



TITLE

Design and Development of Augmented Computational Application Software for Interpretation of Infra-Red Spectrum of Organic Compounds

NAME OF PI/CO-PI:

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COLLABORATOR (S), IF ANY:

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DURATION OF PROPOSAL:

3 Months

- ❖ Infrared (IR) spectroscopy is one of the most common and widely used spectroscopic techniques , but due there's unavailability of computer programs for its accurate interpretation .
- ❖ Infrared spectra are “fingerprints” of molecules and eventually it leads imprecise predictions.
- ❖ If an expert looks at the infrared spectrum, there's difficulty to interpret it.
- ❖ Software are being commercialized on H-NMR but there's no such structural based software.
- ❖ Generally spectral interpretation is easily possible for simple compounds, but it is time consuming, expensive and generally limited for more complicated compounds.
- ❖ The proposed idea state benefits over theoretical basis as well prediction of vibrational frequency which depends upon force constant and reduced mass .

RATIONALE OF IDEA



- ❖ Although the traditional method of analyzing infra red spectrum has flaws as follows :
 - **Difficulties to interpret.**
 - **Manual mistakes.**
 - **Overlapping spectrum of functional groups**
 - **Budding graduates who had fresh exposure to IR spectrum.**
 - **Hunt and peak issues** , it has to be ascertained by modern established scientific tool.
- ❖ The main advantage is that virtual IR spectral SEARCH is fast and can be used by less qualified personal.
- ❖ Limited not only for pharmaceuticals but also by Basic sciences.

AIM :- Design and Development of Augmented Computational Application Software for

Interpretation of Infra-Red Spectrum of Organic Compounds

OBJECTIVES :-

- ✓ To obtain IR spectrum of organic compounds without actual instrumentation which illustrates the vibrational frequency as well as intensity of absorption of the bands of the functional group associated with organic compounds.
- ✓ To create their own spectral libraries.
- ✓ To obtain desired spectrum with customized structured of organic compounds .
- ✓ To understand the factors influencing vibrational frequency like bond strength, mass of atom, electronegativity, hybridization state of the atom constituted with the bond.

IMPORTANCE IN CURRENT CONTEXT

1

OFFLINE EXCESS :
Application can work in different areas having fluctuating internet.

2

CONTENT SIMILARITY AND ACCURACY :
Output has variable buttons to access specific data .

3

DATA LIBRARIES:
Data being processed will be stored in files and easy accessible whenever need.

4

USER FRIENDLY :
IR patterns can be easily access without actual instrumentations .

5

CONCEPT CLARITY:
Probable hydrogen bonding and shifting of IR band accordingly.

WORK PLAN

1. CONCEPTS OF HOOKS LAW:

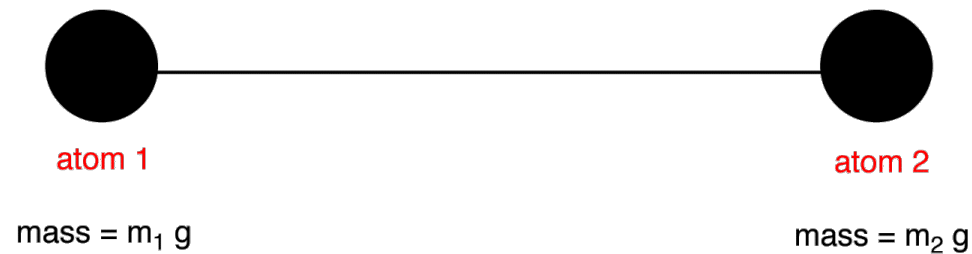
$$\bar{\nu} = \frac{1}{2\pi c} \sqrt{\frac{K}{\mu}}$$

