Manual for TWINLAW

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This program reads two orientation matrices from two different files. The orientation matrices should be specified as a 3x3 matrix in free format. The single values should be separated by at least one blank character. The resulting twin law is written the a file called hklf5.dat and a short listing is written to twinlaw.out.

An example of the input and output data:

Input file containing orientation matrix 1 (a.dat):

```
 -0.02578019  0.13485431 -0.02626642
  0.16684957  0.10632220  0.04471096
  0.09166711 -0.00579784 -0.06533389
```

Input file containing orientation matrix 2 (b.dat):

```
  0.00949118 -0.14715500 -0.02624292
 -0.13885245 -0.08545577  0.04480172
 -0.13216658 -0.02449844 -0.06526571
```

Output file containing the twin law (hklf5.dat):

```
        -0.998962820         0.000807962         0.000507880
         0.000423545        -1.000509977         0.000203392
         0.621302366         0.464893550         0.999651015
```

Output logfile of the program (twinlaw.out):

```
Matrix 1:
      -0.025780190         0.134854317        -0.026266420
       0.166849568         0.106322199         0.044710960
       0.091667108        -0.005797840        -0.065333888

Matrix 2:
       0.009491180        -0.147155002        -0.026242919
      -0.138852447        -0.085455768         0.044801719
      -0.132166579        -0.024498440        -0.065265708


Reciprocal metric tensor 1:
       0.036906257         0.013731772         0.002148190
       0.013731772         0.029523712         0.001590423
       0.002148190         0.001590423         0.006957512

Reciprocal metric tensor 2:
       0.036838088         0.013706943         0.002156040
       0.013706943         0.029557457         0.001632120
       0.002156040         0.001632120         0.006955497


Reciprocal cell parameters:           Direct cell parameters:
     Matrix 1      Matrix 2            Matrix 1      Matrix 2

     0.192110      0.191933            5.751422      5.754688
     0.171825      0.171923            6.411982      6.407566
     0.083412      0.083400           12.120689     12.125757
    83.628845     83.463890           93.511856     93.681694
    82.295799     82.259148           95.581253     95.550331
    65.417824     65.455971          114.034760    113.977692
     0.002477      0.002475          403.787903    403.976593


Twin matrix for transforming the reflection indices (h,k,l)
and the direct cell parameters (a,b,c):

      -0.998962820         0.000807962         0.000507880
       0.000423545        -1.000509977         0.000203392
       0.621302366         0.464893550         0.999651015

h(twin) =  (-0.999 * h)  +  ( 0.001 * k)  +  ( 0.001 * l)
k(twin) =  ( 0.000 * h)  +  (-1.001 * k)  +  ( 0.000 * l)
l(twin) =  ( 0.621 * h)  +  ( 0.465 * k)  +  ( 1.000 * l)


Twin matrix for transforming the atom coordinates (x,y,z)
and the reciprocal cell parameters (ar,br,cr):

      -0.998962820        -0.000423984        -0.621947467
       0.000807962        -1.000509620        -0.465158969
       0.000507880         0.000203607         1.000061512

ar(twin) =  (-0.999 * ar)  +  ( 0.000 * br)  +  (-0.622 * cr)
br(twin) =  ( 0.001 * ar)  +  (-1.001 * br)  +  (-0.465 * cr)
cr(twin) =  ( 0.001 * ar)  +  ( 0.000 * br)  +  ( 1.000 * cr)
```