Supporting information

Triclinic crystal structure distortion of multiferroic $BiMn_7O_{12}$

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3.1. Anisotropic hkl-dependent peakshape in Topas

```
'Anisotropic line asymmetry 1
prm p1  0.0001 min 0.0001
spherical_harmonics_hkl sh1
sh_order  4 load sh_Cij_prm {}
circles_conv = sh1 p1 / Cos(Th);

'Anisotropic line asymmetry  2
prm p2  0.0001 min 0.0001
spherical_harmonics_hkl sh2
sh_order  4 load sh_Cij_prm {}
circles_conv = sh2 p2 / Cos(Th);
```

3.2. Anisotropic hkl-dependent peak broadening in Topas

```
'Anisotropic line broadening due to strain
lor_fwhm = sh3 p3 Tan(Th);

'Anisotropic line broadening due to crystallite size
gauss_fwhm = sh4 p4 / Cos(Th);
```

*3.3. ISODISTORT output file for irreducible representations derived for Im to I*1 *symmetry reduction*

```
!begin distortionFile
#version of isodistort
!isodistortVersion
6.1.11
#string containing parent space group
!parentString
8 Im         Cs-3
#string containing space group setting of parent
!parentSettingString
monoclinic cell choice 3
```

```
#string containing lattice parameters of parent
!lattParamString
a=7.52217, b=7.37005, c=7.53093, alpha=90.00000, beta=91.22340, gamma=90.00000
#for each wyckoff position: string
!wyckoffString
2a (x,0,z), x=0.00137, z=-0.00624
2a (x,0,z), x=-0.48630, z=-0.47580
2a (x,0,z), x=0.02050, z=-0.46790
2a (x,0,z), x=-0.47620, z=0.02210
4b (x,y,z), x=-0.22750, y=-0.24970, z=0.27810
4b (x,y,z), x=0.26140, y=0.23950, z=0.26920
2a (x,0,z), x=0.34000, z=0.18710
2a (x,0,z), x=-0.27730, z=-0.14940
2a (x,0,z), x=0.34600, z=-0.16920
2a (x,0,z), x=-0.29260, z=0.20220
4b (x,y,z), x=0.00880, y=0.18230, z=0.35990
4b (x,y,z), x=-0.46680, y=0.33010, z=0.22220
4b (x,y,z), x=0.19040, y=0.31250, z=0.03670
4b (x,y,z), x=-0.15660, y=-0.30700, z=0.00860
#string containing order parameter and subgroup
!orderParamString
Subgroup:   1 P1, basis={(1/2,1/2,1/2),(-1/2,1/2,-1/2),(-1/2,-1/2,1/2)}, origin=(0.00137,0,-0.0(
#string containing information about distorted structure
!subgroupString
Space group:   1 P1         C1-1, Lattice parameters: a=6.41042, b=6.43765, c=6.50421, alpha=10(
#string containing lattice parameters of undistorted subgroup
!subLattParamString
a=6.42644, b=6.42644, c=6.51987, alpha=108.95839, beta=108.86308, gamma=110.02243
#space group setting of parent
!parentSetting
29
#space group setting: monoclinic axes
!settingAxesM
a(b)c
#space group setting: monoclinic cell
!settingCell
1
#space group setting: origin
!settingOrigin
2
#space group setting: axes for R hexagonal
!settingAxesH
h
#space group setting: axes for orthorhombic
!settingAxesO
abc
#superspace group setting
!settingSSG
standard
#lattice parameters
!lattParam
7.522170    7.370050    7.530930   90.000000   91.223400   90.000000
#number of wyckoff positions
!wyckoffCount
14
#for each wyckoff position: position number
```

3

```
!wyckoffNumber
1  1  1  1  2  2  1  1  1  1  2  2  2  2
#for each wyckoff position: type of atom
!wyckoffAtomType
1  2  2  2  2  2  3  3  3  3  3  3  3  3
#for each wyckoff position: wyckoff position symbol
!wyckoffPos
Bi1
Mn1
Mn2
Mn3
Mn4
Mn5
O1_1
O1_2
O2_1
O2_2
O3_1
O3_2
O4_1
O4_2
#for each wyckoff position: symbol for type of atom
!wyckoffAtom
Bi
Mn
Mn
Mn
Mn
Mn
O
O
O
O
O
O
O
O
#for each wyckoff position: position parameters
!wyckoffParam
0.001370    0.000000   -0.006240
-0.486300    0.000000   -0.475800
0.020500    0.000000   -0.467900
-0.476200    0.000000    0.022100
-0.227500   -0.249700    0.278100
0.261400    0.239500    0.269200
0.340000    0.000000    0.187100
-0.277300    0.000000   -0.149400
0.346000    0.000000   -0.169200
-0.292600    0.000000    0.202200
0.008800    0.182300    0.359900
-0.466800    0.330100    0.222200
0.190400    0.312500    0.036700
-0.156600   -0.307000    0.008600
#for each wyckoff position: occupation
!wyckoffOccupation
1.000000
```

