and computers

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WENT ON - GOTO
...ing statements
... uter coder
...emistry such as

...en write
...mpute pressure(p) from van der waals equation.

$$\Rightarrow \quad P = \frac{nRT}{V - nb} - \frac{n^2 a}{V^2}$$

where n = no. of moles, R = 0.0821 i.e. constant
T = temp or V = vol. of a gas.
a & b = Intermolecular attraction and repulsion respectively.

→ Take a, b, n, V, t as inputs
→ Assign R = 0.0821
→ Take P = as output
→ calculate P as

P = [(n*r*t)/(V-n*b)] - [(n*n*a/V*V)]

→ the flow chart is given as follows.

(START) → [Input a, b] → (A) → [R = 0.0821] → [Input n, v, t] → [P = f(n*r*t)/(v-n*b) - (n*n*a)/(V*V)] → [PRINT pressure P] → (END)

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M.Sc. F.Y.
Sem-I

10) REM: "To calculate pressure from vanderwaals equation.
20) Input a, b
30) LET R=0.0821
40) Input n, v, t
50) P = [(n*r*t)/(v-n*b)] - [(n*n*a)/(v*v)]
60) Print P
70) END

*9] Write a flowchart and compute to vanderwaal constant a & b for a gas by a formula.

$$a = \frac{PV^2}{n^2} \quad \text{and} \quad b = \frac{V}{n}$$

→ Flow chart:-
1) Take P, V and n number of moles as input for the programme & give the information i.e (kind of gas) also as a input for a programme
2) Calculate 'a' as
a = ((P*V*V)/(n*n)) and
b = (V/n)
3) Take calculated values of a & b as o/p hence programme flow chart will be as follows

(Start) → [Input P, V, N] → [a = ((P*V*V)/(n*n)) and b = (V/n)] → [Print a & b] → (END)

programme is as follows
10) REM :- To calculate value of 'a' and 'b' for a given gas (or)
20) Input P, N, V
30) a = ((P*V*V)/(n*n))
40) b = (V/n)
50) PRINT a, b
60) END

7/ PH – Titration :-

Aim: To study the effect of pH on base solu^n by adding an acid solu^n

Theory: The value of PH depends on
1) conc^n of acid
2) volume of base solu^n taken.
3) The PH value increases by addition of small value of acid solu^n (1 ml) at a time.
4) The graph of PH vs vol of acid added in cm³ gives the PH titration curve.
5) If the selected acid is weak it is necessary to give its Pka value.
6) Similarly for a weak base its pKa value should be consider.
7) If you want to draw the titration curve for different acid base solu^n take two set of sample or three set of sample
8) and pKa value are calculated as

$PH = -\log[H^+]$

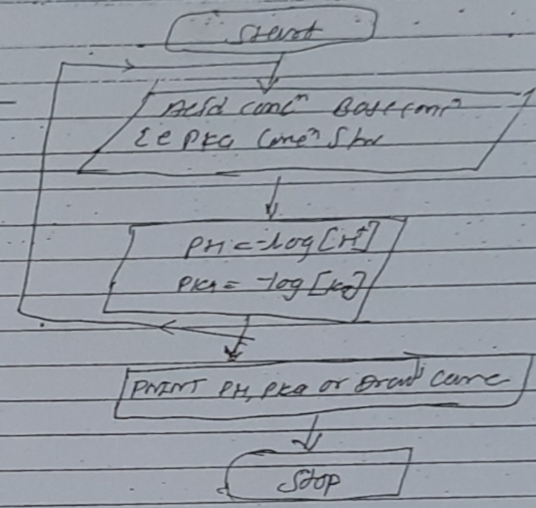
$PKa = -\log[Ka]$

9) Hence to take input for to study titration curve are acid
- Acid strong weak
- Acid concentration
- Base strong weak
- vol of base solu^n used
- pka value

10) If you want to study the PH titration curve for more than one sample of acid and base simultaneously a computer will ask for another sample inputs and it is provided as above
11) Calculate $PH = -\log[H^+]$

$pKa = -\log[Ka]$

12) Take PH and pka as outputs Then programme flow chart is as follows -



Programme:

```
10) REM "To Draw a PH curve OR to Calculate the
    value of PH or pka for acid / Base titration
20) titration
20) LET I = 2 ?
30) INPUT x = A w/s  conc^n pka
         B w/s , conc^n pk
40) Input y = A w/s, conc^n pka
         B w/s, conc^n, pka
50) READ I
60) PH = -log (H+)
    pka = -log [ka]
70) PRINT PH, pka
80) NEXT I
90) END
```

