ISOSUBGROUP: A Web Resource For Generating Isotropy Subgroups

of Crystallographic Space Groups

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ABSTRACT

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Existing web applications that generate lists of isotropy subgroups of crystallographic space groups are either not user friendly or are unnecessarily complicated. We developed a web application, ISOSUBGROUP, which we will show is simple and easy to use. The software development included the assembly of FORTRAN subroutines and an HTML user interface enhanced by CSS, resulting in a visually appealing environment.

Keywords: ISOSUBGROUP,isotropy,crystallographic

ACKNOWLEDGMENTS

I want to thank Dr Stokes for teaching me FORTRAN and many other useful skills, and for being patient enough to listen to and answer all my question. I want to thank him giving me this opportunity in the first place to even do this capstone. I want to thank Dr. Campbell for his help and input on my capstone. Lastly, I want to thank Dr. Hart for taking me into his research group and helping me to enjoy programming.

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Chapter 1

Introduction

1.1 Isotropy Subgroups

Crystallographic materials can be classified in one of 230 different space groups (Hahn, 2006). A space group is a collection of symmetry operations. Materials can undergo distortions. These distortions change the symmetry of the material. As the material goes through a distortion, it loses some of its original symmetry. The new symmetry of the material is a subgroup of the symmetry of the original "parent" space group. All distortions are made up of a linear combination of distortion which can be classified by irreducible representations (IR) of the parent space group. One can calculate new subgroups by selecting IRs of the parent space group that create a distortion. These subgroups are called isotropy subgroups (Stokes and Hatch, 1988). Information about these isotropy subgroups are important to all those who study crystallography.

1.2 Previous Work

At BYU there has been a lot of work to help scientists access information about these isotropy subgroups. Stokes and Hatch wrote a book in 1988 called *Isotropy Subgroups of the 230 Crystal-*

lographic Space Groups (Stokes and Hatch, 1988). This book primarily contains tables of isotropy subgroups. As the World Wide Web began to grow, so did the need to share this information in more accessible ways.

Stokes and Hatch then created software called ISOTROPY to expand the information found in their book (ISOTROPY suite). This software later included both magnetic and incommensurate subgroups as well. However this program was not very easy to use. To operate the program the user needs to type commands into a text box. The syntax is very particular, and the user needs a manual to remember all the possible commands.

Stokes and Campbell later addressed this short coming when they created the software called ISODISTORT (ISOTROPY suite). ISODISTORT was a lot more user friendly. No more long complex commands were needed to operate the program. However the user needs to have a specific material in mind when using ISODISTORT. It works by importing data files about the specific material. For example, a scientist might use it while studying tungsten oxide. The need arose for a program that could generate information about isotropy subgroups without having a particular material in mind and without entering in that information. This was the purpose of developing the program ISOSUBGROUP.

1.3 FORTRAN

ISOSUBGROUP is written using FORTRAN. FORTRAN is a very important programming language that has existed since the 1950s. FORTRAN is rarely used anymore because it is not a simple language. FORTRAN has many unique quirks. The first seven characters of each line are left blank. This is a holdover from when programming was done with punch cards. FORTRAN code on punch cards used these first seven slots to signify different information, e.g., comments, or a continuation from a previous line. These unique features are not intuitive and can sometimes be hard to work with.

Even so, FORTRAN has positive qualities that will prevent it from disappearing. Math is FORTRAN's specialty. FORTRAN can perform calculations faster than many popular languages used today, like Java. Considering ISOSUBGROUP performs many calculations, FORTRAN was a wise choice since even while using FORTRAN some calculation may take more than an hour. Many other languages would not work as well due to the added calculation time needed. FORTRAN is also indispensable because so much code has already been written in it. This is another reason for choosing FORTRAN for the back end of ISOSUBGROUP. Stokes had already created many subroutines used in ISOTROPY and ISODISTORT that would prove crucial to creating ISOSUBGROUP.

There are three important things to keep in mind when reading or writing FORTRAN code. First, as stated earlier, the first seven characters are almost always left blank. Next, functions and subroutines are the two main ways to separate code, especially code that is repeated. Subroutines can return many results, but it does so by changing the parameters sent in the subroutine. Function can also do this, but it returns an additional result through the name of the function. One last difference is that all variables are declared at the beginning of the code before any operations are performed.

