User guide of *TopologicalSupercon* for version 1

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TopologicalSupercon is a subroutine, which can quickly diagnose possible topological and nodal superconductivity based on symmetry-indicator method for any material. Users can use this subroutine just by uploading a particularly formatted result of first-principles calculations. In this document, we explain how to prepare the input file and how to run the program.

Generating inputs

1. *Formatting results of first-principles calculations*

The input file must contain symmetry operations and characters of irreducible representations for each band in a particular format. Although one can make it by oneself, three external programs (*vasp2trace* [1], *irvsp* [2], and *qeirreps* [3]) can automatically generate it. To use our subroutine for superconductors, there are two additional things to do.One is to add the Fermi energy to the first line of the input produced by the above external programs. The other is to compute the characters of the hole-bands below the Fermi energy and include them in the input. In other words, one should take into account the partially filled bands in the computations for superconductors. A sample input of the subroutine for superconductors is shown in Appendix A 1.

2. *Precautions on convention*

When one generates an input, one should pay attention to the convention. In first-principles calculations, one must follow the following settings [5]:

(i) For space groups No. 3–15 (Monoclinic space groups), the rotation axis and the direction perpendicular to the mirror plane are set to the $+y$-axis.

(ii) For space groups No. 75–139 (Tetragonal space groups), the four-fold rotation axis is set to the $+z$-axis.

(iii) For space groups No. 143–194 (Trigonal and Hexagonal space groups), the three-fold or the six-fold rotation axes are set to the $+z$-axis.

(iv) For any space group, the spin-quantization axis is set to the $+z$-axis.

(v) The primitive lattice vectors $(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c})$ are chosen in the same way as Table I.

Running the program

Here, we explain how to use our subroutine given a correctly formatted input.

3. *Uploading the input file*

First, one goes to the page *TopologicalSupercon* (`http://toposupercon.t.u-tokyo.ac.jp/tms`) and uploads the input file by clicking the uploader button and selecting the file.

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TABLE I. **Primitive lattice vectors.** When one performs first-principles calculations, one needs to choose the primitive lattice vectors in the same way as the following table. Here, a, b, c, and γ are independent lattice parameters. In the output of the subroutine, the parameters are set to $a = b = c = 1$ and $\gamma = \pi/2$.

Lattice	$(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c})$	Lattice	$(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c})$
Monoclinic primitive	$\begin{pmatrix} a & 0 & -c\cos(\gamma) \\ 0 & b & 0 \\ 0 & 0 & c\sin(\gamma) \end{pmatrix}$	Monoclinic base-centered	$\begin{pmatrix} \frac{1}{2}a\sin(\gamma) & -\frac{1}{2}a\sin(\gamma) & 0 \\ \frac{b}{2} & \frac{b}{2} & 0 \\ \frac{1}{2}a\cos(\gamma) & -\frac{1}{2}a\cos(\gamma) & c \end{pmatrix}$ or $\begin{pmatrix} \frac{1}{2}a\sin(\gamma) & \frac{1}{2}a\sin(\gamma) & 0 \\ -\frac{b}{2} & \frac{b}{2} & 0 \\ \frac{1}{2}a\cos(\gamma) & -\frac{1}{2}a\cos(\gamma) & c \end{pmatrix}$
Orthorhombic primitive	$\begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix}$	Orthorhombic base-centered	$\begin{pmatrix} \frac{a}{2} & -\frac{a}{2} & 0 \\ \frac{b}{2} & \frac{b}{2} & 0 \\ 0 & 0 & c \end{pmatrix}$ or $\begin{pmatrix} \frac{a}{2} & \frac{a}{2} & 0 \\ -\frac{b}{2} & \frac{b}{2} & 0 \\ 0 & 0 & c \end{pmatrix}$
Orthorhombic body-centered	$\begin{pmatrix} -\frac{a}{2} & \frac{a}{2} & \frac{a}{2} \\ \frac{b}{2} & -\frac{b}{2} & \frac{b}{2} \\ \frac{c}{2} & \frac{c}{2} & -\frac{c}{2} \end{pmatrix}$ or $\begin{pmatrix} \frac{a}{2} & -\frac{a}{2} & \frac{a}{2} \\ \frac{b}{2} & -\frac{b}{2} & -\frac{b}{2} \\ \frac{c}{2} & \frac{c}{2} & -\frac{c}{2} \end{pmatrix}$	Orthorhombic face-centered	$\begin{pmatrix} \frac{a}{2} & 0 & \frac{a}{2} \\ 0 & \frac{b}{2} & \frac{b}{2} \\ \frac{c}{2} & \frac{c}{2} & 0 \end{pmatrix}$ or $\begin{pmatrix} \frac{a}{2} & 0 & \frac{a}{2} \\ 0 & -\frac{b}{2} & -\frac{b}{2} \\ \frac{c}{2} & \frac{c}{2} & 0 \end{pmatrix}$
Tetragonal primitive	$\begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & c \end{pmatrix}$	Tetragonal body-centered	$\begin{pmatrix} -\frac{a}{2} & \frac{a}{2} & \frac{a}{2} \\ \frac{a}{2} & -\frac{a}{2} & \frac{a}{2} \\ \frac{c}{2} & \frac{c}{2} & -\frac{c}{2} \end{pmatrix}$
Rhombohedral	$\begin{pmatrix} \frac{a}{2} & -\frac{a}{2} & 0 \\ \frac{a}{2\sqrt{3}} & \frac{a}{2\sqrt{3}} & -\frac{a}{\sqrt{3}} \\ \frac{c}{3} & \frac{c}{3} & \frac{c}{3} \end{pmatrix}$	Hexagonal	$\begin{pmatrix} a & -\frac{a}{2} & 0 \\ 0 & \frac{\sqrt{3}}{2}a & 0 \\ 0 & 0 & c \end{pmatrix}$
Cubic primitive	$\begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{pmatrix}$	Cubic face-centered	$\begin{pmatrix} 0 & \frac{a}{2} & \frac{a}{2} \\ \frac{a}{2} & 0 & \frac{a}{2} \\ \frac{a}{2} & \frac{a}{2} & 0 \end{pmatrix}$
Cubic body-centered	$\begin{pmatrix} -\frac{a}{2} & \frac{a}{2} & \frac{a}{2} \\ \frac{a}{2} & -\frac{a}{2} & \frac{a}{2} \\ \frac{a}{2} & \frac{a}{2} & -\frac{a}{2} \end{pmatrix}$	A type lattices	$\begin{pmatrix} 0 & 0 & c \\ \frac{a}{2} & -\frac{a}{2} & 0 \\ \frac{b}{2} & \frac{b}{2} & 0 \end{pmatrix}$ or $\begin{pmatrix} c & 0 & 0 \\ 0 & \frac{a}{2} & -\frac{a}{2} \\ 0 & \frac{b}{2} & \frac{b}{2} \end{pmatrix}$

