

NIST Inorganic Crystal Structure Database (NIST ICSD) Data Field Specifications and Conventions



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1. Introduction

The NIST Inorganic Crystal Structure Database (NIST ICSD) is a comprehensive collection of bibliographic, chemical, and crystallographic information covering non-organic materials (including inorganics, ceramics, minerals, pure elements, metals, and intermetallic systems) containing over 210,000 entries and covering the literature from 1913.

NIST ICSD database contains crystallographic information including unit cell data, space group information, Pearson Symbol, formula units per cell, and atomic positions (thermal parameters when available) for full-structure entries, and additional information such as standardized cell and atomic coordinates, reduced cell, structure type, locality for minerals, temperature/pressure of data collections, and editorial remarks for better characterization of the materials.

2. The Data Fields

Specifications and conventions used for the NIST ICSD data fields are described in the following sections.

2.1 Anisotropic Thermal Parameters

U, B, Beta are labels used to designate the anisotropic thermal parameters in the Database. These are the anisotropic atomic displacement components which appear in the corresponding structure-factor term listed below (h, k, l are the Miller indices, and a^*, b^*, c^* are the reciprocal-space cell lengths.).

- Database label U (unit: angstrom squared)

$$\exp(-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*))$$

- Database label B (unit: angstrom squared)

$$\exp(-\frac{1}{4}(B_{11}h^2a^{*2} + B_{22}k^2b^{*2} + B_{33}l^2c^{*2} + 2B_{12}hka^*b^* + 2B_{13}hla^*c^* + 2B_{23}klb^*c^*))$$

- Database label Beta (unitless)

$$\exp(-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl))$$

In the Database, the anisotropic U, B and Beta labels for thermal data are followed by 6 coefficients [for example, (U₁₁ U₂₂ U₃₃ U₁₂ U₁₃ U₂₃), in equation for label U above].

Further details on the nomenclature can be found in the IUCr Report on atomic displacement parameter nomenclature (*K.N. Trueblood, H.-B. Burgi, H. Burzlaff, J.D. Dunitz, C.M. Gramaccioli, H.H. Schulz, U. Shmueli, S.C. Abrahams, Atomic displacement parameter nomenclature, Report of a subcommittee on atomic displacement parameter nomenclature, Acta Cryst. (1996). A52, p770-781*).

2.2 ANX Formula

Elements in the chemical formula are classified according to their oxidation states and the atomic sites they occupy.

For each atomic site, one letter is used to represent all the atom types on that site. Cations and anions, or the same atom types with different oxidation states that occupying the same sites are represented separately.

- Letters A-M are selected (in their alphabetic order) to represent all cations that occupy the same site,
- Letters N-R (also in their alphabetic order) are for neutral atoms
- Letters X, Y, Z, S, T, U, V, W (in the given order) are for anions.

The number follows the letter indicates the number of atoms occupying the site.

Examples:

ANX FORMULA	STRUCTURAL FORMULA
A2B2X11	V2 Re2 O11
AB2X4	(Sr Y) (Co O4)
AB6X3Y6Ta6	Mn C3 S6

2.3 Atomic Site

Fractional coordinates are given for atomic positions. The number of undetermined H atoms bonded to another atom is given in the remarks.

Site Occupancy Factors (SOF) are given in the form of decimals as the probability to find the atom at the site.

An oxidation state of zero is given if it is undetermined.

2.4 Author Name

The author names are generally given in the format of “[Last Name], [Initials of First Name]”, and followed by suffix, if applicable. The names in different languages may have different formats or orders.

Examples:

Cramer, E.M.

Bowman, R.C.jr.

Mel'nikov, O.K. (Melnikov, O.K.)

Wang Yingxia

2.5 Authors' Structure

The structures (unit cell, space group, atom coordinates, thermal parameters, etc.) stored in the database that are reported in the original publication (after correction of errors and typos). They are valuable information for the consideration of the original experiments and settings.

2.6 Centering

The type of non-primitive cell selected to describe the centered lattices, in which the unit cell contains more than one lattice point.

In the case of Rhombohedral Bravais lattice, “Rh” / “Rr” may be used (such as in “Reduced Cell” calculation) to distinguish between Hexagonal and Rhombohedral axes chosen for unit cell.

