



FIZ Karlsruhe

Leibniz Institute for Information Infrastructure

ADVANCING SCIENCE

ICSD Exercise

25th IUCr congress - Joint Workshop for CSD and ICSD

Dr. Stephan Rühl, FIZ Karlsruhe, August 12, 2021

Exercise

Find a structure type in ICSD that includes structures with electrochemical properties and structures with optical properties, and also the structures must contain at least one lanthanoid!

Exercise – Solution

- 1) Find structures containing lanthanoids and which have electrochemical properties:

Chemistry Mask -> Composition: LAN

Bibliography Mask -> Keywords: „electrochemical properties“

- 2) Find structures containing lanthanoids and which have optical properties:
- 3) Combine both queries using boolean operator OR
- 4) Sort the result list by structure type, remove all unnecessary fields and add the field keywords
- 5) Scan through the list until you find a structure type which contains structures for each of the two properties (Perovskite#CaTiO3)

Exercise – Solution: 1st search (electrochemical properties + lanthanoids)



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Content Selection

☒ Experi. inorganic structures
☐ Experi. metal-organic str.
☐ Theoretical structures

Navigation

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

Bibliography Search

Authors

e.g. Jansen

Title of Journal

e.g. Angewandte Chemie

Title of Article

e.g. Super conducting crystals

Year of Publication

e.g. >2008 or 2000-2006 or 2001

Volume

e.g. 10

Page first

e.g. 10

Abstract

e.g. hybrid cage clusters

Keywords

"electrochemical properties"

e.g. Polymorphism

DOI

e.g. 10.1016/0022-4596(76)90194-8

Clear Bibliography Search

Count Bibliography Search

Search Action

Run QueryClear Query

Search Summary

Bibliography:	522
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-
Expert:	-
Combined Results:	522

Query History

Number of queries: 0

Clear Query History

Exercise – Solution: 1st search (electrochemical properties + lanthanoids)

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ICSD links

- ICSD News

Chemistry Search

Composition e.g. Na Cl

Structural Formula e.g. Pb (W O4)

Chemical Name

Mineral Name e.g. Adamite

Mineral Group e.g. Pyroxene

ANX Formula

AB Formula

Formula Weight

Search Action

Search Summary

Bibliography:	522
Cell:	-
Chemistry:	57968
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-
Expert:	-
Combined Results:	116

Query History

Number of queries: 0

Exercise – Solution: Results for the 1st search

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Results: List View # of Hits: 116

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☐	Coll. Code ^	HMS ^	Struct. Form. ^	Struct. Type ^	Title ^	Authors ^	Reference ^	Publication Year ^	CCDC	
☐	230195	P 42/n c m Z	Pr ₂ Ni O ₄ .09		(Nd/Pr) ₂ NiO ₄ +delta. R	Ceretti, Monica; Wahyu	Inorganic Chemistry (2018)	2018		Download
☐	230196	P 42/n c m Z	Nd ₂ Ni O ₄ .10		(Nd/Pr) ₂ NiO ₄ +delta. R	Ceretti, Monica; Wahyu	Inorganic Chemistry (2018)	2018		Download
☐	230197	P 42/n c m Z	Nd ₂ Ni O ₄ .10		(Nd/Pr) ₂ NiO ₄ +delta. R	Ceretti, Monica; Wahyu	Inorganic Chemistry (2018)	2018		Download
☐	230344	F -4 3 m	La Mg Ni ₄	Be ₅ Au#SnMgCu ₄	Solid-gas and electroch	Verbovyskyy, Yu.V.; Sh	Journal of Alloys and C	2018		Download
☐	230345	F -4 3 m	La Mg Ni _{3.5} Co _{0.5}	Be ₅ Au#SnMgCu ₄	Solid-gas and electroch	Verbovyskyy, Yu.V.; Sh	Journal of Alloys and C	2018		Download
☐	230346	F -4 3 m	La Mg Ni ₃ Co ₁	Be ₅ Au#SnMgCu ₄	Solid-gas and electroch	Verbovyskyy, Yu.V.; Sh	Journal of Alloys and C	2018		Download
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☐	230348	F -4 3 m	La _{0.5} Nd _{0.5} Mg Ni _{3.5} Co _{0.5}	Be ₅ Au#SnMgCu ₄	Solid-gas and electroch	Verbovyskyy, Yu.V.; Sh	Journal of Alloys and C	2018		Download
☐	230349	F -4 3 m	La _{0.5} Nd _{0.5} Mg Ni ₃ Co _{0.5}	Be ₅ Au#SnMgCu ₄	Solid-gas and electroch	Verbovyskyy, Yu.V.; Sh	Journal of Alloys and C	2018		Download
☐	230350	F -4 3 m	Nd Mg Ni ₄	Be ₅ Au#SnMgCu ₄	Solid-gas and electroch	Verbovyskyy, Yu.V.; Sh	Journal of Alloys and C	2018		Download