1.4 CSS

Cascading Style Sheets (CSS) is a programming language primarily used to style web pages. Style sheets have existed since the 1980s. CSS was developed in the late 1990s. Style sheets and CSS in particular were designed to separate the design elements of a web page from the rest of the content. This makes editing the content of a web page simpler. Without style sheets, the amount of HyperText Markup Language (HTML) needed for the presentation of a web page would overwhelm the content. CSS can change the look of a web page without cluttering up the HTML. Style sheets also save the web developer from unnecessary code duplication. One style sheet can style a variety of pages for a web domain. There are only a few simple adaptations needed for each unique page.

I suggested the use of Cascading Style Sheets for this web resource because of its ease of use. Upon investigation we decided to use *Twitter Bootstrap*, which is a free resource provided by Twitter (Twitter). It is a collection of adaptable premade CSS and Java Script code. A single CSS document can take several dozen hours to create from scratch, even for those extremely familiar with CSS. Twitter Bootstrap provided a reasonable solution. It allows ISOSUBGROUP access to many contemporary features and styles without the numerous hours of coding.

1.5 Overview

In the next chapter we will share how ISOSUBGROUP uses FORTRAN with HTML, and how CSS was added to improve the look and maintainability. In Chapter 3 we will present a short guide on how to use ISOSUBGROUP. In the final chapter we give our conclusions about this project and our direction for future work.

Chapter 2

Software Design

2.1 HTML and FORTRAN

The ISOSUBGROUP home page was created with HTML. After the user inputs the desired information on the home page, the HTML calls a main FORTRAN program, and it passes parameters based on the options selected by the user. This same FORTRAN program is called every time a user finishes selecting different options on any of ISOSUBGROUP's pages. Each time ISOSUBGROUP passes the FORTRAN program different parameters based on which page the user is on and which options they choose. This FORTRAN code creates new HTML for the next page based on parameters it receives. The program is primarily a big "if else" statement. One of the parameters sent to the FORTRAN tells ISOSUBGROUP which section of code to use to create the correct HTML for the next page.

Within each section of this giant "if else" statement, the HTML is sent to the screen through write statements like

```
write(6,'(a)')'<H1>K Vector</H1>'.
```

This line of code tells the program to send "<H1>k Vector</H1>" to the user's browser. It is then

Subroutine	Number of Lines
get irrepstring	34
get kvecstring	49
get settingstring	45
get argstring	58
input irrep	34
input irrep version	31
input irrep2	40
input irrep count	36
input kvector	200
input kvector2	43
input setting	133
input show	120
input space group	72
put irrep	25
put irrep version	13
put irrep count	12
put kvector	35
put setting	31
put space group	16
request irrep	65
request kvector	55
request show	52
table	836
Total	2035

Figure 2.1

ISOSUBGROUP's subroutines and their length in number of lines.

translated from HTML to what the user sees. Most of the write statements do not appear in the main FORTRAN program. Instead, each section calls a number of different subroutines. The subroutines are the primary writers of the HTML. We either created or heavily modified the 23 subroutines found in Figure 2.1. As the table shows, their sizes vary. Each of these subroutines often access many other subroutines and databases previously provided by Stokes for both ISOTROPY and ISODISTORT. If you add the number of code lines from the subroutines on the table to the 323 lines of FORTRAN code from the main program, you start to see the amount of coding needed to create this web resource, not to mention, the numerous lines from other subroutines, HTML, and CSS files. Appendix A provides a simple example of what one of the FORTRAN subroutine used in ISOSUBGROUP looks like.

2.2 HTML and CSS

After completing the functionality of the web resource, the home page for ISOSUBGROUP looked like Figure 2.2. It is just black text on a white web page. It looks like a page made by a physicist. The next task was to add more visual appeal while keeping the maintenance low and functionality high. We accomplished this through CSS and specifically *Twitter Bootstrap*, which is customizable premade CSS. This keeps the maintenance and hassle down by keeping all of the code in separate CSS files.