4

```
1.000000
1.000000
1.000000
1.000000
1.000000
1.000000
1.000000
1.000000
1.000000
1.000000
1.000000
1.000000
#include pivot atoms
!includePivot
F
#for each wyckoff position:  include displacive distortions
!includeDisplacive
T T T T T T T T T T T T T
#for each wyckoff position:  include ordering distortions
!includeOrdering
F F F F F F F F F F F F F
#for each wyckoff position:  include magnetic distortions
!includeMagnetic
F F F F F F F F F F F F F
#for each wyckoff position:  include rotational distortions
!includeRotational
F F F F F F F F F F F F F
#for each wyckoff position:  include ellipsoidal distortions
!includeEllipsoidal
F F F F F F F F F F F F F
#include strain distortions
!includeStrain
T
#version of irrep matrices
!irrepVersion
3
#number of primary IRs
!irrepCount
0
#isotropy subgroup number
!isoNumber
0
#space group of isotropy subgroup
!subgroup
1
#lattice basis vector and origin of subgroup
!basisOrigin
0   0   1   0   1   0  -1  -1   0   0   0   0   1
#name of file containing modes
!modesFileName
isodistort_33967.iso
#name of file containing information about atomic positions in subgroup
!atomsFileName
isodistort_49625.iso
#maximum number of displacive modes for a single wyckoff position
```

```
!maxDisplaciveModes
6
#for each displacive mode in each wyckoff position: mode coefficient
!displaciveModesCoef
0.000000    0.000000    0.000000    0.000000    0.000000    0.000000
-0.168760    0.491210    0.207840    0.000000    0.000000    0.000000
-0.332400    0.613180    0.147400    0.000000    0.000000    0.000000
-0.354850    0.442270    0.187200    0.000000    0.000000    0.000000
-0.470720    0.787310   -0.038040   -0.033120   -0.056430    0.223570
-0.200500    0.564230    0.218360   -0.064980    0.020760    0.251710
-0.440290    0.386550    0.280060    0.000000    0.000000    0.000000
-0.498780    0.360200    0.184250    0.000000    0.000000    0.000000
-0.455550    0.376760    0.228470    0.000000    0.000000    0.000000
-0.369830    0.304480    0.110550    0.000000    0.000000    0.000000
-0.414120    0.997070    0.002080    0.069720    0.026620    0.203250
-0.436630    1.138690   -0.110480   -0.068580    0.026620    0.119860
-0.279570    0.622260    0.031270    0.026030   -0.026620    0.328320
-0.338330    0.610550   -0.104230   -0.022070   -0.037270    0.364800
#maximum number of ordering modes for a single wyckoff position
!maxOrderingModes
0
#maximum number of magnetic modes for a single wyckoff position
!maxMagneticModes
0
#maximum number of rotational modes for a single wyckoff position
!maxRotationalModes
0
#maximum number of ellipsoidal modes for a single wyckoff position
!maxEllipsoidalModes
0
#for each strain mode: mode coefficient
!strainModesCoef
0.000690    0.001310   -0.004670    0.000900   -0.003120   -0.001410
#atomic radius in applet
!atomicRadius
0.400000
#maximum bond length in applet
!maxBondLength
2.500000
#length of magnetic moment vectors in applet
!angstromsPerMagneton
0.500000
#length of rotational moment vectors in applet
!angstromsPerRadian
4.000000
#default value of Uiso in applet
!uisoDefault
0.040000
#applet width in pixels
!appletWidth
1024
#maximum displacement mode coefficient in applet
!maxDisplaciveModeCoef
1.000000
#maximum strain mode coefficient in applet
!maxStrainModeCoef
```

```
0.100000
#maximum ordering mode coefficient in applet
!maxOrderingModeCoef
1.000000
#maximum magnetic mode coefficient in applet
!maxMagneticModeCoef
1.000000
#maximum rotational mode coefficient in applet
!maxRotationalModeCoef
0.125000
#maximum ellipsoidal mode coefficient in applet
!maxEllipsoidalModeCoef
1.000000
#include strain modes in TOPAS.STR
!includeStrainTopas
F
!end distortionFile

#modes file
!begin modesFile
#maximum number of atoms in applet for each wyckoff position
!maxAtomsApplet
8
#maximum number of displacive modes for each wyckoff position
!maxDisplaciveModes
6
#maximum number of magnetic modes for each wyckoff position
!maxMagneticModes
0
#maximum number of rotational modes for each wyckoff position
!maxRotationalModes
0
#maximum number of ellipsoidal modes for each wyckoff position
!maxEllipsoidalModes
0
#maximum number of ordering modes for each wyckoff position
!maxOrderingModes
0
#number of IRs
!irrepCount
2
#for each wyckoff position: number of atoms in unit cell
!atomCount
1       1       1       1       2       2       1       1       1       1
2       2       2       2
#for each wyckoff position: number of atoms in applet
!atomCountApplet
8       1       1       1       2       2       1       1       1       1
2       2       2       2
#for each wyckoff position: number of displacive modes
!displaciveModesCount
3       3       3       3       6       6       3       3       3       3
6       6       6       6
#for each wyckoff position: number of magnetic modes
!magneticModesCount
0       0       0       0       0       0       0       0       0       0
```

```
0       0       0       0
#for each wyckoff position: number of rotational modes
!rotationalModesCount
0       0       0       0       0       0       0       0       0       0
0       0       0       0
#for each wyckoff position: number of ellipsoidal modes
!ellipsoidalModesCount
0       0       0       0       0       0       0       0       0       0
0       0       0       0
#for each wyckoff position: number of ordering modes
!orderingModesCount
0       0       0       0       0       0       0       0       0       0
0       0       0       0
#number of strain modes
!strainModesCount
6
#for each wyckoff position: number of wyckoff positions in subgroup
!wyckoffSubgroupCount
1       1       1       1       2       2       1       1       1       1
2       2       2       2
#number of incommensurate modulations
!modCount
0
#maximum number of incommensurate modulations for each IR
!maxMod
0
#size of subgroup unit cell
!subgroupCellSize
1
#for each IR: IR number
!irrepNumber
139   140
#for each IR: dimension of matrix
!irrepDim
1  1
#for each IR: magnetic or not
!irrepMagnetic
F F
#for each IR: k vector parameters
!kvecParam
0       0       0       0       0       0       0       0
#for each IR: isotropy subgroup
!isoSubgroup
8     1
#for each IR:  lattice basis vector and origin for isotropy subgroup
!isoBasisOrigin
-1   0   0   0   0   1   0   1   0   0   0   0   1
0   0  -1   0  -1   0  -1   0   1   0   0   0   1
#for each IR: size of unit cell of isotropy subgroup
!isoSubgroupCellSize
1       1
#for each IR: number of degrees of freedom in order parameter
!orderParamFree
1  1
#for each IR: order parameter
!orderParam
```

```
1.00000000   1.00000000
#for each IR: index of isotropy subgroup
!isoSubgroupIndex
1       2
#for each IR: number of incommensurate modulations
!irrepModCount
0       0
#IR for each displacive mode
!displaciveModeIrrep
1     1     2     1     1     2     1     1     2     1     1     2
1     1     1     2     2     2     1     1     1     2     2     2
1     1     2     1     1     2     1     1     2     1     1     2
1     1     1     2     2     2     1     1     1     2     2     2
1     1     1     2     2     2     1     1     1     2     2     2
#IR of wyckoff point group for each displacive mode
!displaciveModePGIrrep
63    63    64    63    63    64    63    63    64    63    63    64
1     1     1     1     1     1     1     1     1     1     1     1
63    63    64    63    63    64    63    63    64    63    63    64
1     1     1     1     1     1     1     1     1     1     1     1
1     1     1     1     1     1     1     1     1     1     1     1
#IR for each strain mode
!strainModeIrrep
1     1     1     1     2     2
#scale for each displacive mode
!displaciveModeScale
1.00000000   1.00000000   1.00000000   1.00000000   1.00000000   1.00000000
1.00000000   1.00000000   1.00000000   1.00000000   1.00000000   1.00000000
1.41421356   1.41421356   1.41421356   1.41421356   1.41421356   1.41421356
1.41421356   1.41421356   1.41421356   1.41421356   1.41421356   1.41421356
1.00000000   1.00000000   1.00000000   1.00000000   1.00000000   1.00000000
1.00000000   1.00000000   1.00000000   1.00000000   1.00000000   1.00000000
1.41421356   1.41421356   1.41421356   1.41421356   1.41421356   1.41421356
1.41421356   1.41421356   1.41421356   1.41421356   1.41421356   1.41421356
1.41421356   1.41421356   1.41421356   1.41421356   1.41421356   1.41421356
1.41421356   1.41421356   1.41421356   1.41421356   1.41421356   1.41421356
#normalization for each displacive mode
!displaciveModeNorm
0.13294036   0.13281600   0.13568429   0.13294036   0.13281600   0.13568429
0.13294036   0.13281600   0.13568429   0.13294036   0.13281600   0.13568429
0.09400303   0.09391509   0.09594328   0.09400303   0.09391509   0.09594328
0.09400303   0.09391509   0.09594328   0.09400303   0.09391509   0.09594328
0.13294036   0.13281600   0.13568429   0.13294036   0.13281600   0.13568429
0.13294036   0.13281600   0.13568429   0.13294036   0.13281600   0.13568429
0.09400303   0.09391509   0.09594328   0.09400303   0.09391509   0.09594328
0.09400303   0.09391509   0.09594328   0.09400303   0.09391509   0.09594328
0.09400303   0.09391509   0.09594328   0.09400303   0.09391509   0.09594328
0.09400303   0.09391509   0.09594328   0.09400303   0.09391509   0.09594328
#normalization for each strain mode
!strainModeNorm
1.00000000   1.41421356   1.00000000   1.00000000   1.41421356   1.41421356
#lattice parameters of subgroup
!subgroupLattParam
6.42644132   6.42644132   6.51986538 108.95838523 108.86308123 110.02242625
#lattice basis vectors and origin of parent wrt subgroup
!parentBasisOrigin
```

```
0.00000000  -1.00000000  -1.00000000   1.00000000   1.00000000   0.00000000
1.00000000   0.00000000   1.00000000  -0.99376000   0.00137000   0.00761000
#nearest neighbor distance
!NearDistance
1.86809632
#components of each strain mode
!strainModes
1.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
0.00000000   0.00000000   0.00000000   0.00000000   1.00000000   0.00000000
0.00000000   1.00000000   0.00000000   0.00000000   0.00000000   0.00000000
0.00000000   0.00000000   1.00000000   0.00000000   0.00000000   0.00000000
0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   1.00000000
0.00000000   0.00000000   0.00000000   1.00000000   0.00000000   0.00000000
#subgroup wyckoff position of each atom in applet
!subgroupWyckoff
1   1   1   1   1   1   1   1   1   1   1   1   2   1   2   1   1   1   1   1
2   1   2   1   2   1   2
#position of each atom in applet
!atomPos
-0.000240000000  -0.000370000000   0.000390000000
-0.000240000000  -0.000370000000   1.000390000000
-0.000240000000   0.999630000000   0.000390000000
-0.000240000000   0.999630000000   1.000390000000
0.999760000000  -0.000370000000   0.000390000000
0.999760000000  -0.000370000000   1.000390000000
0.999760000000   0.999630000000   0.000390000000
0.999760000000   0.999630000000   1.000390000000
0.530200000000   0.487300000000   0.018500000000
0.538100000000   0.980500000000   0.519600000000
0.028100000000   0.477200000000   0.506300000000
0.034400000000   0.978800000000   0.513600000000
0.533800000000   0.478200000000   0.513600000000
0.514700000000   0.979100000000   0.015800000000
0.035700000000   0.500100000000   0.015800000000
0.193100000000   0.661000000000   0.855100000000
0.856600000000   0.278300000000   0.135900000000
0.836800000000   0.655000000000   0.492800000000
0.208200000000   0.293600000000   0.502800000000
0.548200000000   0.174500000000   0.359100000000
0.183600000000   0.809900000000   0.359100000000
0.558300000000   0.797900000000   0.697000000000
0.898100000000   0.137700000000   0.697000000000
0.355200000000   0.123100000000   0.854300000000
0.730200000000   0.498100000000   0.854300000000
0.707600000000   0.850600000000   0.173200000000
0.321600000000   0.464600000000   0.173200000000
#for each displacive mode:  displacement of each atom
!displaciveMode
0.000000000000  -0.132940361624  -0.132940361624
-0.132816000801   0.002839021675  -0.129976979126
0.135684289795   0.135684289795   0.000000000000
0.000000000000  -0.132940361624  -0.132940361624
-0.132816000801   0.002839021675  -0.129976979126
0.135684289795   0.135684289795   0.000000000000
0.000000000000  -0.132940361624  -0.132940361624
-0.132816000801   0.002839021675  -0.129976979126
```