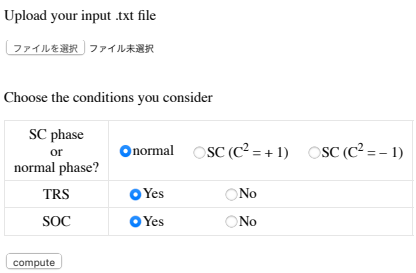

FIG. 1. **A screenshot of *TopologicalSupercon*.** One chooses the conditions and pushes the button 'compute.'

4. Select options

Second, one chooses the following three options as shown in Fig. 1: (i) whether the calculation is performed for the normal conducting phase or for the superconducting phase (for the latter case, one should further specify either $C^2 = +1$ or $C^2 = -1$ for the particle-hole symmetry C), (ii) whether the time reversal symmetry (TRS) is assumed or not, (iii) whether the spin-orbit coupling is taken into account or not. When one chooses 'normal phase,' one immediately obtains the results. On the other hand, if one chooses 'SC ($C^2 = +1$) ' or 'SC ($C^2 = -1$) ', our subroutine performs calculations for all possible pairings belonging to one-dimensional irreducible representations of point groups. To see the result for each pairing, one should select one by clicking the button (see Fig. 2). One can also find the he definition of symbols of one-dimensional irreducible representations of point groups by clicking the link 'irrep of PG,' as shown in Fig. 2.

5. Results

Here we explain the meaning of the results of our subroutine. There are four possible cases: Case I, symmetry-enforced nodal superconductors; Case II, symmetry-diagnosable topological gapped or nodal superconductors; Case III, topologically trivial or not symmetry-diagnosable topological superconductors; Case IV, the case where no BLs can be defined at any high-symmetry momenta. For Case I (symmetry-enforced nodal superconductors), we show the position and symbols ([P], [L], and [S]) of nodes, as listed in Appendix A 2. Here, [P], [L], and [S] denote the shape of nodes such as point, line, and surface nodes. Also, other symbols (A) and (B) represent origins of the nodes (see Ref. [6] for more details). For Case II, one can find an entry of

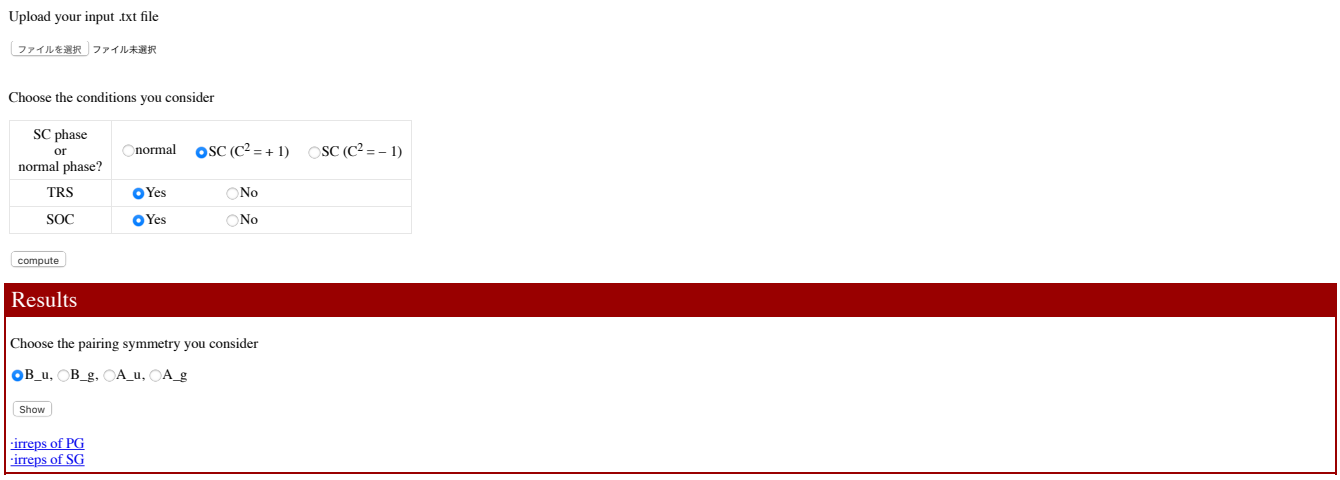

FIG. 2. **A screenshot of *TopologicalSupercon*.** One chooses the pairing and pushes the button 'show.'

symmetry indicators in a particular basis set. As shown in Appendix A 3, we also provide the bases used in the computations. The band labels are arranged in order of the irreducible representations included in 'irrep of SG.'

If you have any problem using this program and/or any question or suggestion, please contact Seishiro Ono at address: toposupercon@gmail.com.

