

EXPLORING PROPERTY DATA WITH REAXYSFILE IN CAS STNEXT

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CAS

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American Chemical Society



Agenda

- REAXYSFILESUB/BIB Content and Coverage
- Property data in REAXYSFILE
- Search Example: Metal Organic Frameworks
- Additional Resources

ReaxysFile Databases on CAS STNNext

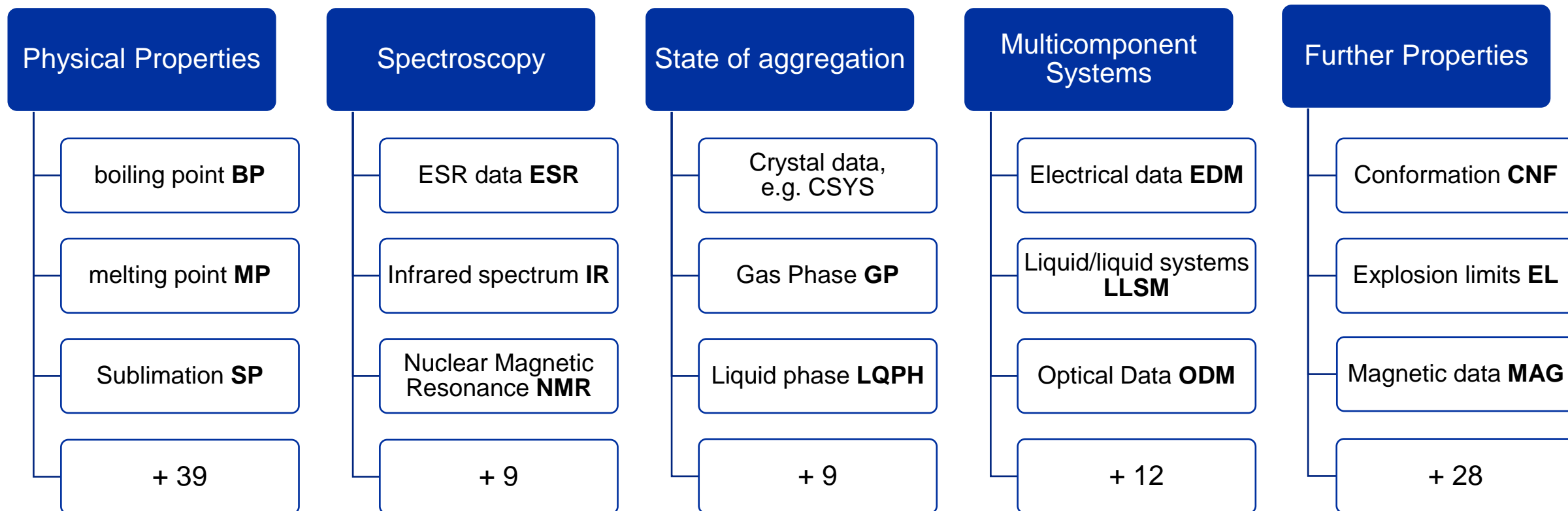
ReaxysFileBIB

- >57 million bibliographic records (2/2024)
- Patent and nonpatent literature records

ReaxysFileSUB

- >51 million chemical substances (2/2024)
 - Properties and reactions available
 - From 1771 to date
 - Both databases are updated twice weekly
- Same database architecture as REG-CAplus, DCR-DWPI - enabling a consistent workflow

Property Sections cover 110 Properties



Consult => **HELP PROPERTIES**
=> **EXPAND A/FA.P**
To see available properties

DISPLAY available properties by category

Kind of Property	Description	Example
PHYS	All physical properties	D PHYS
STATE	All state of aggregation properties	D STATE
FURTHER	All further properties	D FURTHER
MULTI	All multicomponent properties	D MULTI
SPEC	All spectroscopy properties	D SPEC

See all available property types in the database summary sheet

Database summary sheets are the definitive resource for all field codes and file-specific features.

Searching Properties

Properties may be searched in Field Availability, Properties (/FA.P) by using name or code – see table below.

