





Health & Safety Issues

- Clark Science Center is covered by the OSHA Lab Standard
- Our Chemical Hygiene Plan is incorporated into the Clark Science Center Safety Handbook
- The Safety Handbook is available
 - from faculty as hard copy
 - Via www.science.smith.edu/resources/safety/table_contents.html



Basic Emergency Response

- If an emergency, call 800 and give
 - Your name, location including room #, and the nature of the emergency (Fire, spill, etc.)
 - If a student requires first aid, they should also seek a medical opinion regarding whether they should consult a physician (for cuts, burns, etc.)
 - Take the MSDS if a chemical accident.



Be Prepared..

- Locate the fire extinguisher, safety shower, eyewash, pull box, phone, and nearest building exit to the lab before leaving today.
- Locate them again the next time you're here...



Hazardous Operations

- Use of open flames
- Use of any controlled radiation source
- Handling of any quantity of reactive or acutely toxic material
- Handling of more than 4L or 1 kg flammable or corrosive chemicals
- Work on electrical installations which could pose a shock hazard (DC > 40 volts, AC > 24 volts)



Working Alone and “After Hours” Policies...

- “Working Alone”: Defined as when there is no other person within voice contact or in the lab
 - The second person must be aware they are serving as a ‘buddy’
- “After Hours” is defined as when the building is locked
 - Summer open hours 8-5, M-F
 - Academic Year Open Hours: 7AM-11PM M-TH; 7AM-10PM F; 8AM-10PM SAT/SUN
- Students doing research are not allowed to perform any hazardous operations when working alone, and may not work alone after hours, or perform hazardous operations after hours, unless supervised by the faculty member



Where to Go for More H&S Info...

- Aldrich (www.sigma-aldrich.com) and Fisher (www.fishersci.com) provide virtually unlimited free MSDS's
 - Need to register/log in but can ignore request for Smith account #
- www.hazard.com has thousands of MSDS's and you don't need to register
- Safe chemical storage (waste or not) is addressed in CSC Safety Handbook-also handouts
- Compressed gas safe practices:
www.uwm.edu/Dept/EHSRM/LAB/labgascyl.html

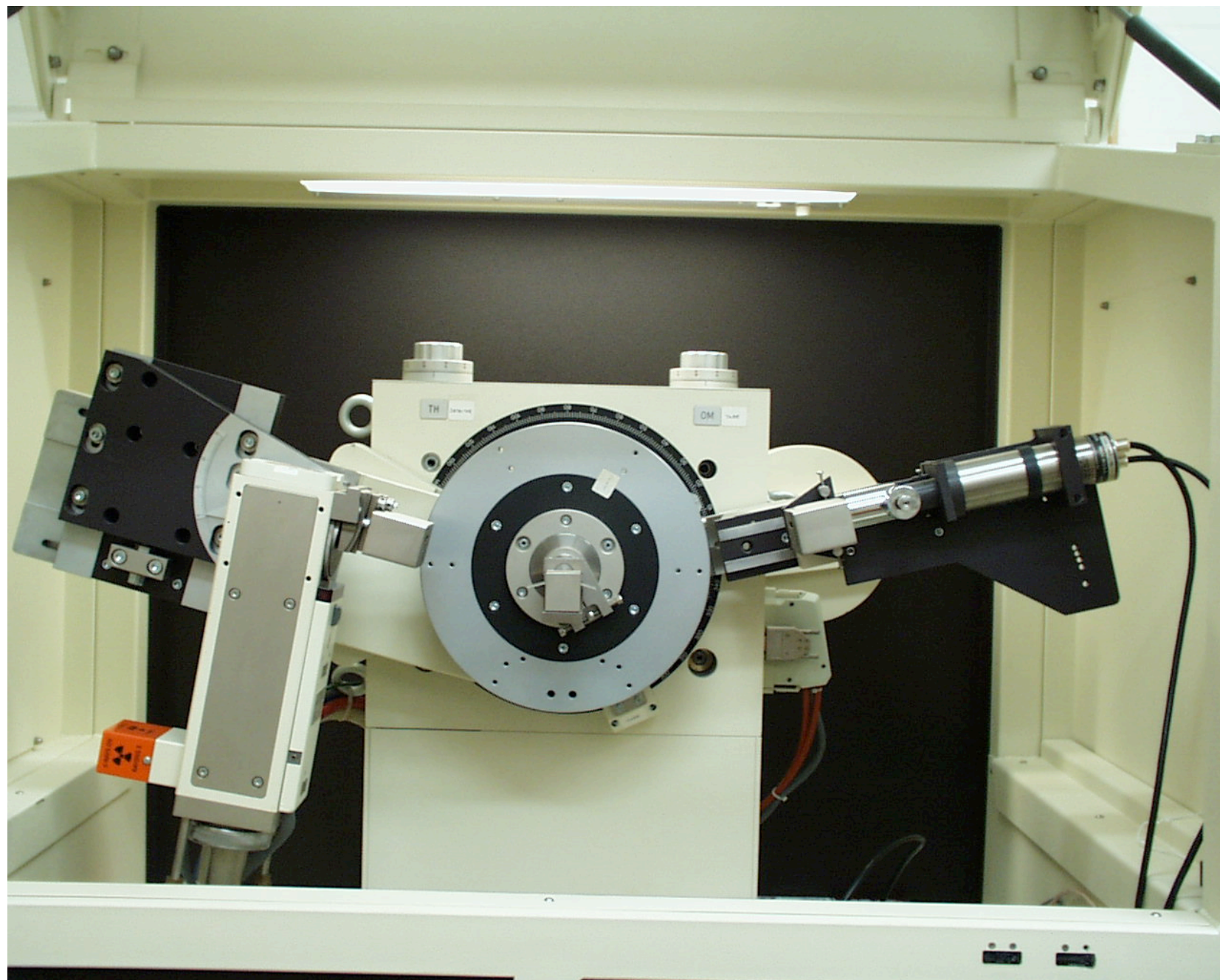
Some Useful URL's for Radiation Safety Information (2004)

<http://www.radsafe.pitt.edu/ManualTraining/SectionIII.htm>

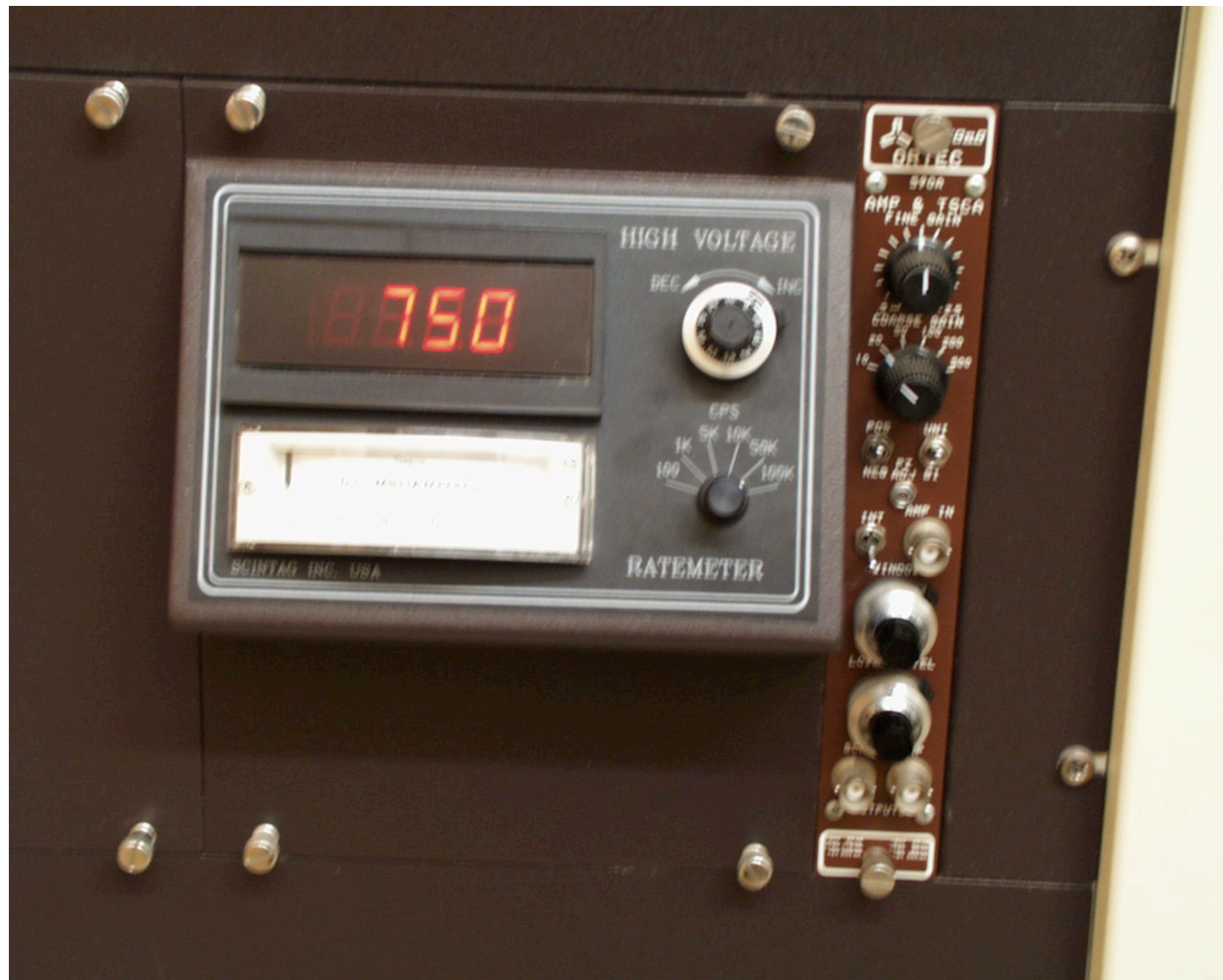
<http://www.ndt-ed.org/EducationResources/CommunityCollege/Radiography/Physics/radiationsafety.htm>

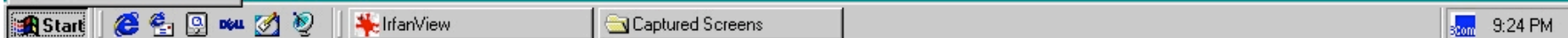
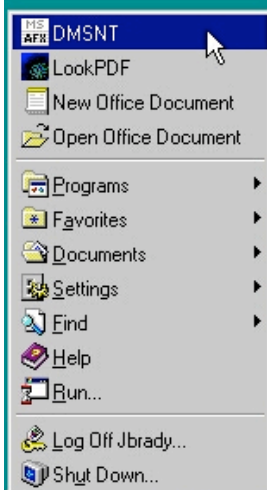
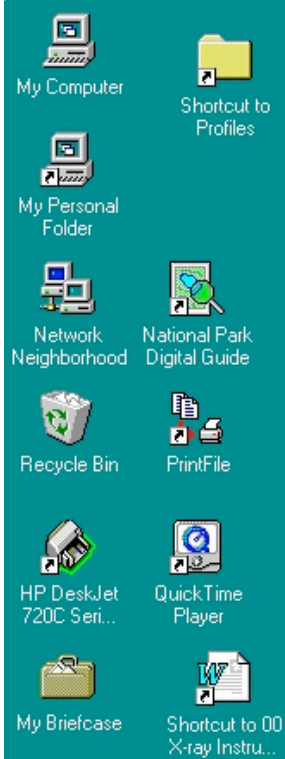
http://www.osha-slc.gov/pls/oshaweb/owadisp.show_document?p_table=STANDARDS&p_id=10098

