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The Pauling File, Binaries Edition

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Abstract

The Pauling File project was launched in 1995 with the aim to create tools for scientists working with inorganic compounds, with particular focus on materials design. As a first step, a comprehensive, phase-oriented database is being built up. It groups four categories of data under the retrieval software: constitution data, crystal structure data, powder diffraction data, and a broad range of physical properties. The project will cover all binary, ternary and multinary, non-organic compounds (no C–H bonds), but the first edition is limited to binary compounds.

Keywords: Pauling File; Database; Inorganic compounds; Crystal structure; Phase diagram; Physical properties

1. Introduction

One of the most challenging tasks in material science is the design of new materials with distinct properties. In general, two different approaches are explored:

1. The first one is to simulate the motion of the atoms in the material, as well as their electronic interactions, as close to reality as possible by using calculations on the quantum-mechanical level. This is an extremely demanding task, especially if the calculation of the property under investigation requires a long-time simulation. However, at least in theory, there is no input other than the laws of quantum mechanics, so using these calculations, the material properties can be understood right away from *first principle*s. Based on this understanding it should be possible to design new materials with distinct properties by computer simulations.
2. The second approach seems to be less challenging at first glance, since it does not ask for the really fundamental principles, but remains on a more pragmatic level. Most of our current knowledge in chemistry and materials science has been collected *empirically*, by searching for patterns and rules in experimental results. During the past 100 years, a huge pile of various types of data like crystal structures, powder diffraction patterns, phase diagrams, and physical properties has been collected for a large variety of compounds. Some of this information is also available in databases. Besides the classical use of databases for analysis, phase identification and teaching purposes, it is worthwhile to use modern computer technology to search for additional rules and correlations in the data and apply them in materials design.

Both approaches have their advantages and problems. While the first one does (at least in principle) not rely on experiments and should result in a deep understanding of fundamental correlations in solids, it is computationally extremely demanding and can currently only be applied to a limited number of rather simple structures. The second approach needs far less computational effort and may thus (at least in the beginning) lead to faster success; however, it is extremely dependent on the availability of a sufficiently large number of experimental data of appropriate quality. An additional problem concerning this second, empirical approach is that, up to now, data have been stored in numerous, relatively small, separate databases, each using its own proprietary retrieval software. This made the investigations

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rather tedious and prohibited the user from performing an overall data analysis in order to discover hidden patterns and correlations. These shortcomings of the empirical approach provided the basic motivation for the initiation of the Pauling File project, which started in 1995 as a collaboration between Japan Science and Technology Corporation (JST), Materials Phases Data System (MPDS), and The University of Tokyo. The project includes three steps:

1. The first goal is to create and maintain a comprehensive materials database for all non-organic (no C–H bonds) solid-state phases, covering phase diagrams, crystallographic data, diffraction patterns, and physical properties. An important aspect, along with completeness, is the quality of the data. The data need to be checked with extreme care, since errors will at least confuse the correlation tools, if not result in the derivation of wrong rules.

