

Calculez les angles de diffraction (sur poudre avec une anticathode de cuivre) suivants :
 - dans le groupe d'espace Pnma pour (h k l) = (0 0 2) et (1 1 0)
 - dans le groupe d'espace P6₃/mmc pour (h k l) = (0 0 2) et (1 0 0) 2 pts

Expliquez le résultat obtenu. 2 pts

Données

r(La) = 1.88 Å ; r(C) = 0.77 Å ; r(Ca) = 1.76 Å ; r(O) = 0.66 Å

Pour le système triclinique : $V = \sqrt{a^2 b^2 c^2 (1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma)}$

Pour le système hexagonal : $d_{hkl} = \frac{a}{\sqrt{\left(\frac{4}{3}(h^2 + k^2 + hk) + l^2 \frac{a^2}{c^2}\right)}}$

$\lambda(\text{Cu}) = 1.5418 \text{ \AA}$

Pnma

D_{2h}^{16}

mmm

Orthorhombic

No. 62

$P 2_1/n 2_1/m 2_1/a$

Patterson symmetry *Pmmm*

Origin at $\bar{1}$ on 12, 1

Asymmetric unit $0 \leq x \leq \frac{1}{2}; 0 \leq y \leq \frac{1}{4}; 0 \leq z \leq 1$

Symmetry operations

- | | | | | | | | |
|---------------|----------------------------|---------------------|----------------------------|-----------|----------------------------|--------------------------------------|---------------------|
| (1) 1 | (2) $2(0, 0, \frac{1}{2})$ | $\frac{1}{4}, 0, z$ | (3) $2(0, \frac{1}{2}, 0)$ | $0, y, 0$ | (4) $2(\frac{1}{2}, 0, 0)$ | $x, \frac{1}{4}, \frac{1}{4}$ | |
| (5) $\bar{1}$ | $0, 0, 0$ | (6) a | $x, y, \frac{1}{4}$ | (7) m | $x, \frac{1}{4}, z$ | (8) $n(0, \frac{1}{2}, \frac{1}{2})$ | $\frac{1}{4}, y, z$ |

Generators selected (1); $t(1, 0, 0)$; $t(0, 1, 0)$; $t(0, 0, 1)$; (2); (3); (5)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

- | | | | | | | |
|---|----------|---|---------------------------------|---|---|---|
| 8 | <i>d</i> | 1 | (1) x, y, z | (2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ | (3) $\bar{x}, y + \frac{1}{2}, \bar{z}$ | (4) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ |
| | | | (5) $\bar{x}, \bar{y}, \bar{z}$ | (6) $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ | (7) $x, \bar{y} + \frac{1}{2}, z$ | (8) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$ |

General:

- $Ok\bar{l} : k + l = 2n$
 $hk0 : h = 2n$
 $h00 : h = 2n$
 $0k0 : k = 2n$
 $00l : l = 2n$

Special: as above, plus

- | | | | | | | |
|---|----------|-------|---------------------|---|---------------------------------|---|
| 4 | <i>c</i> | $.m.$ | $x, \frac{1}{4}, z$ | $\bar{x} + \frac{1}{2}, \frac{3}{4}, z + \frac{1}{2}$ | $\bar{x}, \frac{3}{4}, \bar{z}$ | $x + \frac{1}{2}, \frac{1}{4}, \bar{z} + \frac{1}{2}$ |
|---|----------|-------|---------------------|---|---------------------------------|---|

no extra conditions

- | | | | | | | |
|---|----------|-----------|---------------------|---------------------|-------------------------------|-------------------------------|
| 4 | <i>b</i> | $\bar{1}$ | $0, 0, \frac{1}{2}$ | $\frac{1}{2}, 0, 0$ | $0, \frac{1}{2}, \frac{1}{2}$ | $\frac{1}{2}, \frac{1}{2}, 0$ |
|---|----------|-----------|---------------------|---------------------|-------------------------------|-------------------------------|