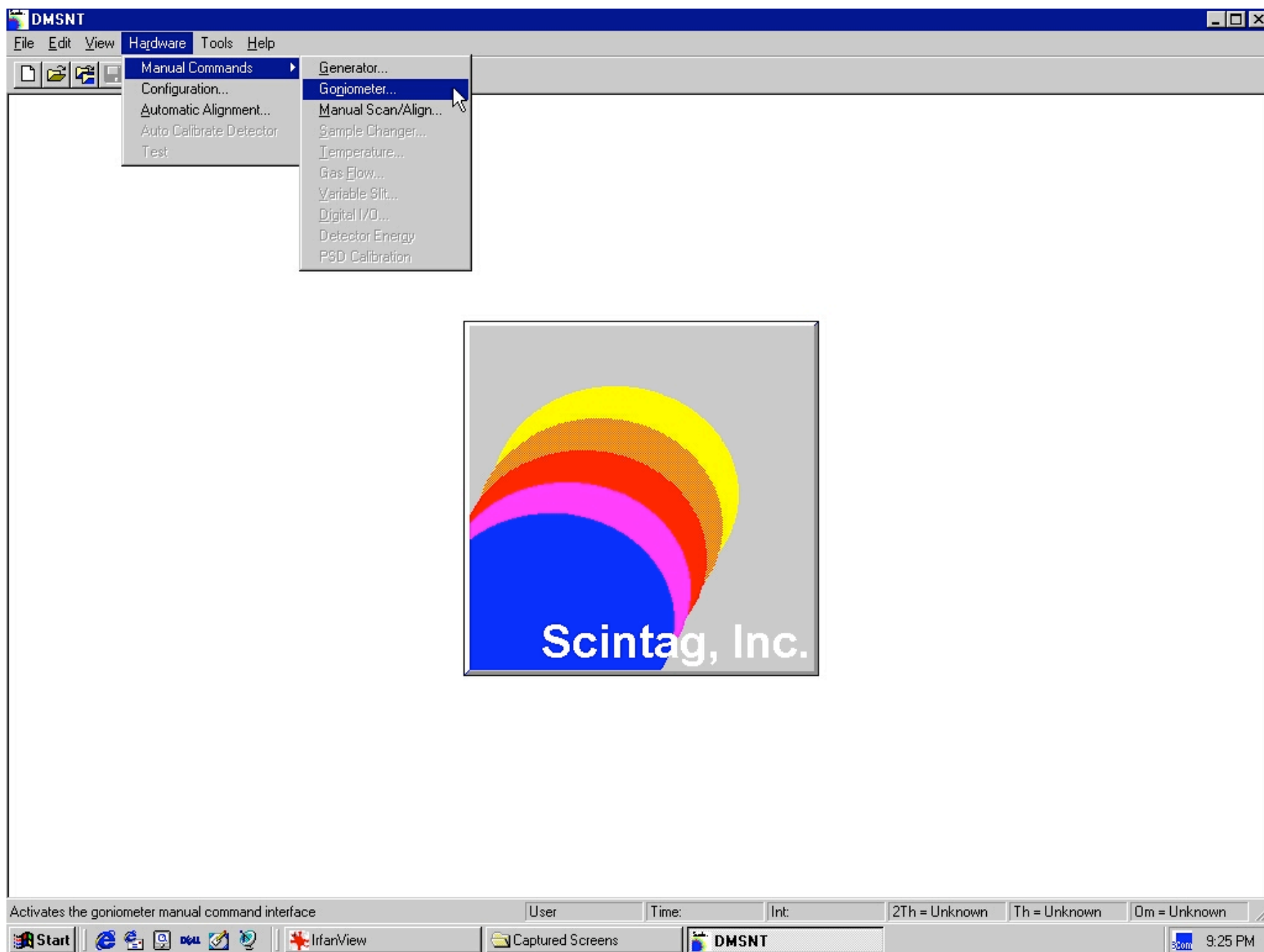


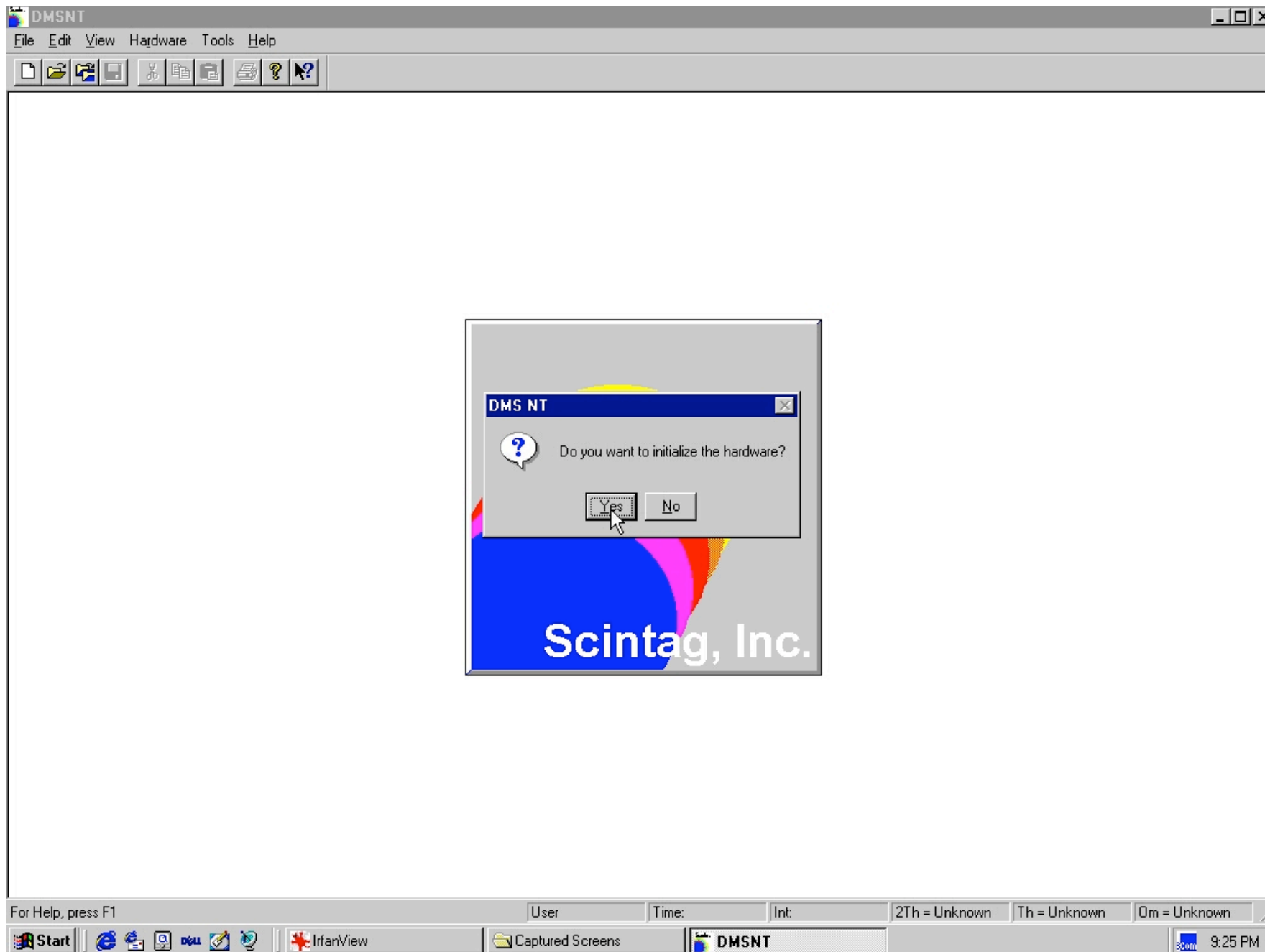














Diffractometer Initialization

Goniometer

Type: Theta-Theta

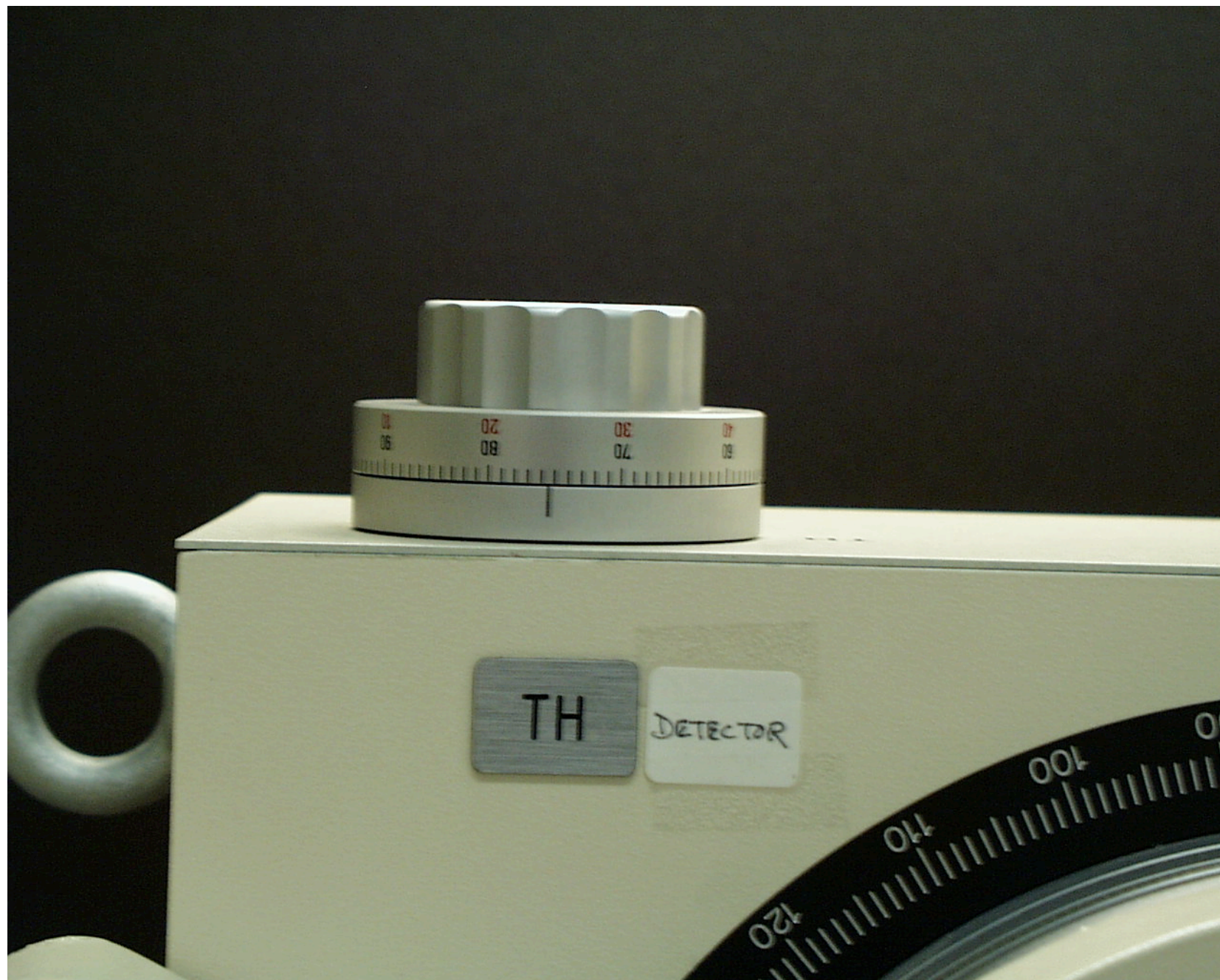
Axis	Current Position
Detector	35.00500000
Tube	35.00500000

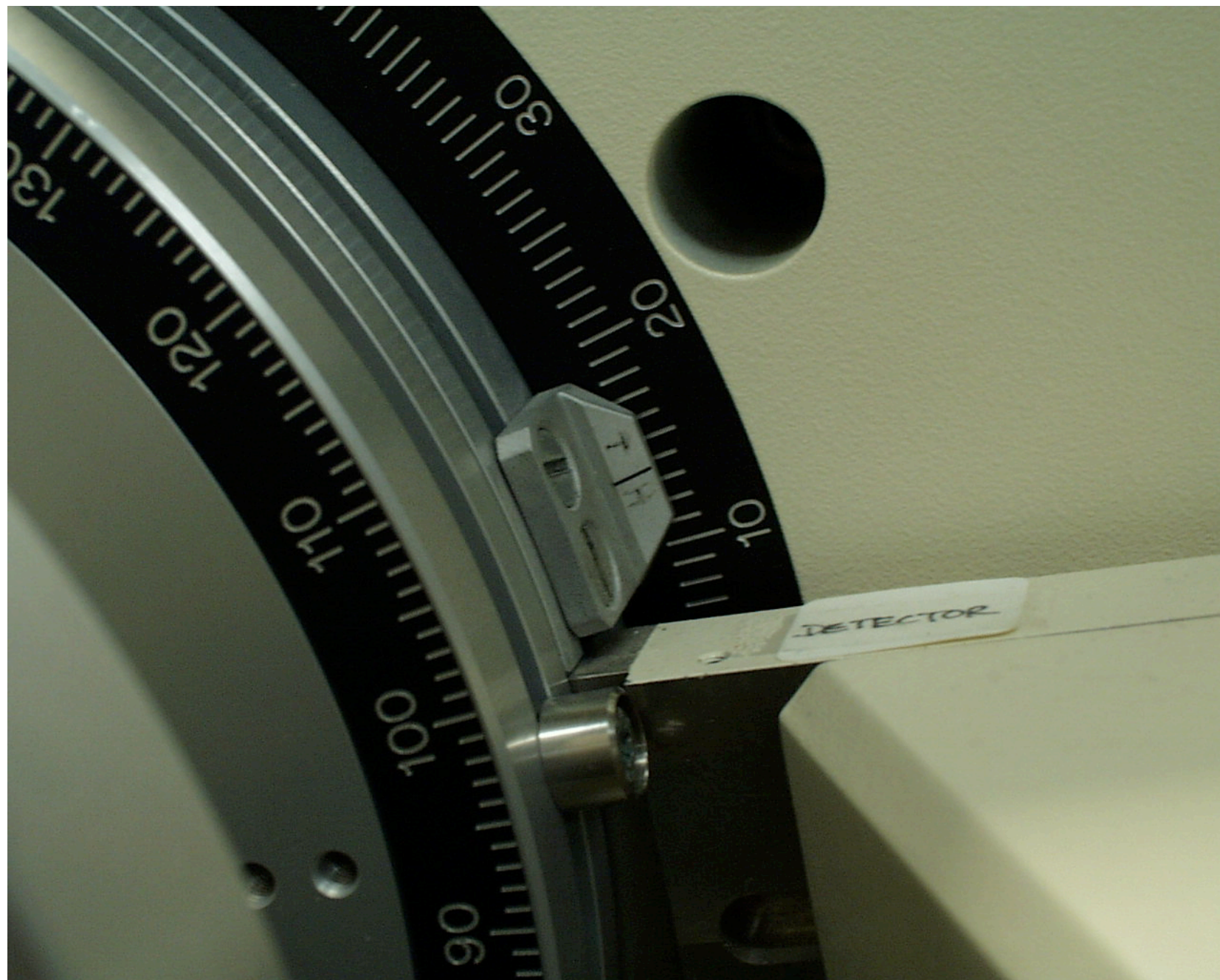
Set Axis Position

Sample Changer

Type: Single Sample

Current Position







Diffractometer Initialization

Goniometer

Type: Theta-Theta

Axis	Current Position
Detector	36.00000000
Tube	54.00000000

Set Axis Position

Sample Changer

Type: Single Sample

Current Position



Goniometer

Physical Axis	Actual Position	User Offset	Next Position
Detector	36.00000000	0.00000000	10.00000000
Tube	36.00000000	0.00000000	10.00000000