These style sheets could be accessed by simple lines of HTML code like

```
<link rel="stylesheet" href="/iso/bootstrap.css">.
```

This line of code links the HTML page to the CSS located in "/iso/bootstrap.css". This line is found in the head of an HTML document. Once the CSS and Java Script had been added in a similar fashion, the only thing needed to change the style of most elements was to add special classes to the HTML tags like

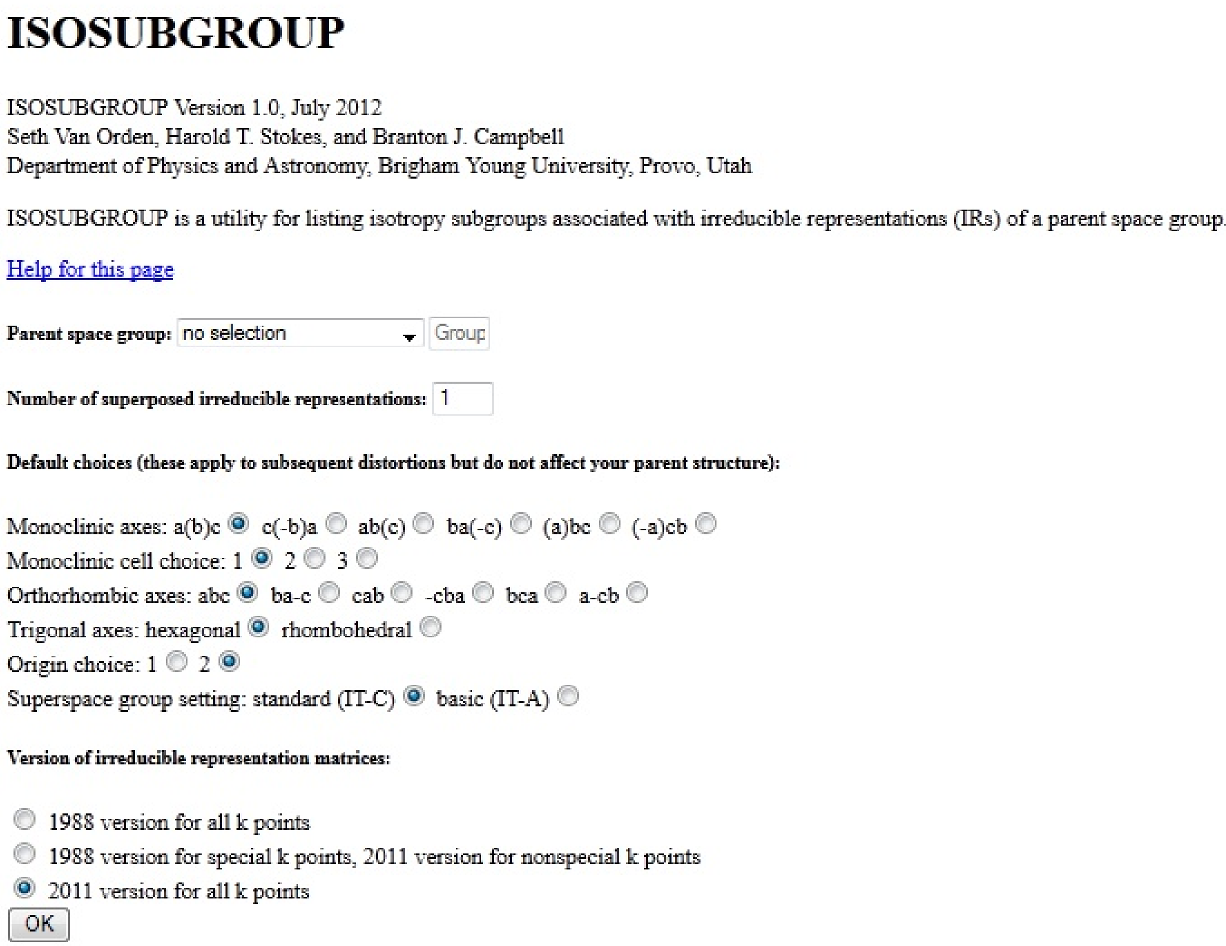


Figure 2.2 ISOSUBGROUP's home page before the CSS addition.

`<div class="container">`.

This line of code connects everything found inside the above div tag to the key word "container" found in the CSS document. However, the CSS conveniently changes many style aspects without the need of classes in tags. The font style and color and similar aspects did not need any manual changes. Some new parts took a little more work. The menu bar at the top of each page took an additional 20 or so lines of code, but its added convenience and style considerably outweighed the inconvenience of adding the extra lines of code.

In the end, it was decided to keep the colors and background simple, so that ISOSUBGROUP would remain easy to use and easy to read. The finished look is displayed in Figure 2.3. It is much improved, yet it still remains easy to read. It is still primarily black on white for those with poor eye sight.

