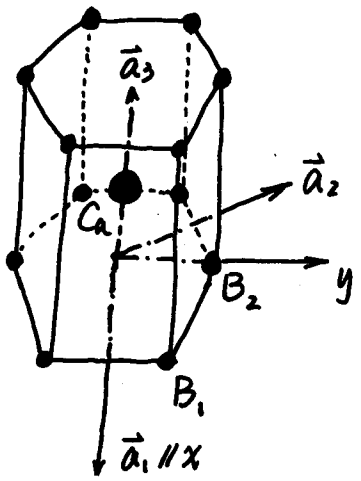
Example: CaB_2

原胞基矢: ($a=6.0940\ a_B$, $C=7.8072\ a_B$)

$\vec{a}_1 = a\vec{i}$, $\vec{a}_2 = a(-\sin 30^\circ \vec{i} + \cos 30^\circ \vec{j})$, $\vec{a}_3 = C\vec{k}$



$\vec{r}_{B_1} = \frac{2}{3}\vec{a}_1 + \frac{1}{3}\vec{a}_2 + 0\vec{a}_3$

$\vec{r}_{B_2} = \frac{1}{3}\vec{a}_1 + \frac{2}{3}\vec{a}_2 + 0\vec{a}_3$

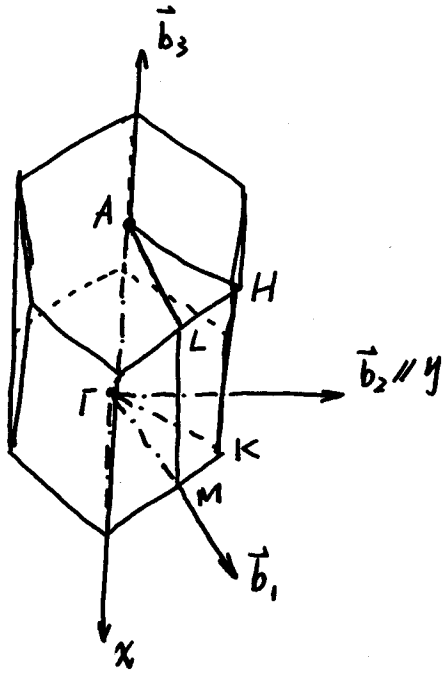
$\vec{r}_{Ca} = 0\vec{a}_1 + 0\vec{a}_2 + \frac{1}{2}\vec{a}_3$

$\vec{b}_1 = \frac{2\pi}{\Omega_c}(\vec{a}_2 \times \vec{a}_3)$

$\vec{b}_2 = \frac{2\pi}{\Omega_c}(\vec{a}_3 \times \vec{a}_1)$

$\vec{b}_3 = \frac{2\pi}{\Omega_c}(\vec{a}_1 \times \vec{a}_2)$

$\Omega_c = |\vec{a}_3 \cdot (\vec{a}_2 \times \vec{a}_1)|$
$= a^2 C \sin 120^\circ$



$\Gamma = 0\vec{b}_1 + 0\vec{b}_2 + 0\vec{b}_3$

$M = \frac{1}{2}\vec{b}_1 + 0\vec{b}_2 + 0\vec{b}_3$

$K = \frac{1}{3}\vec{b}_1 + \frac{1}{3}\vec{b}_2 + 0\vec{b}_3$

$A = 0\vec{b}_1 + 0\vec{b}_2 + \frac{1}{2}\vec{b}_3$

$L = \frac{1}{2}\vec{b}_1 + 0\vec{b}_2 + \frac{1}{2}\vec{b}_3$

$H = \frac{1}{3}\vec{b}_1 + \frac{1}{3}\vec{b}_2 + \frac{1}{2}\vec{b}_3$

需要的文件和程序: (i) Atom_POT. DAT (赝势. 由 Atom. cpi 改名或 copy);
(ii) input (输入参数文件); (iii) paratec_code (计算程序);
(iv) VMLX 或 CD (势能或电子密度的初值文件. optional).

执行语句: /..../paratec_code < input &

考题：计算以下材料的晶格常数和电子能带结构

C 金刚石结构 ($a=3.567\text{Å}$)

C 石墨(六角形结构) ($a=2.46\text{Å}$, $c=6.69\text{Å}$)

Ca (fcc) ($a=5.58\text{Å}$)

Ba (bcc) ($a=5.02\text{Å}$)

BN 金刚石结构 ($a=3.616\text{Å}$)

Si 金刚石结构 ($a=5.430\text{Å}$)

Ga 金刚石结构 ($a=5.658\text{Å}$)

GaAs.

MgB_2.

任选一种材料.