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APPENDICES

APPENDIX A

The Joint Committee for Powder Diffraction Standards (JCPDS) [30]

1. MoO_3, JCPDS file number 05-0508

Name and formula

Reference code:	05-0508
Mineral name:	Molybdite, syn
PDF index name:	Molybdenum Oxide
Empirical formula:	MoO_3
Chemical formula:	MoO_3

Crystallographic parameters

Crystal system:	Orthorhombic
Space group:	Pbnm
Space group number:	62
a (?):	3.9620
b (?):	13.8580
c (?):	3.6970
Alpha (?):	90.0000
Beta (?):	90.0000
Gamma (?):	90.0000

Calculated density (g/cm^3):	4.71
Volume of cell (10^6 pm^3):	202.99
Z:	4.00
RIR:	3.00

Subfiles and Quality

Subfiles:	Inorganic
	Mineral
	Alloy, metal or intermetalic
	Corrosion
	Common Phase
	Educational pattern
	Forensic
	NBS pattern
Quality:	Star (S)

Comments

Color:	Park gray metallic
General comments:	*Merck Index*, 8th Ed., p. 699.
	Color from *Dana's System of Mineralogy, 7th Ed.*,
	I 329.
Sample source:	Sample from Merck Chemical Company.
Analysis:	Spectroscopic analysis: <0.1%, Al, Co, Mn, Si;
	<0.01% Fe; <0.001% Cu, Mg; <0.0001% Ca.
Additional pattern:	To replace 1-706 and 5-506.
Melting point:	1185 C

Temperature: Pattern taken at 26 C.

References

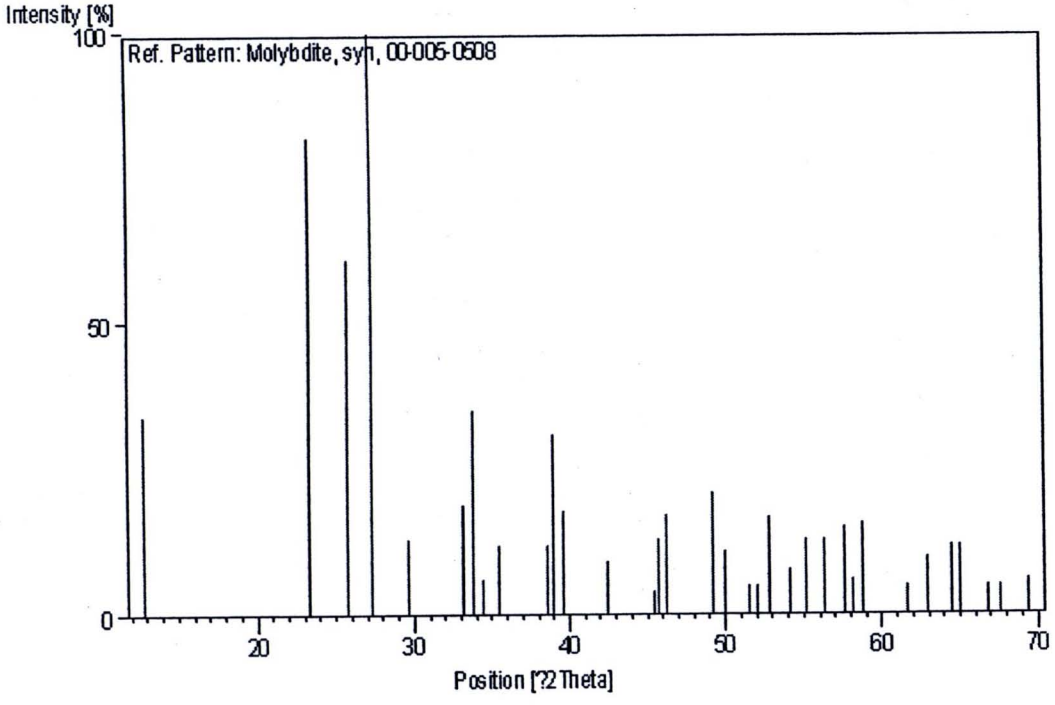
Primary reference: Swanson, Fuyat., *Natl. Bur. Stand. (U.S.), Circ. 539*, **III**, 30, (1954)

