DiSPy Tutorial

Introduction

This tutorial illustrates how DiSPy can be used to perturb a path using irreducible representations (irreps) of its distortion group.

The steps shown below walk through the $Ca_3Ti_2O_7$ example included in the repository. The files required are 'SAMPLE_INPUT', 'PIR_data.txt', and the image files in the 'init_path' folder. These correspond to the DiSPy input file, the tabulation of space group irreps by Stokes *et al.*[2] used by the code, and inital path structure files respectively. Note that the input file and irrep listing file must always be in the same directory when running the program.

Step 1 – Obtain the distortion symmetry group

To obtain the distortion group of the initial path, we first run DiSPy turning off perturbations with the 'PERTURB' flag. The input file for this step is shown below. Note that 'IMAGE_DIR' must be set to the correct location of the image directory.

```
#---Sample DiSPy input file without perturbation

PERTURB=FALSE
INTERPOLATE=FALSE
IMAGES=9
SYMPREC=0.1
ANGLE_TOLERANCE=-1.0
VECTOR_TOLERANCE(A)=0.01,0.01,0.01
GENERAL_TOLERANCE=0.05
IMAGE_DIR=./init_path
INPUT_FORMAT=poscar
OUTPUT_FORMAT=poscar

TRANS_NUM=0
TRANS_MAT=0
OSHIFT=0,0,0
```

Here, we are using an `SPGLIB` symmetry tolerance value ('SYMPREC') of 0.1 and a general tolerance value of 0.05. The former puts a tolerance on the space-group symmetry detection routines in `SPGLIB`, and the latter on identifying and matching matrix-vector representations of symmetry elements when obtaining elements of the distortion group. The general tolerance value here should work for the vast majority of paths. The value of 'SYMPREC' can and should be altered depending on the specific example. The other tolerance values in the input file that have not been mentioned generally do not need to be changed, and are discussed in the instructions manual.

The two other important entries that need to be set in the input file are 'TRANS_NUM', 'TRANS_MAT', and 'OSHIFT'. These control how the linear transformation is chosen that takes the matrix-vector representations of distortion group elements from the basis of the inputted structures to the standard one defined for the isomorphic space group in the International Tables of Crystallography [1]. This is important in order to obtain the correct irrep matrices for each element. Here, setting 'TRANS_NUM' to a value of 0 tells `DiSPy` to try and obtain this transformation using its built in routines.

An alternative method to obtain this is to use the formatted symmetry operations of the distortion group outputted by the code as an input for the IDENTIFY GROUP program of the Bilbao Crystallographic Server (http://www.cryst.ehu.es). This is shown below for this example:

```
-------
------- Symmetry operations in Bilbao IDENTIFY GROUP format:
-------

x,y,z
-x,-y,z+1/2
x,-y,z
-x,y,z+1/2
x+1/2,y+1/2,z
-x+1/2,-y+1/2,z+1/2
x+1/2,-y+1/2,z
-x+1/2,y+1/2,z+1/2
-x,-y,-z
x,y,-z+1/2
-x,y,-z
x,-y,-z+1/2
-x+1/2,-y+1/2,-z
x+1/2,y+1/2,-z+1/2
-x+1/2,y+1/2,-z
x+1/2,-y+1/2,-z+1/2
```

Note that the transformation matrix (**T**) and origin shift (**O**) provided by IDENTIFY GROUP must be converted before being used as values for 'TRANS_MAT' and 'OSHIFT' in the input file. The proper transformation matrix ($\mathbf{T}'$) and origin shift vector ($\mathbf{O}'$) can be calculated as follows:

$$\mathbf{T}' = \mathbf{T}^{-1} \tag{1}$$
$$\mathbf{O}' = -\mathbf{T}^{-1}\mathbf{O} \tag{2}$$

Output Summary:

Afer running `DiSPy`, the output will first show the space-group symmetry of each of the images in the path:

```
==================================================================

-------
-------
------- Symmetry of images:
-------
-------

Image 1: Cmc2_1 (36)
Image 2: Cmc2_1 (36)
Image 3: Cmc2_1 (36)
Image 4: Cmc2_1 (36)
Image 5: Cmcm (63)
Image 6: Cmc2_1 (36)
Image 7: Cmc2_1 (36)
Image 8: Cmc2_1 (36)
Image 9: Cmc2_1 (36)
```

