

# A Shared Semantic Vocabulary as a Path Forward for Harmonized Inventory Data

Content by many people, presented by C. Mutel



DÉPART  
DE SENTIER



Sentier  
.dev

CAULDRON 

# A Shared *Taxonomy*

## Current Practice\*

- chromium steel pipe
- reinforcing steel
- silencer, steel, DN 125
- silencer, steel, DN 315, 50 mm
- spiral-seam duct, steel, DN 125
- spiral-seam duct, steel, DN 400
- steel, chromium steel 18/8
- steel, chromium steel 18/8, hot rolled
- steel, low-alloyed
- steel, low-alloyed, hot rolled
- steel, unalloyed
- tin plated chromium steel sheet, 2 mm
- ventilation duct, steel, 100x50 mm

\* Exclude processes  
(drawing, rolling, etc.) and  
waste

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## Combined Nomenclature

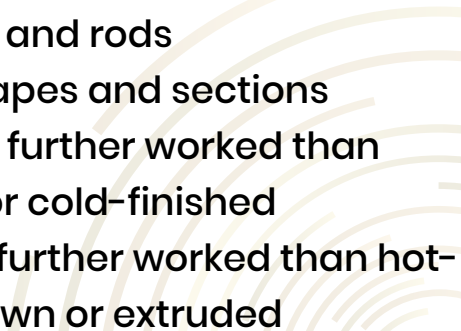
- 7218 Stainless steel in ingots or other primary forms; semi-finished products of stainless steel
- 7219 Flat-rolled products of stainless steel, of a width of 600 mm or more
- 7220 Flat-rolled products of stainless steel, of a width of less than 600 mm
- 7221 Bars and rods, hot-rolled, in irregularly wound coils, of stainless steel
- 7222 Other bars and rods of stainless steel; angles, shapes and sections of stainless steel
- 7223 Wire of stainless steel

\* Exclude processes (drawing, rolling, etc.) and waste



# A Shared *Taxonomy*

## Combined Nomenclature

- 7222 Other bars and rods of stainless steel; angles, shapes and sections of stainless steel
    - 7222 11 Bars and rods, not further worked than hot-rolled, hot-drawn or extruded
    - 7222 20 Bars and rods, not further worked than cold-formed or cold-finished
    - 7222 30 Other bars and rods
    - 7222 40 Angles, shapes and sections
      - 7222 40 50 Not further worked than cold-formed or cold-finished
      - 7222 40 10 Not further worked than hot-rolled, hot-drawn or extruded
- 



# A Shared *Taxonomy*

## Combined Nomenclature

- 7222 Annan stång av rostfritt stål; profiler av rostfritt stål
  - 7222 11 Stång, varmvalsad, varmdragen eller strängpressad men inte vidare bearbetad
  - 7222 20 Stång, tillformad eller färdigbehandlad i kallt tillstånd men inte vidare bearbetad
  - 7222 30 Annan stång
  - 7222 40 Profiler
    - 7222 40 50 Tillformade eller färdigbehandlade i kallt tillstånd men inte vidare bearbetade
- 7222 Other bars and rods of stainless steel; angles, shapes and sections of stainless steel
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# A Shared *Taxonomy*

## Combined Nomenclature

Supplier



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Consumer



- 7222 40 50 Not further worked than cold-formed or cold-finished
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# A Shared Taxonomy

```
1 @prefix skos: <http://www.w3.org/2004/02/skos/core#> .
2 @prefix dc11: <http://purl.org/dc/elements/1.1/> .
3
4 <http://data.europa.eu/xsp/cn2024/721800000010>
5   a skos:Concept ;
6   skos:prefLabel "III. STAINLESS STEEL"@en, "III. ROSTFRITT STÅL"@sv ;
7   skos:inScheme <http://data.europa.eu/xsp/cn2024/cn2024> ;
8   dc11:identifier "721800000010" ;
9   skos:closeMatch <https://glossary.ecoinvent.org/intermediate-exchanges/steel-chromium-steel-18-per-8/> .
```

We can embed links to existing systems with semantically meaningful relationships into the base set of terms.



