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Good luck on your enterprise.
May I suggest a sub-problem
with which you will have to grapple
anyhow, and will help you stage your
work?

This is to "canonicate" a
chemical graph. The procedure
accepts as input $\underline{a}$ description of
a specific structure in arbitrary
form, and outputs one in accord-
ance with the canons of Dendral
order. This is a vital part of the
structure-generator, but does
not yet require a lot of book-keeping
detail needed for stepping from
one to the next radical in
sequence. Please do not hesitate to

Department of Genetics
School of Medicine
Stanford University
Stanford, California 94305

let me know of your problems + successes.