R O T A X : Simon Parsons & Bob Gould, University of Edinburgh
with additions by Richard Cooper (Oxford) and Louis Farrugia (Glasgow)
Version 26th November, 2001
Symmetry element generation for: as19a2
Symmetry element tested: 180.0 degree rotation
Max figure of merit printed = 5.00
Largest index tested = 12
Cell dimensions: 7.2847 9.7400 15.2310 90.0000 94.3860 90.0000
The following thirty data are used to test possible twin laws.
These have the largest values of [F2obs-F2calc]/sigma.

-3	3	3	86.07	-3	4	5	55.69	0	2	3	54.24
0	1	3	48.98	0	1	2	48.89	-3	2	7	45.57
-3	5	3	39.25	0	0	8	37.78	0	2	7	37.41
0	4	0	35.95	-3	6	1	33.18	-3	1	5	32.28
-3	5	8	29.35	-3	1	1	29.20	-3	2	2	28.58
3	1	3	27.78	0	2	2	26.82	-3	1	2	26.55
0	0	4	25.57	-3	3	4	25.10	-3	5	2	25.10
0	2	4	23.78	-3	6	7	22.59	-3	1	6	20.98
-3	3	1	20.00	0	3	3	19.99	-3	5	9	18.65
-3	6	3	17.91	0	1	1	17.59	0	4	7	17.59

Each of these sets of indices is transformed by the printed rotation matrix. How far the transformed indices are from integral values is measured by the figure of merit. The figure of merit is defined as 1000 times the average deviation (in Ang-1) of transformed indices from their nearest reciprocal lattice node. ROTAX tries to minimise the f.o.m. by omitting upto 15 of the largest deviations. A small
figure of merit means that most (or all) of the indices were transformed to integers
and this makes it a likely candidate for a twin law. If only symmetry elements which
occur in the point group of your crystal structure are printed then either your crystal is not a twin, or this program has not worked. Matrices which have a figure
of merit less than 2 are marked with a row of asterisks: **********

180.0 degree rotation about   1. 0. 0. direct lattice direction:
[1.000   0.000   0.000]
[0.000   -1.000   0.000]
[-0.320   0.000   -1.000]
Figure of merit =   1.60 **********
No reflections omitted
Distances in Ang**-1 of transformed indices from integral r.l. points:
d1 = distance of transformed indices to nearest r.l. point
d2 = d1 - distance to r.l. point with rounded transformed indices
In a well-behaved system d2 should be zero, but it could deviate from this value in the case of a highly skew unit cell.

Orig.			Trans.			d1	d2
-3.	3.	3.	-3.	-3.	-2.	0.00267	0.00000
-3.	4.	5.	-3.	-4.	-4.	0.00267	0.00000
0.	2.	3.	0.	-2.	-3.	0.00000	0.00000
0.	1.	3.	0.	-1.	-3.	0.00000	0.00000
0.	1.	2.	0.	-1.	-2.	0.00000	0.00000
-3.	2.	7.	-3.	-2.	-6.	0.00267	0.00000
-3.	5.	3.	-3.	-5.	-2.	0.00267	0.00000
0.	0.	8.	0.	0.	-8.	0.00000	0.00000
0.	2.	7.	0.	-2.	-7.	0.00000	0.00000
0.	4.	0.	0.	-4.	0.	0.00000	0.00000
-3.	6.	1.	-3.	-6.	0.	0.00267	0.00000
-3.	1.	5.	-3.	-1.	-4.	0.00267	0.00000
-3.	5.	8.	-3.	-5.	-7.	0.00267	0.00000
-3.	1.	1.	-3.	-1.	0.	0.00267	0.00000
-3.	2.	2.	-3.	-2.	-1.	0.00267	0.00000
3.	1.	3.	3.	-1.	-4.	0.00267	0.00000
0.	2.	2.	0.	-2.	-2.	0.00000	0.00000
-3.	1.	2.	-3.	-1.	-1.	0.00267	0.00000
0.	0.	4.	0.	0.	-4.	0.00000	0.00000
-3.	3.	4.	-3.	-3.	-3.	0.00267	0.00000
-3.	5.	2.	-3.	-5.	-1.	0.00267	0.00000
0.	2.	4.	0.	-2.	-4.	0.00000	0.00000
-3.	6.	7.	-3.	-6.	-6.	0.00267	0.00000
-3.	1.	6.	-3.	-1.	-5.	0.00267	0.00000
-3.	3.	1.	-3.	-3.	0.	0.00267	0.00000
0.	3.	3.	0.	-3.	-3.	0.00000	0.00000
-3.	5.	9.	-3.	-5.	-8.	0.00267	0.00000
-3.	6.	3.	-3.	-6.	-2.	0.00267	0.00000
0.	1.	1.	0.	-1.	-1.	0.00000	0.00000
0.	4.	7.	0.	-4.	-7.	0.00000	0.00000

