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TABLES OF ISOTOPE EFFECT FUNCTIONS FOR HOMOCOMPETITIVE FIRST-ORDER REACTIONS

M. H. Lietzke
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TABLES OF ISOTOPE EFFECT FUNCTIONS FOR HOMOCOMPETITIVE FIRST-ORDER REACTIONS

M. H. Lietzke and Clair J. Collins

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Abstract

The ORACLE has been employed to determine, for first-order irreversible reactions, the relation between fraction of reaction ($f = 1 - e^{-kt}$) and the accumulated product ratio R ($R = \frac{1 - e^{-k^*t}}{1 - e^{-kt}}$) over a range of values for the isotope effect ($\frac{k^*}{k}$) of 0.05 to 0.99. These data are presented in Tables 1, 2, and 3. Graphic representations of the data are shown in Figures 1, 1A, 2 and 3. Calculations have also been made for f as a function of the ratio (x) of the differentials of the fractions of labeled to unlabeled molecules formed. These latter results are presented graphically in Figures 4 and 5.

The calculations show how the ratio of product from labeled reactant to product from unlabeled reactant varies with the isotope effect. They also illustrate several types of error which can be introduced into tracer experiments, and are useful in assisting the investigator to estimate graphically the value of the isotope effect for a given reaction knowing a) the isotopic ratio of initial reactant, b) the isotopic ratio of the product accumulated at any time t, and c) the fraction f of unlabeled material which has undergone reaction at any time t.

The isotopes of carbon have been widely used as tracers in the study of organic and biochemical reactions.[1] Deuterium and tritium also have been employed in mechanism studies,[2] the tritium being nearly always in trace concentrations.[3] The difference in reaction rate between labeled and unlabeled compounds--that is, the isotope effect--pertains to tracer chemistry in at least three ways: 1) in determinations of the slow or so-called "rate-determining steps" of many reactions;[3,4] 2) in the study of hyperconjugation;[5,6] and 3) because of the possible doubt which might be cast upon the validity of tracer experiments when the manner of operation of the isotope effect is not clearly understood.

The general theory of homocompetitive reactions is well known,[7,8] and has been applied to the field of isotopic chemistry by Bigeleisen[9] and by Melander,[10] who have drawn attention to some of the errors which can arise in tracer experiments because of the "lagging" of the heavy isotope.[10]

In the present report we wish to present the results of calculations carried out with the assistance of the ORACLE,[11] which will show how the ratio of product from labeled reactant to product from unlabeled reactant varies over a wide range of isotope effect values. These calculations illustrate several types of error which can be introduced into tracer experiments; moreover they will be useful in assisting the investigator to estimate the value of the isotope effect for a given reaction knowing a) the isotopic ratio of initial reactant, b) the isotopic ratio of the product accumulated at any time t, and c) the fraction f of unlabeled material which has undergone reaction at any time t.[12]

We shall limit our discussion to irreversible, first-order reactions of the type:

$$A \longrightarrow B$$
$$A^* \longrightarrow B^*$$

in which A and A^* are the unlabeled and labeled reactants, B and B^* are the products arising from the unlabeled and labeled reactants, respectively, and k and k^* are the appropriate specific reaction rate constants. If n and n^* refer to the number of molecules or concentrations of A and A^* in a given reaction at time t, and n_o and n_o^* represent these same molecules at time zero, then:

$$\frac{-dn(t)}{dt} = kn \ ,$$

hence

$$\frac{n}{n_o} = e^{-kt} = \text{fraction of unlabeled molecules remaining at time t.}$$

Then

$$f = 1 - e^{-kt} = \text{fraction of unlabeled molecules which have undergone reaction at time } t.$$

Similarly,

$$f^* = 1 - e^{-k^*t} = \text{fraction of labeled molecules which have undergone reaction at time } t.$$

Thus the ratio of product fraction of the labeled to unlabeled molecules at any time becomes:

$$R = \frac{1 - e^{-k^*t}}{1 - e^{-kt}}$$

Clearly, for very low concentrations of the labeled material, R in the case of radioactive isotopes becomes equal to the ratio of the molar radioactivity of the accumulated product at any time, to the molar radioactivity of reactant at time zero, providing the radioactive atoms go with the product molecules. Although calculation of the points necessary to provide plots of R versus f over a wide range of values for k^*/k would be very time consuming if done by hand, we

have been able to perform the calculations very rapidly through the use of the ORACLE.[11] Given in Table 1 are the values of R for values of k^*/k from 0.05 to 0.80, and of f from 0.05 to 0.99; in Table 2 are presented values of R for values of k^*/k from 0.05 to 0.45 and of f from 0.990 to 0.999; and finally, in Table 3 are given values of R for values of k^*/k from 0.81 to 0.99 and of f from 0.10 to 0.99. All numbers in the tables are in exponentiated form, where e-2 represents, for example, 10^{-2}. Thus 5.00000 e- 2 signifies 0.05.

Given in Fig. 1 are plots of R versus f in which k^*/k has been varied from 0.05 to 0.80 in increments of 0.05 (the deuterium, tritium isotope effect range) for values of f from zero to unity. In Fig. 1A are presented plots of R versus f in which k^*/k has been varied from 0.05 to 0.80 in increments of 0.05 for values of f from 0.90 to 0.99. Given in Fig. 2 are curves representing plots of R versus f for values of k^*/k between 0.05 and 0.45 in increments of 0.05 for values of f between 0.990 and 0.999. Finally, Fig. 3 contains plots of R versus f in which k^*/k has been varied from 0.81 to 0.99 in increments of 0.01 (the carbon-13, carbon-14 isotope effect range) for values of f from zero to unity. In the plots shown in both Fig. 1 and Fig. 3 the intercept of each curve on the R axis at f = 0 corresponds to the value of k^*/k for that particular curve.

Finally it is of interest to consider, in addition to the cumulative ratio R, the ratio[2] of the differentials of the fractions of labeled to unlabeled molecules formed. At any time t the infinitesimal increment of the fraction of unlabeled product formed in the time interval dt for a first-order reaction is:

$$df = \frac{-dn}{n_o} = ke^{-kt}\,dt.$$

The corresponding expression for the labeled product is:

$$df^* = \frac{-dn^*}{n_o^*} = k^* e^{-k^* t}\,dt.$$

Then

$$x \equiv \frac{df^*}{df} = \frac{k^*}{k} \frac{e^{-k^*t}}{e^{-kt}} = \frac{k^*}{k} e^{k(1 - \frac{k^*}{k})t}$$

and

$$\ln x = \ln \frac{k^*}{k} - kt \left(\frac{k^*}{k} - 1\right) .$$

Now the fraction of unlabeled molecules remaining at time $\underline{t}$ is:

$$(1 - f) = \frac{n}{n_o} = e^{-kt}$$

or

$$\ln (1 - f) = \ln \frac{n}{n_o} = -kt.$$

Hence

$$\ln x = \left(\frac{k^*}{k} - 1\right) \ln (1 - f) + \ln \frac{k^*}{k} .$$

By use of the foregoing equation, and with the assistance of the ORACLE,[11] we have made plots of $\underline{x}$ $\underline{\text{versus}}$ $\underline{f}$ (fraction of reaction) for values of $\frac{k^*}{k}$ of 0.05, 0.10 and 0.30 (Fig. 4); and for values of $\frac{k^*}{k}$ of 0.7, 0.8, 0.9 and 0.93 (Fig. 5).[13]

Appendix

It can be demonstrated for any of the curves of Figs. 4 and 5, that the area bounded by the curve and the horizontal line x = 1 to the left of the point where the curve intersects the line x = 1 must equal the area bounded by the curve and the horizontal line x = 1 to the right of the intersection point.

$$\int_{f=o}^{f=1} x\,df = \int_{f=o}^{f=1} \frac{k^*.e^{-k^*t}}{k.e^{-kt}} \left(ke^{-kt}\right) dt = \int_{t=o}^{t=\infty} k^* e^{-k^*t} dt = 1 =$$

the total area under the <u>x</u> <u>versus</u> <u>f</u> curve.

Now
$$\bar{x} = \frac{\int_o^1 x\,df}{\int_o^1 df} = 1 \;;$$

Hence
$$\int_o^1 x\,df = \bar{x} \int_o^1 df = 1 = \text{the total area of the}$$

rectangle (or square if the units of <u>x</u> and <u>f</u> are equal) below the horizontal line x = 1.

Since the two areas, that of the rectangle (or square) and that under the <u>x</u> <u>versus</u> <u>f</u> curve, are equal, it follows that the part of the area under the curve not common to the rectangle (or square) is equal to the part of the area of the rectangle (or square) not common to the area under the curve, i.e.,

$$\int_{o}^{f_1} (1 - x)\, df = \int_{f_1}^{1} (x - 1)\, df$$

or

$$\int_{t = o}^{t = t_1} (1 - x)\, df = \int_{t = t_1}^{t = \infty} (x - 1)\, df$$

where $\underline{f_1}$ and $\underline{t_1}$ are the values of $\underline{f}$ and $\underline{t}$, respectively, where $\underline{x} = 1$. The foregoing theorem is also a consequence of the law of conservation of mass.