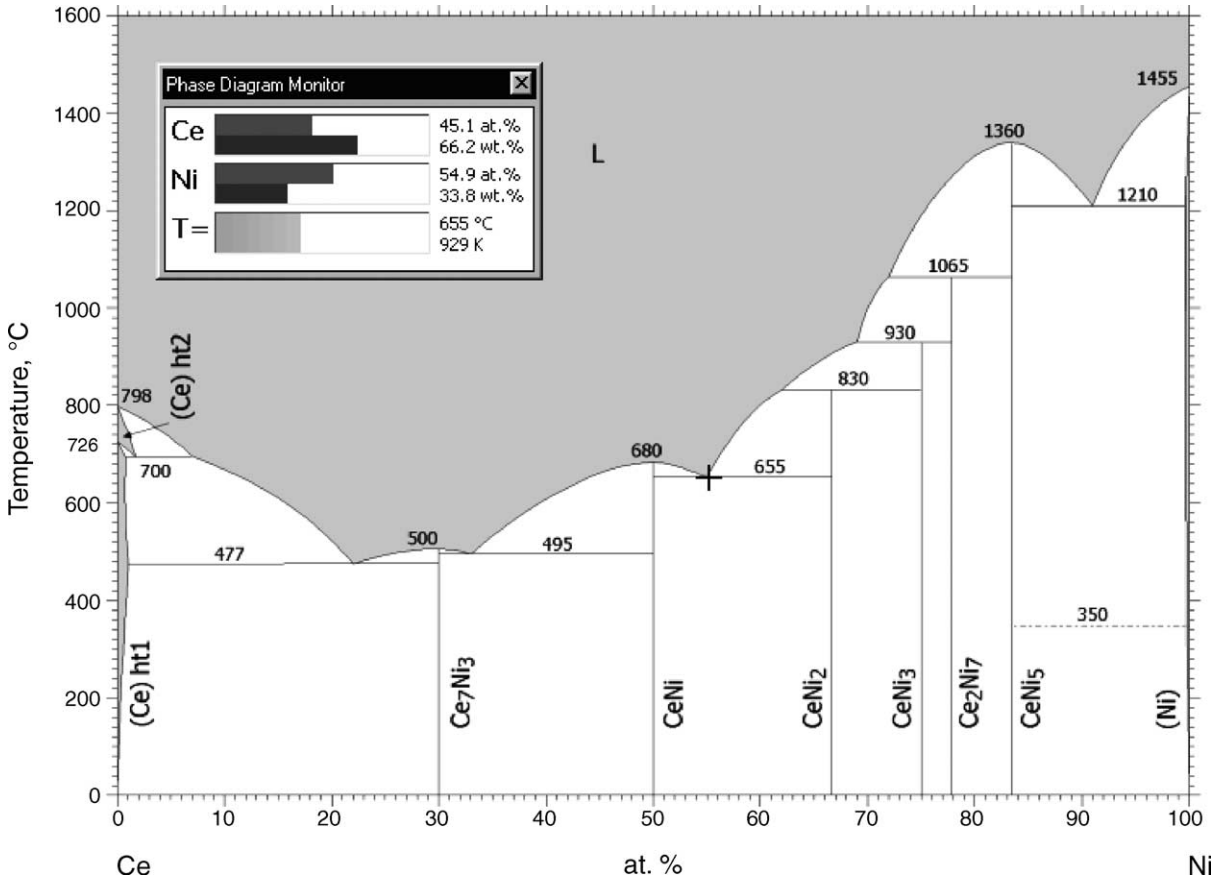


Fig. 1. One of the phase diagrams proposed for the Ce–Ni system in the Pauling File. The monitor indicates the current position of the cursor in composition and temperature.

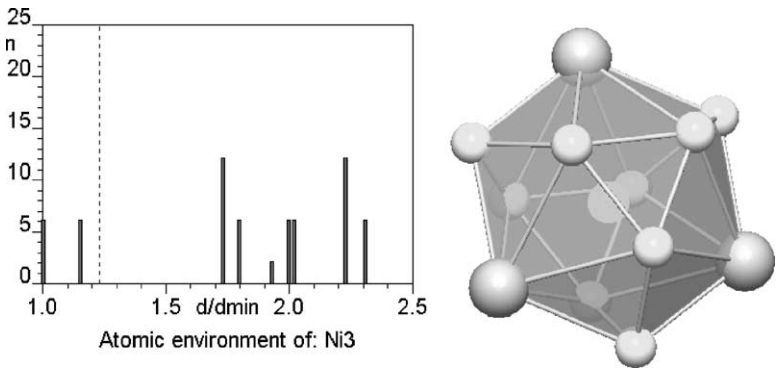


Fig. 2. Histogram of interatomic distances and coordination polyhedron around one of the Ni sites in $CeNi_3$.

2. In parallel to the database creation, appropriate retrieval software is developed, which makes the four different groups of materials data mentioned above accessible by a single user interface.
3. In the longer term, new materials design tools will be created, which will more or less automatically search the database for correlations needed for a purposeful and rapid design of new materials with pre-defined properties.

