Klin, Mikhail; **Rücker, Christoph**; **Rücker, Gerta**; **Tinhofer, Gottfried**

Algebraic combinatorics in mathematical chemistry. Methods and algorithms. I: Permutation groups and coherent (cellular) algebras. (English) Zbl 1029.05151

Match 40, 7-138 (1999).

Summary: Let (G, Ω) be a permutation group of degree n. Let $V(G, \Omega)$ be the set of all square matrices of order n which commute with all permutation matrices corresponding to permutations from (G, Ω). $V(G, \Omega)$ is a matrix algebra which is called the centralizer algebra of (G, Ω). In this paper we introduce the combinatorial analogue of centralizer algebras, namely coherent (cellular) algebras and consider the properties of these algebras. It turns out that coherent algebras provide a very helpful tool for the investigation of the symmetries of graphs of different kinds, in particular, of molecular graphs.

MSC:

05C90	Applications of graph theory
92E10	Molecular structure (graph-theoretic methods, methods of differential topology, etc.)

Software:

nauty