List of Values:

P: Primitive.

I: Body-centered.
F: Face-centered.
A: A-face centered.
B: B-face centered.
C: C-face centered.
R: Rhombohedral.

2.7 Chemical Name

The name of a chemical compound shows its elements and/or constituent components. Chemical names are commonly generated – by scientists worldwide – using the rules and conventions developed by the International Union of Pure and Applied Chemistry (IUPAC).

Caveat: Due to the complexity and 3D character of many structures, it is sometimes difficult or impossible to create a unique chemical name for a compound via the IUPAC rules. Consequently, this non-uniqueness means that “name searches”, though extremely useful, should be carried out with great care.

Examples:

Boron Arsenide (12.2/1.8)

Cesium Gold(III) Bis(sulfate(VI))

Dipotassium Manganese(II) Catena-tetrakis (vanadate)

2.8 Coden / Journal

Codens are six-character bibliographic codes administered by the International CODEN Service. A Journals series may have, in its history, splits / merges, and different publishing language versions, and / or translation versions.

Examples:

CODEN	JOURNAL
-------	---------

ACSEBH	Acta Crystallographica, Section E. Structure Reports Online
--------	---

JCOMEL	Journal of Physics: Condensed Matter
--------	--------------------------------------

NATGAK	Natuurwetenschappelijk tijdschrift (Ghent)
--------	--

2.9 Collection Code

A unique numeric identifier assigned to each database entry.

2.10 Comments

Free text remarks for the structure related information, such as atomic environment, reference structures from other publications, related phases at different experimental conditions, and synthesis conditions, etc.

Examples:

Stable up to 778 K

Cell from powder data at RT: 5.852, 11.716, 8.1997

AE: Ta1: 6p S6: Ta2: 6o S6; S1-4: 3n Ta3 (+3O)

2.11 Crystal Class

The classification of symmetry groups of crystals, which is in one to one correspondence with the types of point groups.

List of 32 Crystal Classes:

1	32	4-2m	622
1-	3m	432	6-m2
2	3-m	4-3m	6mm
2/m	4	4mm	m
222	4-	6	m3-
23	4/m	6-	m3-m
3	4/mmm	6/m	mm2
3-	422	6/mmm	mmm

2.12 Crystal System

According to the symmetry of their unit cells, all crystals – inorganics, minerals & organics – can be classified into one of 7 groups, collectively called Crystal Systems. These systems are designated: Triclinic, Monoclinic, Orthorhombic, Tetragonal, Trigonal, Hexagonal and Cubic.

Caveat: The Trigonal System includes Rhombohedral Crystals that can be based on either a primitive Rhombohedral cell (designated by R or Rr) or a triply primitive Hexagonal cell (designated by Rh).

Crystal Data-Determinative Tables (*Third edition, Volume 2, edited by J.D.H. Donnay and Helen M. Ondik (1973)*) is a classic reference in which crystals are organized within the Crystal Systems for the purpose of identification.

List of 7 Crystal Systems:

Triclinic

Monoclinic

Orthorhombic

Tetragonal

Trigonal / Rhombohedral

Hexagonal

Cubic

2.13 Density

Experimental or calculated density. The calculated density is determined using crystallographic data (the cell volume, formula, and Z) and Avogadro's number.

2.14 Element Count

The number of different element types in the formula. For example, PCl_3 has an element count of 2.

2.15 Formula Weight

Sum of the atomic weights of all atoms in the chemical formula.

2.16 Inversion Center

Centrosymmetric point groups have a symmetry element of $\bar{1}$, which has a Center of Inversion, whose symmetry operation generates an equivalent position of $(\bar{x}, \bar{y}, \bar{z})$ for a given point (x, y, z) .

2.17 Isotropic Thermal Parameters

U and B are labels used to designate the isotropic thermal parameters in the Database. The single atomic displacement component is used for the definition in the following structure-factor terms (λ is the wavelength of the radiation, and θ is the angle between the wave vector of the incident plane wave and the lattice planes).