2. Binaries Edition

The first off-line Pauling File version is called "Binaries Edition" [1] and, as the name already suggests, it is limited to binary compounds. It contains 8000 phase diagrams (with updated phase assignment) covering 2300 binary systems, 28,300 structural data sets (including atom coordinates and displacement parameters, when determined) for more than 10,000 different phases, roughly 3000 experimental and 27,000 calculated diffraction patterns (interplanar spacings, intensities, Miller indices), and around 17,300 physical-property entries (with about 43,100 numerical values and about 10,000 figure descriptions) for some 5000 phases. To reach this result, 21,000 original publications were critically analyzed and processed. Whereas the coverage for crystal structures, diffraction data, and phase diagrams can be considered as satisfactory, it is just the beginning for property data. Nevertheless, the data contained on the CD already equals over 30,000 printed pages, i.e. a 20 volume handbook. In the future, these numbers will increase rapidly when the full (multinary) version of the database will become available as a yearly release in 2007.

Below are given some additional features that distinguish the Pauling File data from other databases and make it particularly valuable.

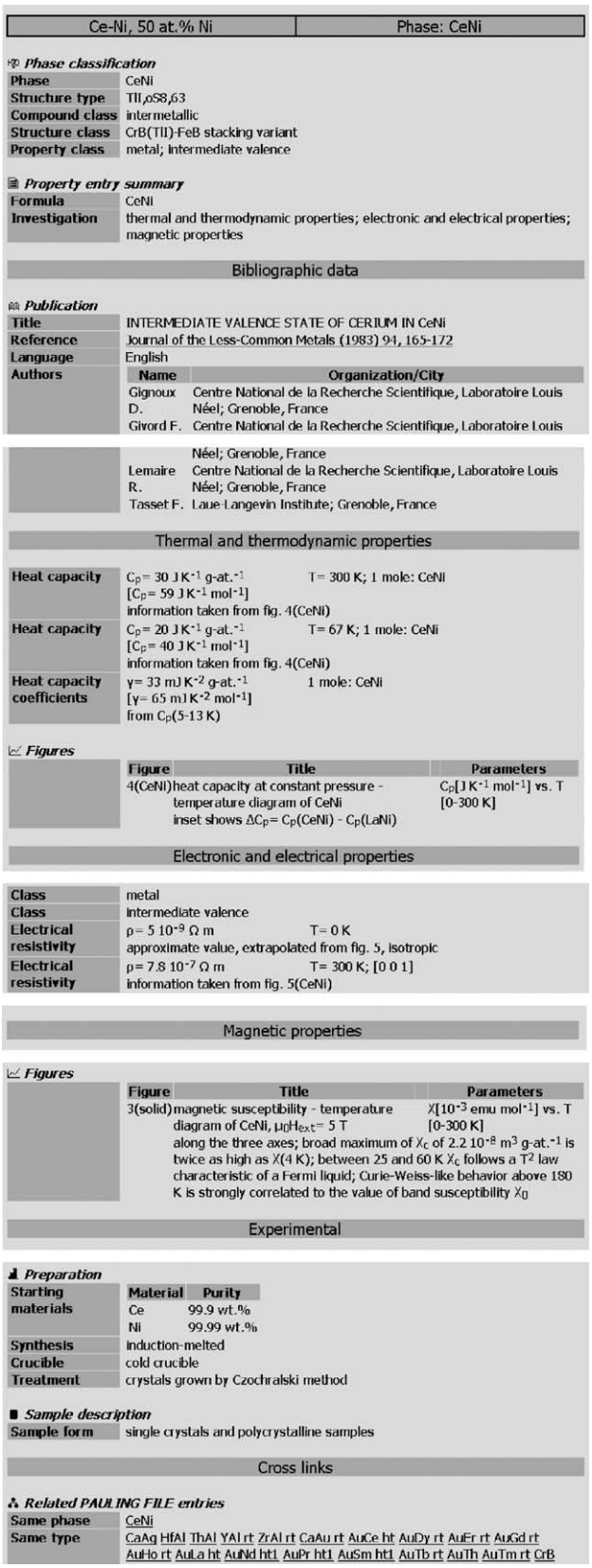
2.1. Distinct phases concept

An individual structure or property entry contains data reported for a particular phase in a given literature reference. A *phase* in the Pauling File is defined by the chemical system and the crystal structure and has been given a unique name by the combination of its chemical formula and modification.