Table 1

Table of Isotope Effect Functions for
$k^*/k = .05 - .80$ and $f = .05 - .99$

k^*/k	f	R
5.00000 e- 2	5.00000 e- 2	5.12275 e- 2
5.00000 e- 2	1.00000 e- 1	5.25415 e- 2
5.00000 e- 2	1.50000 e- 1	5.39535 e- 2
5.00000 e- 2	2.00000 e- 1	5.54758 e- 2
5.00000 e- 2	2.50000 e- 1	5.71246 e- 2
5.00000 e- 2	3.00000 e- 1	5.89189 e- 2
5.00000 e- 2	3.50000 e- 1	6.08824 e- 2
5.00000 e- 2	4.00000 e- 1	6.30447 e- 2
5.00000 e- 2	4.50000 e- 1	6.54433 e- 2
5.00000 e- 2	5.00000 e- 1	6.81273 e- 2
5.00000 e- 2	5.50000 e- 1	7.11616 e- 2
5.00000 e- 2	6.00000 e- 1	7.46348 e- 2
5.00000 e- 2	6.50000 e- 1	7.86727 e- 2
5.00000 e- 2	7.00000 e- 1	8.34607 e- 2
5.00000 e- 2	7.50000 e- 1	8.92893 e- 2
5.00000 e- 2	8.00000 e- 1	9.66490 e- 2
5.00000 e- 2	8.50000 e- 1	1.06466 e- 1
5.00000 e- 2	9.00000 e- 1	1.20832 e- 1
5.00000 e- 2	9.50000 e- 1	1.46430 e- 1
1.00000 e- 1	5.00000 e- 2	1.02323 e- 1
1.00000 e- 1	1.00000 e- 1	1.04807 e- 1
1.00000 e- 1	1.50000 e- 1	1.07470 e- 1
1.00000 e- 1	2.00000 e- 1	1.10336 e- 1
1.00000 e- 1	2.50000 e- 1	1.13433 e- 1
1.00000 e- 1	3.00000 e- 1	1.16796 e- 1
1.00000 e- 1	3.50000 e- 1	1.20467 e- 1
1.00000 e- 1	4.00000 e- 1	1.24499 e- 1
1.00000 e- 1	4.50000 e- 1	1.28959 e- 1
1.00000 e- 1	5.00000 e- 1	1.33934 e- 1
1.00000 e- 1	5.50000 e- 1	1.39538 e- 1
1.00000 e- 1	6.00000 e- 1	1.45927 e- 1
1.00000 e- 1	6.50000 e- 1	1.53322 e- 1
1.00000 e- 1	7.00000 e- 1	1.62045 e- 1
1.00000 e- 1	7.50000 e- 1	1.72599 e- 1
1.00000 e- 1	8.00000 e- 1	1.85825 e- 1
1.00000 e- 1	8.50000 e- 1	2.03297 e- 1
1.00000 e- 1	9.00000 e- 1	2.28524 e- 1
1.00000 e- 1	9.50000 e- 1	2.72490 e- 1

k^*/k	f	R
1.50000 e- 1	5.00000 e- 2	1.53288 e- 1
1.50000 e- 1	1.00000 e- 1	1.56798 e- 1
1.50000 e- 1	1.50000 e- 1	1.60554 e- 1
1.50000 e- 1	2.00000 e- 1	1.64588 e- 1
1.50000 e- 1	2.50000 e- 1	1.68938 e- 1
1.50000 e- 1	3.00000 e- 1	1.73651 e- 1
1.50000 e- 1	3.50000 e- 1	1.78783 e- 1
1.50000 e- 1	4.00000 e- 1	1.84405 e- 1
1.50000 e- 1	4.50000 e- 1	1.90605 e- 1
1.50000 e- 1	5.00000 e- 1	1.97499 e- 1
1.50000 e- 1	5.50000 e- 1	2.05238 e- 1
1.50000 e- 1	6.00000 e- 1	2.14028 e- 1
1.50000 e- 1	6.50000 e- 1	2.24154 e- 1
1.50000 e- 1	7.00000 e- 1	2.36039 e- 1
1.50000 e- 1	7.50000 e- 1	2.50330 e- 1
1.50000 e- 1	8.00000 e- 1	2.68106 e- 1
1.50000 e- 1	8.50000 e- 1	2.91366 e- 1
1.50000 e- 1	9.00000 e- 1	3.24505 e- 1
1.50000 e- 1	9.50000 e- 1	3.81014 e- 1
2.00000 e- 1	5.00000 e- 2	2.04124 e- 1
2.00000 e- 1	1.00000 e- 1	2.08516 e- 1
2.00000 e- 1	1.50000 e- 1	2.13208 e- 1
2.00000 e- 1	2.00000 e- 1	2.18238 e- 1
2.00000 e- 1	2.50000 e- 1	2.23650 e- 1
2.00000 e- 1	3.00000 e- 1	2.29500 e- 1
2.00000 e- 1	3.50000 e- 1	2.35856 e- 1
2.00000 e- 1	4.00000 e- 1	2.42799 e- 1
2.00000 e- 1	4.50000 e- 1	2.50435 e- 1
2.00000 e- 1	5.00000 e- 1	2.58899 e- 1
2.00000 e- 1	5.50000 e- 1	2.68367 e- 1
2.00000 e- 1	6.00000 e- 1	2.79078 e- 1
2.00000 e- 1	6.50000 e- 1	2.91364 e- 1
2.00000 e- 1	7.00000 e- 1	3.05710 e- 1
2.00000 e- 1	7.50000 e- 1	3.22856 e- 1
2.00000 e- 1	8.00000 e- 1	3.44025 e- 1
2.00000 e- 1	8.50000 e- 1	3.71464 e- 1
2.00000 e- 1	9.00000 e- 1	4.10047 e- 1
2.00000 e- 1	9.50000 e- 1	4.74442 e- 1

k^*/k	f	R
2.50000 e- 1	5.00000 e- 2	2.54829 e- 1
2.50000 e- 1	1.00000 e- 1	2.59963 e- 1
2.50000 e- 1	1.50000 e- 1	2.65436 e- 1
2.50000 e- 1	2.00000 e- 1	2.71292 e- 1
2.50000 e- 1	2.50000 e- 1	2.77581 e- 1
2.50000 e- 1	3.00000 e- 1	2.84363 e- 1
2.50000 e- 1	3.50000 e- 1	2.91712 e- 1
2.50000 e- 1	4.00000 e- 1	2.99721 e- 1
2.50000 e- 1	4.50000 e- 1	3.08503 e- 1
2.50000 e- 1	5.00000 e- 1	3.18207 e- 1
2.50000 e- 1	5.50000 e- 1	3.29025 e- 1
2.50000 e- 1	6.00000 e- 1	3.41215 e- 1
2.50000 e- 1	6.50000 e- 1	3.55138 e- 1
2.50000 e- 1	7.00000 e- 1	3.71310 e- 1
2.50000 e- 1	7.50000 e- 1	3.90524 e- 1
2.50000 e- 1	8.00000 e- 1	4.14075 e- 1
2.50000 e- 1	8.50000 e- 1	4.44314 e- 1
2.50000 e- 1	9.00000 e- 1	4.86287 e- 1
2.50000 e- 1	9.50000 e- 1	5.54873 e- 1
3.00000 e- 1	5.00000 e- 2	3.05404 e- 1
3.00000 e- 1	1.00000 e- 1	3.11138 e- 1
3.00000 e- 1	1.50000 e- 1	3.17241 e- 1
3.00000 e- 1	2.00000 e- 1	3.23758 e- 1
3.00000 e- 1	2.50000 e- 1	3.30741 e- 1
3.00000 e- 1	3.00000 e- 1	3.38255 e- 1
3.00000 e- 1	3.50000 e- 1	3.46378 e- 1
3.00000 e- 1	4.00000 e- 1	3.55207 e- 1
3.00000 e- 1	4.50000 e- 1	3.64861 e- 1
3.00000 e- 1	5.00000 e- 1	3.75495 e- 1
3.00000 e- 1	5.50000 e- 1	3.87309 e- 1
3.00000 e- 1	6.00000 e- 1	4.00570 e- 1
3.00000 e- 1	6.50000 e- 1	4.15650 e- 1
3.00000 e- 1	7.00000 e- 1	4.33078 e- 1
3.00000 e- 1	7.50000 e- 1	4.53661 e- 1
3.00000 e- 1	8.00000 e- 1	4.78708 e- 1
3.00000 e- 1	8.50000 e- 1	5.10571 e- 1
3.00000 e- 1	9.00000 e- 1	5.54236 e- 1
3.00000 e- 1	9.50000 e- 1	6.24115 e- 1

k^*/k	f	R
3.50000 e- 1	5.00000 e- 2	3.55849 e- 1
3.50000 e- 1	1.00000 e- 1	3.62045 e- 1
3.50000 e- 1	1.50000 e- 1	3.68627 e- 1
3.50000 e- 1	2.00000 e- 1	3.75641 e- 1
3.50000 e- 1	2.50000 e- 1	3.83142 e- 1
3.50000 e- 1	3.00000 e- 1	3.91195 e- 1
3.50000 e- 1	3.50000 e- 1	3.99880 e- 1
3.50000 e- 1	4.00000 e- 1	4.09294 e- 1
3.50000 e- 1	4.50000 e- 1	4.19560 e- 1
3.50000 e- 1	5.00000 e- 1	4.30832 e- 1
3.50000 e- 1	5.50000 e- 1	4.43312 e- 1
3.50000 e- 1	6.00000 e- 1	4.57267 e- 1
3.50000 e- 1	6.50000 e- 1	4.73067 e- 1
3.50000 e- 1	7.00000 e- 1	4.91237 e- 1
3.50000 e- 1	7.50000 e- 1	5.12570 e- 1
3.50000 e- 1	8.00000 e- 1	5.38343 e- 1
3.50000 e- 1	8.50000 e- 1	5.70833 e- 1
3.50000 e- 1	9.00000 e- 1	6.14796 e- 1
3.50000 e- 1	9.50000 e- 1	6.83725 e- 1
4.00000 e- 1	5.00000 e- 2	4.06165 e- 1
4.00000 e- 1	1.00000 e- 1	4.12685 e- 1
4.00000 e- 1	1.50000 e- 1	4.19598 e- 1
4.00000 e- 1	2.00000 e- 1	4.26949 e- 1
4.00000 e- 1	2.50000 e- 1	4.34795 e- 1
4.00000 e- 1	3.00000 e- 1	4.43199 e- 1
4.00000 e- 1	3.50000 e- 1	4.52241 e- 1
4.00000 e- 1	4.00000 e- 1	4.62017 e- 1
4.00000 e- 1	4.50000 e- 1	4.72647 e- 1
4.00000 e- 1	5.00000 e- 1	4.84283 e- 1
4.00000 e- 1	5.50000 e- 1	4.97123 e- 1
4.00000 e- 1	6.00000 e- 1	5.11425 e- 1
4.00000 e- 1	6.50000 e- 1	5.27548 e- 1
4.00000 e- 1	7.00000 e- 1	5.45999 e- 1
4.00000 e- 1	7.50000 e- 1	5.67534 e- 1
4.00000 e- 1	8.00000 e- 1	5.93368 e- 1
4.00000 e- 1	8.50000 e- 1	6.25641 e- 1
4.00000 e- 1	9.00000 e- 1	6.68770 e- 1
4.00000 e- 1	9.50000 e- 1	7.35043 e- 1