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180.0 degree rotation about   0. 1. 0. direct lattice direction:
[-1.000   0.000   0.000]
[0.000   1.000   0.000]
[0.000   0.000   -1.000]
Figure of merit =   0.00 ***********
No reflections omitted
Distances in Ang**-1 of transformed indices from integral r.l. points:
d1 = distance of transformed indices to nearest r.l. point
d2 = d1 - distance to r.l. point with rounded transformed indices
In a well-behaved system d2 should be zero, but it could deviate from this
value in the case of a highly skew unit cell.

Orig.			Trans.			d1	d2	
-3.	3.	3.	3.	3.	-3.	0.00000	0.00000	
-3.	4.	5.	3.	4.	-5.	0.00000	0.00000	Omitted from fom calculation
0.	2.	3.	0.	2.	-3.	0.00000	0.00000	
0.	1.	3.	0.	1.	-3.	0.00000	0.00000	
0.	1.	2.	0.	1.	-2.	0.00000	0.00000	
-3.	2.	7.	3.	2.	-7.	0.00000	0.00000	
-3.	5.	3.	3.	5.	-3.	0.00000	0.00000	
0.	0.	8.	0.	0.	-8.	0.00000	0.00000	
0.	2.	7.	0.	2.	-7.	0.00000	0.00000	
0.	4.	0.	0.	4.	0.	0.00000	0.00000	
-3.	6.	1.	3.	6.	-1.	0.00000	0.00000	
-3.	1.	5.	3.	1.	-5.	0.00000	0.00000	
-3.	5.	8.	3.	5.	-8.	0.00000	0.00000	Omitted from fom calculation
-3.	1.	1.	3.	1.	-1.	0.00000	0.00000	
-3.	2.	2.	3.	2.	-2.	0.00000	0.00000	
3.	1.	3.	-3.	1.	-3.	0.00000	0.00000	
0.	2.	2.	0.	2.	-2.	0.00000	0.00000	
-3.	1.	2.	3.	1.	-2.	0.00000	0.00000	
0.	0.	4.	0.	0.	-4.	0.00000	0.00000	
-3.	3.	4.	3.	3.	-4.	0.00000	0.00000	
-3.	5.	2.	3.	5.	-2.	0.00000	0.00000	
0.	2.	4.	0.	2.	-4.	0.00000	0.00000	
-3.	6.	7.	3.	6.	-7.	0.00000	0.00000	
-3.	1.	6.	3.	1.	-6.	0.00000	0.00000	
-3.	3.	1.	3.	3.	-1.	0.00000	0.00000	
0.	3.	3.	0.	3.	-3.	0.00000	0.00000	
-3.	5.	9.	3.	5.	-9.	0.00000	0.00000	Omitted from fom calculation
-3.	6.	3.	3.	6.	-3.	0.00000	0.00000	
0.	1.	1.	0.	1.	-1.	0.00000	0.00000	
0.	4.	7.	0.	4.	-7.	0.00000	0.00000	

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180.0 degree rotation about   0. 1. 0. reciprocal lattice direction:
[-1.000   0.000   0.000]
[0.000   1.000   0.000]
[0.000   0.000   -1.000]
Figure of merit =   0.00 ***********
No reflections omitted
Distances in Ang**-1 of transformed indices from integral r.l. points:
d1 = distance of transformed indices to nearest r.l. point
d2 = d1 - distance to r.l. point with rounded transformed indices
In a well-behaved system d2 should be zero, but it could deviate from this
value in the case of a highly skew unit cell.

