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A list of free software for chemical and graph theoretical applications

composed by G. Brinkmann and P.W. Fowler

The following list gives a very short description of some freely available software packages and programs in the area of graph theory and chemical graph theory. Most of the software is authored by or otherwise related to participants of the conference CSD3. We do not give the names of the (sometimes various) authors of the software or list the operating systems on which it runs. This and other detailed information can be obtained via the given links and/or email addresses.

bliss

Function: Given a graph as input, bliss computes a set of generators for the automorphism group of the graph and (optionally) a canonical labeling for the graph.

how to obtain: `http://www.tcs.hut.fi/Software/bliss`

CaGe (the Chemical & abstract Graph environment)

Function: CaGe is a user interface that connects generators for various types of planar/spherical graphs with embedders and visualisation programs that show the graphs in 2 or 3 dimensions or even an unfolding of the 3-dimensional embedding. The generators can be used with the user interface, but also as stand-alone programs. It contains generators for fullerenes, tubetype fullerenes (caps and halftubes), planar polycyclic hydrocarbons, 3-regular planar graphs with given face sizes (see CGF in this list), triangulations and polytopes (see plantri). It is also possible to pipe graphs from other programs or files into CaGe in order to use the embedders and visualisation programs.

how to obtain: `http://www.mathematik.uni-bielefeld.de/~CaGe/`

Cliquer

Function: Cliquer is a set of C routines for finding cliques in an arbitrary weighted graph. It is designed with the aim of being efficient while still being flexible and easy to use. The main features of Cliquer include: support for both unweighted and weighted graphs (faster routines for unweighted graphs), searching for maximum respectively maximum-weight cliques, searching for cliques with size respectively weight within a given range, restricting the search to maximal cliques.

how to obtain it: `http://users.tkk.fi/~pat/cliquer.html`

CGF

Function: CGF generates complete classes of cubic maps with a given genus, a given number of vertices and a given set of face degrees.

how to obtain: `http://www.mathematik.uni-bielefeld.de/~harmuth/Welcome.html` or `http://people.freenet.de/thomas.harmuth/`. It also comes with the CaGe-package.

CPF

Function: CPF generates complete classes of simple cubic planar maps with a given number of vertices and a given set of face degrees.

how to obtain: `http://www.mathematik.uni-bielefeld.de/~harmuth/Welcome.html` or `http://people.freenet.de/thomas.harmuth/`

DART (Decision Analysis by Ranking Techniques)

Function: DART contains several methods for multicriteria decision making.

how to obtain: `http://ecb.jrc.it/`

E-DRAGON

Function: E-DRAGON is a software for molecular descriptor calculations. It calculates 1664 molecular descriptors for different input formats.

how to obtain: `http://www.vcclab.org/lab/edragon/`

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genreg

Function: For given k, n, g the program genreg computes simple connected k-regular graphs on n vertices with girth at least g.

how to obtain: `http://www.mathe2.uni-bayreuth.de/markus/reggraphs.html`

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gradpart

Function: Gradpart computes all isomorphism types of graphs with a given degree sequence.

how to obtain: `http://www.mathe2.uni-bayreuth.de/thomas_g/gradpart.html`

GraPHedron

Function: GraPHedron is a computer-assisted system which helps to obtain conjectures in graph theory. It uses a polyhedral approach to find strongest relations among graph invariants. This approach provides a formal framework allowing to identify interesting and tight relations – under some conditions, these conjectures can be considered as optimal.

The class of graphs under study can be restricted to classes of chemical interest (e.g., chemical graphs or trees) and several chemical invariants are available (e.g., the Randić index).

how to obtain: `www.graphedron.net`

GrInvIn

Function: GrInvIn is an interactive software package for studying graphs, their properties (invariants) and the relations between these properties. One of the intentions is also to use the package in graph theory education (also for chemistry students). GrInvIn includes a graph editor for drawing graphs, so-called 'factories' which create graphs of a certain type and computes invariants and topological indices. The system can also make *guesses* about the relation between the invariants which — when applied in teaching — the students are required to prove or disprove. The intention is similar to Ermelinda DeLaVina's *Graffiti.pc*. Java plugins allow the application to be easily extended.

