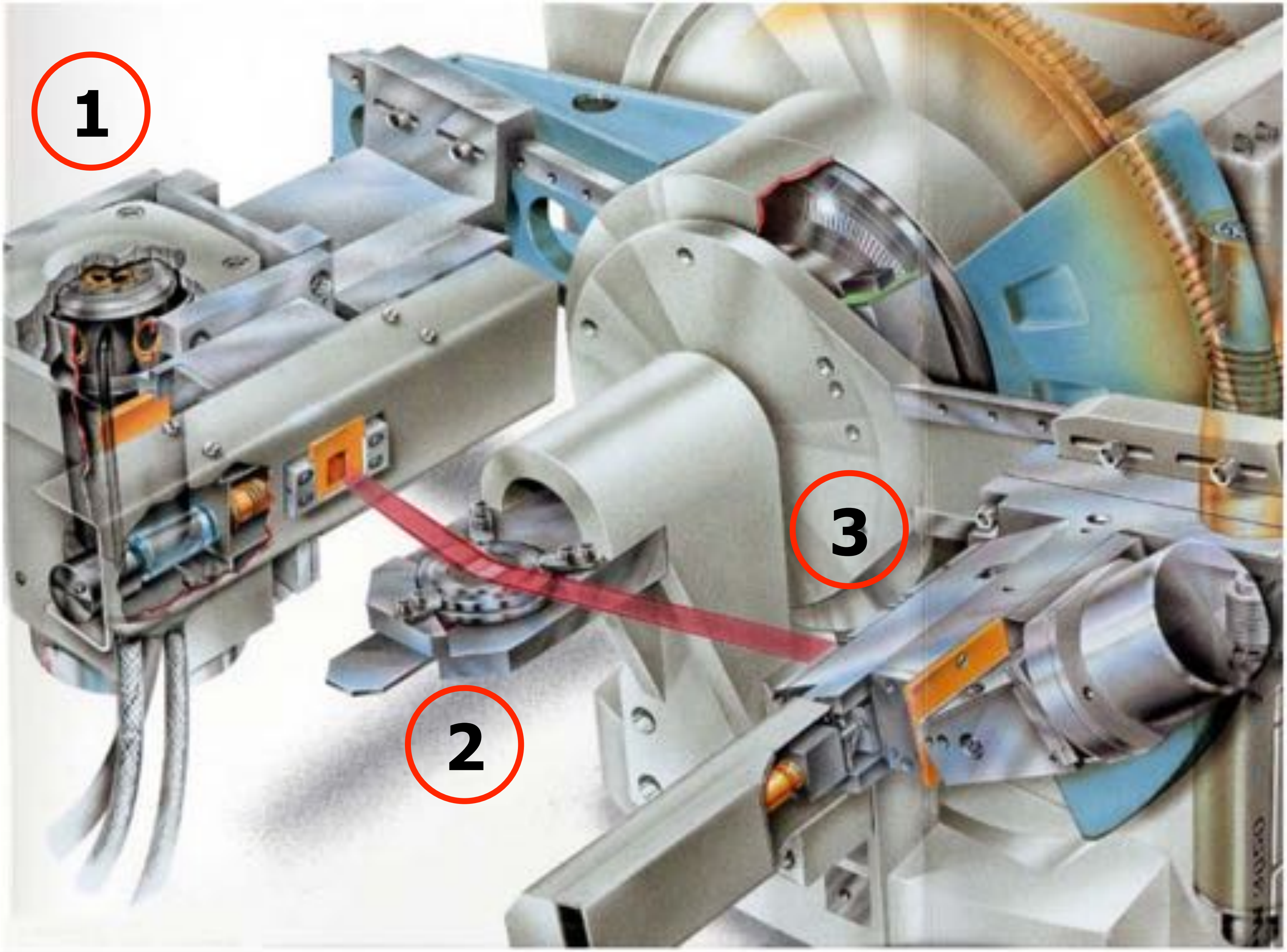
Universidad Nacional Autónoma de México

Facultad de Química

Química del Estado Sólido

5. Difracción de rayos X

Víctor Fabián Ruiz Ruiz.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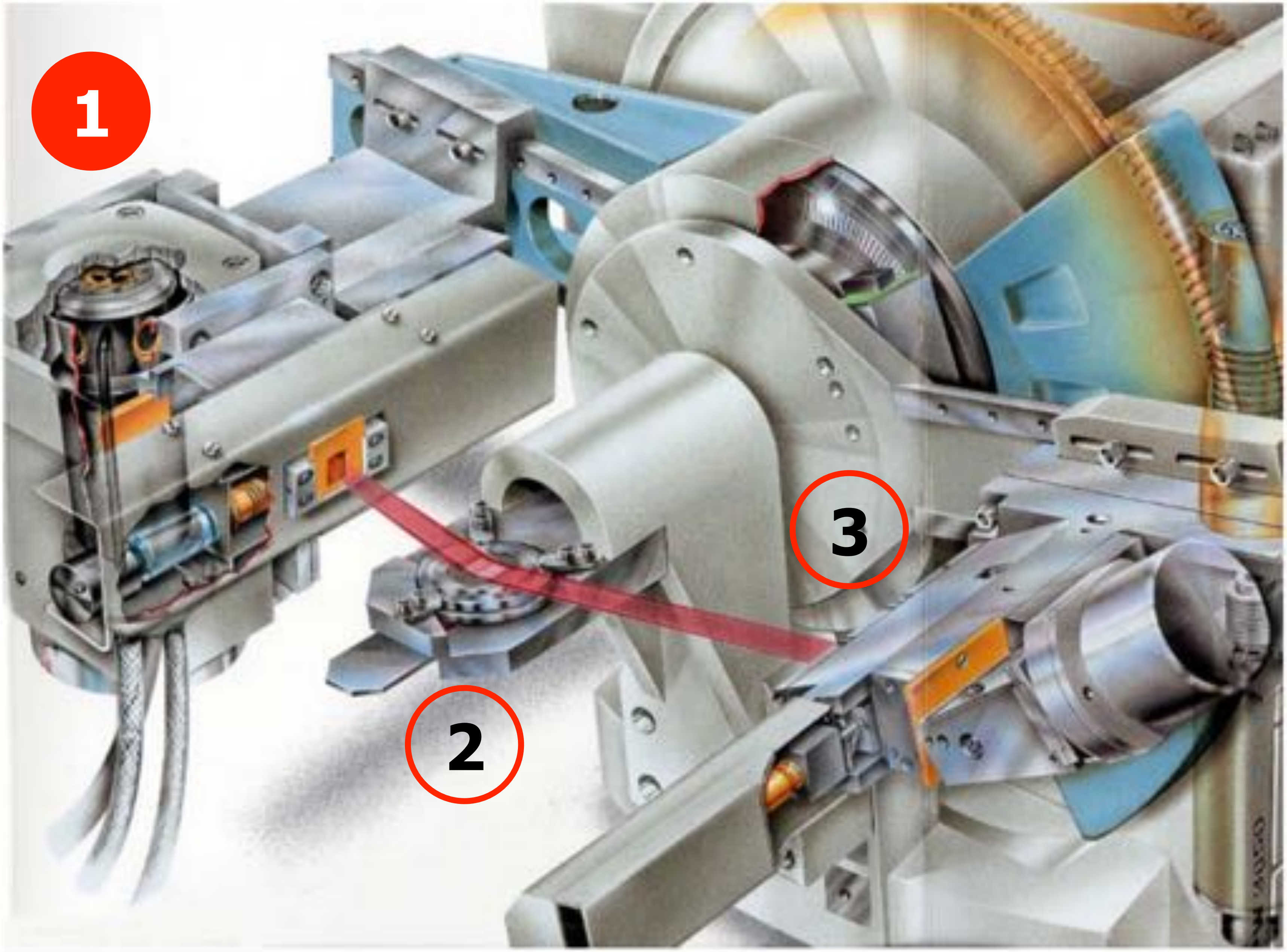
