Calculation for calorimetry

ASSIGN BUSTER

CALCULATIONS Determining the amount Limiting Reagent used. nlimiting reagent = Molarity x Volume or Mass / Molar Mass Example: Limiting reagent is 5mL of 1. 0 M HCl nlimiting reagent = Molarity x Volume nlimiting reagent = (1. 0 [mol/L]) x 0. 005 [L]) = 0. 005 mol Determining the qrxn and qcal. qrxn + qcal = 0 -qrxn = qcal qrxn = ? Hrxn x nlimiting reagent qcal = Ccal ? T qrxn = - Ccal ? T + mcsolid ? T (note: only if there is a precipitate formed in the reaction) Examples: 1) Calibration of the calorimeter given that: ? Hrxn = -55. 8 kJ/mol and nLR = 0. 005 mol qrxn = ? Hrxn x nlimiting reagent qrxn = -55. 8 [kJ/mol] x 0. 005 [mol] = -279 J qcal = -(219 J) = 279 J (2) Determining the qrxn of a given chemical reaction: NH3 (aq) + H+ (aq) ? NH4+ (aq) And given that: ? T = 3. 5 °C and Ccal= 111. 6 J/°C qrxn = - Ccal ? T + mcsolid ? T qrxn = -(111. 6 [kJ/°C] x 3. 5 [°C]) = -390. 6 J qcal = -(-390. 6 J) = 390. 6 Determining the Ccal. Ccal = qcal / ? T Example:

Given qrxn = -279 J and ? T = 2. 5 °C Ccal = -qrxn / ? T Ccal = -(-279 J) / (2. 5 °C) = 111. 6 J/°C Determining the experimental ? Hrxn. ? Hrxn = qrxn / nLR Example: Given: NH3 (aq) + H+ (aq) ? NH4+ (aq) With qrxn = -390. 6 J and nLR = 0. 005 mol ? Hrxn = qrxn / nLR ? Hrxn = -390. 6 J / 0. 005 mol = -78. 1 kJ/mol Determining the theoretical ? Hrxn. ? Hrxn = ? nproductH°f product - ? nreactantH°f reactant Example: Given that: NH3 (aq) + H+ (aq) ? NH4+ (aq) Substance? H°f (kJ/mol) NH3 (aq)-80. 9 H+ (aq)0. 00 NH4+ (aq)-132. 51 ? Hrxn = ? nproductH°f product - ? nreactantH°f reactant ? Hrxn = {-132. 51 kJ/mol}-{-80. 29 kJ/mol} = ? Hrxn = -52. 2 kJ/mol Determining the %error. %error = (|? Hexperimental – ? Htheoretical|) / (? Htheoretical) x 100% Example: Given: ? Hexperimental = -78. 1 kJ/mol and ? Htheoretical = -52. 2 kJ/mol %error = |(? Hexperimental – ? Htheoretical) / (? Htheoretical) | x

100% %error = |(-78. 1 kJ/mol) – (-52. 2 kJ/mol) / -52. 2 kJ/mol| x 100% = 49. 6 %