

# ***PROJECT ONE: CHEM 416***

**Group Name:** Bible Study Class

**Group Members:** Cheng Zhen

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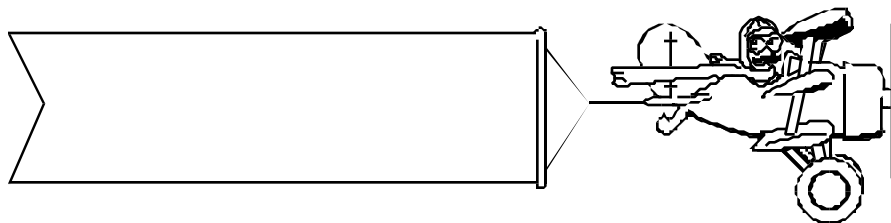
**Group Meetings:**

Twice a week

Place: Chemistry Reading Room

Time: Two Hours

**Project Title and Description (Please see next page)**



# FT-IR Spectroscopy Application in Characterization of Schiff Base (imine) compound

We three are researchers in an organic lab of a pharmaceutical company and intend to develop a kind of pharmaceuticals based on the schiff base.

Schiff base is a kind of compounds that are very useful for developing the new drugs. Their metal complexes have occupied a central roles in the development of coordination chemistry and the studies of their complex based on the ligand  $N_2O_2$  are very popular.

The reaction of carbonyl with the amine can form the imine compound and the synthesis method of imine is described as follows:

Fig1. The reaction of carbonyl with amine and the spectroscopy of FT-IR on-line analyze

This reaction can be analyzed by FT-IR. The reason for us using FT-IR is based on the following facts. First, C=N stretch vibration have strong absorption at  $1690\sim 1640\text{cm}^{-1}$ . This peak is sharp, narrow and easy to be identified. Moreover, the C=O group for the starting materials of the reaction also have a single and strong absorption at  $1720\sim 1700\text{cm}^{-1}$ . So it is very easy to distinguish these two compounds even in the mixture using FT-IR(Fig I). Second, this reaction can not be monitored well by UV because the absorption peak between C=O and C=N may be overlapped, furthermore, the factors which influence the position of their absorption peaks are complicated and also the resolution of the UV is less than that of FT-IR. As for NMR, it is also not a good choice because it is difficult to identify the product in the mixture besides its high expense. FT-IR is a computer automated device and we do not need an operator to drive instrument. Also the temperature control do not needed.

Through *internet web* and *Journal of Analytical Chemistry*, the information about the company which produce the FT-IR Spectrometer is obtained. The major suppliers' name and web addresses is shown in table I:

**Table I: The Company name and their Web Addresses**

Company	Web Site
Nicolet Instrument Corporation	<b>Error! Bookmark not defined.</b>
PERKIN ELMER	<b><u>Error! Bookmark not defined.</u></b>
Analect Instruments, Inc.	<b>Error! Bookmark not defined.</b>
Bruker Analytik GmbH	<b>Error! Bookmark not defined.</b>
Buck Scientific	<b><u>Error! Bookmark not defined.</u></b>
Spectra Tech Inc.	<b><u>Error! Bookmark not defined.</u></b>
MIDAC Corporation	<b><u>Error! Bookmark not defined.</u></b>

After we browsed the introduction about their product of these company. We determined to request the more details about the FT-IR spectrometer of MIDAC and Nicolet through the phone, email and letters. The requirements for the instrument are

- High Resolution:  $1-5\text{cm}^{-1}$
- Spectral Range:  $7,000-450\text{cm}^{-1}$
- Sample Measurement: Solid, Liquid State
- Software: ease to use, strong function,
- Stability, reliability and durability
- Cost: acceptable

Based on these consideration, the Protégé 460. E.S.P. FT-IR Spectrometer (Nicolet Instu. Corp.) and Prospect-IR<sup>TM</sup> Spectrometer (MIDAC Corp.) meet our needs.

These two companies are famous suppliers on this field and have great reputation. Their service is excellent and give us quickly response. So we decided to select the apparatus between them. The comparison of the performance features of them is listed in Table II.

**Table II : Comparison of the performance features of two different modals**

<b>Performance Features</b>	<b>Prospect-IR<sup>TM</sup>(MIDAC)</b>	<b>Protege460(Nicolet)</b>
<b>Signal to noise</b>	The high signal to noise	Better than 20,000/1 peak to peak average SNR in 1 minute measurement time at $4\text{ cm}^{-1}$ resolution with triangular apodization using a KBr

		beamsplitter and DTGS detector
<b>Resolution</b>	1.0cm <sup>-1</sup>	Nominal 1.0cm <sup>-1</sup>
<b>Range</b>	7400-350cm <sup>-1</sup>	Standard KBr 7400-350cm <sup>-1</sup>
<b>Software</b>	GRAM-32 <sup>TM</sup>	OMNIC E.S.P

FT-IR mainly consisted of five parts: Source, Interferometer, Compartment, Detector, Computer system and Software package. The Details are listed below(Quotes List).