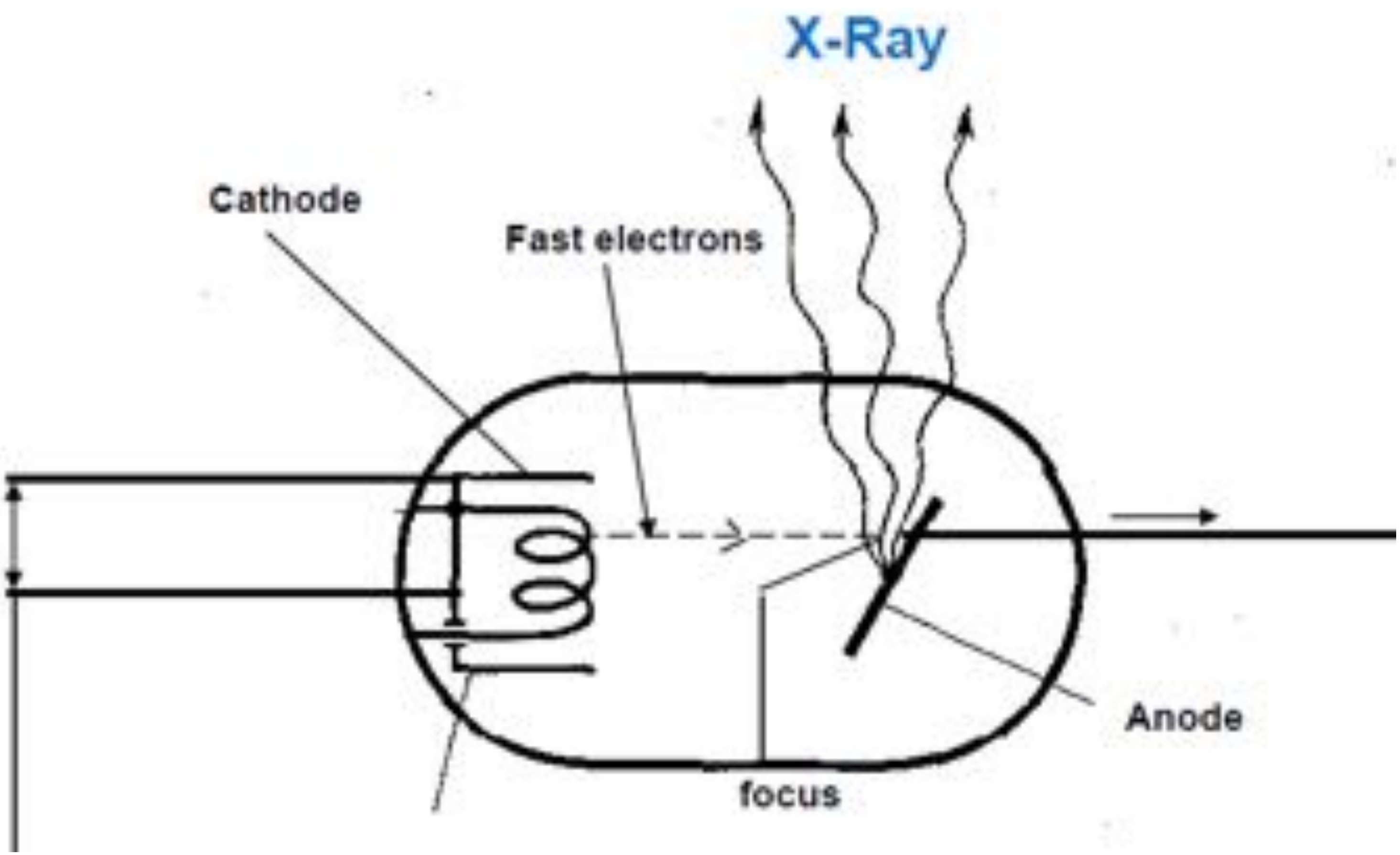
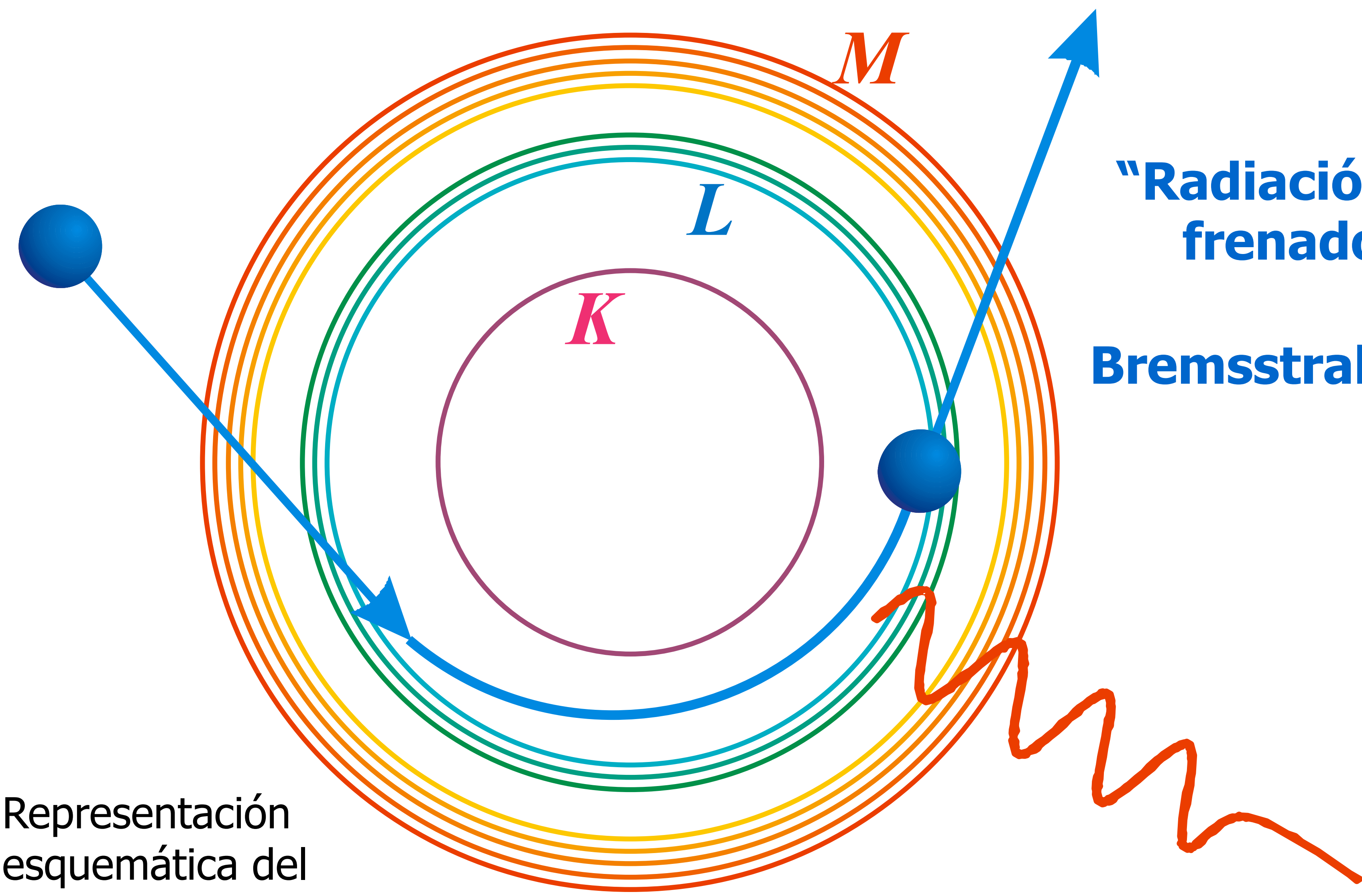
2
3


1
2
3

5.2 Generación de rayos X



GENERACIÓN DE RAYOS X

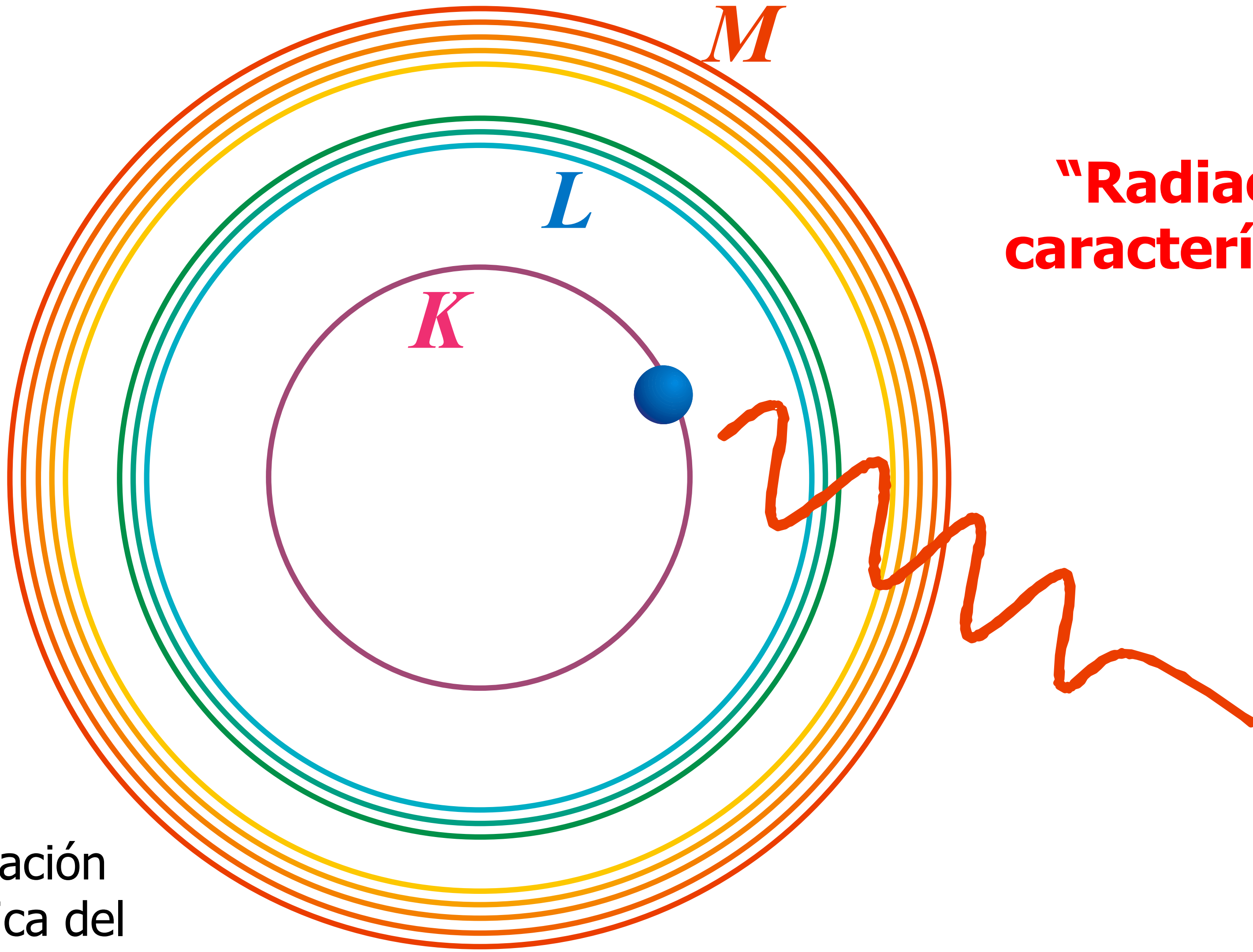


"Radiación de frenado"

