4754709095,-1.371021349
 Li,0,-1.2903162016,1.4615265099,0.0130468095
 Ca,0,0.6175581874,-1.2352294412,0.002225256

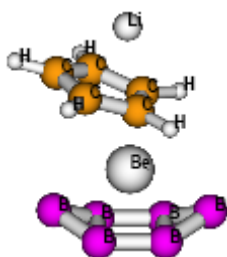
State=1-A\HF=-1027.694964



Charge = 0 Multiplicity = 1^M

B,0,-2.6769227958,-1.8030202901,0.4905228969^M
 B,0,-2.466703802,-0.4585093281,1.1354862013^M
 B,0,-1.7964313261,2.0001504784,-0.5467330854^M
 B,0,-2.9076726931,-0.7714666398,-0.5891824675^M
 B,0,-2.5248340404,0.7642008225,-1.0432532497^M
 B,0,-2.1119835482,1.0740332997,0.6382508391^M
 Li,0,-0.0944693867,2.5210881666,0.6228983801^M
 C,0,2.4325150023,-0.6006064423,-0.8927998871^M
 C,0,2.1680589261,0.7826900727,-0.8161632579^M
 C,0,2.3209749637,-1.1480255894,0.41729493^M
 H,0,2.7269023204,-1.1391897169,-1.7855370906^M
 C,0,1.8770501596,1.0948701712,0.5424017099^M
 H,0,2.2220432402,1.486885644,-1.6364257303^M
 C,0,1.9839952323,-0.1040454931,1.302858266^M
 H,0,2.5094243505,-2.1776144408,0.6961029377^M
 H,0,1.9015721027,2.0971708493,0.9745572152^M
 H,0,1.8742491086,-0.1900472233,2.3762527501^M
 Ca,0,-0.1611803819,-0.590835382,-0.312032573^M

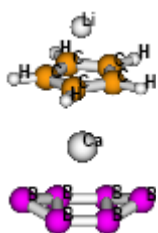
State=1-A\HF=-1027.7035375



Charge = 0 Multiplicity = 1

B,0,-2.3351604649,-1.7125205813,-0.0244404523
 B,0,-2.5095295946,-0.4790170068,-0.8909763746
 B,0,-1.1870498061,1.9872133561,0.0244872573
 B,0,-2.4390269153,-0.523060967,0.9124631324
 B,0,-1.9595632145,1.0621130477,0.9438343726
 B,0,-2.0312618923,1.1063284812,-0.8758959103
 C,0,2.2942717722,0.883639984,-0.1178827192
 C,0,1.9019456486,0.2820356772,1.1030282199
 C,0,1.7273309115,0.1529329349,-1.1806059841
 H,0,2.8500180054,1.8062539888,-0.2134647214
 C,0,1.0991572974,-0.8462561434,0.8123221901
 H,0,2.1234208964,0.6550107925,2.0934853708
 C,0,0.9796675856,-0.9346971306,-0.631094237
 H,0,1.797554694,0.3954909404,-2.231888099
 H,0,0.6808128229,-1.5460043054,1.5242217618
 H,0,0.5419539067,-1.7590886411,-1.1817378717
 Be,0,-0.6848188755,-0.1296411932,-0.0421257918
 Li,0,3.013078441,-1.1547705282,-0.0613594055

State=1-A\HF=-364.769685

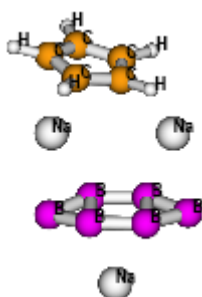


Charge = 0 Multiplicity = 1

B,0,2.3846664113,2.0060977793,0.018007603
 B,0,2.7844410405,0.8372912956,-0.8634770957
 B,0,2.4035285146,-1.9975986999,0.0062623685
 B,0,2.7209135634,0.8344097483,0.9212676913
 B,0,2.733021578,-0.8262142849,0.9134989526
 B,0,2.7951109005,-0.8240247705,-0.8722896993
 C,0,-2.1905417856,0.2920782309,-1.1624015406
 C,0,-2.1854891926,-1.0276829625,-0.6260636238

C,0,-2.1496951811,1.2107099687,-0.0746092966
H,0,-2.2180813321,0.5521027874,-2.2127945731
C,0,-2.1407961906,-0.9250085224,0.7938401189
H,0,-2.1998629734,-1.948094276,-1.1952832964
C,0,-2.1178968125,0.4586009403,1.1332734817
H,0,-2.1272346685,2.2896881017,-0.1522287884
H,0,-2.1133695176,-1.7532522721,1.4893508491
H,0,-2.0750653105,0.8674693087,2.1346745444
Ca,0,0.4060946338,-0.0138460129,-0.0633030843
Li,0,-3.9300579804,0.022338447,0.0672530039