- Database Label U (unit: angstrom squared)

$$\exp(-8\pi^2 U (\frac{\sin\theta}{\lambda})^2)$$

- Database Label B (unit: angstrom squared)

$$\exp(-B (\frac{\sin\theta}{\lambda})^2)$$

$$(B = U \times 78.956835)$$

Further details on the nomenclature can be found in the IUCr Report on atomic displacement parameter nomenclature (*K.N. Trueblood, H.-B. Burgi, H. Burzlaff, J.D. Dunitz, C.M. Gramaccioli, H.H. Schulz, U. Shmueli, S.C. Abrahams, Atomic displacement parameter nomenclature, Report of a subcommittee on atomic displacement parameter nomenclature, Acta Cryst. (1996). A52, p770-781*).

2.18 Laue Class

The classification of the 32 Crystal Classes into eleven classes in terms of diffraction equivalence. A Laue Class contains a point group that is of the crystallographic type of centrosymmetric, and its non-centrosymmetric subgroups.

List of eleven Laue Classes:

1-	4/m	m3-
2/m	4/mmm	m3-m
3-	6/m	mmm
3-m	6/mmm	

2.19 Mineral Group

Minerals are naturally occurring substances with unique unit cells, crystal structures and chemical compositions. The minerals are classified according to their chemical composition. There are seven major groups – Silicates, Oxides, Sulfates, Sulfides, Carbonates, Elements and Halides – and several minor groups.

Examples:

Apatite

Garnet

Zeolite

2.20 Mineral Name

Minerals are named in a variety of ways, due to their great diversity – in structure & chemistry, in their history, and in their place of origin. Many mineral names end in the suffix “ite” which is derived from the Greek word meaning stone. In some cases, a new mineral is named to honor the discoverer (e.g. Mroseite for the geologist Mary Mrose).

Examples:

Hydroxycalciopyrochlore

Mullite, boron-containing

Strontio-orthojoaquinite

2.21 Mineral Origin

The mineral origin commonly refers to where a given mineral was discovered. For example, Whitlockite, a calcium phosphate mineral, was found in guano caves and in meteorites and Mroseite, a calcium tellurite carbonate, was found in a mine in Moctezuma, Sonora Mexico.

Examples:

Ronneburg U deposit, near Gera, Thuringia, Germany

Val Malenco, Italy

Kedykverpakhk Mountain, Lovozero alkaline complex, Kola peninsula, Russia

2.22 Minimal Distance

The shortest distance between two atom types in the structure given in the entry, the default unit used in the database is angstrom.

Examples:

ATOM1-ATOM2	MINIMAL DISTANCE
Nb-Nb	3.5167
Nb-S	2.1493
K-Na	4.3095

2.23 Powder Diffraction File (PDF) Number

The PDF Number is a unique number assigned to an entry in the ICDD Powder Diffraction File. This number is used to cross reference entries in the NIST ICSD with those in the ICDD Powder Diffraction File.

Examples:

CODE	ADDITIONAL COMMENT
PDF	47-1227
PDF	53-1109
PDF	86-1283

2.24 Pearson Symbol

The Pearson symbol consists of three parts: the crystal system code (lower case), the lattice centering code (upper case), and the number of atoms per unit cell.

For monoclinic and orthorhombic space groups, centering code of A, B, C, and (in monoclinic only) I may be given as "S".

Examples:

aP12
mS260
oP26
tI102

2.25 Polar Axis

Point groups that belong to the 10 polar groups, which have an axis of rotation, instead of a unique origin, for all the symmetry operations.

2.26 Pressure

The experimental setting of the pressure, the default value is the standard pressure (≈ 1.01 MPa).

2.27 Reduced Cell

The reduced cell is a unique, primitive cell based on the three shortest noncoplanar vectors of the lattice and satisfies a specified set of mathematical conditions. Because of its uniqueness, reduced cell is the basis for lattice classification, for metric symmetry determination, and for powerful identification systems for crystalline materials (*A. D. Mighell, J. of Appl. Cryst. (1976), v9, p491-498*).

NIST* Lattice program (*V. L. Karen and A. D. Mighell, NIST Technical Note 1290 (1991)*) is used to calculate Reduced Cells.