0.135684289795	0.135684289795	0.000000000000
0.000000000000	-0.132940361624	-0.132940361624
-0.132816000801	0.002839021675	-0.129976979126
0.135684289795	0.135684289795	0.000000000000
0.000000000000	-0.132940361624	-0.132940361624
-0.132816000801	0.002839021675	-0.129976979126
0.135684289795	0.135684289795	0.000000000000
0.000000000000	-0.132940361624	-0.132940361624
-0.132816000801	0.002839021675	-0.129976979126
0.135684289795	0.135684289795	0.000000000000
0.000000000000	-0.132940361624	-0.132940361624
-0.132816000801	0.002839021675	-0.129976979126
0.135684289795	0.135684289795	0.000000000000
0.000000000000	-0.132940361624	-0.132940361624
-0.132816000801	0.002839021675	-0.129976979126
0.135684289795	0.135684289795	0.000000000000
0.000000000000	-0.132940361624	-0.132940361624
-0.132816000801	0.002839021675	-0.129976979126
0.135684289795	0.135684289795	0.000000000000
0.000000000000	-0.132940361624	-0.132940361624
-0.132816000801	0.002839021675	-0.129976979126
0.135684289795	0.135684289795	0.000000000000
0.000000000000	-0.132940361624	-0.132940361624
-0.132816000801	0.002839021675	-0.129976979126
0.135684289795	0.135684289795	0.000000000000
0.000000000000	-0.094003031198	-0.094003031198
-0.093915094816	0.002007491478	-0.091907603338
0.095943281414	0.095943281414	0.000000000000
0.000000000000	-0.094003031198	-0.094003031198
-0.093915094816	0.002007491478	-0.091907603338
0.095943281414	0.095943281414	0.000000000000
0.000000000000	-0.094003031198	-0.094003031198
-0.093915094816	0.002007491478	-0.091907603338
-0.095943281414	-0.095943281414	0.000000000000
0.000000000000	0.094003031198	0.094003031198
0.093915094816	-0.002007491478	0.091907603338
0.095943281414	0.095943281414	0.000000000000
0.000000000000	-0.094003031198	-0.094003031198
-0.093915094816	0.002007491478	-0.091907603338
0.095943281414	0.095943281414	0.000000000000
0.000000000000	-0.094003031198	-0.094003031198
-0.093915094816	0.002007491478	-0.091907603338
0.095943281414	0.095943281414	0.000000000000
0.000000000000	-0.094003031198	-0.094003031198
-0.093915094816	0.002007491478	-0.091907603338
-0.095943281414	-0.095943281414	0.000000000000
0.000000000000	0.094003031198	0.094003031198
0.093915094816	-0.002007491478	0.091907603338
0.095943281414	0.095943281414	0.000000000000
0.000000000000	-0.132940361624	-0.132940361624
-0.132816000801	0.002839021675	-0.129976979126
0.135684289795	0.135684289795	0.000000000000
0.000000000000	-0.132940361624	-0.132940361624
-0.132816000801	0.002839021675	-0.129976979126
0.135684289795	0.135684289795	0.000000000000
0.000000000000	-0.132940361624	-0.132940361624

