CHEM442-001/002 Name ______________________________

College of Charleston

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Exam IV Score ___________ /100

1(20). Calculate $C^{o}_{P,\mathrm{m}}$ for gaseous CO_2 at 298 K. The vibrational frequencies are $\tilde{\nu}/(\mathrm{cm}^{-1})$ = 1384.86, 667.30 (double degenerate), and 2349.30.

For the Shomate equation $C^{o}_{P,\mathrm{m}}/(\mathrm{J\ K^{-1}\ mol^{-1}}) = A + BT + CT^2 + DT^3 + ET^{-2}$, the NIST data base gives $A = 24.99735$, $B = 55.18696 \times 10^{-3}$, $C = -33.69137 \times 10^{-6}$, $D = 7.948387 \times 10^{-9}$, and $E = -0.136638 \times 10^{6}$ for CO_2. Calculate $C^{o}_{P,\mathrm{m}}$ from these data.

Compare the results.

2(30). The electronic thermal energy of a metal is given by

$$E(\text{thermal,electronic}) = \frac{3}{5}NE_{\mathrm{F}}\left[1 + \left(\frac{5\pi^2}{12}\right)\left(\frac{k_{\mathrm{B}}T}{E_{\mathrm{F}}}\right)^2 + \ldots\right]$$

Derive the equation for C_V(electronic).

The value of the Fermi energy can be calculated using

$$E_{\mathrm{F}} = \left(\frac{h^2}{8m_{\mathrm{e}}}\right)\left(\frac{3N}{\pi V_{\mathrm{m}}}\right)^{2/3}$$

where $m_{\mathrm{e}} = 9.11 \times 10^{-31}$ kg. Given the density of Mg at 25 °C is 1.74 g cm^{-3}, calculate E_{F}.

Determine the value of the electronic heat capacity at 25 °C for Mg.

What fraction of the classical limit given by the Law of Dulong-Petit is the electronic heat capacity at 25 °C?

3(10). Starting with $d(\Delta H) = \Delta C_P\, dT$, derive the equation expressing $\Delta_r H_{T_2} - \Delta_r H_{T_1}$ for a chemical reaction assuming the heat capacity data are given by the Shomate equation (see Question 1).

4(10). Calculate the difference between $\Delta_r H$ and $\Delta_r U$ for the chemical reaction between glycine and nitrous acid at 25 °C.

$$NH_2CH_2COOH(aq) + HONO(aq) \rightarrow HOCH_2COOH(aq) + N_2(g) + H_2O(l)$$

5(30). Consider the reversible, isothermal expansion of one mole of Ne acting ideally from a pressure of 10.00 bar to 1.00 bar at 25 ºC. Calculate q, w, ΔU, and ΔH for this process.

Assuming the arm of the piston from the above expansion is connected to a second piston containing one mole of He initially at 25 ºC and that all of the work is used to compress the He reversibly and adiabatically, calculate q, w, ΔU, and ΔH for this process and calculate the final temperature.

Calculate the ratio of the final pressure to the initial pressure for the He after the compression process is completed.