Kinetics of Reaction (K)

Objects:- To derive the order of chemical reaction concentration and time of a data.

data = C, t

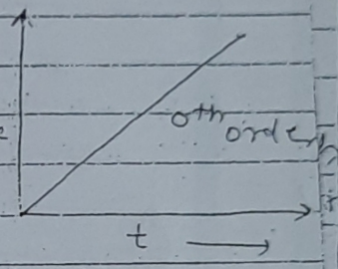
General Remark:- If differential are

$\frac{dx}{dt} = Kc^0$ then reaction is 0th order.

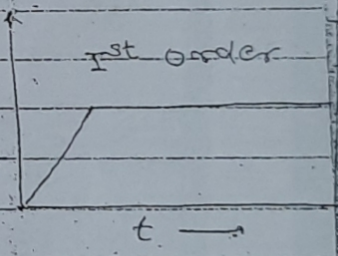
$\frac{dx}{dt} = Kc^1$ then reaction is 1st order.

$\frac{dx}{dt} = Kc^2$ then reaction is IInd order.

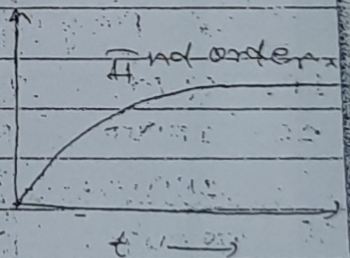
If reaction is 0th order, then graph of concn vs time is a straight line passing through centre.



For 1st order reaction the nature of curve is such that it shows linearity with time.



For second order reaction the reciprocal of concn shows linearity with time.



Therefore programme algorithm as follows:-

1) concn of soln with time is the input for this programme. $t = f(A)$

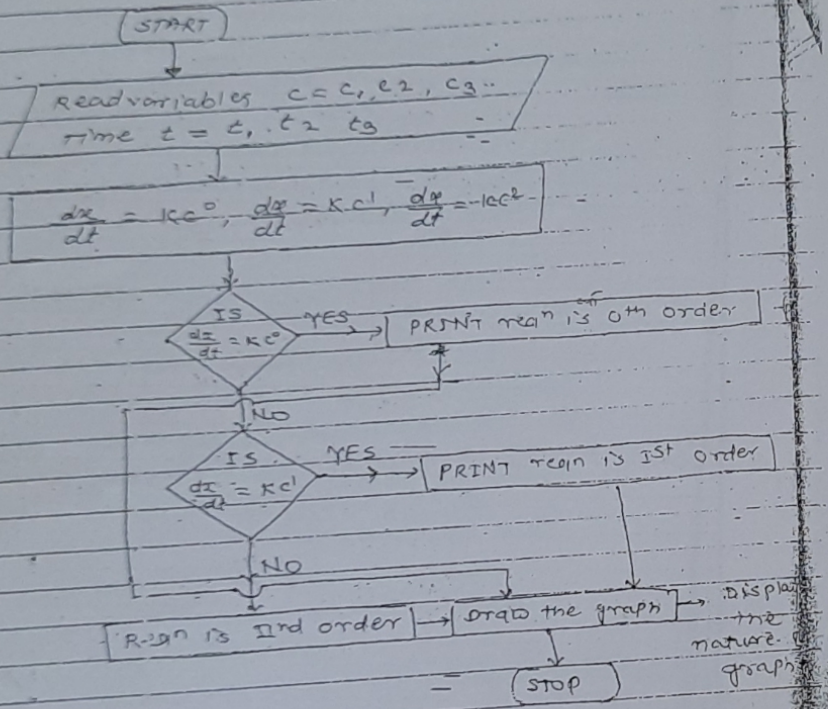
Assign the differential for 0th, 1st, IInd order reaction

i.e. $\frac{dx}{dt} = Kc$

process it to draw the curve.

from nature of graph evaluate the order of reaction it is the output.

Hence programme flow chart will be.



⊙ Programme:-

10. REM:- To study kinetics and find order of reaction
20. INPUT:- Read variables or
INPUT:- $t_1 = t_1, t_2, t_3 \ldots$
30. INPUT: $c = c_1, c_2, c_3 \ldots$
40. LET $\frac{dx}{dt} = kc^0$

$\frac{dx}{dt} = kc^1$

$\frac{dx}{dt} = kc^2$

50. If $dx/dt = kc^0$ THEN PRINT order of Reaction is 0th order.
60. If $\frac{dx}{dt} = kc^1$ THEN PRINT order of Reaction IS Ist order.

