1-APR-75 14:11:48,2485
Date: 1 APR 1975 1411-PST
From: CARHART
Subject: CONGEN comments; A4 problem
To: Lederberg
cc: Carhart
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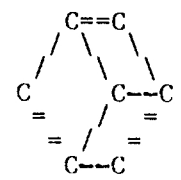
Unfortunately, your interest in CONGEN has taken off just when my pushdown stack overfloweth. I (and Dennis and Sue) have seen your note containing reactions to CONGEN, and we are in the process of digesting and discussing. I hope to compose a reply before I leave for Philadelphia on Sunday.

You will find that the gt40-draw is working somewhat more acurately now, though there are still problems. During the week Peter and I will be polishing this part of the program. By the way, I think it might be helpful if I mentioned the method by which the draw program (the tty draw) works - it may clarify my hesitance at doing away with crossing bonds. The draw program contains a very simple model builder (whose output you see on the GT40 screen) and a "flattener" to spread the molecule out in the plane. The subsequent code extracts a teletype idealization from the flattened model, and of course crossing bonds can occur. We are already running several seconds on moderate-sized molecules, and I feel that any additional jockeying to get the drawing into a planar representation will lead to excessive compute times. Our program contains the Feldmann drawing program, and when that one works, the modelling phase is skipped. Frequently, though, FELDRW fails but my part of the program finds a way to "idealize" the failure. Those strangely twisted large rings result, and sometimes spiro compounds are unbelievably twisted. I am currently going over that section of the draw program,and will see what I can do to detect these situations.

As for A4, Harold is back and we have had a good talk about groups and graphs. I think 22 nodes is about the limit - start with four of the following units



where the node in the center bears the free valence (the alternating double bonds are your idea). now if we bond four of these together as you were doing, we have a solution in 28 nodes. But we can save 6 nodes by merging, rather than bonding, the attachment points. this gives an octahedron with each edge containing C=C-C, and with four of the faces containind the fv-bearing carbons. If the trivalent -C= atoms in the drawing above are used for merging, then they come out as hexavalent nodes in the final graph.

Ray