C455A –Quantum Chemistry and Spectroscopy
Final Exam
June 7, 2005 8:30-10:20 am BAG 154

A SINGLE ***ONE SIDED*** *8.5x11" page of notes is allowed*

-YOU MUST SIT IN YOUR ASSIGNED SEAT TO RECEIVE CREDIT FOR THE EXAM
-ALL ANSWERS MUST BE IN THE ANSWER BOX WHEN PROVIDED
-CROSSED OUT/PARTIALLY ERASED WORK WILL BE IGNORED
-NO PARTIAL CREDIT ON NUMERICAL PROBLEMS WITHOUT A FORMULA
-NO PARTIAL CREDIT ON "PHYSICALLY IMPLAUSIBLE" ANSWERS UNLESS THE ERROR IS RECOGNIZED

Your name:____

Student ID#:____

I have neither received nor provided external assistance of any kind on this exam.
I understand that doing so is serious academic misconduct.

Signature:____

In the following, u and v are functions of x, and a and n and m are real numbers

$$\int u\,dv = uv - \int v\,du$$

$$\int x^n dx = \frac{x^{n+1}}{n+1} \text{ except } n=-1$$

$$\int \frac{dx}{x} = \ln x$$

$$\int e^{ax}dx = \frac{1}{a} e^{ax}$$

$$\int (\sin ax)\,dx = -\frac{1}{a}\cos ax$$

$$\int (\cos ax)\,dx = \frac{1}{a}\sin ax$$

$$\int (\sin^2 ax)\,dx = \frac{1}{2}x - \frac{1}{4a}\sin 2ax$$

$$\int (x \sin^2 ax)\,dx = \frac{x^2}{4} - \frac{\cos 2ax}{8a^2} - \frac{x \sin 2ax}{4a}$$

$$\int (\cos^2 ax)\,dx = \frac{1}{2}x + \frac{1}{4a}\sin 2ax$$

$$\int (x^2 \sin^2 ax)\,dx = \frac{1}{6}x^3 - \left(\frac{1}{4a}x^2 - \frac{1}{8a^3}\right)\sin 2ax - \frac{1}{4a^2}x\cos 2ax$$

$$\int (x^2 \cos^2 ax)\,dx = \frac{1}{6}x^3 + \left(\frac{1}{4a}x^2 - \frac{1}{8a^3}\right)\sin 2ax + \frac{1}{4a^2}x\cos 2ax$$

$$\int x^m e^{ax}dx = \frac{x^m e^{ax}}{a} - \frac{m}{a}\int x^{m-1}e^{ax}dx$$

$$\int \frac{e^{ax}}{x^m}dx = -\frac{1}{m-1}\frac{e^{ax}}{x^{m-1}} + \frac{a}{m-1}\int \frac{e^{ax}}{x^{m-1}}dx$$

$$\int_0^a \sin\left(\frac{n\pi x}{a}\right)\cdot\sin\left(\frac{m\pi x}{a}\right)dx = \int_0^a \cos\left(\frac{n\pi x}{a}\right)\cdot\cos\left(\frac{m\pi x}{a}\right)dx = \frac{a}{2}\delta_{mn}$$

$$\int_0^a \left[\sin\left(\frac{n\pi x}{a}\right)\right]\cdot\left[\cos\left(\frac{n\pi x}{a}\right)\right]dx = 0$$

$$\int_0^\pi \sin^2 mx\,dx = \int_0^\pi \cos^2 mx\,dx = \frac{\pi}{2}$$

$$\int_0^\infty \frac{\sin x}{\sqrt{x}}dx = \int_0^\infty \frac{\cos x}{\sqrt{x}}dx = \sqrt{\frac{\pi}{2}}$$

$$\int_0^\infty x^n e^{-ax}dx = \frac{n!}{a^{n+1}} \quad (a>0,\ n \text{ positive integer})$$

$$\int_0^\infty x^{2n}e^{-ax^2}dx = \frac{1\cdot 3\cdot 5\cdots(2n-1)}{2^{n+1}a^n}\sqrt{\frac{\pi}{a}} \quad (a>0,\ n \text{ positive integer})$$

$$\int_0^\infty x^{2n+1}e^{-ax^2}dx = \frac{n!}{2\,a^{n+1}} \quad (a>0,\ n \text{ positive integer})$$

$$\int_0^\infty e^{-ax^2}dx = \left(\frac{\pi}{4a}\right)^{1/2}$$

$$\frac{d}{dx}(uv) = u\frac{dv}{dx} + v\frac{du}{dx}$$

$$\frac{d}{dx}\frac{u}{v} = \frac{1}{v}\frac{du}{dx} - \frac{u}{v^2}\frac{dv}{dx}$$

$$\frac{d}{dx}(u^n) = nu^{n-1}\frac{du}{dx}$$

$$\frac{d}{dx}\left(\frac{1}{u^n}\right) = -\frac{n}{u^{n-1}}\frac{du}{dx}$$

$$\frac{d}{dx}[f(u)] = \frac{d}{du}[f(u)]\cdot\frac{du}{dx}$$

$$\frac{d}{dx}(u^n v^m) = u^{n-1}v^{n-1}\left(nv\frac{du}{dx} + mu\frac{dv}{dx}\right)$$

