NIST Standard Reference Database 3

NIST Crystal Data

CD-ROM Guide

National Institute of Standards and Technology
Gaithersburg, MD 20899

February 2000

U.S. Department of Commerce
Technology Administration
National Institute of Standards and Technology
Standard Reference Data Program
Gaithersburg, Maryland 20899
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INTRODUCTION

The NIST Crystallographic Data Center collects, evaluates and disseminates data on solid-state materials. NIST Crystal Data is a comprehensive database with chemical, physical and crystallographic information on all classes of well-characterized substances. These materials fall into the following categories: inorganics, organics, organometallics, metals, intermetallics and minerals. For each entry, data types include lattice parameters, crystal system, space group, chemical name, chemical formula, literature reference, among others.

NIST Crystal Data is being distributed in a multi-file format for ease of incorporation in other database management systems and processing by independent software routines. The following documentation describes the content and format of each of the ASCII data files. These files should be processed using column-specified fields, not blank-delimited fields, since there may be internal codes in fields not specified in this documentation. Most of the files contain one line per entry. Note that there may be more than one formula, name, literature reference, or comment per entry; these are unique and separate items and will be qualified by the addition of a sequence number.
### List of files on CDROM

<table>
<thead>
<tr>
<th></th>
<th>File</th>
<th>Lines of Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>au-p1</td>
<td>237671 lines</td>
</tr>
<tr>
<td>2</td>
<td>au-p2</td>
<td>237671 lines</td>
</tr>
<tr>
<td>3</td>
<td>au-p3</td>
<td>237671 lines</td>
</tr>
<tr>
<td>4</td>
<td>cd-p1</td>
<td>237671 lines</td>
</tr>
<tr>
<td>5</td>
<td>cd-p2</td>
<td>237671 lines</td>
</tr>
<tr>
<td>6</td>
<td>cd-trans</td>
<td>237671 lines</td>
</tr>
<tr>
<td>7</td>
<td>cpd-flag</td>
<td>237671 lines</td>
</tr>
<tr>
<td>8</td>
<td>cpd-name</td>
<td>256012 lines</td>
</tr>
<tr>
<td>9</td>
<td>ele-subs</td>
<td>237386 lines</td>
</tr>
<tr>
<td>10</td>
<td>ele-symb</td>
<td>237386 lines</td>
</tr>
<tr>
<td>11</td>
<td>for-chem</td>
<td>241554 lines</td>
</tr>
<tr>
<td>12</td>
<td>for-emp</td>
<td>237386 lines</td>
</tr>
<tr>
<td>13</td>
<td>lit-refs</td>
<td>251782 lines</td>
</tr>
<tr>
<td>14</td>
<td>rd-p1</td>
<td>237671 lines</td>
</tr>
<tr>
<td>15</td>
<td>str-type</td>
<td>222727 lines</td>
</tr>
<tr>
<td>16</td>
<td>comments</td>
<td>181347 lines</td>
</tr>
<tr>
<td>17</td>
<td>process1</td>
<td>27075 lines</td>
</tr>
<tr>
<td>18</td>
<td>process2</td>
<td>237671 lines</td>
</tr>
<tr>
<td>19</td>
<td>codenino</td>
<td>1694 lines</td>
</tr>
<tr>
<td>20</td>
<td>codenorg</td>
<td>950 lines</td>
</tr>
</tbody>
</table>
### au-p1: Authors cell, experimental conditions