how to obtain: `http://grinvin.org/`

Groups & Graphs

Function: (See also the corresponding article in this volume.)
Groups & Graphs is a software package for graphs, digraphs, automorphism groups, graph embeddings, projective configurations, polyhedra, convex hulls, and fractals.

how to obtain: `http://bkocay.cs.umanitoba.ca/G&G/G&G.html`

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gtools

Function: Gtools is a suite of programs for various purposes. Among others it contains very efficient generators for all graphs, all bipartite graphs, all digraphs, and all multigraphs. All of these generators allow various restrictions on the set of graphs to be generated (e.g. maximum degree, number of edges, etc).

how to obtain: `http://cs.anu.edu.au/~bdm/nauty/`

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helicenes

Function: Helicenes is a program to generate all fusenes or benzenoids with a given number of hexagons very efficiently. The generation can be restricted to Kékulean structures.

how to obtain: Email to `Gunnar.Brinkmann@UGent.be` or `Gilles.Caporossi@gerad.ca`

KBGRAPH (Knowledge Base Graph Theory)

Function: (See also the corresponding article in this volume.)
KBGRAPH supports graph-theoretical proofs and helps with the analysis of a given class of graphs.

how to obtain: Email to `t4141ax@mail.lrz-muenchen.de`

MDC (Molecular Descriptors Correlations)

Function: The Molecular Descriptor Correlations is a tool for the analysis of molecular descriptor correlations calculated on 221,860 molecules.

how to obtain: `http://www.disat.unimib.it/chm/download/softwares.htm`

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minibaum

Function: Minibaum is a program specialised on the generation of 3-regular graphs. The generation can be restricted in various ways, e.g. to generate only graphs with a given minimum girth, only bipartite graphs or only snarks.

how to obtain: Email to `Gunnar.Brinkmann@UGent.be`

MTF

Function: MTF generates maximal trianglefree graphs on a given number of vertices – that is trianglefree graphs in which every additional edge would lie in a triangle. It has several options in connection with triangle Ramsey numbers.

how to obtain: Email to `Gunnar.Brinkmann@UGent.be` or `thomas@harmuths.de`

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nauty

Function: Nauty is a C-routine that computes a set of generators for the automorphism group of a graph and (optionally) a canonical labeling for the graph.

how to obtain: `http://cs.anu.edu.au/~bdm/nauty/`

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newGRAPH

Function: NewGRAPH is a fully integrated environment for research in graph theory. Its purpose is to help a researcher pose, verify or disprove a conjecture and to enable him to experiment with graphs. NewGRAPH is also designed to be used in graph theory education.

how to obtain: `http://www.mi.sanu.ac.yu/newgraph/`

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plantri

Function: (See also the corresponding article in this volume.)
Plantri is a program to generate various classes of planar graphs, such as all planar graphs, planar cubic graphs, planar triangulations, planar quadrangulations, polyhedra, and triangulations of the disk. Various options allow to further restrict the class of graphs to be generated.

how to obtain: `http://cs.anu.edu.au/~bdm/plantri/`

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posets

Function: This program generates all non-isomorphic posets on a given number of points.

how to obtain: Email to `Gunnar.Brinkmann@UGent.be` or `bdm@cs.anu.edu.au`

Systre

Function: Systre computes automorphism groups, canonical forms and embeddings of periodic graphs. Examples of periodic graphs are the atom-bond networks of extended crystal structures or the contact graphs of periodic sphere packings. The main computational tool used is a generalization of Tutte's famous barycentric node placement idea. Nodes can be identified by their barycentric positions, which leads to polynomial time algorithms for both the automorphism and the canonical form computation. A small drawback is the fact that, so far, Systre only works if no two nodes have equal barycentric positions. This seems to be a rare case, though, in practical applications and often indicates that the graph in question has a non-crystallographic automorphism group.

how to obtain: www.gavrog.org

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togen

Function: Togen generates cubic toroidal maps with a given number of vertices.

how to obtain: `http://www.mathematik.uni-bielefeld.de/~harmuth/Welcome.html` or `http://people.freenet.de/thomas.harmuth/`

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togen7

Function: Togen7 generates cubic toroidal maps with a given number of vertices where each face has a degree less than or equal to 7.

how to obtain: `http://www.mathematik.uni-bielefeld.de/~harmuth/Welcome.html` or `http://people.freenet.de/thomas.harmuth/`