ReaxysFile on STN: Searching Inorganic Substances and Related Properties

1. Introduction

Inorganic chemistry has a wide range of application – in every aspect of the chemical industry – including catalysis, materials science, pigments, surfactants, coatings, medicine, fuel, and agriculture. E.g. high-throughput techniques aren't just for pharmaceutical and life science research, they are applied in the development of materials of all sorts.

The use and significance of inorganic compounds had been invaluable over decades to, e.g., the medical field. With these compounds, drugs and apparatuses have been available for human benefit. Mercury for instance has been useful for treating various illnesses as well as a major component of some medical instruments. Copper, on the other hand, has been beneficial in treating ulcers, cancers and nervous disorders. Though known to be poisonous, early and current medical sources had identified inorganic arsenic compounds to be useful for medical purposes as well. While some inorganic drugs had been known to be toxic and harmful to health, the ability to develop alternatives has been promoted and enhanced.
Researchers nowadays understand the importance of historical and recent factual data. ReaxysFile has both, combined with powerful search capabilities.
Scientists will find substances relevant to the development of materials such as phosphates, catalysts, polymers and other compounds used in electronics, magnetics, medicine, optics and nanoscience.
The extensive coverage drills deep into the literature. Many different chemical and physical property fields provide detailed information needed to assess new material performance.

2. Search Tips

a. Special Classes of Substances (/CTYPE):

The compound type is used to restrict a search to a specific group of inorganic substances, e.g. alloys or coordination compounds.

```
=> e a/ctype
**** START OF FIELD ****
E3            0 --> A/CTYPE
E4       834171     ACYCLIC/CTYPE
E5       129187     ALLOY/CTYPE
E6        90877     BIOMOLECULE/CTYPE
E7      1498794     COORDINATION COMPOUND/CTYPE
E8        50577     GLASS OR CERAMIC MATERIAL/CTYPE
E9      5532849     HETEROCYCLIC/CTYPE
```

```
E10     3561418      ISOCYCLIC/CTYPE
E11       81029      ISOTOPE OR ISOTOPE CONTAINING COMPOUND/CTYPE
E12      135820      MARKUSH STRUCTURE/CTYPE

=> e
E13        3840      MINERAL/CTYPE
E14      102199      MIXTURE (COMPOSITION COMPLETELY GIVEN)/CTYPE
E15       45830      MIXTURE (COMPOSITION NOT GIVEN)/CTYPE
E16      131220      MIXTURE (COMPOSITION PARTIALLY GIVEN)/CTYPE
E17       56220      POLYMER (MONOMERS GIVEN)/CTYPE
E18       37661      POLYMER (MONOMERS NOT GIVEN)/CTYPE
E19       71727      SOLID SOLUTION/CTYPE
**** END OF FIELD ****
```

b. Ways of Searching

ReaxsyFile offers you different ways of searching inorganic substances

- Structure/substructure

Coordination compounds are the main candidates for structure searches. But not all substances have structures assigned, alloys or ceramics are only identified by molecular formulas and associated fields. If you need to look for a substance there are several other ways than doing a structure query. You can search for all fields within the identification section; it might be useful to search for parts of the molecular formula or the chemical name (keep in mind that not all substances have one).

- Molecular Formula (/MF)

There are a number of fields derived from the molecular formula allowing to search for groups of substances, e.g. element symbol, element count, periodic groups etc.

- CAS Registry Numbers (/RN)

Note: not available for all substances

- Chemical data (incl. reactions) (e.g./RX)

The main topics are reactions and preparations with various sub-fields containing the reaction details.

- Controlled vocabulary (/<prop>.KW)

Many properties are searchable via keywords sub-fields. EXPAND is recommended (see search example 3).
All keywords can be expanded/searched with /AKW.

All these topics can be combined with each other.

For a detailed description of the available properties see:
“Introduction and Property Glossary”

c. Field Availability (/FA)

This field enables the retrieval for the occurrence of a property in the database. Thus you can search for all compounds with mechanical data by entering: => S MEC/FA or combining it with, e.g., substance identifying fields: => S PT/ELS and MEC/FA

A lot of information might be available for well known compounds. Especially in long records it is very useful to employ the Field Availability list to evaluate which fields are of interest.

