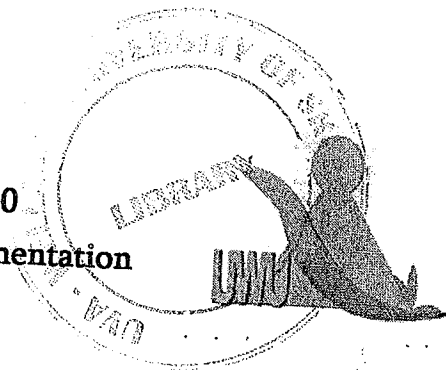


Uva Wellassa University, Sri Lanka  
End Semester Examination – July 2010  
SCT 334-2 Analytical Techniques and Instrumentation



Time: Two (02) hours

Total eight (08) questions

Answer all questions

All questions carry equal marks

Use of scientific calculators is allowed

All symbols carry standard meanings

Use standard notation without a definition in answering

$$(R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1}, h = 6.626 \times 10^{-34} \text{ J s}, m_e = 9.109 \times 10^{-31} \text{ kg}, c = 3.00 \times 10^8 \text{ m s}^{-1})$$

1.

i. Define following terms:

(a) Precision

(b) Accuracy

(c) Random error

ii. The following replicate data were obtained for the concentration of  $\text{SO}_2$  in the air near a paper industry: 1.96, 1.91, 1.88, and 1.94 parts per million (ppm). Calculate the mean and the coefficient of variation of these measurements.

iii. List three sources of errors in instrumental analysis (no details are required).

iv. A new procedure for the determination of sulfur in kerosenes was tested on a sample known from its method of preparation to contain 0.123 % S. The results were  $S = 0.112, 0.118, 0.115, \text{ and } 0.119$  (in %). Do the data indicate the presence of bias in the method at 95% confidence level (hint: what is  $\mu$ )?

2.

i. State briefly with the aid of energy level diagrams, the atomic absorption, emission and fluorescence.

ii. Flames do flicker which shows that there may be significant temperature fluctuations. In order to investigate this sensitivity, calculate the effect of a 10 K variation of the flame temperature on  $N_i/N_0$ , for sodium atoms (hint: calculate  $N_i/N_0$  at 2000 and 2010 K). State the effect of the 10 K temperature rise on emission and absorption intensities.

(For a sodium atom  $E = 203\,000 \text{ J mol}^{-1}$  and  $g_1/g_0 = 2$ )

- iii. State three processes of band broadening mechanisms commonly seen in atomic absorption spectroscopy.
- iv. The spectral line width of the 589.6 nm sodium line has been measured as 0.003 nm at 1000 K and 0.005 nm at 3000 K. Do you think this observation is consistent with the line width being determined by Doppler broadening? Show all work.
- v. Briefly State the meaning of lock and key effect. How emission lines of a given element is generated in a hollow cathode lamp?

3.

- i. Define following units commonly used in X-ray safety measurements
  - (a) Roentgen
  - (b) Gray
  - (c) Sievert

Which of the following is the most dangerous? Give reasons.

- (a) A dose of 3.37 Sv delivered to the elbow in a second
- (b) A constant dose of  $1.07 \times 10^{-7}$  Sv per second for one year to the whole body?

- ii. State Bragg law of diffraction. State all symbols stated in. List the essential components of a powder X-ray diffraction spectrometer.
- iii. The inter-planar spacing and relative intensities derived from the powder pattern of the unknown material are listed below. Using the data given identify the unknown material.

$d/\text{\AA}$	$I/I_1$
2.09	100
1.81	48
1.28	20
1.09	15
1.04	5
0.904	4
0.829	10
0.808	8

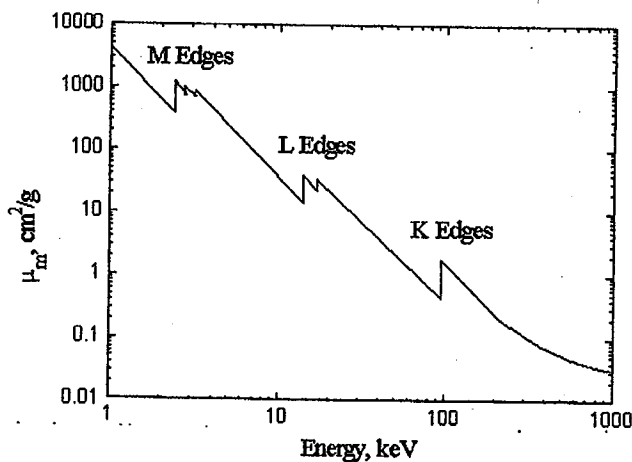
- iv. State the principle of internal standard method as used in XRD for phase quantification of a given material.

