March 26, 1973

Dr. Hartmut Braun
Abt. Prof. Dr. W. Lüttke
Organisch-Chemisches Institut der Universität
34 Göttingen
Windausweg 2
GERMANY

Dear Dr. Braun,

I am deeply embarrassed to have to tell you that your letter of April 26th 1972 was unfortunately mislaid. Please accept my contrite apologies and I hope that we may still be able to be of some service to you in response to your problem which interests us very much.

Our programs are written in the LISP language and it would probably be of little benefit to you to attempt to operate them unless you have an expert who is familiar with this particular kind of computer software. In our experience, unless we are dealing with a colleague who has identical equipment, it would requite about one month's effort to understand and to make minor revisions in the program to enable it to be run on other computer systems. And I am afraid I have to tell you that we are constantly up-dating and correcting the program which I am afraid to say is also some discouragement. However, if you do have such a colleague and he has the means to be able to spend a few weeks with us, we will be glad to give him all possible advice and guidance.

Alternatively we can attempt to run your problem on our system which we would be very glad to do.

I have to tell you right away, however, that in its general form it would simply not be practical to produce a complete list of all of the isomers of $C_{10}H_{10}$. There are over 1,000 of the strictly A-cyclic isomers and many more if one includes all of the possible cycles. I enclose a brief diagram that illustrates the dimensions of the problem and I can also refer you to my chapter in Waller's book "Biochemical Applications of Mass Spectrometry", John Wiley & Sons, New York, pp.193-207, 1972.

I can, however, enclose a set of diagrams of the trivalent planar graphs of orders from 0 to 10 which, indeed, must encompass the example, $C_{10}H_{10}$, with the following possible exceptions: (1) a quadrivalent center, all cases of which are, however, also enumerated up to 8 vertices or (2) a non-planar graph, for which there is not yet any precedent among small molecules.

I will remind you that a vertex is a point of juncture of two simple rings so that the case where $C_{10}H_{10}$ must be mapped onto as many as 10 vertices would represent a physically unrealizable degree of bridging. One can achieve the total enumeration of $C_{10}H_{10}$ cyclic molecules by mapping additional carbon atoms onto the edges of the graphs of lower order.

The most extensive, and essentially trivial,example would be cyclodecane where all 10 carbons would be planted on the single edge (i.e. simple ring) of the graph of vertex or 0. One would then also have to remove sufficient hydrogens, i.e. create unsaturations to match the empirical formula.

I would encourage you to experiment briefly with these kinds of manipulations so as to familiarize yourself with the problem but I do not think it is a profitable way to spend one's time in working out all cases! For this we indeed have some computer programs but they would run for a very long time and have an essentially useless if very voluminous output without anticipating some of the criteria by which one would intend to filter them. If you have given any thought to this problem it might be possible to incorporate those criteria into the program, so that one indeed would be able to generate a usefully restricted list of the possibilities that have not yet been discriminated. For example, it should be possible to get some idea of the total number of double bonds in a particular molecule by observing the results of exhaustive hydrogenation. But in any case I think it would be useful to start a dialogue to discuss the strategies for solving this problem and for this purpose we would be happy to provide help of the kind that the computer programs can give. I do promise that there will be a much shorter interval prior to the next response!

For speed I am enclosing some of the material by first class air mail and will forward some bulky successors by air parcel post.

Sincerely yours,

Joshua Lederberg
Professor of Genetics

JL/rr
Enclosure

P.S. I guess I do have to send you all of the ten vertex figures now since diademane already contradicts my statement that this group would be unbuildable for $C_{10}H_{10}$. It must be very difficult to do this except where there is a high order of symmetry and I am also beginning to think that you may have to give serious consideration to non-planar structures. I have not constructed diagrams for these but I think you can build them yourself if you understand the code for the 13 examples listed. Diademan itself corresponds to BDEBB.