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A PROGRAM FOR CALCULATING Q_{10} VALUES UTILIZING A HEWLETT-PACKARD HP-67 CALCULATOR

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ABSTRACT

Q_{10} values are used to make stability projections from kinetic data. A program to facilitate the computation of Q_{10} values utilizing the Hewlett-Packard HP-67 calculator is presented. In addition, the program may be used to compute incremental changes of Q_{10} as a function of either temperature (dQ_{10}/dT) or activation energy (dQ_{10}/dE_a).

INTRODUCTION

The usefulness of Q_{10} values in stability studies has long been recognized (1,2). Calculation of Q_{10} values, although not difficult, may be cumbersome. Estimates of Q_{10} values at various temperatures and for various activation energies are available (2). We wish to present in this paper a program which, utilizing a Hewlett-Packard HP-67 calculator, facilitates the computation of Q_{10} values.

In addition, it has been pointed out (2) that Q_{10} values are a function of both temperature and actvation energy. The program presented here may also be used for the computation of dQ_{10}/dT and dQ_{10}/dE_a values.

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DISCUSSION

Q_{10} values are an expression of the change in reaction rate constants with a ten degree change in absolute temperature:

$$Q_{10} = k'/k \qquad \text{Eq.1}$$

where k is the rate constant at T °K and k' is the rate constant at T + 10 °K. Clearly any temperature increment could be utilized and a corresponding "Q_T" value could be calculated. However, it has been shown (2) that any such values are easily computed from Q_{10} values.

From the Arrhenius relationship:

$$k = Ae^{-E_a/RT} \qquad \text{Eq.2}$$

where A is a constant, E_a is the activation energy and R is the universal gas constant (1.987 cal/mole-deg), it may be demonstrated that:

$$Q_{10} = e^{E_a/R(1/T - 1/T')} \qquad \text{Eq.3}$$

where T' = T + 10

Substituting T + 10 for T' and differentiating equation 3 with repect to temperature yields, after expansion and simplification:

$$-dQ_{10}/dT = (20E_a/RT^3)e^{10E_a/RT^2} \qquad \text{Eq.4}$$

Since the value of the gas constant is 1.987, when the activation energy is measured in cal/mole, equation 4 simplifies to:

$$-dQ_{10}/dT = (10.1E_a/T^3)e^{5.0E_a/T^2} \qquad \text{Eq.5}$$

At a constant temperature Q_{10} is a function of activation energy. This relationship may be obtained by taking the derivative of Q_{10} with respect to E_a which, from equation 3 yields:

$$dQ_{10}/dE_a = (5.0/T^2)e^{5.0E_a/T^2} \qquad \text{Eq.6}$$

It may be noted that Q_{10} values decrease with increasing temperature, but increase with increasing activation energy. This is due to the fact that at elevated temperatures a small change in temperature will have only a small effect on reaction rates. On the other hand, small changes in temperature will produce more dramatic

TABLE I

Program Steps for Calculating Q_{10}, dQ_{10}/dT and dQ_{10}/dE_a

001 f LBL A	023 9	045 1
002 STO 1	024 8	046 0
003 h RTN	025 7	047 .
004 f LBL B	026 ÷	048 1
005 STO 2	027 g e^x	049 X
006 h RTN	028 h RTN	050 RCL 4
007 f LBL C	029 f LBL D	051 X
008 RCL 1	030 RCL 1	052 h RTN
009 h 1/x	031 g x^2	053 f LBL E
010 STO 3	032 h 1/x	054 RCL 1
011 RCL 1	033 RCL 2	055 g x^2
012 1	034 X	056 h 1/x
013 0	035 5	057 5
014 +	036 X	058 X
015 h 1/x	037 g e^x	059 STO 5
016 CHS	038 STO 4	060 RCL 2
017 RCL 3	039 RCL 1	061 X
018 +	040 3	062 g e^x
019 RCL 2	041 h y^x	063 RCL 5
020 X	042 h 1/x	064 X
021 1	043 RCL 2	065 h RTN
022 .	044 X	

differences in rates of reactions with higher activation energies. This could be important when estimating stability patterns based on Q_{10} values.

Table I presents the program steps required for the computations discussed above. Steps 001 through 006 are general steps for all three computations. Steps 007 through 028 calculate Q_{10}, 029 through 052 calculate dQ_{10}/dT and 053 through 065 calculate dQ_{10}/dE_a. The temperature (^oK) is stored in register A and the activation energy (cal/mole) is stored in register B to initialize the program. Then Q_{10}, dQ_{10}/dT and dQ_{10}/dE_a are found by pressing the keys C, D and E respectively.

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