Reports

An Interpolated Molecular Formula

Abstract. The necessity of counting hydrogen atoms in molecular formulas may be obviated by substituting a "hydrogen reciprocal," which can be obtained more easily.

When molecular formulas are used for searching or filing chemical compounds, handling of the hydrogen atoms proves troublesome. Counting the H's is laborious and is responsible for the majority of errors in these formulas; yet, the sum of the H's does not provide much information about a compound. As a result, this sum has been relegated to the end of the formulas in some collections (*1*) and in others it has been omitted altogether (*2*).

I propose, here, to omit the sum of hydrogen atoms from molecular formulas of covalent compounds and to replace it with the number of rings and the degree of unsaturation of the molecules. It has already been shown that, mathematically, these two expressions are equivalent (*3, 4*).

A few examples of the proposed interpolated formulas are given below, along with their conversion into conventional molecular formulas. In the proposed formulas, the number before the comma represents the number of rings, R, and the number after the comma represents the degree of unsaturation, Δ. This choice of two numbers is arbitrary. One alternative is to use a set of three numbers: f for the number of double bonds connected to hetero atoms (as in $>C{=}O$); s for the number of double bonds linking carbon atoms (as in $>C{=}C<$); and R for the number of rings. Such division is a matter of convenience. If the three numbers f, s, and R are used, the expression will be different for keto and enol tautomers. On the other hand, if R and Δ (which is $f + s + R$) are added to form a single number [Soffer's ρ (*4*), which here may properly be called a hydrogen reciprocal], the expression will remain unaltered even if the represented compound undergoes glycoside formation.

From an equation derived by Soffer (*4*), the conversion formula is obtained. In its general form, it is Eq. 1:

$$n_H = 2 + \Sigma\, n_v(v - 2) - 2(R + \Delta) \quad (1)$$

where n_v is the number of atoms (except hydrogen atoms) of covalence v, the sum of which is taken over all the v's; n_H is the number of hydrogen atoms; R is the number of rings; and Δ is the number of double bonds (one triple bond counts for two double bonds; unsaturated linkages in functions are counted too) (*5*).

In most cases, Eq. 1 will reduce to the following:

$$n_H = 2 + 2n_C + n_{N,P} - n_{Hal} - 2(R + \Delta) \quad (2)$$

where n_C is the number of carbon atoms, $n_{N,P}$ is the number of (trivalent) N and P atoms, and n_{Hal} is the number of halogens. For example:

1) For ergosterol, the interpolated formula is $C_{27}O$-4,3. To find n_H, substitute into Eq. 2 the values $n_C = 27$, $R = 4$, and $\Delta = 3$: $n_H = 2 + 2 \times 27 - 2(4 + 3) = 42$. The molecular formula is $C_{27}H_{42}O$.

2) For riboflavin phosphate, the interpolated formula is $C_{17}N_4O_9P^V$-3,8 (see *5*). To find n_H, substitute into Eq. 2 the values $n_C = 17$, $n_N = 4$, $R = 3$, $\Delta = 8$, and $n_{P^V} = 1$: $n_H = 2 + 2 \times 17 + 4 - 2(3 + 8) + 3 \times 1$ ($= 3n_{P^V}$, Eq. 1) $= 21$. The molecular formula is $C_{17}H_{21}N_4O_9P$.

3) Attention must be paid to abnormal valencies; in carbon monoxide, for instance, $2n_C$ does not apply, since $v = 2$ here and the $n_C(v - 2)$ from Eq. 1 becomes 0.

It is seen that the advantages of interpolated formulas are that no information is lost, and that these formulas are more meaningful, more easily obtained, and less apt to contain errors than conventional formulas. Furthermore, interpolated formulas can be obtained for many compounds with unknown structures, as enough data for their calculation are often available at an early stage. For other compounds, the conventional molecular formulas could be filed, without inconvenience, among interpolated formulas. The presence of hydrogen simply would indicate the lack of other information.

