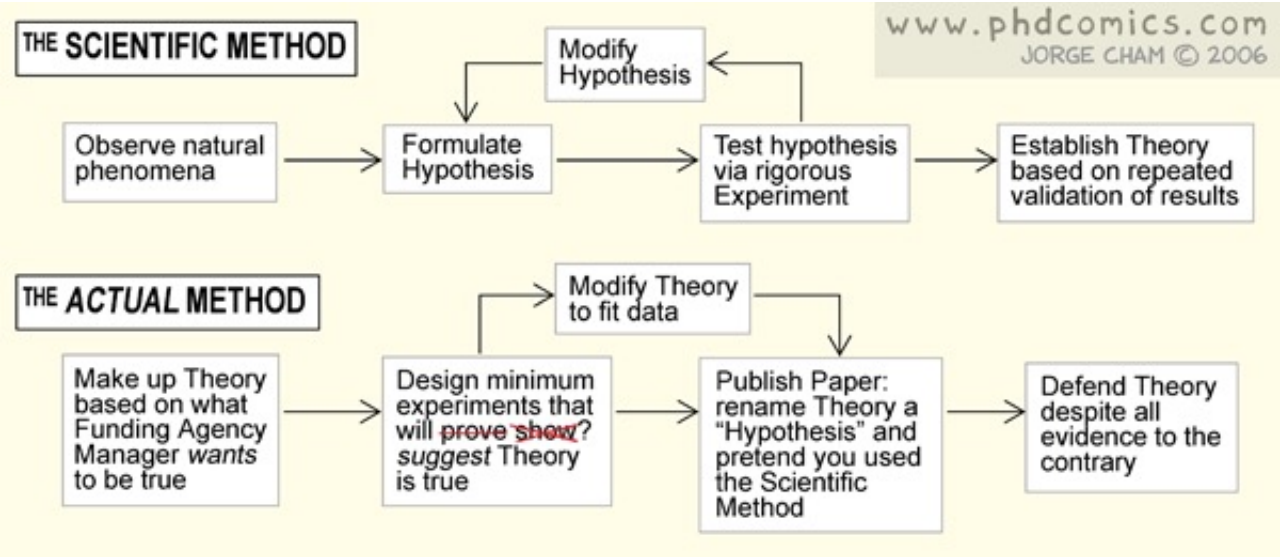
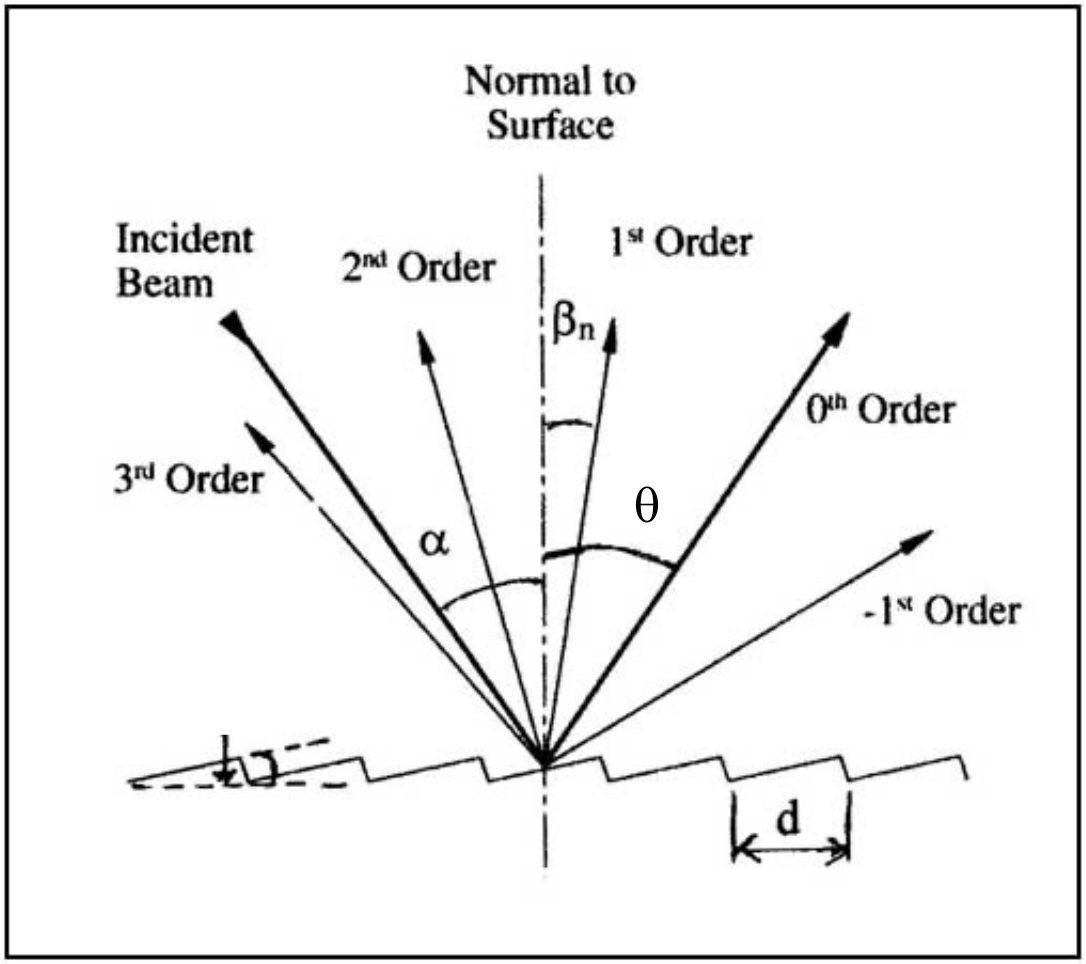
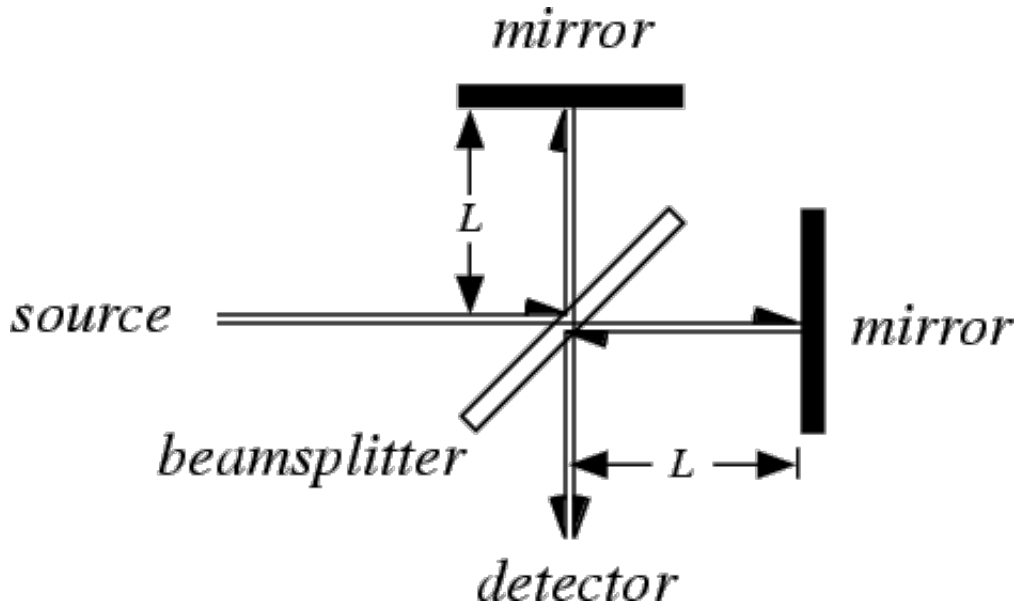
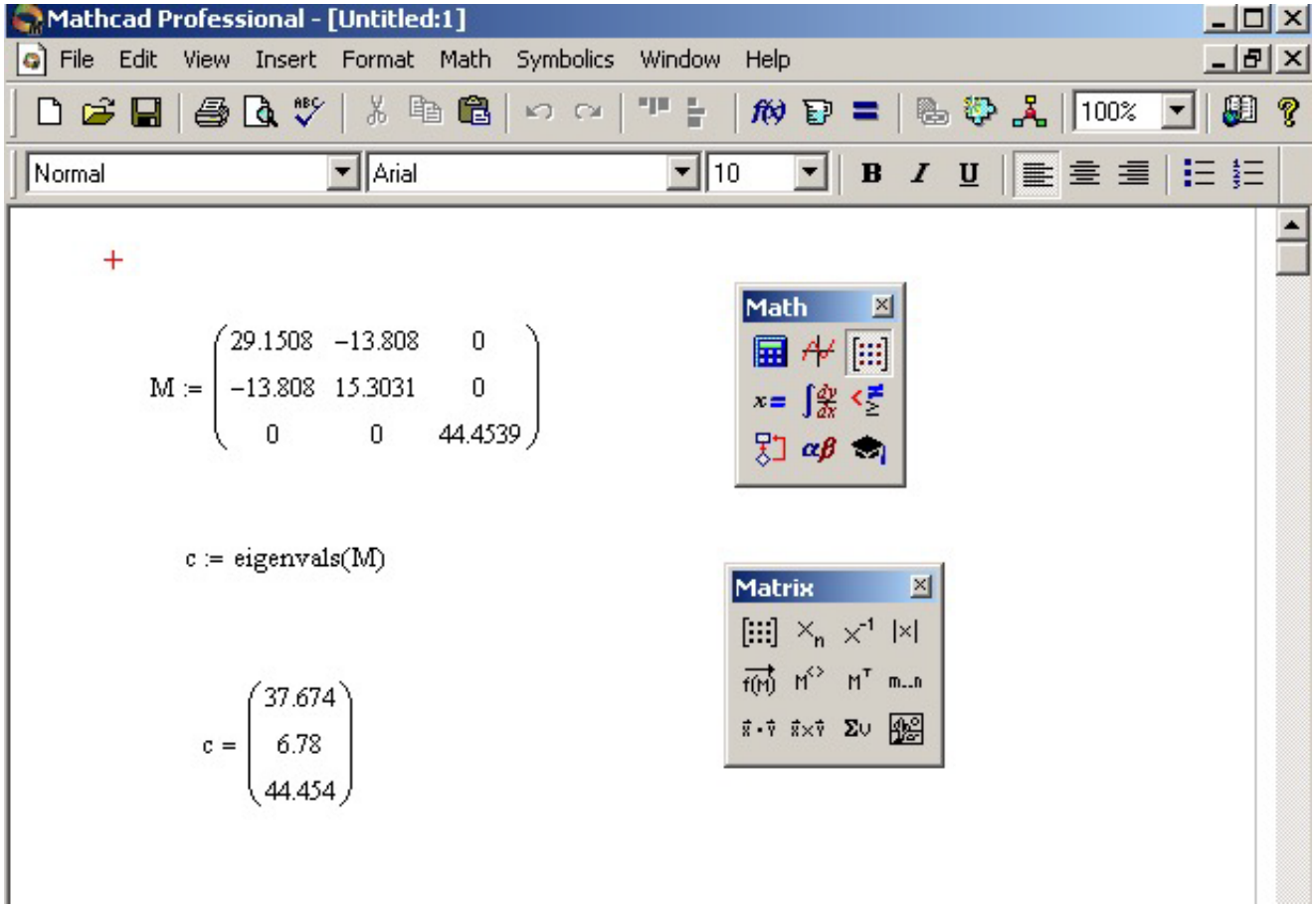

THE SCIENTIFIC METHOD
Modify Hypothesis
Observe natural phenomena
Formulate Hypothesis
Test hypothesis via rigorous Experiment
Establish Theory based on repeated validation of results
www.phdcomics.com
JORGE CHAM © 2006
THE ACTUAL METHOD
Modify Theory to fit data
Make up Theory based on what Funding Agency Manager wants to be true
Design minimum experiments that will prove show? suggest Theory is true
Publish Paper: rename Theory a "Hypothesis" and pretend you used the Scientific Method
Defend Theory despite all evidence to the contrary



