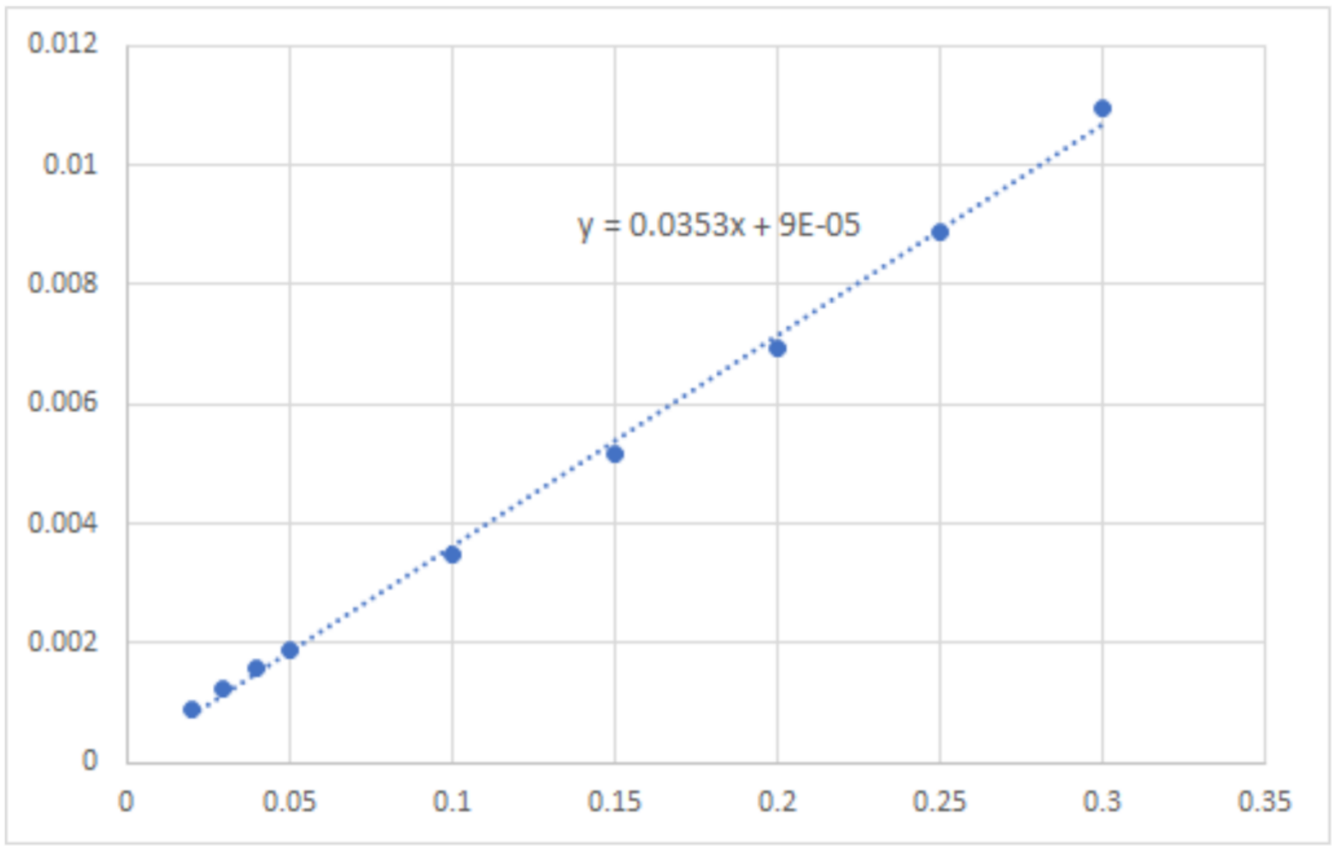
HW5 CH5 P1

(a) BET eqn: $\frac{P}{V_{ads}(P_0-P)} = \frac{1}{CV_m} + \left(\frac{C-1}{CV_m}\right)\frac{P}{P_0}$

$$\frac{P/P_0}{V_{ads}(1-P/P_0)} = \frac{1}{CV_m} + \left(\frac{C-1}{CV_m}\right)\frac{P}{P_0}$$

$\frac{P/P_0}{V_{ads}(1-P/P_0)}$ = y, $\frac{1}{CV_m}$ = b, $\left(\frac{C-1}{CV_m}\right)$ = m, $\frac{P}{P_0}$ = x

plot data in excel:



$\frac{C-1}{CV_m} = 0.0353$ $\quad \frac{1}{CV_m} = 9\times10^{-5}$

$\therefore \quad C-1 = 392.2$ $\quad \boxed{C = 393.2}$

$V_m = 28.26\ cm^3/g$

$\alpha = 0.162 nm^2$ for nitrogen

$$\therefore S = N\alpha = \frac{V_m N_A}{V_g}\alpha = \frac{28.26\times10^{-3}\times6.02\times10^{23}}{22.4} \times 0.162\times10^{-16}$$

$\boxed{= 123\ m^2/g}$ $\quad = 1.23\times10^4\ dm^2/g$

one point BET:

$$\frac{P}{V_{ads}(P_0 - P)} = \left(\frac{1}{V_m}\right)\frac{P}{P_0}, \quad \text{use } \frac{P}{P_0} = 0.25$$

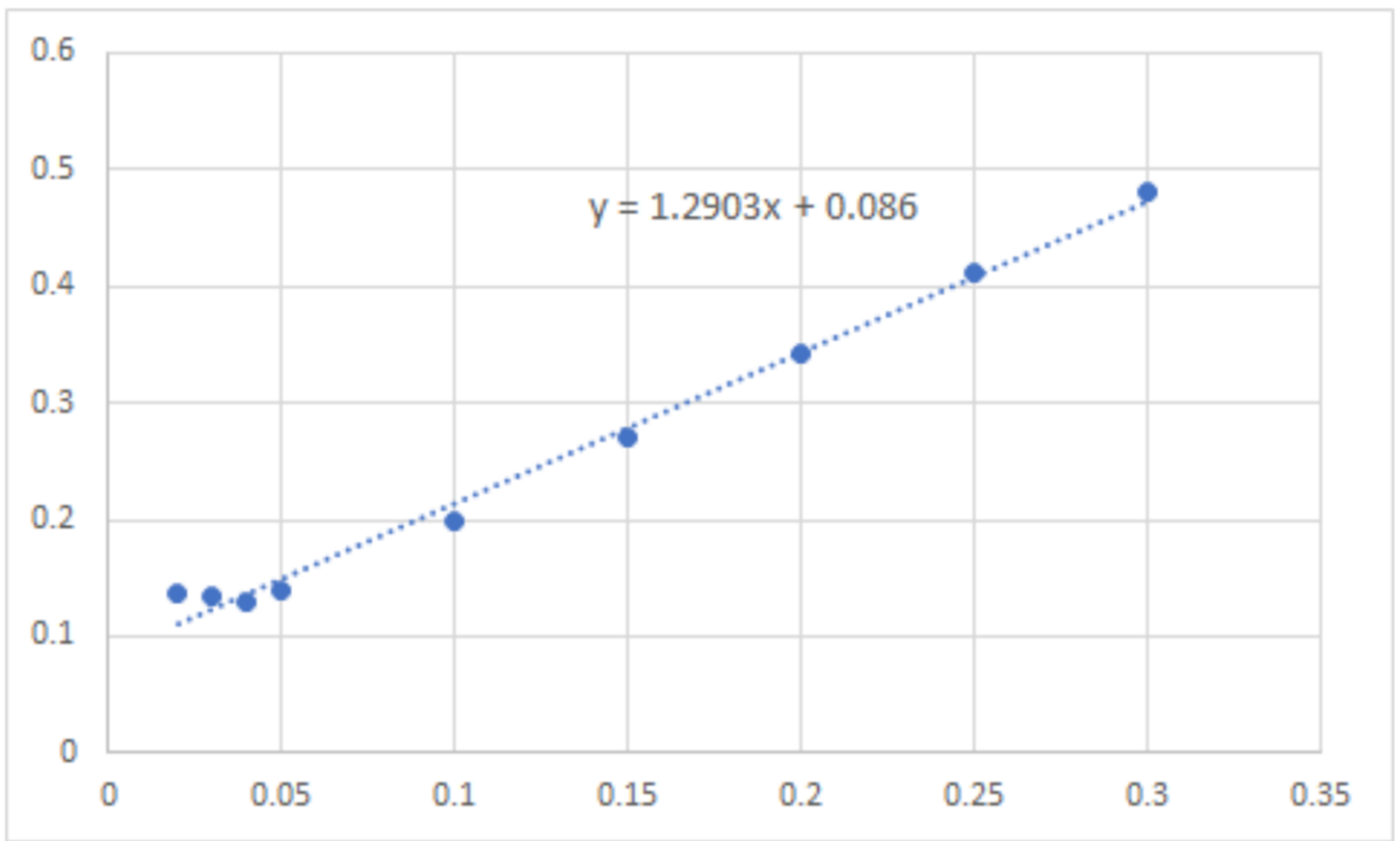
$$V_{ads} = 37.6$$

$$\frac{P/P_0}{V_{ads}(1 - P/P_0)} = \left(\frac{1}{V_m}\right)\frac{P}{P_0}$$

$$\frac{0.25}{37.6(1-0.25)} = \frac{1}{V_m}\,0.25 \qquad V_m = 28.2\ cm^3/g$$

$$\therefore \boxed{S_A = 122.7\ m^2/g}$$

(b) BET eqn. same method as (a)



$$\frac{1}{cV_m} = 0.086 \qquad \frac{c-1}{cV_m} = 1.2903$$

$$c = 16 \qquad V_m = 0.7267\ cm^3/g$$

$\therefore$ $S = 3.162\ m^2/g$

one point BET:

choose $P/P_0 = 0.25$ $V_{ads} = 0.81$

$$\frac{0.25}{0.81(1-0.25)} = \frac{1}{V_m}\ 0.25 \qquad V_m = 0.61\ cm^3/g$$

$\therefore$ $S = 2.654\ m^2/g$

One point BET and BET gave similar S for sample one but have large error for sample 2. This is caused by the small c of sample 2, we can't simplify BET to one point BET when c is small.

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Homework #5 Solution
TA: Weikai Cao

5.7 For the reaction of A to B over a solid catalyst, the reaction rate has the form:

$$r = \frac{k K_A P_A}{(1 + K_A P_A + K_B P_B)^2}$$

However, there is large excess of inert in the reactant stream that is know to readily absorb on the catalyst surface. How will this affect the reaction order with respect to A?