[1] M. G. Vergniory and et al., "A complete catalogue of high-quality topological materials," Nature **566**, 480–485 (2019).
[2] Jiacheng Gao, Quansheng Wu, Clas Persson, and Zhijun Wang, "Irvsp: To obtain irreducible representations of electronic states in the vasp," Computer Physics Communications **261**, 107760 (2021).
[3] Akishi Matsugatani, Seishiro Ono, Yusuke Nomura, and Haruki Watanabe, "qeirreps: An open-source program for quantum espresso to compute irreducible representations of bloch wavefunctions," Computer Physics Communications **264**, 107948 (2021).
[4] L. Elcoro, B. Bradlyn, Z. Wang, M. G. Vergniory, J. Cano, C. Felser, B. A. Bernevig, D. Orobengoa, G. de la Flor, and M. I. Aroyo, "Double crystallographic groups and their representations on the Bilbao Crystallographic Server," J. Appl. Cryst. **50**, 1457–1477 (2017).
[5] These assumptions will be removed from the next update.
[6] Seishiro Ono and Ken Shiozaki, "Symmetry-based approach to nodal structures: Unification of compatibility relations and point-node classifications," , arXiv:2102.07676 (2021).

Appendix A: Example of input and output

1. Input

```
10.0977 (* Fermi energy*)
92
1
4
1  0  0  0  1  0  0  0  1  0.000000  0.000000  0.000000  1.000000  0.000000  0.000000  0.000000  0.000000  0.000000  1.000000  0.000000
-1  0  0  0  1  0  0  0 -1  0.000000  0.500000  0.000000  0.000000  0.000000 -1.000000  0.000000  1.000000  0.000000  0.000000  0.000000
-1  0  0  0 -1  0  0  0 -1  0.000000  0.000000  0.000000  1.000000  0.000000  0.000000  0.000000  0.000000  0.000000  1.000000  0.000000
1  0  0  0 -1  0  0  0  1  0.000000 -0.500000  0.000000  0.000000  0.000000 -1.000000  0.000000  1.000000  0.000000  0.000000  0.000000
8
0.000000  0.000000  0.000000
0.000000  0.000000  0.500000
0.500000  0.000000  0.000000
0.000000  0.500000  0.000000
0.500000  0.500000  0.000000
0.000000  0.500000  0.500000
0.500000  0.000000  0.500000
0.500000  0.500000  0.500000
4
1  2  3  4
1  2 -31.362273  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000  0.000000  0.000000
3  2 -31.361011  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000  0.000000  0.000000
5  2 -19.731624  2.000000  0.000000 -0.000000  0.000000  2.000000  0.000000  0.000000 -0.000000
7  2 -19.700454  2.000000  0.000000 -0.000000  0.000000  2.000000  0.000000 -0.000000  0.000000
9  2 -19.690341  2.000000  0.000000 -0.000000  0.000000 -2.000000  0.000000  0.000000  0.000000
11  2 -19.648876  2.000000  0.000000  0.000000  0.000000 -2.000000  0.000000  0.000000  0.000000
13  2 -19.603224  2.000000  0.000000  0.000000 -0.000000  2.000000  0.000000  0.000000 -0.000000
15  2 -19.597781  2.000000  0.000000 -0.000000  0.000000 -2.000000  0.000000  0.000000 -0.000000
17  2 -19.586202  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000  0.000000  0.000000
19  2 -19.578508  2.000000  0.000000  0.000000 -0.000000 -2.000000  0.000000  0.000000 -0.000000
21  2 -18.523587  2.000000  0.000000 -0.000000 -0.000000  2.000000  0.000000  0.000000 -0.000000
23  2 -18.491918  2.000000  0.000000  0.000000 -0.000000  2.000000  0.000000 -0.000000 -0.000000
25  2 -18.471257  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000  0.000000 -0.000000
27  2 -18.435533  2.000000  0.000000  0.000000  0.000000 -2.000000  0.000000  0.000000  0.000000
29  2 -18.390193  2.000000  0.000000  0.000000 -0.000000 -2.000000  0.000000 -0.000000 -0.000000
31  2 -18.376464  2.000000  0.000000 -0.000000 -0.000000  2.000000  0.000000  0.000000  0.000000
33  2 -18.366340  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000  0.000000  0.000000
35  2 -18.355329  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000  0.000000 -0.000000
37  2 -18.349052  2.000000  0.000000  0.000000 -0.000000 -2.000000  0.000000 -0.000000  0.000000
39  2 -18.342804  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000  0.000000  0.000000
41  2 -18.332066  2.000000  0.000000  0.000000  0.000000 -2.000000  0.000000  0.000000  0.000000
43  2 -18.312703  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000  0.000000  0.000000
45  2 -12.639302  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000  0.000000  0.000000
47  2 -12.628602  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000  0.000000  0.000000
49  2 -12.283273  2.000000  0.000000  0.000000 -0.000000  2.000000  0.000000  0.000000 -0.000000
51  2 -12.269585  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000  0.000000 -0.000000
53  2 -12.233807  2.000000  0.000000 -0.000000  0.000000  2.000000  0.000000 -0.000000 -0.000000
55  2 -12.227327  2.000000  0.000000  0.000000 -0.000000 -2.000000  0.000000 -0.000000 -0.000000
57  2  -1.664309  2.000000  0.000000  0.000000 -0.000000  2.000000  0.000000  0.000000 -0.000000
59  2  -0.831804  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000  0.000000  0.000000
61  2   1.789383  2.000000  0.000000  0.000000  0.000000 -2.000000  0.000000  0.000000  0.000000
63  2   3.713977  2.000000  0.000000 -0.000000  0.000000 -2.000000  0.000000  0.000000 -0.000000
65  2   6.532366  2.000000  0.000000  0.000000 -0.000000  2.000000  0.000000  0.000000  0.000000
67  2   6.786955  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000  0.000000  0.000000
69  2   7.397251  2.000000  0.000000  0.000000 -0.000000  2.000000  0.000000  0.000000  0.000000
71  2   7.655209  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000 -0.000000  0.000000
73  2   7.664034  2.000000  0.000000 -0.000000  0.000000 -2.000000  0.000000  0.000000 -0.000000
75  2   8.115624  2.000000  0.000000 -0.000000 -0.000000  2.000000  0.000000 -0.000000 -0.000000
