| lat.Const=[1]   |            | // latt     | tice constant | , 1x1 real                            |            |           |           |           |
|---|------------|-------------|---------------|---------------------------------------|------------|-----------|-----------|-----------|
| lat.Primitive=  |            |             | mitive vecto  | rs, (3x3/2x2                          | 2/1x1)     |           |           |           |
| [1/2,1/2,0;1/2  |            | _           |               |                                       |            |           |           |           |
| lat.Sublatt=[0,0,0;1/2,1/2,1/2] // sublattice position, (nx3/nx2/nx1/)  |            |             |               |                                       |            |           |           |           |
| lat.Order=[1]   | I          | // Ne       | arest Neighb  | or Order, 1                           | x1 integer |           |           |           |
|   | ==== PiLih | Variable == |               | ===                                   |            |           |           |           |
| ======================================  |            |             |               |                                       |            |           |           |           |
| ORDER= (  |            |             |               |                                       |            |           |           |           |
| 1   | 2 3        |             |               |                                       |            |           |           |           |
| 6.283185  | 6.283185   | -6.283185   |               |                                       |            |           |           |           |
| 6.283185 -6.283185 6.283185   |            |             |               |                                       |            |           |           |           |
| -6.283185   | 6.283185   | 6.283185    |               |                                       |            |           |           |           |
|   | D.Y. 11    |             |               |                                       |            |           |           |           |
| ======================================  |            |             |               |                                       |            |           |           |           |
| lat.surr_site(1), @full, surrouding sites [order, dist, sublatt, n1, n2, n3, x, y, z] ORDER= 0, SIZE=[ 7, 9], TYPE=REAL |            |             |               |                                       |            |           |           |           |
| 1   | 2 3        | 4           | 5 6           | 7                                     | 8 9        | )         |           |           |
| 0.000000  | 0.000000   | 1.000000    | 0.000000      | 0.000000                              | 0.000000   | 0.000000  | 0.000000  | 0.000000  |
| 1.000000  | 0.500000   | 2.000000    | -1.000000     | -1.000000                             | 0.000000   | -0.500000 | 0.000000  | 0.000000  |
| 1.000000  | 0.500000   |             | -1.000000     | 0.000000                              | -1.000000  | 0.000000  | -0.500000 | 0.000000  |
| 1.000000  | 0.500000   | 2.000000    | -1.000000     | 0.000000                              | 0.000000   | 0.000000  | 0.000000  | 0.500000  |
| 1.000000  | 0.500000   | 2.000000    | 0.000000      | -1.000000                             | -1.000000  | 0.000000  | 0.000000  | -0.500000 |
| 1.000000  | 0.500000   | 2.000000    | 0.000000      | -1.000000                             | 0.000000   | 0.000000  | 0.500000  | 0.000000  |
| 1.000000  | 0.500000   | 2.000000    | 0.000000      | 0.000000                              | -1.000000  | 0.500000  | 0.000000  | 0.000000  |
|   | Dil ih     | Variable == |               |                                       |            |           |           |           |
| ======================================  |            |             |               |                                       |            |           |           |           |
|   | ), SIZE=[  |             | PE=REAL       | , , , , , , , , , , , , , , , , , , , | ·,, ,      | J, -1     |           |           |
| 1   | 2 3        | 4           | 5 6           | 7                                     | 8 9        | )         |           |           |
| 0.000000  | 0.000000   | 2.000000    | 0.000000      | 0.000000                              | 0.000000   | 0.500000  | 0.500000  | 0.500000  |
| 1.000000  | 0.500000   | 1.000000    | 0.000000      | 0.000000                              | 1.000000   | 0.000000  | 0.500000  | 0.500000  |
| 1.000000  | 0.500000   | 1.000000    | 0.000000      | 1.000000                              | 0.000000   | 0.500000  | 0.000000  | 0.500000  |
| 1.000000  | 0.500000   | 1.000000    | 0.000000      | 1.000000                              | 1.000000   | 0.500000  | 0.500000  | 1.000000  |
| 1.000000  | 0.500000   | 1.000000    | 1.000000      | 0.000000                              | 0.000000   | 0.500000  | 0.500000  | 0.000000  |
| 1.000000  | 0.500000   | 1.000000    | 1.000000      | 0.000000                              | 1.000000   | 0.500000  | 1.000000  | 0.500000  |
| 1.000000  | 0.500000   | 1.000000    | 1.000000      | 1.000000                              | 0.000000   | 1.000000  | 0.500000  | 0.500000  |
|   |            |             |               |                                       |            |           |           |           |