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HW7:

1. (1) 书2.6: Ne在体心立方与面心立方中结合能比较

$$U = +2\varepsilon N\left(A_{12}\left(\frac{\sigma}{r}\right)^{12} - A_6\left(\frac{\sigma}{r}\right)^6\right)$$

$$\therefore \frac{U_c}{U_f} = \frac{dU}{dr} = 2\varepsilon N\left(-12A_{12}\frac{\sigma^{12}}{r^{13}} + 6A_6\frac{\sigma^6}{r^7}\right) = 0$$

$$\therefore 12A_{12}\frac{\sigma^{12}}{r^{13}} = 6A_6\frac{\sigma^6}{r^7}\, r_0^6$$

$$\therefore r_0 = \left(\frac{2A_{12}\sigma^6}{A_6}\right)^{\frac{1}{6}}$$

$$\therefore U|_{r=r_0} = 2N\varepsilon\left(A_{12}\left(\frac{A_6}{2A_{12}}\right)^{13/6} - A_6\left(\frac{A_6}{2A_{12}}\right)^{6/6}\right)$$

$$= 2N\varepsilon\left(\frac{1}{4}\frac{A_6^2}{A_{12}} - \frac{A_6^2}{2A_{12}}\right) = -\frac{N\varepsilon}{2}\left(A_6^2/A_{12}\right).$$

$$\therefore \frac{U_c}{U_f} = \frac{(A_{6,c}^2/A_{12,c})}{(A_{6,f}^2/A_{12,f})} = \frac{(12.25^2/9.11)}{(14.45^2/12.13)} = 0.957$$

(2) 书2.7, $\varepsilon = 50\times10^{-23}\,J$, $\sigma = 2.96\,Å$

结合化为 $U = -\frac{1}{2}N\varepsilon\left(A_6^2/A_{12}^2\right)$

$$= -\frac{1}{2}\times 6.022\times10^{23}\,mol^{-1}\times 50\times10^{-23}\,J\times\left(\frac{14.45^2}{12.13}\right)$$

$$= -2.58\ kJ\,mol^{-1}$$

与计算值差异在于未考虑零点能.

2. (a) 2-P, 正交点群, 4

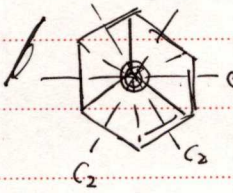
(b) β-P, 六方点群, 2

(c) γ-P, 正交点群, 4

(d) δ-P 正交点群, 8

3. As: 空间点群

$E,\ C_3^1\ C_3^2,\ 3C_2^1\ 3\sigma,\ i,\ iC_3^1,\ iC_3^2$



~~D_{3h}~~ D_{3d}

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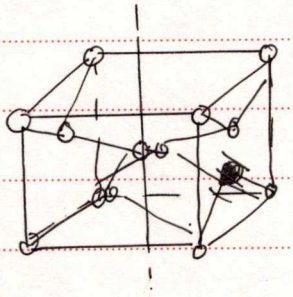
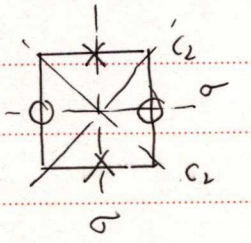
4. 硝酸：点式群为 D_{3d} 群

5. 白磷：



iC_4^1、C_2^1、iC_4^3、E、2σ、$2C_2$



D_{2d} 群