77  2   9.391767  2.000000  0.000000  0.000000 -0.000000  2.000000  0.000000  0.000000 -0.000000
79  2  10.226963  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000  0.000000 -0.000000
81  2  10.577158  2.000000  0.000000  0.000000  0.000000 -2.000000  0.000000  0.000000 -0.000000
83  2  11.328886  2.000000  0.000000  0.000000  0.000000 -2.000000  0.000000  0.000000  0.000000
85  2  11.450807  2.000000  0.000000  0.000000  0.000000 -2.000000  0.000000 -0.000000 -0.000000
87  2  11.859219  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000  0.000000  0.000000
89  2  12.229257  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000  0.000000 -0.000000
91  2  12.776281  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000  0.000000  0.000000
4
1  2  3  4
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9  2 -19.690335  2.000000  0.000000  0.000000 -0.000000  2.000000 -0.000000 -0.000000 -0.000000
11  2 -19.648876  2.000000  0.000000 -0.000000  0.000000 -2.000000 -0.000000  0.000000  0.000000
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17  2 -19.586187  2.000000  0.000000 -0.000000 -0.000000  2.000000  0.000000  0.000000  0.000000
19  2 -19.578507  2.000000  0.000000  0.000000 -0.000000 -2.000000  0.000000  0.000000 -0.000000
21  2 -18.523540  2.000000  0.000000  0.000000  0.000000 -2.000000 -0.000000 -0.000000  0.000000
23  2 -18.492020  2.000000  0.000000  0.000000  0.000000  2.000000 -0.000000 -0.000000  0.000000
25  2 -18.471169  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000  0.000000  0.000000
27  2 -18.435524  2.000000  0.000000 -0.000000  0.000000 -2.000000 -0.000000  0.000000  0.000000
29  2 -18.390244  2.000000  0.000000 -0.000000 -0.000000  2.000000  0.000000 -0.000000  0.000000
31  2 -18.376550  2.000000  0.000000  0.000000 -0.000000 -2.000000 -0.000000  0.000000 -0.000000
33  2 -18.366275  2.000000  0.000000 -0.000000  0.000000 -2.000000 -0.000000  0.000000 -0.000000
35  2 -18.355378  2.000000  0.000000  0.000000  0.000000  2.000000 -0.000000  0.000000 -0.000000
37  2 -18.348940  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000 -0.000000  0.000000
39  2 -18.342956  2.000000  0.000000 -0.000000  0.000000  2.000000  0.000000  0.000000  0.000000
41  2 -18.331879  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000  0.000000  0.000000
43  2 -18.312772  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000  0.000000  0.000000
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47  2 -12.630769  2.000000  0.000000  0.000000 -0.000000  2.000000 -0.000000  0.000000 -0.000000
49  2 -12.280272  2.000000  0.000000 -0.000000  0.000000 -2.000000  0.000000  0.000000 -0.000000
51  2 -12.272459  2.000000  0.000000  0.000000 -0.000000  2.000000 -0.000000  0.000000  0.000000
53  2 -12.232779  2.000000  0.000000  0.000000  0.000000 -2.000000  0.000000 -0.000000  0.000000
55  2 -12.228633  2.000000  0.000000 -0.000000 -0.000000  2.000000  0.000000 -0.000000  0.000000
57  2  -1.448266  2.000000  0.000000  0.000000 -0.000000  2.000000  0.000000  0.000000 -0.000000
59  2  -1.176197  2.000000  0.000000 -0.000000  0.000000 -2.000000 -0.000000  0.000000  0.000000
61  2   2.208205  2.000000  0.000000  0.000000  0.000000  2.000000 -0.000000  0.000000  0.000000
63  2   3.563962  2.000000  0.000000 -0.000000  0.000000 -2.000000  0.000000 -0.000000 -0.000000
65  2   5.767987  2.000000  0.000000 -0.000000  0.000000 -2.000000 -0.000000  0.000000 -0.000000
67  2   6.534182  2.000000  0.000000  0.000000 -0.000000  2.000000  0.000000  0.000000 -0.000000
69  2   7.550560  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000  0.000000  0.000000
71  2   7.693330  2.000000  0.000000  0.000000 -0.000000  2.000000  0.000000  0.000000 -0.000000
```

```
73  2    7.897730  2.000000  0.000000  0.000000 -0.000000 -2.000000  0.000000 -0.000000 -0.000000
75  2    9.152648  2.000000  0.000000  0.000000  0.000000 -2.000000  0.000000  0.000000  0.000000
77  2    9.258516  2.000000  0.000000  0.000000 -0.000000  2.000000 -0.000000  0.000000 -0.000000
79  2    9.823880  2.000000  0.000000 -0.000000  0.000000 -2.000000 -0.000000  0.000000 -0.000000
81  2   10.892466  2.000000  0.000000  0.000000 -0.000000  2.000000 -0.000000 -0.000000  0.000000
83  2   10.940548  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000  0.000000  0.000000
85  2   11.684953  2.000000  0.000000 -0.000000  0.000000  2.000000  0.000000 -0.000000  0.000000
87  2   11.994006  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000  0.000000  0.000000
89  2   12.618764  2.000000  0.000000  0.000000  0.000000 -2.000000  0.000000  0.000000 -0.000000
91  2   12.732885  2.000000  0.000000  0.000000  0.000000  2.000000 -0.000000  0.000000  0.000000
4
1  2  3  4
1  2 -31.361847  2.000000  0.000000 -0.000000  0.000000 -2.000000  0.000000  0.000000  0.000000
3  2 -31.360664  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000  0.000000  0.000000
5  2 -19.731665  2.000000  0.000000 -0.000000 -0.000000  2.000000  0.000000 -0.000000  0.000000
7  2 -19.690940  2.000000  0.000000  0.000000 -0.000000 -2.000000 -0.000000 -0.000000  0.000000
9  2 -19.689939  2.000000  0.000000  0.000000 -0.000000 -2.000000 -0.000000 -0.000000 -0.000000
11  2 -19.654171  2.000000  0.000000  0.000000  0.000000  2.000000 -0.000000 -0.000000  0.000000
13  2 -19.602866  2.000000  0.000000 -0.000000 -0.000000  2.000000  0.000000  0.000000  0.000000
15  2 -19.597810  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000  0.000000  0.000000
17  2 -19.583989  2.000000  0.000000 -0.000000  0.000000 -2.000000  0.000000  0.000000 -0.000000