Next, the matrix-vector representations of the elements in the distortion group are outputted in the crystal basis of the inputted structures:

```
-------
------- Elements of distortion group in the basis of the inputted structures:
-------

Symmetry Element 1 (Unstarred):
Rotation:
[[1 0 0]
[0 1 0]
[0 0 1]]
```

```
Translation:
[0. 0. 0.]
The operation has been identified as the identity.

Symmetry Element 2 (Unstarred):
Rotation:
[[-1  0  0]
[ 0 -1 0]
[ 0  0  1]]
Translation:
[0.  0.  0.5]
The operation has been identified as a twofold rotation along the 0 0 1 axis
    with a translation of [0. 0. 0.5] and an intrinsic screw component of [0.
    0. 1.].

Symmetry Element 3 (Unstarred):
Rotation:
[[ 1  0  0]
[ 0 -1  0]
[ 0  0  1]]
Translation:
[0. 0. 0.]
The operation has been identified as a mirror across the 0 1 0 plane.

Symmetry Element 4 (Unstarred):
Rotation:
[[-1  0  0]
[ 0  1  0]
[ 0  0  1]]
Translation:
[0.  0.  0.5]
The operation has been identified as a mirror across the 1 0 0 plane with a
    translation of [0. 0. 0.5] and an intrinsic glide component of [0. 0. 1.].

Symmetry Element 5 (Unstarred):
Rotation:
[[1 0 0]
[0 1 0]
[0 0 1]]
Translation:
[0.5 0.5 0. ]
The operation has been identified as a translation of [0.5 0.5 0. ].

Symmetry Element 6 (Unstarred):
Rotation:
[[-1  0  0]
[ 0 -1  0]
[ 0  0  1]]
Translation:
```

```
[0.5 0.5 0.5]
The operation has been identified as a twofold rotation along the 0 0 1 axis
    with a translation of [0.5 0.5 0.5] and an intrinsic screw component of
    [0. 0. 1.].

Symmetry Element 7 (Unstarred):
Rotation:
[[ 1  0  0]
 [ 0 -1  0]
 [ 0  0  1]]
Translation:
[0.5 0.5 0. ]
The operation has been identified as a mirror across the 0 1 0 plane with a
    translation of [0.5 0.5 0. ] and an intrinsic glide component of [1. 0.
    0.].

Symmetry Element 8 (Unstarred):
Rotation:
[[-1  0  0]
 [ 0  1  0]
 [ 0  0  1]]
Translation:
[0.5 0.5 0.5]
The operation has been identified as a mirror across the 1 0 0 plane with a
    translation of [0.5 0.5 0.5] and an intrinsic glide component of [0. 1.
    1.].

Symmetry Element 9 (Starred):
Rotation:
[[-1  0  0]
 [ 0 -1  0]
 [ 0  0 -1]]
Translation:
[0. 0. 0.]
The operation has been identified as an inversion.

Symmetry Element 10 (Starred):
Rotation:
[[ 1  0  0]
 [ 0  1  0]
 [ 0  0 -1]]
Translation:
[0.         0.         0.49998689]
The operation has been identified as a mirror across the 0 0 1 plane with a
    translation of [0. 0.      0.49998689] but no intrinsic glide component.

Symmetry Element 11 (Starred):
Rotation:
[[-1  0  0]
```

```
[ 0  1  0]
[ 0  0 -1]]
Translation:
[0. 0. 0.]
The operation has been identified as a twofold rotation along the 0 1 0 axis.

Symmetry Element 12 (Starred):
Rotation:
[[ 1  0  0]
[ 0 -1  0]
[ 0  0 -1]]
Translation:
[0.         0.         0.49998689]
The operation has been identified as a twofold rotation along the 1 0 0 axis
    with a translation of [0. 0.     0.49998689] but no intrinsic screw
    component.

Symmetry Element 13 (Starred):
Rotation:
[[-1  0  0]
[ 0 -1  0]
[ 0  0 -1]]
Translation:
[0.5       0.4999999 0.       ]
The operation has been identified as an inversion with a translation of [0.5
    0.4999999 0.   ] but no intrinsic translation component.

Symmetry Element 14 (Starred):
Rotation:
[[ 1  0  0]
[ 0  1  0]
[ 0  0 -1]]
Translation:
[0.5        0.5        0.49998689]
The operation has been identified as a mirror across the 0 0 1 plane with a
    translation of [0.5 0.5    0.49998689] and an intrinsic glide component of
    [1. 1. 0.].

Symmetry Element 15 (Starred):
Rotation:
[[-1  0  0]
[ 0  1  0]
[ 0  0 -1]]
Translation:
[0.5 0.5 0. ]
The operation has been identified as a twofold rotation along the 0 1 0 axis
    with a translation of [0.5 0.5 0. ] and an intrinsic screw component of
    [0. 1. 0.].
```

```
Symmetry Element 16 (Starred):
Rotation:
[[ 1  0  0]
[ 0 -1  0]
[ 0  0 -1]]
Translation:
[0.5       0.4999999 0.49998689]
The operation has been identified as a twofold rotation along the 1 0 0 axis
    with a translation of [0.5 0.4999999 0.49998689] and an intrinsic screw
    component of [1. 0. 0.].
```