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Exercise – Solution: 2nd search (optical properties + lanthanoids)



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e.g. 10

Abstract

e.g. hybrid cage clusters

Keywords

"optical properties"

e.g. Polymorphism

DOI

e.g. 10.1016/0022-4596(76)90194-8

Clear Bibliography Search

Count Bibliography Search

Search Action

Run Query

Clear Query

Search Summary

Bibliography:	232
Cell:	-
Chemistry:	57968
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-
Expert:	-
Combined Results:	62

Query History

Number of queries: 2	
Clear Query History	
2021-07-29T11:15	62
2021-07-29T11:14	116

Exercise – Solution: Results for the 2nd search

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Results: List View # of Hits: 62

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☐	Coll. Code ^	HMS ^	Struct. Form. ^	Struct. Type ^	Title ^	Authors ^	Reference ^	Publication Year ^	CCDC	
☐	120638	P b n m	Pr ₂ Fe Cr O ₆	Perovskite#GdFeO ₃	Structural, optical and r	Gaikwad, Vishwajit M.;	Journal of Solid State C	2019		↶ ↴
☐	243522	C m c m	(Gd _{0.25} In _{0.25}) Mn _{0.5}	Sr ₂ Ti ₂ O ₅	New metal chalcogenid	Liang, I.C.; Weng, C.Y.;	Dalton Transactions (20	2017		↶ ↴
☐	243523	C m c m	(Gd _{0.375} In _{0.125}) Mn ₀	Sr ₂ Ti ₂ O ₅	New metal chalcogenid	Liang, I.C.; Weng, C.Y.;	Dalton Transactions (20	2017		↶ ↴
☐	243524	C m c m	Gd _{0.50} Mn _{0.75} S _{1.50}		New metal chalcogenid	Liang, I.C.; Weng, C.Y.;	Dalton Transactions (20	2017		↶ ↴
☐	243525	C m c m	Gd _{0.5} Mn S _{1.75}		New metal chalcogenid	Liang, I.C.; Weng, C.Y.;	Dalton Transactions (20	2017		↶ ↴
☐	243840	P n a m	(Ca _{0.995} Ce _{0.005}) Sc ₂	CaV ₂ O ₄ #CaFe ₂ O ₄	Correlating local comp	George, Nathan C.; Br	Chemistry of Materials	2017		↶ ↴
☐	244104	P n n a	Rb Sm ₂ F ₇		Crystal chemistry of hy	McMillen, Colin D.; Con	Acta Crystallographica,	2015		↶ ↴
☐	244105	P n n a	Cs Gd ₂ F ₇		Crystal chemistry of hy	McMillen, Colin D.; Con	Acta Crystallographica,	2015		↶ ↴
☐	244108	F m -3 m	Rb Sm ₃ F ₁₀	Zr ₃ PbO ₄ F ₆	Crystal chemistry of hy	McMillen, Colin D.; Con	Acta Crystallographica,	2015		↶ ↴
☐	244109	P 6 ₃ m c	Rb Gd ₃ F ₁₀	KYb ₃ F ₁₀	Crystal chemistry of hy	McMillen, Colin D.; Con	Acta Crystallographica,	2015		↶ ↴