## Quotes List

### A: Nicolet

Model: Protégé 460. E.S.P. FT-IR Spectrometer

1a	1	912A0377	Protégé 460 E.S.P. Mainframe: <i>Vectra-Plus<sup>TM</sup> Interferometer, Purge Shutters, Sample Compartment Purge Curtain, System, Sample Compartment, and Accessory Purge Ports, Flexible Sample Compartment Door With Slide Port Insert, AT Interface Card and Cable, Alignment-free Toolless sample baseplate, sample compartment size of 8.2" wide× 10.2" deep× 7.09" high, pinned in place user serviceable module components, Integrated Multimedia REAL-TIME Diagnostics &amp; Use Help Videos. Power: 120V,3A,60Hz,or 240V,1.5A,50Hz</i>	\$17,684.42
1b	1	470-151400	Purged System including purge regulator	
1c	1	699-053600	Protégé 460 E.S.P. English Language Kit	
1d	1	840-053900	Mid-IR Optical Configuration <i>Standard Range 7,800-350 cm-1, Germanium beamsplitter on KBr substrate, DTGS detector with KBr Windows, Ever-Glo source</i>	
2a	1	833-009000	Basic OMNIC E.S.P.CD Software Package	\$2,708.74
2b	1	833-000800	OMNIC E.S.P. help and Tutorials CD for Protégé	
4a	1	912A0380	Enhanced Workstation with Windows95 <i>Intel Pentium 200Mhz Processor, 32 Mbytes of EDO RAM, 256K Pipeline Burst Cache RAM on Motherboard, 3Gbyte Hard Drive, 2 Meg 64 bit Accelerated Local Bus Video, 12X CD-ROM and 16 bit Stereo Sound, Internal Travan Style 3.2Gbyte Tape Drive and one Tape 1.44 Mbytes 3.5" Floppy, 2 USB Ports, One 9 Pin Serial Port, One Printer Port, PS/2 Style Keyboard and Mouse, Digital Venturis FX Short Tower Chassis</i>	\$ 1,794.95
5a	1	840-052500	17" SVGA Monitor <i>0.28mm Dot Pitch, Flat Square Picture Tube, MPR2 and Energy Star, Maximum Resolution of 1280× 1024NI, Digital Controls</i>	\$617.75

6a	1	840-047900 HP Deskjet Color Printer 120V* <i>HP Deskjet 690C, Hp IEEE 1284 Cable and Ream of Paper included</i>	\$326.52
Total Protégé 460, FT-IR Spectrometer			\$22,132.38

## **B: MIDAC Corporation**

Model: Prospect-IR<sup>TM</sup> Spectrometer

### 1. General

*Detector(DTGS,room temperature), Opticals(KBr with proprietary Ge coating for moisture protection. Gold coted, diamond turned,permanently aligned mirrors.), Optical Beam(Center focus 2.5" above sample), Image Size(6mm at focal point), Purge(separate internal and sample compartment fittings.) Sample(8"× 11.5"× 7.5" W× D× H). Acess from 3 sides), Compartment(positioning holes for pinned-in-place accessories.), Bench (Size 25"× 12"× 8" W × D× H), Power 110/220 VAC, 50/60Hz, 50W*

### 2. Interferometer

*Type(michelson type with dual mechanical bearings and linear force motor), Mirror cotrol(HeNe laser with quardrature phase detectors), Source(1550° K, air cooled, permantly aligned).*

### 3. Data Systems

*6415 586, 150MHz, 16MB RAM, 1.3GB HD, 2floppy, SVGA*

### 4. Software

*GRAMS-32<sup>TM</sup>, highly optimized 32 bit software from Galactic*

Total Prospect-IR<sup>TM</sup> Spectrometer \$13,600.00

From above discussion, since the basic function of these two Model is similar on resolution and range etc., we decide to purchase the Prospect-IR<sup>TM</sup> Spectrometer (MIDAC) because of its lower price.

In order to finish this project, we have read a great deal of reference such as *Web, Journal of Analytical Chemistry, IR textbook* and product directory. We learn more about both the theory and the instrument of IR. On the other hand, we learn from others and improve our cooperation ability during these days. It is really a good chance for us to do this project. We learn how to plan our schedule and how to search information, use information. But unfortunately it is a time consuming work for us, and it is also difficult for us to face the seller's enthusiastic service. Anyway, all these work is worthy and rewarding. We are looking forward to engage in such group activities again.