$hkl : h + l, k = 2n$

- | | | | | | | |
|---|----------|-----------|-----------|-------------------------------|---------------------|---|
| 4 | <i>a</i> | $\bar{1}$ | $0, 0, 0$ | $\frac{1}{2}, 0, \frac{1}{2}$ | $0, \frac{1}{2}, 0$ | $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ |
|---|----------|-----------|-----------|-------------------------------|---------------------|---|

$hkl : h + l, k = 2n$

Symmetry of special projections

Along [001] *p2gm*
 $a' = \frac{1}{2}a$ $b' = b$
 Origin at $0, 0, z$

Along [100] *c2mm*
 $a' = b$ $b' = c$
 Origin at $x, \frac{1}{4}, \frac{1}{4}$

Along [010] *p2gg*
 $a' = c$ $b' = a$
 Origin at $0, y, 0$

$P6_3/mmc$ D_{6h}^4 $6/mmm$

Hexagonal

No. 194

 $P6_3/m2/m2/c$ Patterson symmetry $P6/mmm$ Origin at centre ($\bar{3}m1$) at $\bar{3}2/mc$

Symmetry operations

(1) 1	(2) $3^+ 0,0,z$	(3) $3^- 0,0,z$
(4) $2(0,0,\frac{1}{2}) 0,0,z$	(5) $6^-(0,0,\frac{1}{2}) 0,0,z$	(6) $6^+(0,0,\frac{1}{2}) 0,0,z$
(7) $2 x,x,0$	(8) $2 x,0,0$	(9) $2 0,y,0$
(10) $2 x,\bar{x},\frac{1}{4}$	(11) $2 x,2x,\frac{1}{4}$	(12) $2 2x,x,\frac{1}{4}$
(13) $\bar{1} 0,0,0$	(14) $\bar{3}^+ 0,0,z; 0,0,0$	(15) $\bar{3}^- 0,0,z; 0,0,0$
(16) $m x,y,\frac{1}{4}$	(17) $\bar{6}^- 0,0,z; 0,0,\frac{1}{4}$	(18) $\bar{6}^+ 0,0,z; 0,0,\frac{1}{4}$
(19) $m x,\bar{x},z$	(20) $m x,2x,z$	(21) $m 2x,x,z$
(22) $c x,x,z$	(23) $c x,0,z$	(24) $c 0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates						Reflection conditions
24 <i>l</i> 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$	General: $hh\bar{2}hl: l=2n$ $000l : l=2n$
	(7) y,x,\bar{z}	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$	(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{1}{2}$	
	(13) \bar{x},\bar{y},\bar{z}	(14) $y,\bar{x}+y,\bar{z}$	(15) $x-y,x,\bar{z}$	(16) $x,y,\bar{z}+\frac{1}{2}$	(17) $\bar{y},x-y,\bar{z}+\frac{1}{2}$	(18) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$	
	(19) \bar{y},\bar{x},z	(20) $\bar{x}+y,y,z$	(21) $x,x-y,z$	(22) $y,x,z+\frac{1}{2}$	(23) $x-y,\bar{y},z+\frac{1}{2}$	(24) $\bar{x},\bar{x}+y,z+\frac{1}{2}$	
12 <i>k</i> . <i>m</i> .	$x,2x,z$	$2\bar{x},\bar{x},z$	x,\bar{x},z	$\bar{x},2\bar{x},z+\frac{1}{2}$	$2x,x,z+\frac{1}{2}$	$\bar{x},2\bar{x},\bar{z}$	Special: as above, plus no extra conditions
	\bar{x},x,\bar{z}	$2\bar{x},\bar{x},\bar{z}+\frac{1}{2}$	$x,2x,\bar{z}+\frac{1}{2}$	$x,\bar{x},\bar{z}+\frac{1}{2}$			
12 <i>j</i> <i>m</i> . .	$x,y,\frac{1}{4}$	$\bar{y},x-y,\frac{1}{4}$	$\bar{x}+y,\bar{x},\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$	$y,\bar{x}+y,\frac{3}{4}$	$x-y,x,\frac{3}{4}$	no extra conditions
	$y,x,\frac{3}{4}$	$x-y,\bar{y},\frac{3}{4}$	$\bar{x},\bar{x}+y,\frac{3}{4}$	$\bar{y},\bar{x},\frac{1}{4}$	$\bar{x}+y,y,\frac{1}{4}$	$x,x-y,\frac{1}{4}$	
12 <i>i</i> .2 .	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$	$hkil : l=2n$
	$\bar{x},0,0$	$0,\bar{x},0$	$x,x,0$	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	
6 <i>h</i> <i>m m</i> 2	$x,2x,\frac{1}{4}$	$2\bar{x},\bar{x},\frac{1}{4}$	$x,\bar{x},\frac{1}{4}$	$\bar{x},2\bar{x},\frac{3}{4}$	$2x,x,\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$	no extra conditions
6 <i>g</i> .2/ <i>m</i> .	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkil : l=2n$
4 <i>f</i> 3 <i>m</i> .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$			$hkil : l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
4 <i>e</i> 3 <i>m</i> .	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$			$hkil : l=2n$
2 <i>d</i> $\bar{6}m2$	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$					$hkil : l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2 <i>c</i> $\bar{6}m2$	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$	$\frac{2}{3},\frac{1}{3},\frac{3}{4}$					
2 <i>b</i> $\bar{6}m2$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil : l=2n$
2 <i>a</i> $\bar{3}m$.	$0,0,0$	$0,0,\frac{1}{2}$					$hkil : l=2n$

