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Chemical Sub-Structural Cluster Expansions.

Molecular structure-property correlation has a long history, and still remains of chemical interest. For an analysis in terms of sub-structures, typically graphs arise with colored vertices and decorated edges. Initially restriction may be to simple graphs, representing singly bonded hydrocarbons, though common mathematical subgraph counting polynomials need extension, particularly for expansions arising in statistical mechanics and many-body quantum mechanics. Focus here is on general sub-structural cluster expansions for a connected graph G belonging to a “universe” U of (molecular) graphs. A real-valued graph invariant is expanded as a linear combination of variables each corresponding to an isomorphism class of subgraphs satisfying “C-subgraph” conditions, which in addition to being a subgraph H of G also include possibilities of H being spanning or connected, and perhaps induced, isometric, or convex (just for the components if disconnected). The general C-subgraphs lead to a complete expansion, for which Möbius inversion is conceivable. In applications the expansions are truncated to subgraphs H of smaller “size”, whence questions arise, say as to rapidity of convergence. (Received September 21, 2010)