Adsorption of $N_2$ on Silica gel

Chem 381
Definitions

Adsorption:
when a fluid accumulates on a solid surface

Desorption: reverse of adsorption

Absorption: NOT the same
when atoms or ions or molecules enter into some bulk phase.

Isotherm:
line of constant temperature in a plot
## Adsorption Processes

<table>
<thead>
<tr>
<th>Physisorption</th>
<th>Chemisorption</th>
</tr>
</thead>
<tbody>
<tr>
<td>No chemical bonds,</td>
<td>Chemical bond formed between</td>
</tr>
<tr>
<td>just van der Waals</td>
<td>adsorbent and adsorbed species</td>
</tr>
<tr>
<td>Multilayer</td>
<td>Monolayer</td>
</tr>
<tr>
<td>Reversible</td>
<td>Can be irreversible</td>
</tr>
</tbody>
</table>

### Comparison of PE’s

![Comparison of PE’s](image)

**E(d)**

**d (nn)**

**Physisorption**

**Chemisorption**
Who is interested in adsorption?

Heterogeneous catalysis:

⇒ Hydrogenation on Platinum surface

⇒ Catalytic converters: oxidize CO

Purification in organic synthesis:

⇒ Activated carbon

Viruses:

⇒ First step for infecting a cell
What are YOU doing?

Adsorption of $N_2$ on Silica Gel

➤ Why?

❖ To calculate the surface area of silica gel
❖ To calculate the heat of adsorption
Procedure

Fill He and N$_2$ in the storage bulbs.
Procedure

Determine the volume of secondary manifold and dead spaces with the He.
Procedure

Get rid of the He from secondary manifold

Introduce amount of $N_2$ and measure change in pressure.
Data Analysis

➢ **Volumes:**

Calculate $V_{\text{man}}$, $V_{\text{ds}}$, and $V_{\text{dc}}$ from ideal gas law

➢ **Amount of adsorption:**

Number of moles entering the bulb is given as

$$n_{\text{sb}} = n_i - n_{\text{ff}}$$

After a series of adsorption

$$N_{\text{ads}_i} = \sum N_{\text{sb}_j} - N_{\text{ds}_i}$$

$N_{\text{ads}_i} =$ # of moles adsorbed after i dose.
$N_{\text{sb}_j} =$ # of moles added in j-th step.
$N_{\text{ds}_i}$ is the dead space after i-th dose.
Some Theories

Langmuir Adsorption Isotherm

Basic Assumptions:

⇒ Monolayer adsorption.
⇒ No interaction among the adsorption sites.
⇒ Binding energy is same for all sites.

Derivation:

\[ R_a = k_a P(1-\theta)N \]
\[ R_d = k_d \theta N \]

\( \theta \) = fraction of sites covered
\( N \) = total number of sites
\( k_a \) = Rate constant of adsorption
\( k_d \) = Rate constant of desorption
At equilibrium:

\[ R_a = R_d \]
\[ k_a P(1-\theta) = k_d \theta \]

Solve for \( \theta \):

\[ \theta = \frac{KP}{1+KP} \]

where \( K = \frac{k_a}{k_d} \)

Define \( V_\infty \) as the volume adsorbed for \( \theta = 1 \):

\[ \theta = \frac{V}{V_\infty} \]

\[ \frac{V_\infty}{V} = \frac{1}{KP} + 1 \]
BET isotherm

BIG Assumptions:

⇒ All sites are equivalent.
⇒ Multilayer adsorption is allowed.
⇒ No interaction between molecules in a layer
⇒ Molecules adsorbed on surface sites are localized.

The isotherm:

\[
\frac{Z}{V(1-Z)} = \frac{1}{cV_m} + \frac{Z(c-1)}{cV_m}
\]

Where \( Z = KP/P^0 \); \( c = P^0/P' \)
Assignment

- Submit a Matlab Program to calculate the various parameters.

- Understand vacuum techniques

- Go through the derivation of BET isotherm
Report

1) All your data

2) Calculations of the volumes i.e., \( V_{\text{man}}, V_{\text{dstot}}, V_{\text{dsc}} \) and \( V_{\text{dsa}} \)

3) Langmuir plot as well as BET plot

4) Surface area of Silica gel (meters\(^2\)/gram)

5) The heat of adsorption.

6) Error analysis for the following:
   
   \( V_{\text{man}} \)
   
   \( N_{\text{adsi}} \)
   
   Slope and intercept of BET isotherm
   
   Surface area
Safety

1) Safety glasses **must** be worn

2) The silica gel compartment should be evacuated before removal of liquid $\text{N}_2$.

3) The valves should be used with care.