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APPENDIX

APPENDIX A

SAMPLE OF CALCULATION

1. Preparation of 8% Ni/Al_2O_3 Catalyst with Incipient Impregnation Method.

Reagent : Nickel Nitrate ($Ni(NO_3)_2.6H_2O$) Analar grade ;
Purity 99.5 % ; Molecular weight = 290.81,
manufactured by Merck Co., Ltd.
(Atomic weight of copper = 63.54)

Support : Alumina (Al_2O_3) ; type KNH-3 ; pore volume = 1.0 cc./gm.
from Sumitomo Aluminium Smelting Co., Ltd.

Calculation for prepared 8% Ni/Al_2O_3 catalyst

basis on : 8% Ni/Al_2O_3 catalyst

Al_2O_3	= 10	gm.
Ni	= (10x8)/(100-8)	gm.
	= 0.87	gm.
Pore Volume of Al_2O_3 (KNH-3)	= 1.0	cc./gm.
Pore volume of Al_2O_3 (KNH-3) 10 gm.		
	= 10 x 1.0	
	= 10	cc.

Nickel nitrate stock solution have 17.4% wt Ni/volume

Use $Ni(NO_3)_2.6H_2O$ solution	= 100x0.87/17.4	cc.
	= 5	cc.

use Nickel nitrate solution 5 cc. and made volume to 10 cc. for impregnating on Al_2O_3 support 10 gm.

2. Preparation of 0.3% Pt-8% Ni/Al_2O_3 Catalyst with Incipient Impregnation Method.

Reagent : Copper(II)Nitrate ($Ni(NO_3)_2.3H_2O$) Analar grade ; Purity 99.5 % ; Molecular weight = 241.6, manufactured by Merck Co.,Ltd.

(Atomic weight of copper = 63.54)

Chloroplatinic acid ($H_2PtCl_6.6H_2O$) ; Molecular weight = 517.92, manufactured by WAKO PURE CHEMICAL INDUSTRIES CO.,LTD.

(Atomic weight of Platinum = 195.1)

Support : Alumina (Al_2O_3) ; type KNH-3 ; pore volume = 1.0 cc./gm. from Sumitomo Aluminium Smelting Co.,Ltd.

Calculation for prepared 0.3% Pt-8% Ni/Al_2O_3 catalyst

basis on : y% Pt-8% Ni/Al_2O_3 catalyst, (%pt/Ni)

y = % of Pt/Ni

Ni	= 0.87	gm.
Pt	= y x 0.87	gm.
Pore Volume of Al_2O_3 (KNH-3)	= 1.0	cc./gm.
Pore Volume of Al_2O_3 (KNH-3) 10 gm.		
	= 10 x 1.0	
	= 10	cc.

Platinum stock solution have 1.48% wt Pt/volume

Volume of Platinum solution	= y x 0.87/1.48	gm.

y	volume of Platinum solution (cm^3)
0.5	0.294
1.0	0.588
1.5	0.882
2.0	1.176

Volume of platinum solution was made to 10 cc. for impregnating on Al_2O_3 support 10 gm.

3. Metal Site Measurement

From Co-adsorption technique

Example data of Co adsorption at 30 °C

peak No.	Volume of Co (cm^3)	High (cm.)
1	0.18	0
2	0.18	65.25
3	0.18	71.15
4	0.18	71.15

From the data Co 0.18 cm^3 give peak high 71.15

adsorption of Co	=	(71-65.25) + (71-0)	cm.
	=	76.75	cm.
Volume of adsorb Co	=	76.75x0.18/71	cm^3
	=	0.1946	cm^3

= 1.946 cm^3/g.cat.

amount of molecule of adsorb Co = $1.946 x 273 x 6.02 x 10^{23} / 303$

= $4.74 x 10^{19}$ mlc./g.cat.

assume :

1 site of catalyst adsorp 1 molecule of Co

amount of active site = $4.74 x 10^{18}$ site/g.cat.

4. Hydrogen Adsorption Measurement

The method of calculation is the same as the calculation of the metal site measurement.

5. Calculation of reactive adsorbed benzene

Peak's weight of 1 cm^3 of mixture (at 30 °C)

(hydrogen : benzene = 85:15) = 235 mg.