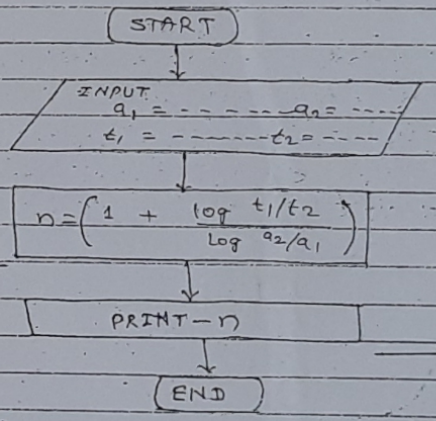
PRINT Reaction is IInd order.
Draw graph.
END.

Another way to compute order of reaction is by using the formula

$$n = 1 + \frac{\log t_1/t_2}{\log a_2/a_1}$$

where a_1 & a_2 are initial concentration of Ist & IInd observations and t_1 & t_2 are the half life period of I and II observations.

So its programme flow chart:-



Programme:-

REM:- To calculate order of reaction.
INPUT:- Enter the initial conc of Ist observation
$a_1 = - - -$
INPUT:- Enter the initial conc of IInd observation
$a_2 = - - -$
Enter the half life period of I obs $t_1 = - - -$
Enter the hal life period of IInd obs $t_2 = - - -$

$$n = \left[1 + \left(\frac{\log t_2/t_1}{\log a_2/a_1}\right)\right]$$

PRINT n
END.

radioactive decay process ym at t=0

Radioactive decay :-

Object :- To study the exponential curve for decay process and calculate decay constant λ, half life period t of any given elements.

$N = N_0 e^{-\lambda t}$

The Law of radioactive decay is that " The no. of atoms of a radioactive atoms or elements disintegrating per sec at any instant is directly proportional to the nature of atom of that substance present at instant".

i.e. $N = N_0^{-\lambda t}$

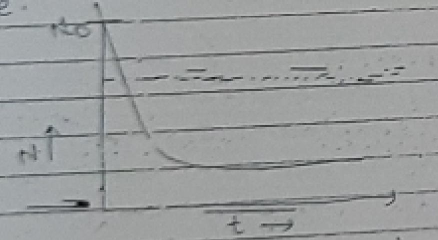
Where,

N_0 = no. of atom present initially

N = no. of atom present at instant t;

λ = decay constants.

The graph N vs t is the radioactive decay curve.



∴ The λ is given as $\lambda = \frac{0.693}{T}$

∴ $T = \frac{0.693}{\lambda}$ and the decay constant at any instant

$\lambda = \frac{2.303}{t} \log \frac{N}{N_0}$

So by observation we can find 'n' i.e. no. of atom present at different interval of time such as $t_1, t_2, ---$

So programme algorithm as follows

N_0 = no. of atoms at time t = 0

$T = t_1 + t_2 + t_3 + ---$

$N = N_1 + N_2 + N_3 + ---$

Take observations of N and T after certain time interval as a point.

By taking different value of N and T, the graph N vs T can be drawn.

λ can be calculated by:

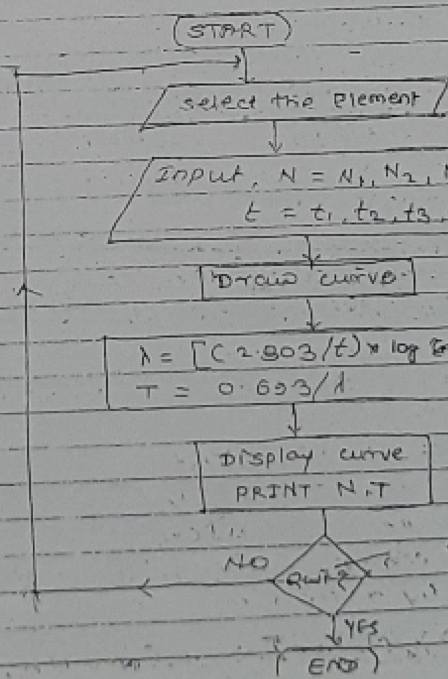
$\lambda = \frac{2.303}{t} \log \frac{N}{N_0}$

T can be calculated by $T = \frac{0.693}{\lambda}$

On graph, value of λ & T can be taken as a O/P.