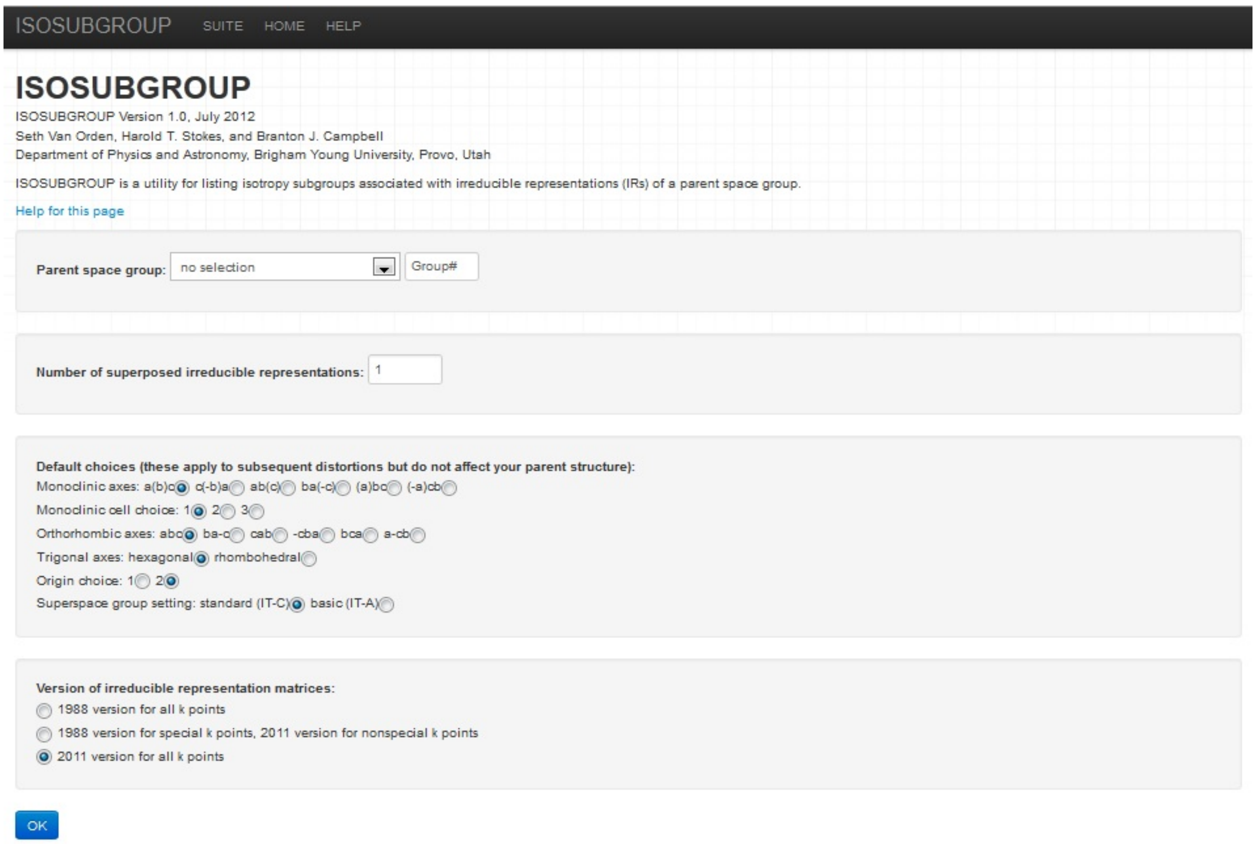


Figure 2.3 ISOSUBGROUP's home page after the CSS addition.

Chapter 3

Guide

3.1 The Home Page

This chapter is written as a user guide for ISOSUBGROUP. We will be addressing the reader as a user with the personal pronoun "you." This information can be accessed by clicking on any of the help links on each page. A screen shot for the home page can be found in Figure 2.3.

For the parent space group you will enter the parent space group symmetry. You may either choose the space group from the drop-down box on the left or enter the space group number in the box on the right. Each line in the drop-down box contains (1) the space-group number from *International Tables*, (2) the short Hermann-Mauguin symbol, and (3) the Schoenflies symbol (Hahn, 2006). The symbols in the drop-down box are generic and do not influence the space-group preferences. If any character is entered into the box on the right, the drop-down box selection will be ignored.

Each IR of the parent space group may produce distortions. You can superpose distortions from different IRs. You first enter in the number of superposed IRs on this page.

