

MAR 22 1965

Mills College



OAKLAND 13, CALIFORNIA

March 20, 1965

Professor Joshua Lederberg
Stanford University School of Medicine
Palo Alto, California

Dear Professor Lederberg:

Thank you for your February 25 letter and your offer of a reprint of your recent NAS paper on Dendral. I shall look forward to receiving it. I also appreciate your offering me Xerox copies of your unpublished tables, but I'm afraid I am innocent of the mathematics I should need to make much use of them.

Mr. Wiswesser has sent me copies of your correspondence of March 8 and 12 and I deduce from this that you may be referring to the "Rule 30" in his 1954 notation manual. My colleagues and I have refined this rule extensively through much pragmatic experience with the notation and we have developed a much more detailed procedure for finding the unique starting point of the longest continuous path of ring atoms. The prism and the bipentagon offer no difficulties.

I, too, have spent much time wrestling with steps that may lead to some logical rigor in approaching ring systems from this point of view. I believe we may now be beginning to see some mathematical basis, however elementary, for our pragmatically based methods. We have not tried to apply our notation to the more esoteric types of polyhedra which may or may not represent possible chemical structures, but we can satisfactorily denote all the ring structures in The Ring Index and both its supplements.

We have discussed this approach in detail in the revision of the Wiswesser notation that I have been writing since 1962, but due to recent revisions I do not now have a copy of our working manuscript that I could simply give you. However, if you would like to see what we have developed, I can lend you a copy that I've been preparing for the purpose of approaching a publisher. I'd be happy to have you make copies of any of the pages which might interest you.

I'm on sabbatical leave this year, so mail will reach me much more quickly at my home--1931 Golden Gate, San Francisco 94115. My telephone number is JOrdan 7-0489.

Sincerely yours

Herbert G. Smith
Professor of Chemistry