Binary mixture of *NiO* and *Mo* were prepared containing 20, 50 and 80 weight percent of *NiO*. 20 g of Al were added to 70 g of these mixtures and to 70 g of an unknown mixture of *NiO* and *Mo*. The X-ray intensities of three suitable reflections were recorded using *Cu K $\alpha$*  radiation. The results are shown below:

Wt% NiO	Wt% Mo	$I(\text{NiO})$	$I(\text{Mo})$	$I(\text{Al})$
20	80	73	639	246
50	50	196	423	261
80	20	508	271	423
Unknown	Unknown	227	364	263

Prepare suitable calibration graphs to determine the composition of unknown sample (hint: normalize the intensities with respect the intensity of the internal standard)

- v. A plot of mass absorption coefficient vs. energy of the X-ray photon for  $^{82}\text{Pb}$  is shown below:



State Beers law of X-ray absorption. Define all terms. Briefly describe the formation of the K edge shown in the figure.

4.

- i. Define following terms:

- |                        |                            |
|------------------------|----------------------------|
| (a) Auger electron     | (b) Satellite photon       |
| (c) X-ray fluorescence | (d) Monochromatic electron |

- ii. Explain the principle of energy and wavelength dispersive modes of X-ray fluorescence spectrometer.

- iii. List the important interactions that occur when an electron beam strikes the sample. Which type/s of interactions are frequently used in SEM? Chromate plated surface was imaged by SEM. State the type of the electron beams monitored in obtaining these images. (Plate A and Plate B shown in page 4)

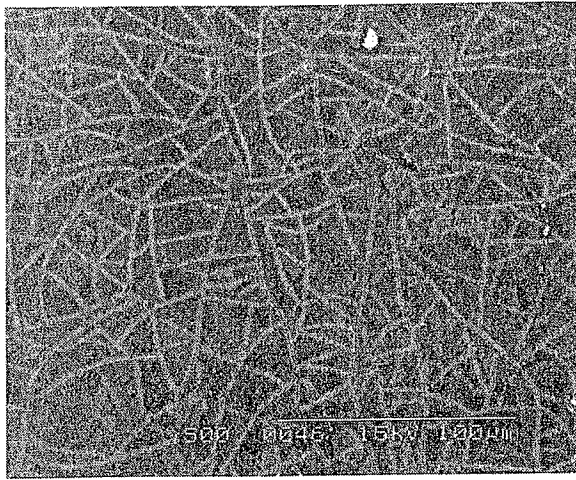


Plate A

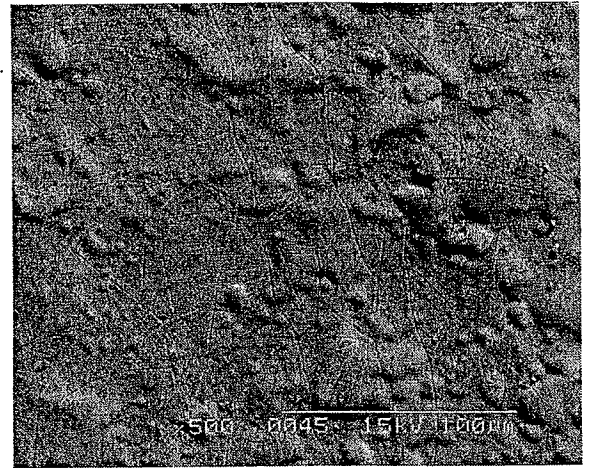


Plate B

- iv. Explain very briefly the photoelectric effect? State the principle of X-ray photo electron spectrometer with a help of the energy level diagram. Write down an expression for the conservation of energy of the electron.

