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Graph6Java: a researcher-friendly Java framework for testing conjectures in chemical graph theory. (English) [Zbl 07410923]

Summary: An important part of a chemical graph theorist’s research work is concerned with making observations and developing intuition about a particular research problem through extensive numerical testing. Research questions in chemical graph theory are often restricted to specific graph classes in which one is either looking for extremal values and extremal graphs of graph invariants, or graphs satisfying certain constraints, or inequalities between different invariants. Many graphs from such classes can nowadays be easily generated or readily downloaded from the web in nauty’s graph6 format. We describe here a Java framework we call Graph6Java for answering the above research questions among sets of graphs given in graph6 format, which represents unification of testing programs that we had used over the years. Graph6Java consists of templates that can be easily customized so that the researcher’s initial work should reduce just to rephrasing a question in hand within a specific template. This way one can quickly prepare numerical calculations to be performed over large sets of graphs and shift focus to more creative research work instead. The use of templates is described in detail and illustrated on several conjectures from chemical graph theory.

MSC:

92E10 Molecular structure (graph-theoretic methods, methods of differential topology, etc.)
68C92 Chemical graph theory
92-04 Software, source code, etc. for problems pertaining to biology

Software:
LEDA; nauty; SymPy; AutoGraphiX; NetworkX; BlueJ; Colt; GrInvIn; plantri; Graph6Java; Mathchem; mpmath; House of Graphs; GraphTheory