Solution: Without inert gas, total active sites

$$[*]_{total} = [*] + [A*] + [B*]$$

However, with inert gas, total active sites

$$[*]_{total} = [*] + [A*] + [B*] + [I*]$$

Thus, the only difference under the inert gas is the denominator

$$r = \frac{k K_A P_A}{(1 + K_A P_A + K_B P_B + K_I P_I)^2}$$

When P_I is much larger than P_A and P_B,

$$r \simeq \frac{k K_A P_A}{(1 + K_I P_I)^2} \simeq 0$$

Therefore, the reaction of A will become very little due to the much occupation of inert gas on active sites.

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Homework # 5 Solution

TA: Weikai Cao

5.4.1 Rework Example 5.4.1 and explain the meaning of steps. Try to get constants for both first and second rxn sequence.

Case I: Cl_2 & CO adsorp onto catalyst then reacted

$Cl_2 + * \xrightleftharpoons{k_1} Cl_2$ — Cl_2 adsorped onto catalyst

$CO + * \xrightleftharpoons{k_2} CO*$ — CO adsorped onto catalyst

$CO* + Cl_2* \xrightarrow{k_3} COCl_2* + *$ — Surface reaction of adsorped species

$COCl_2* \xrightarrow{k_4} COCl_2 + *$ — Products desorped

$$r = \frac{k_1 k_2 k_3 [*][CO][Cl_2]}{(1 + k_1[Cl_2] + k_2[CO] + k_4[COCl_2])^2}$$

Case II:

$Cl_2 + * \xrightleftharpoons{k_1} Cl_2*$ — Cl_2 adsorped onto catalyst

$CO + Cl_2* \xrightarrow{k_2} COCl_2*$ — Surface reaction

$COCl_2* \xrightarrow{k_3} COCl_2 + *$ — Products desorped.

$$r = \frac{k_2 k_1 [*]_{total} [CO][Cl_2]}{1 + k_1[Cl_2] + k_3[COCl_2]}$$

*

	Case I	Case II
k_1	9874	44470
k_2	0.00893	0.0161
k_3	44920	34440
k_4	9373	

* Credit to Sofia's Solution :)