k^*/k	f	R
4.50000 e- 1	5.00000 e- 2	4.56353 e- 1
4.50000 e- 1	1.00000 e- 1	4.63058 e- 1
4.50000 e- 1	1.50000 e- 1	4.70155 e- 1
4.50000 e- 1	2.00000 e- 1	4.77688 e- 1
4.50000 e- 1	2.50000 e- 1	4.85710 e- 1
4.50000 e- 1	3.00000 e- 1	4.94284 e- 1
4.50000 e- 1	3.50000 e- 1	5.03487 e- 1
4.50000 e- 1	4.00000 e- 1	5.13411 e- 1
4.50000 e- 1	4.50000 e- 1	5.24171 e- 1
4.50000 e- 1	5.00000 e- 1	5.35914 e- 1
4.50000 e- 1	5.50000 e- 1	5.48827 e- 1
4.50000 e- 1	6.00000 e- 1	5.63158 e- 1
4.50000 e- 1	6.50000 e- 1	5.79244 e- 1
4.50000 e- 1	7.00000 e- 1	5.97561 e- 1
4.50000 e- 1	7.50000 e- 1	6.18818 e- 1
4.50000 e- 1	8.00000 e- 1	6.44138 e- 1
4.50000 e- 1	8.50000 e- 1	6.75489 e- 1
4.50000 e- 1	9.00000 e- 1	7.16874 e- 1
4.50000 e- 1	9.50000 e- 1	7.79223 e- 1
5.00000 e- 1	5.00000 e- 2	5.06411 e- 1
5.00000 e- 1	1.00000 e- 1	5.13167 e- 1
5.00000 e- 1	1.50000 e- 1	5.20304 e- 1
5.00000 e- 1	2.00000 e- 1	5.27864 e- 1
5.00000 e- 1	2.50000 e- 1	5.35898 e- 1
5.00000 e- 1	3.00000 e- 1	5.44467 e- 1
5.00000 e- 1	3.50000 e- 1	5.53641 e- 1
5.00000 e- 1	4.00000 e- 1	5.63508 e- 1
5.00000 e- 1	4.50000 e- 1	5.74178 e- 1
5.00000 e- 1	5.00000 e- 1	5.85786 e- 1
5.00000 e- 1	5.50000 e- 1	5.98508 e- 1
5.00000 e- 1	6.00000 e- 1	6.12574 e- 1
5.00000 e- 1	6.50000 e- 1	6.28295 e- 1
5.00000 e- 1	7.00000 e- 1	6.46111 e- 1
5.00000 e- 1	7.50000 e- 1	6.66667 e- 1
5.00000 e- 1	8.00000 e- 1	6.90983 e- 1
5.00000 e- 1	8.50000 e- 1	7.20825 e- 1
5.00000 e- 1	9.00000 e- 1	7.59747 e- 1
5.00000 e- 1	9.50000 e- 1	8.17256 e- 1

k^*/k	f	R
5.50000 e- 1	5.00000 e- 2	5.56342 e- 1
5.50000 e- 1	1.00000 e- 1	5.63012 e- 1
5.50000 e- 1	1.50000 e- 1	5.70046 e- 1
5.50000 e- 1	2.00000 e- 1	5.77483 e- 1
5.50000 e- 1	2.50000 e- 1	5.85370 e- 1
5.50000 e- 1	3.00000 e- 1	5.93762 e- 1
5.50000 e- 1	3.50000 e- 1	6.02726 e- 1
5.50000 e- 1	4.00000 e- 1	6.12343 e- 1
5.50000 e- 1	4.50000 e- 1	6.22712 e- 1
5.50000 e- 1	5.00000 e- 1	6.33960 e- 1
5.50000 e- 1	5.50000 e- 1	6.46245 e- 1
5.50000 e- 1	6.00000 e- 1	6.59777 e- 1
5.50000 e- 1	6.50000 e- 1	6.74839 e- 1
5.50000 e- 1	7.00000 e- 1	6.91824 e- 1
5.50000 e- 1	7.50000 e- 1	7.11311 e- 1
5.50000 e- 1	8.00000 e- 1	7.34206 e- 1
5.50000 e- 1	8.50000 e- 1	7.62060 e- 1
5.50000 e- 1	9.00000 e- 1	7.97957 e- 1
5.50000 e- 1	9.50000 e- 1	8.49999 e- 1
6.00000 e- 1	5.00000 e- 2	6.06144 e- 1
6.00000 e- 1	1.00000 e- 1	6.12596 e- 1
6.00000 e- 1	1.50000 e- 1	6.19386 e- 1
6.00000 e- 1	2.00000 e- 1	6.26552 e- 1
6.00000 e- 1	2.50000 e- 1	6.34135 e- 1
6.00000 e- 1	3.00000 e- 1	6.42185 e- 1
6.00000 e- 1	3.50000 e- 1	6.50765 e- 1
6.00000 e- 1	4.00000 e- 1	6.59945 e- 1
6.00000 e- 1	4.50000 e- 1	6.69817 e- 1
6.00000 e- 1	5.00000 e- 1	6.80492 e- 1
6.00000 e- 1	5.50000 e- 1	6.92113 e- 1
6.00000 e- 1	6.00000 e- 1	7.04867 e- 1
6.00000 e- 1	6.50000 e- 1	7.19002 e- 1
6.00000 e- 1	7.00000 e- 1	7.34867 e- 1
6.00000 e- 1	7.50000 e- 1	7.52966 e- 1
6.00000 e- 1	8.00000 e- 1	7.74087 e- 1
6.00000 e- 1	8.50000 e- 1	7.99562 e- 1
6.00000 e- 1	9.00000 e- 1	8.32013 e- 1
6.00000 e- 1	9.50000 e- 1	8.78187 e- 1

k^*/k	f	R
6.50000 e- 1	5.00000 e- 2	6.55819 e- 1
6.50000 e- 1	1.00000 e- 1	6.61919 e- 1
6.50000 e- 1	1.50000 e- 1	6.68327 e- 1
6.50000 e- 1	2.00000 e- 1	6.75076 e- 1
6.50000 e- 1	2.50000 e- 1	6.82203 e- 1
6.50000 e- 1	3.00000 e- 1	6.89753 e- 1
6.50000 e- 1	3.50000 e- 1	6.97780 e- 1
6.50000 e- 1	4.00000 e- 1	7.06347 e- 1
6.50000 e- 1	4.50000 e- 1	7.15535 e- 1
6.50000 e- 1	5.00000 e- 1	7.25439 e- 1
6.50000 e- 1	5.50000 e- 1	7.36186 e- 1
6.50000 e- 1	6.00000 e- 1	7.47937 e- 1
6.50000 e- 1	6.50000 e- 1	7.60907 e- 1
6.50000 e- 1	7.00000 e- 1	7.75395 e- 1
6.50000 e- 1	7.50000 e- 1	7.91832 e- 1
6.50000 e- 1	8.00000 e- 1	8.10884 e- 1
6.50000 e- 1	8.50000 e- 1	8.33671 e- 1
6.50000 e- 1	9.00000 e- 1	8.62364 e- 1
6.50000 e- 1	9.50000 e- 1	9.02453 e- 1
7.00000 e- 1	5.00000 e- 2	7.05367 e- 1
7.00000 e- 1	1.00000 e- 1	7.10983 e- 1
7.00000 e- 1	1.50000 e- 1	7.16872 e- 1
7.00000 e- 1	2.00000 e- 1	7.23062 e- 1
7.00000 e- 1	2.50000 e- 1	7.29585 e- 1
7.00000 e- 1	3.00000 e- 1	7.36480 e- 1
7.00000 e- 1	3.50000 e- 1	7.43793 e- 1
7.00000 e- 1	4.00000 e- 1	7.51580 e- 1
7.00000 e- 1	4.50000 e- 1	7.59906 e- 1
7.00000 e- 1	5.00000 e- 1	7.68856 e- 1
7.00000 e- 1	5.50000 e- 1	7.78534 e- 1
7.00000 e- 1	6.00000 e- 1	7.89079 e- 1
7.00000 e- 1	6.50000 e- 1	8.00669 e- 1
7.00000 e- 1	7.00000 e- 1	8.13555 e- 1
7.00000 e- 1	7.50000 e- 1	8.28094 e- 1
7.00000 e- 1	8.00000 e- 1	8.44836 e- 1
7.00000 e- 1	8.50000 e- 1	8.64693 e- 1
7.00000 e- 1	9.00000 e- 1	8.89415 e- 1
7.00000 e- 1	9.50000 e- 1	9.23344 e- 1

k^*/k	f	R
7.50000 e- 1	5.00000 e- 2	7.54788 e- 1
7.50000 e- 1	1.00000 e- 1	7.59789 e- 1
7.50000 e- 1	1.50000 e- 1	7.65024 e- 1
7.50000 e- 1	2.00000 e- 1	7.70515 e- 1
7.50000 e- 1	2.50000 e- 1	7.76290 e- 1
7.50000 e- 1	3.00000 e- 1	7.82381 e- 1
7.50000 e- 1	3.50000 e- 1	7.88826 e- 1
7.50000 e- 1	4.00000 e- 1	7.95671 e- 1
7.50000 e- 1	4.50000 e- 1	8.02970 e- 1
7.50000 e- 1	5.00000 e- 1	8.10793 e- 1
7.50000 e- 1	5.50000 e- 1	8.19225 e- 1
7.50000 e- 1	6.00000 e- 1	8.28378 e- 1
7.50000 e- 1	6.50000 e- 1	8.38398 e- 1
7.50000 e- 1	7.00000 e- 1	8.49486 e- 1
7.50000 e- 1	7.50000 e- 1	8.61929 e- 1
7.50000 e- 1	8.00000 e- 1	8.76163 e- 1
7.50000 e- 1	8.50000 e- 1	8.92908 e- 1
7.50000 e- 1	9.00000 e- 1	9.13525 e- 1
7.50000 e- 1	9.50000 e- 1	9.41329 e- 1
8.00000 e- 1	5.00000 e- 2	8.04082 e- 1
8.00000 e- 1	1.00000 e- 1	8.08339 e- 1
8.00000 e- 1	1.50000 e- 1	8.12786 e- 1
8.00000 e- 1	2.00000 e- 1	8.17442 e- 1
8.00000 e- 1	2.50000 e- 1	8.22328 e- 1
8.00000 e- 1	3.00000 e- 1	8.27471 e- 1
8.00000 e- 1	3.50000 e- 1	8.32900 e- 1
8.00000 e- 1	4.00000 e- 1	8.38650 e- 1
8.00000 e- 1	4.50000 e- 1	8.44767 e- 1
8.00000 e- 1	5.00000 e- 1	8.51302 e- 1
8.00000 e- 1	5.50000 e- 1	8.58323 e- 1
8.00000 e- 1	6.00000 e- 1	8.65917 e- 1
8.00000 e- 1	6.50000 e- 1	8.74197 e- 1
8.00000 e- 1	7.00000 e- 1	8.83317 e- 1
8.00000 e- 1	7.50000 e- 1	8.93497 e- 1
8.00000 e- 1	8.00000 e- 1	9.05068 e- 1
8.00000 e- 1	8.50000 e- 1	9.18569 e- 1
8.00000 e- 1	9.00000 e- 1	9.35012 e- 1
8.00000 e- 1	9.50000 e- 1	9.56812 e- 1