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```
-0.132816000801   0.002839021675  -0.129976979126
0.135684289795   0.135684289795   0.000000000000
0.000000000000  -0.132940361624  -0.132940361624
-0.132816000801   0.002839021675  -0.129976979126
0.135684289795   0.135684289795   0.000000000000
0.000000000000  -0.094003031198  -0.094003031198
-0.093915094816   0.002007491478  -0.091907603338
0.095943281414   0.095943281414   0.000000000000
0.000000000000  -0.094003031198  -0.094003031198
-0.093915094816   0.002007491478  -0.091907603338
0.095943281414   0.095943281414   0.000000000000
0.000000000000  -0.094003031198  -0.094003031198
-0.093915094816   0.002007491478  -0.091907603338
-0.095943281414  -0.095943281414   0.000000000000
0.000000000000   0.094003031198   0.094003031198
0.093915094816  -0.002007491478   0.091907603338
0.095943281414   0.095943281414   0.000000000000
0.000000000000  -0.094003031198  -0.094003031198
-0.093915094816   0.002007491478  -0.091907603338
0.095943281414   0.095943281414   0.000000000000
0.000000000000  -0.094003031198  -0.094003031198
-0.093915094816   0.002007491478  -0.091907603338
0.095943281414   0.095943281414   0.000000000000
0.000000000000  -0.094003031198  -0.094003031198
-0.093915094816   0.002007491478  -0.091907603338
-0.095943281414  -0.095943281414   0.000000000000
0.000000000000   0.094003031198   0.094003031198
0.093915094816  -0.002007491478   0.091907603338
0.095943281414   0.095943281414   0.000000000000
0.000000000000  -0.094003031198  -0.094003031198
-0.093915094816   0.002007491478  -0.091907603338
0.095943281414   0.095943281414   0.000000000000
0.000000000000  -0.094003031198  -0.094003031198
-0.093915094816   0.002007491478  -0.091907603338
-0.095943281414  -0.095943281414   0.000000000000
0.000000000000   0.094003031198   0.094003031198
0.093915094816  -0.002007491478   0.091907603338
0.095943281414   0.095943281414   0.000000000000
0.000000000000  -0.094003031198  -0.094003031198
-0.093915094816   0.002007491478  -0.091907603338
0.095943281414   0.095943281414   0.000000000000
0.000000000000  -0.094003031198  -0.094003031198
-0.093915094816   0.002007491478  -0.091907603338
0.095943281414   0.095943281414   0.000000000000
0.000000000000  -0.094003031198  -0.094003031198
-0.093915094816   0.002007491478  -0.091907603338
-0.095943281414  -0.095943281414   0.000000000000
0.000000000000   0.094003031198   0.094003031198
0.093915094816  -0.002007491478   0.091907603338
0.095943281414   0.095943281414   0.000000000000
!end modesFile

#atoms file
```

```
!begin atomsFile
6.41042   6.43765   6.50421 108.87173 108.59122 110.36680
Bi1                 Bi
0.00000   0.00000   0.00000
Mn1                 Mn
0.49340   0.53970  -0.02330
Mn2                 Mn
0.47690   0.04680   0.48370
Mn3                 Mn
-0.00500   0.55140   0.49560
Mn4                 Mn
0.47990   0.54650   0.47680
Mn5                 Mn
-0.01620   0.04580   0.49340
Mn6                 Mn
-0.01190   0.51750  -0.02180
Mn7                 Mn
0.50510   0.05070  -0.01340
O1                  O
0.83400   0.37100   0.15500
O2                  O
0.18000   0.75900   0.86300
O3                  O
0.18300   0.35900   0.51200
O4                  O
0.81800   0.74800   0.50400
O5                  O
0.81600   0.19700   0.62900
O6                  O
0.45000   0.84900   0.63700
O7                  O
0.11200   0.87700   0.31500
O8                  O
0.47200   0.22900   0.29700
O9                  O
0.30600   0.54100   0.14300
O10                 O
0.67900  -0.08900   0.15400
O11                 O
0.69800   0.55700   0.82300
O12                 O
0.33400   0.18300   0.82300
!end atomsFile
```

3.4. ISODISTORT output file used in TOPAS (only active modes are refined) at 10 K

```
'Topas .str file generated by ISODISTORT
'Remember to add the appropriate peak shape line when passing this into an input file