If the parent space group symmetry you selected has more than one setting in *International*

Tables, then you should select the desired setting in the Space group preferences section. The same settings are available for both non-magnetic and magnetic space groups.

An IR maps each space-group operator onto a matrix. You can select a version for your IR matrices.

Clicking on "OK" takes you to a page "k vector."

3.2 The k Vector Page

A screen shot for ISOSUBGROUP's k vector page is found in Figure 3.1. Choose a k point in the first Brillouin zone for each superposed IR. The k vector affects the possible superlattices which can result from the distortion. Each line in the drop-down menu contains (1) the label of the k point using the notation of Miller and Love, (2) the label of the k point using the notation of Kovalev (only included for special k points), and (3) the coordinates of the point in terms of the basis vectors of the reciprocal lattice of the conventional lattice defined in *International Tables*. Some k points contain one or more of the parameters a, b, or g (for example, a,0,0). You must enter the values of the parameters needed for fully specifying the position of the k point. If no parameters are needed (for example, the k point (0,0,0)), you do not need to enter any values. You must enter all parameters as rational numbers (for example, 1/2 instead of 0.5).

Incommensurate k-points are points with one or more irrational components. If you want to explore an incommensurate modulation at a given k-point, select "1" for the number of modulations to include (the current version only supports one modulation), and you don't need to enter any values for the parameters a,b,g. An incommensurate distortion arising due to d incommensurate modulations will possess the symmetry of a (3+d)-dimensional superspace group. The isotropy subgroups arising from a single modulation at an incommensurate k-point are listed in a table at the ISO(3+1)D web site (ISOTROPY suite).

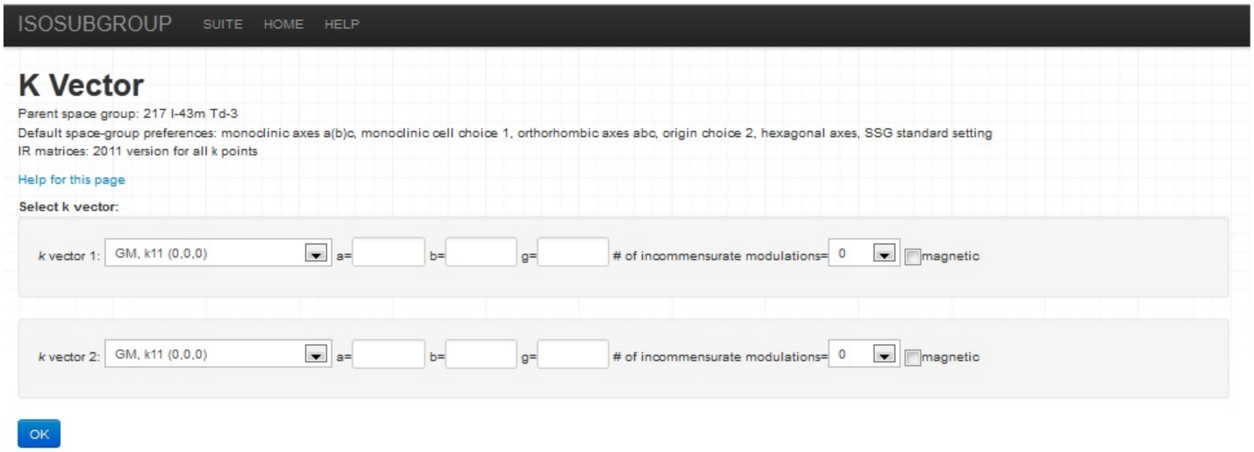


Figure 3.1 ISOSUBGROUP's 2nd page where the user selects the k vector(s).

Figure 3.2 ISOSUBGROUP's 3rd page where the user selects the Irreducible Representation(s).

Use this magnetic checkbox to select which of your k points you would like to be magnetic.

Clicking on "OK" takes you to the page "Irreducible Representaions (IR)."

