DEPARTMENT OF CHEMISTRY
CORNELL UNIVERSITY
ITHACA, NEW YORK
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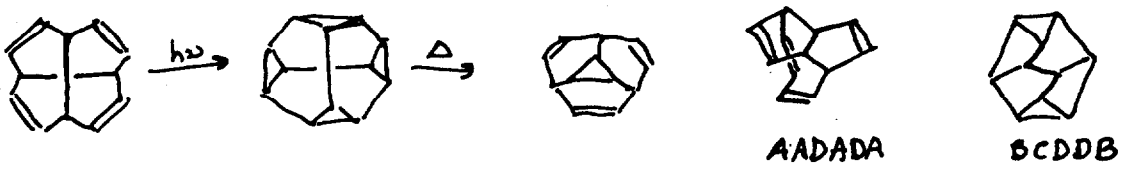
Prof. J.Lederberg
Dept. of Genetics
Stanford University

Dear Prof. Lederberg:

Thank you for sending to me a preliminary version of the DENDRAL-64 writeup. In your listing of the 8 graphs, have you not omitted the gauche ACCC?

My interest in your work stems from an attempt to enumerate all the isomers of $(CH)_{8,10,12}$. The set of trivalent graphs on 8 vertices gives the isomers of cycloctatetraene, etc. (Some isomers, eg. cyclopropenylcyclopentadiene, are of course not strictly cyclic graphs according to your definition). Enumerating by hand some time ago, I obtained about 90% of the 10 vertex graphs, 40% of the 12.

One has to construct models to judge if any of the graphs are of chemical interest. J.Meinwald and I are synthesizing the left-hand $C_{12}H_{12}$ isomer in the series below; there are



some theoretical reasons to expect it might undergo a concerted novel photochemical cyclization to the truncated tetrahedrane which in turn might fall apart thermally. We are also thinking of ways to make the AADADA 12 molecule, which should by a series of facile Cope rearrangements interconvert atoms within two groups of 8 and 4. The BCDDB 10 polyhedron also looks easy to synthesize.

I still have some difficulty with your notation for the graphs with no Hamiltonian circuit. When you have some time, I would appreciate it if you could explain your notation.

Sincerely,

Roald Hoffmann

Roald Hoffmann
Assoc. Prof. of Chemistry