$\bar{\nu}$ = wave number, in cm^{-1} , corresponding to the vibrational frequency of the bond

c = speed of light in cm s^{-1}

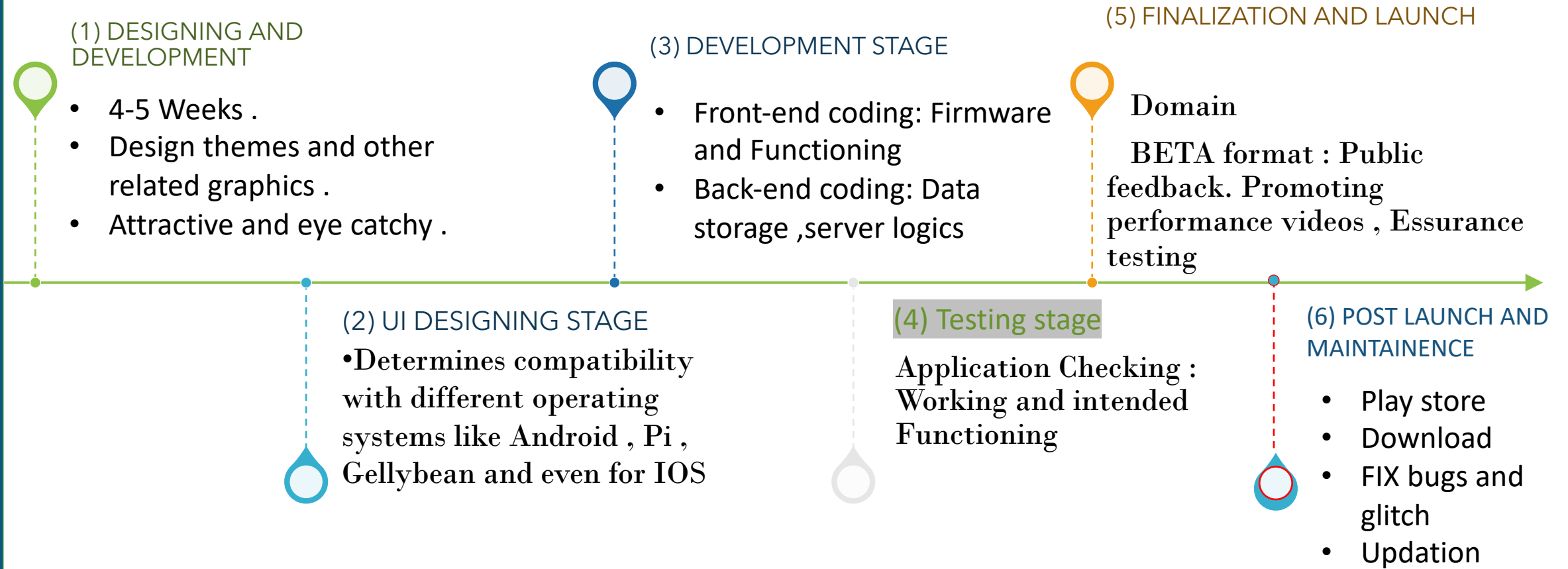
K = force constant in dynes cm^{-1} (a measure of bond strength. The stronger the bond, the larger the K .)