Property Type	Name	Code	Search Examples	Display Code
Physical Property	Boiling Point	BP	S.BP/FA.P	BP
	Bulk Viscosity	BV	S BV/FA.P	BV
	Critical Micelle Concentration	CMC	S CMC/FA.P	CMC
	Density of the Liquid	DEN	S DEN/FA.P	DEN
	Dielectric Constant	DIC	S DIC/FA.P	DIC
	Dissociation Energy	EDIS	S EDIS/FA.P	EDIS
	Dissociation Exponent	DE	S DE/FA.P	DE
	Dynamic Viscosity	DV	S DV/FA.P	DV
	Electrical Data	ELE	S ELE/FA.P	ELE
	Electrical Moment	EM	S EM/FA.P	EM
	Electrolytic Conductivity	ELYC	S ELYC/FA.P	ELYC
	Energy Barriers	EBC	S EBC/FA.P	EBC
	Enthalpies of Other Phase Transitions	HPT	S HPT/FA.P	HPT
	Enthalpy of Combustion	HCOM	S HCOM/FA.P	HCOM
	Enthalpy of Formation	HFOR	S HFOR/FA.P	HFOR
	Enthalpy of Fusion	HFUS	S HFUS/FA.P	HFUS
	Enthalpy of Hydrogenation	HHDG	S HHDG/FA.P	HHDG
	Enthalpy of Sublimation	HSB	S HSB/FA.P	HSB
	Enthalpy of Vaporization	HVAP	S HVAP/FA.P	HVAP
	Flash Point	FP	S FP/FA.P	FP
	Heat Capacity Cp	CP	S CP/FA.P	CP
	Heat Capacity Cp0	CP0	S CP0/FA.P	CP0
	Heat Capacity Cv	CV	S CV/FA.P	CV
	Henry Constant	HNC	S HNC/FA.P	HNC
	Ionization Potential	IP	S IP/FA.P	IP
	Isoelectric Point	IEP	S IEP/FA.P	IEP
	Kinematic Viscosity	KV	S KV/FA.P	KV
	Liquid/Vapor Systems	LVSM	S LVSM/FA.P	LVSM
	Magnetic Susceptibility	MSUS	S MSUS/FA.P	MSUS
	Melting Point	MP	S MP/FA.P	MP

Search Example: Metal-Organic Frameworks

A new class of microporous materials

- Characterized by ultra-high porosity and internal surface area – much higher than zeolites/activated carbon
- Combine attractive features of both organic and inorganic building units
- Pore sizes and topology can be tuned by controlling length and type of organic linkers

Enter REAXYFILESUB and search MOF

```
=> FIL REAXYFILESU
```

```
=> S ((metal?) (2A) (organic?) (2A) (framework)) OR MOF
```

```
817 METAL?
```

```
796 ORGANIC?
```

```
15 FRAMEWORK
```

```
1 FRAMEWORKS
```

```
16 FRAMEWORK
```

```
(FRAMEWORK OR FRAMEWORKS)
```

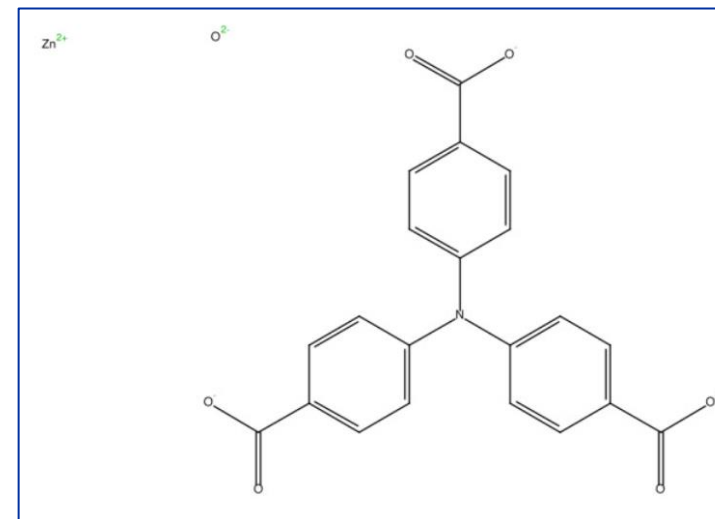
```
4 (METAL?) (2A) (ORGANIC?) (2A) (FRAMEWORK)
```

```
141 MOF
```

```
L1 145 ((METAL?) (2A) (ORGANIC?) (2A) (FRAMEWORK)) OR MOF
```