You can study another element by using the decision in the programme.

So the programme flow chart is as follow




```
10 REM "To study the decay curve and cal. λ
20 Input select element
30 Input N = N1, N2, N3
40 t = t1, t2, t3
50 Draw curve.
60 LET λ = 2.303 / t
70 T = 0.693/λ
80 PRINT N,T Display curve
90 PRINT N,T
100 GOTO 20
110 END
```

programme

```
10. REM :- To study decay curve and calculate
          λ and t
20. Input :- select element
30. INPUT - N = N1, N2, N3, ----
40. INPUT   T = t1, t2, t3, ----
50. DRAW CURVE.
60. λ = (2.303/t) * log of N/No.
70.    T = 0.693/λ
80. Display  curve.
90.   PRINT
100 GO TO 20
110   END.
```

Evaluation of lattice energy from experimental data.

Object :- Evaluate lattice energy of metal halide having different oxidation states on the basis of Haber cycle or

To study enthalpy changes involved in the formation of metal chlorides, having oxidation states 1, 2, 3

① Using Born-Haber cycle total enthalpy changes for formation of metallic chlorides can be calculated.

② The process by which metallic chloride are form are

Ist	oxdn state	NaCl
IInd	—"—	$MgCl_2$
IIIrd	—"—	$AlCl_3$

③ Total enthalpy changes during the formation of NaCl solid by a Hess law is given as

$\Delta H = S_{Na} + D\frac{1}{2}Cl_2 + I_{Na} + E_{Cl} - U_{NaCl}$

[...]ttice energy of metallic halide for min of

where ΔH - change in enthalpy

S_{Na} - sublimation energy of Na

$D\frac{1}{2}Cl_2$ - dissociation of chloride

I = Ionization potential.

E = Electron affinity.

U_{NaCl} = lattice energy of NaCl.

Hence from this eqn Lattice energy of NaCl solid is

$U_{NaCl} = \Delta H - S_{Na} - D\frac{1}{2}Cl_2 + E_{Cl} - I_{Na}$

The another way to calculate U of metals

$$U = \frac{e^2 Z_1 Z_2 N_A}{r_0}\left(1 - \frac{1}{n}\right)$$

where, N - Avogadroes number.

A - Modulus constant

e - electronic charge

Z_1 - charge on cation

Z_2 - charge on anion.

r_0 - dist. betn cation & anion.

in crystal lattice.

n - Born exponent related to repulsive forces betn electron clouds.

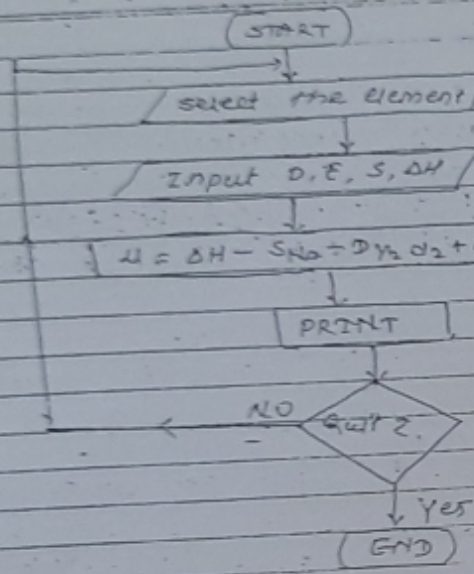
so program algorithm :-

① Give the enthalpy changes involved in different steps of formation of metal oxides as I/p's and other features.

calculate U of NaCl by using formula.

$U = \Delta H - S_{Na} - D\frac{1}{2}Cl_2 + E_{Cl} - I_{Na}$

Take U as output for particular metal you can calculate U of different metals by using the condition in the programme Hence Programm[...]



programme

10. REM :- TO calculate lattice energy of metal oxide.
20. INPUT :- Enter name of metal M = ---
30 - INPUT :- Read, ΔH, S_Na, D, I, E
40. U = ΔH − S_Na − ½ DCl_2 + Ecl − I Na
50. PRINT U
60 GO TO 20
70. STOP

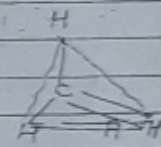
END

Elementary structure features: such as Bond length Bond angle, Bond energy :-

Aim :- To draw the structure of elements and calculate bond energy.