19  2 -19.579893  2.000000  0.000000 -0.000000  0.000000  2.000000  0.000000  0.000000 -0.000000
21  2 -18.523599  2.000000  0.000000  0.000000 -0.000000  2.000000 -0.000000 -0.000000  0.000000
23  2 -18.479709  2.000000  0.000000 -0.000000 -0.000000 -2.000000 -0.000000  0.000000  0.000000
25  2 -18.471290  2.000000  0.000000  0.000000  0.000000 -2.000000 -0.000000 -0.000000  0.000000
27  2 -18.434640  2.000000  0.000000 -0.000000 -0.000000  2.000000 -0.000000  0.000000 -0.000000
29  2 -18.390642  2.000000  0.000000  0.000000  0.000000 -2.000000 -0.000000 -0.000000 -0.000000
31  2 -18.376847  2.000000  0.000000  0.000000 -0.000000  2.000000  0.000000 -0.000000 -0.000000
33  2 -18.365613  2.000000  0.000000 -0.000000 -0.000000  2.000000 -0.000000  0.000000 -0.000000
35  2 -18.362743  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000 -0.000000  0.000000
37  2 -18.355868  2.000000  0.000000  0.000000  0.000000 -2.000000 -0.000000 -0.000000 -0.000000
39  2 -18.342016  2.000000  0.000000 -0.000000  0.000000 -2.000000  0.000000  0.000000 -0.000000
41  2 -18.331391  2.000000  0.000000  0.000000 -0.000000 -2.000000  0.000000  0.000000 -0.000000
43  2 -18.317943  2.000000  0.000000 -0.000000 -0.000000  2.000000 -0.000000  0.000000 -0.000000
45  2 -12.640988  2.000000  0.000000 -0.000000 -0.000000 -2.000000 -0.000000  0.000000 -0.000000
47  2 -12.635479  2.000000  0.000000  0.000000  0.000000  2.000000 -0.000000  0.000000  0.000000
49  2 -12.287163  2.000000  0.000000 -0.000000  0.000000 -2.000000  0.000000  0.000000 -0.000000
51  2 -12.280724  2.000000  0.000000  0.000000 -0.000000  2.000000 -0.000000  0.000000 -0.000000
53  2 -12.233165  2.000000  0.000000  0.000000  0.000000 -2.000000  0.000000 -0.000000 -0.000000
55  2 -12.227737  2.000000  0.000000 -0.000000 -0.000000  2.000000 -0.000000  0.000000  0.000000
57  2  -0.919666  2.000000  0.000000  0.000000 -0.000000  2.000000  0.000000  0.000000 -0.000000
59  2  -0.621864  2.000000  0.000000 -0.000000 -0.000000 -2.000000 -0.000000  0.000000 -0.000000
61  2   1.272418  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000  0.000000 -0.000000
63  2   2.451250  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000  0.000000 -0.000000
65  2   5.567043  2.000000  0.000000  0.000000 -0.000000 -2.000000 -0.000000  0.000000  0.000000
67  2   6.146577  2.000000  0.000000  0.000000 -0.000000  2.000000 -0.000000  0.000000 -0.000000
69  2   7.774926  2.000000  0.000000 -0.000000  0.000000  2.000000 -0.000000 -0.000000 -0.000000
71  2   8.343844  2.000000  0.000000  0.000000  0.000000 -2.000000  0.000000 -0.000000 -0.000000
73  2   8.465382  2.000000  0.000000  0.000000 -0.000000  2.000000 -0.000000  0.000000 -0.000000
75  2   8.759175  2.000000  0.000000  0.000000  0.000000 -2.000000 -0.000000  0.000000 -0.000000
77  2   9.208112  2.000000  0.000000  0.000000  0.000000  2.000000 -0.000000  0.000000  0.000000
79  2  10.294710  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000  0.000000  0.000000
81  2  10.503179  2.000000  0.000000 -0.000000 -0.000000  2.000000  0.000000  0.000000  0.000000
83  2  10.629858  2.000000  0.000000 -0.000000 -0.000000 -2.000000 -0.000000  0.000000  0.000000
85  2  10.833040  2.000000  0.000000  0.000000 -0.000000  2.000000  0.000000  0.000000 -0.000000
87  2  10.922790  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000 -0.000000  0.000000
89  2  12.092028  2.000000  0.000000 -0.000000  0.000000 -2.000000 -0.000000  0.000000 -0.000000
91  2  13.034710  2.000000  0.000000  0.000000  0.000000 -2.000000  0.000000 -0.000000 -0.000000
4
1  2  3  4
1  4 -31.359626  4.000000  0.000000  0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000
5  4 -19.709305  4.000000  0.000000 -0.000000 -0.000000 -0.000000 -0.000000  0.000000 -0.000000
9  4 -19.671153  4.000000  0.000000  0.000000  0.000000  0.000000  0.000000 -0.000000 -0.000000
13  4 -19.599003  4.000000  0.000000  0.000000 -0.000000 -0.000000 -0.000000  0.000000  0.000000
17  4 -19.580366  4.000000  0.000000 -0.000000  0.000000  0.000000 -0.000000 -0.000000  0.000000
21  4 -18.495015  4.000000  0.000000 -0.000000  0.000000 -0.000000  0.000000  0.000000 -0.000000
25  4 -18.454271  4.000000  0.000000 -0.000000  0.000000 -0.000000 -0.000000 -0.000000 -0.000000
29  4 -18.396141  4.000000  0.000000 -0.000000  0.000000 -0.000000  0.000000  0.000000 -0.000000
33  4 -18.369265  4.000000  0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000
37  4 -18.340186  4.000000  0.000000  0.000000 -0.000000  0.000000 -0.000000  0.000000 -0.000000
41  4 -18.323655  4.000000  0.000000  0.000000  0.000000 -0.000000 -0.000000 -0.000000 -0.000000
45  4 -12.641497  4.000000  0.000000  0.000000  0.000000 -0.000000 -0.000000  0.000000 -0.000000
49  4 -12.273172  4.000000  0.000000 -0.000000  0.000000  0.000000  0.000000 -0.000000  0.000000
53  4 -12.256953  4.000000  0.000000 -0.000000  0.000000 -0.000000  0.000000  0.000000  0.000000
57  4   0.340130  4.000000  0.000000  0.000000 -0.000000 -0.000000  0.000000 -0.000000 -0.000000
61  4   0.912366  4.000000  0.000000  0.000000 -0.000000  0.000000  0.000000 -0.000000 -0.000000
65  4   5.595565  4.000000  0.000000  0.000000 -0.000000  0.000000 -0.000000 -0.000000 -0.000000
69  4   8.075724  4.000000  0.000000  0.000000 -0.000000 -0.000000 -0.000000  0.000000 -0.000000
73  4   8.525442  4.000000  0.000000  0.000000  0.000000 -0.000000 -0.000000  0.000000 -0.000000
77  4   9.090748  4.000000  0.000000 -0.000000 -0.000000  0.000000  0.000000  0.000000 -0.000000
81  4   9.953382  4.000000  0.000000 -0.000000 -0.000000  0.000000  0.000000 -0.000000  0.000000