This is followed by the Bilbao formatted operations:

```
-------
------- Symmetry operations in Bilbao IDENTIFY GROUP format:
-------

x,y,z
-x,-y,z+1/2
x,-y,z
-x,y,z+1/2
x+1/2,y+1/2,z
-x+1/2,-y+1/2,z+1/2
x+1/2,-y+1/2,z
-x+1/2,y+1/2,z+1/2
-x,-y,-z
x,y,-z+1/2
-x,y,-z
x,-y,-z+1/2
-x+1/2,-y+1/2,-z
x+1/2,y+1/2,-z+1/2
-x+1/2,y+1/2,-z
x+1/2,-y+1/2,-z+1/2
```

Next, the code will re-print the matrix-vector representations of the distortion group elements in the standard basis:

```
-------
------- Elements of distortion group in the standard basis:
-------

Transformation matrix and origin shift...

Matrix:
[[ 0. -1. 0.]
[ 1.  0.  0.]
[ 0.  0.  1.]]
Origin shift:
[1. 0. 0.]
```

```
Symmetry Element 1 (Unstarred):
Rotation:
[[1. 0. 0.]
[0. 1. 0.]
[0. 0. 1.]]
Translation:
[0. 0. 0.]
The operation has been identified as the identity.

Symmetry Element 2 (Unstarred):
Rotation:
[[-1. 0.  0.]
[ 0. -1. 0.]
[ 0.  0.  1.]]
Translation:
[2.  0.  0.5]
The operation has been identified as a twofold rotation along the 0 0 1 axis
    with a translation of [2. 0. 0.5] and an intrinsic screw component of [0.
    0. 1.].

Symmetry Element 3 (Unstarred):
Rotation:
[[-1. 0.  0.]
[ 0.  1.  0.]
[ 0.  0.  1.]]
Translation:
[2. 0. 0.]
The operation has been identified as a mirror across the 1 0 0 plane with a
    translation of [2. 0. 0.] but no intrinsic glide component.

Symmetry Element 4 (Unstarred):
Rotation:
[[ 1.  0.  0.]
[ 0. -1. 0.]
[ 0.  0.  1.]]
Translation:
[0.  0.  0.5]
The operation has been identified as a mirror across the 0 1 0 plane with a
    translation of [0. 0. 0.5] and an intrinsic glide component of [0. 0. 1.].

Symmetry Element 5 (Unstarred):
Rotation:
[[1. 0. 0.]
[0. 1. 0.]
[0. 0. 1.]]
Translation:
```

```
[-0.5 0.5 0. ]
The operation has been identified as a translation of [-0.5 0.5 0. ].

Symmetry Element 6 (Unstarred):
Rotation:
[[-1. 0. 0.]
[ 0. -1. 0.]
[ 0. 0. 1.]]
Translation:
[1.5 0.5 0.5]
The operation has been identified as a twofold rotation along the 0 0 1 axis
    with a translation of [1.5 0.5 0.5] and an intrinsic screw component of
    [0. 0. 1.].

Symmetry Element 7 (Unstarred):
Rotation:
[[-1. 0. 0.]
[ 0. 1. 0.]
[ 0. 0. 1.]]
Translation:
[1.5 0.5 0. ]
The operation has been identified as a mirror across the 1 0 0 plane with a
    translation of [1.5 0.5 0. ] and an intrinsic glide component of [0. 1.
    0.].

Symmetry Element 8 (Unstarred):
Rotation:
[[ 1. 0. 0.]