Reflection Grating Diffracted Orders


mirror
L
source
mirror
beamsplitter
L
detector

https://www.staff.ncl.ac.uk/j.p.goss/symmetry/Molecules_pov.html


Mathcad Professional - [Untitled:1]
File Edit View Insert Format Math Symbolics Window Help
100%
Normal
Arial
10
Math
Matrix
M := 29.1508 −13.808 0
−13.808 15.3031 0
0 0 44.4539
c := eigenvals(M)
c = 37.674
6.78
44.454

Daniel, F.; Cernicharo, J.; Dubernet, The Excitation of N2H+ in Interstellar Molecular Clouds, The Astrophysical Journal, 648, 461, 2006

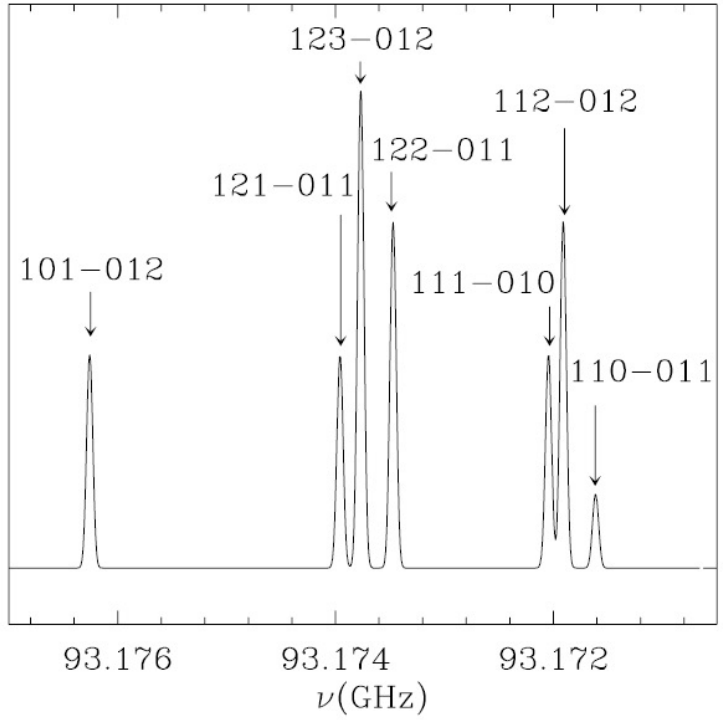
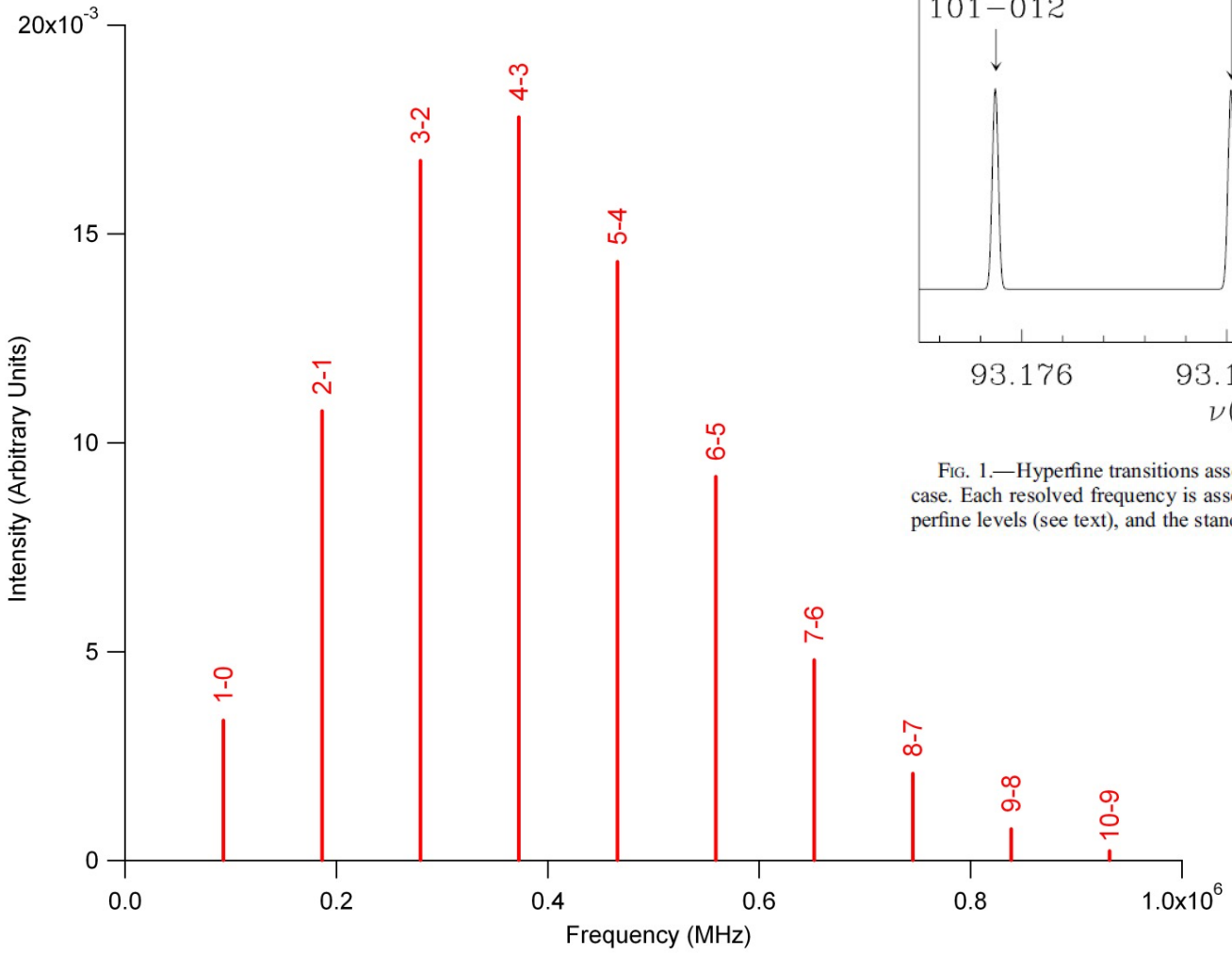
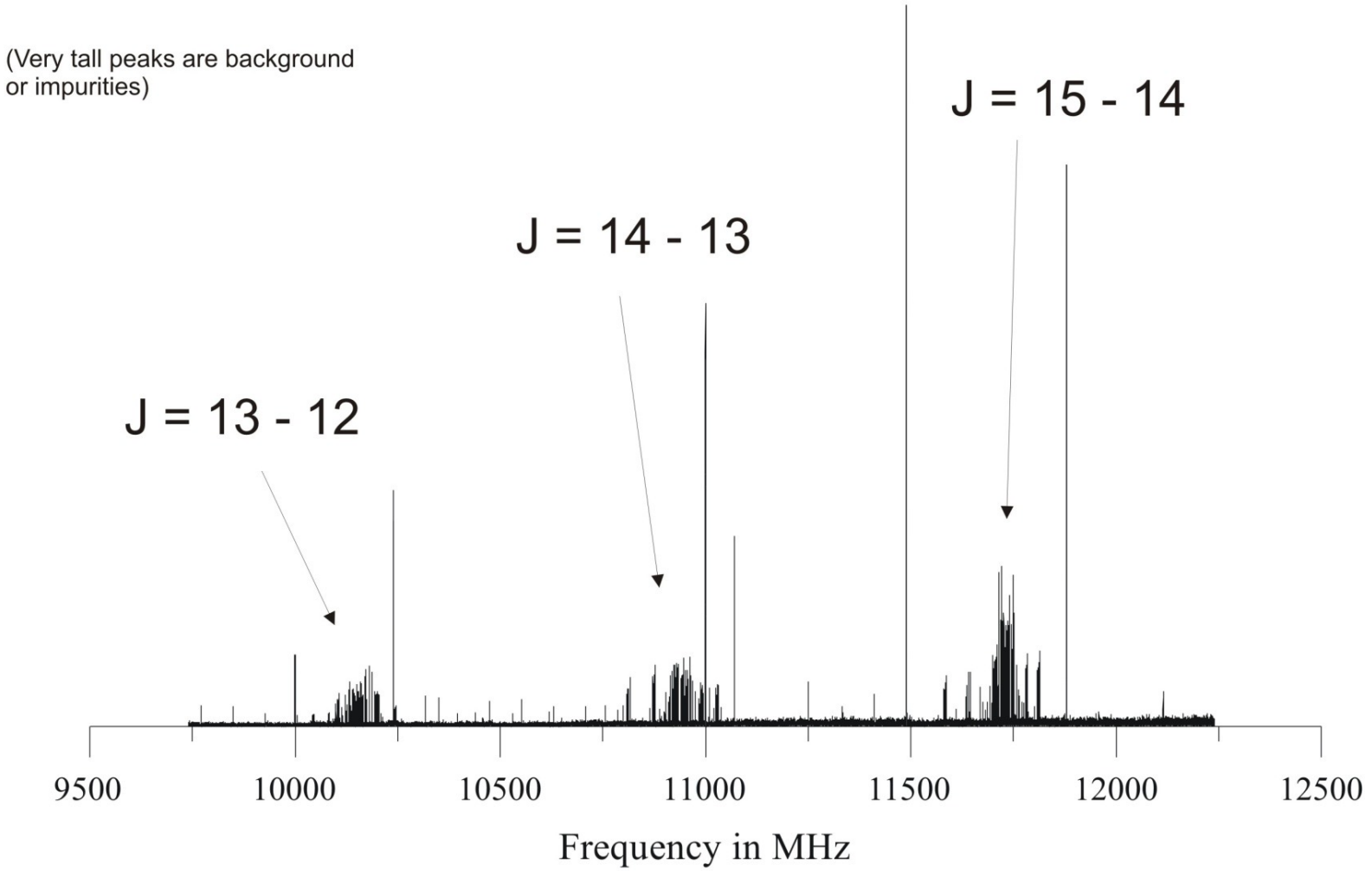


FIG. 1.—Hyperfine transitions associated with $J = 1–0$ in the optically thin case. Each resolved frequency is associated to multiple transitions among hyperfine levels (see text), and the standard labeling of the lines is indicated.



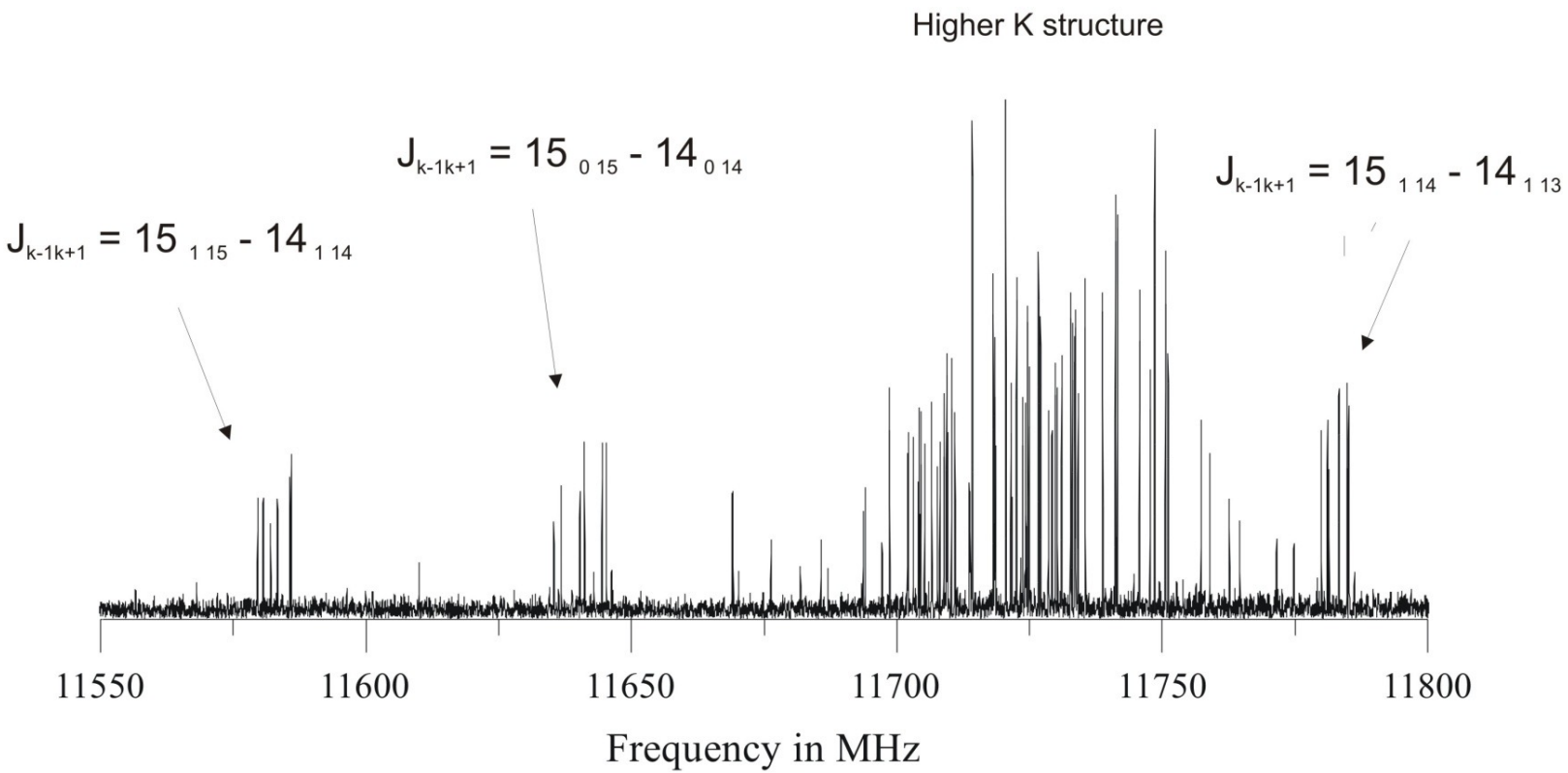
Perfluoro-1-iodopropane (CF3CF2CF2I). Example of a near prolate asymmetric top.