Bremsstrahlung

Representación esquemática del modelo de Bohr

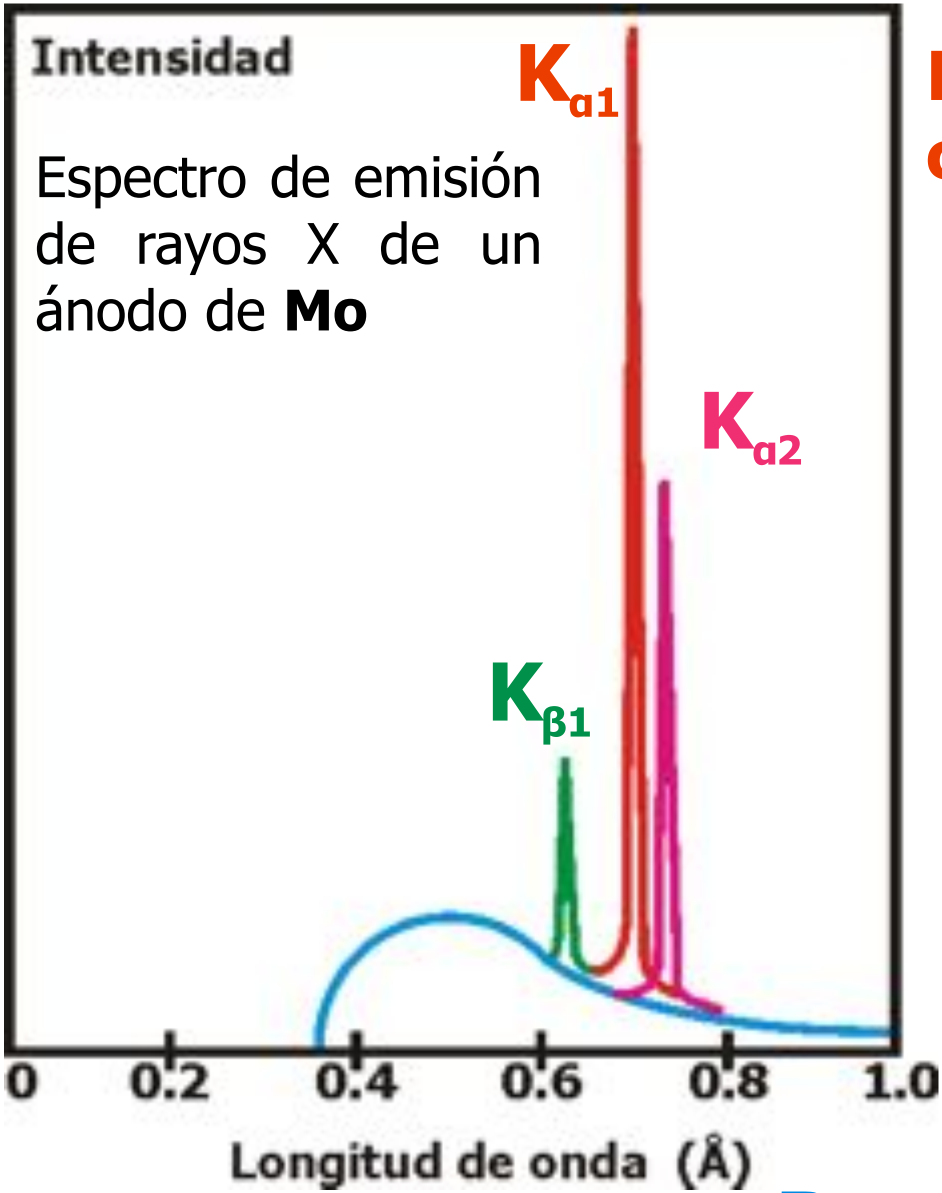
GENERACIÓN DE RAYOS X



"Radiación caracterísitca"

