

Recent developments in the ICSD database: theoretical crystal structure data and related features

D. Zagorac^{1,2}, H. Müller³, S. Rühl³, J. Zagorac^{1,2}, S. Rehme³

¹Technicum Scientific Publishing, Stuttgart, Germany

²Institute of Nuclear Sciences Vinča, Materials Science Laboratory, Belgrade University, Belgrade, Serbia

³FIZ Karlsruhe – Leibniz Institute for Information Infrastructure, Karlsruhe, Germany

Supporting Information

1. Example of the ICSD desktop

Welcome to ICSD-Desktop. FIZ Karlsruhe | Contact

Content Selection

- Experimental Structures only
- Theoretical Structures only
- All Structures

Navigation

- Basic search & retrieve
- Advanced search & retrieve
 - Bibliography
 - Cell
 - Chemistry
 - Symmetry
 - Crystal Chemistry
 - Structure Type
 - Experimental Information**
 - DB Info
- Query Management
 - Manage Queries
 - List Combined Queries
 - Create Combined Query

Experimental Information Search

Temperature: K

Pressure: MPa

Comments: e.g. stable above R-Value:

Radiation Type

- X-Ray
- Electrons
- Neutrons
- Synchrotron

Sample Type

- Powder
- Single Crystal

Additional Properties

- Twinned Crystal Data
- Rietveld Refinement employed
- Anharmonic Temperature Factors given
- Absolute Configuration determined
- Experimental PDF number assigned
- Calculated PDF number assigned
- NMR Data available
- Magnetic Structure available
- Correction of earlier work
- Temperature Factors available
- Cell Constants without s.d.
- Only Cell and Structure Type determined

Calculation Method: Monte Carlo Simulation

Clear Experimental Info Search Count Experimental Info Search

Search Action

Run Query Clear Query

Search Summary

- Bibliography: -
- Cell: -
- Chemistry: -
- Symmetry: -
- Crystal Chemistry: -
- Structure Types: -
- Experimental Info: -
- DB Info: -

Query History

Number of queries: 5

Clear Query History

2018-11-29T19:05	19
2018-11-28T20:50	1
2018-11-28T20:48	99
2018-11-28T20:47	3008
2018-11-28T20:43	66
2018-11-28T20:25	19

Fig. S1. If one chooses *All Structures* in the Content Selection (upper left corner), the interface shows more information in the *Experimental Information Search* mask. In addition to the information for the theoretical structures some more information about experimental structures is now included.

2. The complete list of standardized keywords in the ICSD database (November 2018)

Physical properties

Magnetic properties

- Antiferromagnetism
- Diamagnetism
- Ferrimagnetism
- Ferromagnetism
- Hysteresis
- Magnetic dynamics
- Magnetic exchange interactions
- Magnetic frustration
- Magnetic moment
- Magnetic ordering
- Magnetic refrigeration
- Magnetic structure
- Magnetic susceptibility
- Magnetization
- Magnetization dynamics
- Magnetization relaxation
- Magnetostriction
- Magnetocaloric effect
- Magnetoelectric properties
- Multiferroic
- Paramagnetism, Superparamagnetism
- Spin-chain systems
- Spintronic material

Electrical properties

- Dielectric permittivity
- Dielectric constant
- Electrical conductivity
- Electrical resistivity
- Electrochemical properties
- Ferroelectricity
- Hall effect
- Ionic conductivity
- Magnetoelectric properties
- Piezoelectric constant
- Piezoelectricity
- Proton conduction
- Semiconductor
- Superconductivity
- Superionic conduction
- Thermoelectric properties

Optical properties

- Birefringence

- CIE chromaticity coordinates
- Fluorescence
- Luminescence
- Mechanochromic behavior
- Non-linear optical response
- Photoactivation
- Photoluminescence (PL)
- Photonic material
- Photorefractivity
- Photosensitivity
- Reflectivity
- Refractive index
- Second harmonic generation (SHG)
- Transparency
- Mechanical properties
 - Bimetallic
 - Bulk modulus
 - Compressibility
 - Elastic constants
 - Memory-shape crystal
 - Piezoelectricity
 - Shear modulus
 - Ultra-sonic
 - Vickers hardness
- Thermal properties
 - Anisotropic thermal expansion
 - Heat capacity
 - Negative thermal expansion
 - Seebeck effect
 - Specific heat
 - Thermal conductivity
 - Thermal expansion
 - Thermochromism
 - Thermoelectric properties
- Physicochemical properties
 - Bivalence
 - Catalytic activity
 - Electrochemical properties
 - Kinetic parameters
 - Mixed valence
 - Sensitivity toward impact and friction
 - Stability constants
 - Thermodynamic properties
- Dielectric properties
 - AC electrical conductivity
 - DC electrical conductivity

