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Substitution-reaction posets in chemistry

Substitution-reaction posets represent a chemical reaction placing substituents at different locations of a molecular skeleton. Mathematically, we let G be a permutation group acting on the members of a finite set S representing substitution positions and define a partial ordering of orbits of subsets of S . Chemically, poset members represent substitutional isomers, and the associated Hasse diagram a substitution-reaction network. This self dual, ranked poset has unique maximum and minimum elements and coincidence of three metrics: splinoid fitting, cluster expansion; and flow-network methods. Chemical examples include a 13-member poset for benzene, and a 210-member poset for polychlorinated biphenyls.