85  4  10.353719  4.000000  0.000000 -0.000000  0.000000 -0.000000  0.000000  0.000000  0.000000
89  4  12.092589  4.000000  0.000000  0.000000 -0.000000  0.000000  0.000000 -0.000000  0.000000
4
1  2  3  4
1  4 -31.359345  4.000000  0.000000 -0.000000  0.000000 -0.000000  0.000000  0.000000  0.000000
5  4 -19.709297  4.000000  0.000000 -0.000000  0.000000 -0.000000  0.000000 -0.000000  0.000000
9  4 -19.673282  4.000000  0.000000 -0.000000 -0.000000 -0.000000 -0.000000  0.000000 -0.000000
13  4 -19.598399  4.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
17  4 -19.578968  4.000000  0.000000 -0.000000 -0.000000 -0.000000 -0.000000  0.000000 -0.000000
21  4 -18.495067  4.000000  0.000000  0.000000  0.000000 -0.000000 -0.000000  0.000000 -0.000000
25  4 -18.458707  4.000000  0.000000  0.000000  0.000000  0.000000 -0.000000 -0.000000  0.000000
29  4 -18.395760  4.000000  0.000000  0.000000 -0.000000 -0.000000 -0.000000  0.000000  0.000000
33  4 -18.369261  4.000000  0.000000 -0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
37  4 -18.339180  4.000000  0.000000  0.000000 -0.000000  0.000000 -0.000000  0.000000 -0.000000
41  4 -18.317600  4.000000  0.000000 -0.000000  0.000000  0.000000 -0.000000  0.000000 -0.000000
45  4 -12.645084  4.000000  0.000000 -0.000000  0.000000 -0.000000 -0.000000  0.000000 -0.000000
49  4 -12.278482  4.000000  0.000000 -0.000000 -0.000000 -0.000000  0.000000 -0.000000 -0.000000
53  4 -12.258971  4.000000  0.000000 -0.000000  0.000000  0.000000 -0.000000 -0.000000  0.000000
57  4   0.756887  4.000000  0.000000  0.000000 -0.000000 -0.000000  0.000000 -0.000000  0.000000
61  4   1.023756  4.000000  0.000000  0.000000  0.000000  0.000000 -0.000000  0.000000  0.000000
65  4   5.192389  4.000000  0.000000  0.000000 -0.000000 -0.000000 -0.000000 -0.000000  0.000000
69  4   6.440830  4.000000  0.000000 -0.000000 -0.000000  0.000000 -0.000000  0.000000 -0.000000
73  4   7.358302  4.000000  0.000000 -0.000000 -0.000000 -0.000000  0.000000 -0.000000 -0.000000
77  4   8.191190  4.000000  0.000000 -0.000000  0.000000 -0.000000  0.000000 -0.000000  0.000000
81  4  11.299276  4.000000  0.000000  0.000000 -0.000000  0.000000 -0.000000 -0.000000 -0.000000
85  4  12.717298  4.000000  0.000000  0.000000 -0.000000  0.000000  0.000000  0.000000 -0.000000
89  4  13.189038  4.000000  0.000000 -0.000000  0.000000 -0.000000 -0.000000  0.000000  0.000000
4
1  2  3  4
1  4 -31.359626  4.000000  0.000000 -0.000000 -0.000000 -0.000000 -0.000000  0.000000  0.000000
```

```
5  4 -19.709305  4.000000  0.000000  0.000000  0.000000 -0.000000  0.000000 -0.000000 -0.000000
9  4 -19.671153  4.000000  0.000000 -0.000000 -0.000000 -0.000000 -0.000000  0.000000  0.000000
13  4 -19.598997  4.000000  0.000000 -0.000000  0.000000  0.000000 -0.000000 -0.000000  0.000000
17  4 -19.580370  4.000000  0.000000 -0.000000  0.000000 -0.000000 -0.000000 -0.000000  0.000000
21  4 -18.495025  4.000000  0.000000 -0.000000 -0.000000  0.000000  0.000000 -0.000000 -0.000000
25  4 -18.454268  4.000000  0.000000 -0.000000  0.000000 -0.000000 -0.000000  0.000000  0.000000
29  4 -18.396138  4.000000  0.000000  0.000000  0.000000 -0.000000  0.000000 -0.000000 -0.000000
33  4 -18.369236  4.000000  0.000000  0.000000  0.000000 -0.000000 -0.000000  0.000000 -0.000000
37  4 -18.340237  4.000000  0.000000 -0.000000 -0.000000  0.000000  0.000000 -0.000000  0.000000
41  4 -18.323629  4.000000  0.000000  0.000000  0.000000  0.000000 -0.000000 -0.000000 -0.000000
45  4 -12.641551  4.000000  0.000000 -0.000000 -0.000000  0.000000 -0.000000  0.000000 -0.000000
49  4 -12.273763  4.000000  0.000000 -0.000000 -0.000000  0.000000 -0.000000 -0.000000  0.000000
53  4 -12.256302  4.000000  0.000000  0.000000  0.000000  0.000000  0.000000 -0.000000 -0.000000
57  4   0.482230  4.000000  0.000000 -0.000000 -0.000000 -0.000000  0.000000  0.000000  0.000000
61  4   0.720005  4.000000  0.000000 -0.000000 -0.000000  0.000000  0.000000  0.000000  0.000000
65  4   6.231005  4.000000  0.000000 -0.000000 -0.000000  0.000000  0.000000 -0.000000  0.000000
69  4   7.373860  4.000000  0.000000 -0.000000  0.000000  0.000000 -0.000000 -0.000000 -0.000000
73  4   8.263148  4.000000  0.000000  0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000
77  4   8.487202  4.000000  0.000000 -0.000000 -0.000000 -0.000000 -0.000000  0.000000  0.000000
81  4   9.934743  4.000000  0.000000 -0.000000  0.000000 -0.000000 -0.000000 -0.000000  0.000000
85  4  12.079300  4.000000  0.000000 -0.000000 -0.000000 -0.000000  0.000000  0.000000 -0.000000
89  4  12.237415  4.000000  0.000000 -0.000000  0.000000  0.000000  0.000000  0.000000 -0.000000
4
1  2  3  4
1  2 -31.361846  2.000000  0.000000  0.000000  0.000000  2.000000 -0.000000  0.000000  0.000000
3  2 -31.360665  2.000000  0.000000 -0.000000  0.000000 -2.000000  0.000000  0.000000  0.000000
5  2 -19.731672  2.000000  0.000000  0.000000 -0.000000 -2.000000 -0.000000  0.000000  0.000000
7  2 -19.690502  2.000000  0.000000  0.000000  0.000000  2.000000 -0.000000  0.000000  0.000000
9  2 -19.690367  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000  0.000000  0.000000
11  2 -19.654172  2.000000  0.000000  0.000000 -0.000000  2.000000 -0.000000 -0.000000 -0.000000
13  2 -19.602881  2.000000  0.000000  0.000000 -0.000000 -2.000000 -0.000000  0.000000  0.000000
15  2 -19.597803  2.000000  0.000000  0.000000 -0.000000  2.000000 -0.000000  0.000000  0.000000
17  2 -19.583979  2.000000  0.000000 -0.000000  0.000000 -2.000000 -0.000000  0.000000  0.000000
19  2 -19.579897  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000 -0.000000  0.000000