3. Search Examples

Search Example 1: Crystal Data

Substances containing B5 metals with information on crystal space group and quantum mechanical calculations.

```
=> s b5/pg and csg/fa and qcc/fa
L17         788 B5/PG AND CSG/FA AND QCC/FA

=> d


L17  ANSWER 1 OF 788 REAXYSFILE COPYRIGHT 2012 Elsevier Properties SA. On
     STN

     Accession Number (AN):            21150630
     Lin. Struct. Formula (LSF):      Rb(1+)*La(3+)*Nb2O6F(4-)=RbLaNb2O6F
     Molec. Formula (MF):              F La Nb2 O6 Rb
     Formula Weight (FW):              525.181
     InChi Key: (INCHI):               DQVMPASCERDPOL-UHFFFAOYSA-N
     Alternate InChi Key: (AINCHI):   DQVMPASCERDPOL-NNPLXYKSAV
     Markush Ref. Count (MARKREF):    0
     Entry Date (DED):                 2011/03/21
     Update Date (DUPD):               2011/03/21

     No structure diagram available for this Document

   Field Availability:

     Code      Name                                    Occurrence
     ========================================================
     AN        Accession Number                              1
     LSF       Linearized Structure Formula                  1
     MF        Molecular Formula                             1
     FW        Formula Weight                                1
     INCHI     InChi Key                                     1
     AINCHI    Alternate InChi Key                           1
     MARKREF   Markush Reference Count                       1
     DED       Entry Date                                    1
     DUPD      Update Date                                   1
     CNF       Conformation                                  1
     CRYPH     Crystal Phase                                 1
     CSG       Crystal Space Group                           1
     CSYS      Crystal System                                1
     ELE       Electrical Data (MCS)                         1
     GEO       Interatomic Distances and Angle               1
     QCC       Quantum Chemical Calculations                 1
     USC       Use of Compound                               1

   This substance also occurs in Reaction Documents:

     Code      Name                                    Occurrence
     ========================================================
     RX        Reaction Documents                            2
     RX.RAN    Reactant AN                                   1
     RX.PAN    Product AN                                    1

Crystal Space Group:
CSG
     CSG:                                  129
     Note(s) (.COM):                       a = 3.86575 Angstroem, c = 11.2135
                                           Angstroem
     Reference(s):
     1. Kobayashi, Yoji; Tian, Mingliang; Eguchi, Miharu; Mallouk, Thomas
        E.,Journal of the American Chemical Society, CODEN: JACSAT, 131,
        <2009>,9849 - 9855

Quantum Chemical Calculations:
QCC
     Calculated Properties (.TYP):         Density of states
     Note(s) (.MET):                       Ab initio calcns. (LCAO, GO SCF, DIM,
                                           SAMO, X-alpha, Hartree-Fock)
     Reference(s):
     1. Kobayashi, Yoji; Tian, Mingliang; Eguchi, Miharu; Mallouk, Thomas
        E.,Journal of the American Chemical Society, CODEN: JACSAT, 131,
        <2009>, 9849 - 9855
```

Search Example 2: Pharmacological Data

Physiological behaviour of cis-platin derivatives (if a search with a specific term in the note/comment field is not successful, the combining with PHARM/FA is recommended. Details on, e.g., physiological behaviour are often stored in more than one sub-field).

```
=> e physiological/pharm.com
E1            60      PHYSIOL/PHARM.COM
E2            79      PHYSIOLOG/PHARM.COM
E3         17851 --> PHYSIOLOGICAL/PHARM.COM
E4            12      PHYSIOLOGICALLY/PHARM.COM
E5             3      PHYSIOLOGISCH/PHARM.COM
E6            57      PHYSIOLOGISCHE/PHARM.COM
E7             1      PHYSIOLOGY/PHARM.COM
E8             1      PHYSLIOLOGISCHE/PHARM.COM
E9             1      PHYSOLOGICAL/PHARM.COM
E10           68      PHYSOSTIGMINE/PHARM.COM
E11            5      PHYSYOSTIGMINE/PHARM.COM
E12            2      PHYTATE/PHARM.COM

=> s e3 and pt/els and 2/cl and 2/n and 6/h and 4/elc
L29            3 PHYSIOLOGICAL/PHARM.COM AND PT/ELS AND 2/CL AND 2/N
                 AND 6/H AND 4/ELC

=> d 2


L29  ANSWER 2 OF 3 REAXYSFILE COPYRIGHT 2012 Elsevier Properties SA. on STN

      Accession Number (AN):          11324567
      Basic Pref. RN (BPR):           26035-31-4
      CAS Reg. No. (RN):              26035-31-4, 14913-33-8, 15663-27-1
      Chemical Name (CN):             diammine(dichloro)platinum(II),
                                      dichlorodiammineplatinate(II),
                                      trans-<Pt(NH3)2Cl2>, cis-PtCl2(NH3)2,
                                      cisplatin, <Pta2Cl2>,
                                      cis-dichlorodiamine
                                      platinum (II) (DDP) cisplatin
      Lin. Struct. Formula (LSF):     Cl2H6N2Pt
      Molec. Formula (MF):            Cl2 H6 N2 Pt
      Formula Weight (FW):            300.047
      InChi Key: (INCHI):             LXZZYRPGZAFOLE-UHFFFAOYSA-L
      Alternate InChi Key: (AINCHI):  LXZZYRPGZAFOLE-NLRNZNLACV
      Compound Type (CTYPE):          Coordination compound
      Markush Ref. Count (MARKREF):   0
      Entry Date (DED):               2008/06/16
      Update Date (DUPD):             2011/02/16

      No structure diagram available for this Document

   Field Availability:

      Code      Name                                  Occurrence
      ========================================================
      AN        Accession Number                             1
      BPR       Basic Preferred RN                           1
      RN        CAS Registry Number                          3
      CN        Chemical Name                                7
      LSF       Linearized Structure Formula                 1
      MF        Molecular Formula                            1
      FW        Formula Weight                               1
      INCHI     InChi Key                                    1
      AINCHI    Alternate InChi Key                          1
      CTYPE     Compound Type                                1
      MARKREF   Markush Reference Count                      1
      DED       Entry Date                                   1
      DUPD      Update Date                                  1
      CPD       Crystal Property Description                 1
      FINFO     Further Information                          3
      HFOR      Enthalpy of Formation                        1
      LB        Substance Label                              3
      OPT       Optics                                       1
      PHARM     Pharmacological Data                        36
      PSD       Patent Specific Data                         2
      USC       Use of Compound                             53
      UVS       UV and Visible Spectrum                      1
```

```
   This substance also occurs in Reaction Documents:

      Code      Name                                  Occurrence
      ========================================================
      RX        Reaction Documents                        29
      RX.RAN    Reactant AN                               17
      RX.PAN    Product AN                                12

Pharmacological Data:
PHARM
      Note(s) (.COM):    physiological behaviour discussed
      Reference(s):
      1. Camm, Kenneth D.; El-Sokkary, Ahmed; Gott, Andrew L.; Stockley,
         Peter G.; Belyaeva, Tamara; McGowan, Patrick C.,
         Dalton Transactions, CODEN: DTARAF, <2009>, 10914 - 10925
```