Orig.			Trans.			d1	d2	
-3.	3.	3.	3.	3.	-3.	0.00000	0.00000	
-3.	4.	5.	3.	4.	-5.	0.00000	0.00000	
0.	2.	3.	0.	2.	-3.	0.00000	0.00000	
0.	1.	3.	0.	1.	-3.	0.00000	0.00000	
0.	1.	2.	0.	1.	-2.	0.00000	0.00000	
-3.	2.	7.	3.	2.	-7.	0.00000	0.00000	
-3.	5.	3.	3.	5.	-3.	0.00000	0.00000	
0.	0.	8.	0.	0.	-8.	0.00000	0.00000	
0.	2.	7.	0.	2.	-7.	0.00000	0.00000	
0.	4.	0.	0.	4.	0.	0.00000	0.00000	Omitted from fom calculation
-3.	6.	1.	3.	6.	-1.	0.00000	0.00000	
-3.	1.	5.	3.	1.	-5.	0.00000	0.00000	
-3.	5.	8.	3.	5.	-8.	0.00000	0.00000	
-3.	1.	1.	3.	1.	-1.	0.00000	0.00000	
-3.	2.	2.	3.	2.	-2.	0.00000	0.00000	
3.	1.	3.	-3.	1.	-3.	0.00000	0.00000	
0.	2.	2.	0.	2.	-2.	0.00000	0.00000	
-3.	1.	2.	3.	1.	-2.	0.00000	0.00000	
0.	0.	4.	0.	0.	-4.	0.00000	0.00000	
-3.	3.	4.	3.	3.	-4.	0.00000	0.00000	
-3.	5.	2.	3.	5.	-2.	0.00000	0.00000	
0.	2.	4.	0.	2.	-4.	0.00000	0.00000	
-3.	6.	7.	3.	6.	-7.	0.00000	0.00000	
-3.	1.	6.	3.	1.	-6.	0.00000	0.00000	
-3.	3.	1.	3.	3.	-1.	0.00000	0.00000	
0.	3.	3.	0.	3.	-3.	0.00000	0.00000	
-3.	5.	9.	3.	5.	-9.	0.00000	0.00000	
-3.	6.	3.	3.	6.	-3.	0.00000	0.00000	
0.	1.	1.	0.	1.	-1.	0.00000	0.00000	
0.	4.	7.	0.	4.	-7.	0.00000	0.00000	

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180.0 degree rotation about -6. 0. 1. reciprocal lattice direction:
[0.999   0.000   -0.003]
[0.000   -1.000   0.000]
[-0.333   0.000   -0.999]
Figure of merit =   1.54 ***********
No reflections omitted
Distances in Ang**-1 of transformed indices from integral r.l. points:
d1 = distance of transformed indices to nearest r.l. point
d2 = d1 - distance to r.l. point with rounded transformed indices
In a well-behaved system d2 should be zero, but it could deviate from this value in the case of a highly skew unit cell.

Orig.			Trans.			d1	d2
-3.	3.	3.	-3.	-3.	-2.	0.00107	0.00000
-3.	4.	5.	-3.	-4.	-4.	0.00192	0.00000
0.	2.	3.	0.	-2.	-3.	0.00128	0.00000
0.	1.	3.	0.	-1.	-3.	0.00128	0.00000
0.	1.	2.	0.	-1.	-2.	0.00086	0.00000
-3.	2.	7.	-3.	-2.	-6.	0.00278	0.00000
-3.	5.	3.	-3.	-5.	-2.	0.00107	0.00000
0.	0.	8.	0.	0.	-8.	0.00342	0.00000
0.	2.	7.	0.	-2.	-7.	0.00299	0.00000
0.	4.	0.	0.	-4.	0.	0.00000	0.00000
-3.	6.	1.	-3.	-6.	0.	0.00021	0.00000
-3.	1.	5.	-3.	-1.	-4.	0.00192	0.00000
-3.	5.	8.	-3.	-5.	-7.	0.00321	0.00000
-3.	1.	1.	-3.	-1.	0.	0.00021	0.00000
-3.	2.	2.	-3.	-2.	-1.	0.00064	0.00000
3.	1.	3.	3.	-1.	-4.	0.00150	0.00000
0.	2.	2.	0.	-2.	-2.	0.00086	0.00000
-3.	1.	2.	-3.	-1.	-1.	0.00064	0.00000
0.	0.	4.	0.	0.	-4.	0.00171	0.00000
-3.	3.	4.	-3.	-3.	-3.	0.00150	0.00000
-3.	5.	2.	-3.	-5.	-1.	0.00064	0.00000
0.	2.	4.	0.	-2.	-4.	0.00171	0.00000
-3.	6.	7.	-3.	-6.	-6.	0.00278	0.00000
-3.	1.	6.	-3.	-1.	-5.	0.00235	0.00000
-3.	3.	1.	-3.	-3.	0.	0.00021	0.00000
0.	3.	3.	0.	-3.	-3.	0.00128	0.00000
-3.	5.	9.	-3.	-5.	-8.	0.00364	0.00000
-3.	6.	3.	-3.	-6.	-2.	0.00107	0.00000
0.	1.	1.	0.	-1.	-1.	0.00043	0.00000
0.	4.	7.	0.	-4.	-7.	0.00299	0.00000

