March 8, 1965

Dr. William J. Wiswesser
Research Chemist, Crops Division
U. S. Army Biological Laboratories
Fort Detrick
Frederick, Maryland 21701

Dear Dr. Wiswesser:

I have been reviewing the conjecture concerning fusion locants that underlies Rule 30. As you anticipated, the junctions must play a fundamental role in any systematic treatment of chemical graphs. However, the conventional outlook in counting "rings" is, in my view, already defective, when applied to complex fused systems, since it arbitrarily puts aside one principal face. This tends to obscure the symmetries and especially the isomorphisms of the graphs.

This is perhaps most simply illustrated by the prism - see attachment. (1) and (b) are of course isomorphic. Since the vertices are all equivalent, any one serves as initial locant (for your rule). However, the two projections govern a different choice of path.

Further difficulties arise with the bipentagon, shown on the second attachment. The isomorphic graphs are obtained by choosing, for a base, alternative faces of the polyhedron. This interesting graph has two overtly dissimilar Hamilton circuits (a) and (b). Unless I have misunderstood your rule, they also lead to a different choice of initial locant.

These annoyances are inconsequential to most practical purposes, but I have spent some time wrestling with steps that may lead to some mathematical rigor. At least those trivalent graphs that have Hamilton circuits can be dealt with fairly easily (and in turn the range of chemical graphs mappable on these).

The non-Hamilton graphs have been accommodated by mapping them in turn on polyhedra. The system then seems to work short of a polyhedron lacking a Hamilton circuit; so far Tutte's example with 46 vertices ("24 rings") is the smallest instance: the DENDRAL system has no means of specifying the canonical order of nodes for this particular graph, nor does this seem a tangible limitation. Some rather complex schemes could be laid on.

Where Hamilton circuits are discerned, a rather easy set of symmetry operations (the rotations and reflection) reveals a unique minimum list of chords, and in turn a canonical path, orientation and initial node. But I had better exert myself at completing the writeup of Part II to help clarify this account.

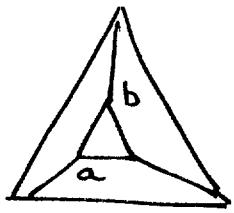
If I have misused or overlooked some aspect of the application of Rule 30, please let me know.

Sincerely yours,

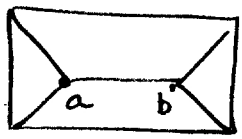
Joshua Lederberg
Professor of Genetics

Attachment 1

PRISM



aaab



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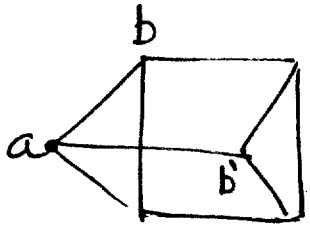
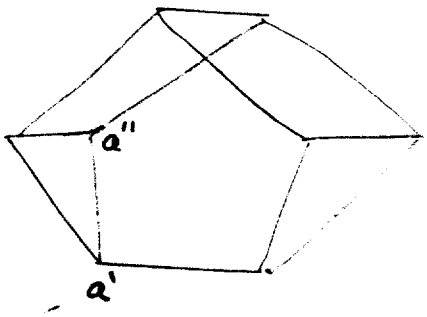
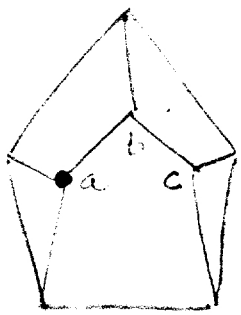
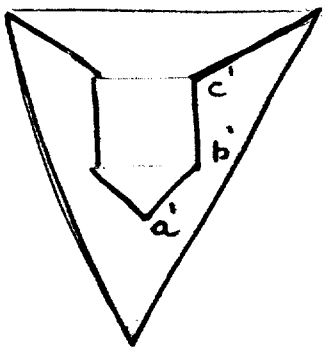


Attachment 2

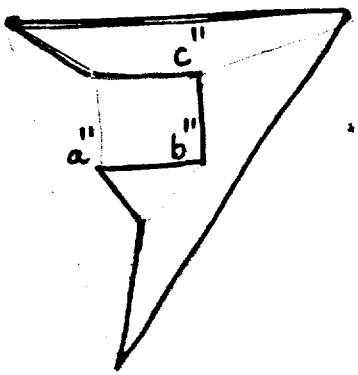




aaabc

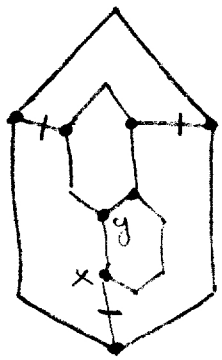


a'a'a'b'c'



a''a''a''b''c''

BICENTROON



Is x or y the initial locant?