Search Example 3: Electrical Data

Superconducting substances which contain Barium, Yttrium and Copper with a special interest in the critical temperature of the superconductivity.

```
=> e superconduction transition/ele.kw
E1          613      PYROELECTRICITY/ELE.KW
E2          234      RELAXATION FREQUENCY/ELE.KW
E3            0 --> SUPERCONDUCTION TRANSITION/ELE.KW
E4        19136      SUPERCONDUCTIVE TRANSITION TEMPERATURE/ELE.KW
E5        19719      SUPERCONDUCTIVITY/ELE.KW
E6         4706      THERMOELECTRICITY/ELE.KW
****  END OF FIELD ****

=> s e4 and ba/els and cu/els and y/els
          19136 "SUPERCONDUCTIVE TRANSITION TEMPERATURE"/ELE.KW
          45333 BA/ELS
         188241 CU/ELS
          35512 Y/ELS
L19        3135 "SUPERCONDUCTIVE TRANSITION TEMPERATURE"/ELE.KW AND BA/ELS
AND CU/ELS AND Y/ELS

=> d


L19   ANSWER 1 OF 3135 REAXYSFILE COPYRIGHT 2012 Elsevier Properties SA. On
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      Accession Number (AN):              20989359
      Lin. Struct. Formula (LSF):         Y0.925Ca0.075Ba2Cu3O6.84
      Molec. Formula (MF):                Ba2 Ca0 Cu3 O6 Y0
      Formula Weight (FW):                659.978
      InChi Key: (INCHI):                 KVWLTSDMFCKXMK-UHFFFAOYSA-N
      Alternate InChi Key: (AINCHI):      KVWLTSDMFCKXMK-NNZOMFNKAM
      Markush Ref. Count (MARKREF):       0
      Entry Date (DED):                   2011/02/17
      Update Date (DUPD):                 2011/02/17

      No structure diagram available for this Document

   Field Availability:

      Code         Name                          Occurrence
      ================================================
      AN           Accession Number                     1
      LSF          Linearized Structure Formula         1
      MF           Molecular Formula                    1
      FW           Formula Weight                       1
      INCHI        InChi Key                            1
      AINCHI       Alternate InChi Key                  1
      MARKREF      Markush Reference Count              1
      DED          Entry Date                           1
      DUPD         Update Date                          1
      CRYPH        Crystal Phase                        1
      CSG          Crystal Space Group                  1
      ELE          Electrical Data (MCS)                2
```

```
   This substance also occurs in Reaction Documents:

     Code        Name                              Occurrence
     ================================================
     RX          Reaction Documents                         1
     RX.PAN      Product AN                                 1


Electrical Data:
   Crit.    |Keyword                     |Ref.
   Temp.    |                            |
   (.CRIT)  |(.KW)                       |
   ==========+============================+====
   -189.16  | Superconductive transition |1
            | temperature                |

Reference(s):
1. Sedky, A.; Abu-Ziad, Bander, Physica C: Superconductivity and its
   Applications (Amsterdam), CODEN: PHYCE6, 470, <2010>, 659 - 668
```