In molecule the atoms are concentrated together by different bonds, such as covalent, ionic, co-ordinate bond. The aim of this programme is to draw the structure of molecule showing structure of Bond length Bond angle in 3-dimentional fig. and calculate the Bond energy.

Eg :- In methane (CH_4) the atom C & H are linked together by co-valent bond. so it is a tetrahedral structure as shown in figure.



Now calculation of C—H Bond energy in methane we have to consider Bond length energy in various cases

$CH_4 \rightarrow CH_3 + H$ $\quad \Delta H_1 = 327$ J
$CH_4 \rightarrow CH_2 + H$ $\quad \Delta H_2 = 318$ J
$CH_4 \rightarrow CH + H$ $\quad \Delta H_3 = 430$ J
$CH_4 \rightarrow C + H$ $\quad \Delta H_4 = 326$ J

and total value of energy is

$\Delta H = \Delta H_1 + \Delta H_2 + \Delta H_3 + \Delta H_4$ and the average bond energy is $\Delta H/4$

the bond angle = 109° 28'

the bond length = 1.04 A°

Hence programme algorithm is

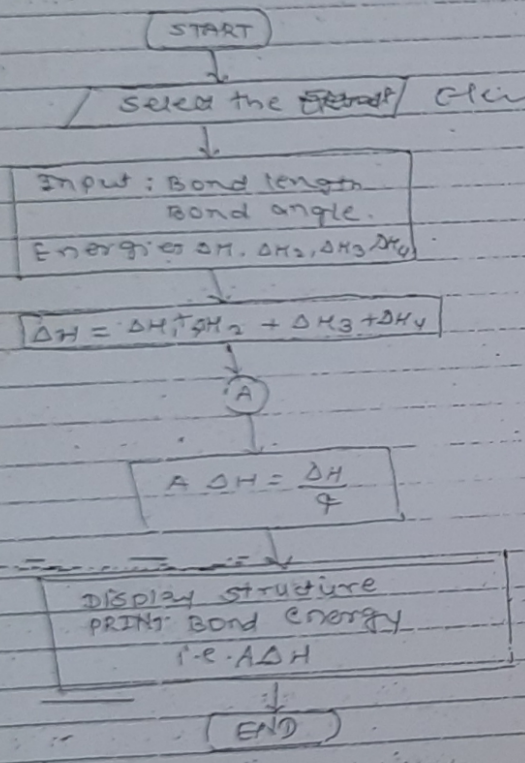
Select the element for study elementary structure at feature and to calculate bond energy provide required data i.e. bond energies in various steps bond length, bond angle as an input

Draw the structure and calculate the bond

for CH is

$\Delta H = \Delta H/4$

(3) Take average ΔH as a O/p for a particular molecule based the programme for particular CH_4 as



10 REM

20 INPUT

30 O/P

Let = Formula $A\Delta H = \Delta H/4$

$\Delta H = \Delta H_1 + \Delta H_2 + \Delta H_3 + \Delta H_4$

Computer

computer is a computing machine (electronic machine) which accept data through input devices in the form of character, words, statements and processing on it and gives the desired result through output device.

Input operation

The computer receive input data from outside world in the form of character word, statement, numericals and then the actual work is done to produce desired result

What is an O.S.?

UNIX

Multiuser Multitasking system

* General account:-

This is an operating system providing the facilities for operating several applns programmes simultaneously on the system of P.C. computer to a super computer. No. of user at a time can perform their application on a supper computer system. Therefore it is regarded as multiuser multitasking unit.

This system is previously designed by Ritzhe and Thomson in 1973 they working in telephone laboratory in USA.

Structure:-

This is considered as a layered structure system. The various units of this system are ① Kernel ② shell ③ pipe facilities etc are shown in fig.