[ 0. -1. 0.]
[ 0. 0. 1.]]
Translation:
[-0.5 0.5 0.5]
The operation has been identified as a mirror across the 0 1 0 plane with a
    translation of [-0.5 0.5 0.5] and an intrinsic glide component of [-1. 0.
    1.].

Symmetry Element 9 (Starred):
Rotation:
[[-1. 0. 0.]
[ 0. -1. 0.]
[ 0. 0. -1.]]
Translation:
[2. 0. 0.]
The operation has been identified as an inversion with a translation of [2. 0.
    0.] but no intrinsic translation component.

Symmetry Element 10 (Starred):
Rotation:
[[ 1. 0. 0.]
```

```
[ 0.  1.  0.]
[ 0.  0. -1.]]
Translation:
[0.         0.         0.49998689]
The operation has been identified as a mirror across the 0 0 1 plane with a
    translation of [0. 0.      0.49998689] but no intrinsic glide component.

Symmetry Element 11 (Starred):
Rotation:
[[ 1.  0.  0.]
[ 0. -1. 0.]
[ 0.  0. -1.]]
Translation:
[0. 0. 0.]
The operation has been identified as a twofold rotation along the 1 0 0 axis.

Symmetry Element 12 (Starred):
Rotation:
[[-1.  0.  0.]
[ 0.  1.  0.]
[ 0.  0. -1.]]
Translation:
[2.         0.         0.49998689]
The operation has been identified as a twofold rotation along the 0 1 0 axis
    with a translation of [2. 0.      0.49998689] but no intrinsic screw
    component.

Symmetry Element 13 (Starred):
Rotation:
[[-1.  0.  0.]
[ 0. -1. 0.]
[ 0.  0. -1.]]
Translation:
[1.5000001 0.5      0.        ]
The operation has been identified as an inversion with a translation of
    [1.5000001 0.5 0.   ] but no intrinsic translation component.

Symmetry Element 14 (Starred):
Rotation:
[[ 1.  0.  0.]
[ 0.  1.  0.]
[ 0.  0. -1.]]
Translation:
[-0.5        0.5        0.49998689]
The operation has been identified as a mirror across the 0 0 1 plane with a
    translation of [-0.5 0.5      0.49998689] and an intrinsic glide component
    of [-1. 1. 0.].

Symmetry Element 15 (Starred):
```

```
Rotation:
[[ 1.  0.  0.]
[ 0. -1. 0.]
[ 0.  0. -1.]]
Translation:
[-0.5 0.5  0. ]
The operation has been identified as a twofold rotation along the 1 0 0 axis
    with a translation of [-0.5 0.5 0. ] and an intrinsic screw component of
    [-1. 0. 0.].

Symmetry Element 16 (Starred):
Rotation:
[[-1.  0.  0.]
[ 0.  1.  0.]
[ 0.  0. -1.]]
Translation:
[1.5000001 0.5       0.49998689]
The operation has been identified as a twofold rotation along the 0 1 0 axis
    with a translation of [1.5000001 0.5 0.49998689] and an intrinsic screw
    component of [0. 1. 0.].
```