21  2 -18.523632  2.000000  0.000000  0.000000  0.000000 -2.000000  0.000000 -0.000000 -0.000000
23  2 -18.479474  2.000000  0.000000 -0.000000 -0.000000 -2.000000 -0.000000  0.000000 -0.000000
25  2 -18.471511  2.000000  0.000000 -0.000000  0.000000  2.000000 -0.000000  0.000000 -0.000000
27  2 -18.434643  2.000000  0.000000  0.000000 -0.000000  2.000000  0.000000  0.000000  0.000000
29  2 -18.390633  2.000000  0.000000 -0.000000 -0.000000  2.000000  0.000000  0.000000 -0.000000
31  2 -18.376782  2.000000  0.000000  0.000000 -0.000000 -2.000000 -0.000000 -0.000000  0.000000
33  2 -18.365534  2.000000  0.000000  0.000000 -0.000000 -2.000000 -0.000000  0.000000  0.000000
35  2 -18.362926  2.000000  0.000000 -0.000000  0.000000  2.000000  0.000000 -0.000000  0.000000
37  2 -18.355895  2.000000  0.000000  0.000000 -0.000000 -2.000000  0.000000 -0.000000  0.000000
39  2 -18.341723  2.000000  0.000000 -0.000000 -0.000000 -2.000000 -0.000000  0.000000  0.000000
41  2 -18.331685  2.000000  0.000000  0.000000  0.000000  2.000000 -0.000000  0.000000 -0.000000
43  2 -18.317862  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000  0.000000  0.000000
45  2 -12.641112  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000  0.000000  0.000000
47  2 -12.635431  2.000000  0.000000 -0.000000  0.000000 -2.000000 -0.000000  0.000000  0.000000
49  2 -12.287320  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000  0.000000 -0.000000
51  2 -12.280669  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000  0.000000  0.000000
53  2 -12.232883  2.000000  0.000000 -0.000000  0.000000  2.000000  0.000000 -0.000000 -0.000000
55  2 -12.227833  2.000000  0.000000 -0.000000  0.000000 -2.000000 -0.000000 -0.000000 -0.000000
57  2  -1.012071  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000  0.000000  0.000000
59  2  -0.447996  2.000000  0.000000  0.000000 -0.000000 -2.000000  0.000000  0.000000  0.000000
61  2   1.110123  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000  0.000000  0.000000
63  2   2.442260  2.000000  0.000000  0.000000 -0.000000  2.000000 -0.000000  0.000000  0.000000
65  2   5.717315  2.000000  0.000000  0.000000 -0.000000  2.000000 -0.000000  0.000000 -0.000000
67  2   7.047574  2.000000  0.000000 -0.000000 -0.000000 -2.000000 -0.000000  0.000000  0.000000
69  2   7.414949  2.000000  0.000000  0.000000 -0.000000  2.000000  0.000000  0.000000 -0.000000
71  2   7.636383  2.000000  0.000000  0.000000 -0.000000 -2.000000 -0.000000 -0.000000 -0.000000
73  2   7.932418  2.000000  0.000000 -0.000000  0.000000 -2.000000 -0.000000  0.000000 -0.000000
75  2   8.768835  2.000000  0.000000  0.000000  0.000000 -2.000000  0.000000 -0.000000  0.000000
77  2   9.750797  2.000000  0.000000 -0.000000 -0.000000 -2.000000  0.000000  0.000000 -0.000000
79  2   9.914865  2.000000  0.000000 -0.000000 -0.000000  2.000000  0.000000  0.000000  0.000000
81  2  10.153468  2.000000  0.000000  0.000000  0.000000  2.000000  0.000000  0.000000 -0.000000
83  2  10.978906  2.000000  0.000000  0.000000 -0.000000  2.000000  0.000000  0.000000 -0.000000
85  2  11.025240  2.000000  0.000000  0.000000 -0.000000 -2.000000  0.000000  0.000000  0.000000
87  2  11.269293  2.000000  0.000000 -0.000000 -0.000000  2.000000 -0.000000 -0.000000 -0.000000
89  2  12.266809  2.000000  0.000000  0.000000  0.000000  2.000000 -0.000000  0.000000  0.000000
91  2  12.969537  2.000000  0.000000 -0.000000  0.000000  2.000000  0.000000  0.000000 -0.000000
4
1  2  3  4
1  4 -31.359345  4.000000  0.000000  0.000000 -0.000000 -0.000000  0.000000 -0.000000  0.000000
5  4 -19.709295  4.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000 -0.000000
9  4 -19.673283  4.000000  0.000000 -0.000000  0.000000  0.000000  0.000000  0.000000 -0.000000
13  4 -19.598404  4.000000  0.000000  0.000000 -0.000000  0.000000 -0.000000  0.000000  0.000000
17  4 -19.578964  4.000000  0.000000 -0.000000 -0.000000  0.000000  0.000000 -0.000000  0.000000
21  4 -18.495065  4.000000  0.000000 -0.000000 -0.000000  0.000000 -0.000000  0.000000 -0.000000
25  4 -18.458705  4.000000  0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000
29  4 -18.395752  4.000000  0.000000  0.000000  0.000000 -0.000000  0.000000  0.000000  0.000000
33  4 -18.369289  4.000000  0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000  0.000000
37  4 -18.339186  4.000000  0.000000  0.000000  0.000000 -0.000000 -0.000000 -0.000000  0.000000
41  4 -18.317580  4.000000  0.000000  0.000000  0.000000 -0.000000  0.000000 -0.000000 -0.000000
45  4 -12.645077  4.000000  0.000000 -0.000000  0.000000 -0.000000 -0.000000 -0.000000  0.000000
49  4 -12.278411  4.000000  0.000000 -0.000000 -0.000000  0.000000 -0.000000 -0.000000  0.000000
53  4 -12.259052  4.000000  0.000000  0.000000  0.000000 -0.000000 -0.000000  0.000000 -0.000000
57  4   0.716517  4.000000  0.000000 -0.000000  0.000000 -0.000000 -0.000000  0.000000 -0.000000
61  4   1.080871  4.000000  0.000000 -0.000000 -0.000000  0.000000 -0.000000  0.000000  0.000000
65  4   5.086642  4.000000  0.000000 -0.000000 -0.000000 -0.000000  0.000000  0.000000  0.000000
69  4   6.308507  4.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
73  4   7.575189  4.000000  0.000000  0.000000  0.000000 -0.000000  0.000000  0.000000  0.000000
77  4   8.524204  4.000000  0.000000 -0.000000  0.000000 -0.000000 -0.000000  0.000000  0.000000
81  4  11.006530  4.000000  0.000000 -0.000000 -0.000000  0.000000 -0.000000  0.000000  0.000000
85  4  12.043615  4.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000 -0.000000
89  4  13.235456  4.000000  0.000000 -0.000000  0.000000  0.000000  0.000000  0.000000 -0.000000
```

