1014-06-582   **Douglas J. Klein*** (`kleind@tamug.edu`), Texas A&M University at Galveston, Galveston, TX 77553. *Partial Orderings in Chemistry: Substitution-Reaction Posets.*

Througout chemistry partial orderings appear ubiquitous, e.g., involving (molecular) branching, acidity, electro-affinity, chemical "aromaticity", or Mendelev's iconic periodic table. Here attention is to progressive reaction networks, as that of successive replacement in benzene of H-atoms by Cl-atoms. Let S be a set (of substitutent positions on a molecular skeleton); let G be a group of permutations acting on the members of S; and consider the minimal G-invariant collections x of subsets of S. Then the substitution-reaction poset P(S,G) of these orbits has x<x' iff there are members C of x and C' of x' such that C is a subset of C'. Chemically x of P(S,G) is a substitutional isomer on skeleton S with symmetry G. Such posets: have unique maximum & minimum elements; are self dual; are ranked; and satisfy certain distance-consistency conditions. Also P(S,G) is related to double-coset structure in the full permutation group acting on S. Such P(S,G) aid in interpolations for properties of molecular species x in P(S,G). (Received September 20, 2005)