Close Help

Set Position

☐ Next Position

☒ Next 2-Theta

☐ User Offset

☐ Current Position

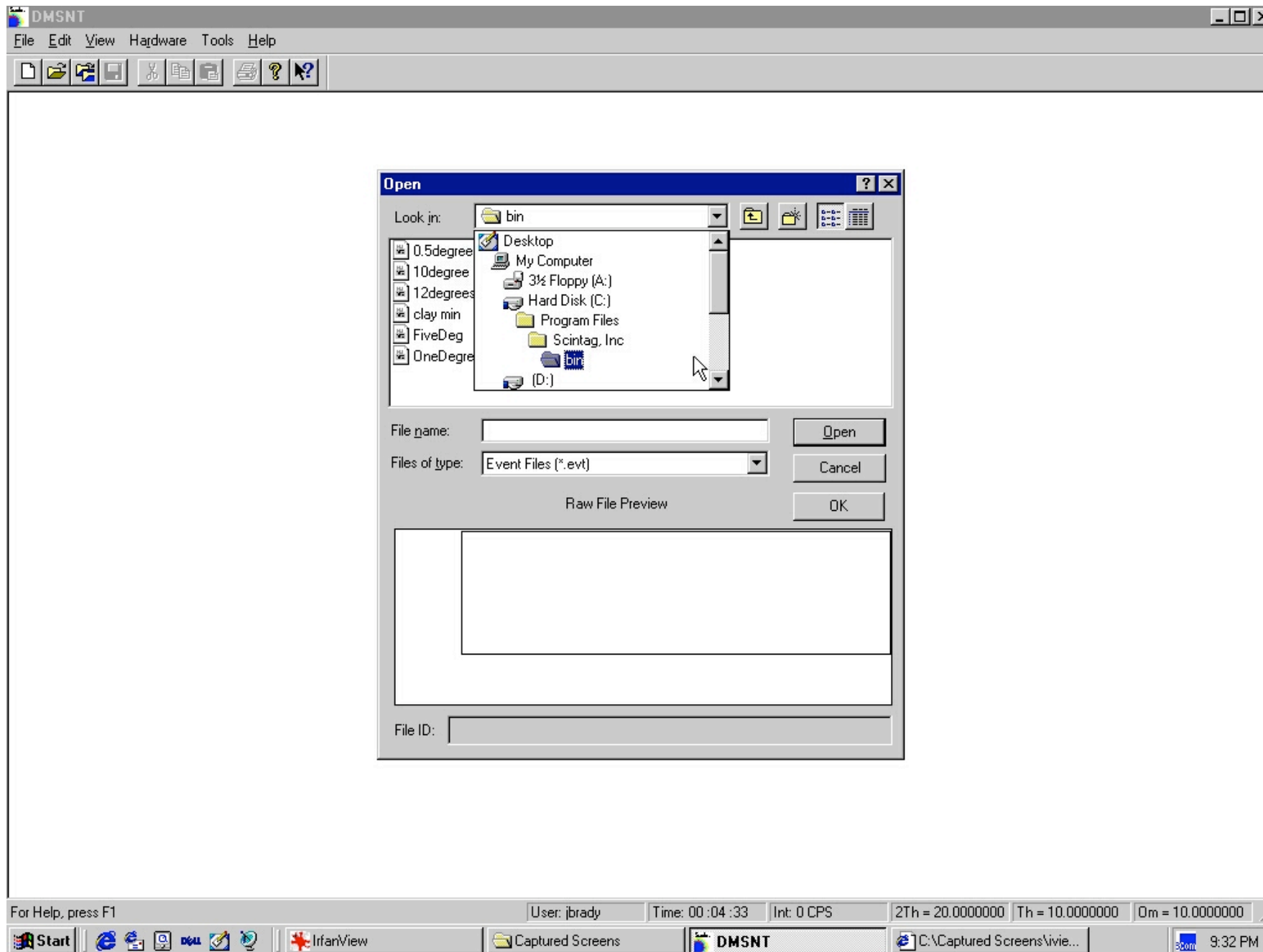
20

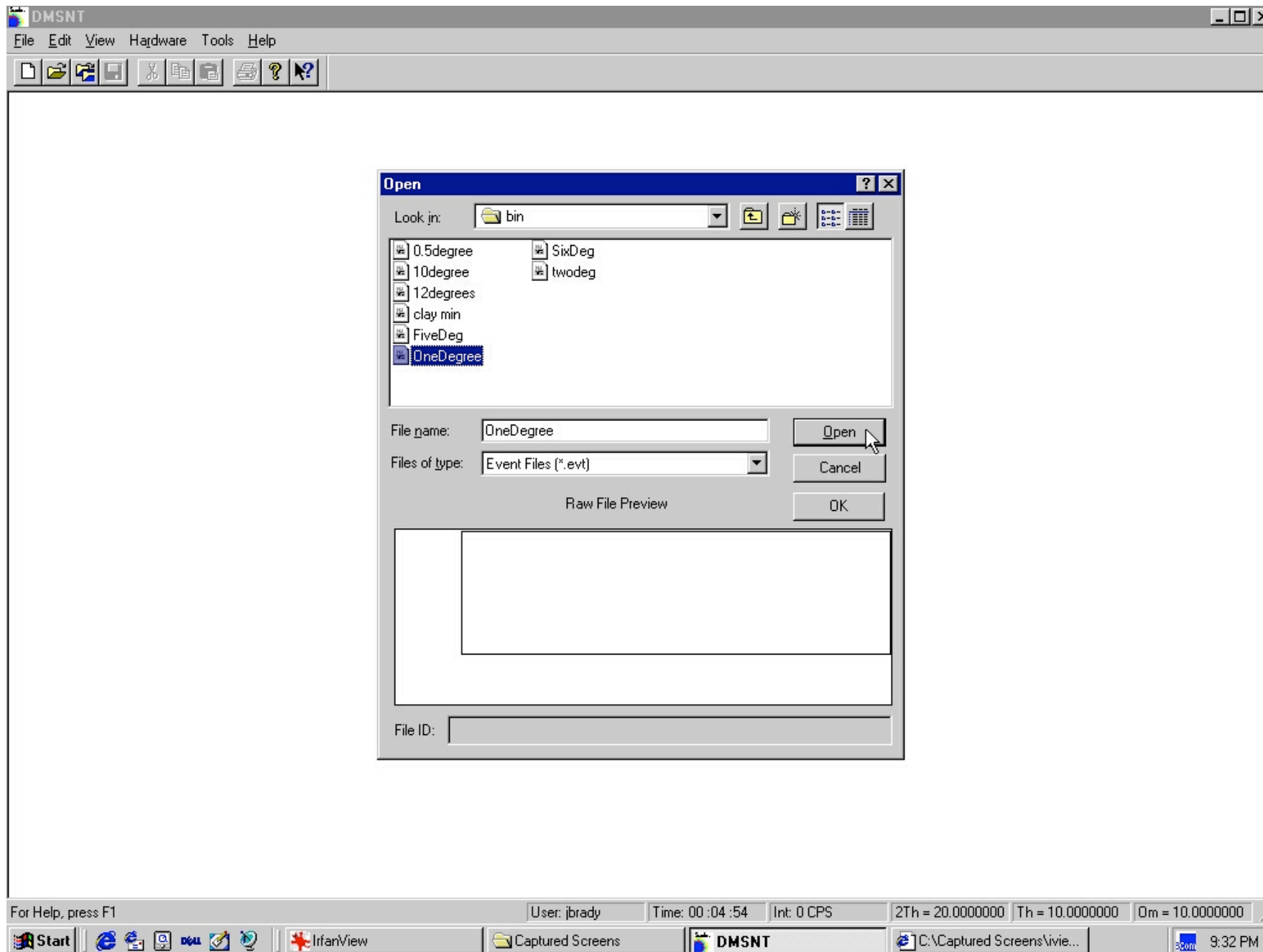
Set

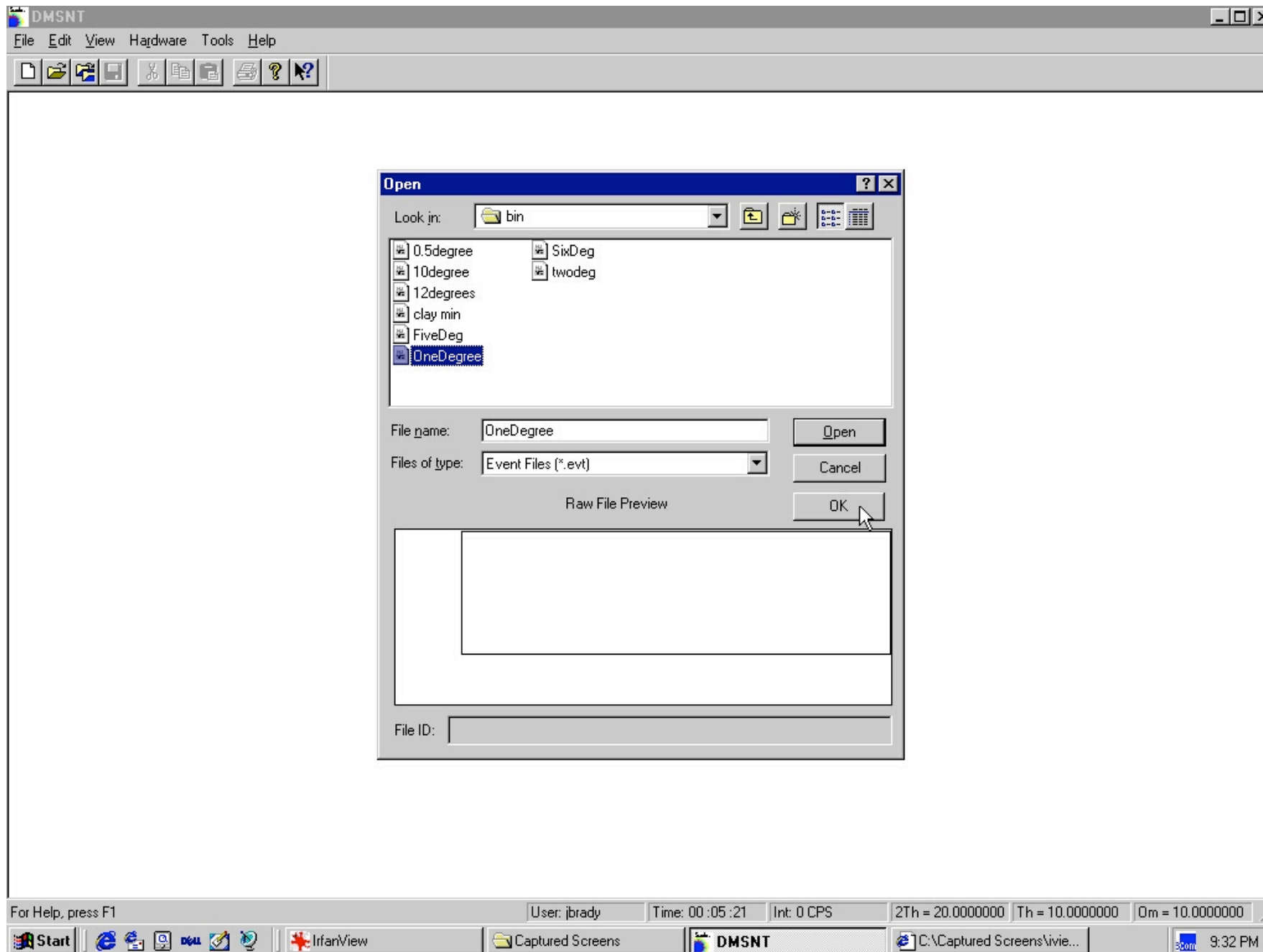
Move Calibrate

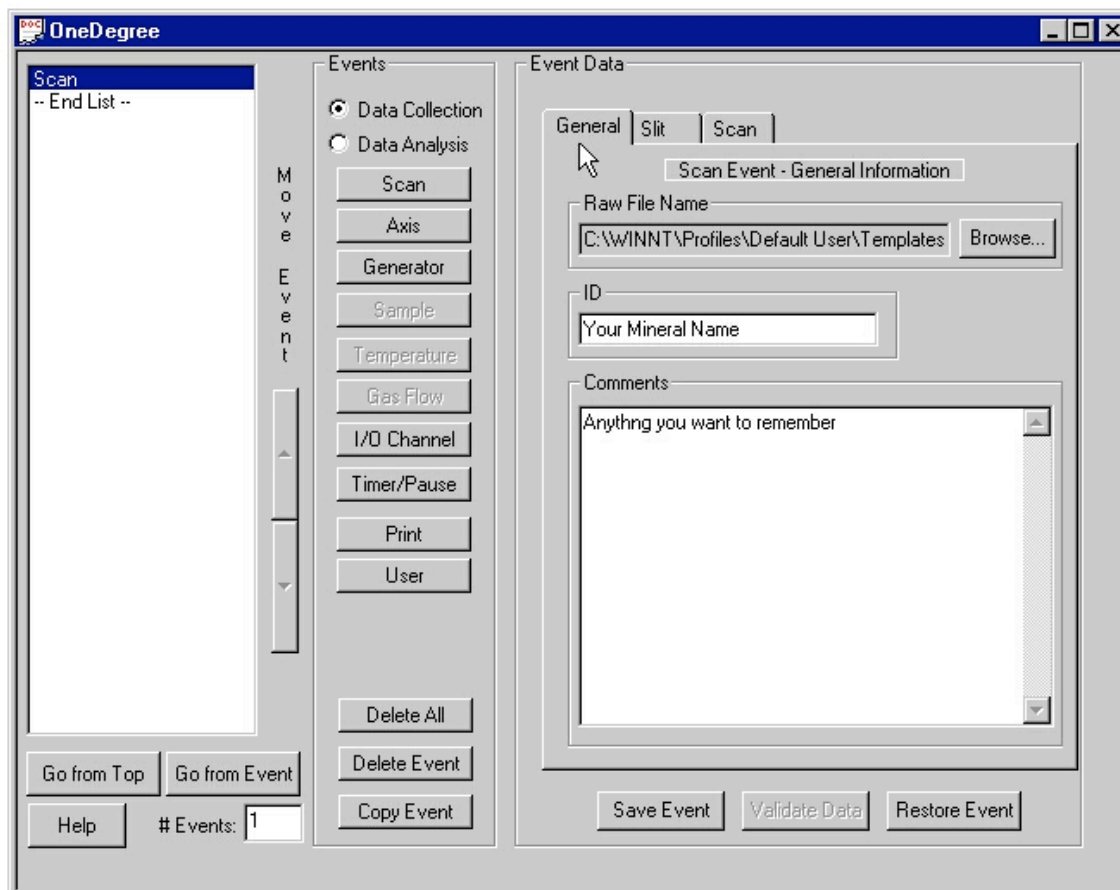
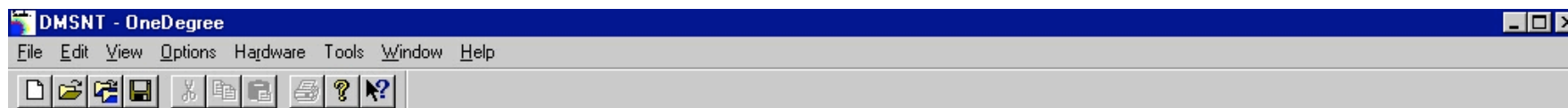
Test Move Set Axes Clear Set Moves Open Shutter Calibrate All Axes Axes Power Off