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References and Notes

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2. H. Skolnik and J. K. Hopkins, *J. Chem. Educ.* **35**, 150 (1958).
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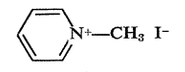
5. In the file now in use in our department at Walter Reed, some simplifications have been introduced. For elements that can exhibit several valencies, the "normal" one is recorded (that is, 3 for N and P, 2 for S), provided that the additional valencies consist of double bonds. These double bonds may then be disregarded. Thus, the formula for $CH_3{-}NO_2$ is CNO_2-0,1; for $CH_3{-}SO_3H$ it is CO_3S-0,0, and for riboflavin phosphate it would be $C_{17}N_4O_9P$-3,7. However, in 1-methylpyridinium iodide,



the additional valencies do not consist of a double bond; therefore, the formula is C_6IN^V-1,3.

2 August 1960

Instructions for preparing reports. Begin the report with an abstract of from 45 to 55 words. The abstract should *not* repeat phrases employed in the title. It should work with the title to give the reader a summary of the results presented in the report proper.

Type manuscripts double-spaced and submit one ribbon copy and one carbon copy.

Limit the report proper to the equivalent of 1200 words. This space includes that occupied by illustrative material as well as by the references and notes.

Limit illustrative material to *one* 2-column figure (that is, a figure whose width equals two columns of text) or to *one* 2-column table or to *two* 1-column illustrations, which may consist of two figures or two tables or one of each.

For further details see "Suggestions to Contributors" [*Science* **125**, 16 (1957)].

Syphacia muris, the Rat Pinworm

Abstract. A migration of gravid *Syphacia muris* pinworms down the large intestine of the rat host is shown to occur from the seventh day on in the worm's life cycle. Eggs obtained from migrating worms have proved to be infective to helminth-free rats after incubation in saline for 30 minutes at room temperature and 4 hours at 37°C.

The pinworm, *Syphacia muris,* is a very common cecal parasite of the laboratory albino rat. Few details of the life history of this pinworm are known, however, mainly because previous workers (*1*) have been unable to obtain infective stages of the parasite for use in experimental infections. These investigators reported that eggs liberated from gravid worms taken from the cecum of infected rats would not continue their development in vitro. Chan (*2*), using the closely related mouse pinworm *S. obvelata,* then demonstrated that eggs obtained from gravid female worms migrating down the colon of the host mice at the conclusion of their life cycle would develop to the infective stage. This suggested that

Table 1. The distribution of *Syphacia muris* in the intestine of albino rats.

T(day)*	Rats (No.)	Worm burdens		Anal swabs
		Cecum	Colon	
1	2	386	0	−
2	2	367	0	−
3	4	635	7	−
4	4	170	0	−
5	4	620	6	−
5½	4	218	0	−
6	4	760	15	−
7	4	270	25	+
7½	4	130	119	+
8	4	133	11	+
9	4	41	3	+
9½	4	61	0	+
10	4	7	3	+

* Time after exposure to infection.

knowledge of the period of migration of *S. muris* down the rat's intestine would greatly facilitate the recovery of large numbers of gravid "migrators" as a source of infective eggs.

Forty-eight helminth-free albino rats, 3 to 5 weeks old, were placed for 24 hours in contaminated cages containing heavily infected *S. muris* "source" rats. This procedure is a modified version of Chan's (*3*) technique for infecting mice with *S. obvelata*. At periodic intervals thereafter, Scotch tape anal swabs were taken from each rat and examined for the presence of *S. muris* eggs, then two or four rats were killed and their pinworm burdens were determined.

Table 1 summarizes the results of this study. The migratory phase of the *S. muris* life cycle began on the sixth to seventh day after infection, as determined by autopsy findings and the presence of eggs on the perianal regions of the rats. During the seventh and eighth days, maximal numbers of gravid migrators were found in the colon of the rats. Many of the migrating female worms spontaneously shed their eggs on exposure to air or to saline solution. In addition, a small number of gravid nonmigrating female worms, from the cecum, also shed their eggs upon exposure. These spontaneously shed eggs were infective to rats after incubation in saline for periods ranging from 30 minutes at room temperature to 4 hours at 37°C (*4*).

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References and Notes

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2. K. F. Chan, *Am. J. Hyg.* **56**, 14 (1952).
3. ———, *ibid.* **56**, 22 (1952).
4. This investigation was carried out in the Columbia University School of Public Health and Administrative Medicine, and was supported in part by research grant No. E-461(C) of the National Institutes of Health, U.S. Public Health Service.

