

# **Chemical Indexing**

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## **Chemical Indexing**

Chemical Indexing is a controlled indexing system intended to provide an effective means for the retrieval of information not normally searchable using key words alone. In this case the information referred to is the inorganic chemicals and material systems<sup>1</sup> discussed in the scientific and technical papers covered by Inspec.

Examples of Barriers to effective searching of chemical information in a database.

- Variation in formula An author can describe substances such as Gallium Aluminium Arsenide, which is used in solid-state physics, in several ways (e.g. GaAlAs, AlGaAs etc.). This variation makes it difficult to ensure comprehensive retrieval of relevant results if relying on keyword searching alone.
- Stoichiometric and Non-Stoichiometric formula Chemicals can be described using stoichiometric formula, where the proportions of each component is fixed (e.g. GaAlAs), or, particularly for semiconductors, non-stoichiometric formula, where the proportion of each component can be varied (e.g. Ga<sub>x</sub>Al<sub>1-x</sub>As or ((GaAs)<sub>0.5</sub>(AlAs)<sub>0.5</sub>)), formulae such as these are not searchable using keywords.
- Upper-case and lower-case characters Chemical symbols are a mixture of Upper and lower case characters. Search platforms commonly do not distinguish between these. They would see no difference between the chemical symbol for Cobalt (Co), and the chemical formula for Carbon Monoxide (CO).
- Ambiguity between chemical symbols and English words Chemical element symbols or molecular formulae can match
  common English words, abbreviations and acronyms. The
  molecular formula for Gallium phosphide is "GaP" which is the
  same as the word "gap". Likewise, the Chemical symbol for
  Beryllium is Be, which is the same as the English verb "to be". It
  is also indistinguishable from the abbreviations for Boltzman
  Equation (BE) and Beta-Emission line (BE).

By standardizing the way inorganic chemicals are represented, and by putting this into a separate field, searchability in Inspec is greatly enhanced. Users can search using chemical symbols, optionally with the inclusion of Roles, in the Chemical Indexing field to achieve a much more complete set of highly relevant results.

<sup>&</sup>lt;sup>1</sup> Some organic compounds, can be searched within the uncontrolled indexing field.

### **Chemical Indexing – Key Facts**

For Searching Inorganic Chemicals and material systems in Inspec that are important to the topics of discussion in a document.

Use Chemical symbols and formulae to search.

Use Roles to search with increased specificity.

Find information in documents published from 1987 to the present.

### **Chemical Indexing Roles**

Roles can be used to limit results to chemical elements, binary systems etc.

### **Table of Chemical Indexing Roles**

<b>Basic Roles</b>	<b>Abbreviation</b>	<b>Function Roles</b>	<b>Abbreviation</b>
Element	EL	Adsorbate	ADS
Binary System	BIN	Dopant	DOP
System of >2 components	SS	Interface System	INT
•		Surface/Substrate	SUR

### **Function Role Definitions**

Role	Example	Criteria
Adsorbate	CO/ads	Used for species being (ads)sorbed.
Dopant	Si:P (Si doped by P)	Used for systems into which an impurity is diffused and those in which the impurity is a probe.
Interface	InGaP-InAlP	Semiconductor junctions, devices, integrated circuits, electrochemical batteries, etc.
Surface	Fe/sur	Used for surface or substrate, e.g. oxidation, corrosion, wear of iron.

### **Indexing Example**

Au-LiNbO<sub>3</sub> (i.e. Gold metal interfaced with Lithium Niobium Oxide). would be indexed as follows:-

- The complete system with its role is e.g. Au-LiNbO3/int
- Substances or material subsystems with their roles e.g. LiNbO3/int Au/int LiNbO3/ss Au/el
- Chemical groups with their roles e.g. NbO3/int NbO3/ss
- Chemical elements with numbers (integers and decimals only) and their roles, e.g. O3/int O3/ss
- Chemical elements with their roles, e.g. Au/int Li/int Nb/int O/int

04788290 INSPEC Abstract Number: A91010684

Title: Linear and nonlinear SH surface acoustic waves

Controlled Indexing: crystal surface and interface vibrations; gold; lithium compounds; surface acoustic waves

**Uncontrolled Indexing:** nonlinear SH surface acoustic waves; linear shear horizontal surface acoustic waves; envelope dark solitons; superimposed linear elastic thermodynamical interface; nonlinear dispersion relation; transverse modal behavior; Au-LiNbO/sub 3/; LiNbO/sub 3/ By

#### **Chemical Indexing:**

Au-LiNbO3 int - LiNbO3 int - NbO3 int - Au int - Li int - Nb int - O3 int - O int - LiNbO3 ss -NbO3 ss - Li ss - Nb ss - O3 ss - O ss - Au el (Elements - 1,3,4) LiNbO3 sur - NbO3 sur - Li sur - Nb sur - O3 sur - O sur - LiNbO3 ss - NbO3 ss - Li ss - Nb ss - O3 ss - O ss (Elements - 3)

Figure 1: Sample Inspec Record - selected fields

By covering all permutations in the Inspec indexing the chances of finding relevant results are maximized for the user.