Complements of Dr. Steve Cooke

Perfluoro-1-iodopropane (CF3CF2CF2I). Example of a near prolate asymmetric top.

Blow up of J = 15 - 14

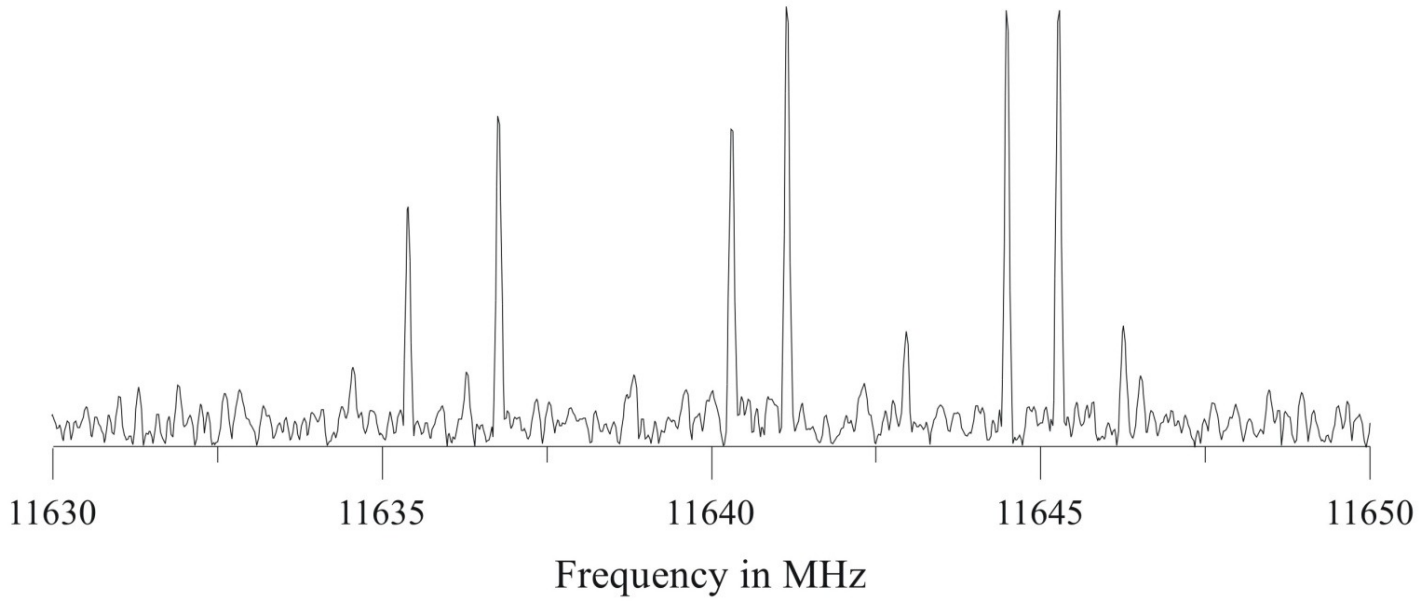


Complements of Dr. Steve Cooke

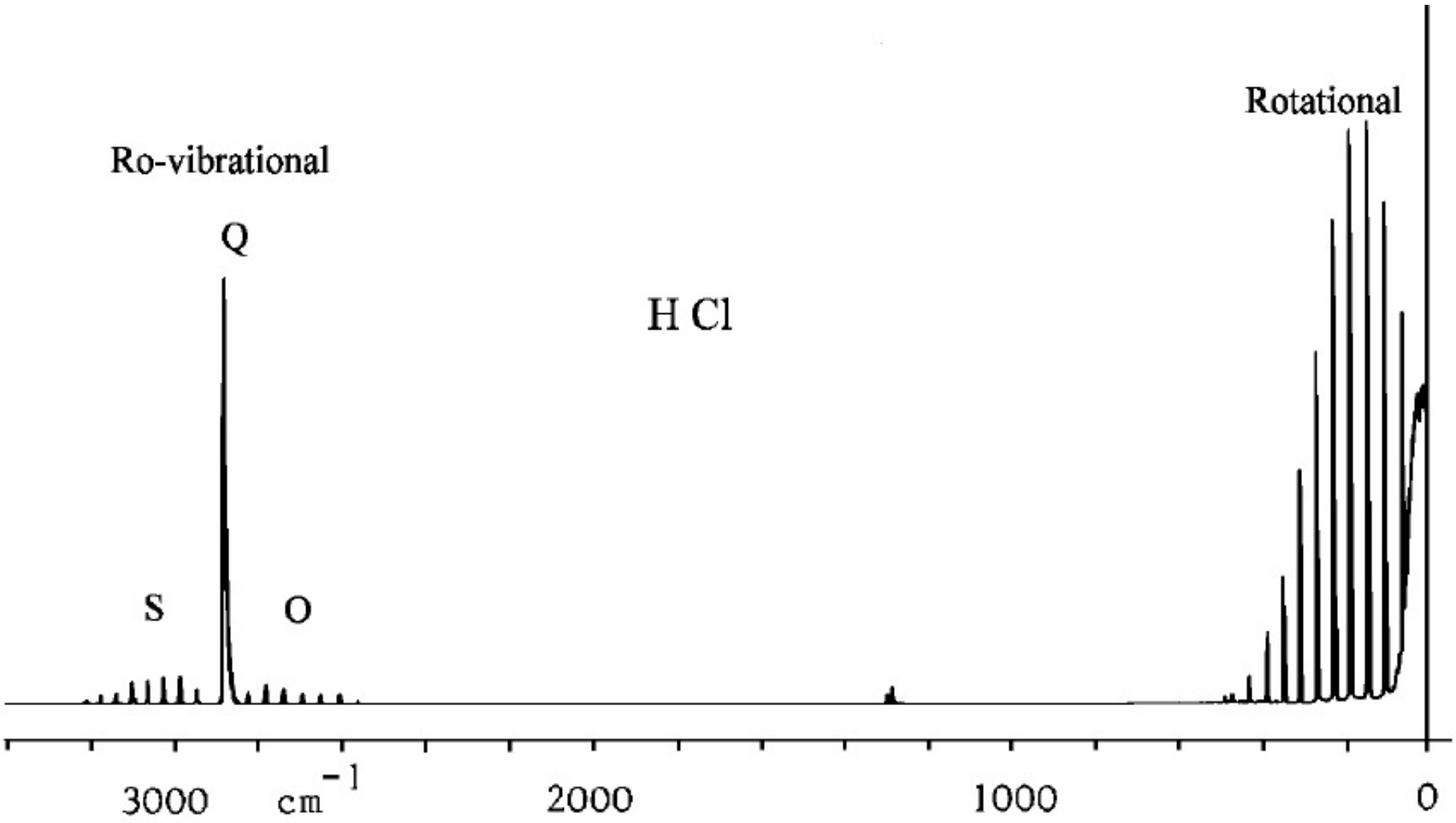
Perfluoro-1-iodopropane (CF3CF2CF2I). Example of a near prolate asymmetric top.

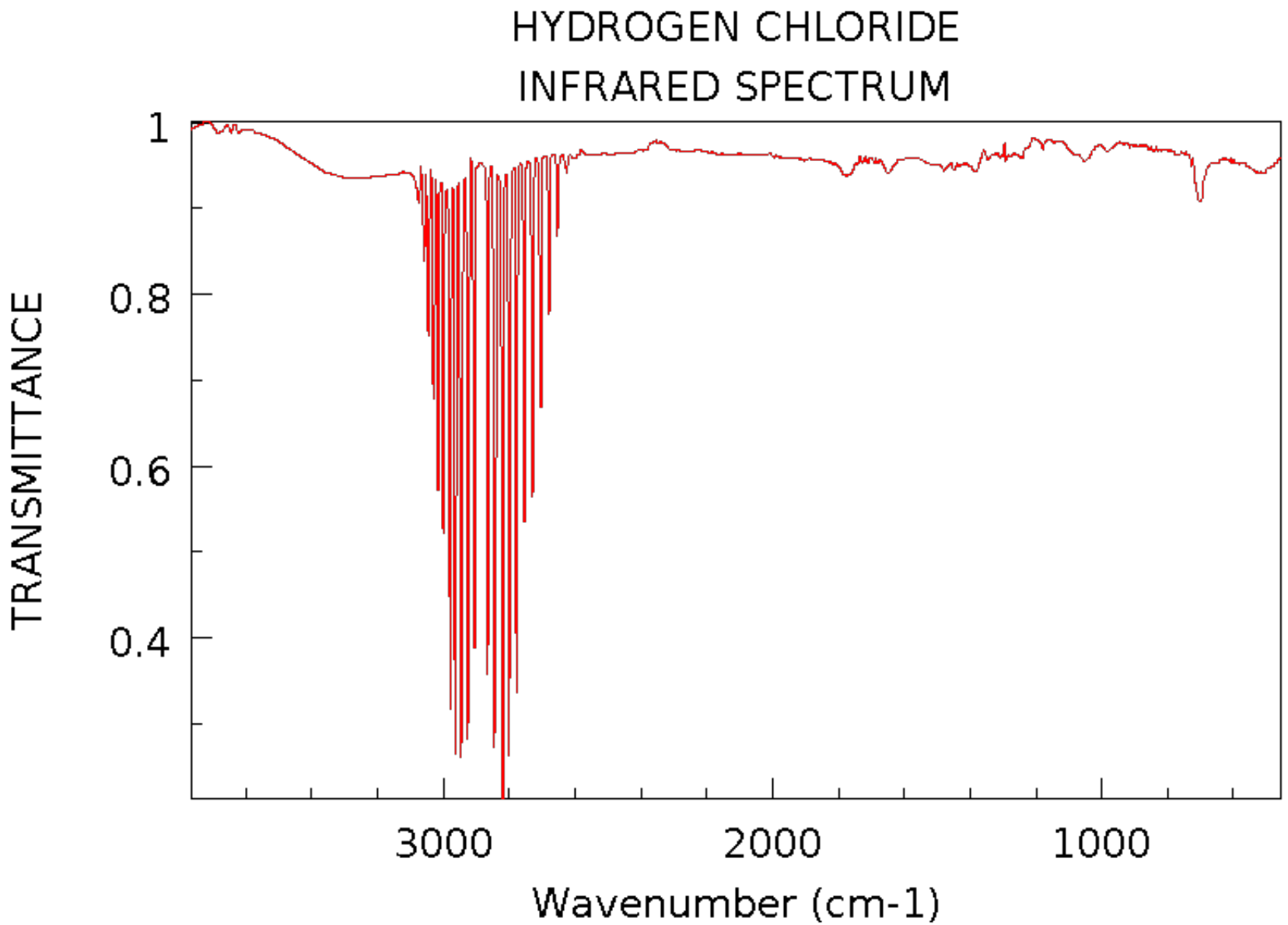
Blow up of $J_{k-1k+1} = 15_{\ 0\ 15} - 14_{\ 0\ 14}$