Peak list

No.	h	k	l	d [A]	2Theta[deg]	I [%]
1	0	2	0	6.93000	12.764	34.0
2	1	1	0	3.81000	23.329	82.0
3	0	4	0	3.46300	25.704	61.0
4	0	2	1	3.26000	27.335	100.0
5	1	3	0	3.00600	29.696	13.0
6	1	0	1	2.70200	33.128	19.0
7	1	1	1	2.65500	33.732	35.0
8	1	4	0	2.60700	34.372	6.0
9	0	4	1	2.52700	35.496	12.0
10	1	3	1	2.33200	38.576	12.0
11	0	6	0	2.30900	38.976	31.0
12	1	5	0	2.27100	39.655	18.0
13	1	4	1	2.13100	42.381	9.0
14	1	6	0	1.99600	45.402	4.0
15	2	0	0	1.98200	45.741	13.0
16	2	1	0	1.96000	46.284	17.0
17	0	0	2	1.84900	49.241	21.0
18	2	3	0	1.82100	50.049	11.0

No.	h	k	l	d [A]	2Theta[deg]	I [%]
19	1	7	0	1.77100	51.564	5.0
20	1	6	1	1.75600	52.038	5.0
21	2	1	1	1.73300	52.781	17.0
22	2	2	1	1.69300	54.129	8.0
23	1	1	2	1.66300	55.187	13.0
24	0	4	2	1.63100	56.366	13.0
25	1	7	1	1.59700	57.677	15.0
26	1	8	0	1.58700	58.075	6.0
27	0	8	1	1.56900	58.806	16.0
28	2	6	0	1.50400	61.617	5.0
29	2	5	1	1.47700	62.870	10.0
30	0	6	2	1.44300	64.528	12.0
31	1	9	0	1.43500	64.931	12.0
32	2	7	0	1.40000	66.763	5.0
33	0	10	0	1.38600	67.528	5.0
34	2	0	2	1.35200	69.465	6.0

Stick Pattern



2. MoO_3, JCPDS file number 21-0569

Name and formula

Reference code:	00-021-0569
PDF index name:	Molybdenum Oxide
Empirical formula:	MoO_3
Chemical formula:	MoO_3

Crystallographic parameters

Crystal system:	Hexagonal
a (?):	10.5310
b (?):	10.5310
c (?):	14.8760
Alpha (?):	90.0000
Beta (?):	90.0000
Gamma (?):	120.0000
Volume of cell (10^6 pm^3):	1428.75

Subfiles and Quality

Subfiles:	Inorganic
	Alloy, metal or intermetalic
	Corrosion
	Common Phase
	Forensic
Quality:	Blank (B)

Comments

Color: White

General comments: Changes to orthorhombic form irreversibly at 450-75 C.

Sample source: Sample from Johnson Matthey Company, Ltd.

References

Primary reference: Spangenberg, Westinghouse Electric Corporation, Horseheads, New York, USA., *Private Communication*