k^*/k	f	R
5.00000 e- 2	9.60000 e- 1	1.54854 e- 1
5.00000 e- 2	9.70000 e- 1	1.65792 e- 1
5.00000 e- 2	9.80000 e- 1	1.81286 e- 1
5.00000 e- 2	9.90000 e- 1	2.07749 e- 1
1.00000 e- 1	9.60000 e- 1	2.86688 e- 1
1.00000 e- 1	9.70000 e- 1	3.04922 e- 1
1.00000 e- 1	9.80000 e- 1	3.30364 e- 1
1.00000 e- 1	9.90000 e- 1	3.72770 e- 1
1.50000 e- 1	9.60000 e- 1	3.98923 e- 1
1.50000 e- 1	9.70000 e- 1	4.21677 e- 1
1.50000 e- 1	9.80000 e- 1	4.52957 e- 1
1.50000 e- 1	9.90000 e- 1	5.03851 e- 1
2.00000 e- 1	9.60000 e- 1	4.94473 e- 1
2.00000 e- 1	9.70000 e- 1	5.19655 e- 1
2.00000 e- 1	9.80000 e- 1	5.53770 e- 1
2.00000 e- 1	9.90000 e- 1	6.07973 e- 1
2.50000 e- 1	9.60000 e- 1	5.75819 e- 1
2.50000 e- 1	9.70000 e- 1	6.01877 e- 1
2.50000 e- 1	9.80000 e- 1	6.36673 e- 1
2.50000 e- 1	9.90000 e- 1	6.90679 e- 1
3.00000 e- 1	9.60000 e- 1	6.45072 e- 1
3.00000 e- 1	9.70000 e- 1	6.70876 e- 1
3.00000 e- 1	9.80000 e- 1	7.04847 e- 1
3.00000 e- 1	9.90000 e- 1	7.56375 e- 1
3.50000 e- 1	9.60000 e- 1	7.04030 e- 1
3.50000 e- 1	9.70000 e- 1	7.28779 e- 1
3.50000 e- 1	9.80000 e- 1	7.60910 e- 1
3.50000 e- 1	9.90000 e- 1	8.08559 e- 1
4.00000 e- 1	9.60000 e- 1	7.54223 e- 1
4.00000 e- 1	9.70000 e- 1	7.77370 e- 1
4.00000 e- 1	9.80000 e- 1	8.07012 e- 1
4.00000 e- 1	9.90000 e- 1	8.50011 e- 1

k^*/k	f	R
4.50000 e- 1	9.60000 e- 1	7.96954 e- 1
4.50000 e- 1	9.70000 e- 1	8.18147 e- 1
4.50000 e- 1	9.80000 e- 1	8.44924 e- 1
4.50000 e- 1	9.90000 e- 1	8.82937 e- 1
5.00000 e- 1	9.60000 e- 1	8.33333 e- 1
5.00000 e- 1	9.70000 e- 1	8.52366 e- 1
5.00000 e- 1	9.80000 e- 1	8.76101 e- 1
5.00000 e- 1	9.90000 e- 1	9.09091 e- 1
5.50000 e- 1	9.60000 e- 1	8.64304 e- 1
5.50000 e- 1	9.70000 e- 1	8.81082 e- 1
5.50000 e- 1	9.80000 e- 1	9.01738 e- 1
5.50000 e- 1	9.90000 e- 1	9.29866 e- 1
6.00000 e- 1	9.60000 e- 1	8.90671 e- 1
6.00000 e- 1	9.70000 e- 1	9.05180 e- 1
6.00000 e- 1	9.80000 e- 1	9.22821 e- 1
6.00000 e- 1	9.90000 e- 1	9.46368 e- 1
6.50000 e- 1	9.60000 e- 1	9.13118 e- 1
6.50000 e- 1	9.70000 e- 1	9.25402 e- 1
6.50000 e- 1	9.80000 e- 1	9.40158 e- 1
6.50000 e- 1	9.90000 e- 1	9.59476 e- 1
7.00000 e- 1	9.60000 e- 1	9.32228 e- 1
7.00000 e- 1	9.70000 e- 1	9.42373 e- 1
7.00000 e- 1	9.80000 e- 1	9.54416 e- 1
7.00000 e- 1	9.90000 e- 1	9.69888 e- 1
7.50000 e- 1	9.60000 e- 1	9.48497 e- 1
7.50000 e- 1	9.70000 e- 1	9.56614 e- 1
7.50000 e- 1	9.80000 e- 1	9.66140 e- 1
7.50000 e- 1	9.90000 e- 1	9.78159 e- 1
8.00000 e- 1	9.60000 e- 1	9.62348 e- 1
8.00000 e- 1	9.70000 e- 1	9.68565 e- 1
8.00000 e- 1	9.80000 e- 1	9.75781 e- 1
8.00000 e- 1	9.90000 e- 1	9.84728 e- 1

Table 2

Table of Isotope Effect Functions for
$k^*/k = .05 - .45$ and $f = .990 - .999$

k^*/k	f	R
5.00000 e- 2	9.90000 e- 1	2.07749 e- 1
5.00000 e- 2	9.91000 e- 1	2.11751 e- 1
5.00000 e- 2	9.92000 e- 1	2.16215 e- 1
5.00000 e- 2	9.93000 e- 1	2.21261 e- 1
5.00000 e- 2	9.94000 e- 1	2.27065 e- 1
5.00000 e- 2	9.95000 e- 1	2.33899 e- 1
5.00000 e- 2	9.96000 e- 1	2.42211 e- 1
5.00000 e- 2	9.97000 e- 1	2.52837 e- 1
5.00000 e- 2	9.98000 e- 1	2.67624 e- 1
5.00000 e- 2	9.99000 e- 1	2.92347 e- 1
1.00000 e- 1	9.90000 e- 1	3.72770 e- 1
1.00000 e- 1	9.91000 e- 1	3.79067 e- 1
1.00000 e- 1	9.92000 e- 1	3.86055 e- 1
1.00000 e- 1	9.93000 e- 1	3.93908 e- 1
1.00000 e- 1	9.94000 e- 1	4.02881 e- 1
1.00000 e- 1	9.95000 e- 1	4.13363 e- 1
1.00000 e- 1	9.96000 e- 1	4.25991 e- 1
1.00000 e- 1	9.97000 e- 1	4.41939 e- 1
1.00000 e- 1	9.98000 e- 1	4.63768 e- 1
1.00000 e- 1	9.99000 e- 1	4.99312 e- 1
1.50000 e- 1	9.90000 e- 1	5.03851 e- 1
1.50000 e- 1	9.91000 e- 1	5.11273 e- 1
1.50000 e- 1	9.92000 e- 1	5.19466 e- 1
1.50000 e- 1	9.93000 e- 1	5.28623 e- 1
1.50000 e- 1	9.94000 e- 1	5.39015 e- 1
1.50000 e- 1	9.95000 e- 1	5.51060 e- 1
1.50000 e- 1	9.96000 e- 1	5.65435 e- 1
1.50000 e- 1	9.97000 e- 1	5.83373 e- 1
1.50000 e- 1	9.98000 e- 1	6.07525 e- 1
1.50000 e- 1	9.99000 e- 1	6.45833 e- 1

k^*/k	f	R
2.00000 e- 1	9.90000 e- 1	6.07973 e- 1
2.00000 e- 1	9.91000 e- 1	6.15736 e- 1
2.00000 e- 1	9.92000 e- 1	6.24263 e- 1
2.00000 e- 1	9.93000 e- 1	6.33739 e- 1
2.00000 e- 1	9.94000 e- 1	6.44423 e- 1
2.00000 e- 1	9.95000 e- 1	6.56711 e- 1
2.00000 e- 1	9.96000 e- 1	6.71240 e- 1
2.00000 e- 1	9.97000 e- 1	6.89154 e- 1
2.00000 e- 1	9.98000 e- 1	7.12886 e- 1
2.00000 e- 1	9.99000 e- 1	7.49561 e- 1
2.50000 e- 1	9.90000 e- 1	6.90679 e- 1
2.50000 e- 1	9.91000 e- 1	6.98277 e- 1
2.50000 e- 1	9.92000 e- 1	7.06583 e- 1
2.50000 e- 1	9.93000 e- 1	7.15760 e- 1
2.50000 e- 1	9.94000 e- 1	7.26040 e- 1
2.50000 e- 1	9.95000 e- 1	7.37774 e- 1
2.50000 e- 1	9.96000 e- 1	7.51519 e- 1
2.50000 e- 1	9.97000 e- 1	7.68270 e- 1
2.50000 e- 1	9.98000 e- 1	7.90106 e- 1
2.50000 e- 1	9.99000 e- 1	8.22995 e- 1
3.00000 e- 1	9.90000 e- 1	7.56375 e- 1
3.00000 e- 1	9.91000 e- 1	7.63498 e- 1
3.00000 e- 1	9.92000 e- 1	7.71246 e- 1
3.00000 e- 1	9.93000 e- 1	7.79759 e- 1
3.00000 e- 1	9.94000 e- 1	7.89236 e- 1
3.00000 e- 1	9.95000 e- 1	7.99971 e- 1
3.00000 e- 1	9.96000 e- 1	8.12432 e- 1
3.00000 e- 1	9.97000 e- 1	8.27443 e- 1
3.00000 e- 1	9.98000 e- 1	8.46702 e- 1
3.00000 e- 1	9.99000 e- 1	8.74983 e- 1

