Beilstein & Gmelin
MDL CrossFire V6/7

Search For:

- **Substances:** Use the Fact and/or Structure Editor.
- **Reactions:** Use the Fact and/or Structure Editor.
  - **? –> A** "how do I make this type of compound"
  - **A –> ?** "what do these starting materials give"
  - **A –> B** "general or specific transformations"
- **Properties:** Use the Fact Editor.
  Electrical, Magnetic, Optical, Physical, Reaction, Solubility, Spectral, Thermal, etc.
- **Citations:** Use the Fact Editor.
- **Text:** Search keywords across both databases simultaneously.

Fact Editor

- Predefined Search Forms for quick and simple searches by specific data fields.
- Double-click in table cells to view choice of field names, field values, and operators.
- Use ***** to expand chemical name segments: ***succinamid*** will retrieve:
  3-hydroxy-2-(4-phenylpiperidino)-5-succinamidotetralin
- Enter molecular formulae in Hill order: carbon, hydrogen, followed by all other elements in alphabetical order.
- Phrases are not searchable, search each phrase element separately.

Structure Editor

- Use the MDL CrossFire Structure Editor (under Options→Select Structure Editor).
- Specify attributes of atoms, bonds and molecules, including: charge, mass, valence, stereo formations, sub-structures, and Markush structures.
- In Reaction Editmode identify reaction roles, conserved atoms, bonds and reaction centers.
- Click on the Crossfire icon to send structure(s) to the Query Builder for searching. 
- Options box in the Query Builder allows further refinement of potential results (exact, free sites, stereochemistry, addl. rings, etc).
- Always use the Structure Editor Icon to return to the editor (V6). 
- Structures can be searched across both databases simultaneously.

Search Results

- Colored hyperlinks and white arrows move between related substance, reaction and citation records.
- Black arrows move between hits.
- Short Display view scans structures of multiple hits.
- Field Availability view displays selected fields.
- Use Hit Only view to see only fields specified in search.

Printing / Exporting

- Display only desired fields before printing (default prints everything).
- Export desired factual and structure information into ASCII, HTML, or modeling program formats.

Documentation – MIMAS Crossfire Service – www.mimas.ac.uk/crossfire/docs.html

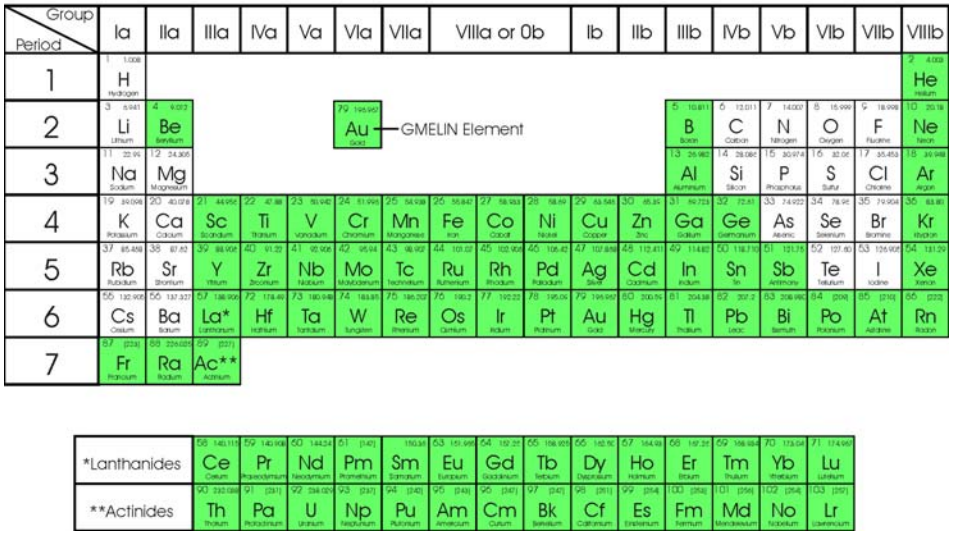
For further assistance with Beilstein Crossfire, please contact a reference librarian at the Physical Sciences Library (pslref@cornell.edu, 255-4016).

3/5/2007– L. R. Solla, Cornell University

MDL CrossFire V6/7 – Database Contents

Database	**Beilstein**	**Gmelin**
Sources	• Beilstein Handbook 1771 – 1959 • Primary literature 1960 – present from 175 journals	• Gmelin Handbook 1772 – 1975 • Primary literature 1975 – present from 62 journals
Scope	• 9.1 million compounds • 10 million reactions • 320 million experimental data facts in 425+ data fields	• 2.2 million compounds • 1.6 million reactions • 300+ million facts in 800+ data fields
Content	**organic compounds** • Substances which contain carbon **and** the non-shaded elements in the periodic table below (and including Boron). Excluding: • Substances which do not contain carbon. • Pure elements • CO, CS, CO2, CS2, COS, C3O2, C3S2 • Carbonic acid and its thio analogs along with their salts with inorganic cations • HCN, HOCN, HSCN and corresponding iso-acids together with all metal salts and complexes of these acids • Dicyanogene • Phosgene • Metal carbides • Metal salts of formic acid, acetic acid, and oxalic acid • Fullerenes, which consist only of carbon • Carboranes	**inorganic and organometallic compounds** • All compounds containing no carbon. • All compounds containing at least one "Gmelin Element" (shaded in the periodic table below). • Additionally: elemental carbon, phosgene, alloys, carbides and carbide oxides, carbonic acid and its thio- and seleno analogues, CO, CS, CO_2, CS_2, COS and multicomponent systems with a carbon component • Including: Coordination compounds Alloys Solid solutions Glasses and ceramics Polymers Minerals

Periodic System of the Elements



Adapted from MDL Crossfire Documentation