Peak's weight of cyclohexane

(from reactive adsorbed benzene) = 170.1 mg./g.cat.

molecule of reactive adsorbed benzene

$$= \frac{0.15 x 273 x 6.02 x 10^{23} x 170}{303 x 22400 x 235} = 2.6 x 10^{18} \text{ mlc/g.cat}$$

6. BET Surface Area Calculation

From BET equation :

$$\frac{X}{v(1-X)} = \frac{1}{v_m C} + \frac{C-1}{V_m C} \times X \qquad (4.1)$$

where : X = ratio of partial pressure P/P_o

P_o = saturated vapour pressure of N_2 (or adsorped gas)

P = equilibrium vapour pressure of N_2

v = amount of adsorption at the equilibrium, c.c. at the NTP/gm of sample

v_m = amount of adsorption to cover the surface, c.c. at the NTP/gm of sample

$$C = \exp(E_1 - E_2 / RT) \qquad (4.2)$$

where : E_1 = heat of adsorption of the first layer

E_2 = heat of condensation of adsorbed gas

assume C ---> ∞, then

$$\frac{X}{v(1-X)} = \frac{1}{v_m C} \times X \qquad (4.3)$$

let : $v_m = v_m'$

v_m' = mean the amount of adsorption to form the N_2 complete monolayer

v = amount of adsorption measuring by G.C.

$X = P/P_o$

$$\frac{P_b V}{273} = \frac{P_t V}{T} \qquad (4.4)$$

where : V = constant volume

P_b = pressure at 0 °C

P_t = pressure at t °C

T = 273.15 + t, K

P_b = $(273.15/T) \times P_t$ = 1 atm

partial pressure

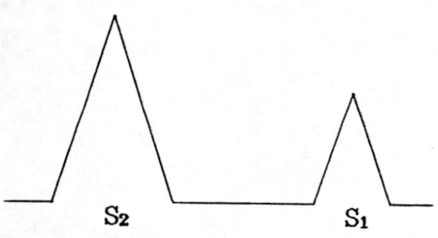
$$P = \frac{[\text{Flow of } (He+N_2) - \text{Flow of He}] \times P_b}{\text{Flow of } (He+N_2)} \qquad (4.5)$$

$$= 0.3 \text{ atm}$$

N_2 saturated vapour pressure, P_o = 1.1 atm = 836 mm.Hg

$$X = P/P_o = P/1.1$$

How to measuring v



1 ml/1 atm at room temperature

desorption of N_2 area

N_2 calibration area

$$v = \frac{S_2}{S_1} \times \frac{1}{w} \times \frac{273.15}{T} \quad \text{c.c./g of catalyst} \qquad (4.6)$$

where : w = weight of sample

$$v_m' = \frac{v[1-(\text{flow of He+N}_2 - \text{flow of He})/1.1]}{\text{flow of He+N}_2} \quad \text{c.c.NTP/g of cat.} \tag{4.7}$$

$$S_b = S \times v_m' \tag{4.8}$$

where : S = surface area from literature of N_2

= 4.373 m^2/c.c. of N_2

so that : S_b = 4.373 v_m' m^2/g of catalyst

APPENDIX B

Table A. Properties of Benzene

Property	Value
formula weight	78.11
mp, °C	5.533
bp, °C	80.100
density, at -3.77 °C, kg/m³	873.7
vapor pressure at 20.6075 °C, kPa (mm Hg)	13.33 (100)
refractive index, n_D^{25}	1.49792
viscosity (absolute) at 20 °C, mPa.s(=cP)	0.6468
surface tension at 25 °C, mN/m (=dyn/cm)	28.18
critical temperature, °C	289.45
critical pressure, kPa (atm)	4924.4 (48.6)
critical density, kg/m³	300.0
flash pount (closed cup), °C	-11.1
ignition temp in air, °C	538
flammability limits in air, vol %	1.5-8.0
heat of fusion, kJ/(kg.mol)[kcal/(kg.mol)]	9847 [2353]
heat of vaporization at 80.100 °C, kJ(kg.mol) [kcal/(kg.mol)]	33871 [8095]
heat of combustion at constant pressure and 25 °C (liquid C_6H_6 to loquid H_2O and gaseous CO_2), kJ/g	41.836 (9.999)
Solubility in water at 25 °C, g/100 g water	0.180
Solubitity of water in benzene at 25 °C, g/100g benzene	0.05

VITA

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