## The CARAT Homepage

CARAT is a computer package which handles enumeration, construction, recognition, and comparison problems for crystallographic groups up to dimension 6. The name CARAT itself is an acronym for Crystallographic AlgoRithms And Tables.

CARAT is a compilation of various programs written in C developed under HP-UX and Linux, and should be portable to most Unices.

In particular CARAT does not come together with an environment, but relies on the ordinary unixes shell and files for input and output. This is one of the points which distiguishes CARAT from most other packages for computer algebra, like <u>GAP</u>. If you would like such a user interface, the current version of GAP comes with an interface to CARAT, which enables one to use the most important functions of CARAT, but not all.

### Some of the features of CARAT

- CARAT can construct any space group up to degree 6 from its build in table of Q-classes,
- CARAT can name a space group R given by generators unily, ie. generate a name which only depends on the isomorphism of R and determines it uniquely.
- Decide Q-, Z- and affine equivalence of finite unimodular groups and space groups resp.
- Calculate the integral normalizer of a finite unimodular group.

# CARAT-introduction and Page of low dimensional Bieberbach groups

- The <u>CARAT-introduction</u> explains all programs and contains several examples!
- The <u>Page of low dimensional Bieberbach groups</u> which enables you to look at all torsion free space groups up to degree 6.

#### Papers

Here we provide some postscript files of papers which are dealing with CARAT or have been written with the help of it:

• J. Opgenorth, W. Plesken, T. Schulz: <u>Crystallographic algorithms and tables</u>, Acta. Cryst (1998), 517-531.

This paper deals with the basic algorithms behind CARAT, and can be viewed as an

introduction to the underlying structures to crystallographic groups from an algorithmic point of view.

- W. Plesken, T. Schulz: <u>Counting crystallographic groups in low dimensions</u>, Experimental Mathematics 9:3 (2000), 407-411 The paper describes the results obtained by CARAT in counting all space groups up to dimension 6.
- C. Cid, T. Schulz: <u>Computation of Five and Six Dimensional Bieberbach Groups</u>, Experimental Mathematics 10:1 (2001), 109-115 This paper is concerned with the computation and classification of 5- and 6-dimensional torsion-free crystallographic groups, also known as Bieberbach groups.

As a result, we have the following table for Crystallographic and Bieberbach groups up to dimension 6:

	1	2	3	4	5	6
No of Q-classes	2	10	32	227	955	7103*
No of Z-classes	2	13	73	710	6079	85308*
No of affine classes	2	17	219	4783	222,018	28,927,915*
No of Bieberbach groups	1	2	10	74	1060	38746

\* in the original version of CARAT, the Q-classes for the group group.7477 and max.22 were in fact the same by accident, hence resulting in these corrected figures.

#### Download

Here you can <u>download CARAT</u> (version 2.1b1 19.07.2008, including some adaptations of the code to recent gcc versions by Franz Gähler, Feb. 2007). For installation, please extract the file downloaded and refer to the file README.install. You can also download <u>historic</u> versions of CARAT.

#### Changes of the new version

- The new function *Graph* calculates the graph of inclusions of a geometric class of space groups.
- The new function *KSubgroups* calculates maximal klassengleich subgroups.
- The new function *KSupergroups* calculates minimal klassengleich supergroups
- The new function *TSubgroups* calculates maximal translationengleich subgroups.
- The new function *TSupergroups* calculates minimal translationengleich supergroupe.
- Bugfixes have been made for *Z\_equiv*, *Name* and *Presentation*.

- *Extract -r -D* writes space groups directly into files. *Conv* now also converts groups and converts to TeX.
- *Name -c* gives the name of a (space-)group in a short form. The Hermann-Mauguin-Symbols can be calculated in dimension 2 and 3 now (*Name -M*).
- Extensions/Vectorsystems -S writes representatives of the affine classes in files.

#### **Contact**

If you have any question concerning CARAT (e.g. installation etc.), or find a bug in the package, please do not hesitate to contact us:

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