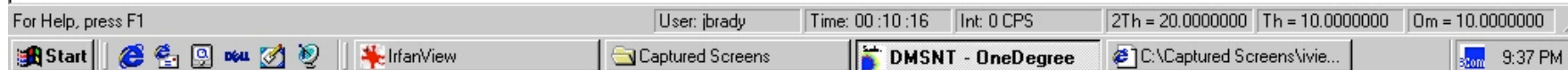
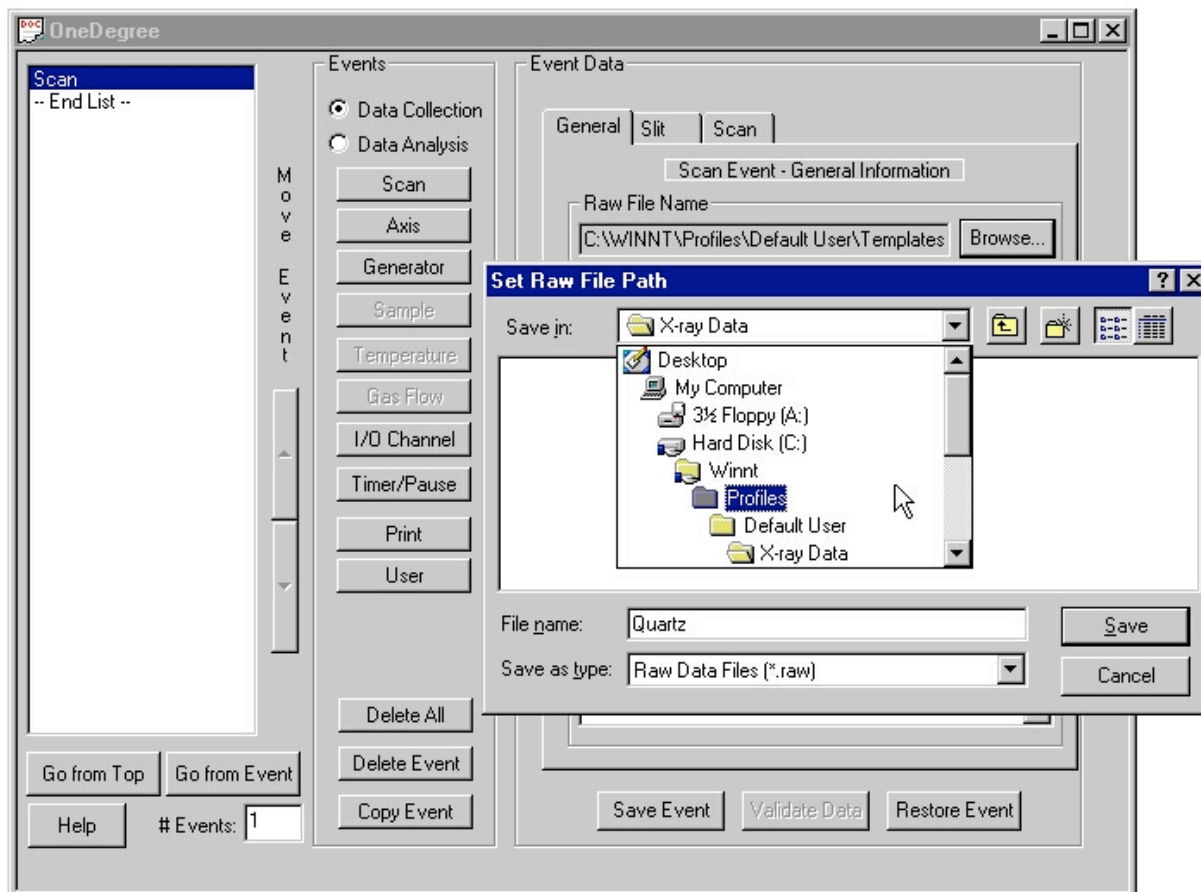
Scintag, Inc.

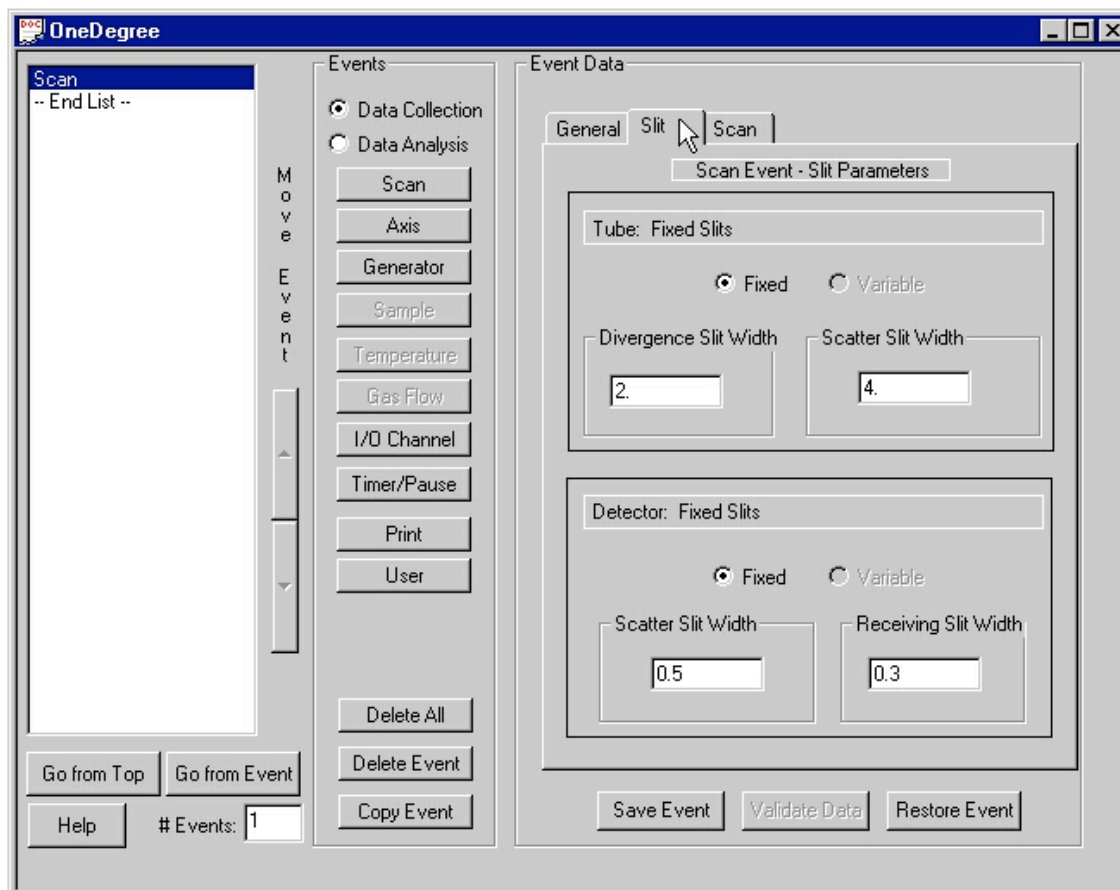
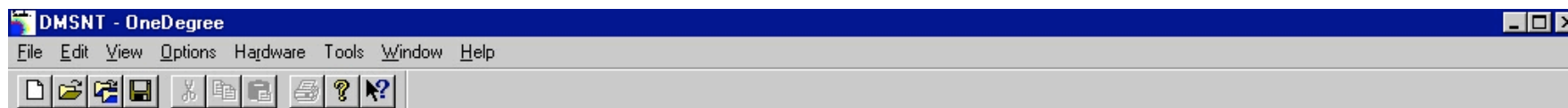


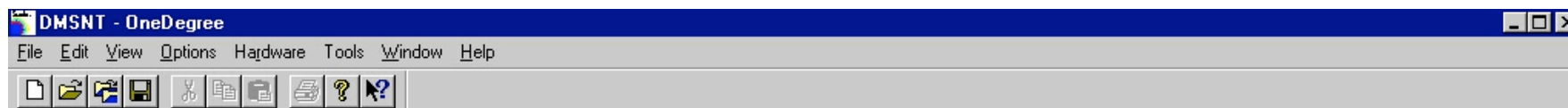












OneDegree

Events

☒ Data Collection
☐ Data Analysis

Scan
-- End List --

Move Event

Scan
Axis
Generator
Sample
Temperature
Gas Flow
I/O Channel
Timer/Pause
Print
User
Delete All
Delete Event
Copy Event

Go from Top
Go from Event
Help
Events: 1

Event Data

General | Slit | Scan

Scan Event - Range Parameters

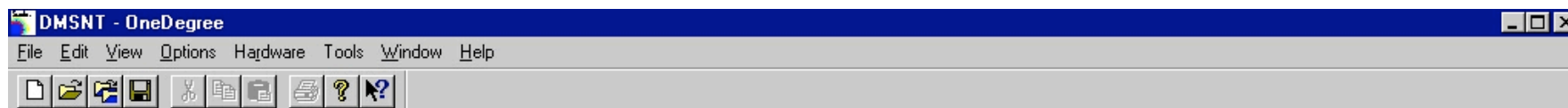
Step Size: 0.02
Type: Normal
Scan Time: 1:10:01

Current Range (2Theta)
Start Angle (deg): 5
Stop Angle (deg): 75
Scan Mode: ☐ Step ☒ Continuous
Time / Step (sec): 1.2
Rate (deg/min): 1.00
Est. Time: 1:10:01

Start Angle	Stop Angle	Scan Mode	Range
5.00000000	75.00000000	Cont	

Set
Add
Restore
Delete

Save Event
Validate Data
Restore Event



OneDegree

Events

☒ Data Collection
☐ Data Analysis

Scan
-- End List --

Move Event

Scan
Axis
Generator
Sample
Temperature
Gas Flow
I/O Channel
Timer/Pause
Print
User

Delete All
Delete Event
Copy Event

Go from Top
Go from Event
Help

Events: 1

Event Data

General Slit Scan

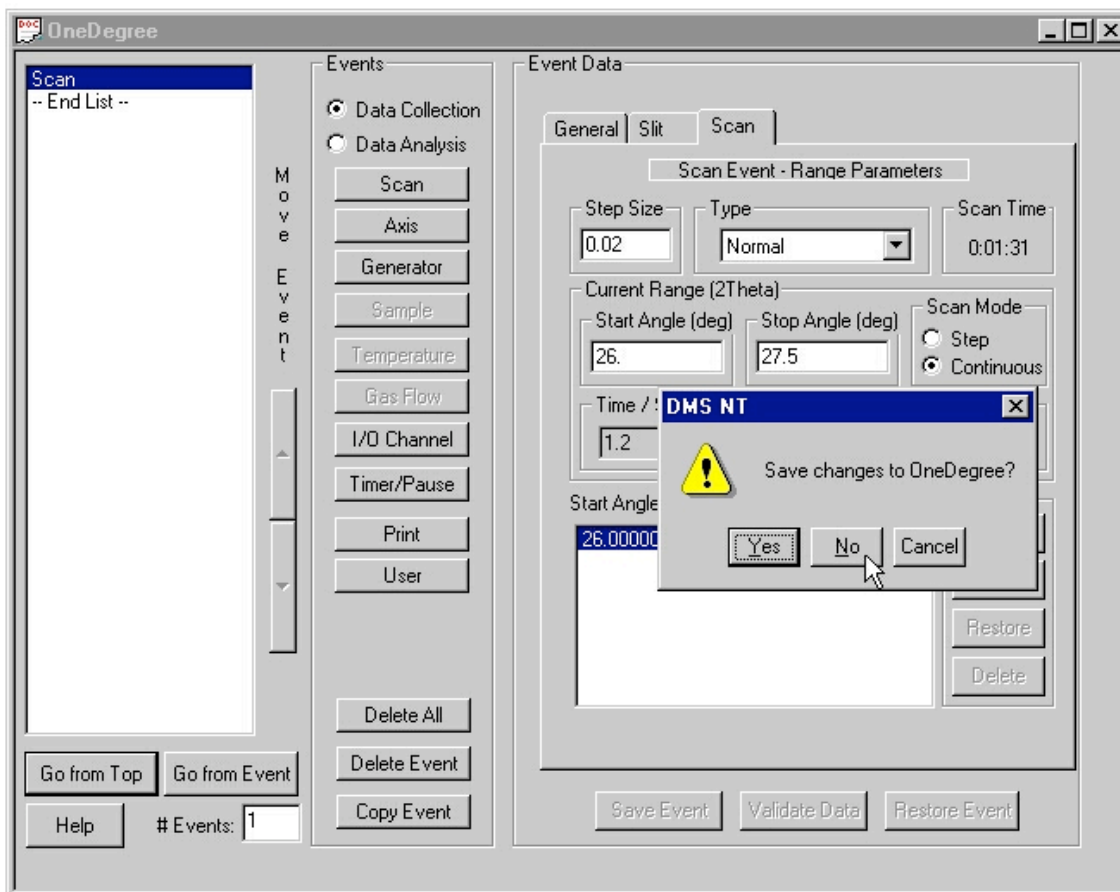
Scan Event - General Information

Raw File Name
C:\WINNT\Profiles\Default User\X-ray Data Browse...

ID
Novaculite Block

Comments
Anything you want to remember

Save Event Validate Data Restore Event



DMSNT - OneDegree - ACTIVE

File Edit View Options Hardware Tools Window Help

OneDegree - ACTIVE

Scan

-- End List --

Move Event

☒ Data Collection

☐ Data Analysis

Scan

Axis

Generator

Sample

Temperature

Gas Flow

I/O Channel

Timer/Pause

Print

User

Delete All

Delete Event

Copy Event

Event Data

General Slit Scan

Scan Event - General Information

Raw File Name

C:\WINNT\Profiles\Default User\X-ray Data

Browse...

ID

Novaculite Block

Comments

Anything you want to remember

Save Event

Validate Data

Restore Event

ABORT

Hold

Events:

1

Scan Status - Quartz.raw

File Name: Quartz.raw

0%

Scan Time Remaining

0:03:02

Realtme Display

For Help, press F1

User: jbrady

Time: 00:14:25

Int: 201 CPS

2Th = 26.0300000

Th = 13.0150000

Om = 13.0150000

Start

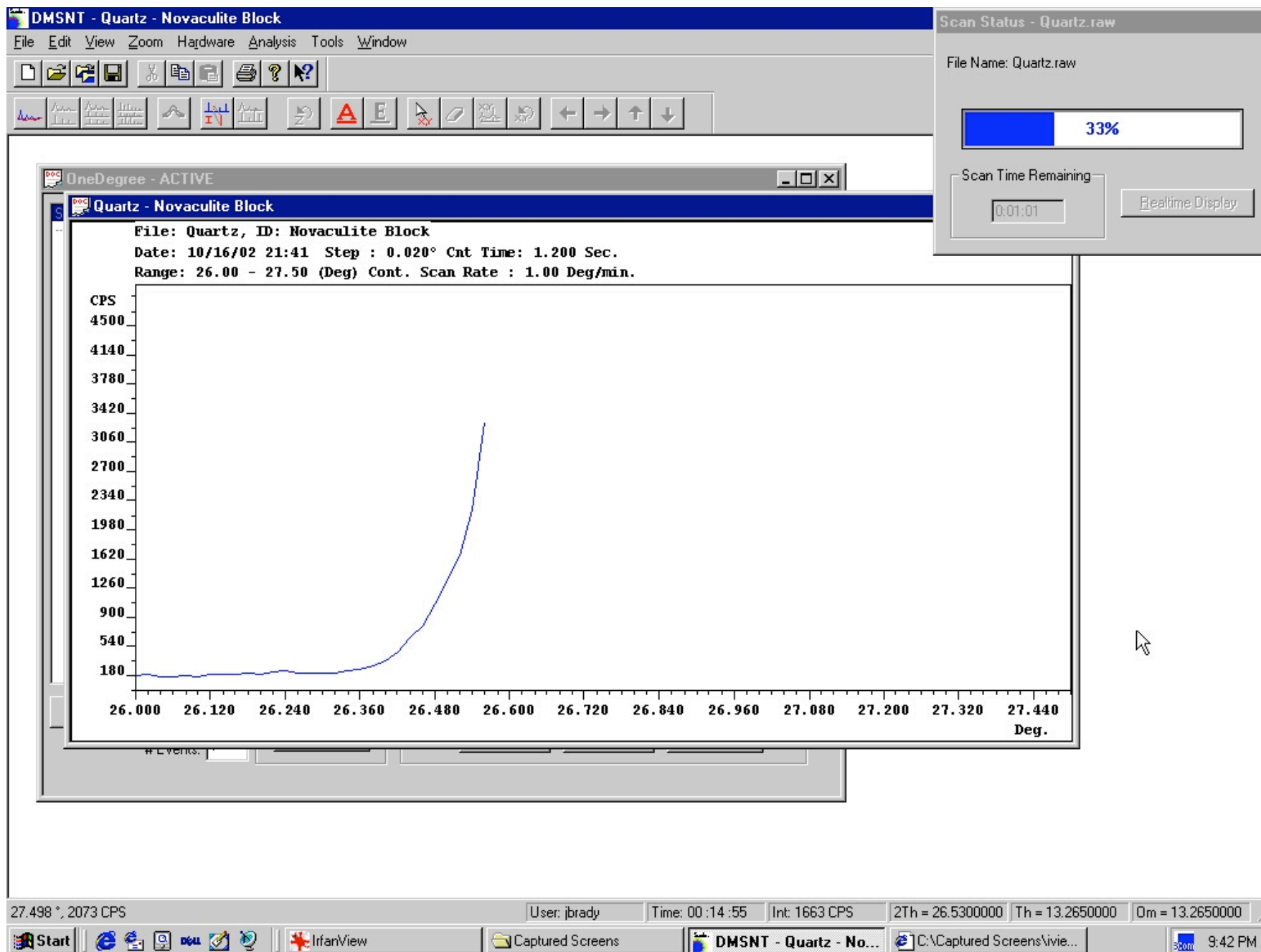
IrfanView

Captured Screens

DMSNT - OneDegree...