These splitting are due to the coupling of the nuclear spin of the iodine nucleus with the end over end rotation of the molecule



Complements of Dr. Steve Cooke


Rotational
Ro-vibrational
Q
H Cl
S
O
3000
cm⁻¹
2000
1000
0



NIST Chemistry WebBook (http://webbook.nist.gov/chemistry)

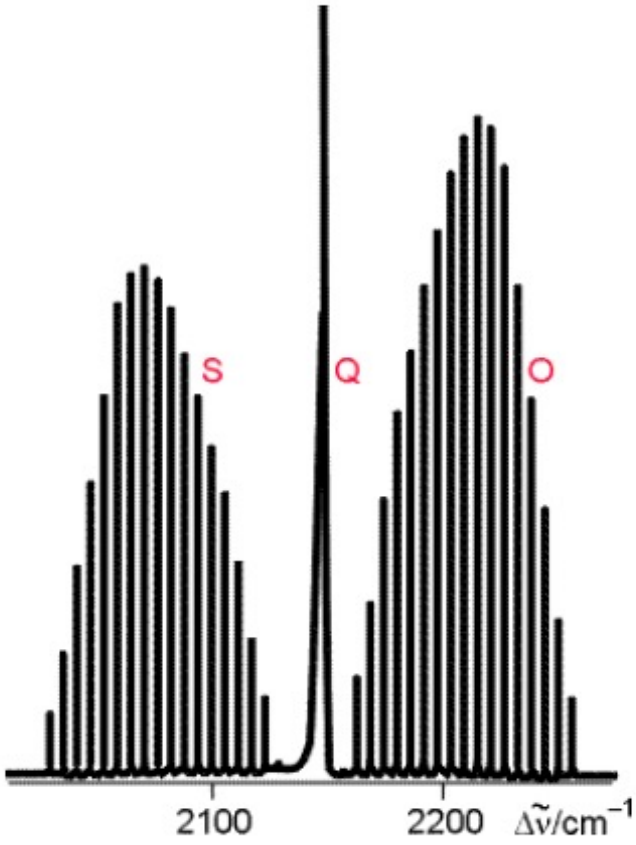
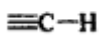
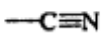
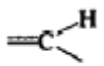
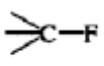
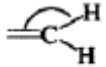
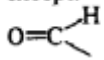
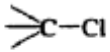
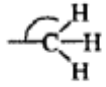
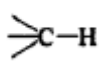
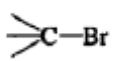
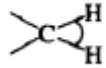
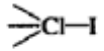
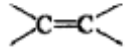
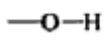
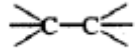
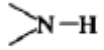
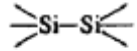
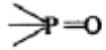
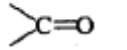
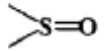
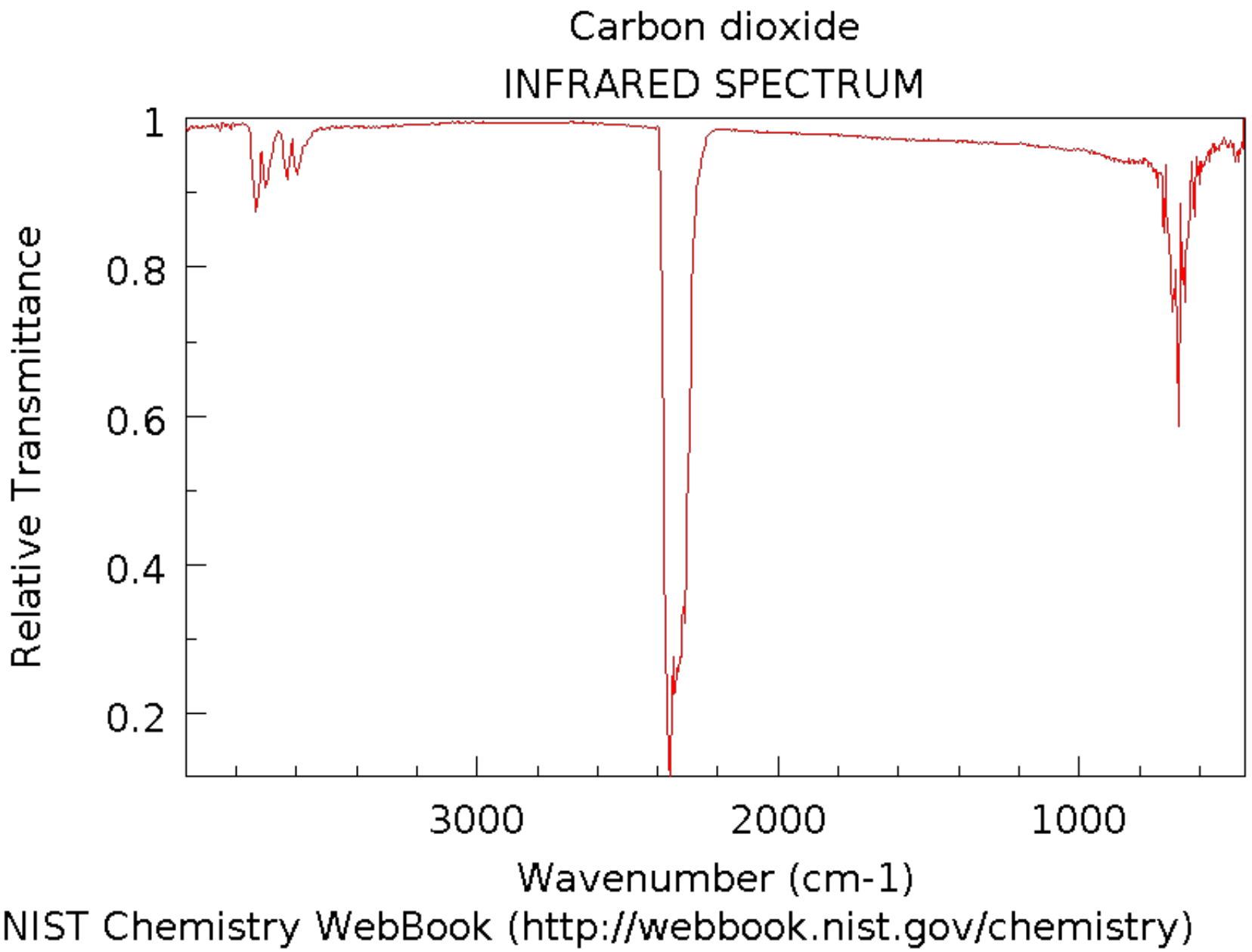
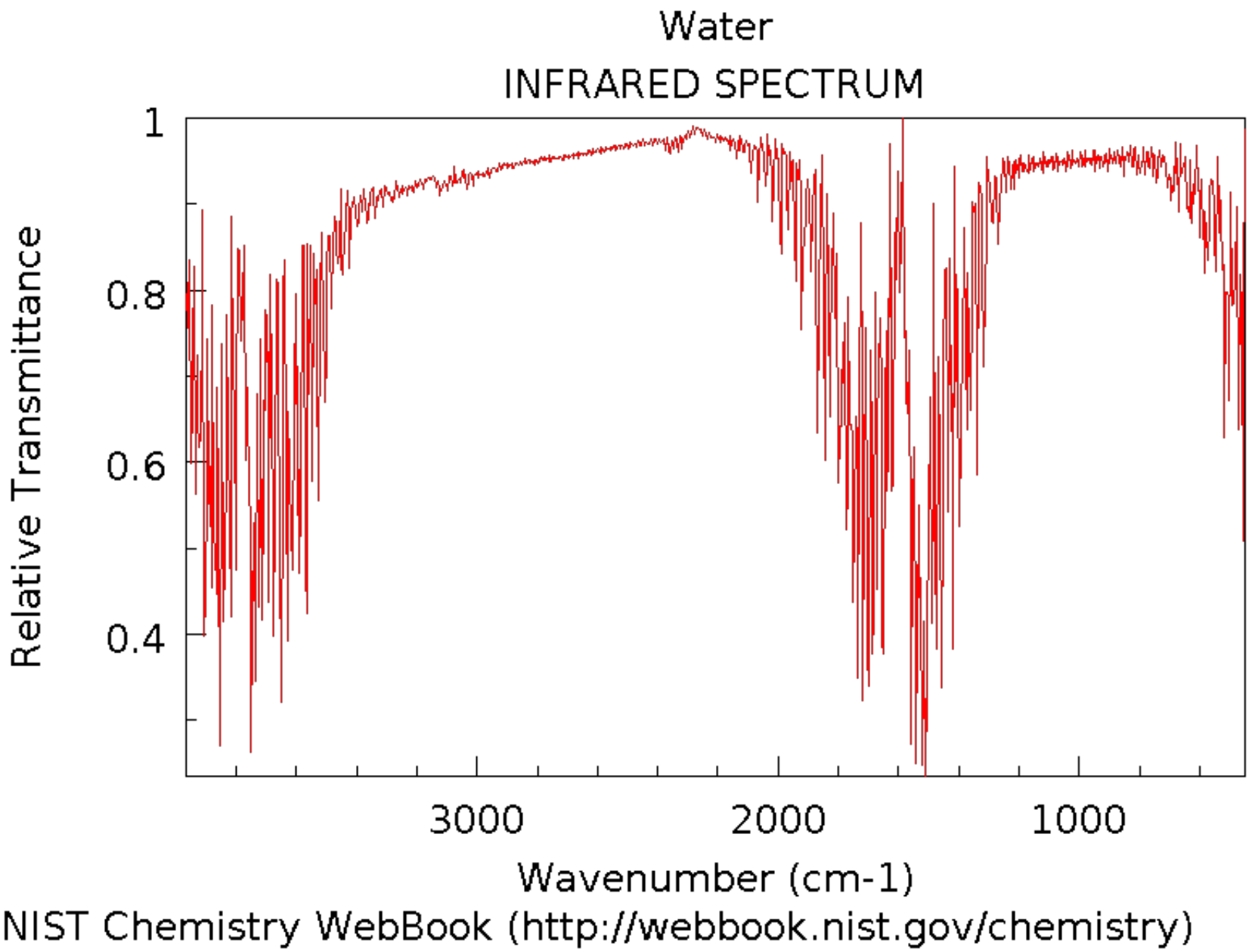

S
Q
O
2100
2200
$\Delta\tilde{\nu}$/cm^{-1}

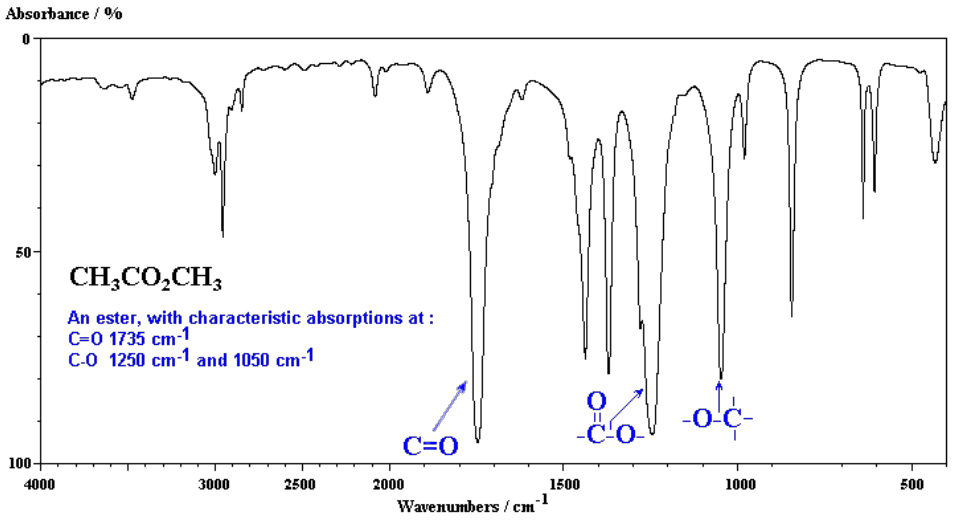
Table 6.3 Typical bond-stretching and angle-bending group vibration wavenumbers ω

