Subduction of coset representations
An application to enumeration of chemical structures

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(Received October 11, 1988; revised March 10,1989/Accepted June 3, 1989)

Summary. Enumerations of compounds based on a parent skeleton with and without the influence of obligatory minimum valency (OMV) are reported. The effect of the OMV is formulated by assigning different weights to the respective orbits of the parent skeleton. This type of enumeration requires introduction of several new concepts that are derived from the subduction of coset representations, e.g., a unit subduced cycle index, a subduced cycle index and the number of suborbits.

Key words: Enumeration of compounds — Table of marks — Coset representation — Unit subduced cycle index

1. Introduction

Enumeration of compounds in chemistry is one of the most important fields to which Pólya’s theorem [1] has been applied. Ruch et al. [2] and later Brocas [3] have proved the concept of double coset to be very convenient for such compound-counting problems. More recently, Hässelbarth [4] has developed an important method in this field. This is based on the concept of “table of marks” that goes back to Burnside [5]. Mead [6] has discussed the relationship between these methods by using common problems as examples.

In previous papers [7] we have reported the counting of organic reactions. The enumeration is based on the manipulation of reaction graphs that are subgraphs of imaginary transition structures. A more specific enumeration has also been accomplished by counting reaction-center graphs. In this enumeration we encountered a problem concerned with obligatory minimum valency (OMV) as discussed below. We have solved the problem by using two or more different
weights that are assigned to the respective orbits of a domain [8]. Although we have restricted ourselves to the case of organic reactions, our results are applicable to the enumeration of chemical structures under the influence of the OMV. A remaining problem is the counting of chemical structures with a given symmetry as well as a given weight, not only in the reaction counting but also in the compound counting.

The present paper deals with the remaining problem, which requires a more general approach than Hässe1barth's one in order to meet the OMV restriction. For this purpose, we clarify the usefulness of subduced representations of a transitive coset representation and of their further reduction into transitive permutation ones. This method provides novel concepts such as a unit subduced cycle index and a subduced cycle index, which are versatile guides for solving enumeration problems.

2. A parent skeleton characterized by a permutation representation and its equivalent positions specified by coset representations

A chemical compound can be considered to be a derivative of a given skeleton which has a skeletal symmetry. The skeleton has several sets (orbits) of equivalent positions. Each orbit is characterized by an obligatory minimum valency. For example, a twistane skeleton (1) has $D_2$ symmetry, which creates three orbits that have different OMVs. Each bridgehead position of the orbit marked with a solid circle has an OMV of 3 and can take C and N from a set of C, N, and O. The other orbits (bridge positions) permit the substitution of all the three atoms because of their OMV of 2. The OMV thus affects the counting of organic structures. The adamantane skeleton (2) has two orbits, one with OMV = 3 and the other with OMV = 2. Hence, substitution patterns on 2 should be restricted by the OMVs.

As a result of the above discussion, our question is formulated as follows: what is the number of compounds, with a given set of substituents (atoms or ligands), on a given skeleton with a specified subsymmetry of the skeleton under the restricting conditions of OMV?

The above discussion shows that our first object is the classification of substitution positions into equivalence classes. This is formulated to obtain the number