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Exercise – Solution: Combine both searches using OR

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Content Selection

☒ Experm. inorganic structures
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☐ Theoretical structures

Navigation

Basic search & retrieve

Advanced search & retrieve

Query Management

ICSD links

Create Combined Query

Name:

Comment:

Available Queries:

☒	Query Name	Date	Query Type	# of hits	Saved
☒	2021-07-29T11:15	2021-07-29T11:15	Advanced	62	
☒	2021-07-29T11:14	2021-07-29T11:14	Advanced	116	

Must have (AND):

☐

No records found.

Must have at least one of (OR):

☐

2021-07-29T11:15

2021-07-29T11:15

Advanced

62

☐

2021-07-29T11:14

2021-07-29T11:14

Advanced

116

Must not have (NOT):

☐

No records found.

Run query

Count query

Clear

Exercise – Solution: Result of combined search

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Results: List View # of Hits: 178

☐	Coll. Code ^	HMS ^	Struct. Form. ^	Struct. Type ^	Title ^	Authors ^	Reference ^	Publication Year ^	CCDC	
☐	120638	P b n m	Pr ₂ Fe Cr O ₆	Perovskite#GdFeO ₃	Structural, optical and r	Gaikwad, Vishwajit M.;	Journal of Solid State C	2019		
☐	230195	P 42/n c m Z	Pr ₂ Ni O _{4.09}		(Nd/Pr) ₂ NiO ₄ +delta. R	Ceretti, Monica; Wahyu	Inorganic Chemistry (20	2018		
☐	230196	P 42/n c m Z	Nd ₂ Ni O _{4.10}		(Nd/Pr) ₂ NiO ₄ +delta. R	Ceretti, Monica; Wahyu	Inorganic Chemistry (20	2018		
☐	230197	P 42/n c m Z	Nd ₂ Ni O _{4.10}		(Nd/Pr) ₂ NiO ₄ +delta. R	Ceretti, Monica; Wahyu	Inorganic Chemistry (20	2018		
☐	230344	F -4 3 m	La Mg Ni ₄	Be ₅ Au#SnMgCu ₄	Solid-gas and electroch	Verbovyskyy, Yu.V.; Sh	Journal of Alloys and C	2018		
☐	230345	F -4 3 m	La Mg Ni _{3.5} Co _{0.5}	Be ₅ Au#SnMgCu ₄	Solid-gas and electroch	Verbovyskyy, Yu.V.; Sh	Journal of Alloys and C	2018		
☐	230346	F -4 3 m	La Mg Ni ₃ Co ₁	Be ₅ Au#SnMgCu ₄	Solid-gas and electroch	Verbovyskyy, Yu.V.; Sh	Journal of Alloys and C	2018		
☐	230347	F -4 3 m	La _{0.5} Nd _{0.5} Mg Ni ₄	Be ₅ Au#SnMgCu ₄	Solid-gas and electroch	Verbovyskyy, Yu.V.; Sh	Journal of Alloys and C	2018		
☐	230348	F -4 3 m	La _{0.5} Nd _{0.5} Mg Ni _{3.5} C	Be ₅ Au#SnMgCu ₄	Solid-gas and electroch	Verbovyskyy, Yu.V.; Sh	Journal of Alloys and C	2018		
☐	230349	F -4 3 m	La _{0.5} Nd _{0.5} Mg Ni ₃ Cc	Be ₅ Au#SnMgCu ₄	Solid-gas and electroch	Verbovyskyy, Yu.V.; Sh	Journal of Alloys and C	2018		

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Exercise – Solution: Sort by structure type/remove unwanted fields