Finally, the code will output the name of the distortion group, and all possible irreps to construct perturbations with in the listing by Stokes *et al.* [2]:

```
-------
------- Distortion group:
-------

Cmcm*

-------
------- Possible irreps of the distortion group:
-------

Irrep #2834: GM1+
Irrep #2835: GM2+
Irrep #2836: GM3+
Irrep #2837: GM4+
Irrep #2838: GM1-
Irrep #2839: GM2-
Irrep #2840: GM3-
Irrep #2841: GM4-
Irrep #2842: DT1
Irrep #2843: DT2
Irrep #2844: DT3
Irrep #2845: DT4
Irrep #2846: LD1
```

```
Irrep #2847: LD2
Irrep #2848: LD3
Irrep #2849: LD4
Irrep #2850: SM1
Irrep #2851: SM2
Irrep #2852: SM3
Irrep #2853: SM4
Irrep #2854: Y1+
Irrep #2855: Y2+
Irrep #2856: Y3+
Irrep #2857: Y4+
Irrep #2858: Y1-
Irrep #2859: Y2-
Irrep #2860: Y3-
Irrep #2861: Y4-
Irrep #2862: Z1
Irrep #2863: Z2
Irrep #2864: R1
Irrep #2865: S1+
Irrep #2866: S2+
Irrep #2867: S1-
Irrep #2868: S2-
Irrep #2869: T1
Irrep #2870: T2
Irrep #2871: A1
Irrep #2872: B1B3
Irrep #2873: B2B4
Irrep #2874: D1
Irrep #2875: D2
Irrep #2876: H1
Irrep #2877: H2
Irrep #2878: H3
Irrep #2879: H4
Irrep #2880: K1
Irrep #2881: K2
Irrep #2882: M1
Irrep #2883: M2
Irrep #2884: P1
Irrep #2885: P2
Irrep #2886: Q1Q2
Irrep #2887: GP1


==================================================
```

Step 2 – Perturb with a particular irreducible representation

Now that we know the distortion group of the path and all of its irreps, we can choose one, generate a symmetry adapted perturbation to the path, and create a new initial path for an NEB calculation. In this case, we choose the Y_{4+} irrep, which is no. 2857 in the listing by Stokes *et al.* [2]. Since the irrep is one-dimentional, and there is only one k-vector in the star of the wave-vector $\{k = (1, 0, 0)\}$, constructing a path perturbation with it will result in a loss of translational symmetry described by operations with fractional translations associated with the C-centering of the group. This is accommodated by the $Ca_3Ti_2O_3$ cell chosen for the images in the path.

To perturb the path, the following input file can be run with `DiSPy`:

```
#---Sample DiSPy input file with perturbation

PERTURB=TRUE
INTERPOLATE=FALSE
IMAGES=9
SYMPREC=0.1
ANGLE_TOLERANCE=-1.0
VECTOR_TOLERANCE(A)=0.01,0.01,0.01
GENERAL_TOLERANCE=0.05
IMAGE_DIR=./init_path
INPUT_FORMAT=poscar
OUTPUT_FORMAT=poscar

TRANS_NUM=0
OSHIFT=0,0,0

MIN_MOVE=0.1

IRR_NUM=2857
IRR_DIM=1
MODE_COEFF=1.0

PERTURB_MAG=0.05
```

Here, the important new quantities are ‘MIN_MOVE’, ‘IRR_NUM’, ‘IRR_DIM’, ‘MODE_COEFF’, and ‘PERTURB_MAG’. ‘MIN_MOVE’ is set to 0.1Å to ensure that only atoms which have displaced a minimum of 0.1Å in any one lattice vector direction are considered when constructing perturbations. ‘IRR_NUM’, ‘IRR_DIM’, and ‘MODE_COEFF’ are used to select the irrep to construct the perturbation with, indicate its dimension, and specify what the coefficients of the order parameter vector are if it has a dimension of two of greater, respectively. Since this is a one-dimensional irrep, these are both set to 1. Lastly, ‘PERTURB_MAG’ is set to 0.05Å to ensure that symmetry-adapted perturbations that are generated are normalized in such a way that the maximum displacement of any one atom in any lattice vector direction is 0.05Å. In general, a value between 0.05-0.1Å has been found to be to be minimally sufficient to induce path instabilities.

Output Summary:

After the the output shown previously in Step 1, `DiSPy` will print the output text shown below:

First the irrep matrices of the elements of the distortion group will be listed:

```
Irrep. #2857 chosen...


------- Irrep. Matrices:

Symmetry Element 1 :
[[1.]]

Symmetry Element 2 :
[[-1.]]

Symmetry Element 3 :
[[-1.]]

Symmetry Element 4 :
[[1.]]

Symmetry Element 5 :
[[-1.]]

Symmetry Element 6 :
[[1.]]

Symmetry Element 7 :
[[1.]]

Symmetry Element 8 :
[[-1.]]

Symmetry Element 9 :
[[1.]]

Symmetry Element 10 :
[[-1.]]

Symmetry Element 11 :
[[-1.]]
```

```
Symmetry Element 12 :
[[1.]]

Symmetry Element 13 :
[[-1.]]

Symmetry Element 14 :
[[1.]]

Symmetry Element 15 :
[[1.]]

Symmetry Element 16 :
[[-1.]]
```