3.3 The Irreducible Representations Page

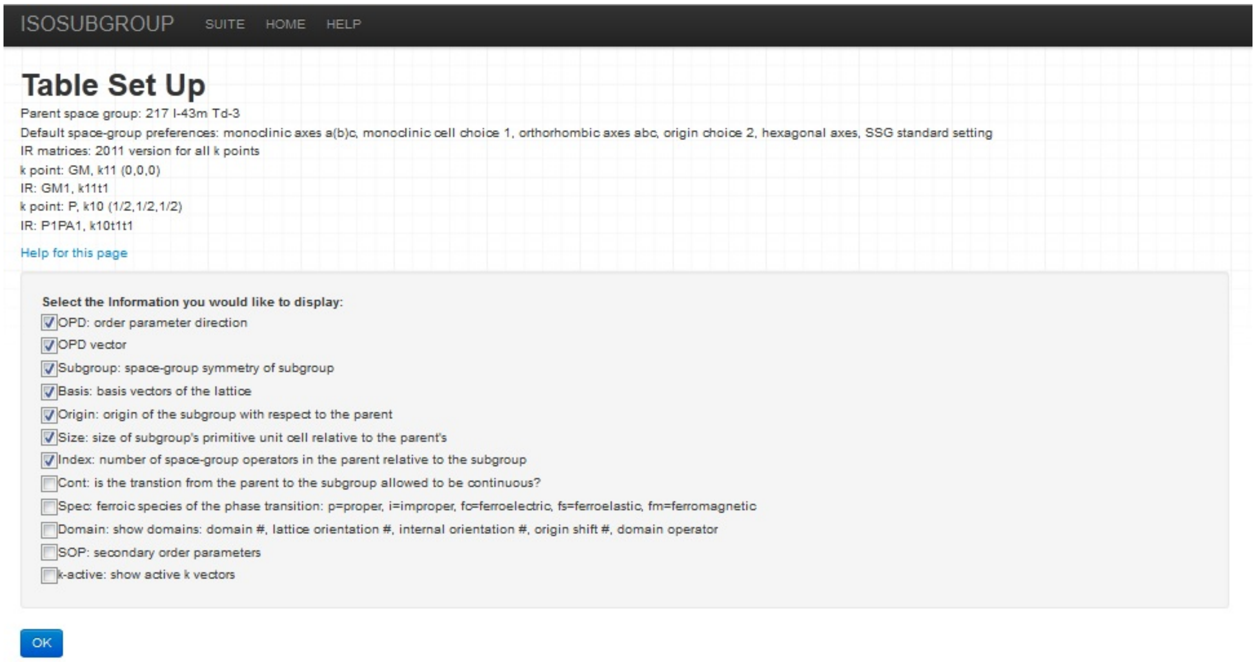
A screen shot for ISOSUBGROUP's irreducible representation page can be seen in Figure 3.2. Choose an irreducible representation (IR) for each superposed IR. The list in the drop-down menu contains IRs associated with the k point you selected. Each line in the drop-down menu contains the label of the IR using the notation of (1) Miller and Love and (2) Kovalev (only included for IRs associated with special k points). Type-2 and type-3 IRs are complex. We want real IRs since distortions induced by the IR must be real. In these cases, we obtain the physical IR from the direct sum of the IR and its complex conjugate. These are indicated in the notation by a pair of IR symbols (for example, P1P1, where P1 is a type-2 IR which is equivalent to its own complex conjugate, and A2A3, where A2 and A3 are type-3 IRs which are complex conjugates of each other). Note that physical IRs are reducible with respect to complex numbers but irreducible with respect to real numbers. When dealing with magnetic distortions, IRs that produce magnetic moments have an "m" prepended to their labels.

Clicking on "OK" takes you to the page "table set up."

3.4 The Table Set Up Page

A screen shot for ISOSUBGROUP's table set up page can be seen in Figure 3.3. This page allows you to select the information you would like to display in the generated table on the next page. Each checkbox represents data that will take the form of columns in the generated table. Check all the boxes for the data you wish to display.

Clicking on "OK" takes you to the page "table."