Representación esquemática del modelo de Bohr

GENERACIÓN DE RAYOS X



Radiación característica = Líneas espectrales

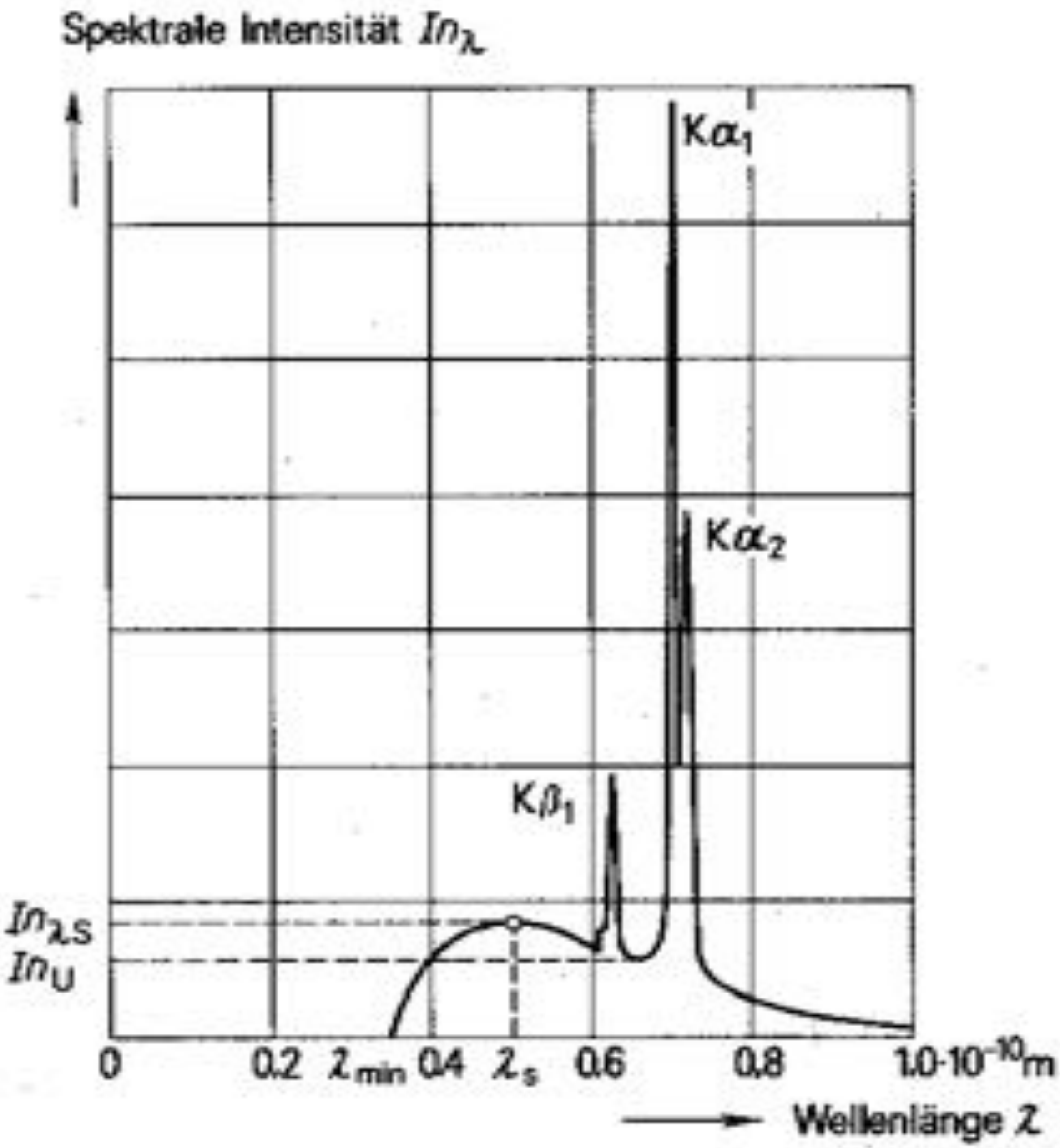
$$E = \frac{hc}{\lambda}$$

Kα1 = 0.7093 Å = 17.48 keV

Kα2 = 0.7135 Å = 17.38 keV

Kβ1 = 0.6322 Å = 19.61 keV

Bremsstrahlung = Espectro continuo



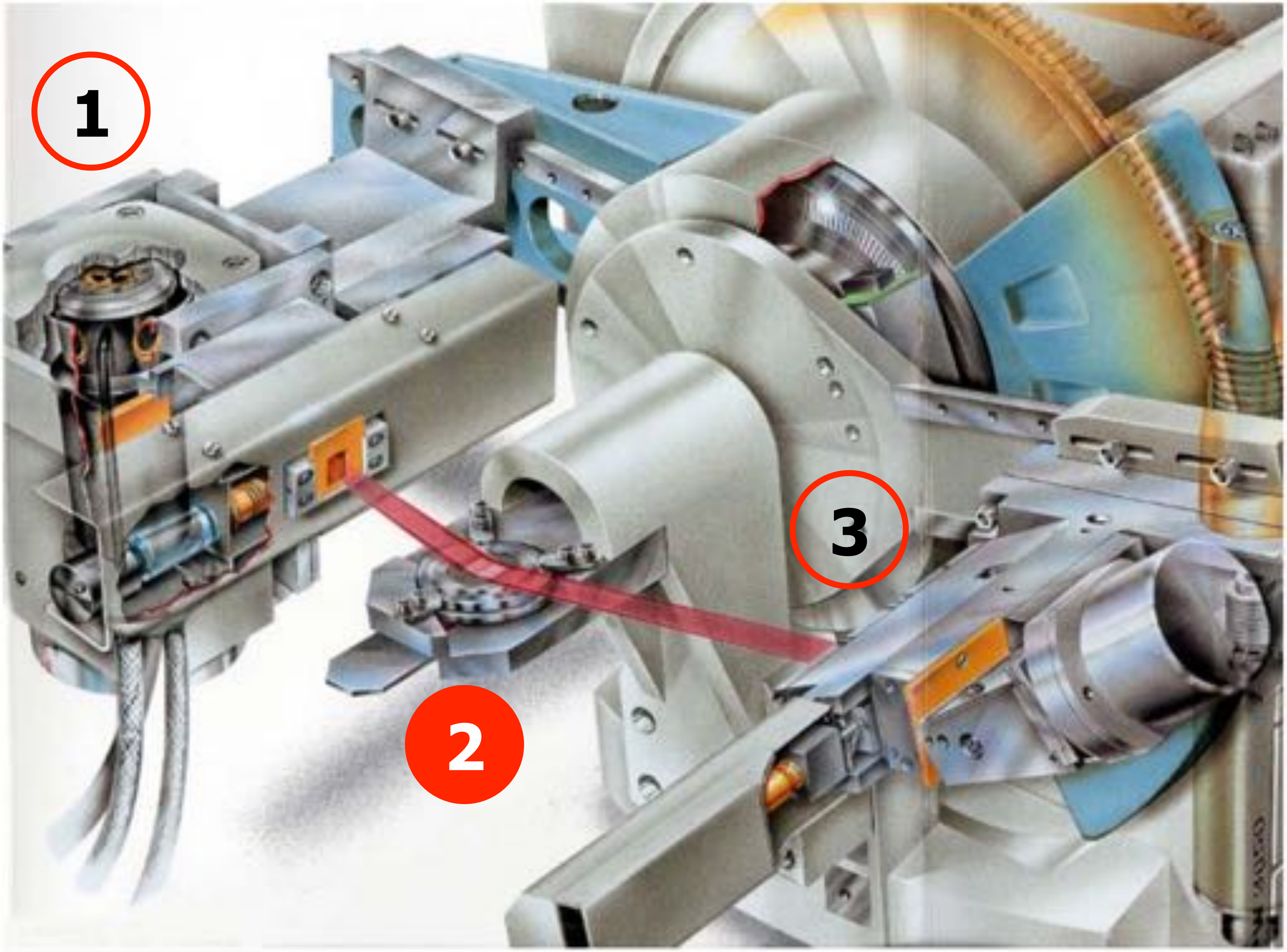
Spektrale Intensität In_λ
$K\alpha_1$
$K\alpha_2$
$K\beta_1$
$In_{\lambda S}$
In_U
0
0.2
λ_{min}
0.4
λ_s
0.6
0.8
$1.0 \cdot 10^{-10}$ m
Wellenlänge λ

GENERACIÓN DE RAYOS X

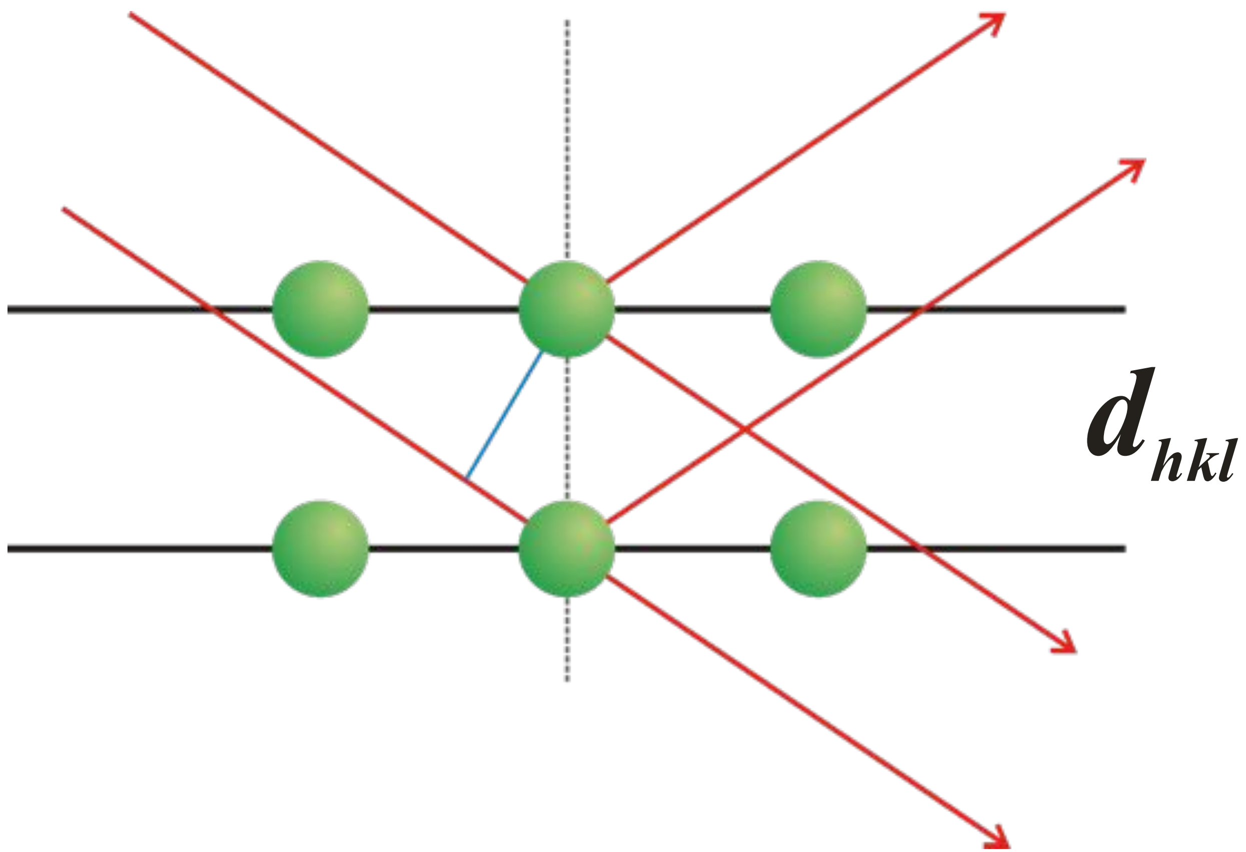
Anode materials and monochromatization of X-rays

atom no.	element	$K\alpha$	$K\alpha_1$	$K\alpha_2$	$K\beta$
24	chromium	2.29092	2.28962	2.29351	2.08480
26	iron	1.93728	1.93597	1.93991	1.75643
27	cobalt	1.79021	1.78892	1.79278	1.62075
28	nickel	1.65912	1.65784	1.66169	1.50010
29	**copper**	**1.54178**	**1.54051**	**1.54433**	**1.39217**
42	**molybdenum**	**0.71069**	**0.70926**	**0.71354**	**0.63225**
47	silver	0.56083	0.55936	0.56378	0.49701
74	tungsten	0.21060	0.20899	0.21381	0.18436

Longitud de onda (en Å) de diferentes líneas de emisión de algunos matales utilizados como ánodos.