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180.0 degree rotation about   0. 0. 1. reciprocal lattice direction:
[-1.000   0.000   0.000]
[0.000   -1.000   0.000]
[0.320   0.000   1.000]
Figure of merit =   1.60 ***********
No reflections omitted
Distances in Ang**-1 of transformed indices from integral r.l. points:
d1 = distance of transformed indices to nearest r.l. point
d2 = d1 - distance to r.l. point with rounded transformed indices
In a well-behaved system d2 should be zero, but it could deviate from this value in the case of a highly skew unit cell.

Orig.			Trans.			d1	d2
-3.	3.	3.	3.	-3.	2.	0.00267	0.00000
-3.	4.	5.	3.	-4.	4.	0.00267	0.00000
0.	2.	3.	0.	-2.	3.	0.00000	0.00000
0.	1.	3.	0.	-1.	3.	0.00000	0.00000
0.	1.	2.	0.	-1.	2.	0.00000	0.00000
-3.	2.	7.	3.	-2.	6.	0.00267	0.00000
-3.	5.	3.	3.	-5.	2.	0.00267	0.00000
0.	0.	8.	0.	0.	8.	0.00000	0.00000
0.	2.	7.	0.	-2.	7.	0.00000	0.00000
0.	4.	0.	0.	-4.	0.	0.00000	0.00000
-3.	6.	1.	3.	-6.	0.	0.00267	0.00000
-3.	1.	5.	3.	-1.	4.	0.00267	0.00000
-3.	5.	8.	3.	-5.	7.	0.00267	0.00000
-3.	1.	1.	3.	-1.	0.	0.00267	0.00000
-3.	2.	2.	3.	-2.	1.	0.00267	0.00000
3.	1.	3.	-3.	-1.	4.	0.00267	0.00000
0.	2.	2.	0.	-2.	2.	0.00000	0.00000
-3.	1.	2.	3.	-1.	1.	0.00267	0.00000
0.	0.	4.	0.	0.	4.	0.00000	0.00000
-3.	3.	4.	3.	-3.	3.	0.00267	0.00000
-3.	5.	2.	3.	-5.	1.	0.00267	0.00000
0.	2.	4.	0.	-2.	4.	0.00000	0.00000
-3.	6.	7.	3.	-6.	6.	0.00267	0.00000
-3.	1.	6.	3.	-1.	5.	0.00267	0.00000
-3.	3.	1.	3.	-3.	0.	0.00267	0.00000
0.	3.	3.	0.	-3.	3.	0.00000	0.00000
-3.	5.	9.	3.	-5.	8.	0.00267	0.00000
-3.	6.	3.	3.	-6.	2.	0.00267	0.00000
0.	1.	1.	0.	-1.	1.	0.00000	0.00000
0.	4.	7.	0.	-4.	7.	0.00000	0.00000

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180.0 degree rotation about -11. 0. 2. reciprocal lattice direction:
[0.998   0.000   -0.010]
[0.000   -1.000   0.000]
[-0.363   0.000   -0.998]
Figure of merit =   4.65
15 reflections omitted
Figure of merit with no omissions =   6.93
Distances in Ang**-1 of transformed indices from integral r.l. points:
d1 = distance of transformed indices to nearest r.l. point
d2 = d1 - distance to r.l. point with rounded transformed indices
In a well-behaved system d2 should be zero, but it could deviate from this
value in the case of a highly skew unit cell.