PERIODIC TABLE OF THE ELEMENTS

GROUP	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
PERIOD	1A	2A	3A	4A	5A	6A	7A	8A	9A	10A	11A	12A	13A	14A	15A	16A	17A	18A
	GROUP NUMBERS IUPAC RECOMMENDATION (1985)	GROUP NUMBERS CHEMICAL ABSTRACT SERVICE (1986)	GROUP NUMBERS IUPAC RECOMMENDATION (1985)	GROUP NUMBERS CHEMICAL ABSTRACT SERVICE (1986)	GROUP NUMBERS IUPAC RECOMMENDATION (1985)	GROUP NUMBERS CHEMICAL ABSTRACT SERVICE (1986)	GROUP NUMBERS IUPAC RECOMMENDATION (1985)	GROUP NUMBERS CHEMICAL ABSTRACT SERVICE (1986)	GROUP NUMBERS IUPAC RECOMMENDATION (1985)	GROUP NUMBERS CHEMICAL ABSTRACT SERVICE (1986)	GROUP NUMBERS IUPAC RECOMMENDATION (1985)	GROUP NUMBERS CHEMICAL ABSTRACT SERVICE (1986)	GROUP NUMBERS IUPAC RECOMMENDATION (1985)	GROUP NUMBERS CHEMICAL ABSTRACT SERVICE (1986)	GROUP NUMBERS IUPAC RECOMMENDATION (1985)	GROUP NUMBERS CHEMICAL ABSTRACT SERVICE (1986)	GROUP NUMBERS IUPAC RECOMMENDATION (1985)	GROUP NUMBERS CHEMICAL ABSTRACT SERVICE (1986)
	ATOMIC NUMBER	SYMBOL																
	RELATIVE ATOMIC MASS (1)		RELATIVE ATOMIC MASS (1)		RELATIVE ATOMIC MASS (1)		RELATIVE ATOMIC MASS (1)		RELATIVE ATOMIC MASS (1)		RELATIVE ATOMIC MASS (1)		RELATIVE ATOMIC MASS (1)		RELATIVE ATOMIC MASS (1)		RELATIVE ATOMIC MASS (1)	
	ELEMENT NAME		ELEMENT NAME		ELEMENT NAME		ELEMENT NAME		ELEMENT NAME		ELEMENT NAME		ELEMENT NAME		ELEMENT NAME		ELEMENT NAME	
1	1 H HYDROGEN	2 He HELIUM	3 Li LITHIUM	4 Be BERYLLIUM	5 B BORON	6 C CARBON	7 N NITROGEN	8 O OXYGEN	9 F FLUORINE	10 Ne NEON	11 Na SODIUM	12 Mg MAGNESIUM	13 Al ALUMINIUM	14 Si SILICON	15 P PHOSPHORUS	16 S SULPHUR	17 Cl CHLORINE	18 Ar ARGON