An XPS electron was found to have a kinetic energy of 1073.5 eV when Mg  $K_{\alpha}$  source was employed ( $\lambda = 9.8900 \text{ \AA}$ ). The electron spectrometer has a work function of 14.7 eV. Calculate the binding energy of the emitted electron (hint: work function of the spectrometer a factor that corrects for the electrostatic environment in which the electron is formed and measured).

- v. Explain the tunneling effect of electrons (no mathematical expressions are need)? Use this information to explain the principle of STM.

## Mathematical formulae

$$CV = \frac{s}{\bar{x}} \times 100$$

$$CL = \bar{x} \pm \frac{z\sigma}{\sqrt{N}}$$

$$CL = \bar{x} \pm \frac{ts}{\sqrt{N}}$$

$$\frac{N_1}{N_0} = \left(\frac{g_1}{g_0}\right) \exp\left(\frac{-\Delta E}{RT}\right)$$

$$\Delta\lambda_{1/2} = \left(\frac{2}{c}\right) \left(\frac{2RT}{A_r}\right)^{3/2} \lambda$$

**t table**

Degrees of freedom (N-1)	confidence level			
	80%	90%	95%	99%
1	3.08	6.31	12.7	63.7
2	1.89	2.92	4.30	9.92
3	1.64	2.35	3.18	5.84
4	1.53	2.13	2.78	4.60
5	1.48	2.02	2.57	4.03
6	1.44	1.94	2.45	3.71
7	1.42	1.90	2.36	3.50
8	1.40	1.86	2.31	3.36
9	1.38	1.83	2.26	3.25
19	1.33	1.73	2.10	2.88
59	1.30	1.67	2.00	2.66
$\infty$	1.29	1.64	1.96	2.58

**z table**

Confidence level	z value
50	0.67
68	1.0
80	1.29
90	1.64
95	1.96
96	2.00
99	2.58
99.7	3.00
99.9	3.29

2.15 - 2.09 (±.01)