Orig.			Trans.			d1	d2	
-3.	3.	3.	-3.	-3.	-2.	0.00691	0.00000	Omitted from fom calculation
-3.	4.	5.	-3.	-4.	-4.	0.00864	0.00000	Omitted from fom calculation
0.	2.	3.	0.	-2.	-3.	0.00415	0.00000	
0.	1.	3.	0.	-1.	-3.	0.00415	0.00000	
0.	1.	2.	0.	-1.	-2.	0.00277	0.00000	
-3.	2.	7.	-3.	-2.	-6.	0.01081	0.00000	Omitted from fom calculation
-3.	5.	3.	-3.	-5.	-2.	0.00692	0.00000	Omitted from fom calculation
0.	0.	8.	0.	0.	-8.	0.01108	0.00000	Omitted from fom calculation
0.	2.	7.	0.	-2.	-7.	0.00969	0.00000	Omitted from fom calculation
0.	4.	0.	0.	-4.	0.	0.00000	0.00000	
-3.	6.	1.	-3.	-6.	0.	0.00603	0.00000	
-3.	1.	5.	-3.	-1.	-4.	0.00864	0.00000	Omitted from fom calculation
-3.	5.	8.	-3.	-5.	-7.	0.01199	0.00000	Omitted from fom calculation
-3.	1.	1.	-3.	-1.	0.	0.00603	0.00000	
-3.	2.	2.	-3.	-2.	-1.	0.00634	0.00000	
3.	1.	3.	3.	-1.	-4.	0.00770	0.00000	Omitted from fom calculation
0.	2.	2.	0.	-2.	-2.	0.00277	0.00000	
-3.	1.	2.	-3.	-1.	-1.	0.00634	0.00000	
0.	0.	4.	0.	0.	-4.	0.00554	0.00000	
-3.	3.	4.	-3.	-3.	-3.	0.00770	0.00000	Omitted from fom calculation
-3.	5.	2.	-3.	-5.	-1.	0.00634	0.00000	
0.	2.	4.	0.	-2.	-4.	0.00554	0.00000	
-3.	6.	7.	-3.	-6.	-6.	0.01081	0.00000	Omitted from fom calculation
-3.	1.	6.	-3.	-1.	-5.	0.00969	0.00000	Omitted from fom calculation
-3.	3.	1.	-3.	-3.	0.	0.00603	0.00000	
0.	3.	3.	0.	-3.	-3.	0.00415	0.00000	
-3.	5.	9.	-3.	-5.	-8.	0.01321	0.00000	Omitted from fom calculation
-3.	6.	3.	-3.	-6.	-2.	0.00692	0.00000	Omitted from fom calculation
0.	1.	1.	0.	-1.	-1.	0.00138	0.00000	
0.	4.	7.	0.	-4.	-7.	0.00969	0.00000	Omitted from fom calculation

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180.0 degree rotation about   1. 0. 6. direct lattice direction:
[-0.999   0.000   0.003]
[0.000   -1.000   0.000]
[0.333   0.000   0.999]
Figure of merit =   1.54 ***********
No reflections omitted
Distances in Ang**-1 of transformed indices from integral r.l. points:
d1 = distance of transformed indices to nearest r.l. point
d2 = d1 - distance to r.l. point with rounded transformed indices
In a well-behaved system d2 should be zero, but it could deviate from this value in the case of a highly skew unit cell.

Orig.			Trans.			d1	d2
-3.	3.	3.	3.	-3.	2.	0.00107	0.00000
-3.	4.	5.	3.	-4.	4.	0.00192	0.00000
0.	2.	3.	0.	-2.	3.	0.00128	0.00000
0.	1.	3.	0.	-1.	3.	0.00128	0.00000
0.	1.	2.	0.	-1.	2.	0.00086	0.00000
-3.	2.	7.	3.	-2.	6.	0.00278	0.00000
-3.	5.	3.	3.	-5.	2.	0.00107	0.00000
0.	0.	8.	0.	0.	8.	0.00342	0.00000
0.	2.	7.	0.	-2.	7.	0.00299	0.00000
0.	4.	0.	0.	-4.	0.	0.00000	0.00000
-3.	6.	1.	3.	-6.	0.	0.00021	0.00000
-3.	1.	5.	3.	-1.	4.	0.00192	0.00000
-3.	5.	8.	3.	-5.	7.	0.00321	0.00000
-3.	1.	1.	3.	-1.	0.	0.00021	0.00000
-3.	2.	2.	3.	-2.	1.	0.00064	0.00000
3.	1.	3.	-3.	-1.	4.	0.00150	0.00000
0.	2.	2.	0.	-2.	2.	0.00086	0.00000
-3.	1.	2.	3.	-1.	1.	0.00064	0.00000
0.	0.	4.	0.	0.	4.	0.00171	0.00000
-3.	3.	4.	3.	-3.	3.	0.00150	0.00000
-3.	5.	2.	3.	-5.	1.	0.00064	0.00000
0.	2.	4.	0.	-2.	4.	0.00171	0.00000
-3.	6.	7.	3.	-6.	6.	0.00278	0.00000
-3.	1.	6.	3.	-1.	5.	0.00235	0.00000
-3.	3.	1.	3.	-3.	0.	0.00021	0.00000
0.	3.	3.	0.	-3.	3.	0.00128	0.00000
-3.	5.	9.	3.	-5.	8.	0.00364	0.00000
-3.	6.	3.	3.	-6.	2.	0.00107	0.00000
0.	1.	1.	0.	-1.	1.	0.00043	0.00000
0.	4.	7.	0.	-4.	7.	0.00299	0.00000