2. Output: Case I

```
This material is a NSC, whose node(s) is (are) located on the following line(s):
{{1/2, 0, 0}, {1/2, 1/2, 0}}[L(B)]
{{1/2, 0, 0}, {1/2, 0, 1/2}}[L(A)]
{{1/2, 0, 1/2}, {0, 0, 0}}[L(A)]
```

```
{{1/2, 0, -1/2}, {0, 0, 0}}[L(A)]
{{0, 0, 0}, {0, 0, -1/2}}[L(A)]
{{0, 0, 0}, {0, 1/2, 0}}[L(B)]

The vector nSC is
nSC = {{0, 1, 0, 1}, {0, 0, 0, 0}, {1, 0, 1, 0}, {0}, {0}, {0}, {1, 1, 1, 1}, {0}}.
```

3. Output: Case II

```
This material is Case II, whose entry of symmetry indicators is {1, 1, 2, 0} in {2, 4, 4, 8}.
The vector nSC is
nSC = {{-3, 3, -3, 3}, {0, 0, 0, 0}, {-1, 1, -1, 1}, {0}, {0}, {0}, {2, -2, 2, -2}, {0}},
and the basis vectors are
{{1, -1, 1, -1}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0}, {0}, {0}, {0, 0, 0, 0}, {0}}
{{0, 0, 0, 0}, {0, 0, 0, 0}, {1, -1, 1, -1}, {0}, {0}, {0}, {0, 0, 0, 0}, {0}}
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0}, {0}, {0}, {1, -1, 1, -1}, {0}}
{{0, 0, 0, 0}, {1, -1, 1, -1}, {0, 0, 0, 0}, {0}, {0}, {0}, {0, 0, 0, 0}, {0}}
```