

Table S2: VASP POSCAR files for the 12 Si structures (4 for each B₄C polytype).

B₄C: B₁₁C^p-CBC-Si-10 equatorial

B C Si

1.0000000000000000

-0.0777610200000000 3.3610142299999999 -4.2438554699999997
2.7708904599999999 -1.5941193800000000 -4.1193430900000001
-2.9190382900000000 -1.5901231000000000 -4.2239891800000002

B C Si

11 3 1

Cartesian

-1.0973856900000001 0.7016022200000001 -4.8883784900000000
-0.1863509800000000 1.2167584700000000 -7.7477722800000004
-0.1490562200000000 -0.8895825400000000 -4.7276686100000003
-1.1020348000000000 -0.3148118700000000 -7.7969556999999998
0.7754282800000000 0.6840597500000000 -4.8323140699999998
1.4266542799999999 -0.7357609200000000 -5.5455747200000003
-1.5740457999999999 0.9212173200000000 -6.6142476700000001
-0.1274214300000000 1.7826419300000000 -6.0268669800000003
-1.5927886899999999 -0.6982712700000000 -5.9786660600000001
1.2851637600000001 0.8010113900000000 -6.6050511600000004
0.1145437600000000 -0.2248090100000000 -0.0499704800000000
0.6492066900000000 -0.2614308700000000 -7.8767738899999999
-0.2241835100000000 -0.0616166200000000 -11.1745607499999995
0.0115440300000000 0.0293841900000000 -1.4752843200000001
0.0297646100000000 -1.6374519900000000 -6.6435307799999999

B₄C: B₁₁C^p-CBC-Si-13 chain end

B C Si

1.0000000000000000

-0.1536305800000000 3.4774369400000000 -4.1569833799999998
2.8211206199999999 -1.6299028900000001 -3.9606249199999999
-3.0892769300000000 -1.6064401100000001 -4.1557262399999999

B C Si

12 2 1

Cartesian

-1.1372940199999999 0.6562293200000000 -4.6480247300000004
-0.2390321700000000 1.2018115300000001 -7.5241264100000000
-0.1838449600000000 -0.9960767900000000 -4.6576294499999999
-1.1608987399999999 -0.3953069200000000 -7.5236247599999997
0.7703637000000000 0.6564564600000000 -4.6583027799999996
1.2714387800000000 -0.7349746400000000 -5.7981131499999998
-1.5524597300000000 0.8956558600000000 -6.3326597400000004
-0.2003546000000000 1.8104971100000000 -5.7879765599999997
-0.2027940300000000 -1.4336196200000000 -6.4137528200000000

-1.6688822999999999 -0.7325218900000000 -5.7875149900000000
1.1394771100000001 0.8909089100000001 -6.4143118599999998
0.2357715400000000 -0.1360029900000000 -0.4133508300000000
0.6489971100000000 -0.3758686600000000 -7.4260988699999997
-0.1561261300000000 0.0904473100000000 -1.7310605400000001
-0.2894335100000000 0.1653457400000000 -10.8246683600000004

B4C: B₁₁Cp-CBC-Si-15 chain center

B C Si

1.0000000000000000
-0.1102250600000000 3.3039660500000001 -4.2078726199999998
2.6959543699999999 -1.5570449500000001 -4.0233867999999999
-2.9169029300000000 -1.5573888000000000 -4.2062723999999996

B C Si

11 3 1

Cartesian

-1.0281422300000000 0.6061736300000000 -4.8416362900000003
-0.0276170100000000 1.1699323300000000 -7.6698043000000000
-0.1168123500000000 -0.9757926000000000 -4.8312483999999998
-1.0162183300000001 -0.5434031600000000 -7.6693938399999997
0.7974614200000000 0.6077495000000001 -4.8322763300000000
1.3146057700000000 -0.7473934600000000 -6.0616686499999997
-1.5294444100000000 0.8948342200000000 -6.6198030000000001
-0.1309484900000000 1.7578043699999999 -5.9260212000000001
-0.1433757500000000 -1.6307640999999999 -6.4485983100000004
-1.5771502500000001 -0.7473024600000000 -5.9253318200000002
1.3501931199999999 0.9563973500000000 -6.4506187300000004
0.7261916500000000 -0.4070697200000000 -7.6265492400000001
-0.1663637200000000 0.1067697300000000 -10.8988766600000009
-0.0523850400000000 0.0428480600000000 -1.6065531200000001
-0.6763879000000000 0.4036922200000000 0.0375669700000000

