March 31, 1975

Dr. Victor Klee
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Dear Victor,

Several times we have discussed possible intersections of deeper mathematical analysis of graphs and our chemistry project. I told you at one time that it was not a matter of urgent chemical necessity to know the smallest non-Hamiltonian graphs, but I hope I did not leave the impression that we felt we had solved all of our problems in that area! While we think we have an adequate catalogue of graphs for the construction of all possible molecules, we are still very much hampered by considerations of efficiency - especially in finding the symmetry groups of arbitrary constructions for labelling problems.

I am enclosing some material that may help tell you where we stand at the present time. I understand there is some possibility that you may be at the Center for Advanced Studies next year and if this is the case, I certainly would hope we may have the opportunity for continued closer interaction.

One issue has come up recently that you might be able to throw some light on. Until now we have given little consideration to the tetrahedral (specifically A_4) symmetry of the carbon atom which is of course extremely important in considerations of stereo-isomerism and the actual three-dimensional conformation of molecules. We hope to incorporate this in the near future.

In trying to patch in this capability into our existing system, it occurred to us to ask what was the simplest trivalent graph that exhibited A_4. Coxeter and Moser have some brief discussion of this which you are probably familiar with referring back to Kempe 1886. This is of course a digraph and the simplest transformation of this into an undirected graph is attached as my Figure 1. In order to obtain useful vertices for simulating the tetrahedral carbon atom, one would make constructions like Figure 2. One can of course make fairly simple variations on these graphs to satisfy particular restrictions like the absence of slings or whatever.

But I wanted to ask you if this is a subject that has been investigated further and if it is known that there are no simpler solutions to this question: what is the simplest graph that displays A_4? I would assume there might also be some fairly interesting more general theory to connect rigid

polyhedral with topological constructions. If you can point me to some moderately elementary discussion of those connections, I would be most appreciative.

The directed triangular subgraphs in Kempe's diagram are of course a surrogate for a particular kind of coloring of the nodes of the tetrahedron. I do not know what more you might wish to make of that but I can assure you that this would be of the greatest interest in the formulaizaiion of organic molecular structure.

I think we can patch in the properties of the group A4 into our own empirical pursuit of the labelling problem but it would certainly be helpful to have a sounder theoretical base than we have at the present time.

Connected with this is my previous remark that we can hardly be satisfied with the present run time efficiency of these programs and I hope to have some opportunity to discuss our strategyms in this area with you.

If it would be of any interest to you to become a collaborator for investigating these problems on the SUMEX system, I would be more than delighted to make the facility available to you. This does not have to involve any very formal commitment and if you would wish to do no more than have some demonstration from your own home terminal of how these systems can be run, we would be more than happy to afford this to you.

Sincerely yours,

Joshua Lederberg
Professor of Genetics

JL/rr
Enclosures