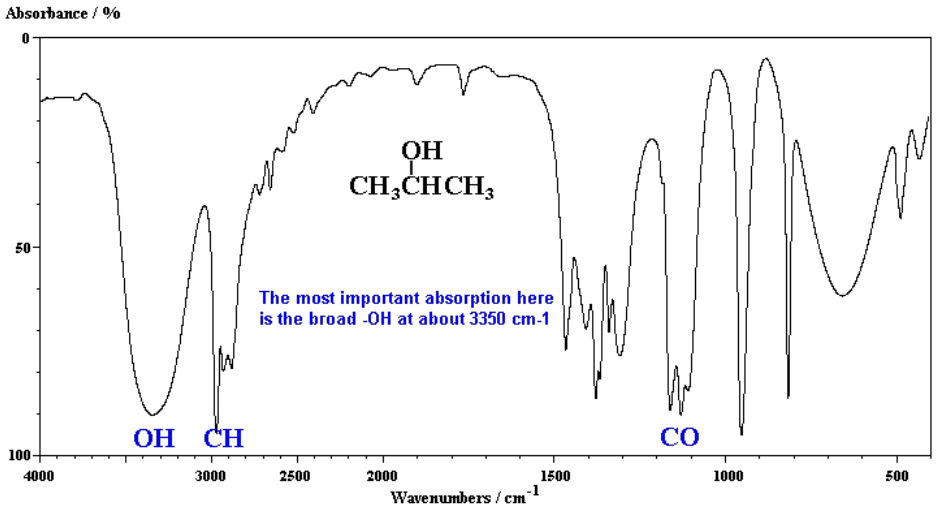
Bond-stretching		Bond-stretching		Angle-bending	
Group	ω/cm^{-1}	Group	ω/cm^{-1}	Group	ω/cm^{-1}
	3300		2100		700
	3020		1100		1100
except: 	2800		650		1000
	2960		560		1450
	2050		500		300
	1650		3600[a]		
	900		3350		
	430		1295		
	1700		1310		

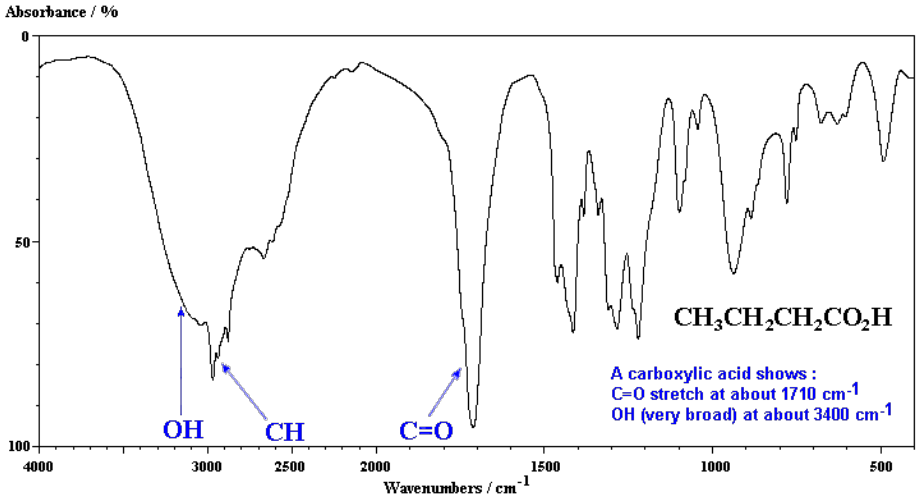
[a] May be reduced in a condensed phase by hydrogen bonding.

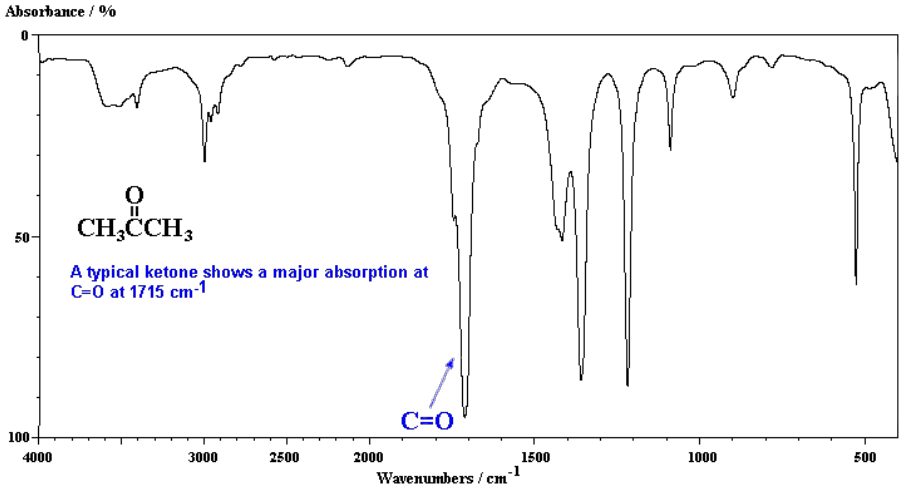

Carbon dioxide
INFRARED SPECTRUM
Relative Transmittance
1
0.8
0.6
0.4
0.2
3000
2000
1000
Wavenumber (cm-1)
NIST Chemistry WebBook (http://webbook.nist.gov/chemistry)

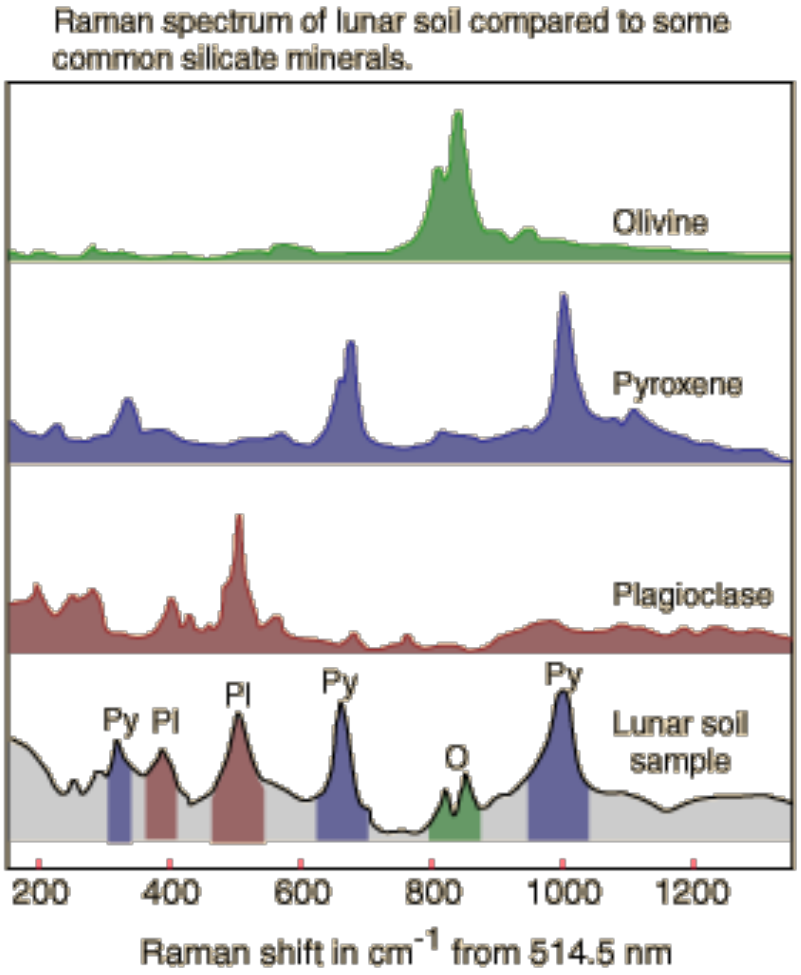

Water
INFRARED SPECTRUM
Relative Transmittance
1
0.8
0.6
0.4
3000
2000
1000
Wavenumber (cm-1)
NIST Chemistry WebBook (http://webbook.nist.gov/chemistry)


Absorbance / %
0
50
100
4000
3000
2500
2000
1500
1000
500
Wavenumbers / cm-1
CH3CO2CH3
An ester, with characteristic absorptions at :
C=O 1735 cm-1
C-O 1250 cm-1 and 1050 cm-1
C=O
O
-C-O-
-O-C-


Absorbance / %
0
50
100
4000
3000
2500
2000
1500
1000
500
Wavenumbers / cm-1
OH
CH3CHCH3
The most important absorption here
is the broad -OH at about 3350 cm-1
OH
CH
CO

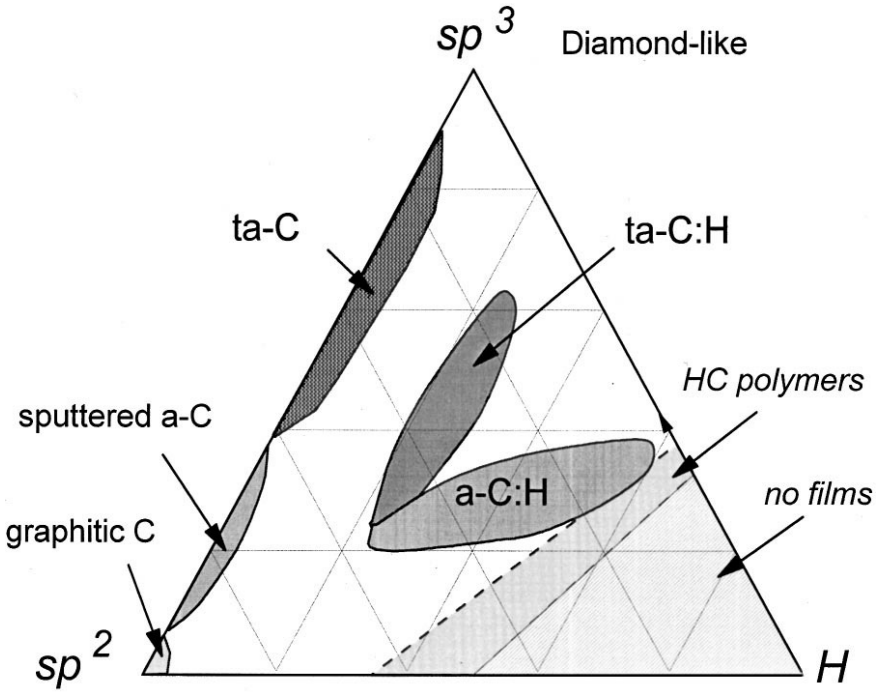

Absorbance / %
0
50
100
4000
3000
2500
2000
1500
1000
500
Wavenumbers / cm-1
CH3CH2CH2CO2H
A carboxylic acid shows :
C=O stretch at about 1710 cm-1
OH (very broad) at about 3400 cm-1
OH
CH
C=O

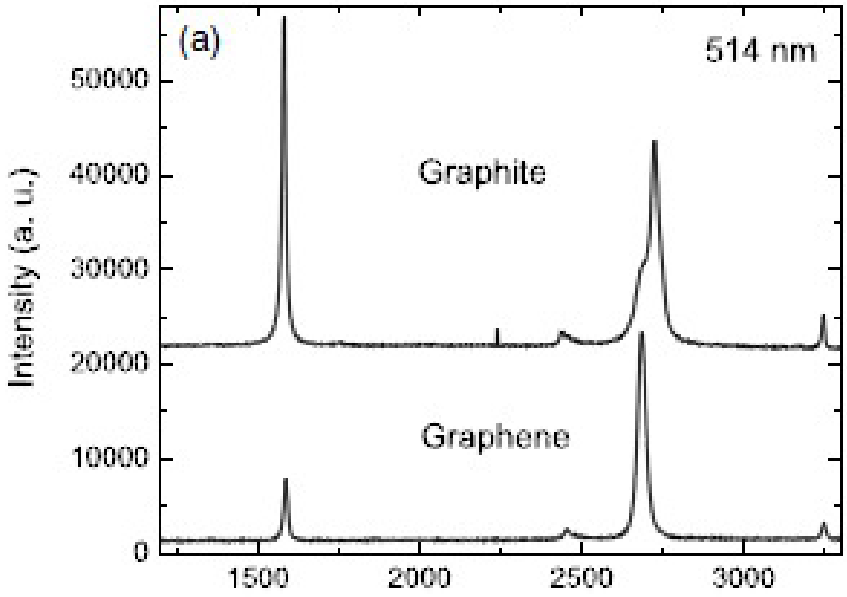

Absorbance / %
0
50
100
4000
3000
2500
2000
1500
1000
500
Wavenumbers / cm-1
O
CH3CCH3
A typical ketone shows a major absorption at
C=O at 1715 cm-1
C=O

