```
# Structural file for the sqrt(3) x sqrt(3) phase of Si(111):Pb

blebleble
H                            10 157 P31m
             RELA
 12.492394 12.492394 57.699840 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 4
Pb1        NPT=  781  R0=0.00000500 RMT= 2.50000     Z:  82.00000
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                    -1.0000000 0.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.00000000 Y=0.68462300 Z=0.06433600
          MULT= 3          ISPLIT= 8
      -2: X=0.31537700 Y=0.31537700 Z=0.06433600
      -2: X=0.68462300 Y=0.00000000 Z=0.06433600
Si1        NPT=  781  R0=0.00010000 RMT= 1.85        Z:  14.00000
LOCAL ROT MATRIX:    0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
ATOM  -3: X=0.00000000 Y=0.00000000 Z=0.09968200
          MULT= 1          ISPLIT= 4
Si2        NPT=  781  R0=0.00010000 RMT= 1.85        Z:  14.00000
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                    -1.0000000 0.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -4: X=0.33333333 Y=0.66666667 Z=0.08570100
          MULT= 2          ISPLIT= 4
      -4: X=0.66666667 Y=0.33333333 Z=0.08570100
Si3        NPT=  781  R0=0.00010000 RMT= 1.85        Z:  14.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -5: X=0.00000000 Y=0.00000000 Z=0.17571500
          MULT= 1          ISPLIT= 4
Si4        NPT=  781  R0=0.00010000 RMT= 1.85        Z:  14.00000
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                    -1.0000000 0.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -6: X=0.33333333 Y=0.66666667 Z=0.16470700
          MULT= 2          ISPLIT= 4
      -6: X=0.66666667 Y=0.33333333 Z=0.16470700
Si5        NPT=  781  R0=0.00010000 RMT= 1.85        Z:  14.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -7: X=0.34188400 Y=0.00000000 Z=0.19408400
          MULT= 3          ISPLIT= 8
      -7: X=0.00000000 Y=0.34188400 Z=0.19408400
      -7: X=0.65811600 Y=0.65811600 Z=0.19408400
Si6        NPT=  781  R0=0.00010000 RMT= 1.85        Z:  14.00000
LOCAL ROT MATRIX:    0.0000000 0.8660254 0.5000000
                     0.0000000-0.5000000 0.8660254
                     1.0000000 0.0000000 0.0000000
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ATOM  -8: X=0.33661100 Y=0.00000000 Z=0.27161100
          MULT= 3          ISPLIT= 8
      -8: X=0.00000000 Y=0.33661100 Z=0.27161100
      -8: X=0.66338900 Y=0.66338900 Z=0.27161100
Si7        NPT=  781  R0=0.00010000 RMT= 1.85        Z:  14.00000
LOCAL ROT MATRIX:    0.0000000 0.8660254 0.5000000
                     0.0000000-0.5000000 0.8660254
                     1.0000000 0.0000000 0.0000000
ATOM  -9: X=0.00000000 Y=0.66867000 Z=0.29732200
          MULT= 3          ISPLIT= 8
      -9: X=0.33133000 Y=0.33133000 Z=0.29732200
      -9: X=0.66867000 Y=0.00000000 Z=0.29732200
Si8        NPT=  781  R0=0.00010000 RMT= 1.85        Z:  14.00000
LOCAL ROT MATRIX:    0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
ATOM -10: X=0.00000000 Y=0.67038400 Z=0.34683500
          MULT= 3          ISPLIT= 8
     -10: X=0.32961600 Y=0.32961600 Z=0.34683500
     -10: X=0.67038400 Y=0.00000000 Z=0.34683500
H 1        NPT=  781  R0=0.00010000 RMT= 0.99        Z:   1.00000
LOCAL ROT MATRIX:    0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
   6      NUMBER OF SYMMETRY OPERATIONS
 1 0 0 0.00000000
 0 1 0 0.00000000
 0 0 1 0.00000000
       1
 0-1 0 0.00000000
 1-1 0 0.00000000
 0 0 1 0.00000000
       2
-1 1 0 0.00000000
-1 0 0 0.00000000
 0 0 1 0.00000000
       3
 0 1 0 0.00000000
 1 0 0 0.00000000
 0 0 1 0.00000000
       4
 1-1 0 0.00000000
 0-1 0 0.00000000
 0 0 1 0.00000000
       5
-1 0 0 0.00000000
-1 1 0 0.00000000
 0 0 1 0.00000000
       6
```

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# Structural file for the 3 x 3 phase of Si(111):Pb

blebleble
H                            26 156 P3m1
             RELA
 21.637459 21.637459 57.699840 90.000000 90.000000120.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.99413158