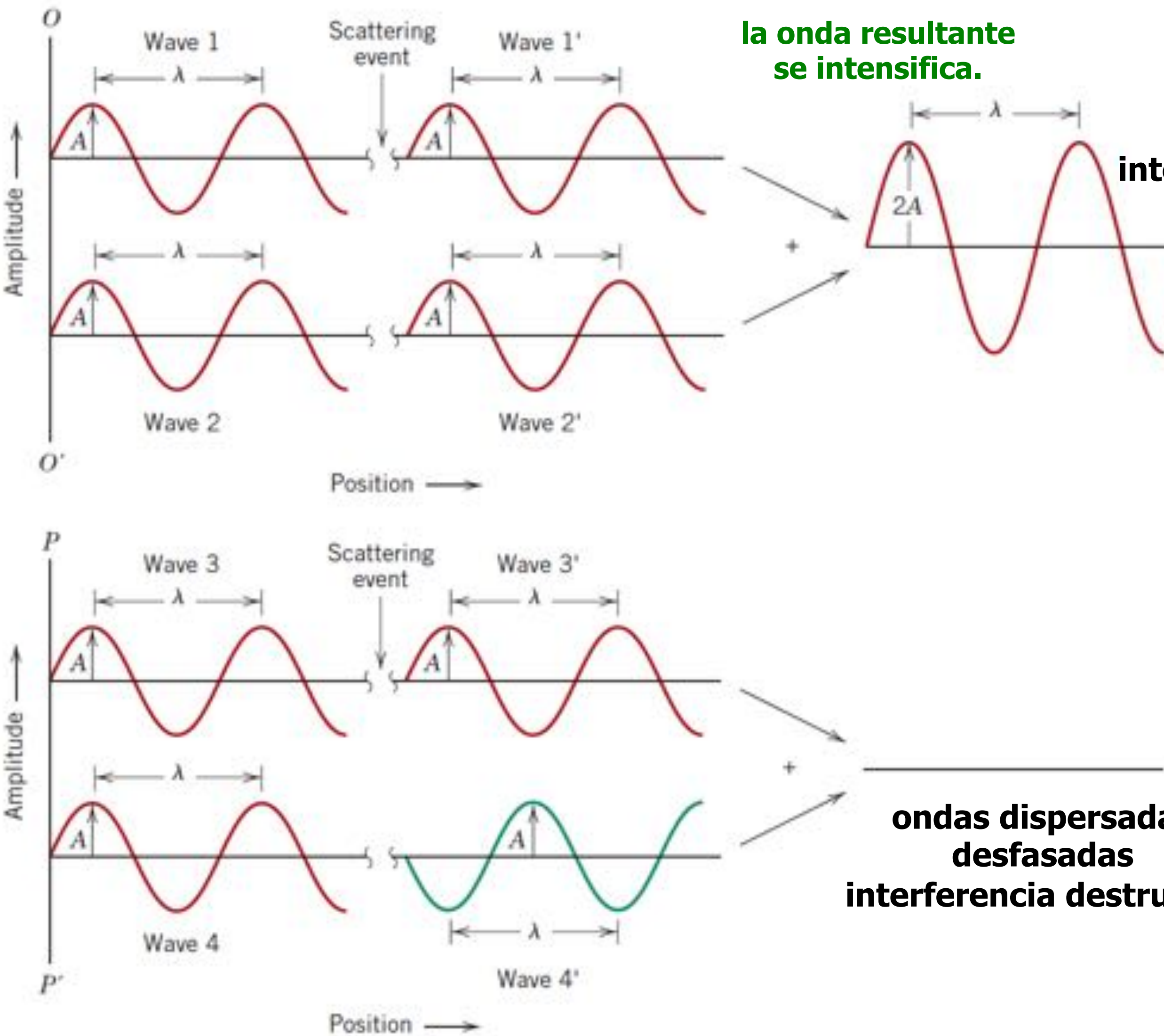

1
2
3

5.1 LEY DE BRAGG



$$2d_{hkl}\,sen\theta = n\lambda$$

5.1 LEY DE BRAGG

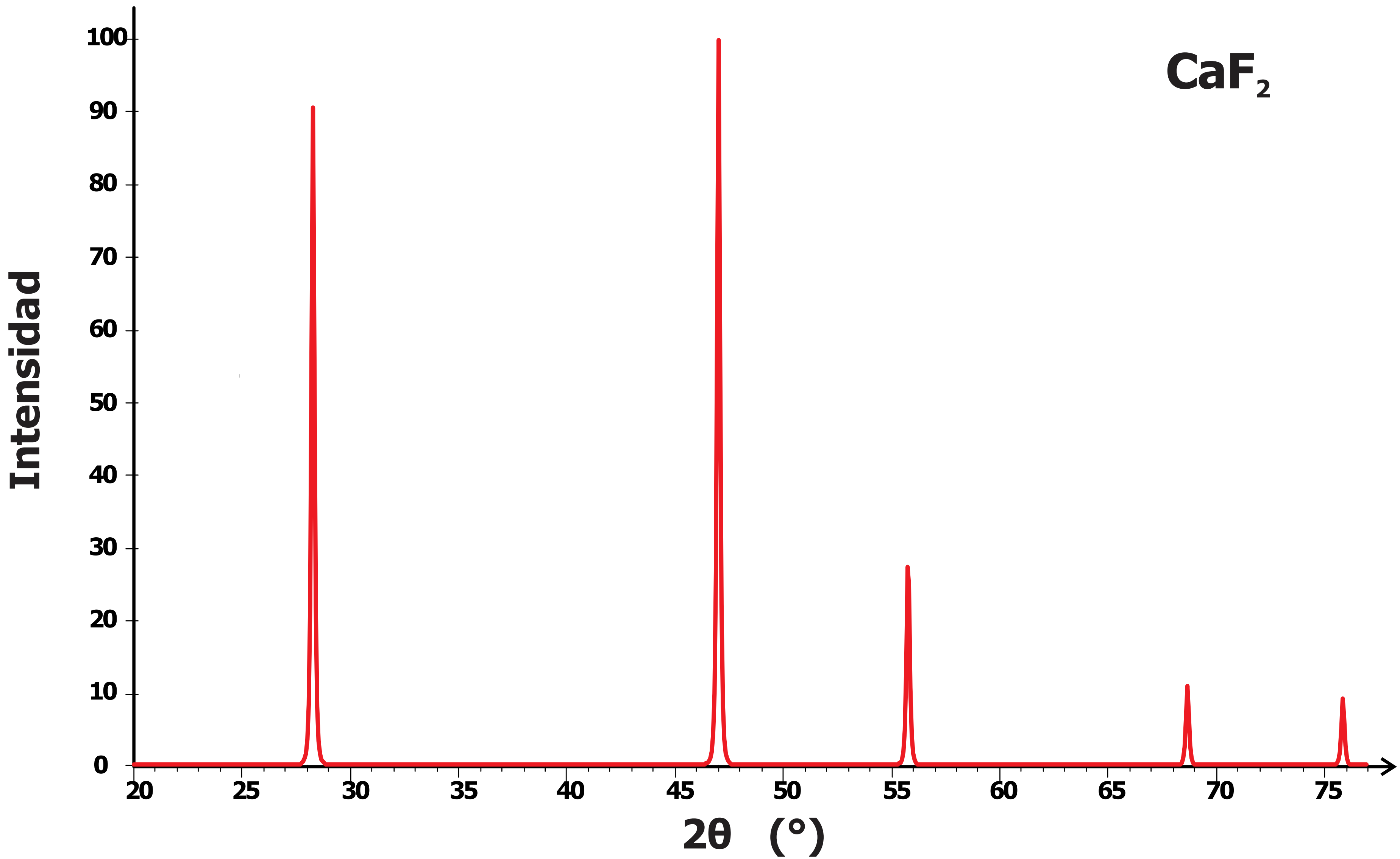


la onda resultante se intensifica.

ondas dispersadas en fase
interferencia constructiva

Esta es una manifestación de difracción, y la referimos como un rayo difractado compuesto de un gran número de ondas dispersadas, que se refuerzan unas con otras.

ondas dispersadas desfasadas
interferencia destructiva



CaF2
Intensidad
2θ (°)
0
10
20
30
40
50
60
70
80
90
100
20
25
30
35
40
45
50
55
60
65
70
75

INTENSIDAD DE UN HAZ DIFRACTADO

La intensidad de los haces difractados dependen básicamente de los siguientes factores:

1. La naturaleza de la radiación.

2. El ángulo de Bragg.

3. El "poder" de difracción de los átomos presentes (**factor de dispersión**).

4. El arreglo de los átomos en el cristal (**factor de estructura**).

5. Vibración térmica de los átomos (factor de temperatura)

6. El espesor, forma y grado de perfección del cristal (factor de forma).

7. El número de planos equivalentes (hkl) presentes (multiplicidad)*

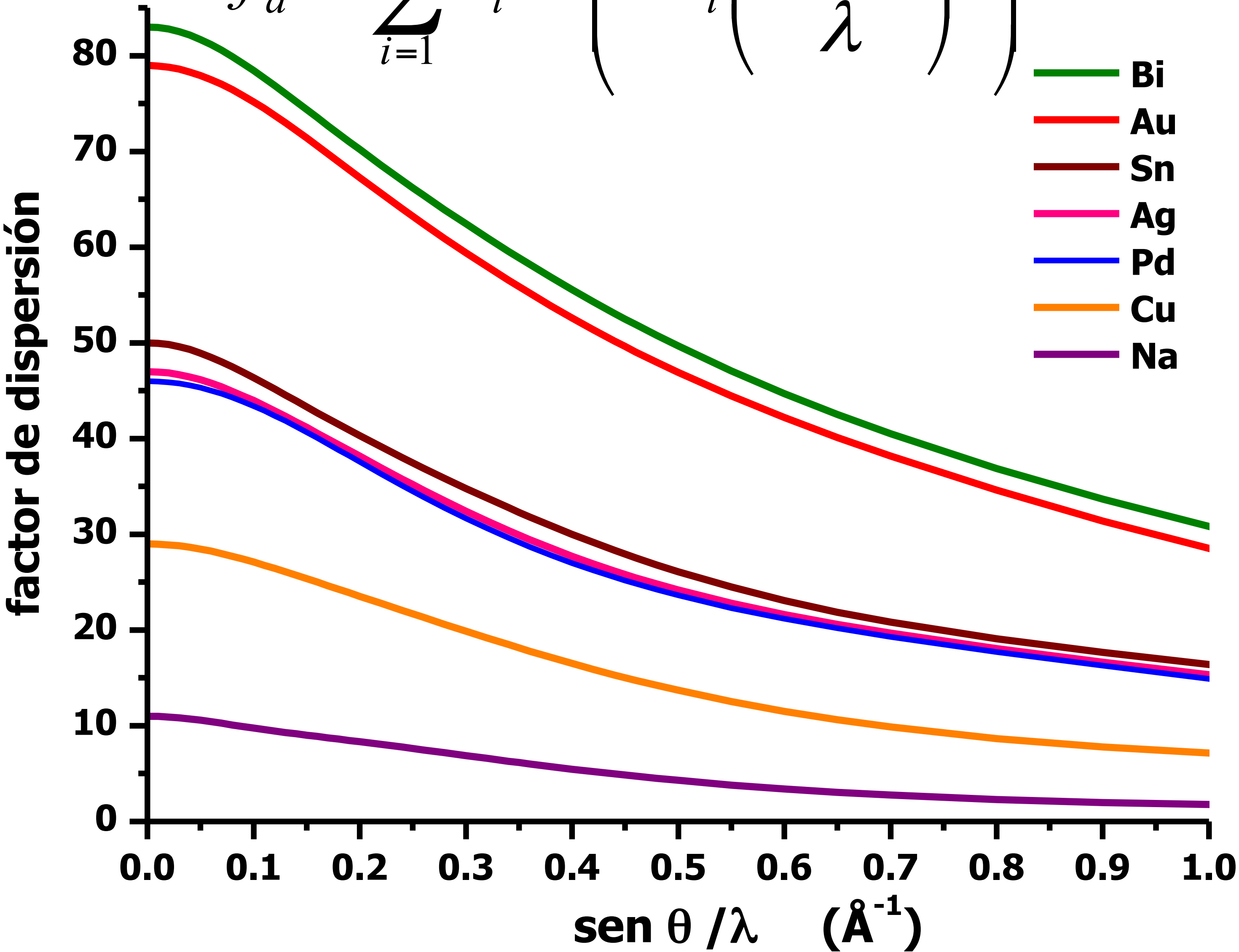
5.3 FACTOR DE DISPERSIÓN

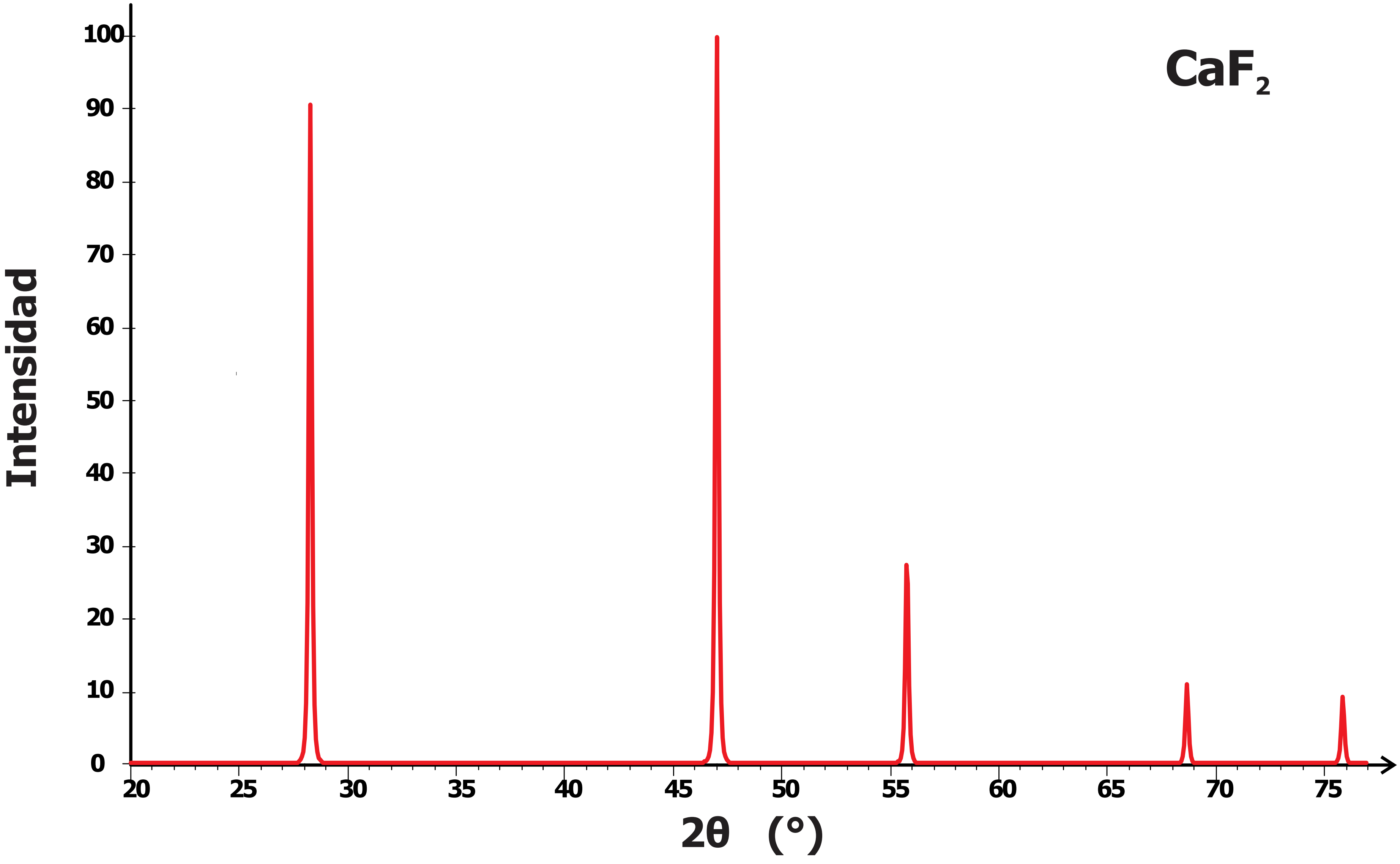
$$f_a = \sum_{i=1}^{4} a_i \cdot e\left(-b_i \left(\frac{sen\theta}{\lambda} \right)^2 \right) + c$$

Coeficientes de **Cromer-Mann**

5.3 FACTOR DE DISPERSIÓN

$$f_a = \sum_{i=1}^{4} a_i \cdot e\left(-b_i\left(\frac{sen\,\theta}{\lambda}\right)^2\right) + c$$





CaF_2
Intensidad
2θ (°)
0
10
20
30
40
50
60
70
80
90
100
20
25
30
35
40
45
50
55
60
65
70
75

5.4 Factor de Estructura

$$F_{hkl} = \sum^{N} f_n \cdot e\left(2\pi i\left(hx_n + ky_n + lz_n\right)\right)$$

Calculando d_{hkl} en los otros sistemas

Cúbico

$$\frac{1}{d_{hkl}^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

(hkl)	d_{hkl}
(100)	
(010)	
(001)	
{100}	

Tetragonal

$$\frac{1}{d_{hkl}^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

(hkl)	d_{hkl}
(100)	
(010)	{100}
(001)	{001}

Ortorrómbico

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

Hexagonal

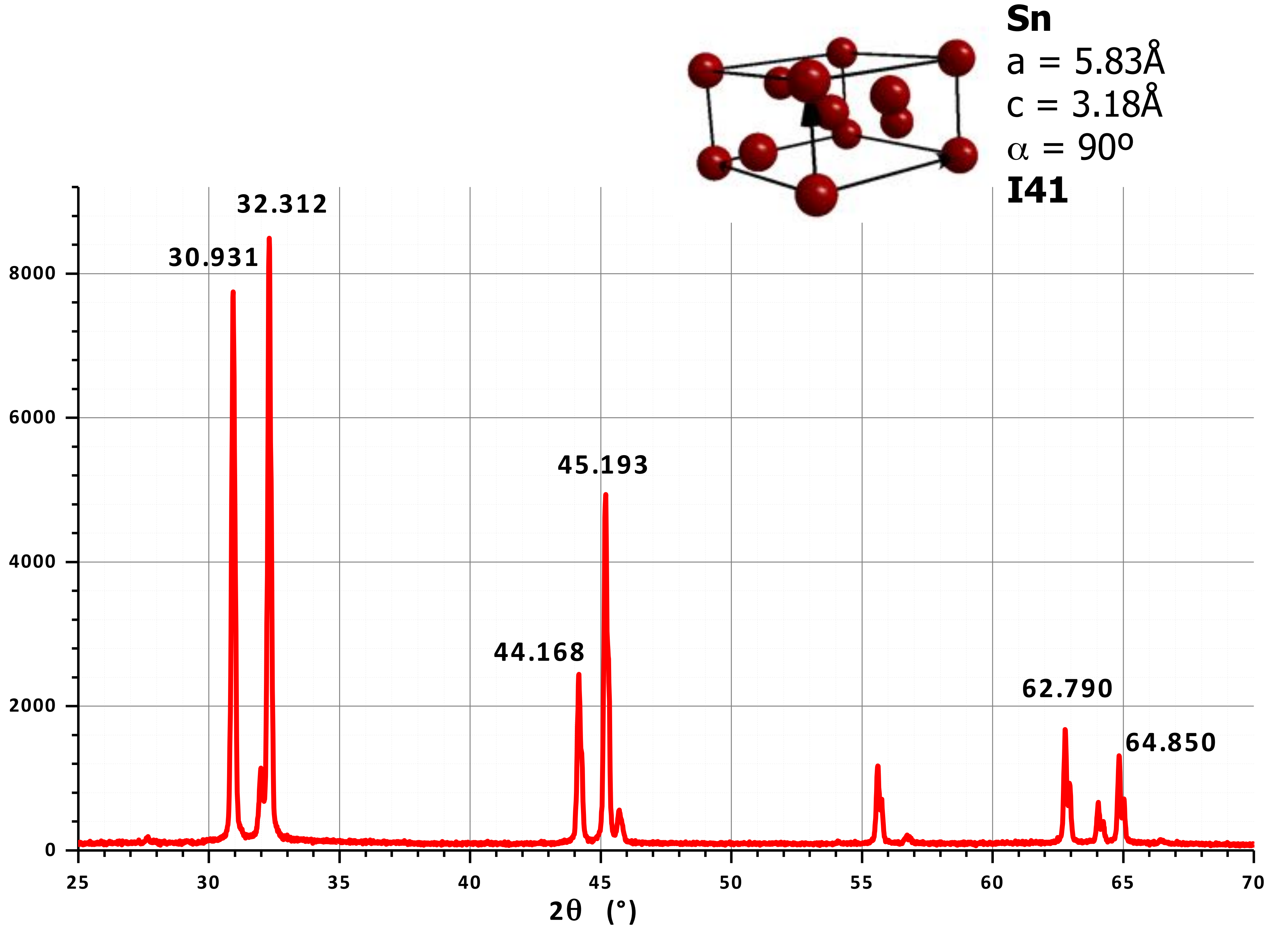
$$\frac{1}{d_{hkl}^2} = \frac{4}{3}\frac{h^2 + hk + k^2}{a^2} + \frac{l^2}{c^2}$$