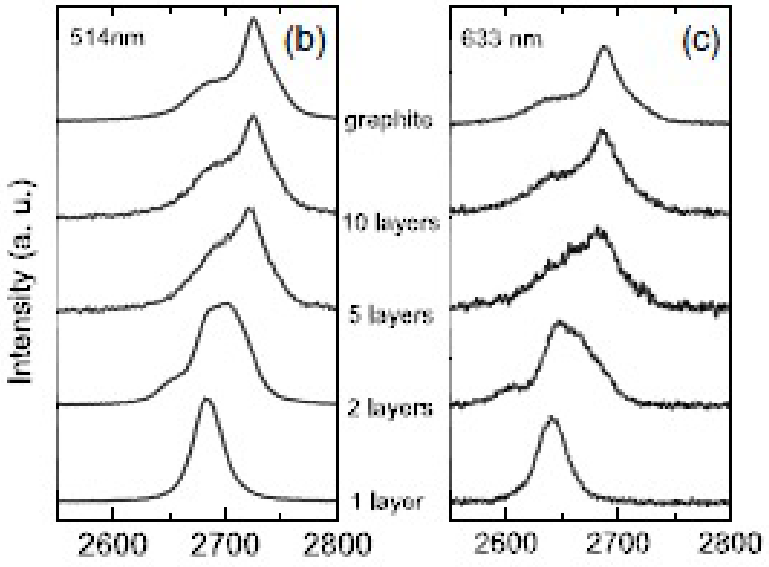


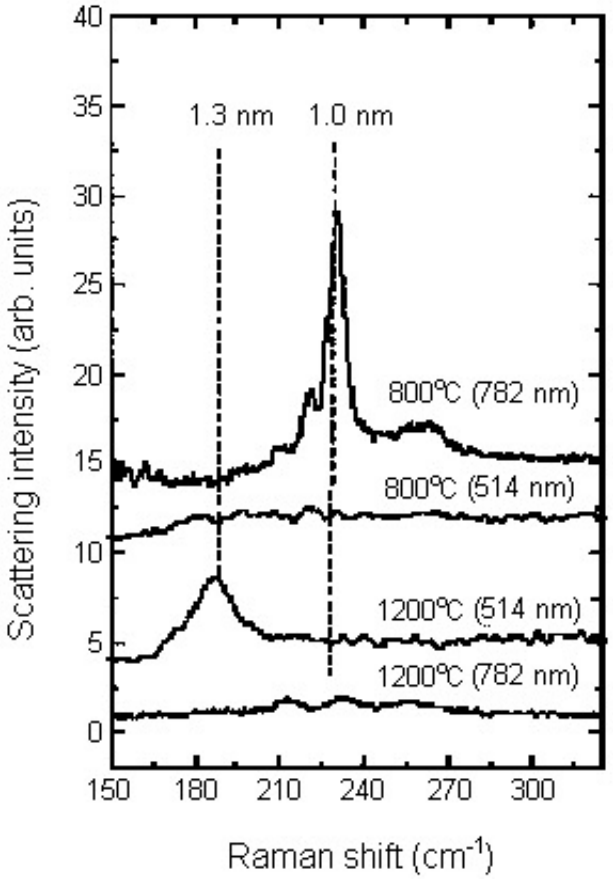
Wang et al., J. Geophys. Res. 100, p21189-21199 (1995).

C. Casiraghi, A. C. Ferrari,* and J. Robertson, PRL, 2000

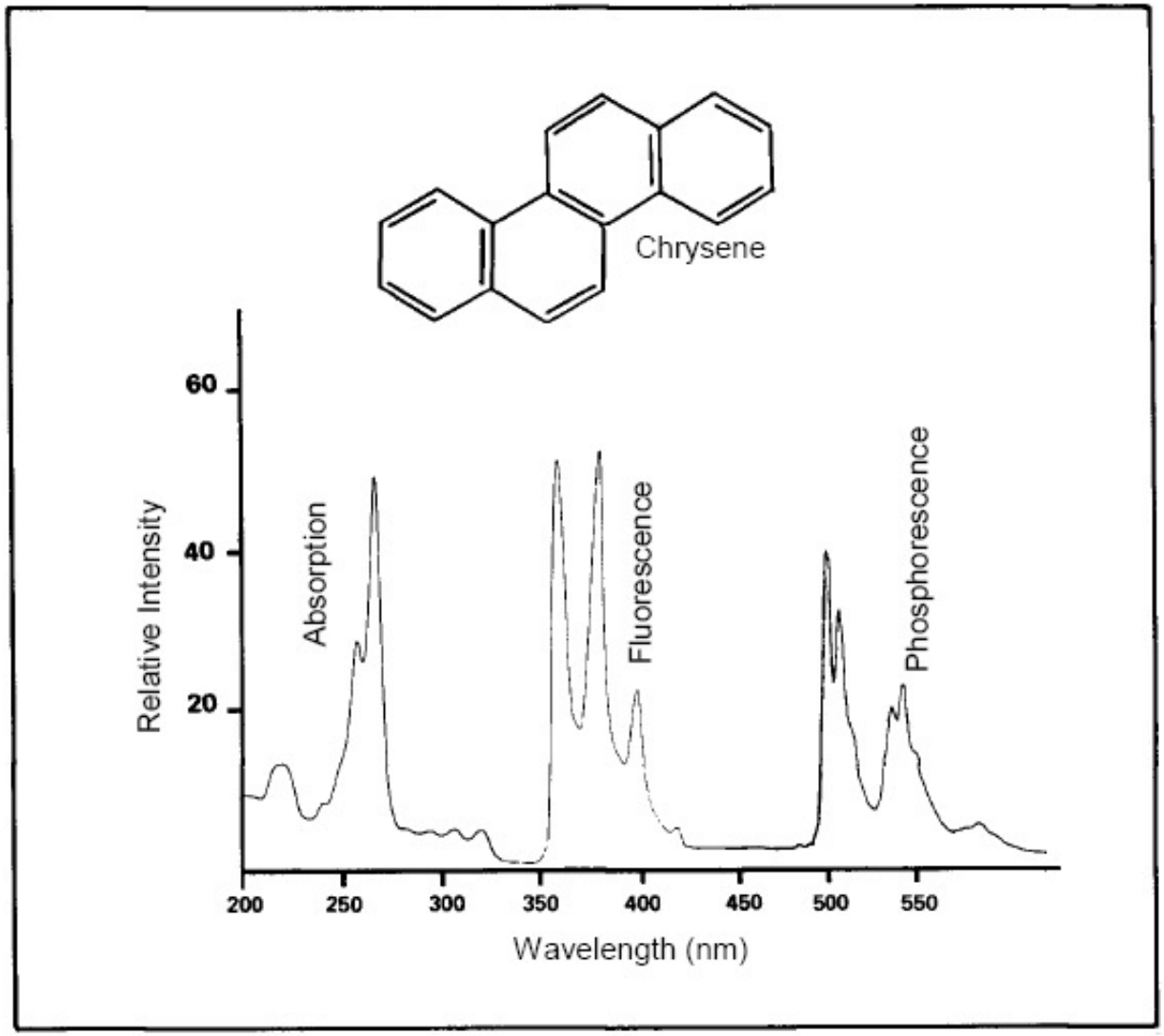




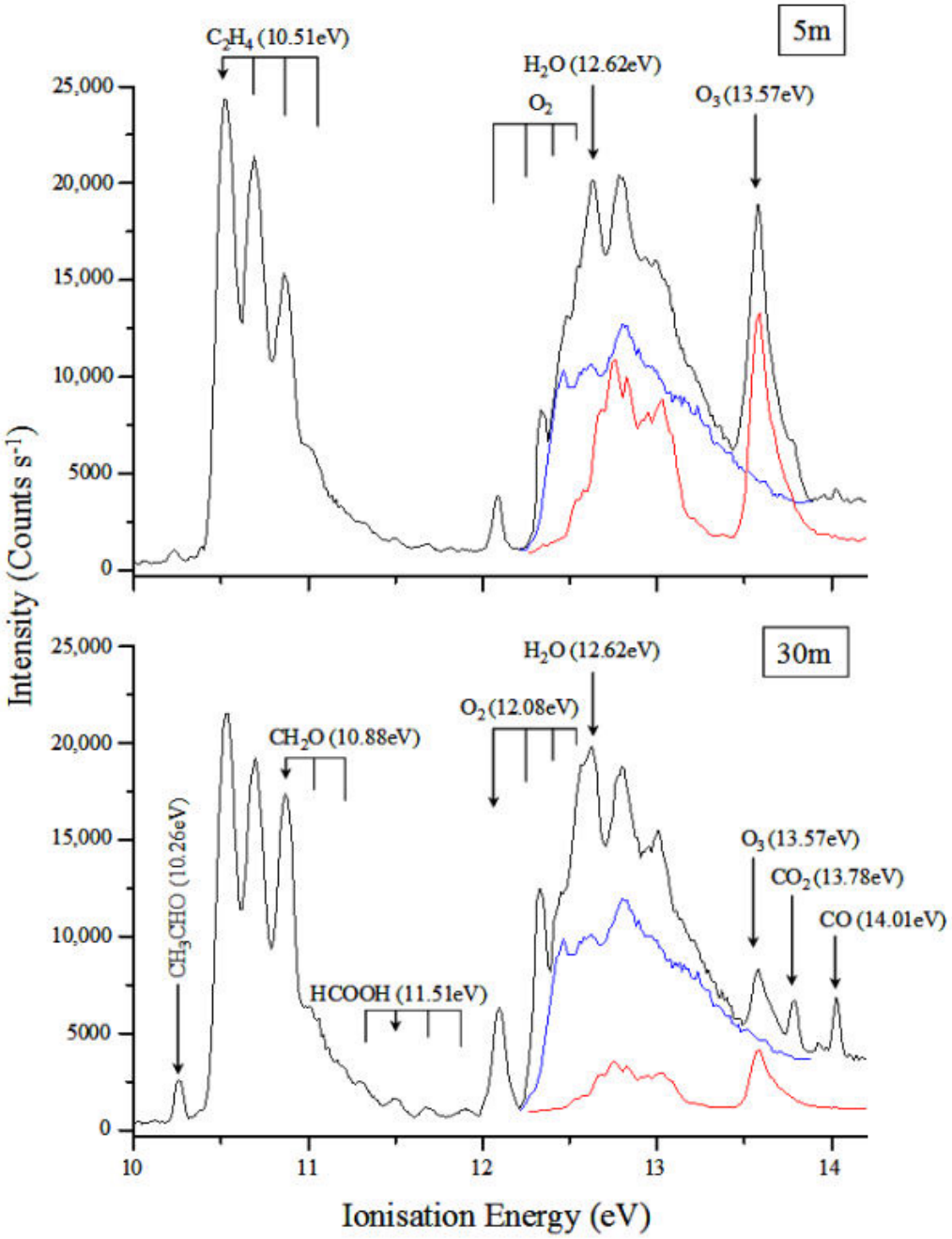




University of Houston • University of Houston-Clear Lake • ISSO Annual Report Y2002—pp. 33-36
Characterization of Carbon Nanotubes Using Raman Spectroscopy: A Parametric Study of Carbon Nanotube Production
Milko N. Iliev (UH), Alexander Litvinchuk (UH), Carl D. Scott (NASA-JSC), Sivaram Arepalli (GB Tech/NASA-JSC), Pavel Nikolaev (GB Tech/NASA-JSC), and Victor G. Hadjiev (UH)


Chrysene
Relative Intensity
60
40
20
Absorption
Fluorescence
Phosphorescence
200
250
300
350
400
450
500
550
Wavelength (nm)