k^*/k	f	R
3.50000 e- 1	9.90000 e- 1	8.08559 e- 1
3.50000 e- 1	9.91000 e- 1	8.15033 e- 1
3.50000 e- 1	9.92000 e- 1	8.22040 e- 1
3.50000 e- 1	9.93000 e- 1	8.29698 e- 1
3.50000 e- 1	9.94000 e- 1	8.38169 e- 1
3.50000 e- 1	9.95000 e- 1	8.47693 e- 1
3.50000 e- 1	9.96000 e- 1	8.58650 e- 1
3.50000 e- 1	9.97000 e- 1	8.71699 e- 1
3.50000 e- 1	9.98000 e- 1	8.88181 e- 1
3.50000 e- 1	9.99000 e- 1	9.11787 e- 1
4.00000 e- 1	9.90000 e- 1	8.50011 e- 1
4.00000 e- 1	9.91000 e- 1	8.55753 e- 1
4.00000 e- 1	9.92000 e- 1	8.61940 e- 1
4.00000 e- 1	9.93000 e- 1	8.68664 e- 1
4.00000 e- 1	9.94000 e- 1	8.76057 e- 1
4.00000 e- 1	9.95000 e- 1	8.84309 e- 1
4.00000 e- 1	9.96000 e- 1	8.93719 e- 1
4.00000 e- 1	9.97000 e- 1	9.04800 e- 1
4.00000 e- 1	9.98000 e- 1	9.18582 e- 1
4.00000 e- 1	9.99000 e- 1	9.37842 e- 1
4.50000 e- 1	9.90000 e- 1	8.82937 e- 1
4.50000 e- 1	9.91000 e- 1	8.87928 e- 1
4.50000 e- 1	9.92000 e- 1	8.93281 e- 1
4.50000 e- 1	9.93000 e- 1	8.99069 e- 1
4.50000 e- 1	9.94000 e- 1	9.05394 e- 1
4.50000 e- 1	9.95000 e- 1	9.12403 e- 1
4.50000 e- 1	9.96000 e- 1	9.20327 e- 1
4.50000 e- 1	9.97000 e- 1	9.29556 e- 1
4.50000 e- 1	9.98000 e- 1	9.40863 e- 1
4.50000 e- 1	9.99000 e- 1	9.56288 e- 1

Table 3

Table of Isotope Effect Functions for
$k^*/k = .81 - .99$ and $f = .10 - .99$

k^*/k	f	R
8.10000 e- 1	1.00000 e- 1	8.18018 e- 1
8.10000 e- 1	2.00000 e- 1	8.26764 e- 1
8.10000 e- 1	3.00000 e- 1	8.36393 e- 1
8.10000 e- 1	4.00000 e- 1	8.47115 e- 1
8.10000 e- 1	5.00000 e- 1	8.59236 e- 1
8.10000 e- 1	6.00000 e- 1	8.73221 e- 1
8.10000 e- 1	7.00000 e- 1	8.89843 e- 1
8.10000 e- 1	8.00000 e- 1	9.10575 e- 1
8.20000 e- 1	1.00000 e- 1	8.27687 e- 1
8.20000 e- 1	2.00000 e- 1	8.36066 e- 1
8.20000 e- 1	3.00000 e- 1	8.45283 e- 1
8.20000 e- 1	4.00000 e- 1	8.55537 e- 1
8.20000 e- 1	5.00000 e- 1	8.67116 e- 1
8.20000 e- 1	6.00000 e- 1	8.80458 e- 1
8.20000 e- 1	7.00000 e- 1	8.96290 e- 1
8.20000 e- 1	8.00000 e- 1	9.15994 e- 1
8.30000 e- 1	1.00000 e- 1	8.37346 e- 1
8.30000 e- 1	2.00000 e- 1	8.45348 e- 1
8.30000 e- 1	3.00000 e- 1	8.54142 e- 1
8.30000 e- 1	4.00000 e- 1	8.63916 e- 1
8.30000 e- 1	5.00000 e- 1	8.74942 e- 1
8.30000 e- 1	6.00000 e- 1	8.87629 e- 1
8.30000 e- 1	7.00000 e- 1	9.02660 e- 1
8.30000 e- 1	8.00000 e- 1	9.21326 e- 1
8.40000 e- 1	1.00000 e- 1	8.46995 e- 1
8.40000 e- 1	2.00000 e- 1	8.54608 e- 1
8.40000 e- 1	3.00000 e- 1	8.62968 e- 1
8.40000 e- 1	4.00000 e- 1	8.72252 e- 1
8.40000 e- 1	5.00000 e- 1	8.82713 e- 1
8.40000 e- 1	6.00000 e- 1	8.94734 e- 1
8.40000 e- 1	7.00000 e- 1	9.08954 e- 1
8.40000 e- 1	8.00000 e- 1	9.26574 e- 1
8.50000 e- 1	1.00000 e- 1	8.56633 e- 1
8.50000 e- 1	2.00000 e- 1	8.63848 e- 1
8.50000 e- 1	3.00000 e- 1	8.71764 e- 1
8.50000 e- 1	4.00000 e- 1	8.80546 e- 1
8.50000 e- 1	5.00000 e- 1	8.90431 e- 1
8.50000 e- 1	6.00000 e- 1	9.01775 e- 1
8.50000 e- 1	7.00000 e- 1	9.15172 e- 1
8.50000 e- 1	8.00000 e- 1	9.31737 e- 1

k^*/k	f	R
8.60000 e- 1	1.00000 e- 1	8.66262 e- 1
8.60000 e- 1	2.00000 e- 1	8.73067 e- 1
8.60000 e- 1	3.00000 e- 1	8.80528 e- 1
8.60000 e- 1	4.00000 e- 1	8.88798 e- 1
8.60000 e- 1	5.00000 e- 1	8.98095 e- 1
8.60000 e- 1	6.00000 e- 1	9.08752 e- 1
8.60000 e- 1	7.00000 e- 1	9.21317 e- 1
8.60000 e- 1	8.00000 e- 1	9.36819 e- 1
8.70000 e- 1	1.00000 e- 1	8.75880 e- 1
8.70000 e- 1	2.00000 e- 1	8.82266 e- 1
8.70000 e- 1	3.00000 e- 1	8.89261 e- 1
8.70000 e- 1	4.00000 e- 1	8.97007 e- 1
8.70000 e- 1	5.00000 e- 1	9.05706 e- 1
8.70000 e- 1	6.00000 e- 1	9.15665 e- 1
8.70000 e- 1	7.00000 e- 1	9.27387 e- 1
8.70000 e- 1	8.00000 e- 1	9.41819 e- 1
8.80000 e- 1	1.00000 e- 1	8.85488 e- 1
8.80000 e- 1	2.00000 e- 1	8.91444 e- 1
8.80000 e- 1	3.00000 e- 1	8.97963 e- 1
8.80000 e- 1	4.00000 e- 1	9.05175 e- 1
8.80000 e- 1	5.00000 e- 1	9.13265 e- 1
8.80000 e- 1	6.00000 e- 1	9.22515 e- 1
8.80000 e- 1	7.00000 e- 1	9.33385 e- 1
8.80000 e- 1	8.00000 e- 1	9.46739 e- 1
8.90000 e- 1	1.00000 e- 1	8.95086 e- 1
8.90000 e- 1	2.00000 e- 1	9.00602 e- 1
8.90000 e- 1	3.00000 e- 1	9.06634 e- 1
8.90000 e- 1	4.00000 e- 1	9.13301 e- 1
8.90000 e- 1	5.00000 e- 1	9.20772 e- 1
8.90000 e- 1	6.00000 e- 1	9.29302 e- 1
8.90000 e- 1	7.00000 e- 1	9.39311 e- 1
8.90000 e- 1	8.00000 e- 1	9.51581 e- 1
9.00000 e- 1	1.00000 e- 1	9.04674 e- 1
9.00000 e- 1	2.00000 e- 1	9.09739 e- 1
9.00000 e- 1	3.00000 e- 1	9.15274 e- 1
9.00000 e- 1	4.00000 e- 1	9.21385 e- 1
9.00000 e- 1	5.00000 e- 1	9.28227 e- 1
9.00000 e- 1	6.00000 e- 1	9.36028 e- 1
9.00000 e- 1	7.00000 e- 1	9.45166 e- 1
9.00000 e- 1	8.00000 e- 1	9.56345 e- 1

k^*/k	f	R
9.10000 e- 1	1.00000 e- 1	9.14252 e- 1
9.10000 e- 1	2.00000 e- 1	9.18856 e- 1
9.10000 e- 1	3.00000 e- 1	9.23883 e- 1
9.10000 e- 1	4.00000 e- 1	9.29429 e- 1
9.10000 e- 1	5.00000 e- 1	9.35630 e- 1
9.10000 e- 1	6.00000 e- 1	9.42692 e- 1
9.10000 e- 1	7.00000 e- 1	9.50952 e- 1
9.10000 e- 1	8.00000 e- 1	9.61034 e- 1
9.20000 e- 1	1.00000 e- 1	9.23820 e- 1
9.20000 e- 1	2.00000 e- 1	9.27953 e- 1
9.20000 e- 1	3.00000 e- 1	9.32462 e- 1
9.20000 e- 1	4.00000 e- 1	9.37431 e- 1
9.20000 e- 1	5.00000 e- 1	9.42982 e- 1
9.20000 e- 1	6.00000 e- 1	9.49295 e- 1
9.20000 e- 1	7.00000 e- 1	9.56668 e- 1
9.20000 e- 1	8.00000 e- 1	9.65647 e- 1
9.30000 e- 1	1.00000 e- 1	9.33377 e- 1
9.30000 e- 1	2.00000 e- 1	9.37029 e- 1
9.30000 e- 1	3.00000 e- 1	9.41010 e- 1
9.30000 e- 1	4.00000 e- 1	9.45393 e- 1
9.30000 e- 1	5.00000 e- 1	9.50283 e- 1
9.30000 e- 1	6.00000 e- 1	9.55839 e- 1
9.30000 e- 1	7.00000 e- 1	9.62315 e- 1
9.30000 e- 1	8.00000 e- 1	9.70187 e- 1
9.40000 e- 1	1.00000 e- 1	9.42925 e- 1
9.40000 e- 1	2.00000 e- 1	9.46085 e- 1
9.40000 e- 1	3.00000 e- 1	9.49527 e- 1
9.40000 e- 1	4.00000 e- 1	9.53314 e- 1
9.40000 e- 1	5.00000 e- 1	9.57534 e- 1
9.40000 e- 1	6.00000 e- 1	9.62322 e- 1
9.40000 e- 1	7.00000 e- 1	9.67895 e- 1
9.40000 e- 1	8.00000 e- 1	9.74654 e- 1
9.50000 e- 1	1.00000 e- 1	9.52463 e- 1
9.50000 e- 1	2.00000 e- 1	9.55121 e- 1
9.50000 e- 1	3.00000 e- 1	9.58015 e- 1
9.50000 e- 1	4.00000 e- 1	9.61195 e- 1
9.50000 e- 1	5.00000 e- 1	9.64735 e- 1
9.50000 e- 1	6.00000 e- 1	9.68747 e- 1
9.50000 e- 1	7.00000 e- 1	9.73408 e- 1
9.50000 e- 1	8.00000 e- 1	9.79050 e- 1