- Dielectric constant
- Nyquist plots
- Applied methods
 - Spectroscopic methods
 - Dielectric spectroscopy
 - ESR
 - EXAFS
 - FTIR
 - Impedance spectroscopy
 - IR
 - Moessbauer
 - NMR
 - NQR
 - Phonon-modes analysis
 - Raman
 - UV/vis
 - UV/vis optical absorbance spectra
 - UV/vis-NIR emission spectroscopy
 - UV/vis-NIR reflectance spectroscopy
 - UV/vis-NIR spectroscopy
 - Vibration-modes analysis
 - X-ray absorption spectroscopy (XAS)
 - X-ray photoelectron spectroscopy (XPS)
 - XANES
 - Calculation methods
 - ab initio calculations
 - Band structure
 - BVS
 - Computational studies
 - DFT
 - DOD, COHP
 - Electronic structure calculations (e.g. DOS)
 - Geometry optimization
 - MAPLE calculations
 - Molecular orbital calculations (MO)
 - Monte Carlo calculations
 - Natural bond orbital analysis (NBO)
 - QTAIM calculations
 - Quantum-chemical calculations
 - TD-DFT
 - Thermodynamic calculations
 - Valence bond analysis
- Thermometry
 - Differential scanning calorimetry (DSC)
 - Differential thermal analysis (DTA)
 - Thermal analysis

- Thermal stability
- Thermogravimetry (TGA, TG)
- Electrochemistry
 - Charge/Discharge curves
 - Cyclovoltammetry (CV)
 - Potentiometry
 - Redox properties
 - Solid electrolytes
- Magnetometry
 - SQUID magnetometry
- Microscopy
 - Atomic force microscopy (AFM)
 - Contact Kelvin Probe Force Microscopy (cKPFM)
 - Electron backscatter diffraction (EBSD)
 - HAADF-STEM
 - High resolution electron microscopy (HREM)
 - Piezoresponse force microscopy (PFM)
 - Scanning electron microscopy (SEM)
 - Selected area electron diffraction (SAED)
 - Transmission electron microscopy (TEM)
- Crystal structure
 - (3+1)D super space group
 - Coordination environment
 - Crystallography instrumentation
 - Doping
 - Electron backscatter diffraction (EBSD)
 - Enantiomorphism, chiral structures
 - Fourier maps
 - Framework structure
 - Group-subgroup relationship
 - Hydrogen bond interactions
 - Interstitial site
 - Layered structures
 - Li+ intercalation
 - Lithiation
 - Modulated structure
 - Nanoparticles (NP)
 - New mineral
 - New structure type
 - Phase diagram
 - Phase transition
 - Polymer structure
 - Polymorphism
 - Polytypism
 - Quasicrystals
 - Rotation electron diffraction (RED)

- Satellite peaks
- Selected area electron diffraction (SAED)
- Single-crystal growth
- Single-crystal to single-crystal transformation (SCSC)
- Stacking variants
- Superflip refinement
- Topology
- Twinning
- Vacancies
- Van-der-Waals interactions
- Chemical composition
 - Doping
 - Electron micro probe analysis (EMPA)
 - Energy-dispersive X-ray spectroscopy (EDX)
 - Intermetallics
 - Phase diagram
 - Polyoxometalates (POM)
- Synthesis
 - Arc-melting
 - Asymmetric synthesis
 - Chemical vapor transport (CVT)
 - Czochralski method
 - Floating zone method
 - Flux-growth
 - HT-HP synthesis
 - Hydrothermal synthesis
 - Ionothermal synthesis
 - Reaction coordinates
 - Reaction mechanism
 - Self-assembly
 - Solid-state synthesis
 - Solvothermal synthesis
 - Synthesis, Molecular Structure, Reaction mechanisms
- Technical Application
 - Optoelectronics
 - Deep-ultraviolet transparent materials (DUV)
 - Laser materials
 - LED technology
 - NLO materials
 - OLED technology
 - Scintillator(radiation detection)
 - White-light emission (WLE)
 - Energy
 - Batteries
 - Fuel cells
 - High-energy-density materials

Hydrogen evolution
 Hydrogen storage
 Ionic conductor
 Optical band gap
 Photovoltaic
 Scintillators
 Semiconductor
 Solar cells
 Solid electrolytes
 Solid oxide fuel cells (SOFC)
 Superconductors
 Thermoelectrics
 Environmental properties
 Actinide extraction
 Cadmium immobilization
 CO₂ emission
 CO₂ fixation/reduction
 Corrosion inhibition
 Environmental pollutants detection
 Explosives
 Ion exchange
 Nuclear fuel cycle
 Organic dyes adsorption/decomposition
 Radionuclide waste disposal
 Catalysis
 Alcohol oxidation
 Alkylation catalysts
 Asymmetric catalysis
 Bond activation
 Catalyst precursors
 Deoxygenation
 Electrocatalytic activity
 Enantioselective catalysts
 Gas absorption
 Hydrogenation catalysts
 N₂ fixation, N₂ activation
 Oxygen reduction reaction (ORR)
 Photocatalysis
 Photoelectrochemical water-splitting
 Polymerization
 Redox properties
 Water oxidation
 Water-splitting
 Spintronics
 Data storage
 Phase-change materials

Zeolites

Ion exchange
Molecular sieve
Gas sorption

Biology

Anti-cancer drugs
Bio-catalysis
Fungicides/Pesticides
Pharmaceutics
Photosynthesis