'{{{mode definitions
prm  !a1      0.00000 min  -1.00 max  1.00 'Im[0,0,0]GM1(a)[Bi1:a:dsp] A'_1(a)
prm  !a2      0.00000 min  -1.00 max  1.00 'Im[0,0,0]GM1(a)[Bi1:a:dsp] A'_2(a)
prm  !a3      0.00000 min  -1.00 max  1.00 'Im[0,0,0]GM2(a)[Bi1:a:dsp] A''(a)
prm  !a4     0.0 min  -1.00 max  1.00 'Im[0,0,0]GM1(a)[Mn1:a:dsp] A'_1(a)
prm  !a5     0.0 min  -1.00 max  1.00 'Im[0,0,0]GM1(a)[Mn1:a:dsp] A'_2(a)
```

```
prm   a6     -0.20116‘_0.00359 min  -1.00 max  1.00 ’Im[0,0,0]GM2(a)[Mn1:a:dsp] A’’(a)
prm   !a7     0.0 min  -1.00 max  1.00 ’Im[0,0,0]GM1(a)[Mn2:a:dsp] A’_1(a)
prm   !a8     0.0 min  -1.00 max  1.00 ’Im[0,0,0]GM1(a)[Mn2:a:dsp] A’_2(a)
prm   a9    -0.15482‘_0.00559 min  -1.00 max  1.00 ’Im[0,0,0]GM2(a)[Mn2:a:dsp] A’’(a)
prm  !a10    0.0 min  -1.00 max  1.00 ’Im[0,0,0]GM1(a)[Mn3:a:dsp] A’_1(a)
prm  !a11    0.0 min  -1.00 max  1.00 ’Im[0,0,0]GM1(a)[Mn3:a:dsp] A’_2(a)
prm   a12    -0.19091‘_0.00530 min  -1.00 max  1.00 ’Im[0,0,0]GM2(a)[Mn3:a:dsp] A’’(a)
prm  !a13    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM1(a)[Mn4:b:dsp] A_1(a)
prm  !a14    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM1(a)[Mn4:b:dsp] A_2(a)
prm  !a15    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM1(a)[Mn4:b:dsp] A_3(a)
prm  !a16    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM2(a)[Mn4:b:dsp] A_1(a)
prm   a17     0.09105‘_0.00539 min  -1.41 max  1.41 ’Im[0,0,0]GM2(a)[Mn4:b:dsp] A_2(a)
prm   a18    -0.22277‘_0.00462 min  -1.41 max  1.41 ’Im[0,0,0]GM2(a)[Mn4:b:dsp] A_3(a)
prm  !a19    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM1(a)[Mn5:b:dsp] A_1(a)
prm  !a20    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM1(a)[Mn5:b:dsp] A_2(a)
prm  !a21    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM1(a)[Mn5:b:dsp] A_3(a)
prm   a22     0.09416‘_0.00507 min  -1.41 max  1.41 ’Im[0,0,0]GM2(a)[Mn5:b:dsp] A_1(a)
prm  !a23    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM2(a)[Mn5:b:dsp] A_2(a)
prm   a24    -0.23076‘_0.00546 min  -1.41 max  1.41 ’Im[0,0,0]GM2(a)[Mn5:b:dsp] A_3(a)
prm  !a25    0.0 min  -1.00 max  1.00 ’Im[0,0,0]GM1(a)[O1_1:a:dsp] A’_1(a)
prm  !a26    0.0 min  -1.00 max  1.00 ’Im[0,0,0]GM1(a)[O1_1:a:dsp] A’_2(a)
prm   a27    -0.23927‘_0.01646 min  -1.00 max  1.00 ’Im[0,0,0]GM2(a)[O1_1:a:dsp] A’’(a)
prm  !a28    0.0 min  -1.00 max  1.00 ’Im[0,0,0]GM1(a)[O1_2:a:dsp] A’_1(a)
prm  !a29    0.0 min  -1.00 max  1.00 ’Im[0,0,0]GM1(a)[O1_2:a:dsp] A’_2(a)
prm   a30    -0.19714‘_0.01710 min  -1.00 max  1.00 ’Im[0,0,0]GM2(a)[O1_2:a:dsp] A’’(a)
prm  !a31    0.0 min  -1.00 max  1.00 ’Im[0,0,0]GM1(a)[O2_1:a:dsp] A’_1(a)
prm  !a32    0.0 min  -1.00 max  1.00 ’Im[0,0,0]GM1(a)[O2_1:a:dsp] A’_2(a)
prm   a33    -0.10635‘_0.01793 min  -1.00 max  1.00 ’Im[0,0,0]GM2(a)[O2_1:a:dsp] A’’(a)
prm  !a34    0.0 min  -1.00 max  1.00 ’Im[0,0,0]GM1(a)[O2_2:a:dsp] A’_1(a)
prm  !a35    0.0 min  -1.00 max  1.00 ’Im[0,0,0]GM1(a)[O2_2:a:dsp] A’_2(a)
prm   a36    -0.22503‘_0.01761 min  -1.00 max  1.00 ’Im[0,0,0]GM2(a)[O2_2:a:dsp] A’’(a)
prm  !a37    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM1(a)[O3_1:b:dsp] A_1(a)
prm  !a38    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM1(a)[O3_1:b:dsp] A_2(a)
prm  !a39    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM1(a)[O3_1:b:dsp] A_3(a)
prm   a40     0.11201‘_0.01808 min  -1.41 max  1.41 ’Im[0,0,0]GM2(a)[O3_1:b:dsp] A_1(a)
prm  !a41    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM2(a)[O3_1:b:dsp] A_2(a)
prm   a42    -0.17725‘_0.01847 min  -1.41 max  1.41 ’Im[0,0,0]GM2(a)[O3_1:b:dsp] A_3(a)
prm  !a43    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM1(a)[O3_2:b:dsp] A_1(a)
prm  !a44    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM1(a)[O3_2:b:dsp] A_2(a)
prm  !a45    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM1(a)[O3_2:b:dsp] A_3(a)
prm   a46    -0.05461‘_0.01842 min  -1.41 max  1.41 ’Im[0,0,0]GM2(a)[O3_2:b:dsp] A_1(a)
prm   a47    -0.08390‘_0.01989 min  -1.41 max  1.41 ’Im[0,0,0]GM2(a)[O3_2:b:dsp] A_2(a)
prm   a48    -0.27467‘_0.01769 min  -1.41 max  1.41 ’Im[0,0,0]GM2(a)[O3_2:b:dsp] A_3(a)
prm  !a49    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM1(a)[O4_1:b:dsp] A_1(a)
prm  !a50    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM1(a)[O4_1:b:dsp] A_2(a)
prm  !a51    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM1(a)[O4_1:b:dsp] A_3(a)
prm   a52     0.12286‘_0.01624 min  -1.41 max  1.41 ’Im[0,0,0]GM2(a)[O4_1:b:dsp] A_1(a)
prm  !a53     0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM2(a)[O4_1:b:dsp] A_2(a)
prm   a54    -0.39245‘_0.01650 min  -1.41 max  1.41 ’Im[0,0,0]GM2(a)[O4_1:b:dsp] A_3(a)
prm  !a55    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM1(a)[O4_2:b:dsp] A_1(a)
prm  !a56    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM1(a)[O4_2:b:dsp] A_2(a)
prm  !a57    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM1(a)[O4_2:b:dsp] A_3(a)
prm  !a58    0.0 min  -1.41 max  1.41 ’Im[0,0,0]GM2(a)[O4_2:b:dsp] A_1(a)
prm   a59     0.12978‘_0.01797 min  -1.41 max  1.41 ’Im[0,0,0]GM2(a)[O4_2:b:dsp] A_2(a)
prm   a60    -0.31657‘_0.01633 min  -1.41 max  1.41 ’Im[0,0,0]GM2(a)[O4_2:b:dsp] A_3(a)
```