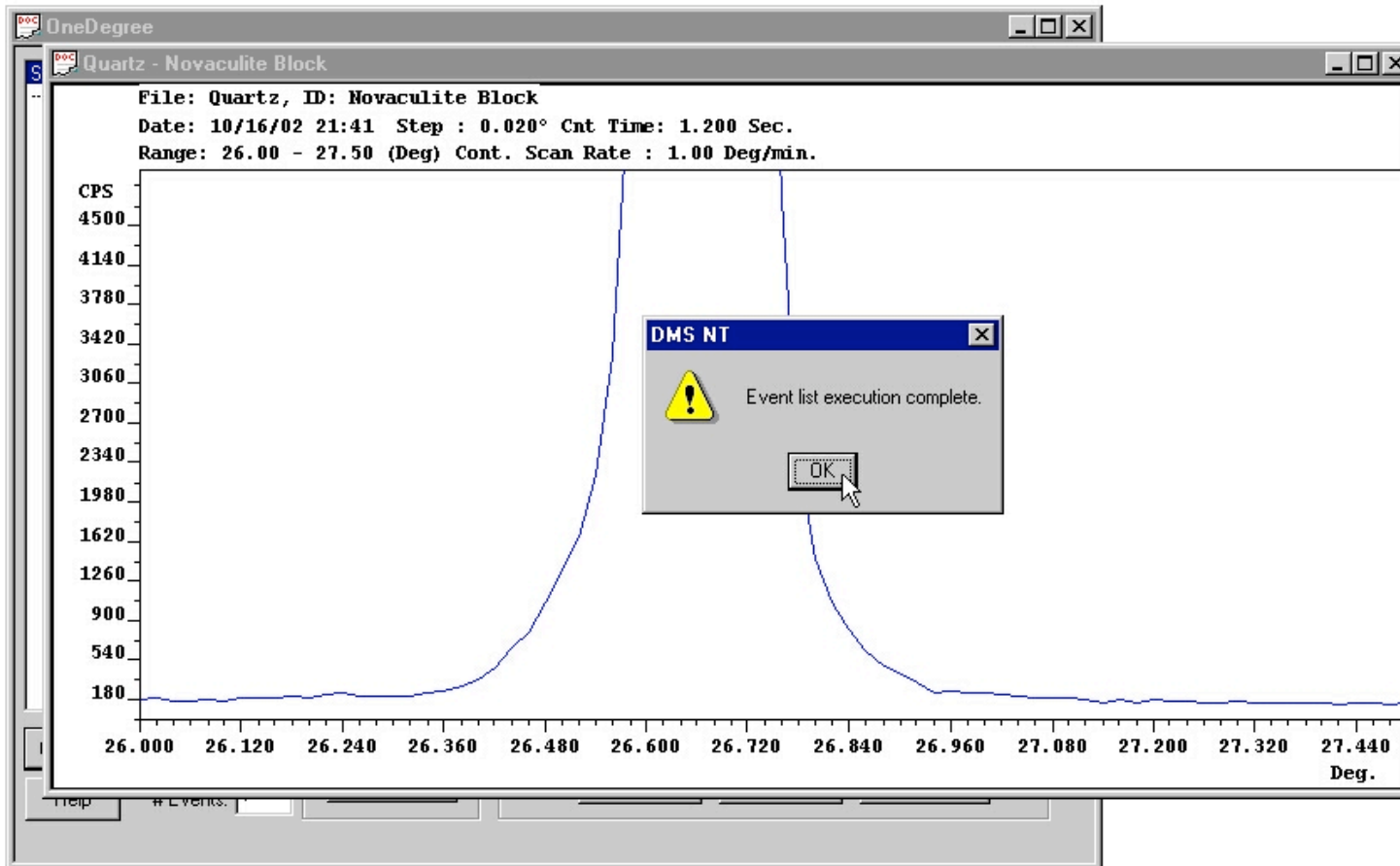
C:\Captured Screens\vie...

9:41 PM



DMSNT - Quartz - Novaculite Block

File Edit View Zoom Hardware Analysis Tools Window Help

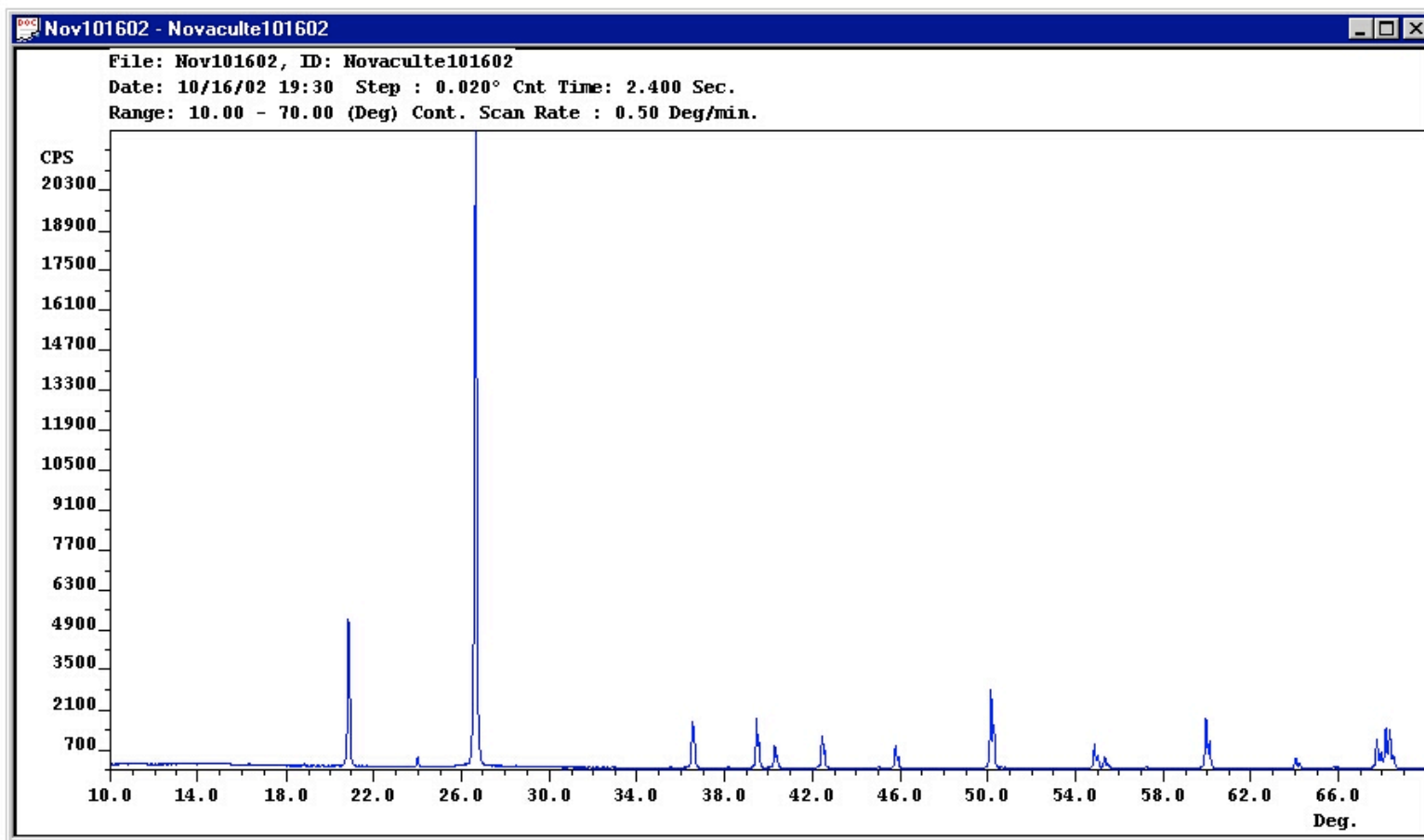
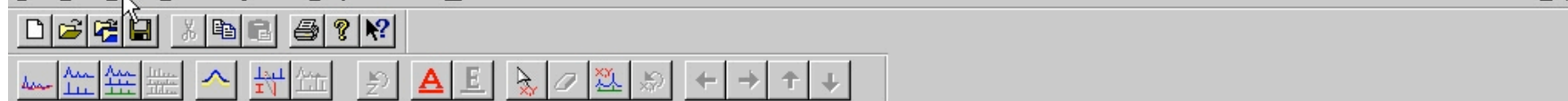


27.498 °, 2073 CPS User: jbrady Time: 00:16:01 Int: 152 CPS 2Th = 27.5100000 Th = 13.7550000 Om = 13.7550000

Start [Icons] IrfanView Captured Screens DMSNT - Quartz - No... C:\Captured Screens\vie... 9:43 PM

DMSNT - Nov101602 - Novaculte101602

File Edit View Zoom Hardware Analysis Tools Window Help



For Help, press F1

User: jbrady

Time: 00:17:17

Int: 152 CPS

2Th = 27.5100000

Th = 13.7550000

Om = 13.7550000

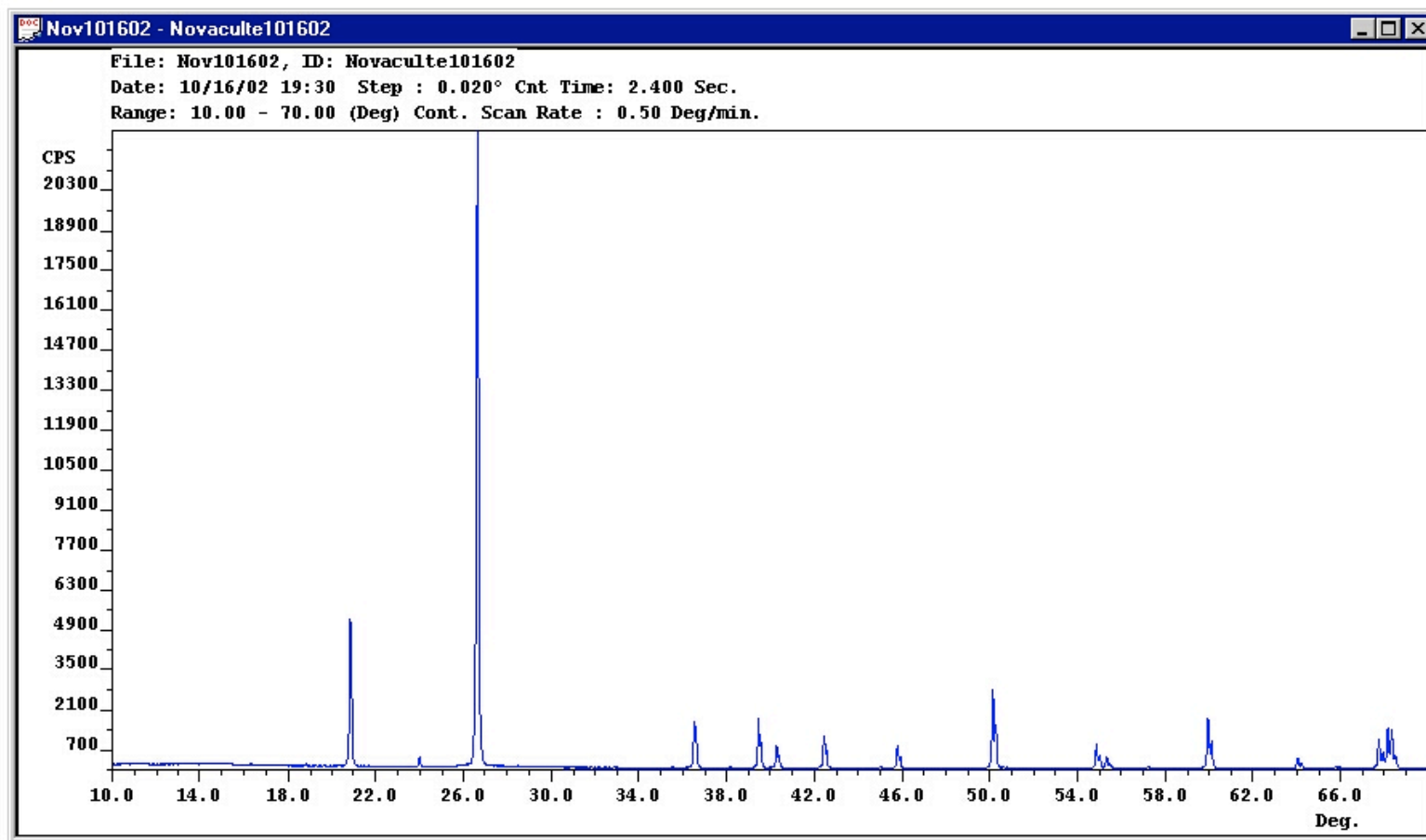
Start | Internet Explorer | Outlook | DMSNT - Nov101602... | C:\Captured Screens\vie... | 9:44 PM

DMSNT - Nov101602 - Novaculte101602

File Edit View Zoom Hardware Analysis Tools Window Help



Background...