Property Data in document records

L4 ANSWER 4 OF 47 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.
 AN 39134933 REAXYSFILESU
 CN MOF-150
 MF 2 C21 H12 N 06 . 0 . 4 Zn
 CMF 2 C21 H12 N 06; 0; 4 Zn
 LSF 2C21H12N06(3-)*4Zn(2+)*O(2-)
 INCHI HXBDHTDDNUNQGS-UHFFFAOYSA-K
 MW 1026.22
 MARKREF.CNT 0
 REC 2
 ED Entered STN: 14 Dec 2021
 Last updated on STN: 21 Aug 2024



Density of the Liquid (1)

Value (DEN) (g*cm**3)	Temp. (.T) (Cel)	Location (.LO)	Ref(s) (REF)
1.224	24.84	supporting informati on	1

- Property Data in Table Format
 - Value(s)
 - Location in document
 - Reference

1. AN 106919542: Journal: Cordova, Kyle E. et al., J. Mater. Chem. A (2021)
 Vol. 9, No.44, pp. 24857 - 24862

Find substances with Aggregation Data

=> S I1 and (CRD or CRP or CRT or CRV or CRYPH or CPTP or CPD or CSG or CSYS or DP or GP or LQPH or LPTP or TP)/FA.P

522 CRD/FA.P
1174 CRP/FA.P
1638 CRT/FA.P
562 CRV/FA.P
1117414 CRYPH/FA.P
27992 CPTP/FA.P
8470855 CPD/FA.P
1131022 CSG/FA.P
1032417 CSYS/FA.P
105493 DP/FA.P
333 GP/FA.P
13609 LQPH/FA.P
47948 LPTP/FA.P
703 TP/FA.P

These property field codes represent different datapoints that describe state of aggregation.

L5 76 L1 AND (CRD OR CRP OR CRT OR CRV OR CRYPH OR CPTP OR CPD OR CSG OR CSYS OR DP OR GP OR LQPH OR LPTP OR TP)/FA.P

State of Aggregation Property Data Examples

L5 ANSWER 2 OF 76 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.

AN 39134933 REAXYSFILESU

CN **MOF**-150

MF 2 C21 H12 N 06 . 0 . 4 Zn

CMF 2 C21 H12 N 06; 0; 4 Zn

LSF 2C21H12N06(3-)*4Zn(2+)*0(2-)

