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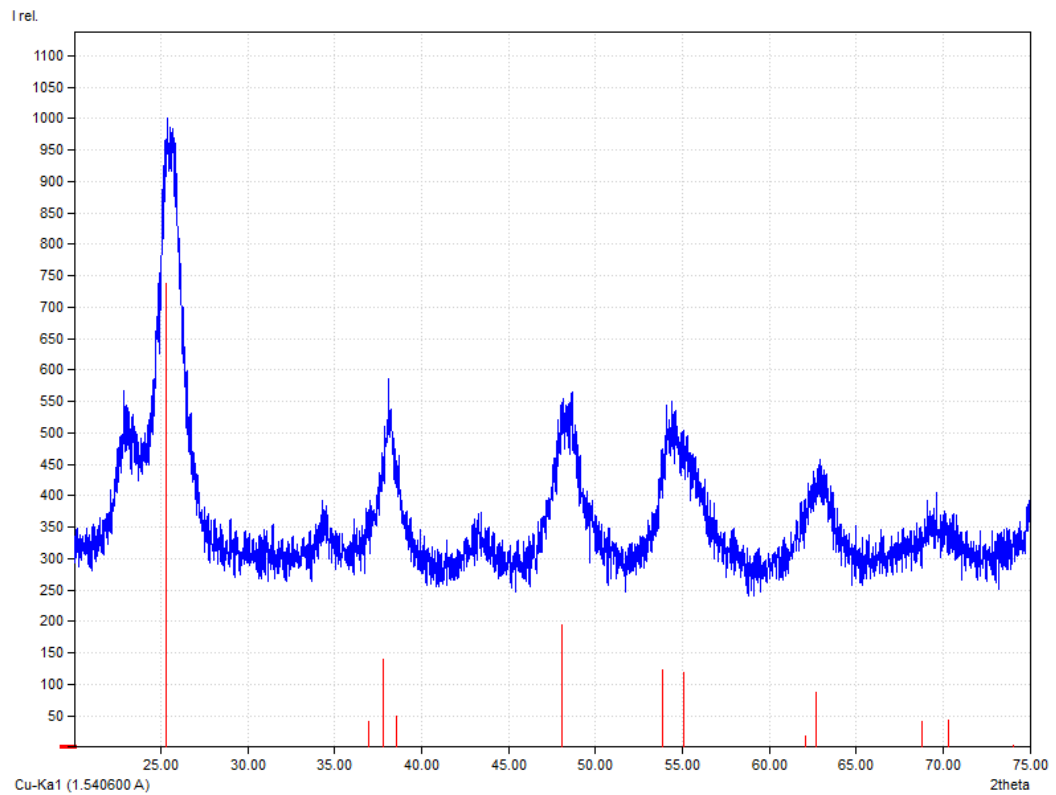
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LAMPIRAN

Lampiran 1: Data X-RD

a. X-RD TiO₂ hasil sintesis



Entry # 96-101-0943

Phase classification

Name	Titanium oxide
Mineral Name	Anatase
Formula	O ₂ Ti
I/Ic	5.600000
Sample Name	1010942
Quality	C (calculated)

References

Publication

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Origin of data

Source of entry [COD \(Crystallography Open Database\)](#)
Link to orig. entry [1010942](#)

Crystal structure

Crystallographic data

Space group I 41/a m d (141)
Crystal system tetragonal
Cell parameters a= 3.73000 Å c= 9.37000 Å
Z 4

Atom coordinates	Element	Oxid.	x	y	z	BI	Focc.
	Ti	4.0	0.000	0.000	0.000	1.000000	1.000000
	O	-2.0	0.000	0.000	0.200	1.000000	1.000000

Diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
3.4655	1000.0	0	1	1	8
2.3947	42.2	0	1	3	8
2.3425	150.3	0	0	4	2
2.2983	75.7	1	1	2	8
1.8650	247.4	0	2	0	4
1.6745	157.9	0	1	5	8
1.6423	157.5	1	2	1	16
1.4714	19.2	1	2	3	16
1.4391	94.9	0	2	4	8
1.3438	66.0	1	1	6	8
1.3188	53.9	2	2	0	4
1.2999	5.5	0	1	7	8
1.2460	83.4	1	2	5	16
1.2325	22.6	0	3	1	8
1.1712	2.1	0	0	8	2
1.1552	4.1	0	3	3	8
1.1492	33.8	2	2	4	8
1.1438	15.7	1	3	2	16
1.0440	6.0	1	2	7	16
1.0360	20.2	0	3	5	8
1.0283	23.1	2	3	1	16