<table>
<thead>
<tr>
<th>Columns</th>
<th>Field</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-7</td>
<td>ID</td>
</tr>
<tr>
<td>11-19</td>
<td>a (Original Data) in Angstroms (1 Å = 10^{-10} m)</td>
</tr>
<tr>
<td>20-28</td>
<td>b</td>
</tr>
<tr>
<td>29-37</td>
<td>c</td>
</tr>
<tr>
<td>38-45</td>
<td>α (Original Data) in degrees</td>
</tr>
<tr>
<td>46-53</td>
<td>β</td>
</tr>
<tr>
<td>54-61</td>
<td>γ</td>
</tr>
<tr>
<td>62</td>
<td>Editorial code for cell</td>
</tr>
<tr>
<td></td>
<td>Blank = cell given by author; normal temperature and pressure</td>
</tr>
<tr>
<td></td>
<td>E = cell inserted by Crystal Data editor</td>
</tr>
<tr>
<td></td>
<td>C = cell is Crystal Data cell (not necessarily the author's original cell)</td>
</tr>
<tr>
<td></td>
<td>T = cell data is at high or low temperature</td>
</tr>
<tr>
<td></td>
<td>P = cell data is at high pressure (may also be at high or low temperature)</td>
</tr>
<tr>
<td>75</td>
<td>Radiation of study</td>
</tr>
<tr>
<td></td>
<td>Blank = not specified</td>
</tr>
<tr>
<td></td>
<td>X = x-ray</td>
</tr>
<tr>
<td></td>
<td>N = neutron</td>
</tr>
<tr>
<td></td>
<td>E = electron</td>
</tr>
<tr>
<td></td>
<td>G = gamma</td>
</tr>
<tr>
<td>77</td>
<td>Source of unit cell data</td>
</tr>
<tr>
<td></td>
<td>Blank = not specified</td>
</tr>
<tr>
<td></td>
<td>S = single crystal</td>
</tr>
<tr>
<td></td>
<td>P = powder diffraction</td>
</tr>
<tr>
<td></td>
<td>R = Rietveld or profile fit analysis</td>
</tr>
<tr>
<td>79</td>
<td>Structure code</td>
</tr>
<tr>
<td></td>
<td>N = no information about structure is given</td>
</tr>
<tr>
<td></td>
<td>L = limited structure information is given (partial structure determined or assigned by type)</td>
</tr>
<tr>
<td></td>
<td>T = total structure determined (excluding H atoms)</td>
</tr>
<tr>
<td>82</td>
<td>Internal update code</td>
</tr>
</tbody>
</table>

NIST Crystal Data 3
Crystal system code
- A = anorthic (triclinic)
- M = monoclinic
- O = orthorhombic
- R = rhombohedral (hexagonal or rhombohedral axes)
- T = tetragonal
- H = hexagonal
- C = cubic

au-p2 : Authors space group, Z, and density

Columns | Field
---|---
2-7 | ID
11-18 | Author's space group, aspect in Laue class, or cell centering (left-justified)
19 | Editorial code for space group
- Blank = space group given by author
- E = space group inserted by Crystal Data editor
- T = space group orientation corresponds to that of the Crystal Data cell (rare; orthorhombic only)
21 | Aspect code
- Blank = Normal
- * = aspect number has been assigned
22-24 | Space group or aspect number
25 | Orientation code for space group or aspect
30-35 | Z (number of formula units per unit cell)
36 | Editorial code for Z
- Blank = Z given by author
- E = Z has been inserted by the Crystal Data editor
- G = Z has been guessed
40-45 | Dm (author's measure density) in Mg/m³ (g/cm³)
48-53 | Dx (author's calculate density) in Mg/m³
71-79 | Input cell volume
82 | Internal update code

NIST Crystal Data 4
au-p3 : Authors standard deviations for cell parameters

Columns | Field
---|---
2-7 | ID
11-19 | $\sigma$ (a)
20-28 | $\sigma$ (b)
29-37 | $\sigma$ (c)
38-45 | $\sigma$ ($\alpha$)
46-53 | $\sigma$ ($\beta$)
54-61 | $\sigma$ ($\gamma$)
63-66 | Average error in axial lengths in parts per $10^5$
67 | Editorial code for average error
   | Blank = standard deviations reported by the authors
   | E = editorial errors assigned
69-79 | Quality index code for cell
82 | Internal update code

cd-p1 : Crystal Data cell, axial ratios

Columns | Field
---|---
2-7 | ID
11-18 | a (Crystal Data cell) in Angstroms
19-26 | b
27-34 | c
35-41 | $\alpha$ (Crystal Data cell) in degrees
42-48 | $\beta$
49-55 | $\gamma$
56-64 | First determinative ratio
   | The first determinative ratio is $a/b$ for the anorthic, monoclinic, and orthorhombic crystal systems; $c/a$ for the tetragonal, hexagonal and rhombohedral (H axes) systems; and $a$ for the cubic system.
65-72 | Second determinative ratio
   | The second determinative ratio is $c/b$ for the anorthic, monoclinic and orthorhombic systems; it is blank for the tetragonal, hexagonal, rhombohedral and cubic systems.
82 | Internal update code

NIST Crystal Data 5
NIST Crystal Data 6
**cd-p2 : Crystal Data space group, Z, and density**