INCHI HXBDHTDDNUNQGS-UHFFFAOYSA-K

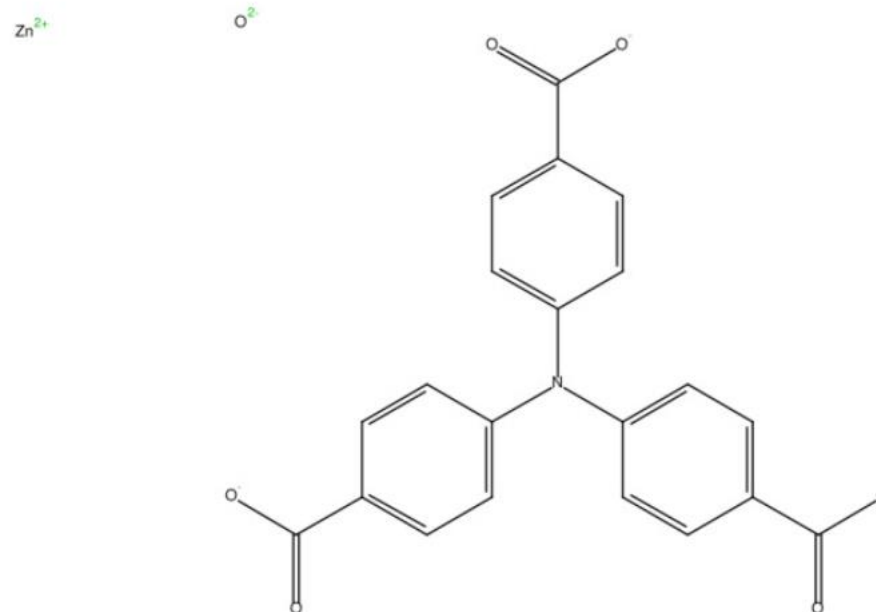
MW 1026.22

MARKREF.CNT 0

REC 2

ED Entered STN: 14 Dec 2021

Last updated on STN: 21 Aug 2024

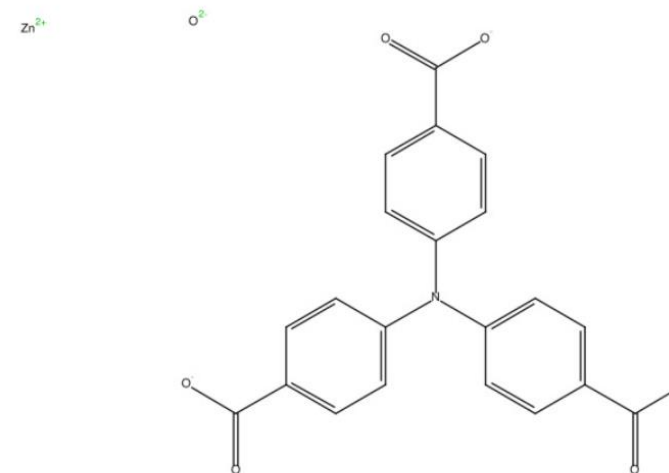


State of Aggregation Property Data Examples

Crystal Space Group (3)

Value (CSG) (--)	Location (.LO)	Comment (.CMT)	Ref(s) (REF)
176	supporting informati on	Method = Single crys tal X-ray diffractio n	1
198	supporting informati on	a = 22.329 0C5;; Z = 8; T = 298 K; Metho d = Single crystal X -ray diffraction; at omic positions avail able a = 0.603 0C5;; Meth od = Powder X-ray di ffraction	2

1. AN 124889770: Journal: Li, Yan et al., Cryst. Growth Des. (2023) Vol. 23, No.5, pp. 3702 - 3710
2. AN 106919542: Journal: Cordova, Kyle E. et al., J. Mater. Chem. A (2021) Vol. 9, No.44, pp. 24857 - 24862



Crystallographic data for this substance, including references

Multi-component substance property data

=> S 11 and (ADSM or ASSM or AZE or BSPM or CPEM or EDM or ENEM or LLSM or LSSM or LVSM or MECM or POW or ODM or SOLM or TRAM)/FA.P

41098 ADSM/FA.P

100394 ASSM/FA.P

1454 AZE/FA.P

7414 BSPM/FA.P

469 CPEM/FA.P

263 EDM/FA.P

5756 ENEM/FA.P

30499 LLSM/FA.P

37354 LSSM/FA.P

4298 LVSM/FA.P

2881 MECM/FA.P

183436 POW/FA.P

815 ODM/FA.P

4866 SOLM/FA.P

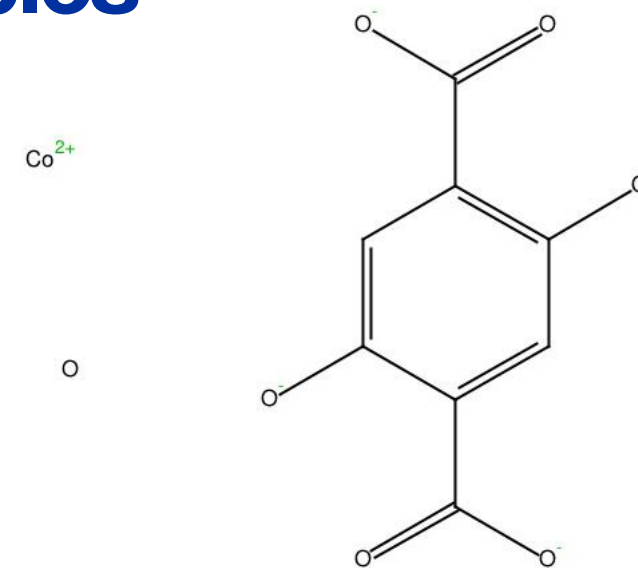
13585 TRAM/FA.P

L6 21 L1 AND (ADSM OR ASSM OR AZE OR BSPM OR CPEM OR EDM OR ENEM OR
LLSM OR LSSM OR LVSM OR MECM OR POW OR ODM OR SOLM OR TRAM)/FA.
P

These property field codes
represent different datapoints that
describe multicomponent systems.

