

## Appendix A

The following consists of a number of programs written specifically for the Nicolet 800 FTIR system for data acquisition and spectra manipulation.

### KK3- Data Acquisition

OMD

Experimental Data Collection

OMD

Prepare to run actual samples:

NSS=NSB

OMD

Which SFN would you like to start with ( $\geq 5$ ) ?

SFN

OMD

How many absorbance measurements would you like to take?

QIT

SRT= SFN

PAU Insert sample and diffusant <ENTER>.

For III=1 TIL QIT

OMD

In the loop...

SCS

RAS

ABS

DSS

TEM=9

NPR

OMD

Just displayed spectra....

SFN=SFN+1

OMD

Adding....

TEM=11

VIØ = {insert # sec. Between scans}

NPR

NXT III

OMD

This set of scans completed for this sample !!!!!

SFN=SFN-1

OMD

Raw data located in files SRT thru SFN/DFN :

PRN SRT

PRN SFN

DSR

QIT=SFN  
END

#### **KK4- Baseline Correction**

OMD

Auto-baseline correction

QIT=SFN

SFN=SRT

OFN=4

DFN=2

MOD

For III=SRT til QIT

DFN=RFN

MOD

PRN=DFN

XSP=4000

XEP=1823

SLG

XSP=1823

XEP=899

SLG

SFN=OFN

FCS=1.0

FCR=1.0

DIF

DSS

OMD

Baseline correction completed for file #.....

PRN SFN

TEM=9

NPR

SFN=SFN+1

OMD

Added and going through loop again....

NXT III

SFN=SFN-1

END