B4C: B₁₁Cp-CBC-Si-1 polar

B C Si

1.0000000000000000
0.0958451900000000 3.2405699200000000 -4.1821215499999997
2.9793325500000001 -1.7185138400000000 -4.3287944899999999
-2.7578541599999999 -1.7021767400000001 -4.1820597599999996

B C Si

12 2 1

Cartesian

-0.6931893700000000 0.3995892100000000 -5.0593148899999996
0.1268791000000000 1.0475508800000000 -7.7334490200000001
0.1516387900000000 -1.1535822099999999 -4.9406479299999999
-0.8438784499999999 -0.6342466600000000 -7.7337800200000002
1.0740943400000000 0.4443293100000000 -4.9403410799999996

1.6347307200000001 -0.9442440000000000 -5.9582091100000003
-1.3072137900000000 0.7540890300000000 -6.6757539799999996
0.1704815900000000 1.6108688400000000 -6.0337234700000000
0.1319039400000000 -1.8161560999999999 -6.6067649599999996
-1.3100788600000000 -0.9538261000000000 -6.0340565499999999
1.6380882900000000 0.7928726100000000 -6.6063734099999998
0.0135139500000000 -0.0099498600000000 0.0324479600000000
0.2538488800000000 -0.1468143900000000 -11.1974965500000003
0.0774160100000000 -0.0456897700000000 -1.4258722600000000
1.1699080799999999 -0.6758850300000000 -7.9336049500000003

B₄C: B₁₂-CBC-Si-chain center

B C Si

1.0000000000000000
-0.0081627100000000 3.2570136700000001 -4.2083386899999997
2.8158744900000001 -1.6355030900000000 -4.2090268100000001
-2.7915540800000000 -1.6110739500000000 -4.2015098599999998

B C Si

12 2 1

Cartesian

0.8417613600000000 -0.5707524800000000 -7.7130570900000004
-0.9392788900000000 0.4946324500000000 -4.8885856700000003
-0.0791797400000000 1.0245058199999999 -7.7126640499999999
-0.0471159800000000 -1.0508003100000001 -4.8892359599999997
-0.9440212700000000 -0.5381123799999999 -7.7656530100000003
0.8666305100000000 0.5068378600000000 -4.8995151000000003
1.4106184500000001 -0.8487324900000000 -5.9850136200000001
-1.4839057400000000 0.8228508500000000 -6.5684705799999996
-0.0350964200000000 1.6558981800000001 -5.9847823499999997
-0.0355449500000000 -1.6864848100000001 -6.5689002900000002
-1.4974022899999999 -0.8576433900000000 -6.1514422299999998
1.4017233000000000 0.8158498199999999 -6.6423358400000003
-0.0293170800000000 -0.0095666000000000 -11.0181941400000003
-0.0515854300000000 -0.0234131800000000 -1.5691178699999999
0.6404940300000000 0.3751227200000000 0.0189066700000000

B₄C: B₁₂-CBC-Si-chain end

B C Si

1.0000000000000000
-0.0054753600000000 3.3080960799999999 -4.0856711099999998
2.9778693600000001 -1.6938118600000001 -4.1174150000000003
-2.9839753700000000 -1.6932669100000000 -4.1158492999999998

B C Si

13 1 1

Cartesian

0.9375988800000000 -0.6921601200000000 -7.6240711699999997

-0.9300597300000000 0.4198353100000000 -4.7773245299999996
 -0.0084365200000000 0.9286919700000000 -7.5962148999999997
 -0.0050985300000000 -1.1430940000000001 -4.7360449800000000
 -0.9545609500000000 -0.6927716700000000 -7.6244950100000004
 0.9180597300000000 0.4212814900000000 -4.7777150800000001
 1.3415187200000001 -0.8652875000000000 -5.8733573699999999
 -1.5288724199999999 0.7527946900000000 -6.5220502500000004
 -0.0068145600000000 1.4311816700000000 -5.8903862199999999
 -0.0064967300000000 -1.8500837000000001 -6.3436241200000003
 -1.3548077400000000 -0.8665515100000000 -5.8723767300000000
 1.5147856600000000 0.7533022100000000 -6.5241410000000002
 0.0060474800000000 1.0556621200000000 0.2706480200000000
 -0.0094072900000000 -0.1449558800000000 -10.8897043199999999
 -0.0044375600000000 -0.0380242700000000 -1.3883753500000000

