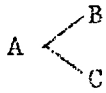
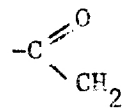
A DENDRAL PRIMER

Rules for reading DENDRAL are very simple and can be applied directly to writing formulas. To be sure these are in canonical form, however, additional rules must be observed which can be implemented either by a trained analyst or the computer. Vernacular forms are unambiguous, but generally not unique.

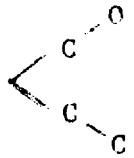
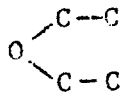
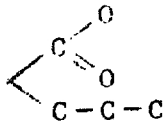
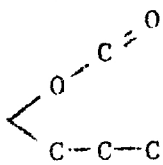
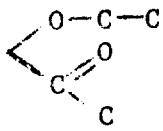
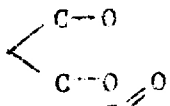
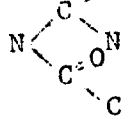
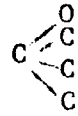
The principal conventions for unringed structures are, besides the familiar atoms:

A..BC		Link(s)
.A B		Leading Link
,A		Repeat
Y		Carboxyl
G		Aceto
Integers, e.g., 3	C.C.C	Alkyl

A SUMMARY OF FORMAL DENDRAL

1. Skeletonize formula: Strip H's; shrink rings to atoms.
2. Define rings, if any.
3. Count skeletal atoms.
4. Identify central apex (unique point of division or central branching).
5. List attached radicals in dictionary order.
6. Dissect each radical, node by node, according to the same rules. Note repeats and use "," notation.
7. Replace strings representing alkyl, carboxy, and aceto radicals by integers, "Y" and "G", respectively.

ELEMENTARY EXAMPLES OF DENDRAL

COMPOUND	CANONICAL SKELETON	VERNACULAR DENDRAL	PROPER DENDRAL
Ethanol		C.C.O 2.0 0.2 C..CO	C..O C
Methanol		C.O	.C O
Propanol		3.0 0.3 C..2 O	.C.O 2
Ethyl Ether		2.0.2 C..C 0.2 0..22	O.,2
Acetic Acid		C.Y O.G	.C Y
Butyric Acid		3.Y O.C:.O2 O.G.2 C..2Y	.Y 3
Propyl Formate		C:.OO.3 3.O.C:O O:C.O.3	.O.C:O 3
Ethyl Acetate		2.O.G O..2G	.O.2 G
Glycol		O.C.C.O C..OC.O .C.OC.O	,C.O
Acetyl urea		N.C:.ON.G	N..C:.ON G
t-Butanol		O.C.,,C C.C..,OCC	C..,,OC