ISOSUBGROUP SUITE HOME HELP

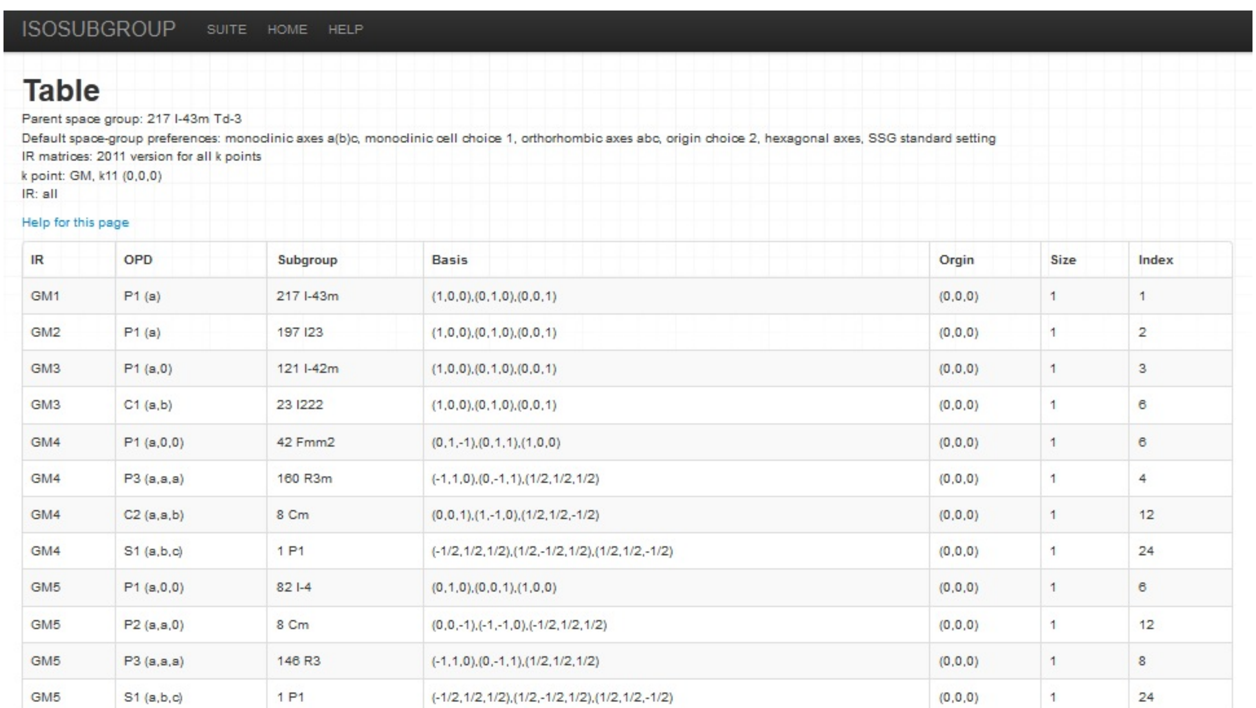
Table Set Up

Parent space group: 217 I-43m Td-3
Default space-group preferences: monoclinic axes a(b)c, monoclinic cell choice 1, orthorhombic axes abc, origin choice 2, hexagonal axes, SSG standard setting
IR matrices: 2011 version for all k points
k point: GM, k11 (0,0,0)
IR: GM1, k11t1
k point: P, k10 (1/2,1/2,1/2)
IR: P1PA1, k10t1t1
Help for this page

Select the Information you would like to display:
- [x] OPD: order parameter direction
- [x] OPD vector
- [x] Subgroup: space-group symmetry of subgroup
- [x] Basis: basis vectors of the lattice
- [x] Origin: origin of the subgroup with respect to the parent
- [x] Size: size of subgroup's primitive unit cell relative to the parent's
- [x] Index: number of space-group operators in the parent relative to the subgroup
- [ ] Cont: is the transtion from the parent to the subgroup allowed to be continuous?
- [ ] Spec: ferroic species of the phase transition: p=proper, i=improper, fc=ferroelectric, fs=ferroelastic, fm=ferromagnetic
- [ ] Domain: show domains: domain #, lattice orientation #, internal orientation #, origin shift #, domain operator
- [ ] SOP: secondary order parameters
- [ ] k-active: show active k vectors

OK

Figure 3.3 ISOSUBGROUP's 4th page where the user selects the which table columns to show.



ISOSUBGROUP SUITE HOME HELP

Table

Parent space group: 217 I-43m Td-3
Default space-group preferences: monoclinic axes a(b)c, monoclinic cell choice 1, orthorhombic axes abc, origin choice 2, hexagonal axes, SSG standard setting
IR matrices: 2011 version for all k points
k point: GM, k11 (0,0,0)
IR: all
Help for this page