B₄C: B₁₂-CBC-Si-equatorial

B C Si

1.0000000000000000
 -0.0284527600000000 3.3356978200000000 -4.1538109600000004
 2.9065887099999999 -1.6782275099999999 -4.1418231800000003
 -2.9030852399999998 -1.6434807899999999 -4.1538186499999998

B C Si

12 2 1

Cartesian

0.8343466600000000 -0.4845196900000000 -7.7270766100000001
 -0.9860899000000000 0.5667155400000000 -4.8252351999999998
 -0.0733317200000000 1.1054339200000001 -7.6398074200000003
 -0.1012182800000000 -1.0322485600000000 -4.7686171499999999
 -0.9965641500000000 -0.4933641600000000 -7.6400569799999998
 0.8410251600000000 0.5998913700000000 -4.7683490400000004
 -1.5207768900000000 0.8752061100000000 -6.5286451200000002
 -0.0214492200000000 1.6680802500000000 -5.9176473999999999
 -0.1026584900000000 -1.6918610900000000 -6.5917125900000002
 -1.4574890199999999 -0.8195736900000000 -5.9177092399999998
 1.4114193700000000 0.9309499500000000 -6.5917989099999996
 0.1266631600000000 -0.0755820000000000 0.0526878900000000
 -0.0502535400000000 0.0261218700000000 -10.9703611799999994
 0.1717113900000000 -0.1018113100000000 -1.3989507900000000
 1.5642817899999999 -0.9057376900000000 -5.8876628899999996

B₄C: B₁₂-CBC-Si-polar

B C Si

1.0000000000000000
 0.0954188300000000 3.2397465099999998 -4.1821117499999998
 2.9782567300000000 -1.7197667100000000 -4.3289299100000003
 -2.7582035700000000 -1.7027134600000000 -4.1820856600000003

B C Si
 12 2 1
 Cartesian
 -0.7047718900000000 0.4019577800000000 -5.0508347400000000
 0.1153179400000000 1.0496395599999999 -7.7257519700000001
 0.1399531600000000 -1.1510683500000001 -4.9321572900000001
 -0.8556851300000000 -0.6320991500000001 -7.7255989999999999
 1.0625782600000000 0.4470544500000000 -4.9320206999999998
 1.6226808600000000 -0.9418418200000001 -5.9497877700000004
 -1.3187255899999999 0.7563559900000000 -6.6676243299999998
 0.1587459600000000 1.6129652999999999 -6.0253535400000002
 0.1203533200000000 -1.8134692500000000 -6.5983603000000004
 -1.3219605800000001 -0.9510748500000000 -6.0252773299999998
 1.6265647299999999 0.7951189500000000 -6.5983192500000003
 0.0019028600000000 -0.0056905900000000 0.0406134800000000
 0.2417550800000000 -0.1443869800000000 -11.1895306699999999
 0.0662614400000000 -0.0431681400000000 -1.4177450199999999
 1.1584980700000000 -0.6736476400000000 -7.9254605700000003

B₄C: B₁₂-CCC-Si-chain center

B C Si
 1.0000000000000000
 -0.0080470000000000 3.2579585199999999 -4.2074398500000001
 2.8155043700000002 -1.6348545100000000 -4.2098714299999997
 -2.7916495700000001 -1.6102134400000001 -4.2016191500000000

B C Si
 12 2 1
 Cartesian
 0.8470278600000000 -0.5667001200000000 -7.7032547800000000
 -0.9340479200000000 0.4980899400000000 -4.8782623200000002
 -0.0742353100000000 1.0284670199999999 -7.7025681400000003
 -0.0418165800000000 -1.0474322899999999 -4.8794648499999997
 -0.9390022900000000 -0.5341675700000000 -7.7559077500000004
 0.8719304100000000 0.5100195500000000 -4.8894764200000003
 1.4159862400000001 -0.8452504000000000 -5.9752113700000002
 -1.4790155100000000 0.8266832400000000 -6.5579375799999999
 -0.0298774200000000 1.6594447600000000 -5.9743067099999996
 -0.0303379000000000 -1.6829309200000000 -6.5598308000000003
 -1.4922028100000000 -0.8541234800000000 -6.1414919000000001
 1.4070071799999999 0.8197234799999999 -6.6323751299999998
 -0.0246172700000000 -0.0047586400000000 -11.0080346900000006
 -0.0459655300000000 -0.0211316400000000 -1.5590367500000000
 0.6472800000000000 0.3751559000000000 0.0289497900000000