Ultraviolet PES



Ozone and ethylene atmosphere RXN

Fundamental XPS Data from Pure Elements, Pure Oxides, and Chemical Compounds

C(1s) BE = 285.0 eV
Charge Referencing

1																		18
1 H 1s H_2° LiH	2											13	14	15	16	17		2 He 1s He+/Be He+/C
3 Li 1s Li° LiOH	4 Be 1s Be° BeO											5 B 1s B° B2O3	6 C 1s HOPG Black	7 N 1s Kapton BN	8 O 1s CuO SiO2	9 F 1s Teflon CaF2		10 Ne 1s Ne+/Be Ne+/C
54.9 (1.65) 285.0 531.8 (1.6)	111.9 113.6 (0.79) (1.73) 286.1 285.0 111.88 531.3 (0.69) (1.47)											187.5 194.0 (0.87) (2.40) 285.2 285.0 187.8 532.5 (1.03) (2.22)	284.5 284.4 (0.42) (1.04)	400.9 398.9 (1.31) (1.10) 285.0 285.0 191.3 (1.03)	529.7 532.5 (0.98) (1.40) 284.9 285.0 934.0 103.0 (1.42) (1.14)	688.9 685.1 (1.8) (1.53) 285.0 285.0 291.9 348.1 (1.6) (1.6)		Ne+/Be Ne+/C
11 Na 1s Na° NaCl	12 Mg 2p Mg° MgO											13 Al 2p Al° Al2O3	14 Si 2p Si° SiO2	15 P 2p P° InP	16 S 2p S° MoS2	17 Cl 2p PVC NaCl	18 Ar 2p Ar+/Be Ar+/C	
1072.0 (1.40) 285.0 199.3 (1.19)	49.7 49.5 (0.58) (1.63) 286.5 285.0 49.77 529.8 (0.60) (1.99)											72.9 74.3 (0.62) (1.41) 284.7 285.0 72.82 531.1 (0.41) (1.56)	99.8 103.0 (0.57) (1.14) 285.3 285.0 99.35 532.5 (0.45) (1.40)	130.13 128.8 (0.67) (0.62) 285.0 285.0 444.7 (0.78)	164.0 162.7 (0.72) (0.39) 285.0 229.7 (0.80)	199.8 199.3 (1.7) (1.19) 285.0 285.0 1072.0 (1.40)		242.1 (0.90) 285.0
19 K 2p3 K° KI	20 Ca 2p3 Ca° CaO	21 Sc 2p3 Sc° Sc2O3	22 Ti 2p3 Ti° TiO2	23 V 2p3 V° V2O5	24 Cr 2p3 Cr° Cr2O3	25 Mn 2p3 Mn° MnO2	26 Fe 2p3 Fe° Fe2O3	27 Co 2p3 Co° Co3O4	28 Ni 2p3 Ni° NiO	29 Cu 2p3 Cu° Cu2O	30 Zn 2p3 Zn° ZnO	31 Ga 3d5 Ga° Ga2O3	32 Ge 3d5 Ge° GeO2	33 As 3d5 As° As2O3	34 Se 3d5 Se° SeOx	35 Br 3d5 KBr	36 Kr 3d5 Kr+/Be Kr+/C	
293.2 (1.11) 285.0 619.2 (1.30)	346.5 347.1 (?) (1.81) 284.6 285.0 346.5 531.5 (1.07) (1.57)	398.6 401.9 (0.9) (1.27) 285.8 285.0 398.46 530.0 (0.69) (1.33)	453.8 458.7 (0.90) (1.09) 285.2 285.0 453.95 530.0 (0.62) (1.18)	512.2 517.3 (0.79) (1.32) 285.0 285.0 512.22 530.2 (0.75) (1.33)	574.2 575.7 (1.05) (1.20) 284.6 285.0 574.37 530.1 (0.89) (1.24)	638.7 641.5 (1.00) (1.12) 286.4 285.0 638.74 529.5 (0.89) (1.02)	706.6 709.8 (0.90) (1.32) 284.9 285.0 706.78 532.9 (0.99) (1.05)	778.1 779.5 (0.99) (1.39) 284.9 285.0 778.26 530.1 (0.85) (1.00)	852.6 853.8 (1.14) (1.42) 284.8 285.0 852.65 529.4 (1.02) (1.03)	932.7 932.5 (1.22) (1.10) 284.6 285.0 932.68 530.5 (0.92) (1.01)	1021.8 1021.7 (1.10) (1.50) 284.8 285.0 1021.76 530.5 (0.97) (1.11)	18.7 20.7 (0.70) (1.37) 285.0 285.0 18.5 531.3 (0.60) (1.51)	29.3 33.2 (0.68) (1.49) 285.0 285.0 29.28 532.2 (0.64) (1.40)	41.8 45.1 (0.67) (1.26) 284.5 285.0 41.69 532.0 (0.67) (1.41)	54.8 59.3 (0.76) (1.09) 284.2 285.0 54.90 532.6 (0.78)	68.8 (0.92) 285.0 293.0 (1.31)	86.94 (0.79) 285.0	
37 Rb 3d5 Rb° RbOAc	38 Sr 3d5 Sr° SrCO3	39 Y 3d5 Y° Y2O3	40 Zr 3d5 Zr° ZrO2	41 Nb 3d5 Nb° Nb2O5	42 Mo 3d5 Mo° MoO3	43 Tc 3d5 Tc°	44 Ru 3d5 Ru° RuO2	45 Rh 3d5 Rh° Rh2O3	46 Pd 3d5 Pd° PdO	47 Ag 3d5 Ag° Ag2O	48 Cd 3d5 Cd° CdO	49 In 3d5 In° In2O3	50 Sn 3d5 Sn° SnO2	51 Sb 3d5 Sb° Sb2O5	52 Te 3d5 Te° TeO2	53 I 3d5 KI	54 Xe 3d5 Xe+/Be Xe+/C	
109.7 (1.40) 285.0 530.9 (1.6)	133.7 (1.63) 285.0 531.5 (1.9)	155.9 156.6 (0.80) (1.25) 286.0 285.0 155.92 531.0 (0.62) (1.30)	179.0 182.4 (0.90) (1.18) 285.3 285.0 178.80 530.3 (0.63) (1.39)	202.1 207.4 (0.78) (1.14) 285.0 285.0 202.35 530.4 (0.57) (1.36)	227.8 233.1 (0.66) (1.05) 285.4 285.0 227.94 531.0 (0.57) (1.20)	Radioactive	280.0 281.1 (0.67) (0.79) --- 285.0 280.11 529.7 (0.59) (0.95)	307.2 308.9 (0.73) (0.80) 284.05 285.0 307.21 530.5 (0.69) (1.05)	335.1 337.0 (0.86) (0.97) 284.5 285.0 335.10 530.7 (0.77) (1.35)	368.2 367.5 (0.64) (1.00) 284.7 285.0 368.28 529.4 (0.62) (0.97)	405.0 404.0 (0.90) (1.38) 285.0 285.0 405.04 528.6 (0.61) (1.28)	443.8 444.3 (1.08) (1.26) 284.9 285.0 443.87 529.9 (0.71) (1.19)	484.9 487.3 (0.81) (1.28) 284.7 285.0 485.01 531.1 (0.68) (1.29)	528.2 529.8 (1.0) (1.10) 284.6 285.0 528.26 531.3 (0.80) (0.86)	572.8 576.5 (1.12) (1.27) 284.2 285.0 572.97 530.7 (0.83) (1.39)		619.2 (1.30) 285.0 293.2 (1.11)	669.6 (1.13) 285.0	
55 Cs 3d5 Cs° CsCl	56 Ba 3d5 Ba° BaOAc	57 La 3d5 La° La2O3	72 Hf 4f7 Hf° HfO2	73 Ta 4f7 Ta° Ta2O5	74 W 4f7 W° WO3	75 Re 4f7 Re° Re2O7	76 Os 4f7 Os° OsO4	77 Ir 4f7 Ir° IrO2	78 Pt 4f7 Pt° PtO2	79 Au 4f7 Au° Au2O3	80 Hg 4f7 Hg° HgO	81 Tl 4f7 Tl° Tl2O3	82 Pb 4f7 Pb° PbO	83 Bi 4f7 Bi° Bi2O3	84 Po 4f7	85 At 4f7	86 Rn 4f7	
724.6 (2.08) 285.0 199.2	780.0 (1.80) 285.0 531.4 (1.83)	834.7 (3.0) 285.0 529.2 (1.6)	14.4 17.1 (0.63) (1.26) 285.7 285.0 14.32 530.5 (0.62) (1.68)	21.8 26.8 (0.80) (1.12) 285.0 285.0 21.78 531.0 (0.56) (1.46)	31.4 35.8 (0.58) (1.01) 285.3 285.0 31.38 530.6 (0.53) (1.27)	40.3 46.8 (0.67) (1.64) 285.3 285.0 40.30 532.1 (0.54) (1.58)		60.8 62.0 (0.80) (0.98) 284.4 285.0 60.88 530.2 (0.82) (0.97)	71.0 75.1 (0.96) (1.16) 284.3 285.0 71.15 531.3 (0.88) (1.74)	84.1 88.1 (0.83) (1.12) 284.1 285.0 83.98 531.6 (0.68) (1.13)	99.8 100.7 --- (1.06) 285.0 (285.0) 99.81 532.9 (0.65) (0.96)	117.8 117.4 (0.97) (1.01) 285.1 285.0 117.77 528.9 (0.66) (1.10)	136.9 137.5 (0.67) (1.10) 284.9 285.0 136.95 528.9 (0.63) (1.07)	157.0 158.8 (0.73) (1.11) 284.6 285.0 157.05 529.6 (0.62) (1.58)	Radioactive	Radioactive	Radioactive	
87 Fr 4f7	88 Ra 4f7	89 Ac 4f7																
Radioactive	Radioactive	Radioactive																

Atomic Number of Element
Abbreviation for Element
Al (2p3) BE of Al° under Native Oxide
Al (2p3) FWHM of Al° under Native Oxide
C (1s) BE of Hydrocarbons Captured by Ion Etched Al°
Reliable Reference BE for Ion Etched, Pure Al°
Al (2p3) FWHM of Ion Etched , Pure Al°

13 Al 2p3	
Al°	Al2O3
72.9	74.3
(0.62)	(1.41)
284.7	285.0
72.82	531.1
(0.41)	(1.56)

Main XPS Signal for Element of Interest
Most Common Oxide or Chemical Compound of Element
Al (2p3) BE of Major Oxide Species in Pure Oxide
Al (2p3) FWHM of Major Oxide Species in Pure Oxide
C (1s) BE Defined to be at 285.0 eV
O (1s) BE of Major Oxygen Species in Pure Oxide
O (1s) FWHM of Major Oxygen Species in Pure Oxide

All non-conductive materials were referenced to adventitious hydrocarbon with C (1s) BE at 285.0eV. Energy resolution settings for pure oxide data gave FWHM <0.75 eV for Ag (3d5) of ion etched Ag°. All non-conductors were analyzed with the Flood-Gun Mesh-Screen 0.5-1.0 mm above the specimen. C (1s) BEs for "hydrocarbons" on elements were collected from carbon captured by ion etched elements. Carbon from the cryo-pumped vacuum (3x10(-9) torr) was analyzed >10 hours after ion etching. Energy resolution settings for ion etched elements gave FWHM <0.50 eV forAg (3d5) of ion etched Ag°. Calibration was: Cu (2p3) at 932.67 ±0.05 eV, Cu (3s) at 122.45 ±0.05 eV, and Au(4f7) at 83.98 eV.