```
'}}}

'{{{mode-amplitude to delta transformation
prm  Bi1_dx   = -  0.13282*a2 +  0.13568*a3;:  0.00000
prm  Bi1_dy   = -  0.13294*a1 +  0.00284*a2 +  0.13568*a3;:  0.00000
prm  Bi1_dz   = -  0.13294*a1 -  0.12998*a2;: -0.00000
prm  Mn1_dx   = -  0.13282*a5 +  0.13568*a6;: -0.02729`_0.00049
prm  Mn1_dy   = -  0.13294*a4 +  0.00284*a5 +  0.13568*a6;: -0.02729`_0.00049
prm  Mn1_dz   = -  0.13294*a4 -  0.12998*a5;: -0.00000
prm  Mn2_dx   = -  0.13282*a8 +  0.13568*a9;: -0.02101`_0.00076
prm  Mn2_dy   = -  0.13294*a7 +  0.00284*a8 +  0.13568*a9;: -0.02101`_0.00076
prm  Mn2_dz   = -  0.13294*a7 -  0.12998*a8;: -0.00000
prm  Mn3_dx   = -  0.13282*a11 +  0.13568*a12;: -0.02590`_0.00072
prm  Mn3_dy   = -  0.13294*a10 +  0.00284*a11 +  0.13568*a12;: -0.02590`_0.00072
prm  Mn3_dz   = -  0.13294*a10 -  0.12998*a11;: -0.00000
prm  Mn4_dx   = -  0.09392*a14 -  0.09594*a15 +  0.09392*a17 +  0.09594*a18;: -0.01282`_0.00067
prm  Mn4_dy   = -  0.09400*a13 +  0.00201*a14 -  0.09594*a15 +  0.09400*a16 -  0.00201*a17 +  0.
prm  Mn4_dz   = -  0.09400*a13 -  0.09191*a14 +  0.09400*a16 +  0.09191*a17;:  0.00837`_0.00050
prm  Mn5_dx   = -  0.09392*a14 +  0.09594*a15 -  0.09392*a17 +  0.09594*a18;: -0.02992`_0.00067
prm  Mn5_dy   = -  0.09400*a13 +  0.00201*a14 +  0.09594*a15 -  0.09400*a16 +  0.00201*a17 +  0.
prm  Mn5_dz   = -  0.09400*a13 -  0.09191*a14 -  0.09400*a16 -  0.09191*a17;: -0.00837`_0.00050
prm  Mn6_dx   = -  0.09392*a20 -  0.09594*a21 +  0.09392*a23 +  0.09594*a24;: -0.02214`_0.00052
prm  Mn6_dy   = -  0.09400*a19 +  0.00201*a20 -  0.09594*a21 +  0.09400*a22 -  0.00201*a23 +  0.
prm  Mn6_dz   = -  0.09400*a19 -  0.09191*a20 +  0.09400*a22 +  0.09191*a23;:  0.00885`_0.00048
prm  Mn7_dx   = -  0.09392*a20 +  0.09594*a21 -  0.09392*a23 +  0.09594*a24;: -0.02214`_0.00052
prm  Mn7_dy   = -  0.09400*a19 +  0.00201*a20 +  0.09594*a21 -  0.09400*a22 +  0.00201*a23 +  0.
prm  Mn7_dz   = -  0.09400*a19 -  0.09191*a20 -  0.09400*a22 -  0.09191*a23;: -0.00885`_0.00048
prm  O1_dx    = -  0.13282*a29 +  0.13568*a30;: -0.02675`_0.00232
prm  O1_dy    = -  0.13294*a28 +  0.00284*a29 +  0.13568*a30;: -0.02675`_0.00232
prm  O1_dz    = -  0.13294*a28 -  0.12998*a29;: -0.00000
prm  O2_dx    = -  0.13282*a26 +  0.13568*a27;: -0.03246`_0.00223
prm  O2_dy    = -  0.13294*a25 +  0.00284*a26 +  0.13568*a27;: -0.03246`_0.00223
prm  O2_dz    = -  0.13294*a25 -  0.12998*a26;: -0.00000
prm  O3_dx    = -  0.13282*a35 +  0.13568*a36;: -0.03053`_0.00239
prm  O3_dy    = -  0.13294*a34 +  0.00284*a35 +  0.13568*a36;: -0.03053`_0.00239
prm  O3_dz    = -  0.13294*a34 -  0.12998*a35;: -0.00000
prm  O4_dx    = -  0.13282*a32 +  0.13568*a33;: -0.01443`_0.00243
prm  O4_dy    = -  0.13294*a31 +  0.00284*a32 +  0.13568*a33;: -0.01443`_0.00243
prm  O4_dz    = -  0.13294*a31 -  0.12998*a32;: -0.00000
prm  O5_dx    = -  0.09392*a44 -  0.09594*a45 +  0.09392*a47 +  0.09594*a48;: -0.03423`_0.00252
prm  O5_dy    = -  0.09400*a43 +  0.00201*a44 -  0.09594*a45 +  0.09400*a46 -  0.00201*a47 +  0.
prm  O5_dz    = -  0.09400*a43 -  0.09191*a44 +  0.09400*a46 +  0.09191*a47;: -0.01284`_0.00252
prm  O6_dx    = -  0.09392*a44 +  0.09594*a45 -  0.09392*a47 +  0.09594*a48;: -0.01847`_0.00252
prm  O6_dy    = -  0.09400*a43 +  0.00201*a44 +  0.09594*a45 -  0.09400*a46 +  0.00201*a47 +  0.
prm  O6_dz    = -  0.09400*a43 -  0.09191*a44 -  0.09400*a46 -  0.09191*a47;:  0.01284`_0.00252
prm  O7_dx    = -  0.09392*a38 -  0.09594*a39 +  0.09392*a41 +  0.09594*a42;: -0.01700`_0.00177
prm  O7_dy    = -  0.09400*a37 +  0.00201*a38 -  0.09594*a39 +  0.09400*a40 -  0.00201*a41 +  0.
prm  O7_dz    = -  0.09400*a37 -  0.09191*a38 +  0.09400*a40 +  0.09191*a41;:  0.01053`_0.00170
prm  O8_dx    = -  0.09392*a38 +  0.09594*a39 -  0.09392*a41 +  0.09594*a42;: -0.01700`_0.00177
prm  O8_dy    = -  0.09400*a37 +  0.00201*a38 +  0.09594*a39 -  0.09400*a40 +  0.00201*a41 +  0.
prm  O8_dz    = -  0.09400*a37 -  0.09191*a38 -  0.09400*a40 -  0.09191*a41;: -0.01053`_0.00170
prm  O9_dx    = -  0.09392*a56 -  0.09594*a57 +  0.09392*a59 +  0.09594*a60;: -0.01818`_0.00230
prm  O9_dy    = -  0.09400*a55 +  0.00201*a56 -  0.09594*a57 +  0.09400*a58 -  0.00201*a59 +  0.
prm  O9_dz    = -  0.09400*a55 -  0.09191*a56 +  0.09400*a58 +  0.09191*a59;:  0.01193`_0.00165
prm  O10_dx   = -  0.09392*a56 +  0.09594*a57 -  0.09392*a59 +  0.09594*a60;: -0.04256`_0.00230
prm  O10_dy   = -  0.09400*a55 +  0.00201*a56 +  0.09594*a57 -  0.09400*a58 +  0.00201*a59 +  0.
```