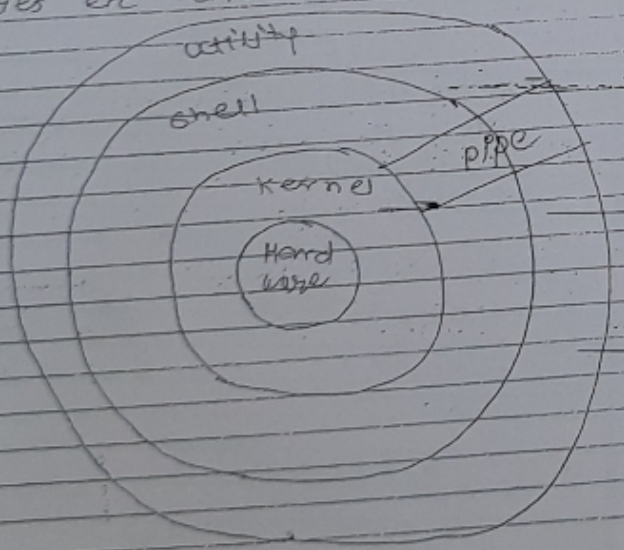


fig:- structure of UNIX operating system

① Kernel:-

this is the inner part of the unix O.S. this unit communicates the programme in relation with the user & hardware component of computer system.

It control the resources of computer and allow the co-ordination of these resources as in house.

it control the operation of peripheral devices such as hard disk, key board, monitor etc. so that required tasks can be performed by this.

The Kernel of unix O.S. provides files which can store data and programe useful handling the files - various functions renaming, moving of files, stored into system.

Shell:-

It is a next layer of unix O.S. code of a strong command interpreter.

This consist of a very large no. of useful commands stored in a file. The user can also creates his own commands. unix shell with the help of certain programmes is used to perform various duties as read instructions through input it also provide a very ideal called pipe.

pipe:- unix O.S. introduce a new in the form of pipe, this is used output of first programe to other as its input without storing the output in the temporary

A line connecting two or more such a programme is known as pipe line.

) **utility:-**
The outermost layer contains the utility programes eg. language compiler are available in this part of system. This system makes particularly use of the instructions written by the user in C language these are popular & easily understandable high language to the user

One of the unique feature & compiler of this system is they have common object code with the help of which easy mixing of high level language is possible.

Imp. formula –

$\lambda = \frac{h}{\sqrt{2mVe}}$ $\lambda = \frac{h}{\sqrt{2mVe}}$

$n\lambda = 2d\sin\theta$

1 esu = 300 V

$e = 4.8 \times 10^{-10}$ esu

$e = \frac{4.8}{300} \times 10^{-10}$ volt

calculate the wavelength of electron beam if it's accelerated by an applied potential diff of 20,000 volts to produce a diffraction pattern

$\frac{20,000 \text{ volt}}{300 \text{ esu}}$

1 esu = 300 volts

Given =

we know

$\lambda = \frac{h}{\sqrt{2mVe}}$

$\lambda = 6.626 \times 10^{-27}$ erg/sec

$\sqrt{2 \times 9.11 \times 10^{-28} \times 66.67 \times 4.8 \times 10^{-10}}$

$= \frac{6.}{\sqrt{1213.4 \times 10^{-38}}}$

$= \frac{6.626 \times 10^{-27}}{3.4834 \times 10^{-18}}$

$= \frac{6.626}{3.4834} \times 10^{-9}$

$= 1.902 \times 10^{-9}$

$\lambda = 19.02 \times 10^{-10}$ m

$\lambda = 19.02 A^{0}$

$\rightarrow = \frac{6.626 \times 10^{-27}}{\sqrt{5.830.69 \times 10^{-38}}}$

$\frac{6.626 \times 10^{-27}}{7.6359}$

$= 8.677 \times 10^{-10}$

II) $\lambda = \frac{12.2 \times 10^{-8}}{\sqrt{V}}$

$= \frac{12.2 \times 10^{-8}}{\sqrt{20,000}}$

$\frac{12.2 \times 10^{-8}}{141.43}$

Right method ?

0.086×10^{-8} cm

8.6×10^{-10} cm

8.627×10^{-10}

10^{-10} m

10^{-8} cm $= A^{0}$

0.086×10^{-10}

4. A: First order reflection (111) plane of KCl crystal was observed at a glancing angle 7.37° when CuKα x ray of wavelength 1.5 A° were used. Calculate interplanar distance.

$$\Rightarrow 2d\sin\theta = n\lambda$$

$$n\lambda = 2d\sin\theta$$

$n = 1$

$$d = \frac{2d\sin\theta}{}$$

~~$\lambda = 2\lambda$~~

$$d = \frac{n\lambda}{2\sin\theta} = \frac{1.5}{2\times\sin 7.37}$$

~~$\frac{6.62\times10^{-27}}{5\times\sin}$~~

$$= \frac{1.5}{2\times 0.885} = 1285$$

$$= \frac{1.5}{1.77}$$

$$= 0.84\ A^{\circ}$$