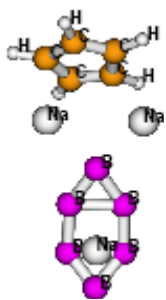
State=1-A\HF=-1027.682278



Charge = 0 Multiplicity = 1

B,0,-1.8061846727,-2.0608594374,-0.0025562351
B,0,-1.8705098547,-0.8375473209,0.889355563
B,0,-2.4749523321,1.9819156962,0.000144107
B,0,-1.8753498589,-0.8372522967,-0.8936866666
B,0,-2.1754524909,0.7939760138,-0.8919318146
B,0,-2.1708152261,0.7936108879,0.8901291096
Na,0,-4.3581159421,-0.5505368126,0.0055922917
Na,0,0.1598244325,2.030313523,-0.0050823217
Na,0,0.8052522368,-1.4797997031,-0.0115944782
C,0,2.4606816219,0.9267087614,-0.7051616169
C,0,2.4538938251,0.919707157,0.7198191501
C,0,2.9604778166,-0.3226533891,-1.1438094788
H,0,2.2992990703,1.7838550273,-1.3564652247
C,0,2.9493661091,-0.3337752308,1.1508674418
H,0,2.2835531617,1.7697177173,1.3780444754
C,0,3.2782189792,-1.0926093876,0.0013461856
H,0,3.1360675498,-0.6058601097,-2.1745801091
H,0,3.114000051,-0.627453372,2.1805071252
H,0,3.7410042323,-2.0734915233,-0.0012170831

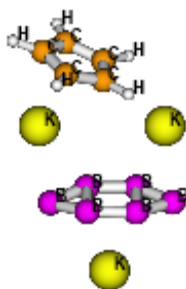
State=1-A\HF=-829.4811829



Charge = 0 Multiplicity = 1

B,0,-4.5825355828,-0.1797546485,1.4302948262
 B,0,-3.3898045076,-0.9966154592,0.9946294916
 B,0,-1.1121244048,0.1098297899,-0.6809125057
 B,0,-3.5140767729,0.8111032282,1.0340697729
 B,0,-2.1560925746,0.8997580117,0.11233753
 B,0,-2.0352489501,-0.8508032776,0.0752178762
 C,0,3.3966324473,-1.2494140216,0.0688191269
 C,0,3.4618322128,-0.3468943194,-1.0229974034
 C,0,3.086697988,-0.5077822758,1.2375004972
 H,0,3.6373961247,-2.3068903559,0.0334127974
 C,0,3.2296903148,0.9560548133,-0.5253941608
 H,0,3.7301148776,-0.5965204677,-2.0428065907
 C,0,2.9965848393,0.856034645,0.8765910346
 H,0,3.018943732,-0.9011786727,2.2448817634
 H,0,3.3618174995,1.873977723,-1.092306934
 H,0,2.9181577092,1.683231643,1.5771717103
 Na,0,0.7377774405,1.747984329,-0.1614554998
 Na,0,-4.3849344103,-0.106818082,-1.2799740768
 Na,0,0.943007625,-1.3655481689,-0.3181751752

State=1-A\HF=-829.4786452

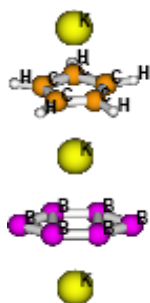


Charge = 0 Multiplicity = 1

B,0,1.7703093506,-2.0102150958,-0.0010761676
 B,0,1.8825489959,-0.78610079,-0.887801983
 B,0,2.5853034857,2.0122447757,0.0007456159
 B,0,1.8820313503,-0.7867813499,0.8866528944
 B,0,2.2396094262,0.8313457085,0.8867911411
 B,0,2.240132981,0.8320305464,-0.8864163006

K,0,4.7876189118,-0.6191821826,0.0003035687
K,0,-0.3945866675,2.3778857718,-0.0001755069
K,0,-1.2808670192,-1.7524140012,-0.0015036308
C,0,-2.955197662,0.7985175479,0.7134689656
C,0,-2.9559145262,0.8000660587,-0.710360344
C,0,-3.678212199,-0.3378010318,1.1457355499
H,0,-2.6114268128,1.5856853285,1.3811394369
C,0,-3.6793705792,-0.3352896248,-1.1444598489
H,0,-2.613311717,1.5889039291,-1.3766655973
C,0,-4.126713114,-1.0335980445,0.0000891006
H,0,-3.8940901004,-0.5934833761,2.1767930836
H,0,-3.8964265843,-0.588561944,-2.1758624418
H,0,-4.7431135302,-1.9260345183,-0.0005852104

State=1-A\HF=-2142.4092514



Charge = 0 Multiplicity = 1

B,0,3.2584624007,-2.0431380559,0.0084555901
B,0,3.1956204681,-0.8120527456,0.889837518
B,0,3.2165168727,2.0769602423,-0.0073005892
B,0,3.1933473553,-0.8190002654,-0.8823744776
B,0,3.1762805726,0.8448553954,-0.8885923448
B,0,3.1785479016,0.8517902132,0.8836479952
C,0,-2.5892698057,1.1489026566,0.3228559503
C,0,-2.5935104856,0.6540368893,-1.0069224457
C,0,-2.5916676371,0.036687685,1.2043675567
H,0,-2.5465563327,2.1924035208,0.6138198606
C,0,-2.5979163078,-0.763878314,-0.9473410703
H,0,-2.5566119469,1.2540917282,-1.9092191051
C,0,-2.5967990007,-1.1455567685,0.4192126303
H,0,-2.5548623941,0.0821320296,2.2871216061
H,0,-2.5650873296,-1.4376333078,-1.7961736498
H,0,-2.5614268405,-2.161365648,0.796470769
K,0,0.2962271342,-0.0158837998,0.0047338907
K,0,-5.2314981823,-0.0037827313,0.0088448421

K,0,5.9383824476,0.0437204429,-0.0024545906
State=1-A\HF=-2142.3986603