E.g. References to sulphuric acid (H<sub>2</sub>SO<sub>4</sub>) can be retrieved with any of the strategies below.:

- H<sub>2</sub>SO<sub>4</sub> Any system where H<sub>2</sub>SO<sub>4</sub> is a component
- SO<sub>4</sub> Any substance containing an SO<sub>4</sub> group
   H<sub>2</sub> Any substance containing the H<sub>2</sub>
- H, S and O Any substance containing H, S, and O

Some strategies are more specific to H2SO4 than others. E.G. searching SO4 would result in any compound containing a sulphate group being retrieved.

N.B. If a given system contains two elements, then it is a binary system even if one of the elements is only a very minor component like a dopant.

# Other Methods for Searching Chemical Information in Inspec

Controlled and uncontrolled can be useful for searching Chemical information. The controlled indexing field contains terms from the Inspec Thesaurus. The uncontrolled indexing field contains formulae rather than names of the substance, and uses the author's own terminology from the original document.

### **Inspec Thesaurus Terms<sup>2,3,4</sup>**

A thesaurus term exists for each element of the periodic table (e.g. HYDROGEN, GALLIUM, etc.).

Many terms exist for compounds (e.g. ALUMINIUM COMPOUNDS, MERCURY COMPOUNDS etc.)

Terms exist within hierarchies comprising Broader and narrower terms (e.g. ALKALI METAL COMPOUNDS, GALLIUM ARSENIDE, MIXED VALENCE COMPOUNDS, etc.)

N.B. Inspec indexers apply the most specific Thesaurus Terms they can from a hierarchy to a document. Searching a broader term such as ALKALI METALS will only retrieve records which contain general references to Alkali metals and not specific Alkali Metals such as Sodium. To retrieve records with references to all Alkali Metals it is necessary to search the Broader Terms in combination with the all of it's narrower terms.

Search ALKALI METALS to find results with general references to Alkali Metals

Search ALKALI METALS OR LITHIUM OR SODIUM OR POTASSIUM OR RUBIDIUM OR CAESIUM OR FRANCIUM to find results for all references to Alkali Metals

<sup>&</sup>lt;sup>2</sup> Several Inspec Vendor platforms allow thesaurus terms to be "exploded" i.e. for broader terms to be automatically searched along with its narrower terms. Consult the Inspec Thesaurus for appropriate search terms and to see whether a chosen Vendor offers the "explode" feature.

<sup>&</sup>lt;sup>3</sup> Inspec thesaurus terms can be used to search for chemical information back to 1969

<sup>&</sup>lt;sup>4</sup> Inspec Thesaurus Terms uses British English spelling and terminology. (e.g. search SULPHUR to retrieve results related to sulphur and sulfur, search ALUMINIUM to retrieve results related to aluminium and aluminum, etc.).

## **Inspec Chemical Indexing Search Guides**

## **Tables of Vendor Search Examples<sup>5</sup>**

Vendor Platform	Database File Name	Chemical Indexing Search Field	Chemical Indexing Roles	Search Examples
ProQuest Dialog	(1898 ->) (1969 ->)	CI	EL BIN SS ADS DOP INT SUR	Search a single component:  CI(BE - EL) CI(SI) – for the component in any role  Search multiple components within a multicomponent system:  CI("GA - SS" and "AL - SS" and "AS - SS")

<sup>&</sup>lt;sup>5</sup> Examples shown use advanced search mode on each Vendor platform

Vendor Platform	Database File Name	Chemical Indexing Search Field	Chemical Indexing Roles	Search Examples
EBSCOHost	Inspec	CI	/EL /BIN /SS /ADS /DOP /INT /SUR	Search a single component:  CI BE/EL CI SI - – for the component in any role  Search multiple components within a multicomponent system:  CI GA/SS N5 AL/SS N5 AS/SS  where N5 indicates within the same indexing field and with up to five words between terms in any order

Vendor Platform	Database File Name	Chemical Indexing Search Field	Chemical Indexing Roles	Search Examples
Elsevier Engineering Village	Inspec	WN CI	/EL /BIN /SS /ADS /DOP /INT /SUR	Search a single component:  BE/EL WN CI SI WN CI - for the component with any role  Search multiple components within a multicomponent system:  (GA/SS NEAR/2 AS/SS NEAR/2 AS/SS) WN CI  where NEAR/2 indicates within the same indexing sentence and up to 2 terms in between.  Note: Only available in Expert search.