										File No.	I/c
o	2.09x	1.88 <sub>1</sub>	1.20 <sub>1</sub>	2.21 <sub>1</sub>	1.80 <sub>1</sub>	1.73 <sub>1</sub>	1.27 <sub>2</sub>	1.25 <sub>2</sub>	Fe <sub>3</sub> V <sub>2</sub> Si <sub>2</sub>	23-1134	
	2.08x	1.88 <sub>1</sub>	1.18 <sub>1</sub>	1.37 <sub>1</sub>	1.18 <sub>1</sub>	4.02 <sub>1</sub>	2.84 <sub>1</sub>	2.72 <sub>1</sub>	Os(Te <sub>1-9</sub> Sb <sub>0-1</sub> )	14- 572	
	2.14 <sub>1</sub>	1.87 <sub>1</sub>	2.34x	1.28 <sub>1</sub>	1.26 <sub>1</sub>	1.22 <sub>1</sub>	1.43 <sub>1</sub>	1.40 <sub>1</sub>	(Mo(Ga <sub>0-7</sub> Ge <sub>0-3</sub> ) <sub>2</sub> ) <sub>245</sub>	19- 489	
	2.14 <sub>1</sub>	1.87x	1.99 <sub>1</sub>	1.46 <sub>1</sub>	1.26 <sub>1</sub>	1.15 <sub>1</sub>	0.00 <sub>1</sub>	0.00 <sub>1</sub>	(Fe,Ni) <sub>2</sub> H	26- 790	
*	2.13 <sub>1</sub>	1.87 <sub>1</sub>	2.33x	1.90 <sub>1</sub>	1.40 <sub>1</sub>	1.21 <sub>2</sub>	1.27 <sub>1</sub>	2.48 <sub>1</sub>	(FeGe <sub>2</sub> ) <sub>12U</sub>	25- 357	
	2.08 <sub>1</sub>	1.87 <sub>1</sub>	3.37x	3.45 <sub>1</sub>	2.67 <sub>1</sub>	2.26 <sub>1</sub>	4.84 <sub>1</sub>	4.33 <sub>1</sub>	K <sub>2</sub> B <sub>2</sub> O <sub>3</sub> F <sub>4</sub> OH	21- 646	
*	2.16x	1.86 <sub>1</sub>	3.54x	1.19 <sub>1</sub>	2.18 <sub>1</sub>	1.40 <sub>1</sub>	1.26 <sub>1</sub>	1.24 <sub>1</sub>	Li <sub>7</sub> MnAs <sub>4</sub>	14- 43	
	2.16x	1.86 <sub>1</sub>	2.13 <sub>1</sub>	3.37 <sub>1</sub>	2.29 <sub>2</sub>	2.48 <sub>2</sub>	1.56 <sub>1</sub>	1.31 <sub>1</sub>	(VSi <sub>2</sub> ) <sub>9H</sub>	13- 260	
	2.15 <sub>1</sub>	1.86 <sub>1</sub>	2.63x	0.88x	1.67 <sub>1</sub>	1.52 <sub>1</sub>	3.72 <sub>1</sub>	1.18 <sub>1</sub>	(SmAl) <sub>2</sub> C	17- 712	
	2.15 <sub>1</sub>	1.86x	2.61 <sub>2</sub>	2.31 <sub>1</sub>	1.95 <sub>1</sub>	3.72 <sub>1</sub>	2.95 <sub>1</sub>	1.84 <sub>1</sub>	(Be <sub>17</sub> Hf <sub>2</sub> ) <sub>38H</sub>	14- 457	
o	2.15x	1.86 <sub>1</sub>	2.36x	1.24 <sub>1</sub>	1.76 <sub>1</sub>	1.22 <sub>1</sub>	1.06 <sub>1</sub>	1.28 <sub>1</sub>	(Fe,Ni) <sub>23</sub> C <sub>4</sub>	25- 405	
	2.13x	1.86x	1.83 <sub>1</sub>	1.31x	1.30x	0.00 <sub>1</sub>	0.00 <sub>1</sub>	0.00 <sub>1</sub>	FeMn <sub>3</sub>	3- 970	
	2.13x	1.86 <sub>1</sub>	1.22 <sub>2</sub>	1.11 <sub>2</sub>	2.63 <sub>1</sub>	1.50 <sub>1</sub>	1.30 <sub>1</sub>	1.07 <sub>1</sub>	(CuSn) <sub>2</sub> T	17- 865	
i	2.11x	1.86 <sub>1</sub>	2.45 <sub>1</sub>	1.27 <sub>1</sub>	1.29 <sub>1</sub>	1.23 <sub>1</sub>	1.20 <sub>1</sub>	2.74 <sub>1</sub>	((Fe,Ir) <sub>23</sub> B <sub>6</sub> )F	26-1132	