The linkage of the four different groups of data was considered most important, therefore the Pauling File was designed as a phase-oriented materials database using a fully relational database system. This was achieved by the creation of a *distinct phases* table as well as all required internal links. In practice this means that each chemical system has been evaluated and the distinct phases identified based on all information available on phase diagrams, crystal structures, etc. Finally, every entry has been linked to such a distinct phase.

2.2. Constitution data

The 8000 phase diagrams contained in the constitution part of the Pauling File include APDIC diagrams and cal-



Ce-Ni, 50 at.% Ni | Phase: CeNi

Phase classification

Phase	CeNi
Structure type	TII,oS8,63
Compound class	intermetallic
Structure class	CrB(TII)-FeB stacking variant
Property class	metal; intermediate valence

Property entry summary

Formula	CeNi
Investigation	thermal and thermodynamic properties; electronic and electrical properties; magnetic properties

Bibliographic data

Publication

Title	INTERMEDIATE VALENCE STATE OF CERIUM IN CeNi
Reference	Journal of the Less-Common Metals (1983) 94, 165-172
Language	English

Authors	Name	Organization/City
	Gignoux D.	Centre National de la Recherche Scientifique, Laboratoire Louis Néel; Grenoble, France
	Givord F.	Centre National de la Recherche Scientifique, Laboratoire Louis Néel; Grenoble, France
	Lemaire R.	Centre National de la Recherche Scientifique, Laboratoire Louis Néel; Grenoble, France
	Tasset F.	Laue-Langevin Institute; Grenoble, France

Thermal and thermodynamic properties

Heat capacity	C_p= 30 J K^{-1} g-at.$^{-1}$ [C_p= 59 J K^{-1} mol^{-1}] information taken from fig. 4(CeNi)	T= 300 K; 1 mole: CeNi
Heat capacity	C_p= 20 J K^{-1} g-at.$^{-1}$ [C_p= 40 J K^{-1} mol^{-1}] information taken from fig. 4(CeNi)	T= 67 K; 1 mole: CeNi
Heat capacity coefficients	γ= 33 mJ K^{-2} g-at.$^{-1}$ [γ= 65 mJ K^{-2} mol^{-1}] from C_p(5-13 K)	1 mole: CeNi

Figures

Figure	Title	Parameters
4(CeNi)	heat capacity at constant pressure - temperature diagram of CeNi inset shows $\Delta C_p = C_p$(CeNi) - C_p(LaNi)	C_p[J K^{-1} mol^{-1}] vs. T [0-300 K]

Electronic and electrical properties

Class	metal
Class	intermediate valence
Electrical resistivity	ρ= 5 10^{-9} Ω m; T= 0 K; approximate value, extrapolated from fig. 5, isotropic
Electrical resistivity	ρ= 7.8 10^{-7} Ω m; T= 300 K; [0 0 1]; information taken from fig. 5(CeNi)

Magnetic properties

Figures

Figure	Title	Parameters
3(solid)	magnetic susceptibility - temperature diagram of CeNi, $\mu_0 H_{ext}$= 5 T; along the three axes; broad maximum of χ_c of 2.2 10^{-8} m^3 g-at.$^{-1}$ is twice as high as χ(4 K); between 25 and 60 K χ_c follows a T^2 law characteristic of a Fermi liquid; Curie-Weiss-like behavior above 180 K is strongly correlated to the value of band susceptibility χ_0	χ[10^{-3} emu mol^{-1}] vs. T [0-300 K]