Smooth data, correct data, and remove background signal

User: jbrady

Time: 00:17:26

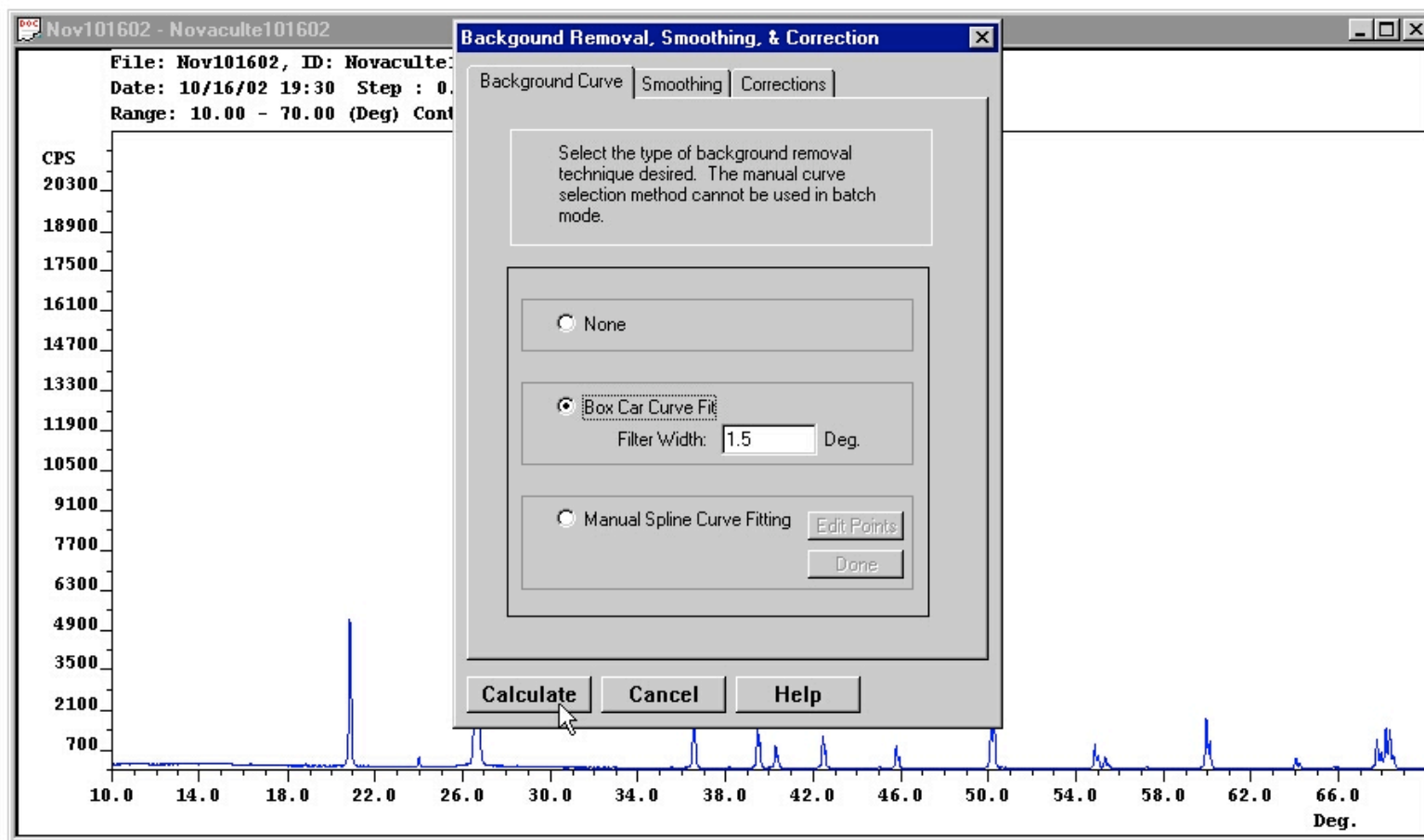
Int: 152 CPS

2Th = 27.5100000

Th = 13.7550000

Om = 13.7550000

Start | Internet Explorer | Dell | IrifarView | Captured Screens | DMSNT - Nov101602... | C:\Captured Screens\vie... | 9:44 PM



24.6 °, 7072 CPS

User: jbrady

Time: 00:17:41

Int: 152 CPS

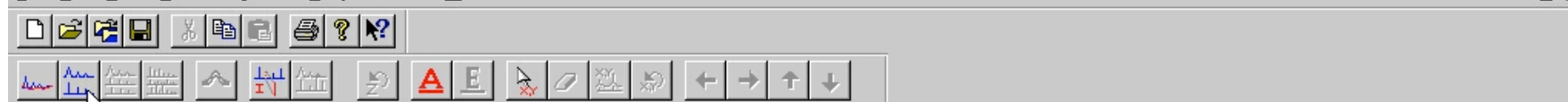
2Th = 27.5100000

Th = 13.7550000

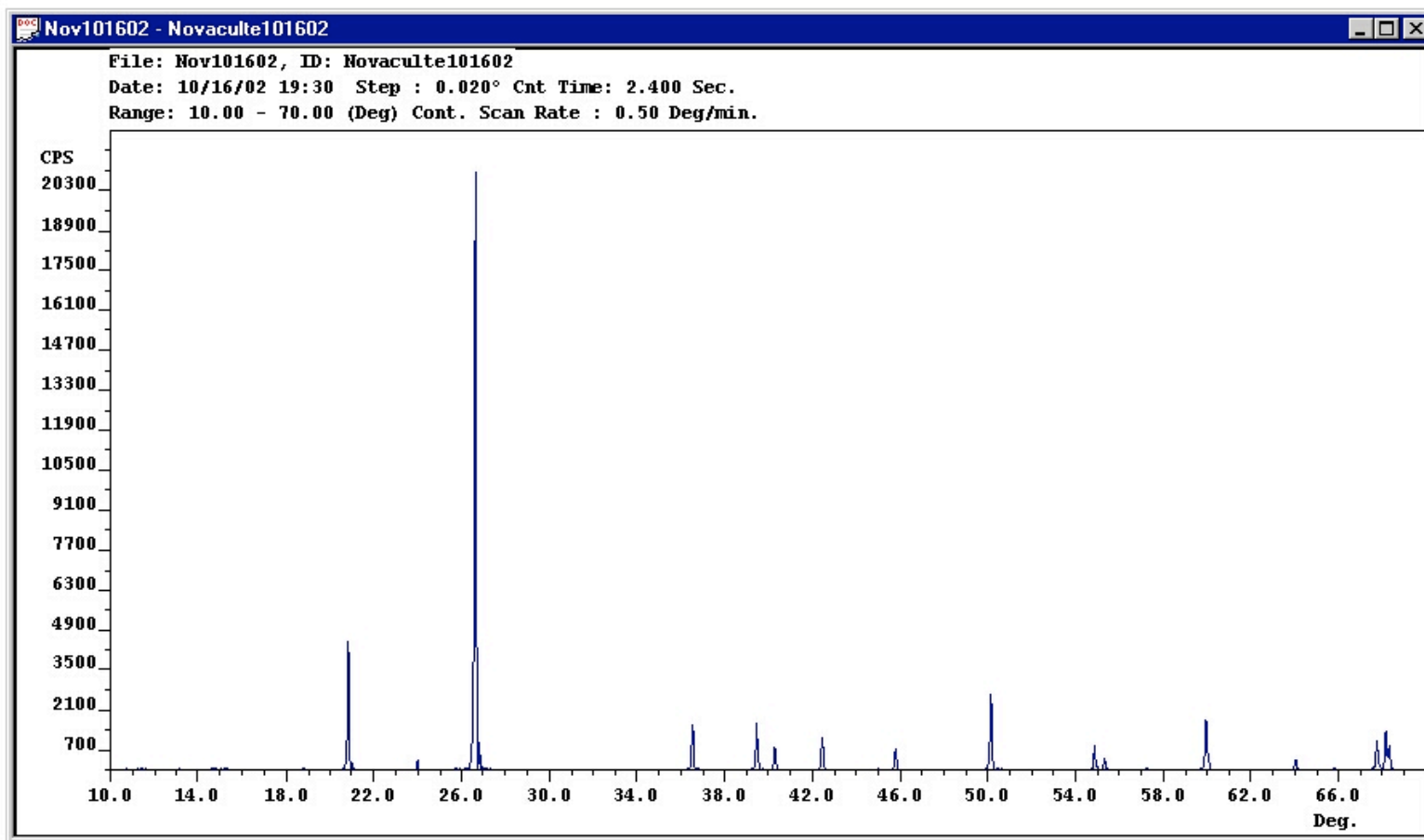
Om = 13.7550000

DMSNT - Nov101602 - Novaculte101602

File Edit View Zoom Hardware Analysis Tools Window Help

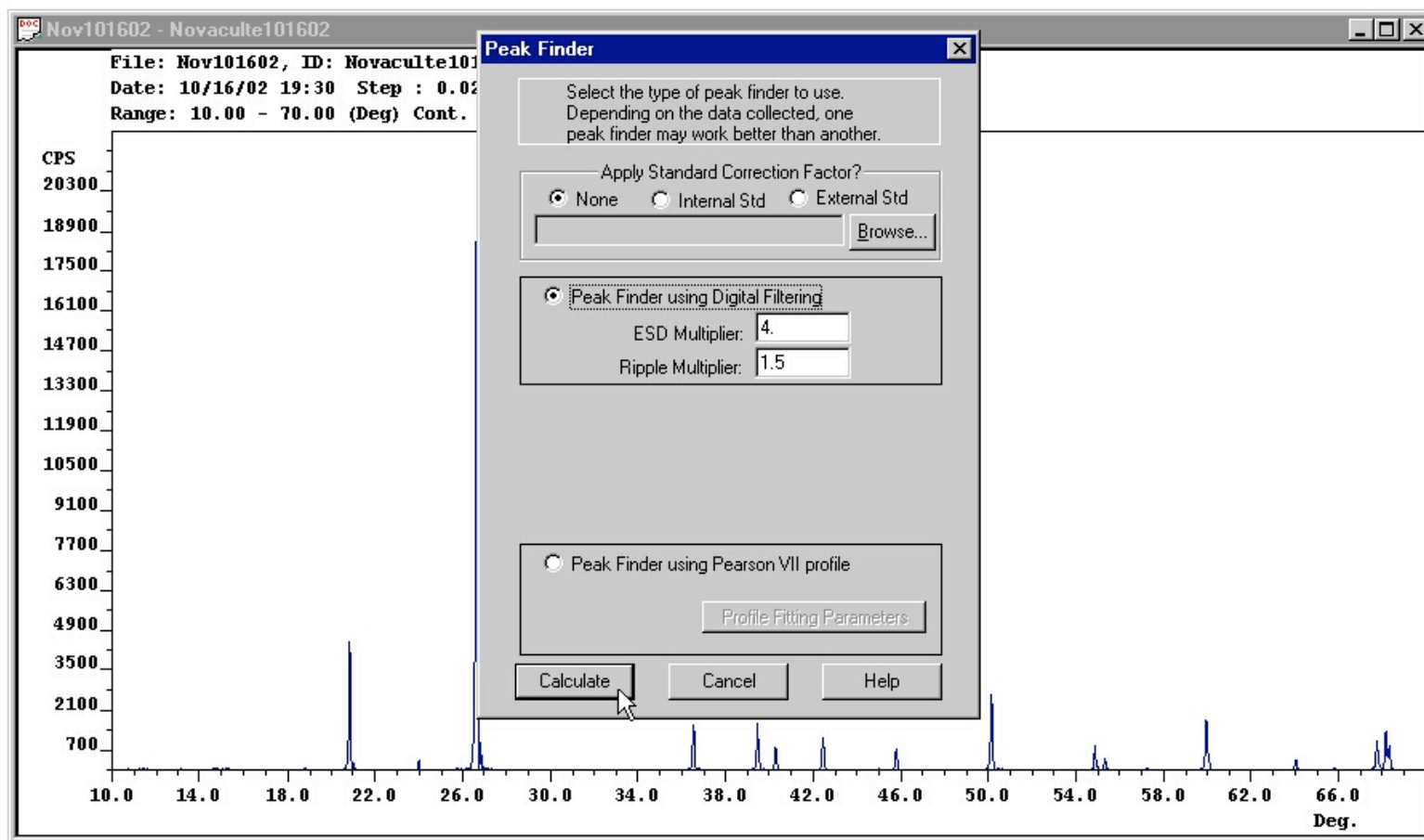
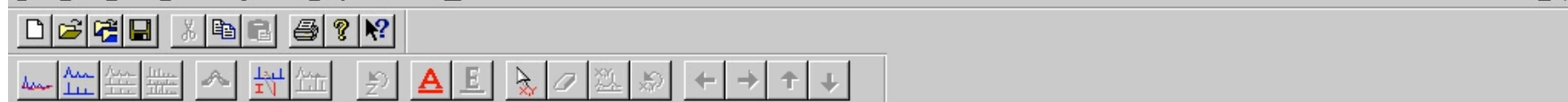


Peak Finder



Find peaks in the Net Intensity data User: jbrady Time: 00:17:53 Int: 152 CPS 2Th = 27.5100000 Th = 13.7550000 Om = 13.7550000

Start IrfanView Captured Screens DMSNT - Nov101... C:\Captured Screens\... 9:45 PM