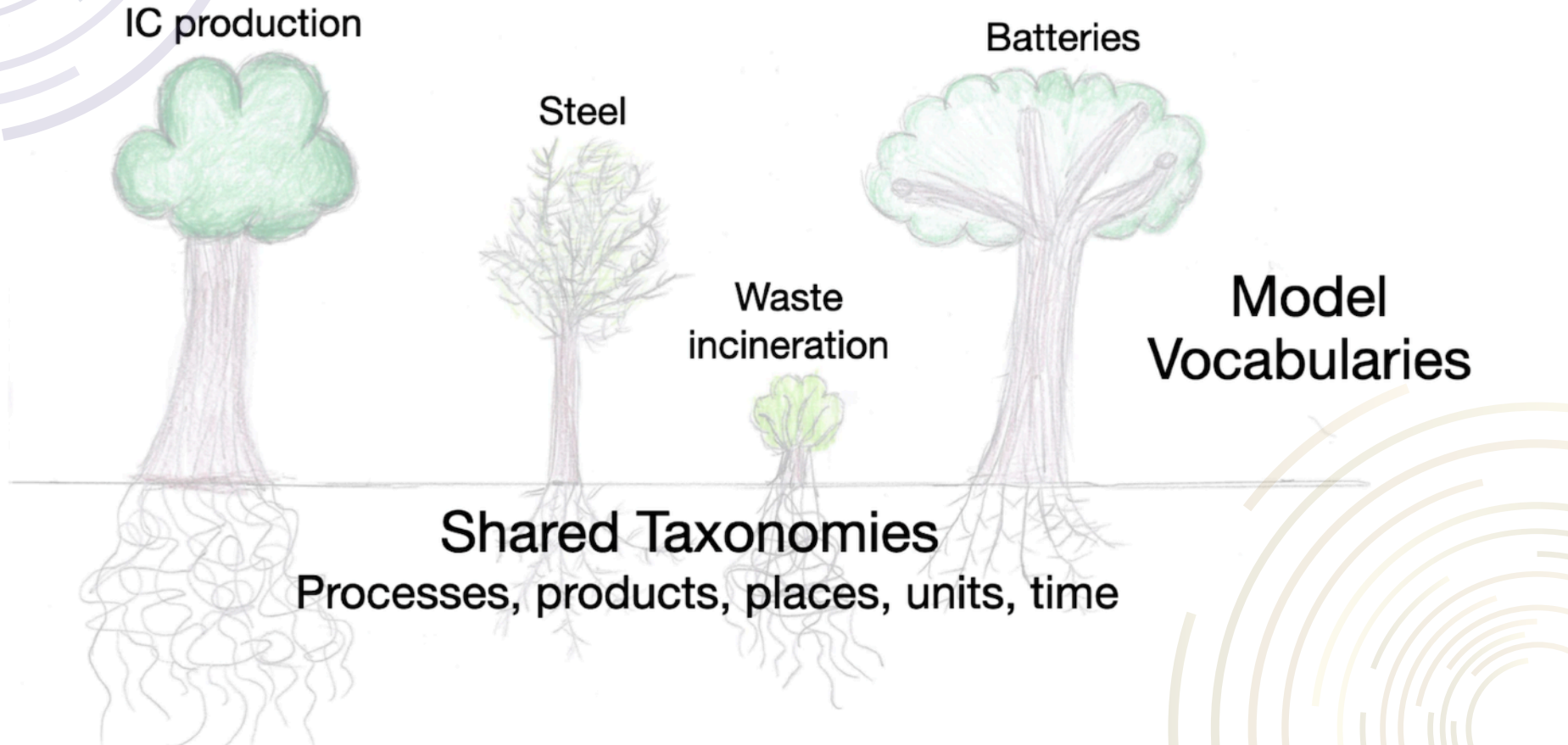
# A Shared Taxonomy

```
1 @prefix skos: <http://www.w3.org/2004/02/skos/core#> .
2 @prefix dc11: <http://purl.org/dc/elements/1.1/> .
3
4 <http://data.europa.eu/xsp/cn2024/721800000010>
5   a skos:Concept ;
6   skos:prefLabel "III. STAINLESS STEEL"@en, "III. ROSTFRITT STÅL"@sv ;
7   skos:inScheme <http://data.europa.eu/xsp/cn2024/cn2024> ;
8   dc11:identifier "721800000010" ;
9   skos:closeMatch <https://glossary.ecoinvent.org/intermediate-exchange> .
```

- exactMatch
- closeMatch
- relatedMatch
- broadMatch
- narrowMatch

We can embed links to existing systems with semantically meaningful relationships into the base set of terms.