Next, all of the atoms included in the perturbation basis are outputted:

```
------- Atoms included in basis:
Ca Yes
Ca Yes
Ca Yes
Ca Yes
Ca Yes
Ca Yes
Ca Yes
Ca Yes
Ca Yes
Ca Yes
Ca Yes
Ca Yes
Ti No
Ti No
Ti No
Ti No
Ti No
Ti No
Ti No
Ti No
O Yes
O Yes
O Yes
O Yes
O Yes
O Yes
O Yes
O Yes
O Yes
O Yes
```

```
0 Yes
0 Yes
0 Yes
0 Yes
0 Yes
0 Yes
0 Yes
0 Yes
0 Yes
0 Yes
0 Yes
0 Yes
0 Yes
0 Yes
0 Yes
0 Yes
0 Yes
0 Yes
```

Finally, the same data described in Section 1 is shown again, but for the newly perturbed path:

```
-------
-------
------- Symmetry of images:
-------
-------

Image 1: Cmc2_1 (36)
Image 2: Pca2_1 (29)
Image 3: Pca2_1 (29)
Image 4: Pca2_1 (29)
Image 5: Pbcn (60)
Image 6: Pca2_1 (29)
Image 7: Pca2_1 (29)
Image 8: Pca2_1 (29)
Image 9: Cmc2_1 (36)

-------
------- Elements of distortion group in the basis of the inputted structures:
-------

Symmetry Element 1 (Unstarred):
Rotation:
[[1 0 0]
[0 1 0]
[0 0 1]]
Translation:
[0. 0. 0.]
```

```
The operation has been identified as the identity.

Symmetry Element 2 (Unstarred):
Rotation:
[[-1  0  0]
 [ 0  1  0]
 [ 0  0  1]]
Translation:
[0.  0.  0.5]
The operation has been identified as a mirror across the 1 0 0 plane with a
    translation of [0. 0. 0.5] and an intrinsic glide component of [0. 0. 1.].

Symmetry Element 3 (Unstarred):
Rotation:
[[-1  0  0]
 [ 0 -1  0]
 [ 0  0  1]]
Translation:
[0.5 0.5 0.5]
The operation has been identified as a twofold rotation along the 0 0 1 axis
    with a translation of [0.5 0.5 0.5] and an intrinsic screw component of
    [0. 0. 1.].

Symmetry Element 4 (Unstarred):
Rotation:
[[ 1  0  0]
 [ 0 -1  0]
 [ 0  0  1]]
Translation:
[0.5 0.5 0. ]
The operation has been identified as a mirror across the 0 1 0 plane with a
    translation of [0.5 0.5 0. ] and an intrinsic glide component of [1. 0.
    0.].

Symmetry Element 5 (Starred):
Rotation:
[[-1  0  0]
 [ 0 -1  0]
 [ 0  0 -1]]
Translation:
[0. 0. 0.]
The operation has been identified as an inversion.

Symmetry Element 6 (Starred):
Rotation:
[[ 1  0  0]
 [ 0  1  0]
 [ 0  0 -1]]
Translation:
```

```
[0.5        0.5        0.49998689]
The operation has been identified as a mirror across the 0 0 1 plane with a
    translation of [0.5 0.5    0.49998689] and an intrinsic glide component of
    [1. 1. 0.].

Symmetry Element 7 (Starred):
Rotation:
[[-1  0  0]
[ 0  1  0]
[ 0  0 -1]]
Translation:
[0.5 0.5 0. ]
The operation has been identified as a twofold rotation along the 0 1 0 axis
    with a translation of [0.5 0.5 0. ] and an intrinsic screw component of
    [0. 1. 0.].

Symmetry Element 8 (Starred):
Rotation:
[[ 1  0  0]
[ 0 -1  0]
[ 0  0 -1]]
Translation:
[0.         0.         0.49998689]
The operation has been identified as a twofold rotation along the 1 0 0 axis
    with a translation of [0. 0.     0.49998689] but no intrinsic screw
    component.

-------
------- Elements of distortion group in the standard basis:
-------

Transformation matrix and origin shift...

Matrix:
[[ 0. -1.  0.]
[-1.  0.  0.]
[ 0.  0. -1.]]
Origin shift:
[1. 1. 0.]



Symmetry Element 1 (Unstarred):
Rotation:
[[1. 0. 0.]
[0. 1. 0.]
[0. 0. 1.]]
Translation:
[0. 0. 0.]
```

```
The operation has been identified as the identity.

Symmetry Element 2 (Unstarred):
Rotation:
[[ 1. 0.  0.]
[ 0. -1. 0.]
[ 0. 0.  1.]]
Translation:
[ 0.  2.  -0.5]
The operation has been identified as a mirror across the 0 1 0 plane with a
    translation of [ 0. 2. -0.5] and an intrinsic glide component of [ 0. 0.
    -1.].

Symmetry Element 3 (Unstarred):
Rotation:
[[-1. 0.  0.]
[ 0. -1. 0.]
[ 0. 0.  1.]]
Translation:
[ 1.5 1.5 -0.5]
The operation has been identified as a twofold rotation along the 0 0 1 axis
    with a translation of [ 1.5 1.5 -0.5] and an intrinsic screw component of
    [ 0. 0. -1.].

Symmetry Element 4 (Unstarred):
Rotation:
[[-1. 0.  0.]
[ 0. 1.  0.]
[ 0. 0.  1.]]
Translation:
[ 1.5 -0.5 0. ]
The operation has been identified as a mirror across the 1 0 0 plane with a
    translation of [ 1.5 -0.5 0. ] and an intrinsic glide component of [ 0.
    -1. 0.].

Symmetry Element 5 (Starred):
Rotation:
[[-1. 0.  0.]
[ 0. -1. 0.]
[ 0. 0. -1.]]
Translation:
[2. 2. 0.]
The operation has been identified as an inversion with a translation of [2. 2.
    0.] but no intrinsic translation component.

Symmetry Element 6 (Starred):
Rotation:
[[ 1. 0.  0.]
[ 0. 1.  0.]
```

```
[ 0.  0. -1.]]
Translation:
[-0.5       -0.5       -0.49998689]
The operation has been identified as a mirror across the 0 0 1 plane with a
    translation of [-0.5 -0.5    -0.49998689] and an intrinsic glide component
    of [-1. -1. 0.].

Symmetry Element 7 (Starred):
Rotation:
[[ 1.  0.  0.]
[ 0. -1. 0.]
[ 0.  0. -1.]]
Translation:
[-0.5 1.5  0. ]
The operation has been identified as a twofold rotation along the 1 0 0 axis
    with a translation of [-0.5 1.5 0. ] and an intrinsic screw component of
    [-1. 0. 0.].

Symmetry Element 8 (Starred):
Rotation:
[[-1.  0.  0.]
[ 0.  1.  0.]
[ 0.  0. -1.]]
Translation:
[ 2.         0.        -0.49998689]
The operation has been identified as a twofold rotation along the 0 1 0 axis
    with a translation of [ 2. 0.      -0.49998689] but no intrinsic screw
    component.


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------- Distortion group:
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Pbcn*


==================================================
```

As can be seen, the new distortion group of the path after perturbation is $Pbcn^*$. This result can be confirmed by looking at the isotropy subgroup for the Y_{4+} irrep of the isomorphic space group of the unperturbed path ($Cmcm$) using the ISOSUBGROUP program by Stokes *et al.* (http://iso.byu.edu). Perturbed image files can now be taken from './results/output_structures' and used as images of an initial path for an NEB calculation.

References

[1] T. Hahn, editor. *International Tables for Crystallography*, volume A of *International Tables for Crystallography.* International Union of Crystallography, Chester, England, Oct. 2006.

[2] H. T. Stokes, B. J. Campbell, and R. Cordes. Tabulation of irreducible representations of the crystallographic space groups and their superspace extensions. *Acta Crystallographica Section A Foundations of Crystallography*, 69(4):388–395, July 2013.