++

180.0 degree rotation about   2. 0. 11. direct lattice direction:
[-0.998   0.000   0.010]
[0.000   -1.000   0.000]
[0.363   0.000   0.998]
Figure of merit =   4.65
15 reflections omitted
Figure of merit with no omissions =   6.93
Distances in Ang**-1 of transformed indices from integral r.l. points:
d1 = distance of transformed indices to nearest r.l. point
d2 = d1 - distance to r.l. point with rounded transformed indices
In a well-behaved system d2 should be zero, but it could deviate from this
value in the case of a highly skew unit cell.

Orig.			Trans.			d1	d2	
-3.	3.	3.	3.	-3.	2.	0.00692	0.00000	Omitted from fom calculation
-3.	4.	5.	3.	-4.	4.	0.00864	0.00000	Omitted from fom calculation
0.	2.	3.	0.	-2.	3.	0.00415	0.00000	
0.	1.	3.	0.	-1.	3.	0.00415	0.00000	
0.	1.	2.	0.	-1.	2.	0.00277	0.00000	
-3.	2.	7.	3.	-2.	6.	0.01081	0.00000	Omitted from fom calculation
-3.	5.	3.	3.	-5.	2.	0.00692	0.00000	Omitted from fom calculation
0.	0.	8.	0.	0.	8.	0.01108	0.00000	Omitted from fom calculation
0.	2.	7.	0.	-2.	7.	0.00969	0.00000	Omitted from fom calculation
0.	4.	0.	0.	-4.	0.	0.00000	0.00000	
-3.	6.	1.	3.	-6.	0.	0.00603	0.00000	
-3.	1.	5.	3.	-1.	4.	0.00864	0.00000	Omitted from fom calculation
-3.	5.	8.	3.	-5.	7.	0.01199	0.00000	Omitted from fom calculation
-3.	1.	1.	3.	-1.	0.	0.00603	0.00000	
-3.	2.	2.	3.	-2.	1.	0.00634	0.00000	
3.	1.	3.	-3.	-1.	4.	0.00770	0.00000	Omitted from fom calculation
0.	2.	2.	0.	-2.	2.	0.00277	0.00000	
-3.	1.	2.	3.	-1.	1.	0.00634	0.00000	
0.	0.	4.	0.	0.	4.	0.00554	0.00000	
-3.	3.	4.	3.	-3.	3.	0.00770	0.00000	Omitted from fom calculation
-3.	5.	2.	3.	-5.	1.	0.00634	0.00000	
0.	2.	4.	0.	-2.	4.	0.00554	0.00000	
-3.	6.	7.	3.	-6.	6.	0.01081	0.00000	Omitted from fom calculation
-3.	1.	6.	3.	-1.	5.	0.00969	0.00000	Omitted from fom calculation
-3.	3.	1.	3.	-3.	0.	0.00603	0.00000	
0.	3.	3.	0.	-3.	3.	0.00415	0.00000	
-3.	5.	9.	3.	-5.	8.	0.01321	0.00000	Omitted from fom calculation
-3.	6.	3.	3.	-6.	2.	0.00692	0.00000	Omitted from fom calculation
0.	1.	1.	0.	-1.	1.	0.00138	0.00000	
0.	4.	7.	0.	-4.	7.	0.00969	0.00000	Omitted from fom calculation

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