2.28 R Value

A measure of agreement between the amplitudes of the structure factors calculated from a crystallographic model and those from the original diffraction experiment.

$$R = \frac{\sum |F_{obs} - F_{calc}|}{\sum |F_{obs}|}$$

2.29 Space Group

The Space Group numbers correspond to those given in the *IUCr International Tables for Crystallography* (2006). Authors' Structures may have settings of Space Group deviates from the conventions used in the International Tables.

Some Space Groups in orthorhombic, tetragonal, and cubic Crystal Systems may have two choices for the position of the origin, and these space group symbols will have a suffix of "S"

(choice 1) or “Z” (choice 2) to indicate whether it is the choice of inversion center as defined in the International Tables.

For Rhombohedral Space Groups that have hexagonal axes, the Space Group Symbols will have a suffix of “H”, or “HR” for reverse setting, to distinguish from those that have Rhombohedral axes.

Examples:

```
C m m a
P m c 21
F d -3 m S
P b a n Z
R 3 2 HR
```

2.30 Standard Remarks

Additional information related to the experimental settings, sample preparation and conditions, defects, disorders, and other structure related information, etc. A standard 3 or 4-letter code is associated with the type of information provided, and can be searched based on the code.

Examples:

CODE	ADDITIONAL COMMENT
DIS	Oxygen and fluorine statistical spread over three positions
XDS	X-ray diffraction from single crystal
DFT	Density functional theory

2.31 Standardized Structure

Programs and routines, such as Structure Tidy (*L.M. Gelato and E. Parthe, J. Appl. Cryst. (1987), v20, p139-143*), are used to obtain structure(s) defined according to the definitions and conventions used by International Tables for Crystallography.

The “Standardized” Structures, including Unit Cell, Space Group, Pearson’s Symbol, and Wyckoff Sequences, etc., are equivalent descriptions to Authors’ Structures. The resulted

structures make it easier to compare and evaluate experimental structures, or to identify materials with similar structures.

2.32 Structure Type

The structure type given will usually be the formula or name of the isostructural type material.

A number of structure descriptors, including Space Group, Wyckoff sequences, Pearson's Symbol, ANX formula, c/a Ratio, cell parameters, and Beta range, etc., are used to determine the closeness of structural similarities. (*Rudolf Allmanna & Roland Hinek, Acta Cryst. (2007). A63, p412–417*)

Examples:

CODE	ADDITIONAL COMMENT
TYP	Wurtzite-ZnS (2H)
TYP	Elpasolite-K ₂ NaAlF ₆
TYP	Perovskite-Ba ₂ LaRuO ₆
TYP	La ₂ SrCu ₂ O ₆

2.33 Structural Formula

The formula is expressed by a sequence of discrete structure units based on the occupancy of atomic sites. The information is obtained from the full structure data.

Examples:

```
(Sr0.5 Ca0.5) (Mn0.5 Ru0.5) O3  
Ca (Mn0.5 Ru0.5) O3  
K Zn4 (Sb3 O12)
```

2.34 Sum Formula

A set of chemical symbols showing the elements present in the Structural Formula and their relative proportions. Element symbols are presented in alphabetical order. Each element type can appear only once – i.e. elements of the same type appearing multiple times in the structural formula are summed together in the Sum Formula.

The relative proportions are set such that the total number of atoms in the Sum and in the Structural Formulas are identical.

Examples:

La3 O7 Ta1

B2 Mg5 O10 Sn0.9 Ti0.1

F1 K2 Nb5 O14 Sr1

2.35 Temperature

The experimental setting of temperature. The default value is at room temperature (≈ 293 K).

2.36 Unit Cell

The Unit Cell is a primitive or centered cell, with cell parameters assigned on the basis of the symmetry elements of the crystal system.

2.37 Wyckoff / Multiplicity

The multiplicity of a site is the number of equivalent atom positions produced by the symmetry of a space group from a single site noted in structure descriptions.

2.38 Wyckoff Sequence

The occupied Wyckoff sites are sorted alphabetically using the corresponding Wyckoff letter, followed by the count of atom sites that belongs to the same Wyckoff letter.

Examples:

d c2 b

i h g3 e

h g2 c b a

2.39 Z

The number of formula units presented in the unit cell.