	2.16x	1.85 <sub>1</sub>	3.53x	1.40 <sub>1</sub>	1.25 <sub>1</sub>	1.18 <sub>1</sub>	1.76 <sub>1</sub>	1.53 <sub>1</sub>	(Be <sub>4</sub> AlMn) <sub>2</sub> C	18- 7	
i	2.16x	1.85 <sub>1</sub>	1.91 <sub>1</sub>	1.33 <sub>1</sub>	1.31 <sub>1</sub>	1.17 <sub>1</sub>	1.25 <sub>1</sub>	1.24 <sub>1</sub>	(Fe <sub>2</sub> GeN <sub>0-1</sub> ) <sub>18U</sub>	22- 345	
*	2.16x	1.85 <sub>1</sub>	1.25 <sub>1</sub>	3.53 <sub>1</sub>	1.41 <sub>1</sub>	1.04 <sub>1</sub>	0.93 <sub>1</sub>	1.18 <sub>1</sub>	ZnIn <sub>2</sub> Te <sub>4</sub>	8- 276	
	2.15 <sub>1</sub>	1.85 <sub>1</sub>	3.02x	1.91 <sub>1</sub>	6.03 <sub>1</sub>	3.48 <sub>1</sub>	4.35 <sub>2</sub>	2.81 <sub>2</sub>	NdPO <sub>3</sub>	4- 644	
*	2.16 <sub>1</sub>	1.84 <sub>1</sub>	3.52x	1.24 <sub>1</sub>	1.40 <sub>2</sub>	3.05 <sub>1</sub>	1.52 <sub>1</sub>	1.17 <sub>1</sub>	(GaSb) <sub>8</sub> F	7- 215	
*	2.16 <sub>1</sub>	1.84 <sub>1</sub>	3.52x	1.40 <sub>1</sub>	3.05 <sub>1</sub>	1.25 <sub>1</sub>	1.53 <sub>1</sub>	1.17 <sub>1</sub>	(ZnTe) <sub>8</sub> F	15- 746	
	2.16x	1.84 <sub>1</sub>	3.51x	1.25 <sub>1</sub>	1.77 <sub>1</sub>	1.41 <sub>1</sub>	1.53 <sub>2</sub>	1.37 <sub>2</sub>	(Cu <sub>2</sub> Te) <sub>12</sub> F	7- 106	
	2.15 <sub>1</sub>	1.84 <sub>1</sub>	3.70x	1.41 <sub>1</sub>	4.66 <sub>1</sub>	2.89 <sub>1</sub>	2.63 <sub>1</sub>	2.52 <sub>1</sub>	KPr(Ru(CN) <sub>6</sub> ) <sub>6</sub> ·6H <sub>2</sub> O	24- 889	
*	2.15 <sub>1</sub>	1.84 <sub>1</sub>	3.51x	3.04 <sub>1</sub>	1.40 <sub>1</sub>	1.24 <sub>1</sub>	1.52 <sub>1</sub>	1.76 <sub>1</sub>	HgSe	8- 469	
	2.15 <sub>1</sub>	1.84 <sub>1</sub>	3.51x	3.04 <sub>1</sub>	1.40 <sub>2</sub>	1.24 <sub>2</sub>	6.09 <sub>1</sub>	4.96 <sub>1</sub>	Li <sub>2</sub> TiAs <sub>2</sub>	21- 956	
i	2.13 <sub>1</sub>	1.84 <sub>1</sub>	4.35x	1.81 <sub>1</sub>	3.07 <sub>1</sub>	1.91 <sub>1</sub>	3.24 <sub>1</sub>	2.31 <sub>1</sub>	CoAl <sub>2</sub> (F,OH) <sub>6</sub>	5- 307	
*	2.13 <sub>1</sub>	1.84 <sub>1</sub>	3.49x	3.07 <sub>2</sub>	2.17 <sub>2</sub>	1.75 <sub>1</sub>	1.38 <sub>1</sub>	1.79 <sub>1</sub>	ZnI <sub>2</sub>	10- 72	
	2.12x	1.84 <sub>1</sub>	1.30 <sub>1</sub>	1.11 <sub>1</sub>	1.06 <sub>1</sub>	3.70 <sub>2</sub>	2.59 <sub>2</sub>	1.65 <sub>2</sub>	(Fe <sub>2</sub> Ge) <sub>4</sub> C	17- 129	