$\bar{k}^*/k$	f	R
9.60000 e- 1	1.00000 e- 1	9.61990 e- 1
9.60000 e- 1	2.00000 e- 1	9.64137 e- 1
9.60000 e- 1	3.00000 e- 1	9.66472 e- 1
9.60000 e- 1	4.00000 e- 1	9.69035 e- 1
9.60000 e- 1	5.00000 e- 1	9.71886 e- 1
9.60000 e- 1	6.00000 e- 1	9.75112 e- 1
9.60000 e- 1	7.00000 e- 1	9.78855 e- 1
9.60000 e- 1	8.00000 e- 1	9.83376 e- 1
9.70000 e- 1	1.00000 e- 1	9.71508 e- 1
9.70000 e- 1	2.00000 e- 1	9.73133 e- 1
9.70000 e- 1	3.00000 e- 1	9.74899 e- 1
9.70000 e- 1	4.00000 e- 1	9.76836 e- 1
9.70000 e- 1	5.00000 e- 1	9.78988 e- 1
9.70000 e- 1	6.00000 e- 1	9.81420 e- 1
9.70000 e- 1	7.00000 e- 1	9.84237 e- 1
9.70000 e- 1	8.00000 e- 1	9.87633 e- 1
9.80000 e- 1	1.00000 e- 1	9.81015 e- 1
9.80000 e- 1	2.00000 e- 1	9.82109 e- 1
9.80000 e- 1	3.00000 e- 1	9.83296 e- 1
9.80000 e- 1	4.00000 e- 1	9.84597 e- 1
9.80000 e- 1	5.00000 e- 1	9.86041 e- 1
9.80000 e- 1	6.00000 e- 1	9.87670 e- 1
9.80000 e- 1	7.00000 e- 1	9.89555 e- 1
9.80000 e- 1	8.00000 e- 1	9.91822 e- 1
9.90000 e- 1	1.00000 e- 1	9.90513 e- 1
9.90000 e- 1	2.00000 e- 1	9.91064 e- 1
9.90000 e- 1	3.00000 e- 1	9.91663 e- 1
9.90000 e- 1	4.00000 e- 1	9.92318 e- 1
9.90000 e- 1	5.00000 e- 1	9.93044 e- 1
9.90000 e- 1	6.00000 e- 1	9.93863 e- 1
9.90000 e- 1	7.00000 e- 1	9.94809 e- 1
9.90000 e- 1	8.00000 e- 1	9.95944 e- 1

k^*/k	f	R
8.10000 e- 1	8.50000 e- 1	9.23416 e- 1
8.10000 e- 1	9.00000 e- 1	9.39020 e- 1
8.10000 e- 1	9.50000 e- 1	9.59640 e- 1
8.20000 e- 1	8.50000 e- 1	9.28171 e- 1
8.20000 e- 1	9.00000 e- 1	9.42938 e- 1
8.20000 e- 1	9.50000 e- 1	9.62385 e- 1
8.30000 e- 1	8.50000 e- 1	9.32837 e- 1
8.30000 e- 1	9.00000 e- 1	9.46766 e- 1
8.30000 e- 1	9.50000 e- 1	9.65048 e- 1
8.40000 e- 1	8.50000 e- 1	9.37416 e- 1
8.40000 e- 1	9.00000 e- 1	9.50507 e- 1
8.40000 e- 1	9.50000 e- 1	9.67633 e- 1
8.50000 e- 1	8.50000 e- 1	9.41908 e- 1
8.50000 e- 1	9.00000 e- 1	9.54162 e- 1
8.50000 e- 1	9.50000 e- 1	9.70142 e- 1
8.60000 e- 1	8.50000 e- 1	9.46316 e- 1
8.60000 e- 1	9.00000 e- 1	9.57735 e- 1
8.60000 e- 1	9.50000 e- 1	9.72576 e- 1
8.70000 e- 1	8.50000 e- 1	9.50641 e- 1
8.70000 e- 1	9.00000 e- 1	9.61226 e- 1
8.70000 e- 1	9.50000 e- 1	9.74939 e- 1
8.80000 e- 1	8.50000 e- 1	9.54885 e- 1
8.80000 e- 1	9.00000 e- 1	9.64638 e- 1
8.80000 e- 1	9.50000 e- 1	9.77232 e- 1
8.90000 e- 1	8.50000 e- 1	9.59049 e- 1
8.90000 e- 1	9.00000 e- 1	9.67972 e- 1
8.90000 e- 1	9.50000 e- 1	9.79457 e- 1
9.00000 e- 1	8.50000 e- 1	9.63135 e- 1
9.00000 e- 1	9.00000 e- 1	9.71231 e- 1
9.00000 e- 1	9.50000 e- 1	9.81617 e- 1

$\bar{k}^*/k$	f	R
9.10000 e- 1	8.50000 e- 1	9.67144 e- 1
9.10000 e- 1	9.00000 e- 1	9.74415 e- 1
9.10000 e- 1	9.50000 e- 1	9.83713 e- 1
9.20000 e- 1	8.50000 e- 1	9.71078 e- 1
9.20000 e- 1	9.00000 e- 1	9.77526 e- 1
9.20000 e- 1	9.50000 e- 1	9.85747 e- 1
9.30000 e- 1	8.50000 e- 1	9.74938 e- 1
9.30000 e- 1	9.00000 e- 1	9.80567 e- 1
9.30000 e- 1	9.50000 e- 1	9.87721 e- 1
9.40000 e- 1	8.50000 e- 1	9.78725 e- 1
9.40000 e- 1	9.00000 e- 1	9.83538 e- 1
9.40000 e- 1	9.50000 e- 1	9.89636 e- 1
9.50000 e- 1	8.50000 e- 1	9.82441 e- 1
9.50000 e- 1	9.00000 e- 1	9.86442 e- 1
9.50000 e- 1	9.50000 e- 1	9.91495 e- 1
9.60000 e- 1	8.50000 e- 1	9.86087 e- 1
9.60000 e- 1	9.00000 e- 1	9.89280 e- 1
9.60000 e- 1	9.50000 e- 1	9.93300 e- 1
9.70000 e- 1	8.50000 e- 1	9.89665 e- 1
9.70000 e- 1	9.00000 e- 1	9.92053 e- 1
9.70000 e- 1	9.50000 e- 1	9.95051 e- 1
9.80000 e- 1	8.50000 e- 1	9.93176 e- 1
9.80000 e- 1	9.00000 e- 1	9.94763 e- 1
9.80000 e- 1	9.50000 e- 1	9.96750 e- 1
9.90000 e- 1	8.50000 e- 1	9.96620 e- 1
9.90000 e- 1	9.00000 e- 1	9.97412 e- 1
9.90000 e- 1	9.50000 e- 1	9.98399 e- 1

k^*/k	f	R
8.10000 e- 1	9.50000 e- 1	9.59640 e- 1
8.10000 e- 1	9.60000 e- 1	9.64860 e- 1
8.10000 e- 1	9.70000 e- 1	9.70714 e- 1
8.10000 e- 1	9.80000 e- 1	9.77493 e- 1
8.10000 e- 1	9.90000 e- 1	9.85870 e- 1
8.20000 e- 1	9.50000 e- 1	9.62385 e- 1
8.20000 e- 1	9.60000 e- 1	9.67293 e- 1
8.20000 e- 1	9.70000 e- 1	9.72789 e- 1
8.20000 e- 1	9.80000 e- 1	9.79140 e- 1
8.20000 e- 1	9.90000 e- 1	9.86961 e- 1
8.30000 e- 1	9.50000 e- 1	9.65048 e- 1
8.30000 e- 1	9.60000 e- 1	9.69649 e- 1
8.30000 e- 1	9.70000 e- 1	9.74792 e- 1
8.30000 e- 1	9.80000 e- 1	9.80723 e- 1
8.30000 e- 1	9.90000 e- 1	9.88002 e- 1
8.40000 e- 1	9.50000 e- 1	9.67633 e- 1
8.40000 e- 1	9.60000 e- 1	9.71930 e- 1
8.40000 e- 1	9.70000 e- 1	9.76726 e- 1
8.40000 e- 1	9.80000 e- 1	9.82245 e- 1
8.40000 e- 1	9.90000 e- 1	9.88997 e- 1
8.50000 e- 1	9.50000 e- 1	9.70142 e- 1
8.50000 e- 1	9.60000 e- 1	9.74139 e- 1
8.50000 e- 1	9.70000 e- 1	9.78594 e- 1
8.50000 e- 1	9.80000 e- 1	9.83710 e- 1
8.50000 e- 1	9.90000 e- 1	9.89947 e- 1
8.60000 e- 1	9.50000 e- 1	9.72576 e- 1
8.60000 e- 1	9.60000 e- 1	9.76278 e- 1
8.60000 e- 1	9.70000 e- 1	9.80397 e- 1
8.60000 e- 1	9.80000 e- 1	9.85118 e- 1
8.60000 e- 1	9.90000 e- 1	9.90854 e- 1
8.70000 e- 1	9.50000 e- 1	9.74939 e- 1
8.70000 e- 1	9.60000 e- 1	9.78350 e- 1
8.70000 e- 1	9.70000 e- 1	9.82139 e- 1
8.70000 e- 1	9.80000 e- 1	9.86471 e- 1
8.70000 e- 1	9.90000 e- 1	9.91720 e- 1

