

MAR 18 1975

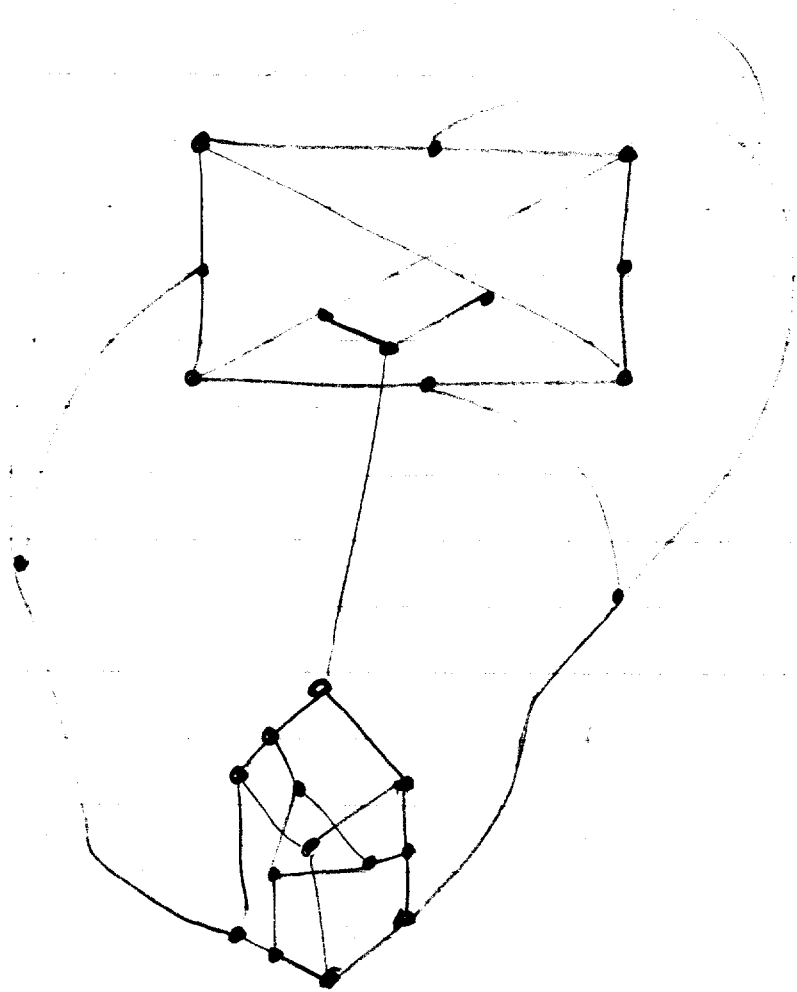
Dear Victor

Thank you for sending me Jim Lawrence's answer to the problem I posed to you in my letter of 3/31/75 (copy enclosed.) Hardly anything bearing exactly on this question has been published: the 2 enclosed reports may say something of the background (labelling; COORD).

The molecular structures that COORD handles ignore stereoisomerism (for the present): i.e., they classify the C atom as S_4 . At one time I wanted to categorize some stereoisomers. Instead of re-writing the basic program, I thought I would substitute an A4 graph in place of C; the program would then calculate the appropriate symmetries, albeit at some cost in computational efficiency.

Hence the question: what is the smallest A4.

You should note that Ray Carhart had already produced a 26-node graph, and I thought I had sent that to you. We did not know whether this was the smallest. With slings (—••—) and higher values we also found one at 22 nodes;



Lawrence -
Klee

A4 [complex]
graph

MAR 18 1976

26 nodes

how about putting it in
congen to prove it
is A4 (and verify the program
again)

JMK