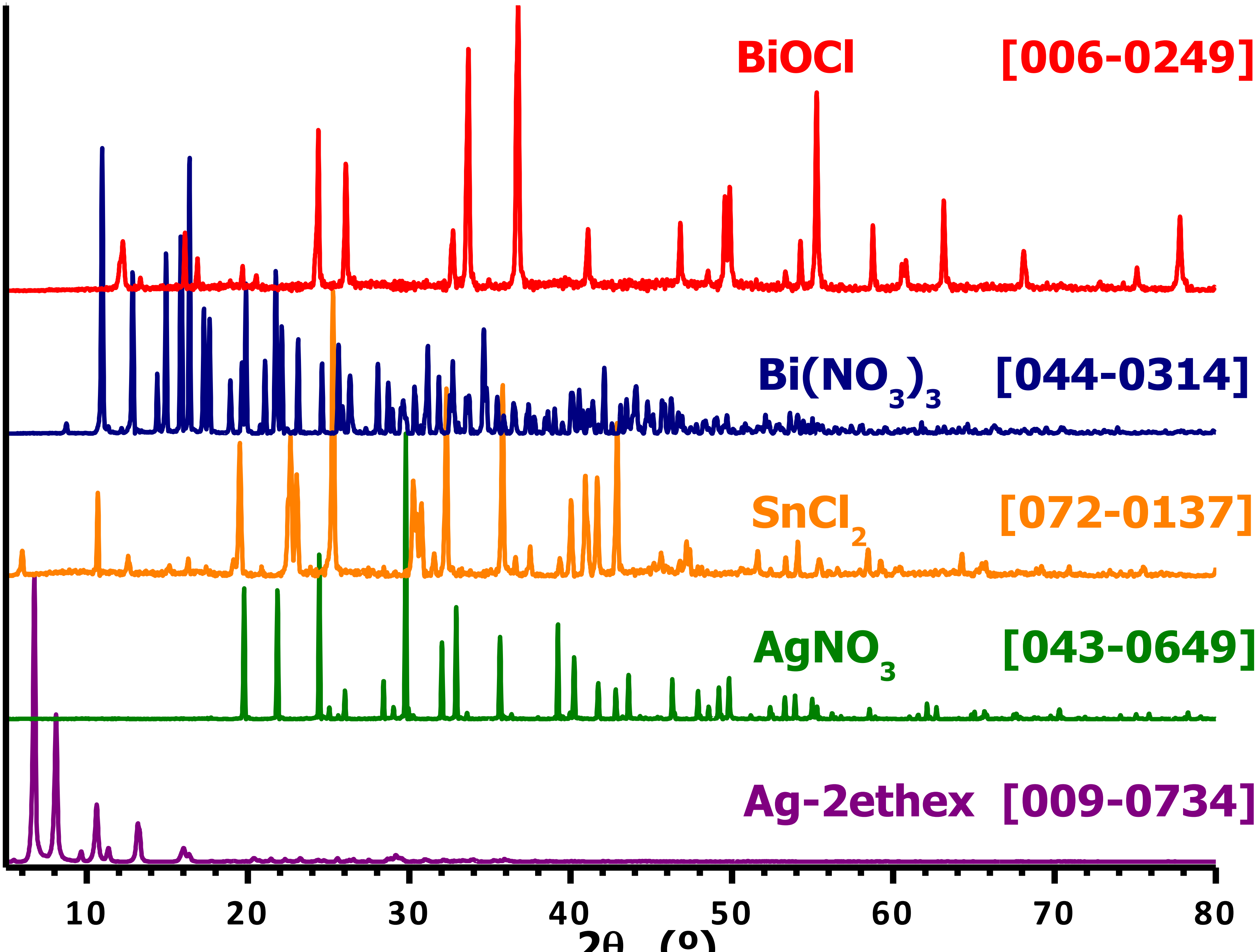
Trigonal (R)

$$\frac{1}{d_{hkl}^2} = \frac{(h^2 + k^2 + l^2)\sin\alpha^2 + 2(hk + kl + hl)(\cos\alpha^2 - \cos\alpha)}{a^2(1 - 3\cos\alpha^2 + 2\cos\alpha^2)}$$

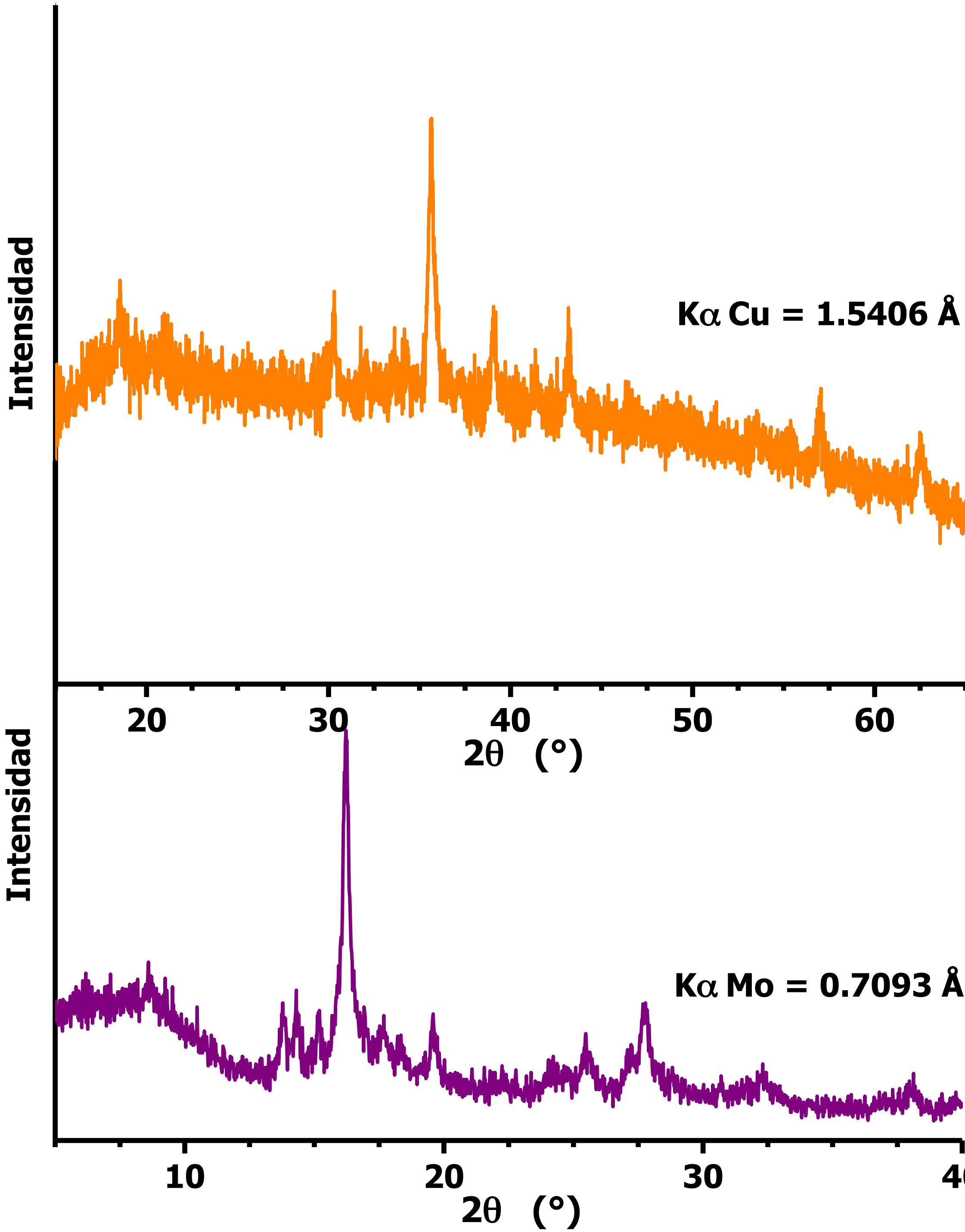
Monoclínico

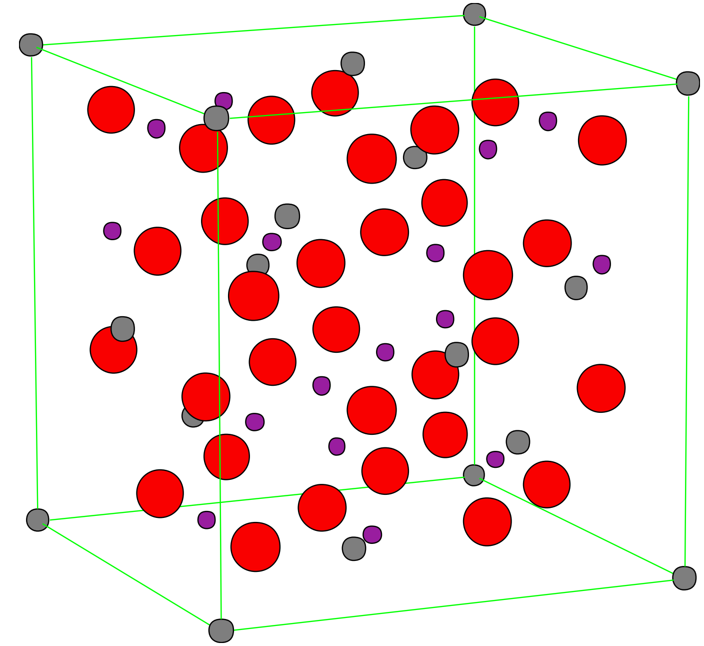
$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2\sin\beta^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2\sin\beta^2} - \frac{2hl\cos\beta}{ac\ \sin\beta^2}$$


