

Manual for HKLF5

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This program reads

- 1) a file containing a twin law for transforming the reflection indices of two twin components,
- 2) a file containing the untwinned reflection data [The reflections should be corrected for absorption (if necessary) and merged.],
- 3) and optionally two files containing the orientation matrices corresponding to the two twin domains. These two files are only necessary if the reflections do not perfectly overlap.

Then the kind of overlap between reflections of the two twin domains must be specified:

- 1) Perfect overlap (see example 1).
- 2) Two reflections are assumed to be overlapping if their distance in reciprocal space is less than a predefined value. A default of 0.01 \AA^{-1} is set, but may be altered (see example 2).

For refinement with SHELXL, the modified reflection file should be read in using the HKLF5 option and an additional parameter should be introduced (BASF).

Example 1 of the input and output data:

Input file containing the twin law (hk1f51.dat):

1	0	0
0	-1	0
-0.25	0	-1

Input file containing the untwinned (shortened) reflection data (orig1.hkl):

-5	-5	4	44.53	8.00
-5	-5	5	70.55	8.98
-5	-5	6	76.42	8.31
-4	-5	11	408.20	11.52
-4	-5	10	167.04	8.96

Output file containing the modified reflection data (twin1.hkl):

```
-5 -5 4 44.53 8.00 1
-5 -5 5 70.55 8.98 1
-5 -5 6 76.42 8.31 1
-4 5 -10 408.20 11.52 -2
-4 -5 11 408.20 11.52 1
-4 5 -9 167.04 8.96 -2
-4 -5 10 167.04 8.96 1
```

Example 2 of the input and output data:

Input 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
```

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
```

Input file containing the untwinned (shortened) reflection data (orig.hkl):

```
3 0 0 125.90 26.36
4 0 0 1650.95 22.62
5 0 0 7.45 4.15
6 0 0 28.39 4.34
-7 1 0 732.64 14.64
```

Output file containing the modified reflection data (twin.hkl):

```
3 0 0 125.90 26.36 1
4 0 0 1650.95 22.62 1
-5 0 3 7.45 4.15 -2
5 0 0 7.45 4.15 1
6 0 0 28.39 4.34 1
7 -1 -4 732.64 14.64 -2
-7 1 0 732.64 14.64 1
```