          MULT= 1          ISPLIT= 4
Pb1        NPT=  781  R0=0.00000500 RMT= 2.50000     Z:  82.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.33333333 Y=0.66666667 Z=0.00140432
          MULT= 1          ISPLIT= 4
Pb2        NPT=  781  R0=0.00000500 RMT= 2.50000     Z:  82.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -3: X=0.66666667 Y=0.33333333 Z=0.00143096
          MULT= 1          ISPLIT= 4
Pb3        NPT=  781  R0=0.00000500 RMT= 2.50000     Z:  82.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -4: X=0.77285951 Y=0.22714049 Z=0.06464506
          MULT= 3          ISPLIT= 8
      -4: X=0.77285951 Y=0.54571902 Z=0.06464506
      -4: X=0.45428098 Y=0.22714049 Z=0.06464506
Si1        NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    0.0000000 0.5000000 0.8660254
                     0.0000000-0.8660254 0.5000000
                     1.0000000 0.0000000 0.0000000
ATOM  -5: X=0.43961483 Y=0.56038517 Z=0.06458439
          MULT= 3          ISPLIT= 8
      -5: X=0.43961483 Y=0.87922966 Z=0.06458439
      -5: X=0.12077034 Y=0.56038517 Z=0.06458439
Si2        NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    0.0000000 0.5000000 0.8660254
                     0.0000000-0.8660254 0.5000000
                     1.0000000 0.0000000 0.0000000
ATOM  -6: X=0.79453703 Y=0.89726851 Z=0.06084092
          MULT= 3          ISPLIT= 8
      -6: X=0.10273149 Y=0.89726851 Z=0.06084092
      -6: X=0.10273149 Y=0.20546297 Z=0.06084092
Si3        NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
ATOM  -7: X=0.00000000 Y=0.00000000 Z=0.09907526
          MULT= 1          ISPLIT= 4
Si4        NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
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ATOM  -8: X=0.33333333 Y=0.66666667 Z=0.09865712
          MULT= 1          ISPLIT= 4
Si5        NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -9: X=0.66666667 Y=0.33333333 Z=0.09880781
          MULT= 1          ISPLIT= 4
Si6        NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM -10: X=0.32924123 Y=0.99807733 Z=0.08501628
          MULT= 6          ISPLIT= 8
     -10: X=0.00192267 Y=0.33116390 Z=0.08501628
     -10: X=0.66883610 Y=0.67075877 Z=0.08501628
     -10: X=0.00192267 Y=0.67075877 Z=0.08501628
     -10: X=0.66883610 Y=0.99807733 Z=0.08501628
     -10: X=0.32924123 Y=0.33116390 Z=0.08501628
Si7        NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM -11: X=0.00000000 Y=0.00000000 Z=0.17439369
          MULT= 1          ISPLIT= 4
Si8        NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM -12: X=0.33333333 Y=0.66666667 Z=0.17530497
          MULT= 1          ISPLIT= 4
Si9        NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM -13: X=0.66666667 Y=0.33333333 Z=0.17534516
          MULT= 1          ISPLIT= 4
Si10       NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM -14: X=0.33272054 Y=0.00032393 Z=0.16435634
          MULT= 6          ISPLIT= 8
     -14: X=0.99967607 Y=0.33239661 Z=0.16435634
     -14: X=0.66760339 Y=0.66727946 Z=0.16435634
     -14: X=0.99967607 Y=0.66727946 Z=0.16435634
     -14: X=0.66760339 Y=0.00032393 Z=0.16435634
     -14: X=0.33272054 Y=0.33239661 Z=0.16435634
Si11       NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM -15: X=0.22650804 Y=0.11325402 Z=0.19448932
          MULT= 3          ISPLIT= 8
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     -15: X=0.88674598 Y=0.11325402 Z=0.19448932
     -15: X=0.88674598 Y=0.77349196 Z=0.19448932
Si12       NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
ATOM -16: X=0.21925394 Y=0.78074606 Z=0.19387431
          MULT= 3          ISPLIT= 8
     -16: X=0.21925394 Y=0.43850788 Z=0.19387431
     -16: X=0.56149212 Y=0.78074606 Z=0.19387431
Si13       NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    0.0000000 0.5000000 0.8660254
                     0.0000000-0.8660254 0.5000000
                     1.0000000 0.0000000 0.0000000