Sn
a = 5.83Å
c = 3.18Å
α = 90o
I41
32.312
30.931
45.193
44.168
62.790
64.850
8000
6000
4000
2000
0
25
30
35
40
45
50
55
60
65
70
2θ (°)



BiOCl [006-0249]
Bi(NO3)3 [044-0314]
SnCl2 [072-0137]
AgNO3 [043-0649]
Ag-2ethex [009-0734]
10
20
30
40
50
60
70
80
2θ (o)

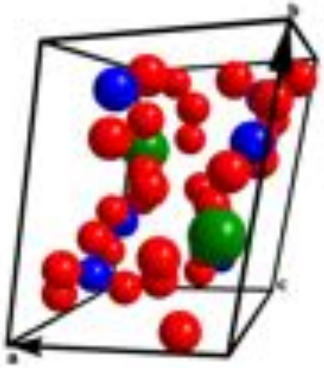




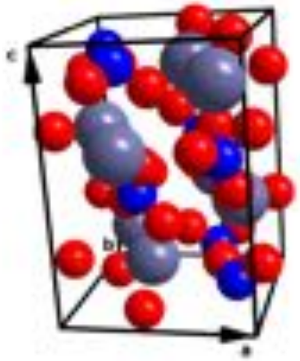
$CuFe_2O_4$

a = 8.370 Å

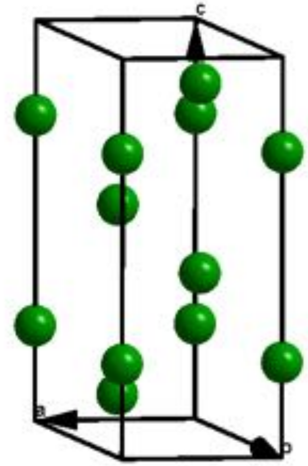
Fd-3m



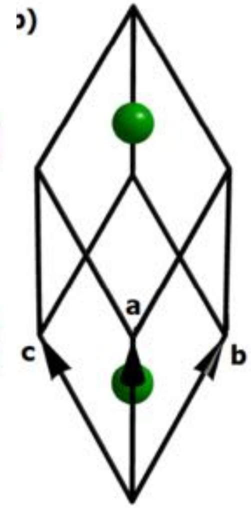
a = 6.52 Å
b = 8.64 Å
c = 10.68 Å
α = 100.8º
β = 80.8º
γ = 104.7º
P-1



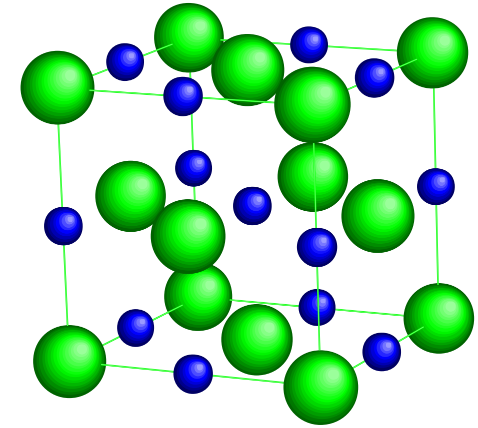
a = 6.99 Å
b = 7.34 Å
c = 10.12 Å
α = 90º
Pbca



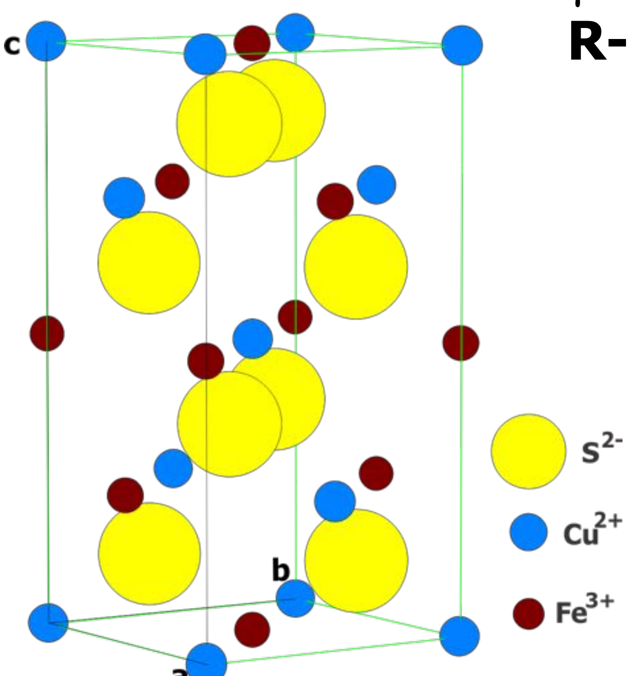
a = 4.55 Å
c = 11.85 Å
α = 90º
γ = 120º
R-3m (H)



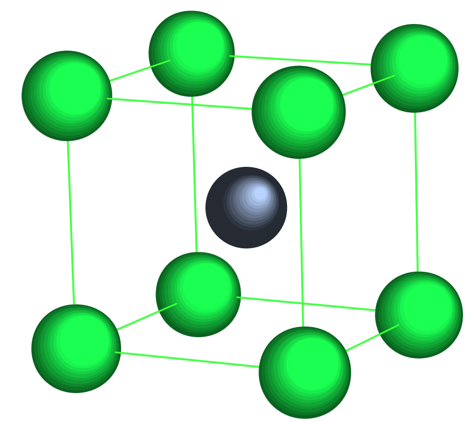
a = 4.75 Å
α = 57.23º
R-3m (R)



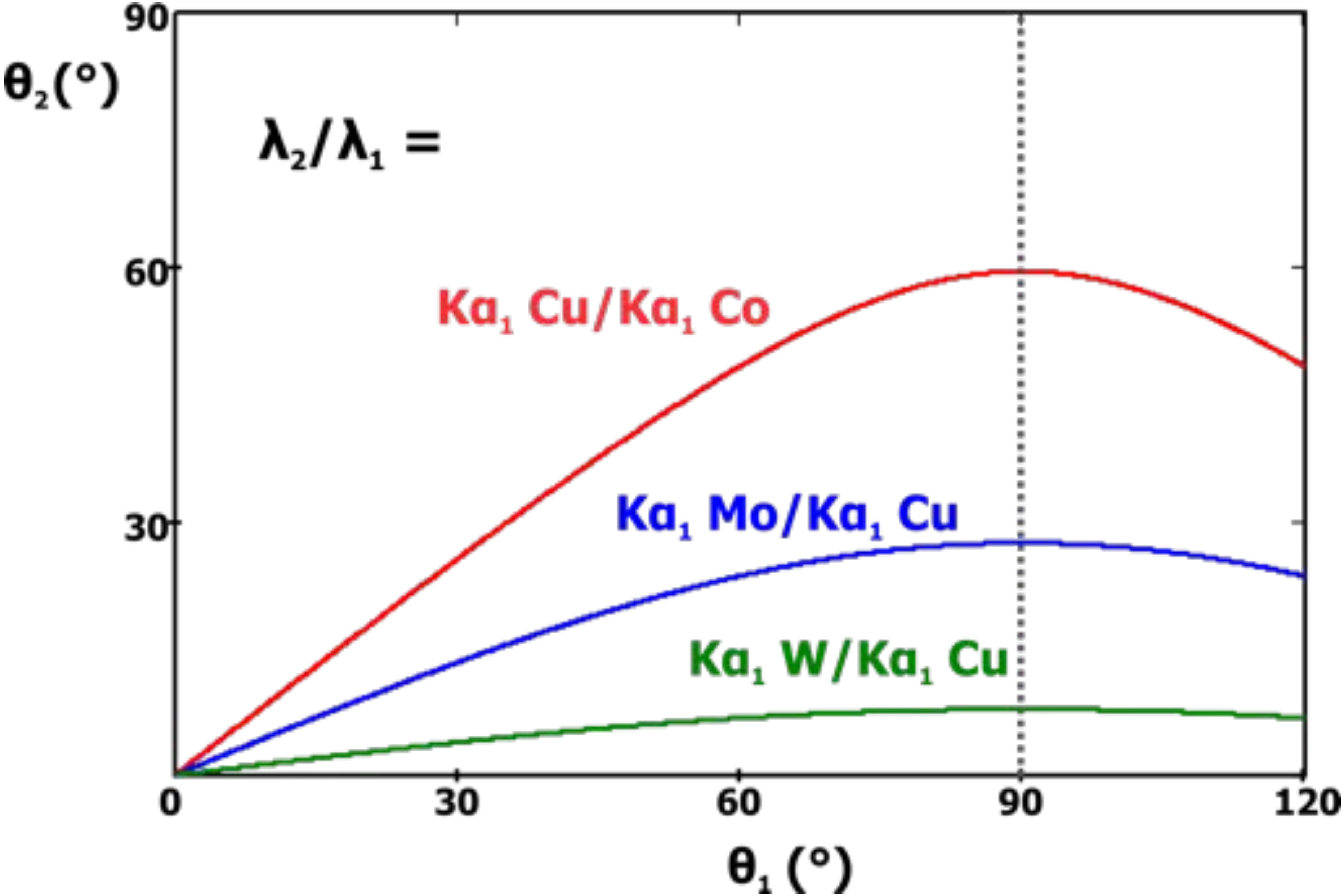
a = 5.64 Å
Fm-3m



a = 5.277 Å
c = 10.441 Å
I-42d



a = 4.12 Å
Pm3m


90
θ2(°)
λ2/λ1 =
60
Kα1 Cu/Kα1 Co
30
Kα1 Mo/Kα1 Cu
Kα1 W/Kα1 Cu
0
30
60
90
120
θ1 (°)