

FEB 20 1965

Dear Professor Klee--

I was quite delighted to receive your note, and look forward to studying the report you mentioned. The prospect of opening up this kind of communication is of course the main purpose of ~~publishing~~ publishing notes like that in the PNAS and I do hope to see it flourish. It may be rather informal, but it is convenient to pass on some more background on what we are doing in the form of the enclosed copies of other material.

At this moment I am just in the course of final revision of part 2 of the DENDRAL system, and do not know whether I will be able to assimilate your new information into it, but will surely make every effort to do so in writing up the later parts. I hope you will give me the privilege of quoting it as a forthcoming publication.

Having assured ourselves to a practical certainty that the graphs through 18 vertices either have Hamiltonian circuits, or are unions of graphs of lower order, we can therefore feel somewhat comfortable that we can anticipate all the graphs of practical consequence in organic chemistry, and in this sense the problem is solved for our immediate purposes. However, I am sure there are deeper generalizations than I know how to deal with, and which might simplify many aspects of programming the hypothesis-generator, and also the problem of efficient search techniques for matching substructures (which I have just not attempted to deal with-- perhaps you know of Sussenguth's work on this). I also have some immediate problems in dealing with symmetries of the various graphs so as to produce an economical generator for the canonical forms without undertaking the intolerable labor of retrospectively checking the isomorphism of various mappings.

Unless this is already cited in your report, could you send me Bouwkamp's initials and full address, as I would indeed like to follow up your reference to his compilation. I feel we have the trivalent graphs fairly well in hand now even up to 18 vertices, but he may well have a much more attractive to our approach to quadrivalent vertices-- (I will have to send you a draft of part 2/dendral which has progressed somewhat over the pnas note.)

Sincerely,

Joshua Lederberg

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Dear
Klee
12/11/64
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