<table>
<thead>
<tr>
<th>Columns</th>
<th>Field</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-7</td>
<td>ID</td>
<td></td>
</tr>
<tr>
<td>11-18</td>
<td>Crystal Data space group, aspect, or centering</td>
<td>(left-justified)</td>
</tr>
<tr>
<td>19</td>
<td>Editorial code for space group</td>
<td>Blank = normal, E = original space group is editorial</td>
</tr>
<tr>
<td>21</td>
<td>Aspect code</td>
<td>Blank = normal, * = aspect number assigned</td>
</tr>
<tr>
<td>22-24</td>
<td>Space group number or aspect number</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>Orientation code for space group or aspect</td>
<td></td>
</tr>
<tr>
<td>30-35</td>
<td>Z for Crystal Data cell</td>
<td></td>
</tr>
<tr>
<td>36</td>
<td>Editorial code for Crystal Data Z</td>
<td>Blank = normal, E = original Z is editorial, G = original Z is guessed</td>
</tr>
<tr>
<td>40-44</td>
<td>Density approximated by atomic volumes in Mg/m³</td>
<td></td>
</tr>
<tr>
<td>45</td>
<td>A (editorial code for approximate density)</td>
<td></td>
</tr>
<tr>
<td>48-53</td>
<td>Dx (program calculated density)</td>
<td></td>
</tr>
<tr>
<td>54</td>
<td>Editorial code for Dx</td>
<td>Blank = normal, G = Dx is questionable due to guessed or missing Z, or to approximation of empirical formula</td>
</tr>
<tr>
<td>61-68</td>
<td>Molecular or formula weight</td>
<td></td>
</tr>
<tr>
<td>69</td>
<td>Editorial code for molecular weight</td>
<td>Blank = normal, G = molecular weight is questionable due to approximation of empirical formula</td>
</tr>
<tr>
<td>71-79</td>
<td>Volume of Crystal Data cell</td>
<td></td>
</tr>
<tr>
<td>82</td>
<td>Internal update code</td>
<td></td>
</tr>
</tbody>
</table>

*NIST Crystal Data 7*
cd-trans : Matrix for authors cell → Crystal Data cell

Columns | Field
---|---
2-7 | ID
11-14 | Determinant of transformation matrix
15 | :
17-34 | First row of transformation matrix
35 | /
36-53 | Second row of transformation matrix
54 | /
55-72 | Third row of transformation matrix
82 | Internal update code

cpd-flag : Material, class and registration indicators

Columns | Field
---|---
2-7 | ID
11 | I for inorganic material (blank if not)
12 | O for organic material (blank if not)
13 | M for mineral (blank if not)
14 | A for alloy, metal, intermetallic material (blank if not)
35-62 | Chemical class indicators (organic) or mineral group codes (inorganic)
64-74 | Chemical Abstracts Service (CAS) registry number
82 | Internal update code

cpd-name : Compound name

Columns | Field
---|---
2-7 | ID
9 | Sequence number
11 | Index code
    | Blank = Crystal Data index name
    | M = mineral name
    | N = chemical name for a mineral
    | C = common or trivial name
    | D = name to be omitted from index

NIST Crystal Data 8
13-end  Compound name

**ele-subs : Element subscript**

Columns  Field

2-7  ID
10-11  Element count
13-17  Number of atoms for element symbol #1
19-23  Number of atoms for element symbol #2
25-29  Number of atoms for element symbol #3

.  .  .

End  Number of atoms for element symbol # = element count

**ele-symb : Element symbol**

Columns  Field

2-7  ID
10-11  Element count
13-15  Element symbol #1
17-19  Element symbol #2
21-23  Element symbol #3

.  .  .

End  Element symbol # = element count

(Note: the symbols Ln or TR may be used for unspecified rare earth elements.)
for-chem : Chemical formula

Columns Field

2-7 ID
9 Sequence number
11 Formula approximation code
   Blank = normal
   G  = editor has simplified formula or composition
       is approximate (e.g. for minerals)
13 Formula editorial code
   Blank = normal
   A  = formula is absent
   D  = omit from index
   X  = pseudo-empirical formula index (organic only)
   P  = permuted formula index (organic only)
15-end Chemical formula

(Note: the symbols Ln or TR may be used for unspecified rare earth elements.)

for-emp : Empirical formula

Columns Field

2-7 ID
9 Approximation code
   Blank = normal
   G  = formula is approximate or simplified
11 Editorial code
   Blank = empirical formula was generated from the chemical formula
   E  = empirical formula inserted by editor
13-end Empirical formula

NIST Crystal Data 10
### lit-refs: Literature reference

<table>
<thead>
<tr>
<th>Columns</th>
<th>Field</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-7</td>
<td>ID</td>
</tr>
<tr>
<td>9-10</td>
<td>Sequence number</td>
</tr>
<tr>
<td>12-13</td>
<td>Code for reference</td>
</tr>
<tr>
<td></td>
<td>Blank = primary journal reference</td>
</tr>
<tr>
<td></td>
<td>CD = reference from Volume 1 or 2 of Crystal Data Determinative Tables</td>
</tr>
<tr>
<td>15-20</td>
<td>CODEN</td>
</tr>
<tr>
<td>22-25</td>
<td>Volume number</td>
</tr>
<tr>
<td>27-31</td>
<td>Page number</td>
</tr>
<tr>
<td>33-36</td>
<td>Year</td>
</tr>
<tr>
<td>38-end</td>
<td>Authors</td>
</tr>
</tbody>
</table>