Multi-component property data examples

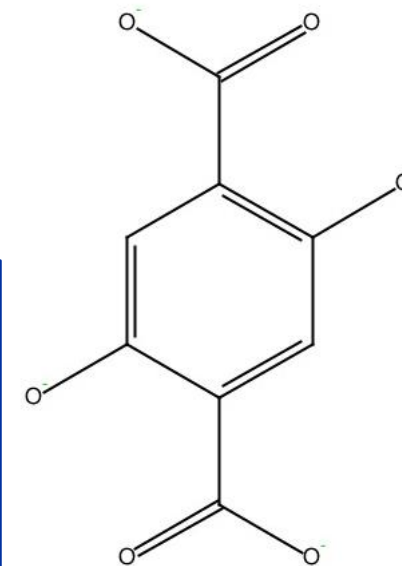
L6 ANSWER 1 OF 21 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.
AN 47041467 REAXYSFILESU
CN $[\text{Co}(\text{sub})2(\text{/sub})(\text{dtp})(\text{H}(\text{sub})2(\text{/sub})\text{O})(\text{sub})2(\text{/sub})]$; MOF-74-Co;
 $\text{Co}(\text{sub})2(\text{/sub})(\text{dhtp}) * 2\text{H}(\text{sub})2(\text{/sub})\text{O}$
MF C8 H2 O6 . 2 Co . 2 H2 O
CMF C8 H2 O6; 2 Co; 2 H2 O
LSF C8H2O6(4-)*2Co(2+)*2H2O
INCHI VMRPLKZAZLKBBL-UHFFFAOYSA-J
MW 348.117
MARKREF.CNT 0
REC 3
ED Entered STN: 26 Jan 2023
Last updated on STN: 14 Jun 2024



Multi-component property data examples

L6 ANSWER 1 OF 21 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.
 AN 47041467 REAXYSFILESU
 CN

Co²⁺



Adsorption (MCS) (5)

Part 1 | Keyword
 of 2 | (.KW)

=====+

LSF	1	Adsorption
INCHI	2	
MW	3	Adsorption
MARKRE	4	
REC	5	Adsorption
ED	6	
	7	Adsorption a
	8	ption isothe
	9	Adsorption a
	10	ption isothe

Adsorption (MCS) (5)

Part 2 | Location | Ref(s)
 of 2 | (.LO) | (REF)

=====+

1	supporting informati	1
2	on	
3	supporting informati	1
4	on	
5	supporting informati	1
6	on	
7	supporting informati	1
8	on	
9	supporting informati	1
10	on	

1. AN 127800797: Journal: Lee, Sujeong et al., Dalton Trans. (2023) Vol. 52, No.34, pp. 12143 - 12151

Search for specific types of property data, including spectroscopy

=> S l1 and (ESR or FLUS or IR or LUM or MS or NMR or NQR or OSM or PHOS or RAS or ROT or UVS)/FA.P

139603 ESR/FA.P

306381 FLUS/FA.P

6665264 IR/FA.P

233674 LUM/FA.P

12908234 MS/FA.P

15448301 NMR/FA.P

10219 NQR/FA.P

100253 OSM/FA.P

21952 PHOS/FA.P

121288 RAS/FA.P

7979 ROT/FA.P

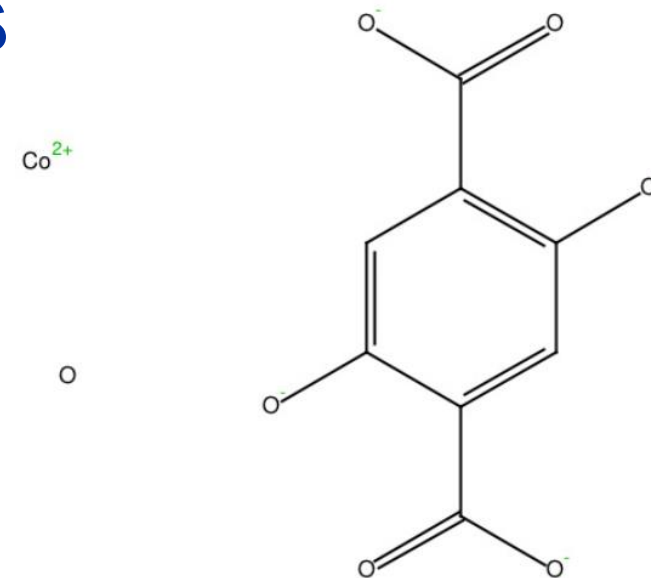
1846685 UVS/FA.P

L7 78 L1 AND (ESR OR FLUS OR IR OR LUM OR MS OR NMR OR NQR OR OSM OR
PHOS OR RAS OR ROT OR UVS)/FA.P

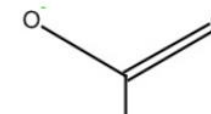
These property field codes represent different datapoints that describe results of spectroscopic studies, with results