Experimental

Preparation

Starting materials	Ce	99.9 wt.%
	Ni	99.99 wt.%
Synthesis	induction-melted	
Crucible	cold crucible	
Treatment	crystals grown by Czochralski method	

Sample description

Sample form	single crystals and polycrystalline samples

Cross links

Related PAULING FILE entries

Same phase	CeNi
Same type	CaAg HfAl ThAl YAl rt ZrAl rt CaAu rt AuCe ht AuDy rt AuEr rt AuGd rt AuHo rt AuLa ht AuNd ht1 AuPr ht1 AuSm ht1 AuTb rt AuTh AuTm rt CrB

Fig. 3. Extract from a Pauling File property data sheet for the phase CeNi.

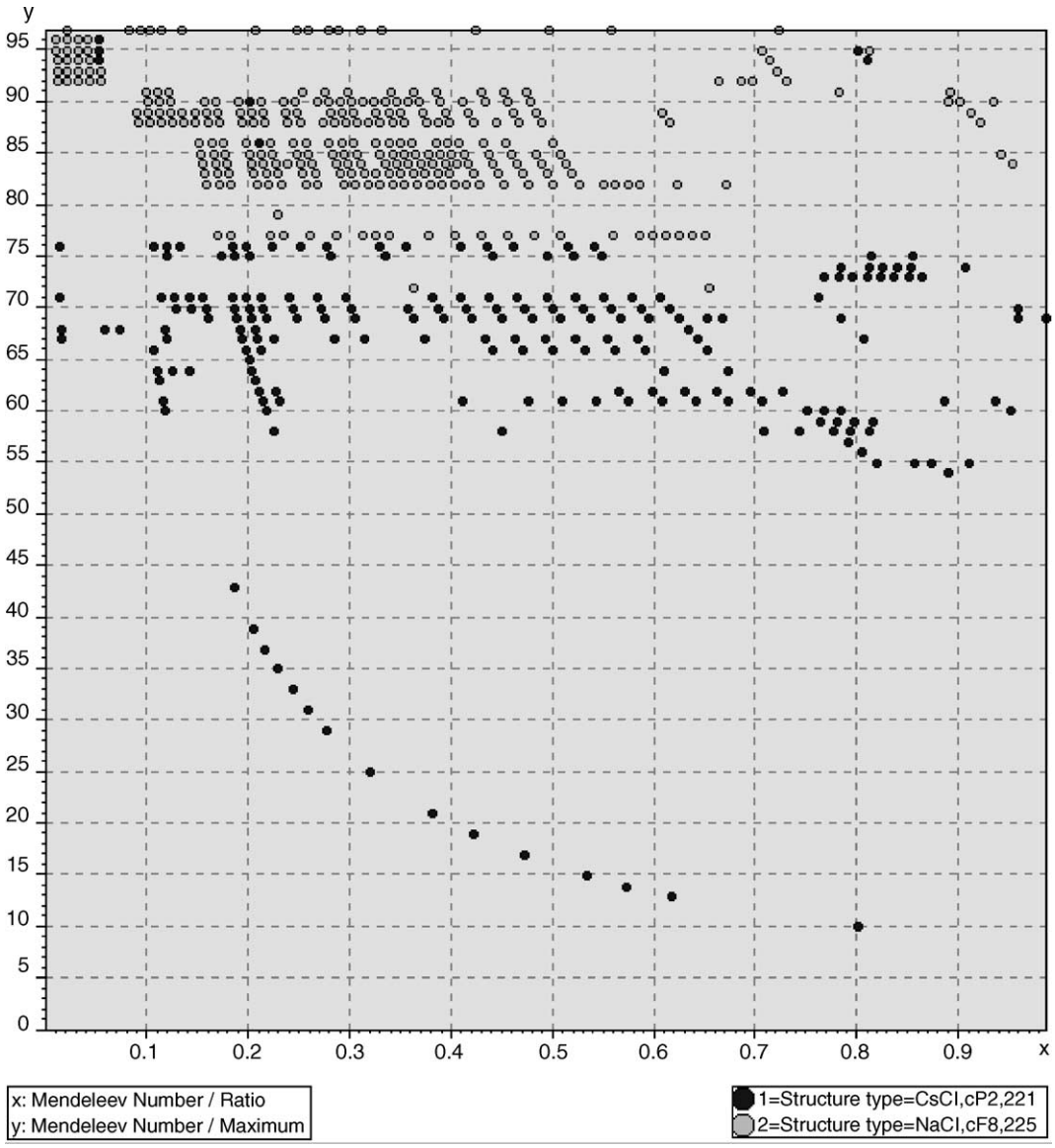


Fig. 4. A structure map Mendeleev number *MN* vs. ratio of Mendeleev numbers MN_{min}/MN_{max} prepared using Discovery. It shows the separation of binary phases crystallizing with the structure types CsCl and NaCl under ambient conditions.

culated diagrams (see example in Fig. 1). All have been redrawn from the original papers. The format has been standardized by converting wt.% and other expressions for composition to at.%. The diagrams are interactive so that, by clicking on a phase label, for instance, the user has access to all the data linked to that phase. The temperature range of existence for each phase and the type of formation reaction are stored.

2.3. Structure data

The structural part of the database contains cell parameters, space group, positional and displacement parameters, the minimal requirement being a complete set of cell parameters reported for a well-defined composition. The crystallographic data are accompanied by information about sample preparation and experimental conditions for the structure determination. The cell parameters and atom coordinates are presented as published, but also standardized, in order to facilitate the comparison of isotypic compounds. The latter data are prepared in a three-step procedure:

- The symmetry is checked and the data transformed into a space group of higher symmetry, when relevant.
- The data are standardized [2], applying criteria for the choice of the space group setting, origin of the coordinate system, representative triplets, etc.
- Data sets for isotypic compounds are compared and, if necessary, adjusted by applying an origin shift, etc.

As far as possible, a structure type has been assigned to the crystallographic data, following criteria defined in TYPIX [3]. When positional coordinates were not published but the structure type could be identified, atom coordinates of the type-defining entry are proposed as a first approximation. Atomic environment types (AET) have been investigated and can easily be visualized and modified, including more, or less atoms (Fig. 2).