2	19 K POTASSIUM	20 Ca CALCIUM	21 Sc SCANDIUM	22 Ti TITANIUM	23 V VANADIUM	24 Cr CHROMIUM	25 Mn MANGANESE	26 Fe IRON	27 Co COBALT	28 Ni NICKEL	29 Cu COPPER	30 Zn ZINC	31 Ga GALLIUM	32 Ge GERMANIUM	33 As ARSENIC	34 Se SELENIUM	35 Br BROMINE	36 Kr KRYPTON
3	37 Rb RUBIDIUM	38 Sr STRONTIUM	39 Y YTRIUM	40 Zr ZIRCONIUM	41 Nb NIOBIUM	42 Mo MOLYBDENUM	43 Tc TECHNETIUM	44 Ru RUTHENIUM	45 Rh RHODIUM	46 Pd PALLADIUM	47 Ag SILVER	48 Cd CADMIUM	49 In INDIUM	50 Sn TIN	51 Sb ANTIMONY	52 Te TELLURIUM	53 I IODINE	54 Xe XENON
4	55 Cs CAESIUM	56 Ba BARIUM	57-71 La-Lu Lanthanide	72 Hf HAFNIUM	73 Ta TANTALUM	74 W TUNGSTEN	75 Re RHENIUM	76 Os OSMIUM	77 Ir IRIDIUM	78 Pt PLATINIUM	79 Au GOLD	80 Hg MERCURY	81 Tl THALLIUM	82 Pb LEAD	83 Bi BISMUTH	84 Po POLONIUM	85 At ASTATINE	86 Rn RADON
5	87 Fr FRANCIUM	88 Ra RADIUM	89-103 Ac-Lr Actinide	104 Rf RUTHERFORDIUM	105 Db DUBNIUM	106 Sg SEABORGIUM	107 Bh BOHRIUM	108 Hs HASSIUM	109 Mt MEITNERIUM	110 Ds DARMSTADTIUM	111 Rg ROENTGENIUM	112 Cn COPERNICIUM	113 Nh NIHONIUM	114 Fl FLEROVIUM	115 Mc MOSCOVIUM	116 Lv LIVERMORIUM	117 Ts TENNESSINE	118 Og OGANESSON

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57	58	59	60	61	62	63	64	65	66	67	68	69	70	71
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
LANTHANIDE	LANTHANIDE	LANTHANIDE	LANTHANIDE	LANTHANIDE	LANTHANIDE	LANTHANIDE	LANTHANIDE	LANTHANIDE	LANTHANIDE	LANTHANIDE	LANTHANIDE	LANTHANIDE	LANTHANIDE	LANTHANIDE
138.91	140.12	140.91	144.24	(145)	150.36	151.96	157.25	158.93	162.50	164.93	167.26	168.93	173.05	174.97
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
ACTINIDE	THORIUM	PROTACTINIUM	URANIUM	NEPTUNIUM	PLUTONIUM	AMERICIUM	CURIUM	BERKELIUM	CALIFORNIUM	EINSTEINIUM	FERMIUM	MENDELEVIUM	NOBELIUM	LAWRENCIUM



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(1) Atomic weights of the elements 2013, Pure Appl. Chem., 85, 265-291 (2016)