Experimental

Physical Properties

Calc. density 4.06900 g/cm³

Remarks

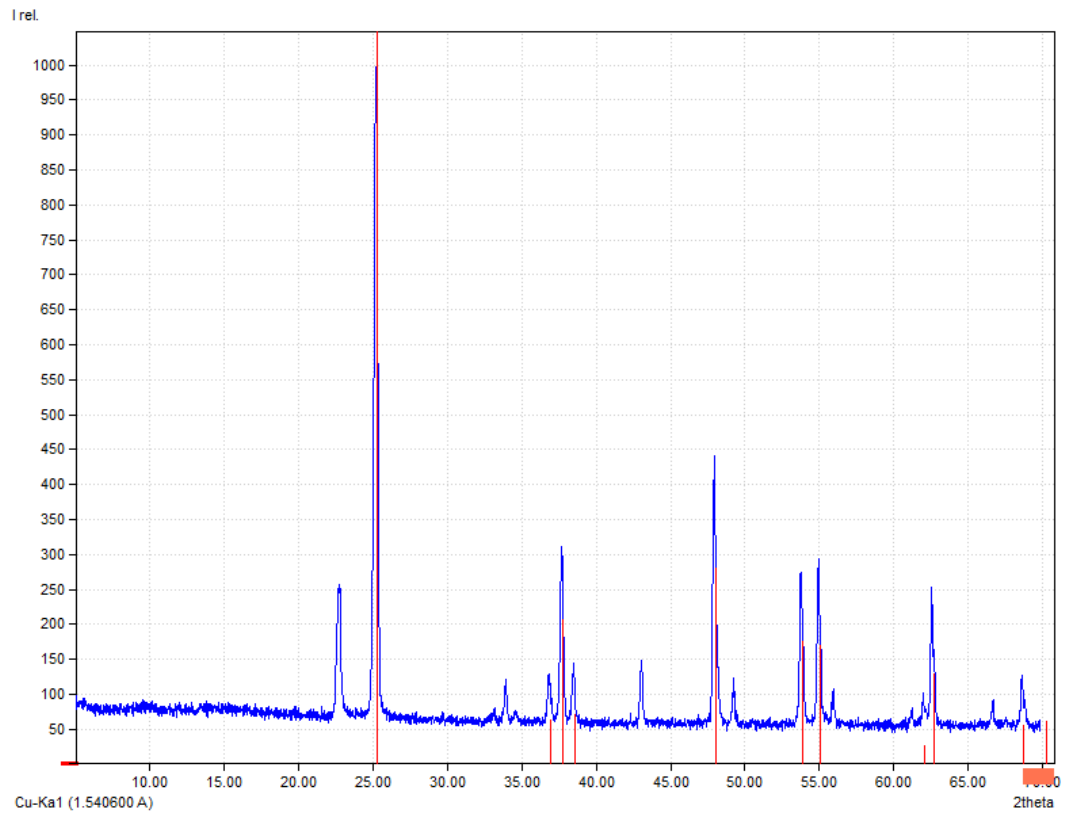
Remarks

Comments - Diffraction pattern calculated by Matchl.
 - I/Ic calculated by Matchl.
 - Space group has been derived from given symmetry operations.



Optimization Software:
www.balesio.com

b. X-RD TiO₂ Komersil



Entry # 96-901-5930

Phase classification

Name	
Mineral Name	Anatase
Formula	O ₂ Ti
I/Ic	5.310000
Sample Name	9015929
Quality	C (calculated)

References

Publication

Bibliography Howard C. J., Sabine T. M., Dickson F., "Structural and thermal parameters for rutile and anatase", Acta Crystallographica, Section B **47(4)**, 462-468 (1991)

Origin of data

Source of entry [COD \(Crystallography Open Database\)](#)

Link to orig. entry [9015929](#)

Crystal structure

Crystallographic data

Space group	I 41/a m d (141)												
Crystal system	tetragonal												
Cell parameters	a= 3.78450 Å c= 9.51430 Å												
Atom coordinates	Element	Oxld.	x	y	z	Bl	Focc	U11	U22	U33	U12	U13	U23
	Ti	0.000	0.000	0.000	1.000000	1.000000	0.005200	0.000000	0.000000	0.005200	0.000000	0.000000	0.007000
	O		0.000	0.000	0.208	1.000000	1.000000	0.011700	0.000000	0.000000	0.002700	0.000000	0.007200

Diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
3.5165	1000.0	0	1	1	8
2.4308	59.9	0	1	3	8
2.3786	197.0	0	0	4	2
2.3323	67.0	1	1	2	8
1.8922	267.0	0	2	0	4
1.7001	167.4	0	1	5	8
1.6663	161.9	1	2	1	16
1.4932	25.5	1	2	3	16
1.4808	123.1	0	2	4	8
1.3642	52.5	1	1	6	8
1.3380	58.7	2	2	0	4
1.2792	4.2	0	1	7	8
1.2646	88.7	1	2	5	16
1.2500	23.4	0	3	1	8
1.1893	3.8	0	0	8	2
1.1722	5.2	0	3	3	8
1.1662	43.1	2	2	4	8
1.1606	15.1	1	3	2	16
1.0598	4.7	1	2	7	16
1.0514	21.1	0	3	5	8
1.0433	23.5	2	3	1	16
1.0182	15.8	0	1	9	8
1.0069	9.1	0	2	8	8

Experimental

Physical Properties

Calc. density 3.89400 g/cm³

Remarks

Remarks

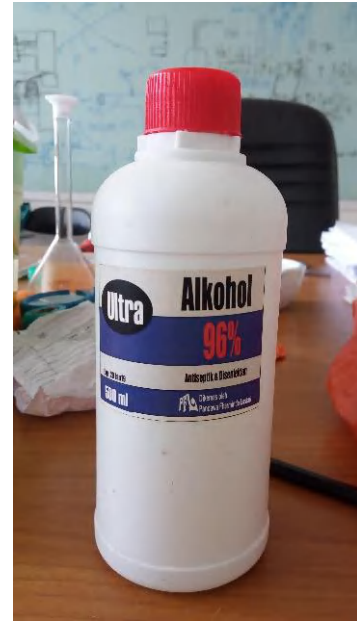
Comments

- Synthetic
- Diffraction pattern calculated by Matchl.
- I/Ic calculated by Matchl.
- Space group has been derived from given symmetry operations.



Lampiran 3: Dokumentasi Penelitian





Optimization Software:
www.balesio.com