2.4. Diffraction data

Diffraction data for X-rays can be computed on the spot [4] for all 7000 structure entries with refined atom coordinates, but also for another 19,000 entries with assigned structure type, using the atom coordinates of the type-defining entry. The software contains a search-and-match option based on the strongest diffraction lines.

2.5. Physical properties

A broad range of mechanical (e.g. bulk modulus, elastic stiffness coefficients), thermal (e.g. heat capacity, enthalpy of formation, thermal conductivity), electrical (e.g. resistivity, energy gap, density of states at the Fermi level, electron/hole mobility), optical (e.g. permittivity, refractive indices), magnetic (e.g. magnetic ordering temperatures, magnetization, anisotropy coefficients), and superconductor properties (e.g. superconducting transition temperature, critical field) are included in the database. Both experimental and calculated data are considered. Numerical values are presented as published, and converted to standard, usually SI, units. Values defined with respect to a quantity of material are normalized to 1 gram-atom When relevant, the property entries also contain information about sample preparation, experimental conditions or calculation methods. An extract of the data stored for the phase CeNi from a particular publication is shown in Fig. 3. It is possible to search for groups of properties, as well as to define ranges of numerical values for selected properties.

2.6. Search possibilities

The Pauling File is a fully relational database. The Binaries Edition comes with an innovative software package for data retrieval, which enables the user to perform tasks from simple queries to complex searches. Most of the tasks can be done using the so-called “Browser”, which is also able to

- display and navigate through phase diagrams,
- visualize crystal structures,
- explore atomic environments, interatomic distances and angles,
- perform a search-and-match phase identification from powder patterns.

The package includes the “Discovery” software (Fig. 4) in an early prototype version. This tool is able to search for correlations between any kind of Pauling File data for selected phases and various expressions of atomic properties of their constituting chemical elements.

Acknowledgements

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