Spectroscopic Property Data Examples

L7 ANSWER 2 OF 78 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.
AN 47041467 REAXYSFILESU
CN [Co(sub)2(/sub)(dptp)(H(sub)2(/sub)O)(sub)2(/sub)]; MOF-74-Co;
Co(sub)2(/sub)(dhtp)*2H(sub)2(/sub)O
MF C8 H2 O6 . 2 Co . 2 H2 O
CMF C8 H2 O6; 2 Co; 2 H2 O
LSF C8H2O6(4-)*2Co(2+)*2H2O
INCHI VMRPLKZAZLKBBL-UHFFFAOYSA-J
MW 348.117
MARKREF.CNT 0
REC 3
ED Entered STN: 26 Jan 2023
Last updated on STN: 14 Jun 2024



Spectroscopic Property Data Examples



ANSWER 2 OF 78 RE		NMR spectroscopy (1)			
Keyword	(.KW)	Nucleus	Location	Ref(s)	
(.KW)		(.NUC)	(.LO)	(REF)	
=====+=====+=====+=====					
Chemical shifts; Spe		1H	supporting informati	1	
ctrum			on		
Luminescence sp		Other Spectroscopic Methods (1)			
Keyword	(.KW)	Location	Ref(s)		
(.KW)		(.LO)	(REF)		
=====+=====+=====					
ESCA		supporting informati	1		
		on			
1. AN 127800797: Journal: Lee, Sujeong et al., Dalton Trans. (2023) Vol. 52, No.34, pp. 12143 - 12151					

Search Further Properties and combine sets

=> S I1 and (SOUND or AIT or CDER or CDIC or CMP or CNF or XS or ELP or ELCB or POT or ELCH or CIP or EL or FINFO or FINFO1 or FINFO2 or FINFO3 or IDA or INP or MAG or MEC or DFM or ORD or OPT or OTHE)/FA.P

=> S I1 and (PSD or PUR or QCC or RSTR or LB or TRAN)/FA.P

=> S L8 OR L9

L10 82 L8 OR L9

Further Properties include those that do not fall into one of the already-mentioned categories

Further Properties Data Examples

Further Information (1)

Key

(.KW)

Cat

Further Information (1)

Keyword | Ref(s) | Location

Substance Label (1)

Label | Ref(s)

(.LB) | (REF)

=====+=====

RBC-MOF-HRP NP | 1

1. AN 117081537: Journal: Wang, Shuyan et al., Angew. Chem. Int. Ed. (2022)

Vol. 61, No.24 arn.E202203115

1. A

1. AN 117081537: Journal: Wang, Shuyan et al., Angew. Chem. Int. Ed. (2022)

Vol. 61, No.24 arn.E202203115

Searchable Keywords within Property Data

```
=> S L7 AND (ELECTROSPRAY? OR ESI)/KW
```

```
6649358 ELECTROSPRAY?/KW
```

```
6649401 ESI/KW
```

```
L11          1 L7 AND (ELECTROSPRAY? OR ESI)/KW
```

The Keyword (/KW) field contains text terms from the document. These can be searched to refine results

/KW field allows further refinement of results

L11 ANSWER 1 OF 1 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.

AN 237238 REAXYSFILESU

RN 145370-50-9

CN ST057649; 7-hydroxy-3'-methoxyflavone; 7-H-3'-MOF;

7-hydroxy-2-(3-methoxy-phenyl)-chromen-4-one

7-Hydroxy-2-(3-methoxy-

7-Hydroxy-2-(3-methoxy-

SD heterocyclic

MF C16 H12 O4

CMF C16 H12 O4

LSF C16H12O4

INCHI PTXIWVJSAQPKEY-UHFFFAOY

AINCHI PTXIWVJSAQPKEY-UHFFFAOY

MW 268.269

Mass Spectrometry (1)

Keyword	Location	Ref(s)
(.KW)	(.LO)	(REF)

electrospray ionisation (ESI); spectrum	supporting information	1
---	------------------------	---