For Help, press F1

User: jbrady

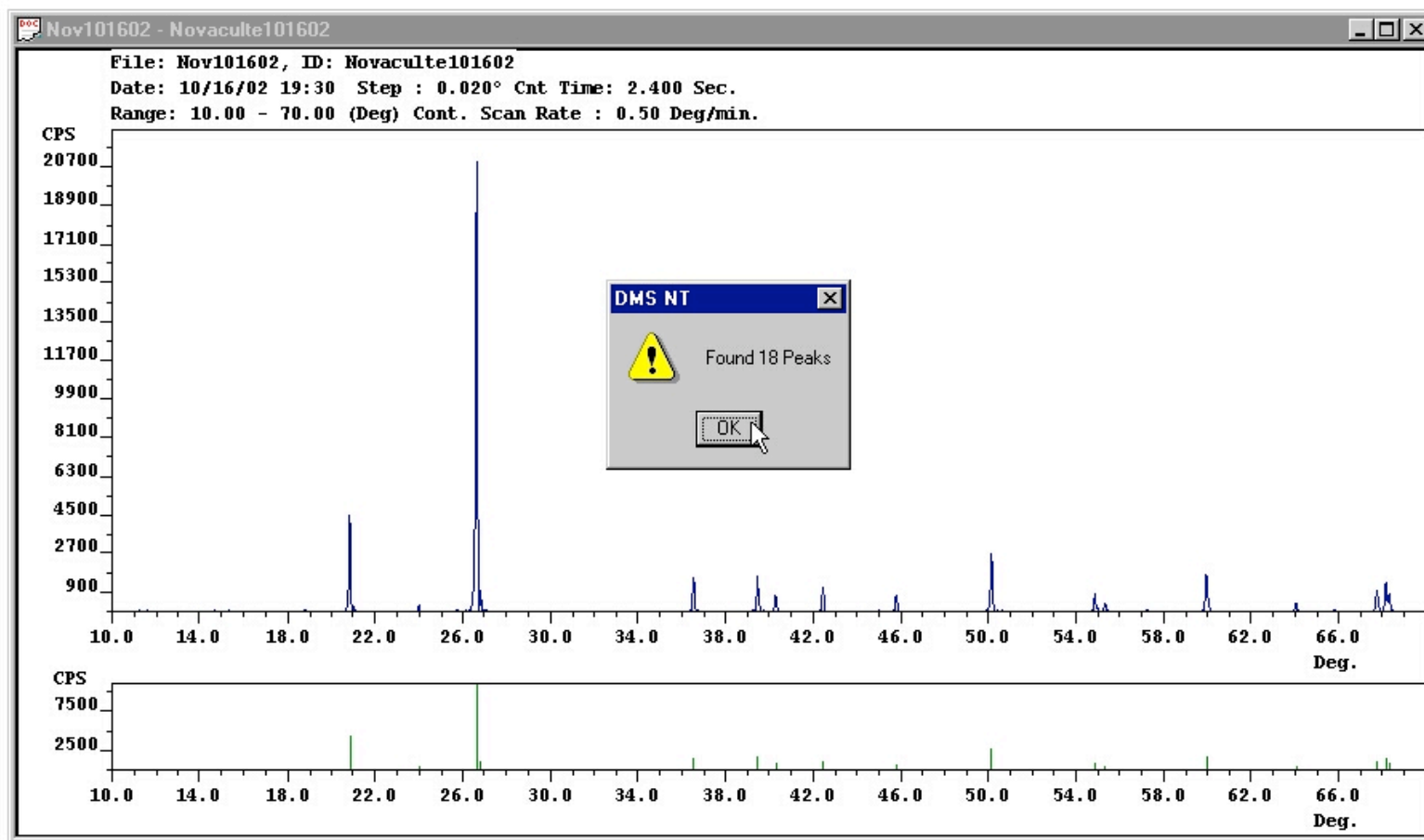
Time: 00:23:44

Int: 152 CPS

2Th = 27.5100000

Th = 13.7550000

Om = 13.7550000



For Help, press F1

User: jbrady

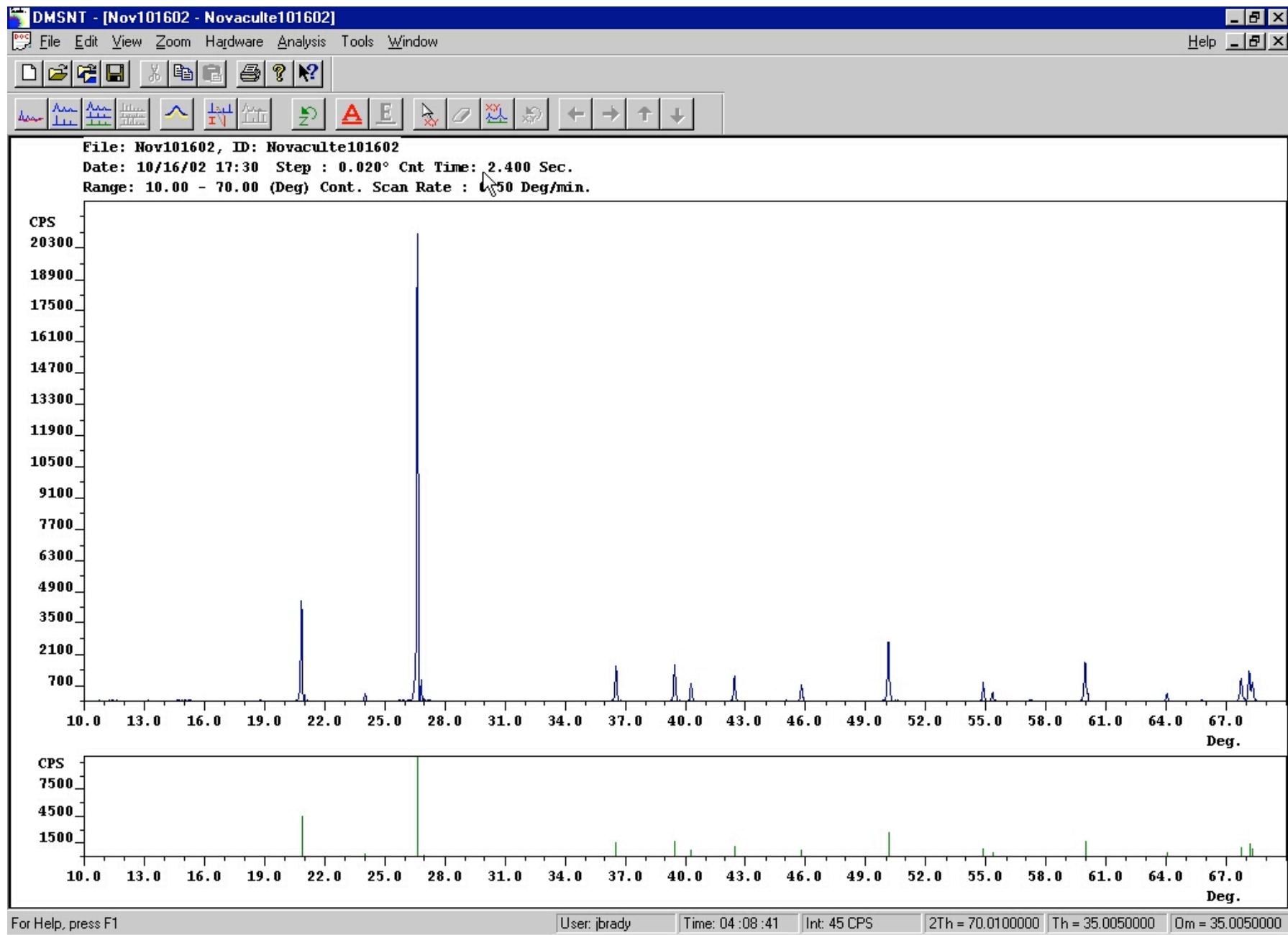
Time: 00:23:56

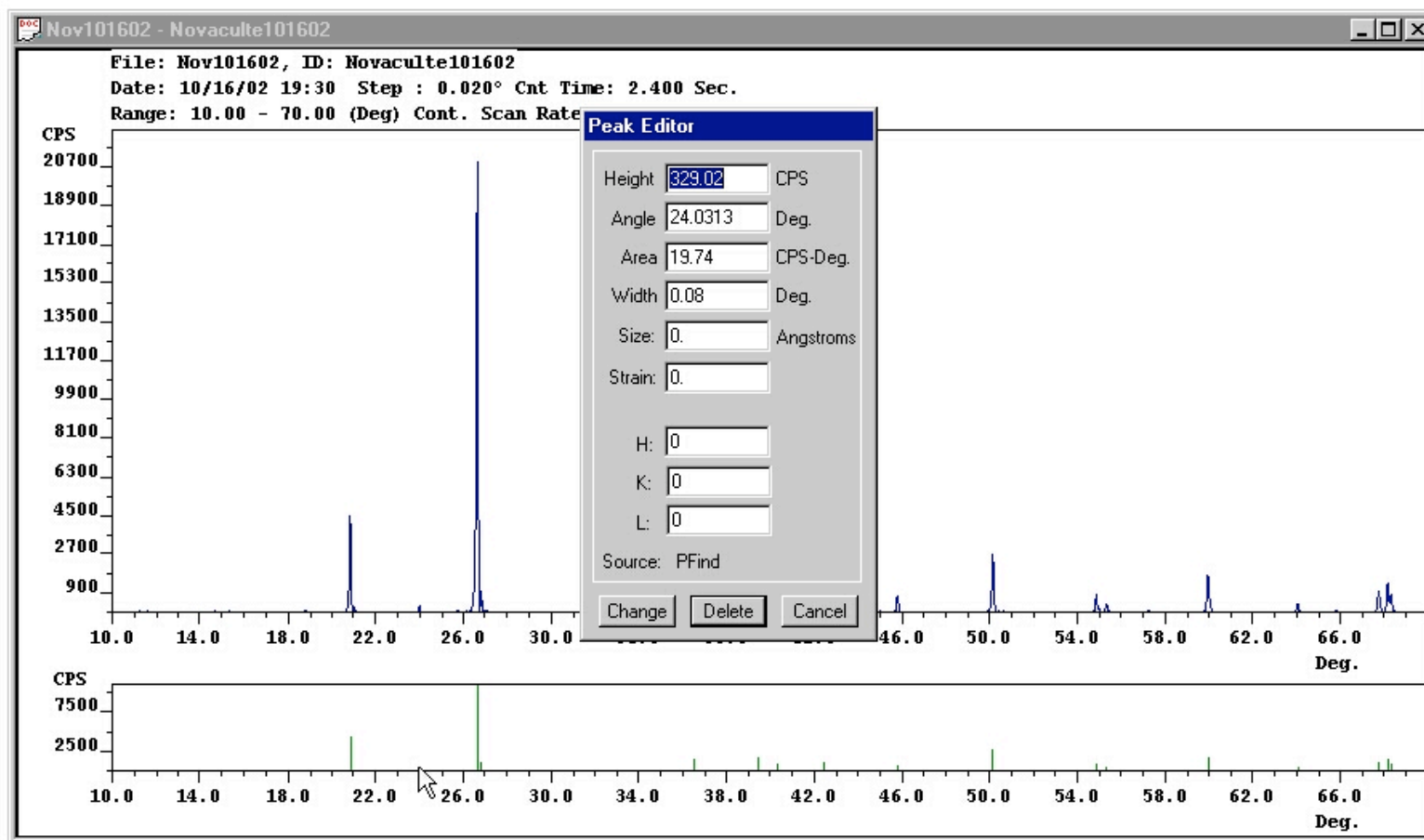
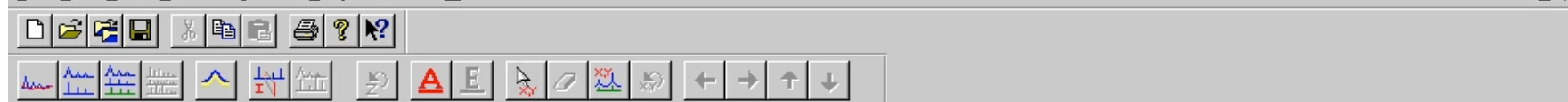
Int: 152 CPS