	2.11x	1.84 <sub>1</sub>	2.14 <sub>1</sub>	1.20x	1.31 <sub>1</sub>	1.27 <sub>1</sub>	3.32 <sub>2</sub>	2.24 <sub>2</sub>	(MnAl <sub>0-7</sub> Si <sub>1-23</sub> ) <sub>9</sub> H	18- 37	
	2.10 <sub>1</sub>	1.84 <sub>1</sub>	2.30x	1.19 <sub>1</sub>	1.25 <sub>1</sub>	3.72 <sub>1</sub>	2.18 <sub>1</sub>	1.41 <sub>1</sub>	(MoAl <sub>1-3</sub> Si <sub>0-7</sub> ) <sub>245</sub>	17- 423	
*	2.16x	1.83 <sub>1</sub>	3.52x	1.24x	1.40 <sub>1</sub>	2.14 <sub>1</sub>	1.25 <sub>1</sub>	1.86 <sub>2</sub>	Li <sub>3</sub> MnAs <sub>2</sub>	14- 42	
	2.16x	1.83 <sub>1</sub>	2.79x	1.67 <sub>1</sub>	1.15 <sub>1</sub>	1.54 <sub>1</sub>	1.47 <sub>1</sub>	1.40 <sub>1</sub>	Cr <sub>2</sub> Se <sub>2</sub> Te	20- 968	
*	2.15x	1.83x	3.52x	1.40 <sub>1</sub>	1.25 <sub>1</sub>	1.53 <sub>1</sub>	1.57 <sub>1</sub>	1.47 <sub>1</sub>	Cu <sub>2</sub> HgI <sub>4</sub>	18- 450	
	2.15 <sub>1</sub>	1.83 <sub>1</sub>	3.51x	1.39 <sub>1</sub>	1.24 <sub>1</sub>	1.52 <sub>1</sub>	1.17 <sub>1</sub>	1.08 <sub>1</sub>	(CdSe) <sub>8</sub> F	19- 191	
*	2.15 <sub>1</sub>	1.83 <sub>1</sub>	3.51x	3.04 <sub>1</sub>	1.03 <sub>1</sub>	1.24 <sub>1</sub>	0.96 <sub>1</sub>	0.93 <sub>1</sub>	Li <sub>2</sub> CdP	25- 470	
	2.14 <sub>1</sub>	1.83 <sub>1</sub>	3.50x	0.79 <sub>1</sub>	3.03 <sub>1</sub>	1.39 <sub>1</sub>	1.23 <sub>1</sub>	0.81 <sub>1</sub>	(Li <sub>3</sub> SiAs <sub>2</sub> ) <sub>12</sub> F	7- 148	
*	2.14 <sub>1</sub>	1.83 <sub>1</sub>	3.50x	1.24 <sub>1</sub>	0.81 <sub>2</sub>	1.39 <sub>1</sub>	1.51 <sub>1</sub>	1.17 <sub>1</sub>	(InAs) <sub>8</sub> F	15- 869	
	2.14x	1.83 <sub>1</sub>	3.50 <sub>1</sub>	1.24 <sub>1</sub>	1.39 <sub>2</sub>	1.17 <sub>2</sub>	1.07 <sub>2</sub>	1.51 <sub>1</sub>	(Be <sub>3</sub> (FeAl)) <sub>24</sub> F	18- 5	
	2.14x	1.83 <sub>1</sub>	3.49x	3.01 <sub>1</sub>	1.39 <sub>1</sub>	1.24 <sub>1</sub>	1.74 <sub>1</sub>	1.51 <sub>1</sub>	(Be <sub>4</sub> AlFe) <sub>2</sub> C	18- 6	
i	2.12x	1.83 <sub>1</sub>	2.07 <sub>2</sub>	1.06 <sub>1</sub>	1.11 <sub>1</sub>	1.38 <sub>1</sub>	1.36 <sub>1</sub>	0.00 <sub>1</sub>	(Cu,Zn) <sub>12</sub> H	25- 322	
o	2.10x	1.83 <sub>1</sub>	1.28 <sub>1</sub>	1.81 <sub>1</sub>	1.29 <sub>1</sub>	2.74 <sub>1</sub>	1.93 <sub>1</sub>	2.63 <sub>1</sub>	Cu-Be	9- 213	
	2.08 <sub>1</sub>	1.83 <sub>1</sub>	2.27x	1.24g	1.18 <sub>1</sub>	2.17 <sub>1</sub>	1.40 <sub>1</sub>	1.35 <sub>1</sub>	(Go <sub>2</sub> Ru) <sub>245</sub>	23- 261	
	2.08 <sub>1</sub>	1.83x	2.24 <sub>1</sub>	1.85 <sub>1</sub>	2.76 <sub>1</sub>	1.99 <sub>1</sub>	2.60 <sub>1</sub>	3.22 <sub>1</sub>	(Rh <sub>2</sub> Te <sub>2</sub> ) <sub>20Q</sub>	19-1057	