Vendor Platform	Database File Name	Chemical Indexing Search Field	Chemical Indexing Roles	Search Examples
ProQuest Academic	Inspec	<in>CI</in>	/EL /BIN /SS /ADS /DOP /INT /SUR	Search a single component:  Be/EL <in>CI Si<in>CI – for the component with any role  Search multiple components within a multicomponent system:  (Ga/SS and AI/SS AND As)<in>SS</in></in></in>

Vendor Platform	Inspec File Name	Chemical Indexing Search Field		Search Examples
Clarivate Web of Science	Inspec	CH=	/EL /BIN /SS	Search a single component: CH=(Be/EL)
			/ADS /DOP /INT /SUR	for the component with any role: CH(SI)
				Search multiple components within a multicomponent system: CH=(GA/SS SAME AI/SS SAME AS/SS)

Vendor Platform	Database File Name	Chemical Indexing Search Field	Chemical Indexing Roles	Search Examples
Ovid SP	Inspec	.CH.	-EL -BIN -SS -ADS -DOP -INT -SUR	Search a single component:  BE-EL.CH.SI.CH. – for the component with any role  Search multiple components within a multicomponent system:  (GA-SS ADJX AL-SS ADJ10 AS-SS).CH.  where ADJ10 is a proximity operator indicating that search terms should be within X words of each other, in any order.  X can be any number (e.g. where X=5 the search terms could be within 5 words of each other in any direction

STN Inspec /CHI EL Search a single	Vendor Platform	Database File Name	Chemical Indexing Search Field	Chemical Indexing Roles	
SS  S BE EL/CHI  ADS S SI/CHI – for the component with any role.  Search multiple components within a multicomponent system:  S (AL SS(S)AL SS(S)AS SS)/CHI  where (S) is a proximity operator indicating that search terms should be within the same indexing sentence.  N.B.: Additional STN generated fields may be used, ELC for Element Count and ET for Element Count and ET for Element Terms. Use ELC to limit a search of, for example, 3 components to systems that only have 3 elements in total, i.e. 3/ELC. Use (L) to link CHI to ELC, e.g.	STN	Inspec	/CHI	BIN SS ADS DOP INT	component:  S BE EL/CHI S SI/CHI – for the component with any role.  Search multiple components within a multicomponent system:  S (AL SS(S)AL SS(S)AS SS)/CHI  where (S) is a proximity operator indicating that search terms should be within the same indexing sentence.  N.B.: Additional STN generated fields may be used, ELC for Element Count and ET for Element Terms. Use ELC to limit a search of, for example, 3 components to systems that only have 3 elements in total, i.e. 3/ELC. Use (L) to link CHI to ELC, e.g.  S (AL SS(S)GA SS(S)AS

### **Table of Chemical Elements and Their Symbols**

Element	Symbol	Element	Symbol	Element	Symbol
Actinium	Ac	hafnium*	Hf	praseodymium	Pr
Aluminium	Al	hahnium	На	promethium	Pm
Americium	Am	(now dubnium)	(now Db)	protactinium	Pa
Antimony	Sb	hassium	Hs	radium	Ra
Argon	Ar	Helium	He	radon	Rn
Arsenic	As	holmium*	Но	rhenium	Re
Astatine	At	hydrogen	Н	rhodium	Rh
Barium	Ва	see also		roentgenium	Rg
Berkelium	Bk	deuterium,		rubidium	Rb
Beryllium	Ве	tritium		ruthenium	Ru
Bohrium	Bh	indium*	In	rutherfordium	Rf
Bismuth	Bi	Iodine	I	samarium	Sm
Boron	В	Iridium	Ir	scandium*	Sc
Bromine	Br	Iron	Fe	seaborgium	Sg
Cadmium	Cd	krypton	Kr	selenium	Se
caesium*	Cs	lanthanum	La	silicon*	Si
Calcium	Ca	lawrencium	Lr	silver	Ag
californium*	Cf	lead*	Pb	sodium	Na
Carbon	С	Lithium	Li	strontium	Sr
Cerium	Ce	lutetium	Lu	sulphur	S
Chlorine	Cl	magnesium	Mg	tantalum	Та
Chromium	Cr	manganese	Mn	technetium	Tc
cobalt*	Со	meitnerium	Mt	tellurium	Te
Copper	Cu	mendelevium	Md	terbium	Tb
Curium	Cm	mercury	Hg	thallium	TI
deuterium	D	molybdenum	Мо	thorium	Th
see also		neodymium	Nd	thulium	Tm
hydrogen		Neon	Ne	tin*	Sn
Darmstadtium	Ds	neptunium*	Np	titanium	Ti
Dubnium	Db	nickel*	Ni	tritium	Т
Dysprosium	Dy	niobium*	Nb	see also	
Einsteinium	Es	nitrogen	N	hydrogen	
Erbium	Er	nobelium*	No	tungsten	W
Europium	Eu	osmium*	Os	uranium	U
Fermium	Fm	oxygen	0	vanadium	V
Fluorine	F	palladium	Pd	xenon	Xe