IR	OPD	Subgroup	Basis	Orgin	Size	Index
GM1	P1 (a)	217 I-43m	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	1
GM2	P1 (a)	197 I23	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	2
GM3	P1 (a,0)	121 I-42m	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	3
GM3	C1 (a,b)	23 I222	(1,0,0),(0,1,0),(0,0,1)	(0,0,0)	1	6
GM4	P1 (a,0,0)	42 Fmm2	(0,1,-1),(0,1,1),(1,0,0)	(0,0,0)	1	6
GM4	P3 (a,a,a)	160 R3m	(-1,1,0),(0,-1,1),(1/2,1/2,1/2)	(0,0,0)	1	4
GM4	C2 (a,a,b)	8 Cm	(0,0,1),(1,-1,0),(1/2,1/2,-1/2)	(0,0,0)	1	12
GM4	S1 (a,b,c)	1 P1	(-1/2,1/2,1/2),(1/2,-1/2,1/2),(1/2,1/2,-1/2)	(0,0,0)	1	24
GM5	P1 (a,0,0)	82 I-4	(0,1,0),(0,0,1),(1,0,0)	(0,0,0)	1	6
GM5	P2 (a,a,0)	8 Cm	(0,0,-1),(-1,-1,0),(-1/2,1/2,1/2)	(0,0,0)	1	12
GM5	P3 (a,a,a)	146 R3	(-1,1,0),(0,-1,1),(1/2,1/2,1/2)	(0,0,0)	1	8
GM5	S1 (a,b,c)	1 P1	(-1/2,1/2,1/2),(1/2,-1/2,1/2),(1/2,1/2,-1/2)	(0,0,0)	1	24

Figure 3.4 ISOSUBGROUP's final page where the results are shown in a table.

3.5 The Table Page

A screen shot for ISOSUBGROUP's table page can be seen in Figure 3.4. ISOSUBGROUP uses precomputed data tables containing the isotropy subgroups for single IRs at special k points and for single IRs associated with incommensurate k points. For any other case (IRs at non-special k points or superposed IRs), the isotropy subgroups must be generated on demand and saved to a temporary file on the server. The generation of isotropy subgroups may take anywhere from a few seconds to many hours. Be prepared to wait while they are being generated. Factors that increase the time required include a high-symmetry parent, a low-symmetry distortion, or the coupling of multiple IRs. Calculations on the server are automatically shut off if they have not run to completion within one hour, and all temporary files on the server are automatically deleted once a week.

Chapter 4

Conclusion

4.1 Conclusion

ISOSUBGROUP is fully functional and ready to be placed online. ISOSUBGROUP is user friendly just like ISODISTORT without having a specific material in mind. I have learned a great deal from creating it. Before starting this project, I did not know HTML, FORTRAN or CSS, and I have learned a great deal about all three. Everyone will be able to access ISOSUBGROUP online soon.

4.2 Direction for Future Work

ISOSUBGROUP will be made available to crystallographers everywhere as soon as a paper is written about its release. There will most certainly be updates as bugs are found and improvements are needed. The CSS was found to be beneficial enough that Stokes and Campbell decided to add it to ISOTROPY and ISODISTORT. This will be added by Campbell after I have cleaned it up and simplified it for maintenance sake. The future looks bright for crystallographers everywhere.

Appendix A

Appendix: Code

The following code is a single subroutine in ISOSUBGROUP written in FORTRAN. The lines starting with an asterisk represent comments. This subroutine creates a string containing a desired IR.

A.1 FORTRAN Code

```
* get irrepstring
      subroutine  isosubgroup_get_irrepstring(irrpointer,magnetic_irrep,
     $     irrepstring)
* arguments:
*   irrpointer (input): pointer to irrep in data_little.bin
*   magnetic irrep (input): true if irrep is magnetic
*   irrepstring (output): string containing irrep

      implicit none
      integer i,m,irrpointer
      logical magnetic_irrep
```

```
character irrepstring*(*)
include 'declare_irreps.f'
include 'declare_little.f'
irrepstring=' '
m=0
if(magnetic_irrep)then
  irrepstring(m+1:m+1)='m'
  m=m+1
endif
irrepstring(m+1:m+8)=little_irr_full_label(irrpointer)
m=len_trim(irrepstring)
i=little_irr_old(irrpointer)
if(i.ne.0)then
  irrepstring(m+1:m+2)=', '
  m=m+2
  if(magnetic_irrep)then
    irrepstring(m+1:m+1)='m'
    m=m+1
  endif
  irrepstring(m+1:m+8)=irrep_label_kov(i)
  m=len_trim(irrepstring)
endif
end
```

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Twitter. Twitter Bootstrap. (http://twitter.github.io/bootstrap/).

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