# *An Extendible Taxonomy*



```
[1]: from sentier_data_tools import UnitIRI, ProductIRI, get_conversion_factor
```

```
[4]: UnitIRI("https://vocab.sentier.dev/units/unit/KiloGM").narrower()[15]
```

08:36:49 [info] Retrieved 53 triples from <https://fuseki.d-d-s.ch/skosmos/query>

```
[4]: [<https://vocab.sentier.dev/units/unit/AMU>: Atomic mass unit (unit),  
<https://vocab.sentier.dev/units/unit/CARAT>: Carat (unit),  
<https://vocab.sentier.dev/units/unit/CWT_LONG>: Long Hundred Weight (unit),  
<https://vocab.sentier.dev/units/unit/CWT_SHORT>: Hundred Weight - Short (unit),  
<https://vocab.sentier.dev/units/unit/CentiGM>: Centigram (unit),  
<https://vocab.sentier.dev/units/unit/DRAM_UK>: Dram (UK) (unit),  
<https://vocab.sentier.dev/units/unit/DRAM_US>: Dram (US) (unit),  
<https://vocab.sentier.dev/units/unit/DWT>: Penny Weight (unit),  
<https://vocab.sentier.dev/units/unit/DecaGM>: Decagram (unit),  
<https://vocab.sentier.dev/units/unit/DeciGM>: Decigram (unit),  
<https://vocab.sentier.dev/units/unit/DeciTONNE>: DeciTonne (unit),  
<https://vocab.sentier.dev/units/unit/DeciTON_Metric>: Metric DeciTON (unit),  
<https://vocab.sentier.dev/units/unit/EarthMass>: Earth mass (unit),  
<https://vocab.sentier.dev/units/unit/FemtoGM>: FemtoGram (unit),  
<https://vocab.sentier.dev/units/unit/GM>: Gram (unit)]
```

```
[3]: get_conversion_factor(  
    "https://vocab.sentier.dev/units/unit/KiloGM",  
    "https://vocab.sentier.dev/units/unit/EarthMass"  
)
```

```
[3]: 1.6744276387723765e-25
```

```
[1]: from sentier_data_tools import ProductIRI
```

```
[2]: ProductIRI("http://data.europa.eu/xsp/cn2024/721900000080").narrower()
```

08:40:26 [info] Retrieved 37 triples from <https://fuseki.d-d-s.ch/skosmos/query>

```
[2]: [<http://data.europa.eu/xsp/cn2024/721990000080>: Other (product),  
<http://data.europa.eu/xsp/cn2024/721911000010>: Not further worked than hot-rolled, in coils (product),  
<http://data.europa.eu/xsp/cn2024/721921000010>: Not further worked than hot-rolled, not in coils (product),  
<http://data.europa.eu/xsp/cn2024/721931000010>: Not further worked than cold-rolled (cold-reduced) (product),  
<http://data.europa.eu/xsp/cn2024/721990200080>: Perforated (product),  
<http://data.europa.eu/xsp/cn2024/721990800080>: Other (product),  
<http://data.europa.eu/xsp/cn2024/721911000080>: Of a thickness exceeding 10 mm (product),  
<http://data.europa.eu/xsp/cn2024/721912000080>: Of a thickness of 4,75 mm or more but not exceeding 10 mm (product),  
<http://data.europa.eu/xsp/cn2024/721913000080>: Of a thickness of 3 mm or more but less than 4,75 mm (product),  
<http://data.europa.eu/xsp/cn2024/721914000080>: Of a thickness of less than 3 mm (product),  
<http://data.europa.eu/xsp/cn2024/721923000080>: Of a thickness of 3 mm or more but less than 4,75 mm (product),  
<http://data.europa.eu/xsp/cn2024/721924000080>: Of a thickness of less than 3 mm (product),  
<http://data.europa.eu/xsp/cn2024/721921000080>: Of a thickness exceeding 10 mm (product),  
<http://data.europa.eu/xsp/cn2024/721922000080>: Of a thickness of 4,75 mm or more but not exceeding 10 mm (product),  
<http://data.europa.eu/xsp/cn2024/721931000080>: Of a thickness of 4,75 mm or more (product),  
<http://data.europa.eu/xsp/cn2024/721932000080>: Of a thickness of 3 mm or more but less than 4,75 mm (product),  
<http://data.europa.eu/xsp/cn2024/721933000080>: Of a thickness exceeding 1 mm but less than 3 mm (product),  
<http://data.europa.eu/xsp/cn2024/721934000080>: Of a thickness of 0,5 mm or more but not exceeding 1 mm (product),  
<http://data.europa.eu/xsp/cn2024/721935000080>: Of a thickness of less than 0,5 mm (product),  
<http://data.europa.eu/xsp/cn2024/721912100080>: Containing by weight 2,5 % or more of nickel (product),  
<http://data.europa.eu/xsp/cn2024/721912900080>: Containing by weight less than 2,5 % of nickel (product),  
<http://data.europa.eu/xsp/cn2024/721913100080>: Containing by weight 2,5 % or more of nickel (product),  
<http://data.europa.eu/xsp/cn2024/721913900080>: Containing by weight less than 2,5 % of nickel (product),  
<http://data.europa.eu/xsp/cn2024/721914100080>: Containing by weight 2,5 % or more of nickel (product),  
<http://data.europa.eu/xsp/cn2024/721914900080>: Containing by weight less than 2,5 % of nickel (product),  
<http://data.europa.eu/xsp/cn2024/721921100080>: Containing by weight 2,5 % or more of nickel (product),
```