	2.08 <sub>1</sub>	1.83 <sub>1</sub>	1.92x	3.13 <sub>1</sub>	2.65 <sub>1</sub>	3.01 <sub>1</sub>	1.33 <sub>1</sub>	1.38 <sub>1</sub>	CuCrSe <sub>2</sub>	9- 299	
	2.16 <sub>1</sub>	1.82 <sub>1</sub>	2.78x	1.17 <sub>1</sub>	1.15 <sub>1</sub>	1.68 <sub>1</sub>	1.52 <sub>1</sub>	1.10 <sub>1</sub>	FeSe	26- 795	
*	2.14 <sub>1</sub>	1.82 <sub>1</sub>	3.49x	3.03x	1.39 <sub>1</sub>	1.24 <sub>1</sub>	1.51 <sub>1</sub>	1.16 <sub>1</sub>	CuI	6- 246	
	2.13 <sub>1</sub>	1.82 <sub>1</sub>	1.97x	3.69 <sub>1</sub>	3.49 <sub>1</sub>	3.26 <sub>1</sub>	2.54 <sub>1</sub>	1.78 <sub>2</sub>	(Be <sub>2</sub> Cr) <sub>12</sub> H	12- 588	
	2.09x	1.82 <sub>1</sub>	3.28 <sub>1</sub>	2.45 <sub>1</sub>	2.22 <sub>1</sub>	2.12 <sub>1</sub>	1.53 <sub>1</sub>	1.29 <sub>1</sub>	(CrSi <sub>2</sub> ) <sub>9</sub> H	12- 596	
	2.08 <sub>1</sub>	1.82 <sub>1</sub>	2.29x	1.31 <sub>1</sub>	1.19 <sub>1</sub>	2.13 <sub>1</sub>	1.39 <sub>1</sub>	1.36 <sub>1</sub>	TiSi <sub>2</sub>	2-1120	
	2.13x	1.81 <sub>1</sub>	3.47x	3.00 <sub>1</sub>	1.38 <sub>1</sub>	1.23 <sub>1</sub>	1.16 <sub>1</sub>	1.73 <sub>1</sub>	(Be <sub>4</sub> AlNi) <sub>2</sub> C	18- 8	
	2.13 <sub>1</sub>	1.81 <sub>1</sub>	2.76x	1.38 <sub>1</sub>	5.82 <sub>1</sub>	2.91 <sub>1</sub>	1.65 <sub>1</sub>	1.52 <sub>1</sub>	Cr <sub>0-66</sub> Se	21- 241	
i	2.12 <sub>1</sub>	1.81 <sub>1</sub>	3.46x	3.00 <sub>2</sub>	1.38 <sub>2</sub>	1.73 <sub>1</sub>	1.50 <sub>1</sub>	1.23 <sub>1</sub>	(CuInAl <sub>2</sub> Te) <sub>7</sub> F	24- 346	
	2.12 <sub>1</sub>	1.81 <sub>1</sub>	3.43x	1.38 <sub>1</sub>	1.23 <sub>1</sub>	0.80 <sub>1</sub>	0.78 <sub>1</sub>	2.98 <sub>1</sub>	Zn <sub>3</sub> As	15- 477	
	2.12x	1.81 <sub>1</sub>	3.00 <sub>1</sub>	1.73 <sub>2</sub>	0.00 <sub>1</sub>	0.00 <sub>1</sub>	0.00 <sub>1</sub>	0.00 <sub>1</sub>	Ag <sub>1-2</sub> Cu <sub>0-8</sub> S	12- 154	
i	2.12 <sub>1</sub>	1.81 <sub>1</sub>	2.75x	5.77 <sub>1</sub>	2.89 <sub>1</sub>	1.64 <sub>1</sub>	1.53 <sub>1</sub>	1.51 <sub>1</sub>	Cr <sub>0-66</sub> Se	23- 931	
	2.12 <sub>1</sub>	1.81 <sub>1</sub>	2.04x	1.74 <sub>1</sub>	1.21 <sub>1</sub>	1.18 <sub>1</sub>	1.16 <sub>1</sub>	2.30 <sub>1</sub>	(Cr,Fe) <sub>2</sub> C <sub>3</sub>	5- 720	
o	2.11 <sub>1</sub>	1.81 <sub>1</sub>	3.33x	1.20 <sub>1</sub>	1.37 <sub>1</sub>	1.18 <sub>1</sub>	1.18 <sub>1</sub>	1.54 <sub>1</sub>	(Re <sub>0-74</sub> Nb <sub>0-12</sub> Co <sub>0-14</sub> )	23- 448	