```
prm  O10_dz   = -  0.09400*a55 -  0.09191*a56 -  0.09400*a58 -  0.09191*a59;: -0.01193`_0.00165
prm  O11_dx   = -  0.09392*a50 -  0.09594*a51 +  0.09392*a53 +  0.09594*a54;: -0.03765`_0.00158
prm  O11_dy   = -  0.09400*a49 +  0.00201*a50 -  0.09594*a51 +  0.09400*a52 -  0.00201*a53 +  0.
prm  O11_dz   = -  0.09400*a49 -  0.09191*a50 +  0.09400*a52 +  0.09191*a53;:  0.01155`_0.00153
prm  O12_dx   = -  0.09392*a50 +  0.09594*a51 -  0.09392*a53 +  0.09594*a54;: -0.03765`_0.00158
prm  O12_dy   = -  0.09400*a49 +  0.00201*a50 +  0.09594*a51 -  0.09400*a52 +  0.00201*a53 +  0.
prm  O12_dz   = -  0.09400*a49 -  0.09191*a50 -  0.09400*a52 -  0.09191*a53;: -0.01155`_0.00153

'}}}

'{{{distorted parameters
prm  Bi1_x    =    0.00000 + Bi1_dx;:  0.00000
prm  Bi1_y    =    0.00000 + Bi1_dy;:  0.00000
prm  Bi1_z    =    0.00000 + Bi1_dz;: -0.00000
prm  Mn1_x    =    0.53020 + Mn1_dx;:  0.50291`_0.00049
prm  Mn1_y    =    0.48730 + Mn1_dy;:  0.46001`_0.00049
prm  Mn1_z    =    0.01850 + Mn1_dz;:  0.01850
prm  Mn2_x    =    0.53810 + Mn2_dx;:  0.51709`_0.00076
prm  Mn2_y    =   -0.01950 + Mn2_dy;: -0.04051`_0.00076
prm  Mn2_z    =    0.51960 + Mn2_dz;:  0.51960
prm  Mn3_x    =    0.02810 + Mn3_dx;:  0.00220`_0.00072
prm  Mn3_y    =    0.47720 + Mn3_dy;:  0.45130`_0.00072
prm  Mn3_z    =    0.50630 + Mn3_dz;:  0.50630
prm  Mn4_x    =    0.53380 + Mn4_dx;:  0.52098`_0.00067
prm  Mn4_y    =    0.47820 + Mn4_dy;:  0.45664`_0.00044
prm  Mn4_z    =    0.51360 + Mn4_dz;:  0.52197`_0.00050
prm  Mn5_x    =    0.03440 + Mn5_dx;:  0.00448`_0.00067
prm  Mn5_y    =   -0.02120 + Mn5_dy;: -0.04239`_0.00044
prm  Mn5_z    =    0.51360 + Mn5_dz;:  0.50523`_0.00050
prm  Mn6_x    =    0.03570 + Mn6_dx;:  0.01356`_0.00052
prm  Mn6_y    =    0.50010 + Mn6_dy;:  0.48681`_0.00071
prm  Mn6_z    =    0.01580 + Mn6_dz;:  0.02465`_0.00048
prm  Mn7_x    =    0.51470 + Mn7_dx;:  0.49256`_0.00052
prm  Mn7_y    =   -0.02090 + Mn7_dy;: -0.05189`_0.00071
prm  Mn7_z    =    0.01580 + Mn7_dz;:  0.00695`_0.00048
prm  O1_x     =    0.85660 + O1_dx;:  0.82985`_0.00232
prm  O1_y     =    0.27830 + O1_dy;:  0.25155`_0.00232
prm  O1_z     =    0.13590 + O1_dz;:  0.13590
prm  O2_x     =    0.19310 + O2_dx;:  0.16064`_0.00223
prm  O2_y     =    0.66100 + O2_dy;:  0.62854`_0.00223
prm  O2_z     =    0.85510 + O2_dz;:  0.85510
prm  O3_x     =    0.20820 + O3_dx;:  0.17767`_0.00239
prm  O3_y     =    0.29360 + O3_dy;:  0.26307`_0.00239
prm  O3_z     =    0.50280 + O3_dz;:  0.50280
prm  O4_x     =    0.83680 + O4_dx;:  0.82237`_0.00243
prm  O4_y     =    0.65500 + O4_dy;:  0.64057`_0.00243
prm  O4_z     =    0.49280 + O4_dz;:  0.49280
prm  O5_x     =    0.89810 + O5_dx;:  0.86387`_0.00252
prm  O5_y     =    0.13770 + O5_dy;:  0.10638`_0.00242
prm  O5_z     =    0.69700 + O5_dz;:  0.68416`_0.00252
prm  O6_x     =    0.55830 + O6_dx;:  0.53983`_0.00252
prm  O6_y     =    0.79790 + O6_dy;:  0.77651`_0.00242
prm  O6_z     =    0.69700 + O6_dz;:  0.70984`_0.00252
prm  O7_x     =    0.18360 + O7_dx;:  0.16660`_0.00177
prm  O7_y     =    0.80990 + O7_dy;:  0.80342`_0.00246
prm  O7_z     =    0.35910 + O7_dz;:  0.36963`_0.00170
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prm  O8_x     =    0.54820 + O8_dx;:  0.53120`_0.00177
prm  O8_y     =    0.17450 + O8_dy;:  0.14697`_0.00246
prm  O8_z     =    0.35910 + O8_dz;:  0.34857`_0.00170
prm  O9_x     =    0.32160 + O9_dx;:  0.30342`_0.00230
prm  O9_y     =    0.46460 + O9_dy;:  0.43397`_0.00157
prm  O9_z     =    0.17320 + O9_dz;:  0.18513`_0.00165
prm  O10_x    =    0.70760 + O10_dx;:  0.66504`_0.00230
prm  O10_y    =    0.85060 + O10_dy;:  0.82049`_0.00157
prm  O10_z    =    0.17320 + O10_dz;:  0.16127`_0.00165
prm  O11_x    =    0.73020 + O11_dx;:  0.69255`_0.00158
prm  O11_y    =    0.49810 + O11_dy;:  0.47200`_0.00220
prm  O11_z    =    0.85430 + O11_dz;:  0.86585`_0.00153
prm  O12_x    =    0.35520 + O12_dx;:  0.31755`_0.00158
prm  O12_y    =    0.12310 + O12_dy;:  0.07390`_0.00220
prm  O12_z    =    0.85430 + O12_dz;:  0.84275`_0.00153