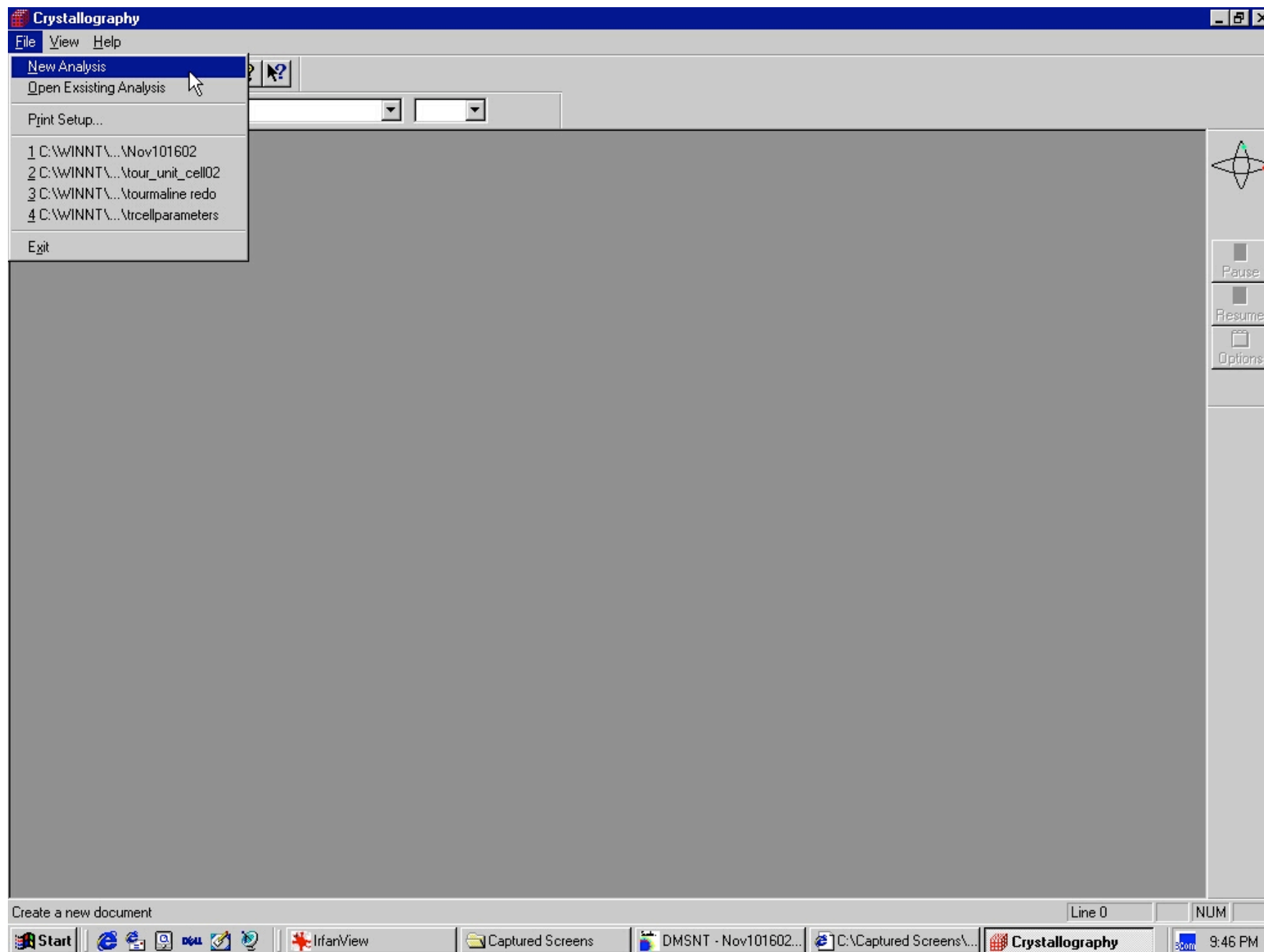
2Th = 27.5100000

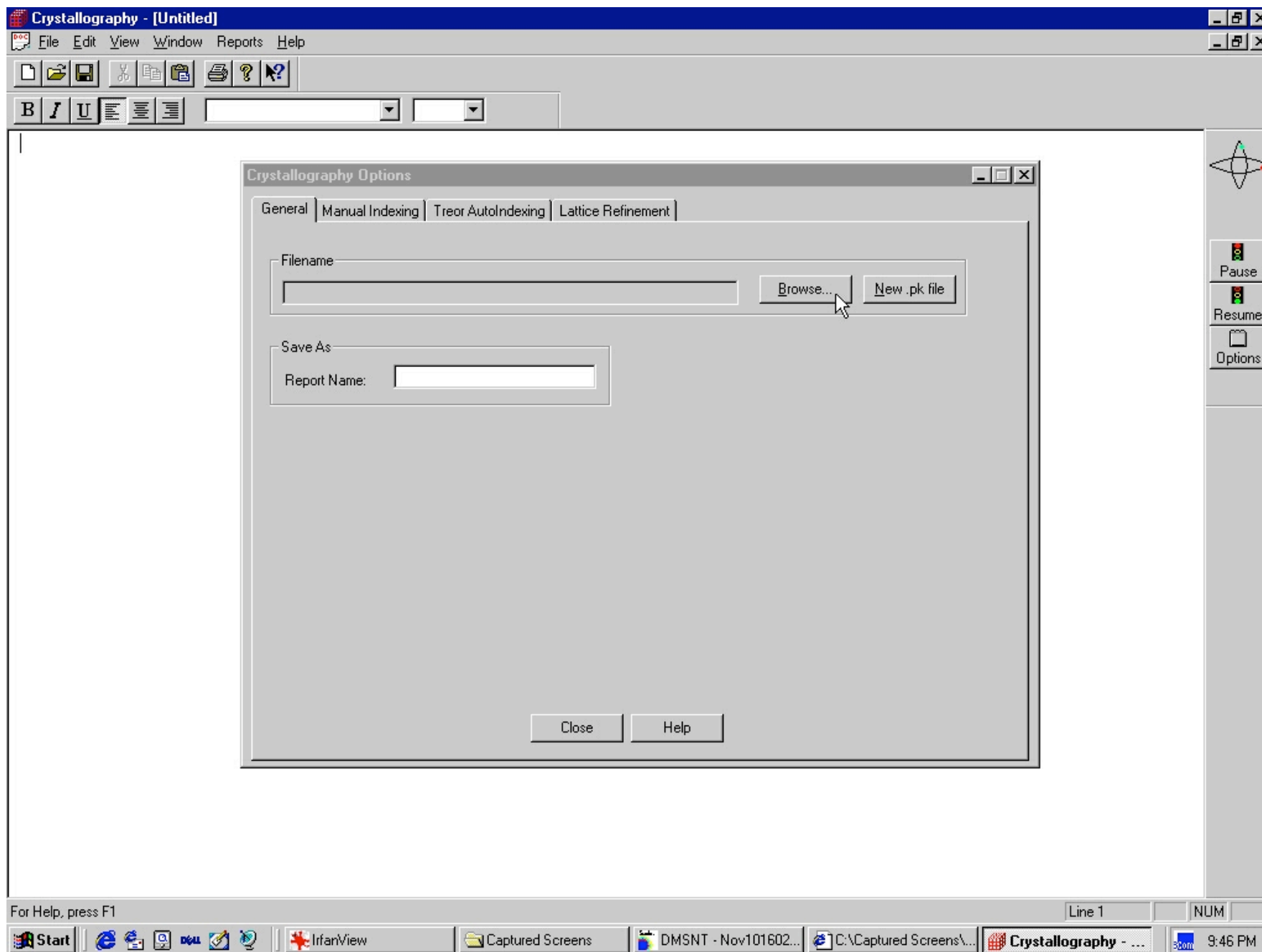
Th = 13.7550000

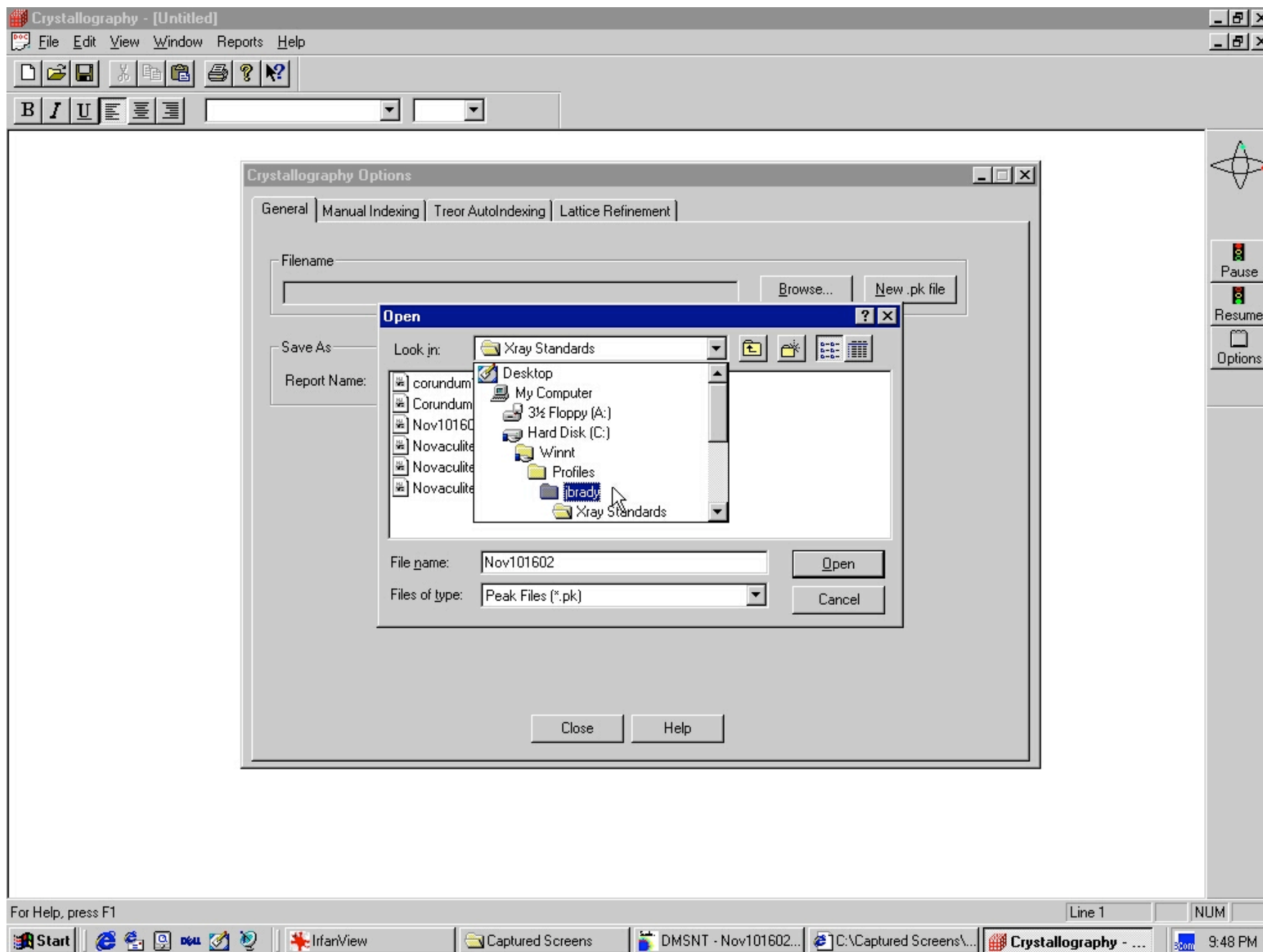
Om = 13.7550000











Crystallography - [Untitled]

File Edit View Window Reports Help

B *I* U

Crystallography Options

General Manual Indexing Treor AutoIndexing Lattice Refinement

Wavelength: KAlpha1: ☒ 1.540562 KAlpha1,2: ☐ 1.54183 KBeta: ☐ 1.392218 User Wavelength: 0

Input Mode: ☒ 2-Theta ☐ D-Spacing Sort By: ☒ 2-Theta ☐ Intensity Intensity: ☒ Absolute ☐ Relative Max Int: 20933

2-Theta Value	Intensity (CPS)	H Index	K Index	L Index
20.858749	4431	1	0	0
26.646875	20933	1	0	1
36.553123	1551	1	1	0
39.478127	1615	1	0	2
40.300625	771	1	1	1
42.460625	1074	2	0	0
45.803749	730	2	0	1
50.150002	2710	1	1	2
54.880001	803	2	0	2
55.336250	361	1	0	3
59.965626	1733	2	1	1

Add New Peak Reset Peaks

Save Save As Done



Pause

Resume

Options

For Help, press F1

Line 1

NUM

Start | Internet Explorer | Outlook | InfranView | Captured Screens | DMSNT - Nov101602... | C:\Captured Screens\... | Crystallography - ... | 9:48 PM

Crystallography Options

General Manual Indexing Treor AutoIndexing Lattice Refinement

Sample Identifier:

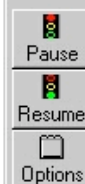
Crystal System

- CUBIC
- CUBIC
- HEXAGONAL
- MONOCLINIC 1
- MONOCLINIC 2
- MONOCLINIC 3
- ORTHORHOMBIC
- RHOMBOHEDRAL
- TETRAGONAL

2-Theta	Intensity	H	K	L
20.858749	4431	1	0	0
26.646875	20933	1	1	0
36.553123	1551	1	1	1
39.478127	1615	1	1	0
40.300625	771	1	1	1
42.460625	1074	2	0	0
45.803749	730	2	0	1
50.150002	2710	1	1	2
54.880001	803	2	0	2
55.336250	361	1	0	3
59.965626	1733	2	1	1
64.044373	355	1	1	3
67.751877	994	2	1	2
68.158127	1359	2	0	3

Refine Cell Parameters Select All Invert Selection

Begin Report Cancel





Crystallography Options

General | Manual Indexing | Treor AutoIndexing | Lattice Refinement

Sample Identifier:

Crystal System: **HEXAGONAL**

2-Theta	Intensity	H	K	L
20.858749	4431	1	0	0
26.646875	20933	1	0	1
36.553123	1551	1	1	0
39.478127	1615	1	0	2
40.300625	771	1	1	1
42.460625	1074	2	0	0
45.803749	730	2	0	1
50.150002	2710	1	1	2
54.880001	803	2	0	2
55.336250	361	1	0	3
59.965626	1733	2	1	1
64.044373	355	1	1	3
67.751877	994	2	1	2
68.158127	1359	2	0	3

Buttons: Refine Cell Parameters, Select All, Invert Selection, Begin Report, Cancel



Pause

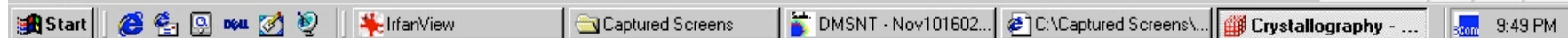
Resume

Options

For Help, press F1

Line 1

NUM





Crystallography Options

General | Manual Indexing | Treor AutoIndexing | Lattice Refinement

Sample Identifier:

Crystal System: **HEXAGONAL**

2-Theta	Intensity	H	K	L
20.858749	4431	1	0	0
26.646875	20933	1	0	1
36.553123	1551	1	1	0
39.478127	1615	1	0	2
40.300625	771	1	1	1
42.460625	1074	2	0	0
45.803749	730	2	0	1
50.150002	2710	1	1	2
54.880001	803	2	0	2
55.336250	361	1	0	3
59.965626	1733	2	1	1
64.044373	355	1	1	3
67.751877	994	2	1	2
68.158127	1359	2	0	3

Buttons: Refine Cell Parameters, Select All, Invert Selection, Begin Report, Cancel



Pause

Resume

Options

For Help, press F1

Line 1

NUM



9:49 PM

Crystallography - [Untitled]

File Edit View Window Reports Help

Crystallography - [Untitled]

*
* SCINTAG/USA LATTICE REFINEMENT PROGRAM *
* 3.00-WINNT *

CELL PARAMETERS:

A = 4.913139 B = 4.913139 C = 5.403852
ESD A = .000201 ESD B = .000201 ESD C = .000349

ALPHA = 90.000 BETA = 90.000 GAMMA = 120.000
ESD ALPHA = .000 ESD BETA = .000 ESD GAMMA = .000

VOLUME = 112.97

CRYSTAL SYMMETRY SYSTEM:

HEXAGONAL

H	K	L	2-THETA (DEG)			Q = (1/D**2)			INT(CPS)
			OBS	CALC	DELTA	OBS	CALC	DELTA	
1	0	0	20.8587	20.8600	-.0012	.05523	.05524	-.00001	4431
1	0	1	26.6469	26.6432	.0037	.08950	.08948	.00002	20933
1	1	0	36.5531	36.5478	.0054	.16575	.16571	.00005	1551
1	0	2	39.4781	39.4747	.0035	.19225	.19221	.00003	1615
1	1	1	40.3006	40.2951	.0055	.20000	.19995	.00005	771
2	0	0	42.4606	42.4544	.0062	.22100	.22094	.00006	1074
2	0	1	45.8037	45.7990	.0047	.25524	.25519	.00005	730
1	1	2	50.1500	50.1475	.0025	.30271	.30269	.00003	2710
2	0	2	54.8800	54.8817	-.0017	.35790	.35792	-.00002	803
1	0	3	55.3363	55.3389	-.0027	.36341	.36344	-.00003	361
2	1	1	59.9656	59.9644	.0012	.42091	.42090	.00002	1733
1	1	3	64.0444	64.0474	-.0030	.47387	.47391	-.00004	355
2	1	2	67.7519	67.7513	.0005	.52364	.52363	.00001	994
2	0	3	68.1581	68.1560	.0022	.52917	.52915	.00003	1359
3	0	1	68.3044	68.3186	-.0142	.53117	.53137	-.00019	805

H	K	L	2-THETA (DEG)			D - SPACINGS			INT(CPS)
			OBS	CALC	DELTA	OBS	CALC	DELTA	
1	0	0	20.8587	20.8600	-.0012	4.25515	4.25490	.00024	4431
1	0	1	26.6469	26.6432	.0037	3.34254	3.34300	-.00046	20933
1	1	0	36.5531	36.5478	.0054	2.45677	2.45657	.00020	1551

Crystallography - [Untitled]

Line 33 NUM

Start

InfraView

Captured Screens

DMSNT - Nov101602...

C:\Captured Screens\...

Crystallography - ...

9:50 PM