k^*/k	f	R
8.80000 e- 1	9.50000 e- 1	9.77232 e- 1
8.80000 e- 1	9.60000 e- 1	9.80355 e- 1
8.80000 e- 1	9.70000 e- 1	9.83820 e- 1
8.80000 e- 1	9.80000 e- 1	9.87773 e- 1
8.80000 e- 1	9.90000 e- 1	9.92547 e- 1
8.90000 e- 1	9.50000 e- 1	9.79457 e- 1
8.90000 e- 1	9.60000 e- 1	9.82297 e- 1
8.90000 e- 1	9.70000 e- 1	9.85443 e- 1
8.90000 e- 1	9.80000 e- 1	9.89025 e- 1
8.90000 e- 1	9.90000 e- 1	9.93338 e- 1
9.00000 e- 1	9.50000 e- 1	9.81617 e- 1
9.00000 e- 1	9.60000 e- 1	9.84178 e- 1
9.00000 e- 1	9.70000 e- 1	9.87010 e- 1
9.00000 e- 1	9.80000 e- 1	9.90229 e- 1
9.00000 e- 1	9.90000 e- 1	9.94092 e- 1
9.10000 e- 1	9.50000 e- 1	9.83713 e- 1
9.10000 e- 1	9.60000 e- 1	9.85999 e- 1
9.10000 e- 1	9.70000 e- 1	9.88524 e- 1
9.10000 e- 1	9.80000 e- 1	9.91387 e- 1
9.10000 e- 1	9.90000 e- 1	9.94813 e- 1
9.20000 e- 1	9.50000 e- 1	9.85747 e- 1
9.20000 e- 1	9.60000 e- 1	9.87762 e- 1
9.20000 e- 1	9.70000 e- 1	9.89985 e- 1
9.20000 e- 1	9.80000 e- 1	9.92501 e- 1
9.20000 e- 1	9.90000 e- 1	9.95501 e- 1
9.30000 e- 1	9.50000 e- 1	9.87721 e- 1
9.30000 e- 1	9.60000 e- 1	9.89470 e- 1
9.30000 e- 1	9.70000 e- 1	9.91396 e- 1
9.30000 e- 1	9.80000 e- 1	9.93571 e- 1
9.30000 e- 1	9.90000 e- 1	9.96158 e- 1
9.40000 e- 1	9.50000 e- 1	9.89636 e- 1
9.40000 e- 1	9.60000 e- 1	9.91123 e- 1
9.40000 e- 1	9.70000 e- 1	9.92758 e- 1
9.40000 e- 1	9.80000 e- 1	9.94601 e- 1
9.40000 e- 1	9.90000 e- 1	9.96785 e- 1

k^*/k	f	R
9.50000 e- 1	9.50000 e- 1	9.91495 e- 1
9.50000 e- 1	9.60000 e- 1	9.92724 e- 1
9.50000 e- 1	9.70000 e- 1	9.94073 e- 1
9.50000 e- 1	9.80000 e- 1	9.95591 e- 1
9.50000 e- 1	9.90000 e- 1	9.97385 e- 1
9.60000 e- 1	9.50000 e- 1	9.93300 e- 1
9.60000 e- 1	9.60000 e- 1	9.94275 e- 1
9.60000 e- 1	9.70000 e- 1	9.95343 e- 1
9.60000 e- 1	9.80000 e- 1	9.96543 e- 1
9.60000 e- 1	9.90000 e- 1	9.97957 e- 1
9.70000 e- 1	9.50000 e- 1	9.95051 e- 1
9.70000 e- 1	9.60000 e- 1	9.95776 e- 1
9.70000 e- 1	9.70000 e- 1	9.96569 e- 1
9.70000 e- 1	9.80000 e- 1	9.97459 e- 1
9.70000 e- 1	9.90000 e- 1	9.98503 e- 1
9.80000 e- 1	9.50000 e- 1	9.96750 e- 1
9.80000 e- 1	9.60000 e- 1	9.97229 e- 1
9.80000 e- 1	9.70000 e- 1	9.97753 e- 1
9.80000 e- 1	9.80000 e- 1	9.98339 e- 1
9.80000 e- 1	9.90000 e- 1	9.99025 e- 1
9.90000 e- 1	9.50000 e- 1	9.98399 e- 1
9.90000 e- 1	9.60000 e- 1	9.98637 e- 1
9.90000 e- 1	9.70000 e- 1	9.98896 e- 1
9.90000 e- 1	9.80000 e- 1	9.99186 e- 1
9.90000 e- 1	9.90000 e- 1	9.99524 e- 1

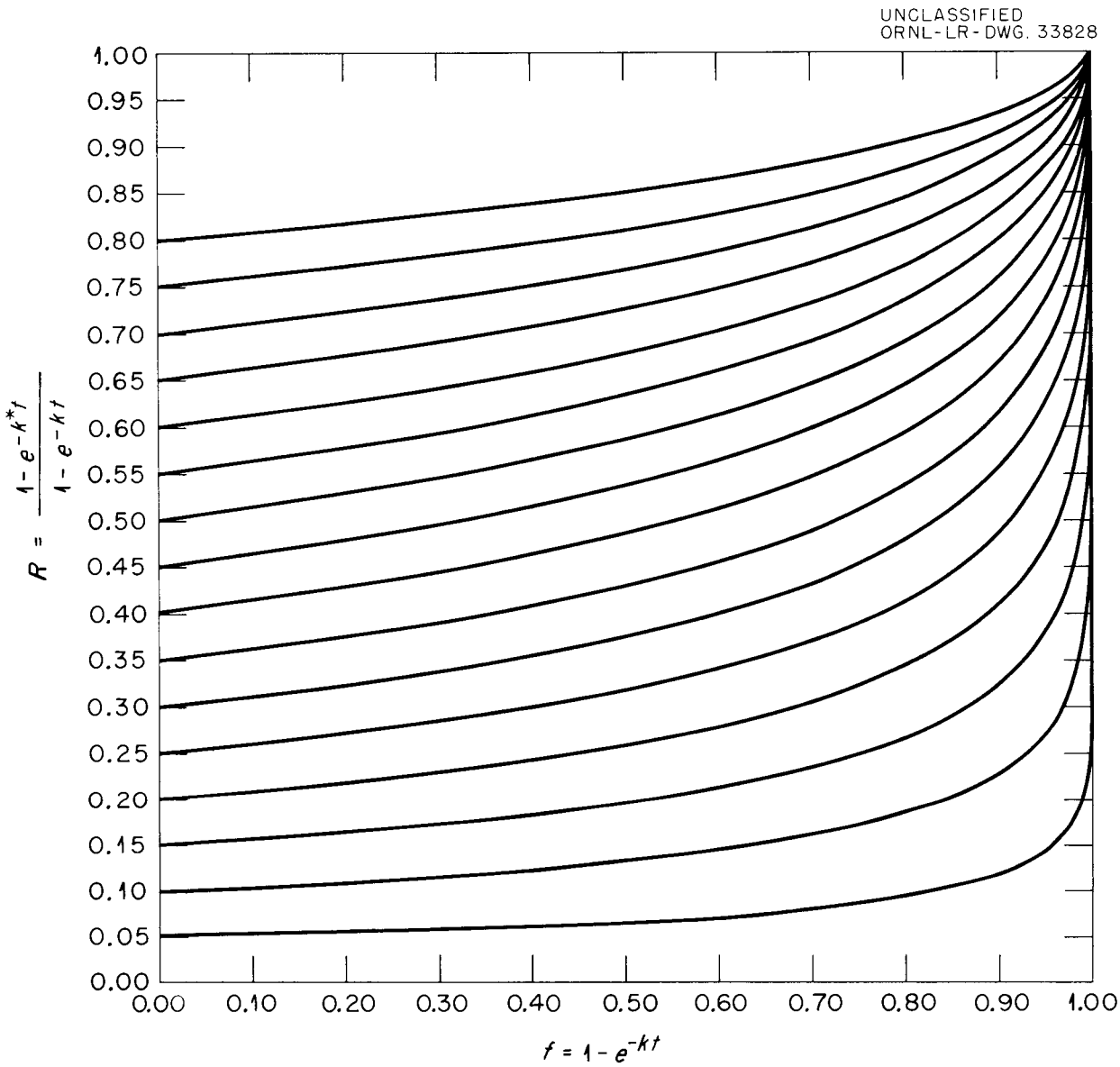
UNCLASSIFIED
ORNL-LR-DWG. 33828
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
$R = \frac{1 - e^{-k^* t}}{1 - e^{-kt}}$
0.00
0.10
0.20
0.30
0.40
0.50
0.60
0.70
0.80
0.90
1.00
$f = 1 - e^{-kt}$

Figure 1

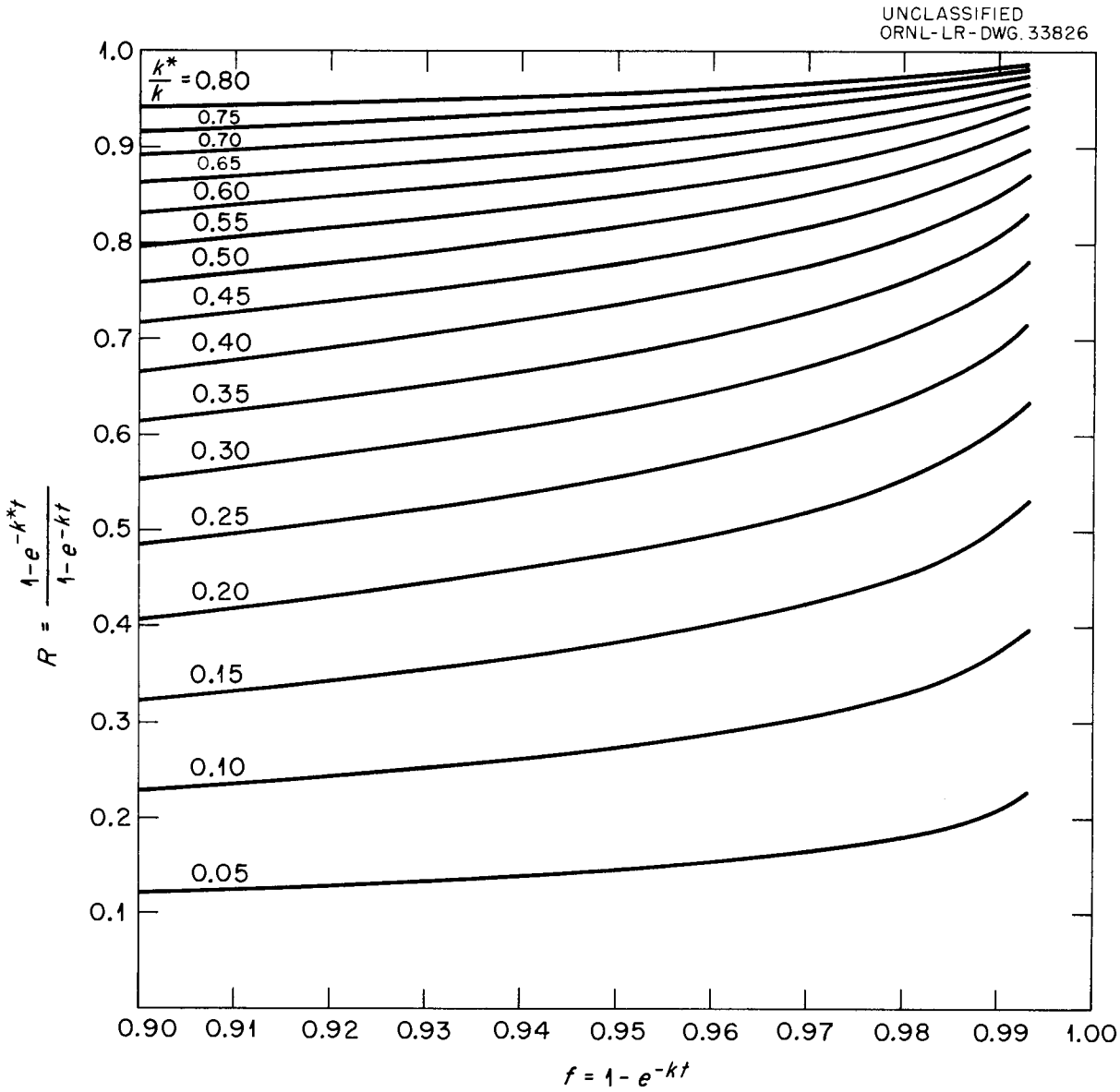
UNCLASSIFIED
ORNL-LR-DWG. 33826
$\frac{k^*}{k}$ = 0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
$R = \frac{1-e^{-k^*t}}{1-e^{-kt}}$
0.90
0.91
0.92
0.93
0.94
0.95
0.96
0.97
0.98
0.99
1.00
$f = 1 - e^{-kt}$