ATOM -17: X=0.55247016 Y=0.10494033 Z=0.19371103
          MULT= 3          ISPLIT= 8
     -17: X=0.89505967 Y=0.44752984 Z=0.19371103
     -17: X=0.55247016 Y=0.44752984 Z=0.19371103
Si14       NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    0.0000000-0.5000000 0.8660254
                     0.0000000-0.8660254-0.5000000
                     1.0000000 0.0000000 0.0000000
ATOM -18: X=0.22476540 Y=0.11238270 Z=0.27203995
          MULT= 3          ISPLIT= 8
     -18: X=0.88761730 Y=0.11238270 Z=0.27203995
     -18: X=0.88761730 Y=0.77523460 Z=0.27203995
Si15       NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
ATOM -19: X=0.55784842 Y=0.77892421 Z=0.27173982
          MULT= 3          ISPLIT= 8
     -19: X=0.22107579 Y=0.77892421 Z=0.27173982
     -19: X=0.22107579 Y=0.44215158 Z=0.27173982
Si16       NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
ATOM -20: X=0.55460989 Y=0.10921979 Z=0.27170261
          MULT= 3          ISPLIT= 8
     -20: X=0.89078021 Y=0.44539011 Z=0.27170261
     -20: X=0.55460989 Y=0.44539011 Z=0.27170261
Si17       NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    0.0000000-0.5000000 0.8660254
                     0.0000000-0.8660254-0.5000000
                     1.0000000 0.0000000 0.0000000
ATOM -21: X=0.11030226 Y=0.88969774 Z=0.29791032
          MULT= 3          ISPLIT= 8
     -21: X=0.11030226 Y=0.22060452 Z=0.29791032
     -21: X=0.77939548 Y=0.88969774 Z=0.29791032
Si18       NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    0.0000000 0.5000000 0.8660254
                     0.0000000-0.8660254 0.5000000
                     1.0000000 0.0000000 0.0000000
```

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ATOM -22: X=0.44596332 Y=0.22298166 Z=0.29795535
          MULT= 3          ISPLIT= 8
     -22: X=0.77701834 Y=0.22298166 Z=0.29795535
     -22: X=0.77701834 Y=0.55403668 Z=0.29795535
Si19       NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
ATOM -23: X=0.44371513 Y=0.88743027 Z=0.29760186
          MULT= 3          ISPLIT= 8
     -23: X=0.11256973 Y=0.55628487 Z=0.29760186
     -23: X=0.44371513 Y=0.55628487 Z=0.29760186
Si20       NPT=  781  R0=0.00010000 RMT= 1.84        Z:  14.00000
LOCAL ROT MATRIX:    0.0000000-0.5000000 0.8660254
                     0.0000000-0.8660254-0.5000000
                     1.0000000 0.0000000 0.0000000
ATOM -24: X=0.77511490 Y=0.22488510 Z=0.34736823
          MULT= 3          ISPLIT= 8
     -24: X=0.77511490 Y=0.55022980 Z=0.34736823
     -24: X=0.44977020 Y=0.22488510 Z=0.34736823
H 1        NPT=  781  R0=0.00010000 RMT= 0.99        Z:   1.00000
LOCAL ROT MATRIX:    0.0000000 0.5000000 0.8660254
                     0.0000000-0.8660254 0.5000000
                     1.0000000 0.0000000 0.0000000
ATOM -25: X=0.44248609 Y=0.55751391 Z=0.34702569
          MULT= 3          ISPLIT= 8
     -25: X=0.44248609 Y=0.88497217 Z=0.34702569
     -25: X=0.11502783 Y=0.55751391 Z=0.34702569
H 2        NPT=  781  R0=0.00010000 RMT= 0.99        Z:   1.00000
LOCAL ROT MATRIX:    0.0000000 0.5000000 0.8660254
                     0.0000000-0.8660254 0.5000000
                     1.0000000 0.0000000 0.0000000
ATOM -26: X=0.78138476 Y=0.89069238 Z=0.34732485
          MULT= 3          ISPLIT= 8
     -26: X=0.10930762 Y=0.89069238 Z=0.34732485
     -26: X=0.10930762 Y=0.21861524 Z=0.34732485
H 3        NPT=  781  R0=0.00010000 RMT= 0.99        Z:   1.00000
LOCAL ROT MATRIX:    0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
                     1.0000000 0.0000000 0.0000000
   6      NUMBER OF SYMMETRY OPERATIONS
 1 0 0 0.00000000
 0 1 0 0.00000000
 0 0 1 0.00000000
       1
 0-1 0 0.00000000
 1-1 0 0.00000000
 0 0 1 0.00000000
       2
-1 1 0 0.00000000
-1 0 0 0.00000000
 0 0 1 0.00000000
       3
 0-1 0 0.00000000
```

```
-1 0 0 0.00000000
 0 0 1 0.00000000
       4
-1 1 0 0.00000000
 0 1 0 0.00000000
 0 0 1 0.00000000
       5
 1 0 0 0.00000000
 1-1 0 0.00000000
 0 0 1 0.00000000
       6
```