## Stainless steel grades listed in the international standard ISO 15510:2010

Comparative designations of grades with similar composition from other important standards.

(listed by type of steel structure and by increasing intermediate 3-digits code of the ISO name)



Type	ISO-Name (1)	ISO Designation	EN	UNS	AISI	JIS	GB(国标)
M	4119-410-92-C	X13CrMo13	1.4119()			SUS410J1	S45710
M	4024-410-09-E	X15Cr13	1.4024			SUS410	
M	4006-410-00-I	X12Cr13	1.4006	S41000	410	SUS410	S41010
M	4415-415-92-E	X2CrNiMoV13-5-2	1.4415				
M	4313-415-00-I	X3CrNiMo13-4	1.4313	S41500		SUSF6NM	S41595
M	4642-416-72-J	X13CrPb13	1.4642()			SUS410F2	
M	4005-416-00-I	X12CrS13	1.4005	S41600	416	SUS416	S41617
M	4038-420-00-I	X52Cr13	1.4038()	S42000			
M	4039-420-09-I	X60Cr13	1.4039()				
M	4419-420-97-E	X38CrMo14	1.4419				S35830
M	4110-420-69-E	X55CrMo14	1.4110				
M	4116-420-77-E	X50CrMoV15	1.4116				
M	4035-420-74-E	X46CrS13	1.4035				
M	4034-420-00-I	X46Cr13	1.4034	S42000			S42040
M	4643-420-72-J	X33CrPb13	1.4643()			SUS420F2	
M	4029-420-20-I	X33CrS13	1.4029	S42020	420F	SUS420F	S42037
M	4031-420-00-I	X39Cr13	1.4031	S42000	420		S42040
M	4028-420-00-I	X30Cr1 3	1.4028	S42000	420	SUS420J2	S42030
M	4021-420-00-I	X20Cr13	1.4021	S42000	420	SUS420J1	S42020
M	4923-422-77-E	X22CrMoNiV12-1	1.4923				
M	4929-422-00-I	X23CrMoWMnNiV12-1-1	1.4929()	S42200	422	SUH616	S47220
M	4058-429-99-J	X33Cr16	1.4058()			SUS429J1	
M	4019-430-20-I	X14CrS17	1.4019,1.4104	S43020	430F		S11717
M	4418-431-77-E	X4CrNiMo16-5-1	1.4418				
M	4123-431-77-E	X40CrMoVN16-2	1.4123				
M	4057-431-00-X	X17CrNi16-2	1.4057	S43100	431	SUS431	S43120