	2.10 <sub>1</sub>	1.81 <sub>1</sub>	2.74x	2.18 <sub>2</sub>	1.61 <sub>1</sub>	2.22 <sub>1</sub>	1.96 <sub>1</sub>	0.00 <sub>1</sub>	(MnAs <sub>0-9</sub> Po <sub>0-1</sub> ) <sub>8</sub> O	23- 807	
*	2.09x	1.81 <sub>1</sub>	1.28 <sub>1</sub>	1.09 <sub>2</sub>	0.83 <sub>1</sub>	0.81 <sub>1</sub>	1.04 <sub>1</sub>	0.90 <sub>1</sub>	Cu	4- 836	
i	2.08 <sub>1</sub>	1.81x	3.42 <sub>1</sub>	1.35 <sub>1</sub>	1.74 <sub>1</sub>	2.13 <sub>1</sub>	1.71 <sub>1</sub>	1.38 <sub>1</sub>	BaAgF <sub>4</sub>	26- 181	
	2.16x	1.80 <sub>1</sub>	2.76x	1.53 <sub>1</sub>	2.98 <sub>1</sub>	1.67 <sub>1</sub>	1.67 <sub>1</sub>	1.55 <sub>1</sub>	Ti <sub>3</sub> Se <sub>6</sub>	17- 583	
*	2.15x	1.80x	2.99x	2.06x	2.04x	3.60 <sub>1</sub>	2.69 <sub>1</sub>	1.70 <sub>1</sub>	Cu(NH <sub>3</sub> ) <sub>6</sub> Br <sub>2</sub>	20- 346	
*	2.15 <sub>1</sub>	1.80 <sub>1</sub>	2.75x	2.97 <sub>2</sub>	1.67 <sub>2</sub>	1.67 <sub>2</sub>	5.92 <sub>1</sub>	5.50 <sub>1</sub>	FeTi <sub>2</sub> Se <sub>4</sub>	20-1302	
	2.13x	1.80x	3.47x	3.00 <sub>1</sub>	1.38 <sub>1</sub>	1.34 <sub>1</sub>	1.23 <sub>1</sub>	1.16 <sub>1</sub>	SiI <sub>4</sub>	4- 487	
*	2.12 <sub>1</sub>	1.80 <sub>1</sub>	3.46x	1.22 <sub>1</sub>	0.80 <sub>7</sub>	1.01 <sub>1</sub>	0.95 <sub>1</sub>	2.99 <sub>1</sub>	Li <sub>2</sub> VP <sub>4</sub>	10- 214	
	2.12 <sub>1</sub>	1.80 <sub>1</sub>	2.74x	1.65 <sub>1</sub>	1.09 <sub>1</sub>	5.81 <sub>1</sub>	1.50 <sub>1</sub>	1.37 <sub>1</sub>	VCl <sub>2</sub>	15- 215	
*	2.11x	1.80 <sub>1</sub>	3.45x	1.22 <sub>1</sub>	1.01 <sub>1</sub>	1.06 <sub>1</sub>	1.15 <sub>1</sub>	1.37 <sub>1</sub>	Li <sub>7</sub> MnP <sub>4</sub>	14- 45	
	2.11 <sub>1</sub>	1.80 <sub>1</sub>	3.45x	2.99 <sub>1</sub>	1.72 <sub>1</sub>	1.49 <sub>1</sub>	1.37 <sub>1</sub>	1.33 <sub>1</sub>	K <sub>2</sub> UF <sub>6</sub>	12- 42	
	2.11 <sub>1</sub>	1.80 <sub>1</sub>	3.44x	2.99 <sub>2</sub>	1.22 <sub>2</sub>	1.37 <sub>1</sub>	1.01 <sub>1</sub>	1.49 <sub>1</sub>	Li <sub>0-66</sub> V <sub>1-12</sub> P <sub>4</sub>	21- 535	
	2.11 <sub>1</sub>	1.80 <sub>1</sub>	3.44x	1.22 <sub>2</sub>	2.98 <sub>2</sub>	1.37 <sub>2</sub>	1.49 <sub>1</sub>	1.15 <sub>1</sub>	Li <sub>0-66</sub> Ti <sub>1-02</sub> P <sub>4</sub>	21- 529	
	2.11x	1.80 <sub>1</sub>	2.74x	1.64 <sub>1</sub>	1.51 <sub>1</sub>	1.37 <sub>1</sub>	1.21 <sub>1</sub>	1.53 <sub>1</sub>	CrSe	2- 883	
	2.11 <sub>1</sub>	1.80 <sub>1</sub>	2.73x</								