

# [Pw\_forum] Monkhorst Pack k points

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On Tuesday 30 May 2006 11:39, Cyrille Barreteau wrote:

```
> I am generating the k points by the following input:
>
> K_POINTS automatic
> n1 n2 1 0 0 0
>
> According to the manual the code is using MP k points but I am a bit
> surprised to find that the Gamma= 0,0,0 point is always present in
> the k points list whatever the parity of the integers n1 and n2.
```

```
K_POINTS automatic
n1 n2 n3 j1 j2 j3
yields a grid of k-points:
k(i1,i2,i3) = (i1+j1/2) * g1/n1 + (i2+j2/2) * g2/n2 + (i3+j3/2) * g3/n3
where g1, g2, g3 are the vectors that generate the reciprocal lattice;
the indices i1, i2, i3, run from 0 to n1-1, n2-1, n3-1 respectively;
j1, j2, j3 can be either 0 (no offset, k=0 in the grid) or 1 (with offset,
k=0 not in the grid). What is usually referred to as "Monkhorst-Pack"
grid has offset and does not contain k=0 . Of course, only inequivalent
k-points are actually used
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Paolo

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