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☐	☐	Coll. Code ↕	Struct. Form. ↕	Struct. Type ▲	Keywords ↕	
☐		627166	Dy Cu S2	AgErSe2	Electrical properties; Magnetic properties; Optical properties;	
☐		627965	Ho Cu S2	AgErSe2	Electrical properties; Magnetic properties; Optical properties;	
☐		628311	Lu Cu S2	AgErSe2	Electrical properties; Magnetic properties; Optical properties;	
☐		628974	Yb Cu S2	AgErSe2	Electrical properties; Magnetic properties; Optical properties;	
☐		622338	Ce Zn11	BaCd11	Thermodynamic properties; Electrochemical properties; Batteries, Electrode materials; Chemical bonding; Coordination e	
☐		649486	Pr Zn11	BaCd11	Thermodynamic properties; Electrochemical properties; Batteries, Electrode materials; Chemical bonding; Coordination e	
☐		619662	Ce Cd11	BaHg11	Thermodynamic properties; Electrochemical properties; Batteries, Electrode materials; Chemical bonding; Coordination e	
☐		620191	Nd Cd11	BaHg11	Thermodynamic properties; Electrochemical properties; Batteries, Electrode materials; Chemical bonding; Coordination e	
☐		230682	La4 Ba Cu3 Co2 O13.47	BaLa4Cu5O13+x	Solid oxide fuel cells (SOFC); Impedance spectroscopy; Electrical conductivity; Electrochemical properties;	
☐		257289	Nd Ba Mn2 O5	BaLaMn2O5(tP18)	Electrochemical properties; SOFC;	

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Exercise – Solution: Scan through the hits

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☐	Coll. Code	Struct. Form.	Struct. Type	Keywords	
☐	253367	K (Mg0.90 Eu0.02 Gd0.08) F3	Perovskite#CaTiO3	Optical properties; Luminescence;;Energy transfer; Jablonksi diagram; Rare earth doping; Short-wave laser material; UV.	
☐	253366	K (Mg0.92 Eu0.02 Gd0.06) F3	Perovskite#CaTiO3	Optical properties; Luminescence;;Energy transfer; Jablonksi diagram; Rare earth doping; Short-wave laser material; UV.	
☐	253365	K (Mg0.94 Eu0.02 Gd0.04) F3	Perovskite#CaTiO3	Optical properties; Luminescence;;Energy transfer; Jablonksi diagram; Rare earth doping; Short-wave laser material; UV.	
☐	253364	K (Mg0.96 Eu0.02 Gd0.02) F3	Perovskite#CaTiO3	Optical properties; Luminescence;;Energy transfer; Jablonksi diagram; Rare earth doping; Short-wave laser material; UV.	
☐	253363	K (Mg0.98 Eu0.02) F3	Perovskite#CaTiO3	Optical properties; Luminescence;;Energy transfer; Jablonksi diagram; Rare earth doping; Short-wave laser material; UV.	
☐	230417	Nd0.1 Sr0.9 Fe0.3 Co0.7 O2.55	Perovskite#CaTiO3	Solid oxide fuel cells (SOFC); Electrical conductivity; Phase diagram; Electrochemical properties;	
☐	230416	Nd0.1 Sr0.9 Fe0.5 Co0.5 O2.55	Perovskite#CaTiO3	Solid oxide fuel cells (SOFC); Electrical conductivity; Phase diagram; Electrochemical properties;	
☐	230415	Nd0.1 Sr0.9 Fe0.7 Co0.3 O2.55	Perovskite#CaTiO3	Solid oxide fuel cells (SOFC); Electrical conductivity; Phase diagram; Electrochemical properties;	
☐	230414	Nd0.1 Sr0.9 Fe0.9 Co0.1 O2.55	Perovskite#CaTiO3	Solid oxide fuel cells (SOFC); Electrical conductivity; Phase diagram; Electrochemical properties;	
☐	230413	Nd0.2 Sr0.8 Fe0.1 Co0.9 O2.60	Perovskite#CaTiO3	Solid oxide fuel cells (SOFC); Electrical conductivity; Phase diagram; Electrochemical properties;	

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Tipp: Scanning through the list is much easier for 50 hits per page!

Contact

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