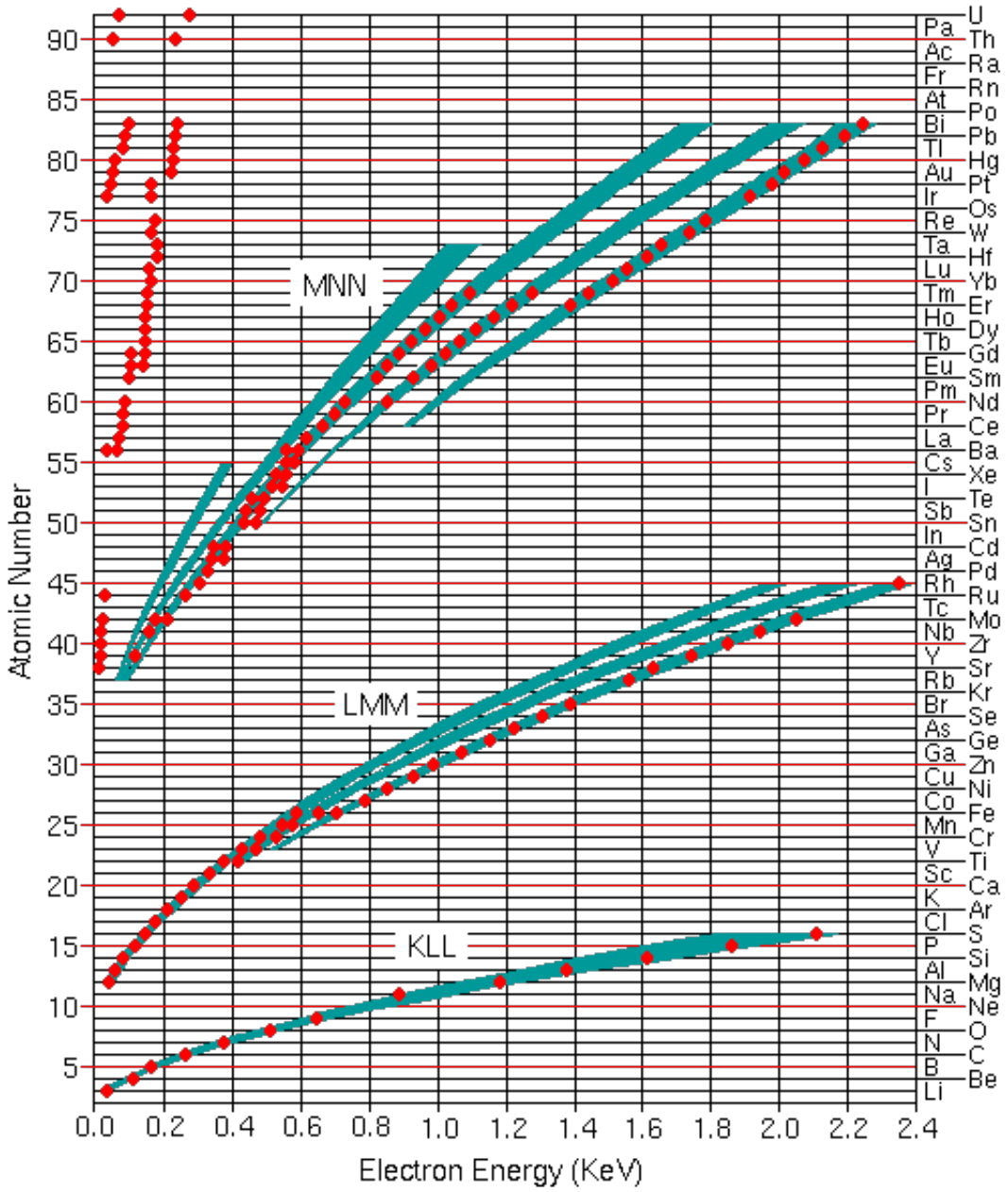
The FWHM and BE values presented in this table were all obtained by one scientist using two SSI XPS systems, which yield a theoretical energy resolution limit of about 0.1 eV and were equipped with monochromatic Aluminum X-ray sources which have a theoretical energy resolution limit of about 0.16 eV. The BEs for the ion etched elements can be used as reliable secondary energy reference values within a standard deviation of 0.055. All other BE values are <±0.15 eV.

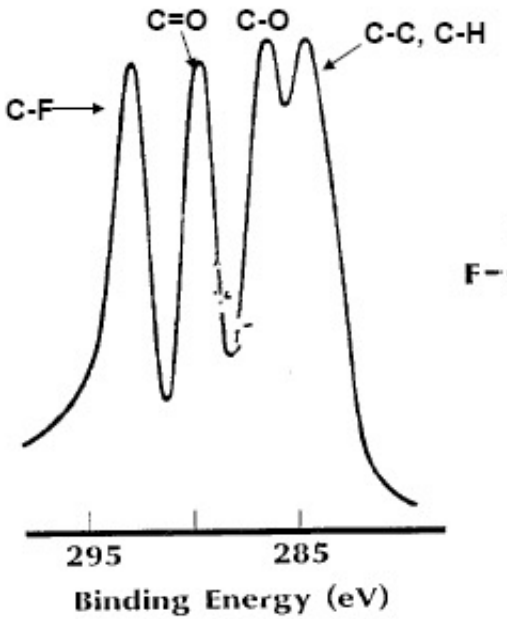
3	4	5	6	7	8	9	10	11	12

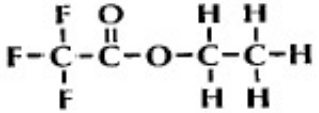
58 Ce 3d5 Ce° CeO2	59 Pr 3d5 Pr° Pr2O5	60 Nd 3d5 Nd° Nd2O3	61 Pm 4d5 Pm° Pm2O3	62 Sm 4d5 Sm° Sm2O3	63 Eu 4d5 Eu° Eu2O3	64 Gd 4d5 Gd° Gd2O3	65 Tb 4d5 Tb° Tb3O7	66 Dy 4d5 Dy° Dy2O3	67 Ho 4d5 Ho° Ho2O3	68 Er 4d5 Er° Er2O3	69 Tm 4d5 Tm° Tm2O3	70 Yb 4f7 Yb° Yb2O3	71 Lu 4f7 Lu° Lu2O3
882.1 (2.0) 285.0 529.6 (2.00)	(931.98) 933.1 --- (4.4) --- 285.0 111.2 528.2 (2.17) (1.4)	(980.86) --- --- 118.0 (1.80)	Radioactive	--- (134.9) --- (10) --- 285.0 123.2 531.7 (2.57) (2.4)	128.2 135.6 --- (3.7) 284.3 285.0 128.18 529.2 (1.08) (1.4)	140.2 (1186.8) --- (5.4) 281.4 285.0 140.33 529.0 (1.02) (1.7)	145.9 (149.9) --- (?) --- 285.0 146.02 529.5 (1.33) (1.6)	152.4 (156.1) --- (?) --- 285.0 152.30 529.2 (1.88) (1.7)	159.8 161.3 --- ((6.0) --- 285.0 159.58 529.3 (1.50) (1.7)	167.7 168.5 --- (3.8) --- 285.0 167.25 529.2 (1.93) (1.9)	175.3 176.3 --- (3.4) 285.3 285.0 175.37 529.6 (1.92) (1.7)	1.07 184.9 --- (3.4) 285.6 285.0 (182.39) 529.4 (0.61) (2.0)	7.10 8.4 --- (3.0) 284.6 285.0 7.1 529.6 (0.69) (1.8)
90 Th 4f7 Th° ThO2	91 Pa 4f7	92 U 4f7 U° U2O3	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr
	Radioactive		Radioactive	Radioactive	Radioactive	Radioactive	Radioactive	Radioactive	Radioactive	Radioactive	Radioactive	Radioactive	Radioactive

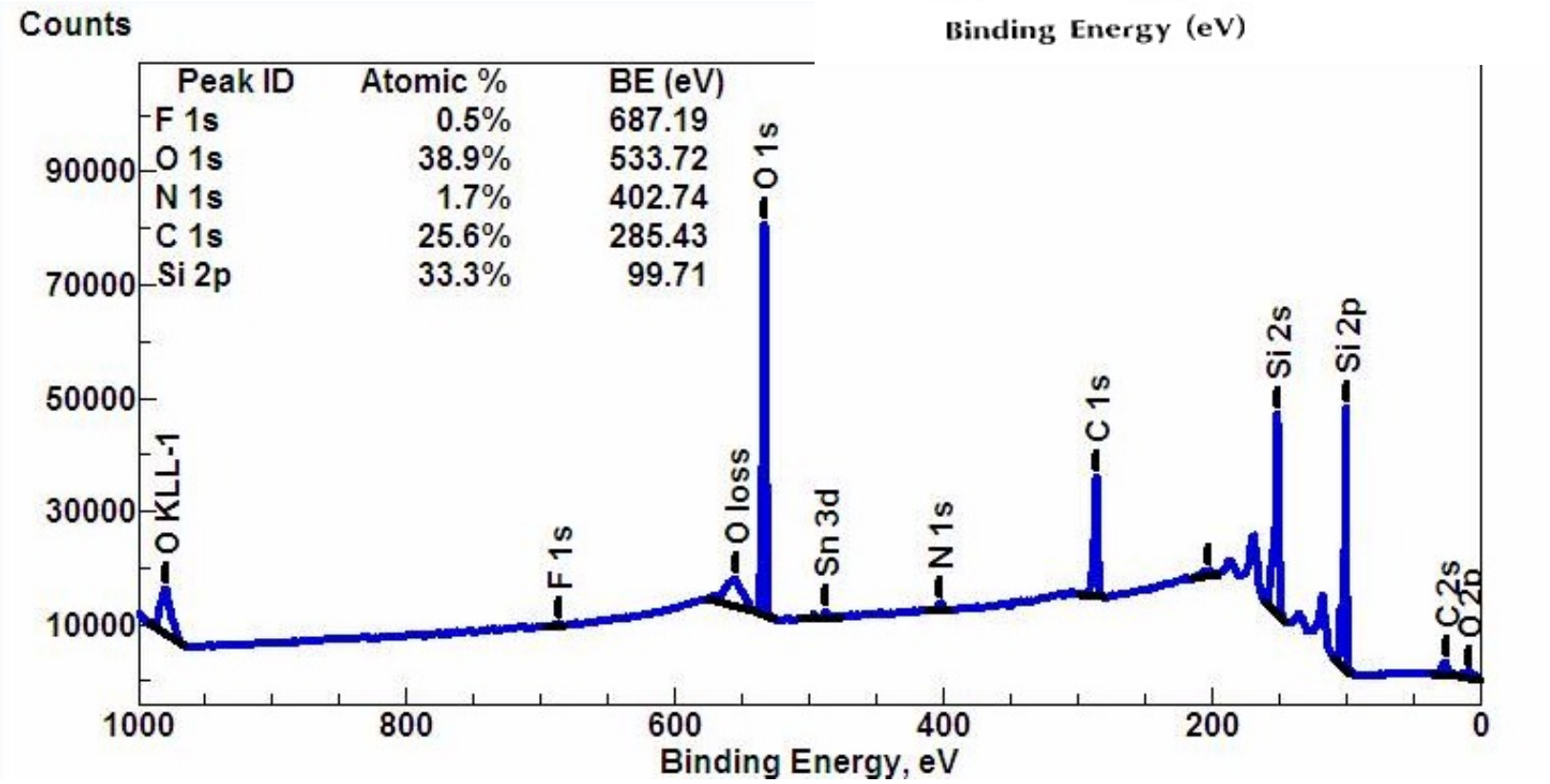
XPS International LLC: www.xpsdata.com

B. Vincent Crist
Last Update 4-28-97


MNN
LMM
KLL
Atomic Number
Electron Energy (KeV)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
2.2
2.4
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80
85
90
U
Pa Th
Ac Ra
Fr Rn
At Po
Bi Pb
Tl Hg
Au Pt
Ir Os
Re W
Ta Hf
Lu Yb
Tm Er
Ho Dy
Tb Gd
Eu Sm
Pm Nd
Pr Ce
La Ba
Cs Xe
I Te
Sb Sn
In Cd
Ag Pd
Rh Ru
Tc Mo
Nb Zr
Y Sr
Rb Kr
Br Se
As Ge
Ga Zn
Cu Ni
Co Fe
Mn Cr
V Ti
Sc Ca
K Ar
Cl S
P Si
Al Mg
Na Ne
F O
N C
B Be
Li


C=O
C-O
C-C, C-H
C-F
295
285
Binding Energy (eV)




Counts
Peak ID Atomic % BE (eV)
F 1s 0.5% 687.19
O 1s 38.9% 533.72
N 1s 1.7% 402.74
C 1s 25.6% 285.43
Si 2p 33.3% 99.71
90000
70000
50000
30000
10000
O KLL-1
F 1s
O loss
O 1s
Sn 3d
N 1s
C 1s
Si 2s
Si 2p
C 2s
O 2p
1000
800
600
400
200
0
Binding Energy, eV

Circular Dichroism