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Low Temperature Induced Male Sterility in Male-Fertile Pennisetum clandestinum

Abstract. Controlled environment studies of *Pennisetum clandestinum* showed that at 10°C stamens of the male-fertile strain were not exserted from the floret although stigmas emerged normally. At higher temperatures both stamens and stigmas were exserted. Pollen abortion was high at 10°C and was increased by lengthening photoperiod. Flowering of the male-sterile strain was not changed by any temperature or photoperiod. These responses to temperature may explain the natural sterility during the cool season.

Pennisetum clandestinum, introduced to the United States about 1920, consists of male-sterile and male-fertile strains. The inflorescences of the two strains have been described by Edwards (*1*) and Narayan (*2*). Anthers of the male-sterile strain are retained in the leaf sheath enclosing the flower and contain no viable pollen. Anthers of the male-fertile strain are exserted from the enveloping sheath on long filaments. Stigmas are exserted in both strains throughout the year in the Los Angeles area, but few or no stamens emerge during the winter in the male-fertile strain. I observed approximately 25 percent nonstaining (sterile) pollen during the summer and 50 percent or more in the winter in the fertile strain. No stainable pollen was observed in the sterile strain at any season (*3*).

Anther abortion in wheat by chilling was demonstrated by Suneson (*4*). Nitsch *et al.* (*5*) reported deformed male flowers in Cucurbitaceae as well as a reduction in the proportion of male flowers when temperatures were reduced from 26°C to 20°C. The purpose of this study was to determine if the seasonal changes in sex expression of *P. clandestinum* were caused by changes in temperature or photoperiod.

Plants of *P. clandestinum* were propagated in 5-in. pots from a male-sterile and a male-fertile clone. All plants were kept in a 21°C minimum temperature greenhouse. As the plants developed they were clipped frequently to stimulate flowering (*6*). At full flowering, they were transferred to controlled environment growing chambers under 8- and 16-hour photoperiods at the following temperatures centigrade: 27°, 10°, and 21° minimum for days to 10° for nights. Plants, given the alternating temperature and 16-hour photoperiod, received 8 hours of light at the day temperature and 8 hours at the night temperature. In addition, two lots of plants were given continuous light at 27° and 10°C. Five plants of each clone were placed in each treatment.

Flowering behavior was noted periodically as the treatment progressed. After 4 weeks in the growing chambers, pollen fertility was determined by staining with acetocarmine (*7*). Three inflorescences from each plant were examined.

Observation of the male-fertile strain showed a pronounced reduction in the number of florets with exserted stamens between the second and third week in the 10°C treatments. Table 1 shows that by the fourth week there were no stamens visible on any plants in these treatments, but numerous stigmas were still exserted. All fertile plants in the other treatments continued to flower in a normal manner, producing numerous stamens.

Flowering was not affected by the photoperiods within the temperature treatments. Exsertion of stamens stopped at the same time in the 8-, 10-, and 24-hour light periods at 10°C. In all other temperature-photoperiod treatments, exsertion of new stamens continued during the treatment period of 8 weeks. Normal-appearing stigmas developed on all plants in all treatments throughout the entire period.

Flowering behavior of the male-sterile strain did not appear to be altered in any way by any of the treatments. Stigmas but no stamens emerged under all temperatures and photoperiods.

Plants of both strains receiving continuous light developed shoots with long internodes and few branches; thus the total number of inflorescenses per plant was lower than for plants under the 8- and 16-hour photoperiods.

Pollen sterility was nearly complete in the male-sterile strain regardless of treatment. Anthers were flat, containing only shrunken nonstaining pollen grains. As shown in Table 1, anthers from male-fertile plants grown at 27° and 21°C days to 10°C nights contained high percentages of stainable pollen. These percentages are comparable to those observed in field grown plants during summer.

Anthers on short filaments, removed from plants grown at 10°C, contained a much lower percentage of stainable

Table 1. Appearance of florets, after 4 weeks of treatment, in fertile *P. clandestinum*.

Day length (hr)	Stamens	Fertile pollen (%)
	Temperature 27°C	
8	Exserted	89 ± 16
16	Exserted	65 ± 11
24	Exserted	71 ± 13
	Temperature 10°C	
8	Nonexserted	36 ± 5
16	Nonexserted	21 ± 6
24	Nonexserted	0.4 ± 0.2
Temperature	*21°C (day) to 10°C (night)*	
8	Exserted	72 ± 13
16	Exserted	82 ± 16