$$\frac{d}{dx}(e^u) = e^u\frac{du}{dx}$$

$$\frac{d\sin x}{dx} = \cos x$$

$$\frac{d\cos x}{dx} = -\sin x$$

$$\frac{d\sin u}{dx} = \frac{du}{dx}\cos u$$

$$\frac{d\cos u}{dx} = -\frac{du}{dx}\sin u$$

$$\sin\alpha\sin\beta = \frac{1}{2}\cos(\alpha-\beta) - \frac{1}{2}\cos(\alpha+\beta)$$

$$\cos\alpha\cos\beta = \frac{1}{2}\cos(\alpha-\beta) + \frac{1}{2}\cos(\alpha+\beta)$$

$$\sin(\alpha\pm\beta) = \sin\alpha\cos\beta \pm \cos\alpha\sin\beta$$

$$\cos(\alpha\pm\beta) = \cos\alpha\cos\beta \mp \sin\alpha\sin\beta$$

Some H-Atom wave functions:

$$\psi_{100}(r,\theta,\phi) = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$$

$$\psi_{200}(r,\theta,\phi) = \frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_0}\right)^{3/2}\left(2-\frac{r}{a_0}\right)^{3/2} e^{-r/2a_0}$$

$$\psi_{310}(r,\theta,\phi) = \frac{1}{81}\sqrt{\frac{2}{\pi}}\left(\frac{1}{a_0}\right)^{3/2}\left(6\frac{r}{a_0}-\frac{r^2}{a_0{}^2}\right)^{3/2} e^{-r/3a_0}\cos(\theta)$$

Some H-Atom radial wave functions:

$$R_{10}(r) = 2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$$

$$R_{20}(r) = \frac{1}{\sqrt{8}}\left(2-\frac{r}{a_0}\right)^{3/2} e^{-r/2a_0}$$

Total Points: 200

Question 1:_________/20

Question 2:_________/20

Question 3:_________/35

Question 4:_________/30

Question 5:_________/20

Question 6:_________/30

Question 7:_________/30

Question 8:_________/35

Total: _____________/200

The First Few Spherical Harmonics

$$Y_0^0 = \frac{1}{(4\pi)^{1/2}}$$

$$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$$

$$Y_1^1 = \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta e^{i\phi}$$

$$Y_1^{-1} = \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta e^{-i\phi}$$

$$Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2\theta - 1)$$

$$Y_2^1 = \left(\frac{15}{8\pi}\right)^{1/2} \sin\theta\cos\theta e^{i\phi}$$

$$Y_2^{-1} = \left(\frac{15}{8\pi}\right)^{1/2} \sin\theta\cos\theta e^{-i\phi}$$

$$Y_2^2 = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta e^{2i\phi}$$

$$Y_2^{-2} = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta e^{-2i\phi}$$

Potentially Useful Information:

Workfunctions of Metals:

Li	2.3 eV
Ca	2.87 eV
Al	4.28 eV
Au	5.1 eV

Values of Some Physical Constants

Constant	Symbol	Value
Atomic mass constant	*amu*	$1.660\ 5402 \times 10^{-27}$ kg
Avogadro constant	N_A	$6.022\ 1367 \times 10^{23}$ mol^{-1}
Bohr magneton	$\mu B = eh/2m_e$	$9.274\ 0154 \times 10^{-24}$ J · T^{-1}
Bohr radius	$a_0 = 4\pi\varepsilon_0^2/r_e e^2$	$5.291\ 772\ 49 \times 10^{-11}$ m
Boltzmann constant	k_B	$1.380\ 658 \times 10^{-23}$ J · K^{-1}
		0.695 038 cm^{-1}
Electron rest mass	m_e	$9.109\ 3897 \times 10^{-31}$ kg
Gravitational constant	G	$6.672\ 59 \times 10^{-11}$ · m^3 · kg^{-1} · s^{-2}
Molar gas constant	R	8.3145101 J · K^{-1} · mol^{-1}
		0.083 1451 dm^3 · bar K^{-1} · mol^{-1}
		0.082 0578 dm^3 · atm K^{-1} · mol^{-1}
Molar volume, ideal gas		
(one bar, 0^0C)		22.711 08L · mol^{-1}
(one atm, 0^0C)		22.414 09 L · mol^{-1}
Nuclear magneton	$\mu_N = e\hbar/2m_p$	$5.050\ 7866 \times 10^{-27}$ J · T^{-1}
Permittivity of vacuum	ε_0	$8.854\ 187\ 816 \times 10^{-12}$ C^2 · J^{-1} · m^{-1}
	$4\pi\varepsilon_0$	$1.112\ 650\ 056 \times 10^{-10}$ C^2 · J^{-1} · m^{-1}
Planck constant	h	$6.626\ 0755 \times 10^{-34}$ J · s
	$\hbar$	$1.054\ 572\ 66 \times 10^{-34}$ J · s
Proton charge	e	$1.602\ 177\ 33 \times 10^{-19}$ C
Proton magnetogyric ratio	γ_p	$2.675\ 221\ 28 \times 10^{8}$ s^{-1} · T^{-1}
Proton rest mass	m_p	$1.672\ 6231 \times 10^{-27}$kg
Rydberg constant (Bohr)	$R_\infty = m_e e^4/8\varepsilon_0^2 h^2$	$2.179\ 8736 \times 10^{-23}$ J
		109 737.31534 cm^{-1}
Rydberg constant for H	R_H	109677.581 cm^{-1}
Speed of light in vacuum	c	299 792 458 m · s^{-1} (defined)
Stefan-Boltzmann constant	$\sigma = 2\pi^5 k_B^4/15h^3c^2$	$5.670\ 51 \times 10^{-8}$ J · m^{-2} · K^{-4} · s^{-1}