μ = reduced mass in g atom^{-1}

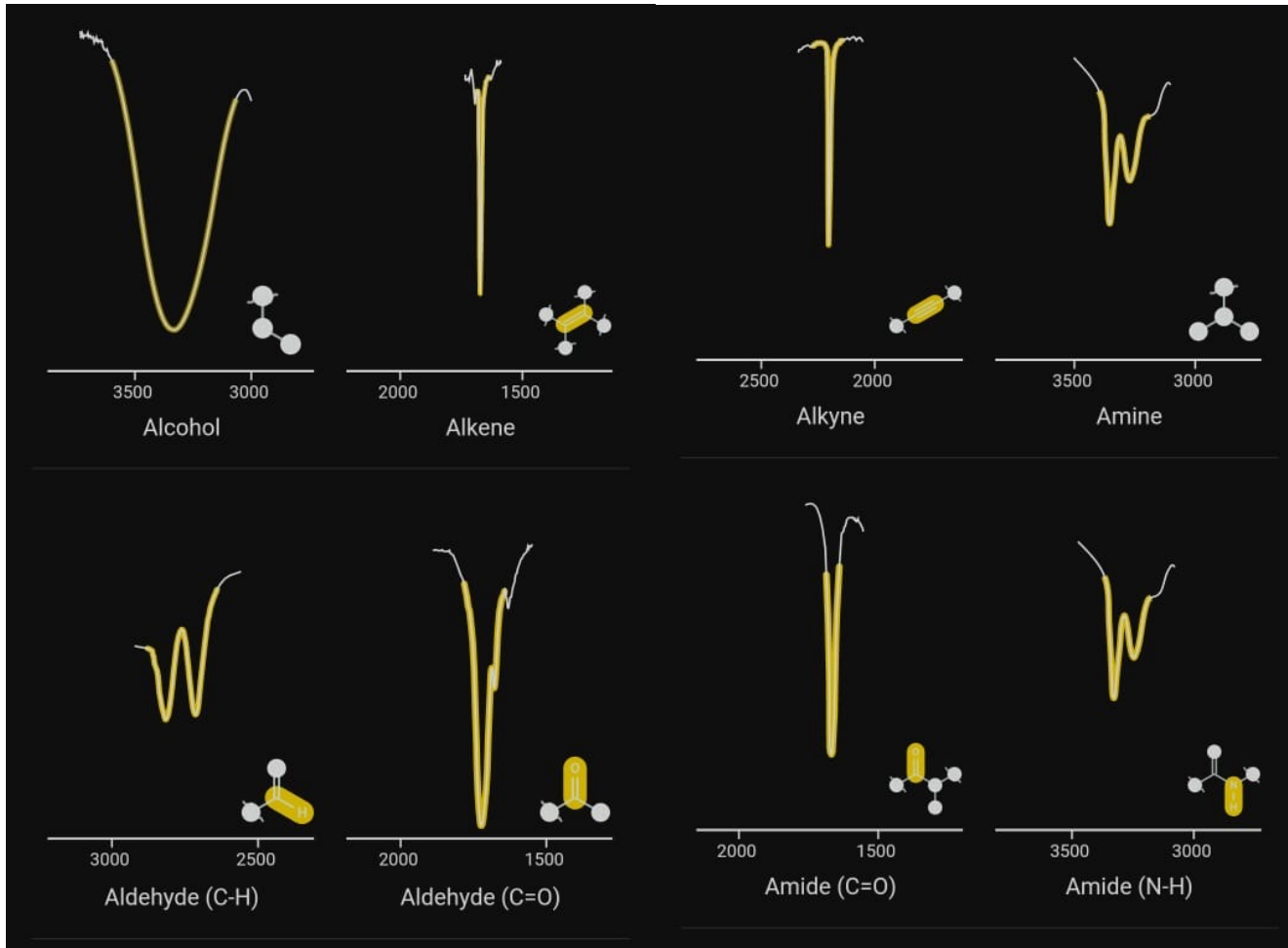


$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

2. CODING:



EXPECTED OUTCOME

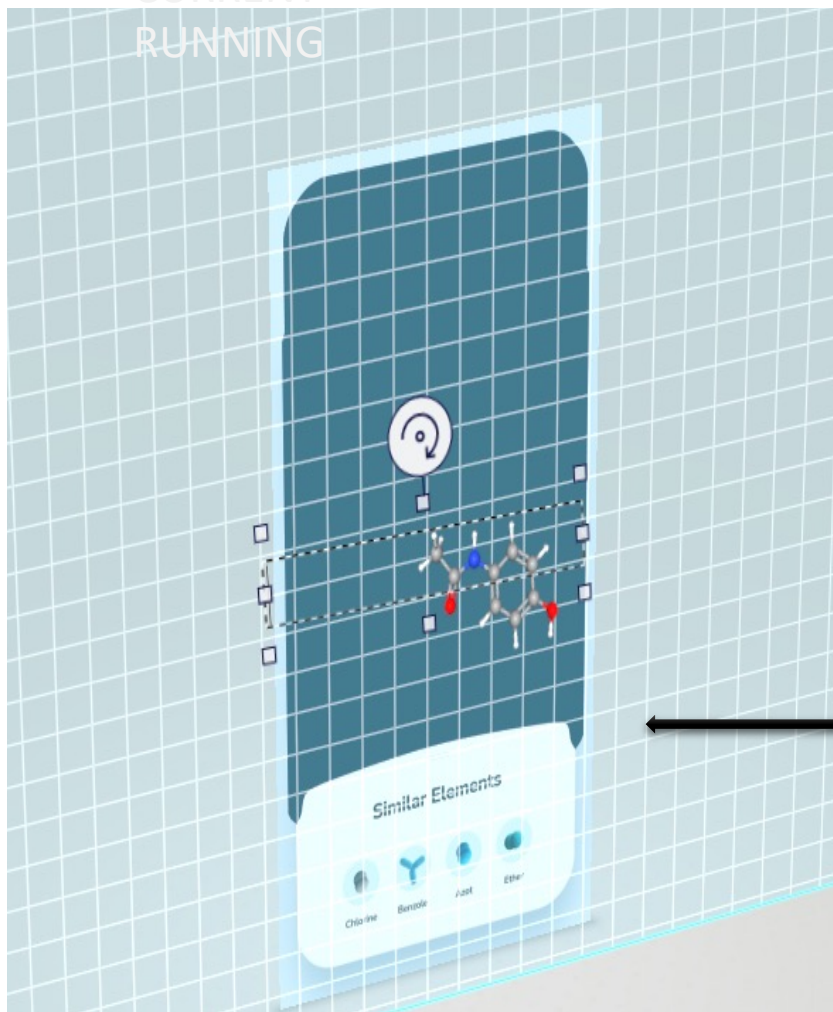


- Different functional groups of a molecule (like -CH_3 , COOH , NH_2) exhibit peaks at different ranges of wavenumbers.
- The peak position gives you information about sample and depends on the symmetry of the molecule, atom weight and bond strength .
- Peak intensity gives you quantitative information and depends on concentration.
- Peaks from 1400 – 650 nm can be obtained with labelling of frequencies which commercial instrument can't show.

PILOT STUDY RESULTS



CURRENT
RUNNING



GLIMSE OF
CODING

A 3D demo of
molecular structure
obtained after
sketching our pre-
intended INPUT
Accessible 3D
Movement

```
> <PUBCHEM_ATOM_DEF_STEREO_COUNT>
0
> <PUBCHEM_ATOM_UDEF_STEREO_COUNT>
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> <PUBCHEM_BOND_UDEF_STEREO_COUNT>
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> <PUBCHEM_CACTVS_TAUTO_COUNT>
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> <PUBCHEM_MMFF94_ENERGY>
29.3225
> <PUBCHEM_FEATURE_SELFOverlap>
20.297
> <PUBCHEM_SHAPE_FINGERPRINT>
10219947 1 18113338621837817764
11062470 55 18411419518204251026
12032990 46 18411707547554542334
12932764 1 17203596078260793835
13380535 76 18408886260652285810
14144814 61 18411136913877994947
14325111 11 18410856538196653569
15775835 57 18272936041829235069
16945 1 18410575114838704230
17844478 74 18113625564592914661
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PILOT STUDY RESULTS

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RECEIPT NO : 68590
FILING DATE : 11/12/2022
BRANCH : Delhi
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S.No	Form	Diary No.	Request No	Title	Amount (Rupees)
1	Form-XIV	25758/2022-CO/SW	70698	DESIGN AND DEVELOPMENT OF AUGMENTED COMPUTENTIONAL SOFTWARE BASED ON INFRA-RED SPECTRUM TO INTERPRET ORGANIC COMPOUND	500
Amount in Words			Rupees Five Hundreds		500

PAYMENT MODE	Transaction Id	CIN
Online	C-0000079342	1112220004488

(Administrative Officer)

THANK YOU