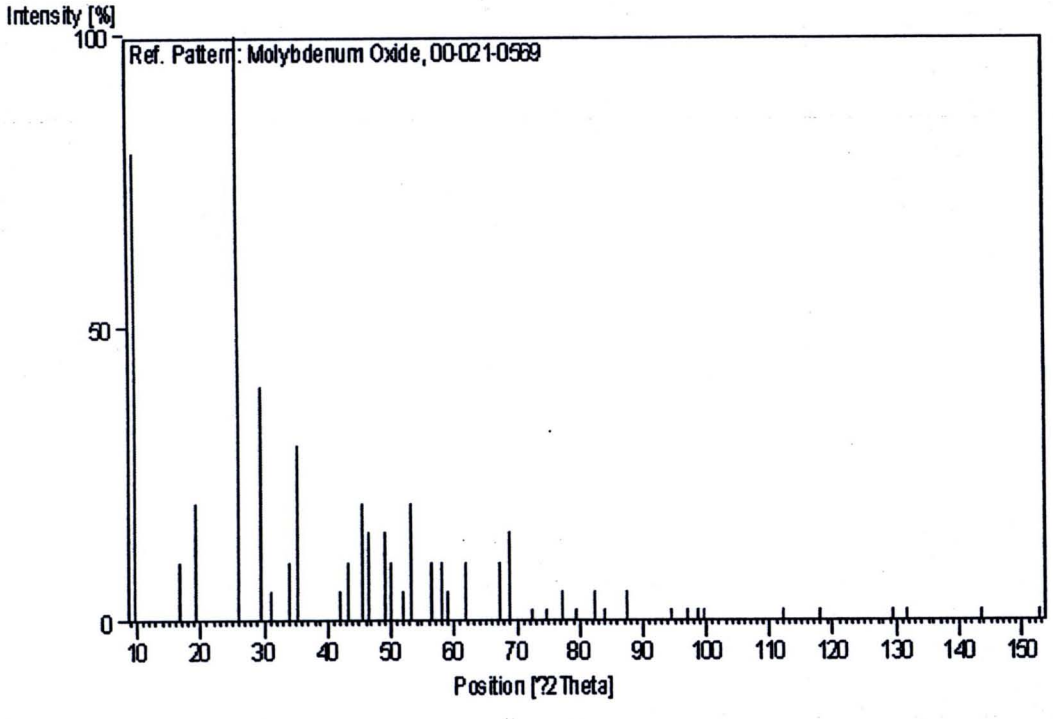
Peak list

No.	h	k	l	d [A]	2Theta[deg]	I [%]
1	1	0	0	9.12000	9.690	80.0
2	1	1	0	5.29000	16.746	10.0
3	2	0	0	4.56000	19.451	20.0
4	2	1	0	3.45000	25.803	100.0
5	3	0	0	3.04000	29.356	40.0
6	2	0	4	2.88000	31.027	5.0
7	2	2	0	2.63000	34.062	10.0
8	3	1	0	2.53000	35.452	30.0
9	2	2	4	2.14700	42.051	5.0
10	3	2	0	2.09700	43.103	10.0
11	4	1	0	1.99300	45.474	20.0
12	4	0	4	1.94700	46.611	15.0
13	0	0	8	1.86000	48.930	15.0

No.	h	k	l	d [A]	2Theta[deg]	I [%]
14	5	0	0	1.82400	49.961	10.0
15	3	3	0	1.75500	52.070	5.0
16	4	2	0	1.72400	53.078	20.0
17	2	1	8	1.63400	56.253	10.0
18	3	3	4	1.59000	57.955	10.0
19	4	2	4	1.56600	58.930	5.0
20	4	3	0	1.50200	61.708	10.0
21	6	1	0	1.39200	67.198	10.0
22	5	2	4	1.36200	68.883	15.0
23	7	0	0	1.30400	72.416	2.0
24	4	1	9	1.26900	74.748	2.0
25	3	0	11	1.23400	77.251	5.0
26	1	1	12	1.20700	79.315	2.0
27	5	4	0	1.16900	82.438	5.0
28	5	0	10	1.15100	84.018	2.0
29	7	2	0	1.11600	87.297	5.0
30	2	2	13	1.04900	94.499	2.0
31	4	4	9	1.02800	97.063	2.0
32	2	1	14	1.01500	98.738	2.0
33	6	4	4	1.00800	99.669	2.0
34	2	2	15	0.92830	112.156	2.0
35	5	2	13	0.89980	117.758	2.0
36	8	2	9	0.85170	129.492	2.0

No.	h	k	l	d [A]	2Theta[deg]	I [%]
37	6	1	14	0.84420	131.696	2.0
38	9	0	11	0.81090	143.585	2.0
39	8	5	3	0.79250	152.813	2.0

Stick Pattern



APPENDIX B

Material Safety Data Sheet [50]

Material Safety Data Sheet
Molybdenum trioxide MSDS

Section 1: Chemical Product and Company Identification

Product Name: Molybdenum trioxide

Catalog Codes: SLM4291

CAS#: 1313-27-5

RTECS: QA4725000

TSCA: TSCA 8(b) inventory: Molybdenum trioxide

CI#: Not available.

Synonym:

Chemical Name: Not available.

Chemical Formula: MoO3

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Molybdenum trioxide	1313-27-5	100

Toxicological Data on Ingredients: Molybdenum trioxide: ORAL (LD50): Acute: 125 mg/kg [Rat]. 2689 mg/kg [Rat]. DUST (LC50): Acute: 5841 ppm 4 hour(s) [Rat].

Section 3: Hazards Identification

Potential Acute Health Effects:
Hazardous in case of eye contact (irritant), of ingestion, of inhalation. Slightly hazardous in case of skin contact (irritant). Severe over-exposure can result in death.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance is toxic to lungs, mucous membranes. Repeated or prolonged exposure to the substance can produce target organs damage. Repeated exposure to an highly toxic material may produce general deterioration of health by an accumulation in one or many human organs.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used. Do not use an eye ointment. Seek medical attention.