Search Example 4: Chemical Data

Iron-based substances as potential catalysts (EXPAND recommended for "all keywords" /AKW).

```
= > s fe/els and alloy/ctype and behaviour as catalyst/akw
         236377 FE/ELS
         129187 ALLOY/CTYPE
          56257 BEHAVIOUR AS CATALYST/AKW
L18         155 FE/ELS AND ALLOY/CTYPE AND BEHAVIOUR AS CATALYST/AKW

=> d


L18  ANSWER 1 OF 155 REAXYSFILE COPYRIGHT 2012 Elsevier Properties SA. On
     STN

     Accession Number (AN):           21085615
     Lin. Struct. Formula (LSF):     Cu65.5Fe34.5
     Molec. Formula (MF):             Cu65 Fe34
     Formula Weight (FW):             6088.98
     InChi Key: (INCHI):              URFQZDXFKHDAQB-UHFFFAOYSA-N
     Alternate InChi Key: (AINCHI):  URFQZDXFKHDAQB-UHFFFAOYAK
     Compound Type (CTYPE):           Alloy
     Markush Ref. Count (MARKREF):   0
     Entry Date (DED):                2011/02/27
     Update Date (DUPD):              2011/02/27

     No structure diagram available for this Document

   Field Availability:

     Code        Name                           Occurrence
     ================================================
     AN          Accession Number                        1
     LSF         Linearized Structure Formula            1
     MF          Molecular Formula                       1
     FW          Formula Weight                          1
     INCHI       InChi Key                               1
     AINCHI      Alternate InChi Key                     1
     CTYPE       Compound Type                           1
     MARKREF     Markush Reference Count                 1
     DED         Entry Date                              1
     DUPD        Update Date                             1
     FINFO       Further Information                     1

   This substance also occurs in Reaction Documents:

     Code        Name                           Occurrence
     ================================================
     RX          Reaction Documents                      1
     RX.PAN      Product AN                              1
```

```
Further Information:
FINFO
      Description (.KW):                Behaviour as catalyst
      Reference(s):
      1. Srivastava, Pratibha; Dubey, Reena; Kapoor, I. P. S.; Singh, G.,
      Indian Journal of Chemistry, Section A: Inorganic, Physical,
      theoretical & Analytical Chemistry, CODEN: ICACEC, 49, <2010>,
      1339 - 1344
```

Reactions

The role of a substance (reactant or product) can be defined in the search query.
Thus you can search for the following reaction types:

? => B "how do I make this type of compound" (Preparations)
A => ? "what do these starting materials give" (Reactions)
A => B general or specific transformations, reaction conditions, yields and more.

Search Example 5:

Reaction or preparation? How to restrict to preparations.
Find Fullerene type compounds of C70 or greater that have information on preparation.

```
=> s c/els and 1/elc and atc>69 and rx/fa
       15864973 RX/FA
                  (RX/FA.RX)
L4          128 C/ELS AND 1/ELC AND ATC>69 AND RX/FA

=> sel an
E129 THROUGH E256 ASSIGNED

=> s e129-256/rx.pan
L5          217 (10520367/RX.PAN…)

=> d rx


L5    ANSWER 1 OF 217 REAXYSFILE COPYRIGHT 2012 Elsevier Properties SA. On
      STN

Reaction:
RX
      Reaction ID:                        30107949
      Reactant AN (.RAN):                 21115974
      Reactant (.RCT):                    C70*2(mesitylene)
      Product AN (.PAN):                  6843004
      Product (.PRO):                     fullerene C70
      React. Struct. Keywords (.SKW):     nonmapped reaction
      Record type (.RTYP):                full reaction, has preparation
      Number of Bond Changes (.NBC):      0
      No. of React. Details (.NVAR):      1
      Preparation reactants (.BLB):       21115974, 6843004
      Det. React. reactants (.BLC):       21115974, 6843004
      No. of References (.NUMREF):        1

Reaction Details:
RX
      Reaction RID (.RID):                30107949.1
      Reaction Classification (.CL):      Preparation
      Solvent (.SOL):                     neat (no solvent)
      Number of R. steps (.STP):          1
      Reference(s):
      1. Park, Chibeom; Yoon, Eunjin; Kawano, Masaki; Joo, Taiha; Choi, Hee
         Cheul, Angewandte Chemie, International Edition, CODEN: ACIEF5, 49,
         <2010>, 9670 - 9675, Angewandte Chemie, CODEN: ANCEAD, 122, <2010>,
         9864 - 9869xx
```

For more information and further support please contact your STN Helpdesk.