prm !Bi1_occ  = 1;:  1.00000
prm !Mn1_occ  = 1;:  1.00000
prm !Mn2_occ  = 1;:  1.00000
prm !Mn3_occ  = 1;:  1.00000
prm !Mn4_occ  = 1;:  1.00000
prm !Mn5_occ  = 1;:  1.00000
prm !Mn6_occ  = 1;:  1.00000
prm !Mn7_occ  = 1;:  1.00000
prm !O1_occ   = 1;:  1.00000
prm !O2_occ   = 1;:  1.00000
prm !O3_occ   = 1;:  1.00000
prm !O4_occ   = 1;:  1.00000
prm !O5_occ   = 1;:  1.00000
prm !O6_occ   = 1;:  1.00000
prm !O7_occ   = 1;:  1.00000
prm !O8_occ   = 1;:  1.00000
prm !O9_occ   = 1;:  1.00000
prm !O10_occ  = 1;:  1.00000
prm !O11_occ  = 1;:  1.00000
prm !O12_occ  = 1;:  1.00000
'}}}

'{{{mode-dependent sites
site Bi1  x = Bi1_x;  y = Bi1_y;  z = Bi1_z;  occ Bi = Bi1_occ;  ADPs { @  0.00232`_0.00038 @  (
site Mn2  x = Mn2_x;  y = Mn2_y;  z = Mn2_z;  occ Mn = Mn2_occ;  beq BMn  0.32646`_0.01847
site Mn1  x = Mn1_x;  y = Mn1_y;  z = Mn1_z;  occ Mn = Mn1_occ;  beq BMn  0.32646`_0.01847
site Mn3  x = Mn3_x;  y = Mn3_y;  z = Mn3_z;  occ Mn = Mn3_occ;  beq BMn  0.32646`_0.01847
site Mn4  x = Mn4_x;  y = Mn4_y;  z = Mn4_z;  occ Mn = Mn4_occ;  beq BMn  0.32646`_0.01847
site Mn5  x = Mn5_x;  y = Mn5_y;  z = Mn5_z;  occ Mn = Mn5_occ;  beq BMn  0.32646`_0.01847
site Mn6  x = Mn6_x;  y = Mn6_y;  z = Mn6_z;  occ Mn = Mn6_occ;  beq BMn  0.32646`_0.01847
site Mn7  x = Mn7_x;  y = Mn7_y;  z = Mn7_z;  occ Mn = Mn7_occ;  beq BMn  0.32646`_0.01847
site O1   x = O1_x;   y = O1_y;   z = O1_z;   occ O  = O1_occ;   beq BO  0.23309`_0.08112
site O2   x = O2_x;   y = O2_y;   z = O2_z;   occ O  = O2_occ;   beq BO  0.23309`_0.08112
site O3   x = O3_x;   y = O3_y;   z = O3_z;   occ O  = O3_occ;   beq BO  0.23309`_0.08112
site O4   x = O4_x;   y = O4_y;   z = O4_z;   occ O  = O4_occ;   beq BO  0.23309`_0.08112
site O5   x = O5_x;   y = O5_y;   z = O5_z;   occ O  = O5_occ;   beq BO  0.23309`_0.08112
site O6   x = O6_x;   y = O6_y;   z = O6_z;   occ O  = O6_occ;   beq BO  0.23309`_0.08112
site O7   x = O7_x;   y = O7_y;   z = O7_z;   occ O  = O7_occ;   beq BO  0.23309`_0.08112
site O8   x = O8_x;   y = O8_y;   z = O8_z;   occ O  = O8_occ;   beq BO  0.23309`_0.08112
site O9   x = O9_x;   y = O9_y;   z = O9_z;   occ O  = O9_occ;   beq BO  0.23309`_0.08112
```

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site O10  x = O10_x;  y = O10_y;  z = O10_z;  occ O  = O10_occ;  beq BO  0.23309`_0.08112
site O11  x = O11_x;  y = O11_y;  z = O11_z;  occ O  = O11_occ;  beq BO  0.23309`_0.08112
site O12  x = O12_x;  y = O12_y;  z = O12_z;  occ O  = O12_occ;  beq BO  0.23309`_0.08112
```