### rd-p1: Reduced cell, metric symmetry

<table>
<thead>
<tr>
<th>Columns</th>
<th>Field</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-7</td>
<td>ID</td>
</tr>
<tr>
<td>11-18</td>
<td>a (reduced cell) in Angstroms</td>
</tr>
<tr>
<td>19-26</td>
<td>b</td>
</tr>
<tr>
<td>27-34</td>
<td>c</td>
</tr>
<tr>
<td>35-41</td>
<td>α (reduced cell) in degrees</td>
</tr>
<tr>
<td>42-48</td>
<td>β</td>
</tr>
<tr>
<td>49-55</td>
<td>γ</td>
</tr>
<tr>
<td>56-64</td>
<td>Volume (reduced cell)</td>
</tr>
<tr>
<td>76-77</td>
<td>Reduced form number</td>
</tr>
<tr>
<td>78</td>
<td>Metric symmetry code</td>
</tr>
<tr>
<td></td>
<td>Blank = normal</td>
</tr>
<tr>
<td></td>
<td>X = metric symmetry exceeds crystal symmetry</td>
</tr>
<tr>
<td>82</td>
<td>Internal update code</td>
</tr>
</tbody>
</table>
**str-type : Structure type**

Columns | Field
---|---
2-7 | ID
11-19 | Pearson symbol for alloys, metals, and intermetallics
20 | Editorial code for Pearson symbol
    | Blank = normal (generated from empirical formula and Z)
    | E = Pearson symbol inserted by Crystal Data editor
28-77 | Structure type (formula, name, or Strukturbericht designation)
82 | Internal update code

**comments : Comments**

Columns | Field
---|---
2-7 | ID
9-10 | Sequence number
12-13 | Comment code
    | Blank = General comment
    | SM = Sample source or locality
    | PR = Sample preparation
    | ST = Structure
    | CL = Color
    | AN = Analysis
    | OP = Optical data
    | PM = Polymorphism
    | AD = Additional pattern
    | MP = Melting point
    | CR = Cross-reference (added at production time)
    | LN = Additional diffraction line(s)
    | AX = Axial ratio data
    | UC = Unit cell data
    | TM = Temperature of data collected
    | PD = Powder data
    | HK = Footnotes for hkl and superlattice d-spacings
    | OO = Reason 'O' quality was assigned (PDF code)
    | FN = Footnote for d-spacings
    | DB = Deleted by or rejected by

**NIST Crystal Data 12**
AT = Atomic positions  
TH = Thermal parameters  
FF = Scattering factors  
SC = Scale factors  

15-end Comment

process1: Update or revision

Columns  Field

2-7 ID  
11-18 Revision date (year/month/day)  
20-22 Initials (revision by)  
24-78 Information on items revised or corrected  
82 Internal update code

process2: Processing history

Columns  Field

2-7 ID  
11-18 Entry date (inorganic) or accession date (organic) in the form year/month/day  
21-28 Keyboarding date (inorganic) or modification date (organic) (year/month/day)  
30-32 Initials of keyboarder  
34-41 Processing date (year/month/day)  
42-44 Number of warnings  
45-47 Number of errors  
49-50 Processing program revision number  
52-59 Revision date (year/month/day)  
61-67 PDF number (reference to the Powder Diffraction File of the International Centre for Diffraction Data)  
69-76 Alternate reference code (Cambridge code, metals code, or inorganic structural code)  
82 Internal update code

NIST Crystal Data 13
Journal CODENS

NIST Crystal Data contains the journal CODEN as given by Chemical Abstracts or as assigned by the Crystal Data editors when no published CODEN was available. The journal names have been abbreviated according to conventions of Chemical Abstracts or the Bibliographic Guide for Editors and Authors published by the American Chemical Society.

codenino : Journal CODEN for inorganic data

Columns Field
1-6 CODEN
8-end Journal name

codenorg : Journal CODEN for organic data

Columns Field
1-6 CODEN
8-end Journal name

NIST Crystal Data 14
CONTACTS

If you have comments or questions about the database, the Standard Reference Data Program would like to hear from you. Also, if you should have any problems with the CD-ROM, please let us know by contacting:

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Fax: (301) 975-5334  
Email: vicky.karen@nist.gov