**Possible Oral Final Topics: Physical Chemistry**

1)Origins of need for quantum theory

Be able to talk about PE effect; black body uv catastrophe; H atom issues; Stern-Gernlach dilemma

2) Old theory

* what are the main pieces leading to Bohr’s model ?
* general form of Bohr’s En
* Failures of Bohr model

3)Schrodinger’s Quantum theory formulation: the quantum operator model

* Be able to describe eigen value formalism …requirements for `solving’
* basic requirement of `good’ wave functions
* provide notion of underlying source/meaning of Heisenburg uncertainty

4) particle-in-a box

* Describe the picture and set up Hamiltonian
* Conditions for box ?
* E form and Ψ form ( varies with n how ? basic function for Ψ)

5)vibration and rotation

* 2-body🡪 1 body pictures [bonus if you can show how either vibrational of rotational picture leads to reduced mass formula μ = m1\*m2/{m1+ m2} )
* Energies for both ?
* Describe vibrational rotational transition and HO vs. Morse potential well
* Selection rules
* How did you analyze HCl spectrum for constants ?

6) H atom…

* Why spherical coordinates ?
* Qualitatively describe overall process of converting Ψ(r,θ,φ) 🡪 R(r)Θ(θ)Φ(φ) …1 three variable problem into three 1 variable problems
* Quantum number relationships of solution n=> L= ?, L=> mL= ?
* Show how above generates Periodic table

7) Approximation (Variational) method

* Why can’t we solve even He exactly ?
* Variational theorem states…what ?
* Describe qualitatively how we use variational model to estimate Ψ
* Be able to write out a qualitative version of secular equation determinant …and explain why it =0
* Modern QM (Spartan QChem) …what are wave functions ? what is HF approximation, Born-Oppenheimer approximation; how do we escape the correlation issue ?

8. First and second law

* Statements of…
* Express work and heat for simple expansions/contractions of ideal gas
* State functions, adiabatic,
* First law uses (what is Hess law calc; ε(bond energies); heat capacity spectra