# Elementary Flows

- Name
- Synonyms
- Reference unit
- CAS Number
- *Properties*

# Ni<sup>2+</sup>

	ILCD	Ecoinvent 3.8	Ecoinvent 3.10	FedEFL
Name	nickel (ii)	Nickel, ion	Nickel II	Nickel(II)
Synonyms		Ni+2	Ni+2, Nickel, Nickel ion, Nickel (+2)	Ni++
Reference Unit	kg	kg	kg	kg
CAS Number	14701-22-5	014701-22-5	014701-22-5	14701-22-5
Properties		Water mass, carbon content, wet mass, dry mass	Elemental content, water mass, carbon content, wet mass, dry mass	Broken link to CompTox Chemicals Dashboard



Main

ChEBI Ontology

Automatic Xrefs

Reactions

Pathways

Models



ChEBI Name	<b>nickel(2+)</b>
ChEBI ID	<b>CHEBI:49786</b>
Definition	A nickel cation in which the nickel carries a double positive charge.
Stars	☆☆☆ This entity has been manually annotated by the ChEBI Team
Secondary ChEBI IDs	CHEBI:49785, CHEBI:25517
Supplier Information	No supplier information found for this compound.
Download	<a href="#">Molfile</a> <a href="#">XML</a> <a href="#">SDF</a>

- [Find compounds which contain this structure](#)
- [Find compounds which resemble this structure](#)
- [Take structure to the Advanced Search](#)

Formula	Ni
Net Charge	+2
Average Mass	58.69340
Monoisotopic Mass	57.93424
InChI	InChI=1S/Ni/q+2
InChIKey	VEQPNABPJHWN SG-UHFFFAOYSA-N
SMILES	[Ni++]

- Data quality indicator
- Formula
- Net charge
- Average Mass
- Monoisotopic Mass
- InChi
- InChiKey
- SMILES





# ChEBI

## IUPAC Names i

nickel(II) cation

nickel(2+)

nickel(2+) ion

## Synonyms i

Ni2+

Ni<sup>2+</sup>

Ni<sup>2+</sup>

NICKEL (II) ION

Nickel, ion (Ni2+)

nickelous ion

## Registry Numbers i

[14701-22-5](#)

6859

- Synonyms
  - KEGG
  - IUPAC
  - UniProt
  - ChemIDplus
  - ChEBI
- Registry numbers
  - CAS
  - Gmelin

## Sources

KEGG COMPOUND

IUPAC

[UniProt](#)

PDBeChem

ChemIDplus

ChEBI

## Sources

ChemIDplus

Gmelin



## Roles Classification

### cofactor

An organic molecule or ion (usually a metal ion) that is required by an enzyme for its activity. It may be attached to the enzyme by a covalent bond or by a non-covalent interaction (via [nickel cation](#) )

### Biological Role(s):

#### allergen

A chemical compound, or part thereof, which causes the onset of an allergic reaction by interacting with any of the immune system components (via [metal cation allergen](#) )

[View more via ChEBI Ontology](#)

## ChEBI Ontology

### Outgoing

nickel(2+) ([CHEBI:49786](#)) **has role** cofactor ([CHEBI:23357](#))  
nickel(2+) ([CHEBI:49786](#)) **is a** divalent metal cation ([CHEBI:60240](#))  
nickel(2+) ([CHEBI:49786](#)) **is a** metal cation allergen ([CHEBI:88186](#))  
nickel(2+) ([CHEBI:49786](#)) **is a** monoatomic dication ([CHEBI:30412](#))  
nickel(2+) ([CHEBI:49786](#)) **is a** nickel cation ([CHEBI:25516](#))


### Incoming

ammonium nickel sulfate ([CHEBI:86151](#)) **has part** nickel(2+) ([CHEBI:49786](#))  
nickel sulfate ([CHEBI:53001](#)) **has part** nickel(2+) ([CHEBI:49786](#))

- Biological roles
- Cofactor roles
- Allergen roles
- Chemical relationships
- Nickel 2+ is a part of compounds



# ChEBI Linked Data

- Nickel 2+ is a Nickel cation
  - Nickel cation is a nickel ion
  - Nickel cation is a Transition element cation
  - Nickel ion is an Inorganic ion
  - Nickel 1+ is a Nickel cation
  - Nickel 3+ is a Nickel cation
  - etc.
- 

Call to  
action

<https://better.d-d-s.ch>





DdS Hackathon  
June 2024

Thanks to many, many  
people!



Spring School  
May 2024



Eaternity workshop  
April 2024

Brightcon 2024  
Hackathon



Autumn School  
October 2024



cauldron.ch