173° was obtained. The elementary analysis indicated that it was an acetate of 3-hydroxy-4-pteridinone.

Anal. Calcd. for $C_8H_6N_4O_3$: C, 46.6; H, 2.93; N, 27.2. Found: C, 46.5; H, 2.93; N, 27.2.

Acknowledgment.—We wish to express our gratitude to Mr. O. Sundberg and his associates for the microanalyses and to Mr. J. Morath for the photometric data.

BOUND BROOK LABORATORIES
RESEARCH DIVISION
AMERICAN CYANAMID COMPANY
BOUND BROOK, NEW JERSEY

COMMUNICATIONS TO THE EDITOR

THE STRUCTON NUMBER RULE

Sir:

A theory according to which many properties of solids and liquids can be related to the numbers and properties of the "structons" present, recently has been outlined.[1] A "structon" is defined as an atom or ion or molecule or group of atoms of a given kind, surrounded in a specified manner. A "structon number rule," relating the minimum number of structon types (S) to the number of degrees of composition freedom (F), was presented.

Application was made specifically to sodium silicate glasses. When the theory is extended to other systems, including liquid solutions, it appears advisable to express the structon number rule somewhat differently. One can still use the same equation, but now C denotes the number of types of contact between unlike structon centers. In the

$$S = C + F + 2 \qquad (1)$$

Na_2O–SiO_2 system, C is two, there being only Na–O and Si–O contacts. In a solution composed of two molecular species, forming strong contacts with each other (*e.g.*, by hydrogen-bonding), C is one, regardless of whether or not *like* molecules also form strong contacts.

To determine the number of each of S types of structons requires S equations. For each of the C types of contact between different types of structon centers (A, B), there is one equation, equating the number of contacts between A-type structon centers and B neighbors to the number of contacts between B-type structon centers and A neighbors. Thus, in the high-silica region of the sodium silicate system

$$2N_{O(2Si)} + 2N_{O(2Si,Na)} + N_{O(Si,3Na)} = 4N_{Si(40)} \qquad (2)$$

$$N_{O(2Si,Na)} + 3N_{O(Si,3Na)} = 6N_{Na(60)} \qquad (3)$$

There is one normalizing equation. In the sodium silicate example, it expressed the fact that the total number of oxygen-centered structons equals unity (since the quantity of glass being considered was that containing a single atom of oxygen)

$$N_{O(2Si)} + N_{O(2Si,Na)} + N_{O(Si,3Na)} = 1 \qquad (4)$$

In molecular solutions, the normalizing equation may show that the sum of the mole fractions equals unity.

There is also another equation, in many cases, expressing the over-all neutrality or valence-balancing requirement; *e.g.*

$$N_{Na(60)} + 4N_{Si(40)} = 2[N_{O(2Si)} + N_{O(2Si,Na)} + N_{O(Si,3Na)}] \qquad (5)$$

The number of degrees of composition freedom gives the number of additional equations required to fix the numbers of all structons present. This, with the other relationships just given, leads to eq. (1).

In molecular solutions, the neutrality equation is no longer of use, hence eq. (1) must be replaced by

$$S = C + F + 1 \qquad (6)$$

This is also the equation to use if all the structon charges (see ref. 1) are zero, since then the neutrality equation is not independent; it can be obtained by appropriate addition of the structon-contact equations, such as eqs. (2) and (3). This applies, for example, to pure silica.

Application of structon theory and the structon number rule to molecular solutions will be made in another paper.

RESEARCH LABORATORIES
EASTMAN KODAK COMPANY
ROCHESTER 4, NEW YORK
MAURICE L. HUGGINS

RECEIVED JUNE 7, 1955

(1) M. L. Huggins, *J. Phys. Chem.*, **58**, 1141 (1954).

A CARCINOGENIC OXIDATION PRODUCT OF CHOLESTEROL

Sir:

The observation[1] that a crude progesterone preparation prepared[2] by permanganate oxidation of cholesterol dibromide and debromination produced tumors in 32% of the mice tested initiated an extended investigation in which various products of oxidation of cholesterol have been prepared in Cambridge and tested for carcinogenicity in Santa Barbara. Some of the compounds submitted for assay were suggested by specific hypotheses (an abnormal cholesteryl ester,[3] an epoxide derived from a 7,8,-9,11-diene,[4] Δ^5-cholestene-3-one[4]), others were empirically observed known or new[5] products of

(1) F. Bischoff and J. J. Rupp, *Cancer Research*, **6**, 403 (1946).
(2) M. A. Spielman and R. K. Meyer, THIS JOURNAL, **61**, 893 (1939).
(3) L. F. Fieser and W. P. Schneider, *ibid.*, **74**, 2254 (1952).
(4) L. F. Fieser, *Bull. soc. chim.*, **21**, 541 (1954); *Science*, **119**, 3099 (1954).
(5) L. F. Fieser, THIS JOURNAL, **75**, 4377, 4386, 4395 (1953).