1. AN 70696020: Journal: Zhang, Guoning et al., Eur. J. Med. Chem. (2017) Vol. 129, pp. 303 - 309

Search for Preparation Reactions

```
=> S L4 AND PREPARATION/RX.CL
```

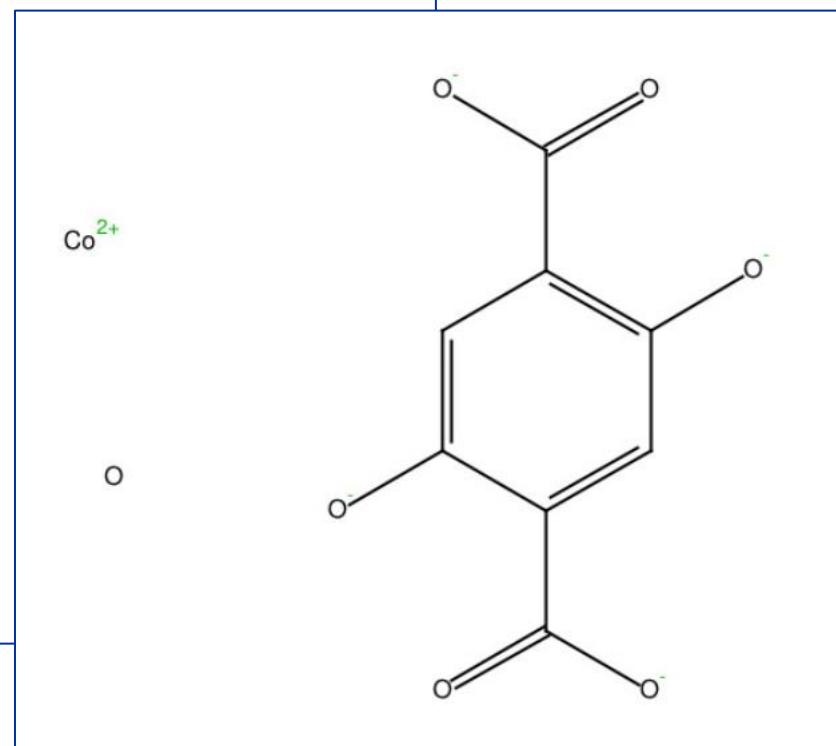
```
24595404 PREPARATION/RX.CL
```

```
L12          43 L4 AND PREPARATION/RX.CL
```

Searching in /RX.CL retrieves only records where “preparation” is noted as the type of reaction.

Substances with Preparation reaction data available

L12 ANSWER 1 OF 43 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.
AN 47041467 REAXYSFILESU
CN [Co(sub)2(/sub)(dptp)(H(sub)2(/sub)O)(sub)2(/sub)); MOF-74-Co;
Co(sub)2(/sub)(dhtp)*2H(sub)2(/sub)O
MF C8 H2 O6 . 2 Co . 2 H2 O
CMF C8 H2 O6; 2 Co; 2 H2 O
LSF C8H2O6(4-)*2Co(2+)*2H2O
INCHI VMRPLKZAZLKBBL-UHFFFAOYSA-J
MW 348.117
MARKREF.CNT 0
REC 3
ED Entered STN: 26 Jan 2023
Last updated on STN: 14 Jun 2024



Substances with Preparation reaction data available

Reaction:

Reaction ID: 62198643
Reactant AN (.RAN): 13149477; 2696052
Reactant (.RCT): cobalt(II) nitrate hexahydrate;
2,5-dihydroxy-1,4-benzenedicarboxylic
acid

Product AN (.PAN)
Product (.PRO):

Reference Count:

Reaction Details:

Reaction RID: 62198643.1
Reaction Classification (.CL): **Preparation**
Solvent AN (.SOLAN): 1718733; 3587155; 605365
Solvent: ethanol; water; N,N-dimethyl-formamide
Temperature: 100 Cel
Reference(s): 121669304: Journal: Xiong, Jiabin et al.,
RSC Adv. (2022) Vol. 12, No.46, pp. 30051
- 30055

Crossover to REAXYSFILEBIB

=> FIL REAXYSFILEBIB; S L10 AND PATENT/DT

1616 L10

43532065 PATENT/DT

L13

57 L10 AND PATENT/DT

Crossfile searching in
REAXYSFILEBIB retrieves 57
patent literature results

Patent Results

L13 ANSWER 1 OF 5
 AN 135336219
 TI Multivariate
 frameworks
 IN Peterson, Gre
 PA U.S. Army Cor
 Center, APG,
 PI PATENT NO.

