# Inorganic Material Database "AtomWork-Adv"

## **Data Platform Group**

Yibin XU, Junko HOSOYA, Isao KUWAJIMA and Yuta SAKAIRI

XU.Yibin@nims.go.jp



Outline



This database offers crystal structure, X-ray diffraction, material properties and phase diagrams extracted from approx. 1,000 of science and technology journals.

### New features (planned)

1. Download the data list displayed by "Property Chart"



Contents	Data	Crystalline structures: 318,837	
		X-ray diffractions: 577,449	
		Properties: 390,263	
		Type of properties: 480	
		Phase diagrams: 43,498	
		As of Sep. 2019.	
		To be upgraded and expanded.	
	Tools	Search functions	
		Material matrix	
		Property chart	
How to use	Website access		
Contact type	Free tr	ial use	

#### 2. Added display items on the detail page

Detail of Material	Detail of Material			
	▼ Substatnce Classification			
	Substance Phase Formula Modifier Structure Type Pearson Symbol Space Group			
Phase Formula Modifier Structure Type Pearson Symbol Space Grou	<u>CsyAs7</u> rt CsyAs7 oP80 Pbca (61)			
Cs-As- rt Cs-As- 080 Pbra (61)	Substance Name cristobalite low			
cisto alla città della città d	Compound Class arsenate; hydroxide; orthophosphate; orthosilicate; hexaoxotellurate(VI); oxid			
cristopante low	Structure Class CaCu <sub>5-2</sub> Cr <sub>4</sub> Al <sub>3</sub> intergrowth, CaCu <sub>5-2</sub> Cr <sub>4</sub> Al <sub>3</sub> intergrowth			
arsenate; hydroxide; orthophosphate; orthosilicate; hexaoxotellui (VI); or CaCu <sub>5</sub> -Zr <sub>4</sub> Al <sub>3</sub> intergrowth; CaCu <sub>5</sub> -Zr <sub>4</sub> Al <sub>3</sub> intergrowth	▼ Material			
	Chemical Formula AgEes/MoOda			
sampic	▼ Preparation Ion   Starting Materials Material   An-MoO₄ 99.98   99.9 % pow			
Material Description	Synthesis t 9 ( for 2			
Cs 99.9 wt.%				
As 99.99 wt %	▼ Bibliography			
melted at 973 K, cooled to 573 K at a rate of 5 K h <sup>-1</sup> , then to rt at rate of 25 K h <sup>-1</sup>	Publication     Balsanova L.V., Mikhallova D.A., Senyshyn A., Trots D.M., Fuess H., Lottermoser W., Ehrenberg H. (2009). Structure and properties of α-AgFe <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub> .       Solid State Sci., 11, 1137-1143.			
	▼ valence [-]			
	Symbol valence [-] Lower Upper Temperature [K] Temperature [K] Direction Additional Parameter Formula Remark			
	v 2.5 for Fe average value; for Fe; from Mössbauer spectroscopy			
	v 6 for Mo for Mo is to calculate average valence of Fe			

structure

literature

(72 hours, browsing only.)

Fixed annual rate

(Academic discounts available.)

Preparation					MoOg
Starting Materials	Material	Description	Synth	esis	
	Cs	99.9 wt.%			
	As	99.99 wt.%	▼ Biblio	graphy	
Synthesis	melted at 973 K, cooled to	573 K at a rate of 5 K h <sup>-1</sup> , then to rt at rate of 25 K h <sup>-1</sup>	Publi	cation	Balsan Solid S
			valen	ce [-]	
			Symbol	valence [-]	Lower Temperature [K
			v	2.5	
			×.	6	

Substatnce Classifie

Compound Class Structure Class

 Material Chemical Formul

#### Data details

Crystalling			Dronortios	
Crystaline Structure Structure	Substance information	Substance name and chemical composition, structure type, Pearson symbol, space group name and number	Sector Work (AS)	Substance information
N     NO     NO </td <td>Sample information</td> <td>Raw material, synthesis process</td> <td>6     HSS ort     216     Semanta     32     6.6.5 for     110<sup>3</sup>     110<sup>3</sup></td> <td>Property data</td>	Sample information	Raw material, synthesis process	6     HSS ort     216     Semanta     32     6.6.5 for     110 <sup>3</sup>	Property data
K Mg-04-h-Th W ① 13 SrTbs:Nbg:203.ft CaTO3 CP5 221 - 2 2 4 SH3b:217b:23WG:24O3 CaTO3 CP5 221 - 1 1	Cell parameters determination	Sample condition, experiment method, temperature	Phase Diagram	Summary
Mn2     0.2797       Mn2     0.2797       Mn2     0.2797       Bi1     0.2669       Bi1     0.2669       Bi2     0.2763       Mod     0.2669       Bi2     0.2669       Bi3     0.2669       Bi3     0.2669     439       Control     0.2675     10     0.00965     439       Control     0.2675     10     10     0.00965     439       Control     0.2675     10     10     10     10 <td>Cell parameters determination</td> <td>Sample condition, experiment method, spectrum</td> <td></td> <td>Phase</td>	Cell parameters determination	Sample condition, experiment method, spectrum		Phase
A - K = K     b (m)     c (m)     0 [1]     p [1]     v [1]     mm (m)     m (m)     mm (m)     m (m)	Cell structure	Lattice constant, atomic	CayAy H CayAy Charles and Carlos	information



Cell structure information (Standardized)

configuration

Other information Interatomic distance, literature



symbol, space group name, space group number, maximum and minimum temperature, link to crystal structure data

Substance name, chemical

space group name, space

group No., link to crystal

Type of phase diagram,

composition range,

composition, structure type,

Property values, temperature,

temperature range, generation

Phases, structure type, Pearson

Literature

method

<section-header></section-header>	X-ray diffraction graph with specified X-ray source	x axis: 2θ, y axis: intensity
	X-ray diffraction data (Tabular form)	2θ, Miller index, diffraction intensity, lattice spacing

User support: atomwork-adv@ml.nims.go.jp Website : https://atomwork-adv.nims.go.jp