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<sup>&</sup>lt;sup>6</sup>Certain element symbols when searched with the binary role, give ambiguous results, e.g. the letters c and o in a binary system could be the element cobalt within a binary system, or the binary system carbon monoxide. To differentiate the binary system, it is good practice to search both the binary system whole and one of the elements within the binary system, e.g. search CO/BIN AND C/BIN which will retrieve records where a carbon binary system is indexed, that system being CO. Alternatively combine the Chemical Indexing search with a search of the appropriate Inspec Thesaurus Term, e.g. (CO/BIN), and the thesaurus term CARBON COMPOUNDS. Searches of binary and multicomponent systems using the element symbols indicated by \* in the table above need searching this way.

<sup>&</sup>lt;sup>7</sup> Where an element symbol or a molecular formula matches a database field label or search system proximity operator, it may be necessary to enclose the search in quotes. For example, on OCLC the title field label is TI. This is the same as the element symbol for titanium. On OCLC search it as CI: "TI" W El. See individual Vendor Inspec data sheets for details.

Francium	Fr	phosphorus	Р	ytterbium*	Yb
Gadolinium	Gd	platinum	Pt	yttrium	Υ
Gallium	Ga	plutonium	Pu	Zinc	Zn
Germanium	Ge	polonium*	Ро	zirconium	Zr
Gold	Au	potassium	K		

## **Table of Chemical Groups and Their Formulae**

<b>Chemical Group</b>	Chemical	<b>Chemical Group</b>	Chemical
Name	Group	Name	Group
	<b>Formula</b>		<b>Formula</b>
Alumina	Al2O3	iron garnet	Fe5O12
aluminium garnet	Al5O12	see also ferrite	
Arsenate	AsO4	Magnesite	MgO3
Arsenate	As2O3	Manganate	MnO4
Bismuthate	Bi2O3	Molybdate	MoO4
Borate	BO4	Niobite	NbO3
Borate	B2O3	Niobite	Nb2O5
Borate	B3O6	Niobite	Nb2O7
borate (per-)	BO3	Nitrate	NO3
Bromate	BrO3	Nitrite	NO2
Carbonate	CO3	phosphate (ortho-)	PO4
Carbonyl	CO	Phosphate	P2O5
chromate (di-)	Cr207	phosphate (pyro-)	P2O7
chromate (per-)	CrO3	Phosphite	PO3
/cyanide	CN	Phosphite	P4O12
Ferrite	Fe2O3	Selenite	SeO4
Ferrite	Fe2O4	Selenite	SeO3
Ferrite	Fe3O4	Silica	SiO2
ferrite (ortho)	FeO3	Silicate	SiO4
see also iron garnet		Sulphate	SO4
gallium garnet	Ga5O12	sulphate (thio-)	S2O3
garnet (aluminium)	Al5O12	Sulphite	SO3
garnet (gallium)	Ga5O12	Tantalite	TaO3
garnet (iron)	Fe5O12	Titanate	TiO3
Germanate	GeO2	Tungstate	WO3
Germanate	GeO3	Tungstate	WO4
Hydroxyl	OH	Vanadate	V2O5
hydroxyl (deuterated)	OD	vanadate (meta-)	VO3
Iodate	IO3	vanadate (ortho-)	VO4
		Zirconate	ZrO3

## **Table of Abbreviations and Their Corresponding Formulae**

<b>Abbreviation</b>	Formula	<b>Abbreviation</b>	Formula
ADP	NH4N2PO4	KSP	KSnOPO4
AG	Al5O12	KTP	KTiOPO4
BBO	BaB2O4	LMN	PbMgO3NbO3
BEL	La2Be2O5	NASI <i>or</i>	NaZrSiO4PO4
BPSG	B2O3-P2O5-SiO2	NASICON	
BSG	B2O3-SiO2	PLZT	PbLaZrO3TiO3
BSN	NaBaNb2O6	PMN	PbMgO3NbO3
BSO	Bi12SiO20	PSG	P2O5-SiO2
DKDP	KD2PO4	PZT	PbZrO3TiO3
GG	Ga5O12	SBN	SrBaNb2O6
IG	Fe5O12	YAP	YAIO3
ITO	InSnO	YLF	LiYF4
KDP	KH2PO4	ZBLAN	ZrF4-BaF2-LaF3-
			AlF3-NaF
KNSBN	KNaSrBaNb2O6	ZBLANP	ZrF4-BaF2-LaF3-
			AIF3-NaF-PbF2