 US 11459342
 US 11987594
 US 12012423
 US 12037347
 * = indexed patent


L13 ANSWER 4 OF 57 REAXYSFILEBI COPYRIGHT 2024 ELSEVIER INC. on STN.
 AN 133876256
 TI Method fo
 polymeriz
 IN ZHANG QI
 PA UNIV GUAN
 PI PATENT NO.

 CN 117976
 * = index
 DT Patent
 LA Chinese
 SL English
 ED Entered S
 Last upda

L13 ANSWER 7 OF 57 REAXYSFILEBI COPYRIGHT 2024 ELSEVIER INC. on STN.
 AN 123857016 REAXYSFILEBI [Full-text](#)
 TI CONTROLLING METAL-ORGANIC FRAMEWORK MORPHOLOGY THROUGH COORDINATIVE
 MIMICRY
 IN JACKSON, Megan N.; LONG, Jeffrey R.; FALKOWSKI, Joseph M.
 PA THE REGENTS OF THE UNIVERSITY OF CALIFORNIA; EXXONMOBIL TECHNOLOGY AND
 ENGINEERING COMPANY
 PI PATENT NO. KIND DATE APPLICATION NO. DATE

 WO 2023014513 * A1 20230209 WO 2022-US37901 20220721
 WO 2023014513 A9 20230330
 KR 2024042474 A 20240402
 CN 118076618 A 20240524
 EP 4380944 A1 20240612
 * = indexed patent
 DT Patent

Link to Full Text via Espacenet



Espacenet
Patent search

Office/Language ▾

My Espacenet Help Classification search Results Advanced search Filters Popup tips Report data error Feedback

Home > Results > **US11459342B1**

1. >

☆ **US11459342B1** Multivariate carboxylate derivatized phenyl-based metal-organic frameworks

Available in ▾ Patent Translate ▾ ⋮

Bibliographic data Description Claims Drawings Original document Citations Legal events Patent family

Global Dossier ↗

Applicants COMBAT CAPABILITIES DEV COMMAND CHEMICAL BIOLOGICAL CENTER [US]; US ARMY [US] +

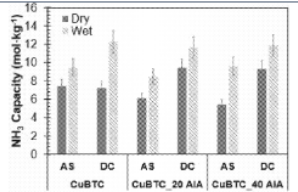
Inventors PETERSON GREGORY W [US]; EPPS III THOMAS H [US] +

Classifications

IPC **B01D53/58; B01D53/62; B01D67/00; B01D69/12; B01D71/02; B01D71/82; B01J20/22; B01J20/28; B01J31/16; B01J31/22; B01J35/02; B01J35/04; B01J35/08; B01J35/10; B01J37/04; B01J37/10; C07F1/08;**

CPC **B01D53/04 (EP); B01D53/228 (EP); B01D53/58 (US); B01D53/62 (US); B01D67/0079 (EP,US); B01D69/12 (EP,US); B01D71/022 (EP,US); B01D71/82 (US); B01J20/226 (EP); B01J20/321 (EP); B01J20/3212 (EP); B01J20/3236 (EP);**

Front-page drawing from US11459342B1



Sample	Dry Capacity (mol.kg ⁻¹)	Wet Capacity (mol.kg ⁻¹)
AS CuBTC	~7	~10
DC CuBTC	~7	~12
AS CuBTC_20 AIA	~7	~10
DC CuBTC_20 AIA	~9	~12
AS CuBTC_40 AIA	~5	~10
DC CuBTC_40 AIA	~9	~12

Summary

- REAXYSFILESub contains more than 51 million records and covers all types of organic and inorganic substances, including alloys, coordination compounds, minerals, mixtures, polymers, and salts
- Substance properties and reaction data are now included in REAXYSFILESUB's biweekly updates
- Simplified property and reaction searching and displays allow for efficient and thorough retrieval
- Crossfile searching harmonized with all other structure/bibliographic pairs in CAS STNext

Additional Resources and Materials

- User Guide:

<https://www.cas.org/sites/default/files/documents/CAS-STNext-ReaxysfileSUB-User%20Guide%20Properties-Reactions-2024-1.pdf>

- Database Summary Sheet: [REAXYSFILESU.pdf](#)

- Recorded training sessions:

<https://www.cas.org/training/solution/stn>

For more information...

CONTACT

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