Skin Contact:
After contact with skin, wash immediately with plenty of water. Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases and groin. Cover the irritated skin with an emollient. If irritation persists, seek medical attention.

Serious Skin Contact: Not available.

Inhalation: Allow the victim to rest in a well ventilated area. Seek immediate medical attention.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek medical attention.

Ingestion:
Do not induce vomiting. Examine the lips and mouth to ascertain whether the tissues are damaged, a possible indication that the toxic material was ingested; the absence of such signs, however, is not conclusive. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek immediate medical attention.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Non-flammable.

Auto-Ignition Temperature: Not applicable.

Flash Points: Not applicable.

Flammable Limits: Not applicable.

Products of Combustion: Not available.

Fire Hazards in Presence of Various Substances: Not applicable.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions: Not applicable.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill: Use appropriate tools to put the spilled solid in a convenient waste disposal container.

Large Spill:
Use a shovel to put the material into a convenient waste disposal container. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep locked up Do not ingest. Do not breathe dust. Avoid contact with eyes Wear suitable protective clothing In case of insufficient ventilation, wear suitable respiratory equipment If ingested, seek medical advice immediately and show the container or the label.

Storage:
Keep container tightly closed. Keep in a cool, well-ventilated place. Highly toxic or infectious materials should be stored in a separate locked safety storage cabinet or room.

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection:
Splash goggles. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Dust respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 5 CEIL: 10 (mg/m3) from ACGIH [1995] Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid.

Odor: Not available.

Taste: Not available.

Molecular Weight: 143.94 g/mole

Color: Not available.

pH (1% soln/water): Not available.

Boiling Point: 1155°C (2111°F)

Melting Point: 795°C (1463°F)

Critical Temperature: Not available.

Specific Gravity: 4.696 (Water = 1)

Vapor Pressure: Not applicable.

Vapor Density: Not available.

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: Not available.

Solubility: Very slightly soluble in cold water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.
Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances: Not available.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: Not available.

Polymerization: No.

Section 11: Toxicological Information

Routes of Entry: Eye contact. Inhalation. Ingestion.

Toxicity to Animals:
WARNING: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE. Acute oral toxicity (LD50): 125 mg/kg [Rat]. Acute toxicity of the dust (LC50): 34386.6 mg/m 4 hour(s) [Rat]. 3

Chronic Effects on Humans: The substance is toxic to lungs, mucous membranes.

Other Toxic Effects on Humans:
Hazardous in case of ingestion, of inhalation. Slightly hazardous in case of skin contact (irritant).

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: Not available.

Special Remarks on other Toxic Effects on Humans: Not available.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are as toxic as the original product.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

DOT Classification: CLASS 6.1: Poisonous material.

Identification: : Toxic solid, inorganic, n.o.s. (Molybdenum trioxide) : UN3288 PG: III

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
Pennsylvania RTK: Molybdenum trioxide Massachusetts RTK: Molybdenum trioxide TSCA 8(b) inventory: Molybdenum trioxide SARA 313 toxic chemical notification and release reporting: Molybdenum trioxide

Other Regulations: OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200).

Other Classifications:

WHMIS (Canada):
CLASS D-1B: Material causing immediate and serious toxic effects (TOXIC). CLASS D-2A: Material causing other toxic effects (VERY TOXIC).

DSCL (EEC):
R25- Toxic if swallowed. R36- Irritating to eyes.

HMIS (U.S.A.):

Health Hazard: 3

Fire Hazard: 0

Reactivity: 0

Personal Protection: E

National Fire Protection Association (U.S.A.):

Health: 3

Flammability: 0

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

CURRICULUM VITAE

Name Miss Hathai Sinaim

Date of Birth 7 February 1987

Education Background

2005 - 2008 Bachelor of Science (Chemistry),
Chiang Mai University

Scholarship

2009 - 2011 The Center of Excellence for Innovation in Chemistry (PERCH-CIC)

Experiences

2009 - 2010 Undergraduate Teaching Assistant, General Chemistry Laboratory, Chiang Mai University,

Conference presentations

1. Hathai Sinaim, Titipun Thongtem, Anukorn Phuruangrat, and Somchai Thongtem, Synthesis of α-MoO_3 nanobelts by facile hydrothermal method and its optical properties, The 28th Annual Conference of the Microscopy Society of Thailand, 5-7 January 2011, Mae Fha Luang University, Chiang Rai, Thailand.