

系別：化學學系(化學組)

科目：物理化學

准帶項目請打「V」	
V	計算機

本試題共 1 頁，5 大題

- Show that $\langle p \rangle = 0$ for all state of a particle in a 1-D box with length a .
 - What are the degeneracies of the first three energy levels of a particle in a 3-D box with $a = b = 1.5c$.
- Determine the term symbol of the ground state electron configuration of B_2 .
 - Show that $\psi_{sp} = \frac{1}{\sqrt{2}}(2s \pm 2p_z)$ is normalized.
- Integrate the rate equation $-\frac{dC}{dt} = kC^{1/2}$.
 - What are the units of k .
 - Derive the expression for $t_{1/2}$ in terms of k and C_0 .
- Determine the normal modes of vibration for C_{20} molecule and indicate the IR active and Raman active. (Hint: the C_{20} has I_h symmetry with the carbon is located in the center of equivalent triangle of icosahedron)
- Calculate the entropy change if 2.0 mol of monatomic gas ($C_{p,m} = \frac{5}{2}R$) is heated from 300K to 400K and the pressure increases from 2.5 atm to 3.5 atm.
 - Describe a Carnot engine being one mole of ideal gas, write the expression for the work done in each step.

每題二十分

11. The Icosahedral Groups*

I_h	E	$12C_5$	$12C_5^2$	$20C_3$	$15C_2$	i	$12S_{10}$	$12S_{10}^3$	$20S_6$	15σ	
A_g	1	1	1	1	1	1	1	1	1	1	(R_x, R_y, R_z) $x^2 + y^2 + z^2$
T_{1g}	3	$\frac{1}{2}(1 + \sqrt{5})$	$\frac{1}{2}(1 - \sqrt{5})$	0	-1	3	$\frac{1}{2}(1 - \sqrt{5})$	$\frac{1}{2}(1 + \sqrt{5})$	0	-1	
T_{2g}	3	$\frac{1}{2}(1 - \sqrt{5})$	$\frac{1}{2}(1 + \sqrt{5})$	0	-1	3	$\frac{1}{2}(1 + \sqrt{5})$	$\frac{1}{2}(1 - \sqrt{5})$	0	-1	
G_g	4	-1	-1	1	0	4	-1	-1	1	0	
H_g	5	0	0	-1	1	5	0	0	-1	1	
A_u	1	1	1	1	1	-1	-1	-1	-1	-1	(x, y, z) $(2z^2 - x^2 - y^2,$ $x^2 - y^2,$ $xy, yz, zx)$
T_{1u}	3	$\frac{1}{2}(1 + \sqrt{5})$	$\frac{1}{2}(1 - \sqrt{5})$	0	-1	-3	$-\frac{1}{2}(1 - \sqrt{5})$	$-\frac{1}{2}(1 + \sqrt{5})$	0	1	
T_{2u}	3	$\frac{1}{2}(1 - \sqrt{5})$	$\frac{1}{2}(1 + \sqrt{5})$	0	-1	-3	$-\frac{1}{2}(1 + \sqrt{5})$	$-\frac{1}{2}(1 - \sqrt{5})$	0	1	
G_u	4	-1	-1	1	0	-4	1	1	-1	0	
H_u	5	0	0	-1	1	-5	0	0	1	-1	

*For the pure rotation group I , the outlined section in the upper left is the character table; the g subscripts should, of course, be dropped and (x, y, z) assigned to the T_1 representation.