B₄C: B₁₂-CCC-Si-chain-end

B C Si

1.0000000000000000
0.1147362000000000 3.4940846600000000 -3.9371399199999999
3.0736222999999998 -1.6400798800000000 -3.9485175199999998
-3.2158854500000000 -1.8443844000000000 -3.8795929400000002

B C Si

12 2 1

Cartesian

0.9010829700000000 -0.5392394900000000 -7.4010159299999998
-0.9690660900000000 0.5357252600000000 -4.5825205100000002
-0.0332279100000000 1.0819104799999999 -7.3974669899999999
-0.0354880400000000 -1.0841862799999999 -4.5861737900000001
-1.0282077300000001 -0.5711644500000000 -7.3651434699999996
0.9423721200000000 0.5581776100000000 -4.5586388600000003
1.3920760800000000 -0.7891175900000000 -5.6148790699999997
-1.3980778100000000 0.8692266900000000 -6.3165285300000003
0.0001608900000000 1.6261779700000001 -5.6096022899999998
0.0345509900000000 -1.6169571199999999 -6.3219067200000003
-1.4406807699999999 -0.8125133600000000 -5.6445107999999999
1.3025448799999999 0.7696250600000000 -6.3214518000000002
-0.6744642500000000 -0.3601540300000000 -10.5439291500000003
0.4510373900000000 0.2620771000000000 1.1591519200000000
0.0676737400000000 0.0472419300000000 -1.3503825300000001

B₄C: B₁₂-CCC-Si-equatorial

B C Si

1.0000000000000000

-0.0249325000000000 3.3317496000000002 -4.1514122300000000
2.9087197800000002 -1.6695952000000001 -4.1370554000000004
-2.9008453599999999 -1.6365795500000000 -4.1451482000000004

B C Si

11 3 1

Cartesian

0.8599159600000000 -0.4792843600000000 -7.7224377999999998
-0.9510773900000000 0.5642922300000000 -4.8078909500000000
-0.0404367800000000 1.0996775200000000 -7.6321035300000002
-0.0627366000000000 -1.0235429400000000 -4.7445596300000004
-0.9583073600000001 -0.4897655900000000 -7.6317095100000003
0.8682389300000000 0.5878662200000000 -4.7469430299999997
-1.4765156500000001 0.8677252300000000 -6.5230805199999997
0.0117823800000000 1.6539929499999999 -5.9010201999999996
-0.0690127200000000 -1.6782713400000000 -6.5845670399999996
-1.4115568400000000 -0.8132448100000000 -5.9023942600000003
1.4319475100000001 0.9207278900000000 -6.5800286699999999
-0.0103105300000000 0.0196372800000000 -11.0326736499999996
0.2288855900000000 -0.1135209200000000 -1.3176166300000001
0.0910766900000000 -0.0453664200000000 0.0423735900000000

1.6003962500000000 -0.9112359600000000 -5.8758135600000001

B₄C: B₁₂-CCC-Si-polar

B C Si

1.0000000000000000

0.1580441500000000 3.1997799200000001 -4.1563757800000003

3.0077101399999999 -1.7353682600000000 -4.3761539400000000

-2.6916831299999999 -1.7359625900000000 -4.1561408100000001

B C Si

11 3 1

Cartesian

-0.6362285500000000 0.3688233500000000 -5.0646959699999998

0.2237437600000000 0.9904529600000000 -7.7309840000000003

0.2098273500000000 -1.1871421200000001 -4.9549489700000002

-0.7446155200000000 -0.6866057700000000 -7.7308845399999999

1.1341693900000000 0.4136632000000000 -4.9552812399999997

1.6945440599999999 -0.9768629100000000 -5.9567359499999997

-1.2209131900000001 0.7064114000000000 -6.7008575400000003

0.2391829800000000 1.5547733399999999 -6.0410642000000001

0.2093267300000000 -1.8414429900000000 -6.6167150799999996

-1.2258153599999999 -0.9823334800000000 -6.0414826399999999

1.7004564200000001 0.7412065100000000 -6.6180059900000003

0.3428534400000000 -0.1961755300000000 -11.2869379100000007

0.1363663000000000 -0.0778972000000000 -1.3597336099999999

-0.0085618000000000 0.0100610200000000 0.0113377300000000

1.2724001199999999 -0.7342125000000000 -7.9648846200000003