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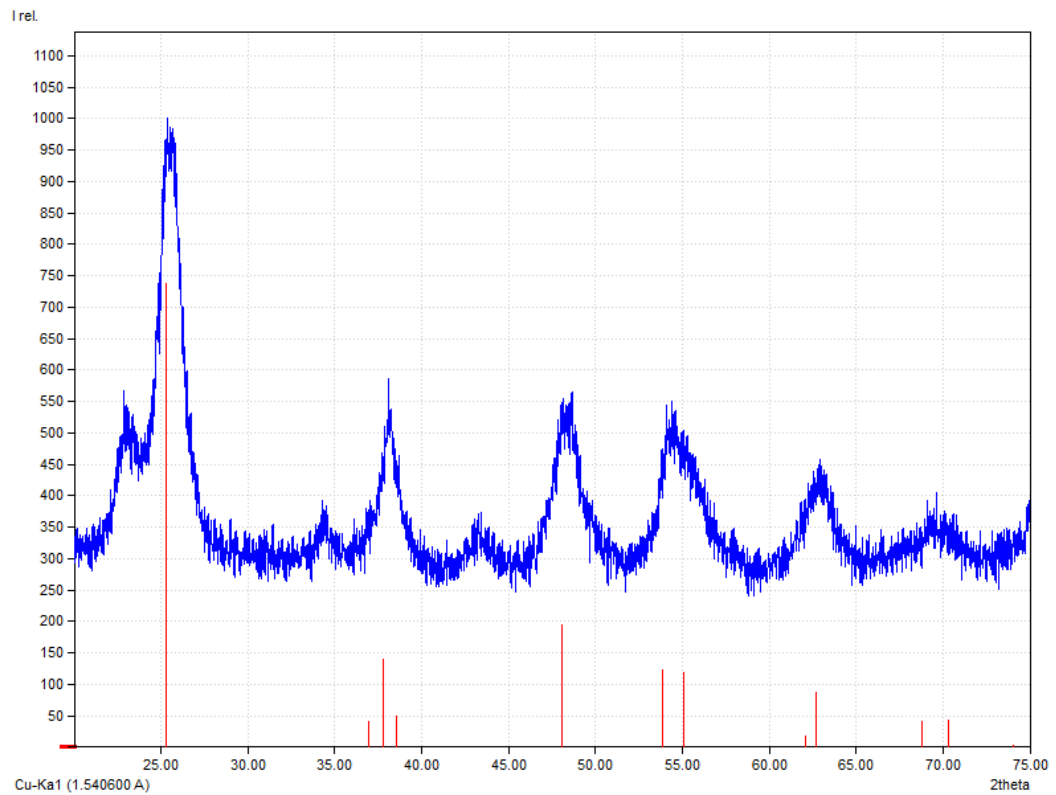
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## LAMPIRAN

### Lampiran 1: Data X-RD

#### a. X-RD TiO<sub>2</sub> hasil sintesis



Entry # 96-101-0943

**Phase classification**

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

References

**Publication**

**Bibliography** Parker R.L., "Zur Kristallstruktur von Anatas und Rutil. (II. Teil. Die Anatasstruktur).", Zeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie (-144,1977) **59**, 1-54 (1924)

**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	<b>Element</b>	<b>Oxid.</b>	<b>x</b>	<b>y</b>	<b>z</b>	<b>BI</b>	<b>Focc.</b>
	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** 4.00900 g/cm<sup>3</sup>

Remarks

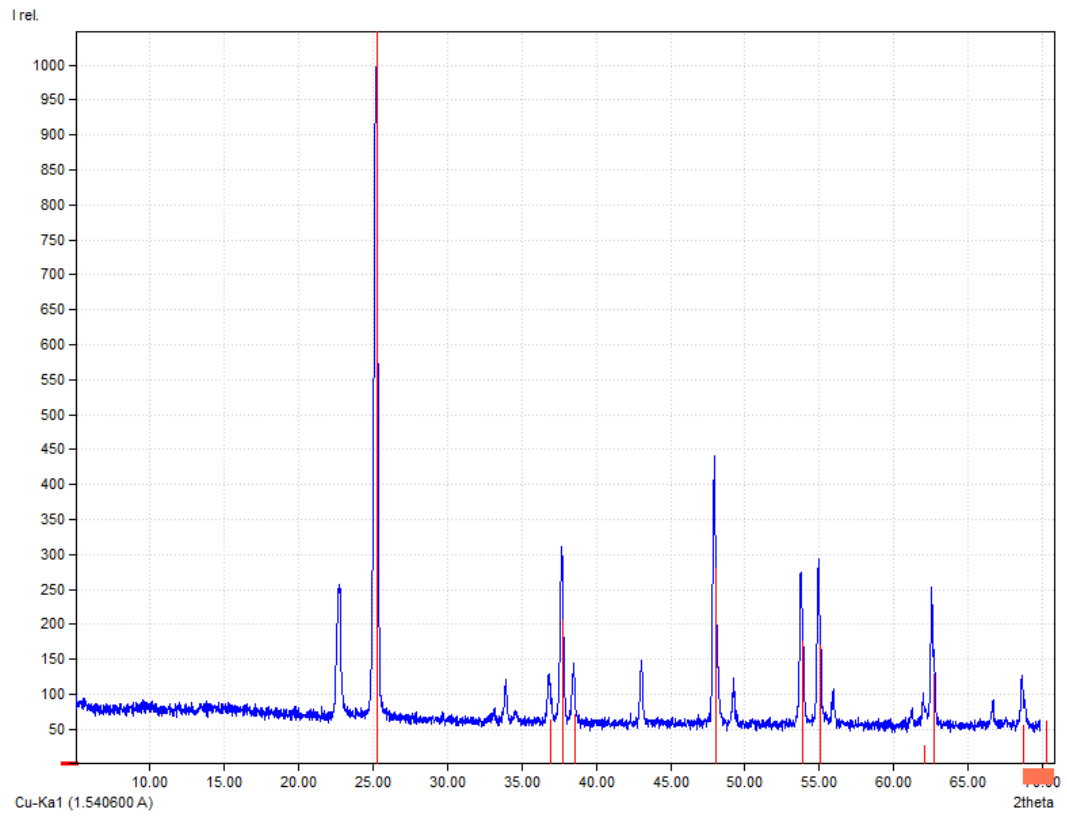
**Remarks**

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



Optimization Software:  
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## b. X-RD TiO<sub>2</sub> Komersil



## Entry # 96-901-5930

## Phase classification

Name	
Mineral Name	Anatase
Formula	O <sub>2</sub> 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	Element	Oxid.	x	y	z	BI	Focc	U11	U22	U33	U12	U13	U23
coordinates	Ti		0.000	0.000	0.000	1.000000	1.000000	0.005200	0.000000	0.000000	0.005200	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/cm<sup>3</sup>

## 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







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[www.balesio.com](http://www.balesio.com)