Figure 1A

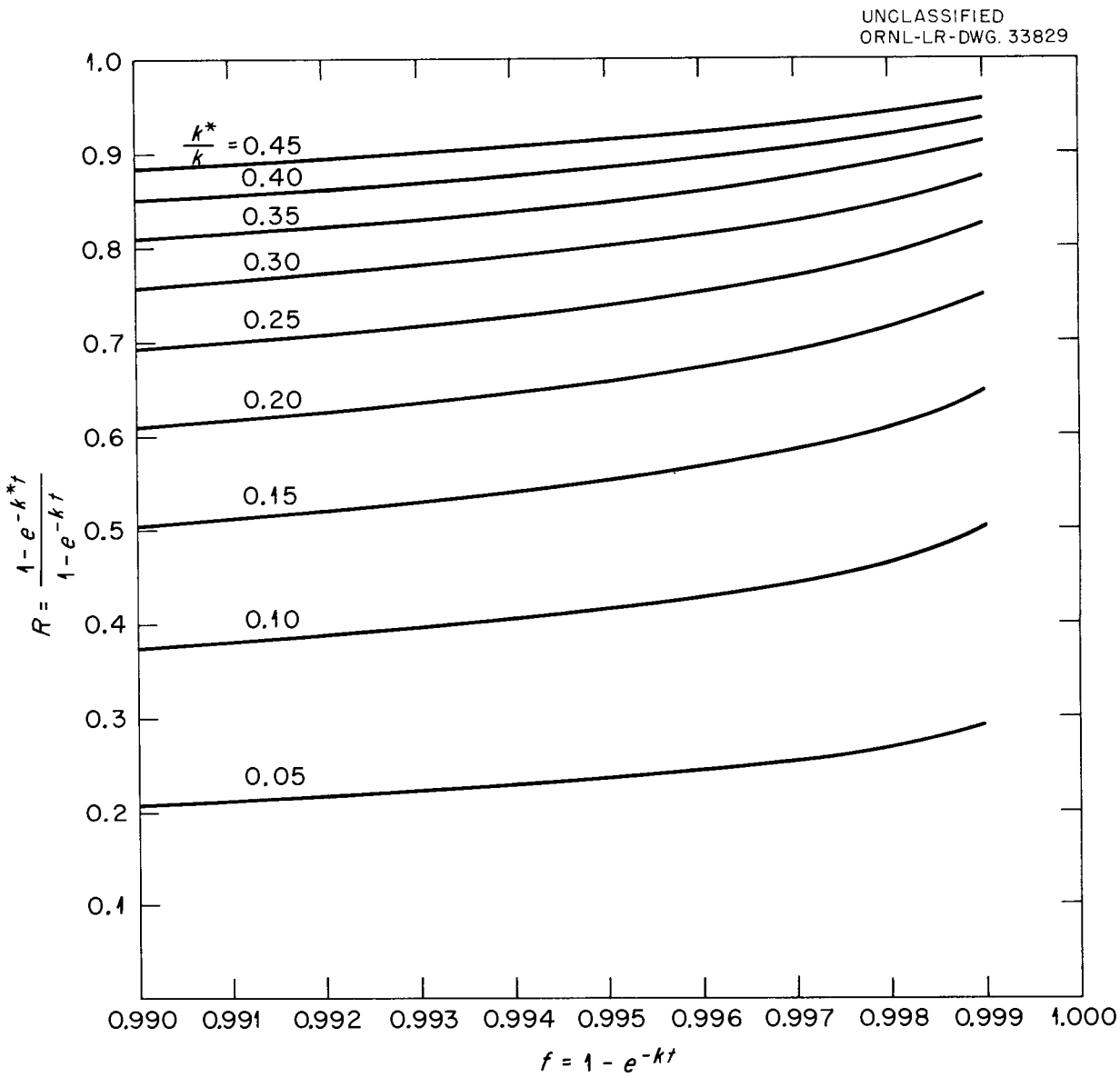
UNCLASSIFIED
ORNL-LR-DWG. 33829
$\frac{k^*}{k}$ = 0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
$R = \frac{1-e^{-k^*t}}{1-e^{-kt}}$
0.990
0.991
0.992
0.993
0.994
0.995
0.996
0.997
0.998
0.999
1.000
$f = 1 - e^{-kt}$

Figure 2

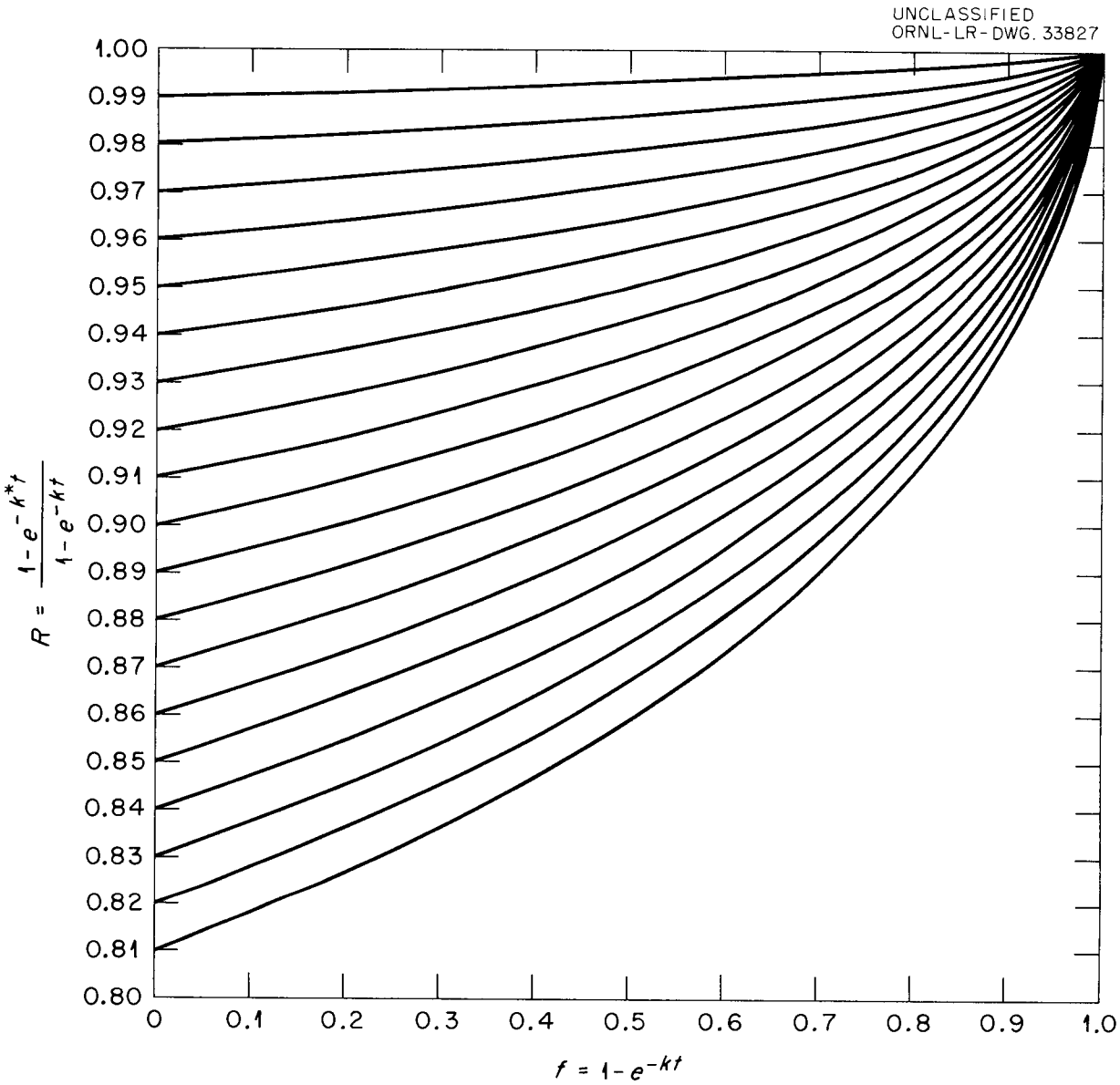
UNCLASSIFIED
ORNL-LR-DWG. 33827
1.00
0.99
0.98
0.97
0.96
0.95
0.94
0.93
0.92
0.91
0.90
0.89
0.88
0.87
0.86
0.85
0.84
0.83
0.82
0.81
0.80
$R = \frac{1-e^{-k^*t}}{1-e^{-kt}}$
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
$f = 1-e^{-kt}$

Figure 3

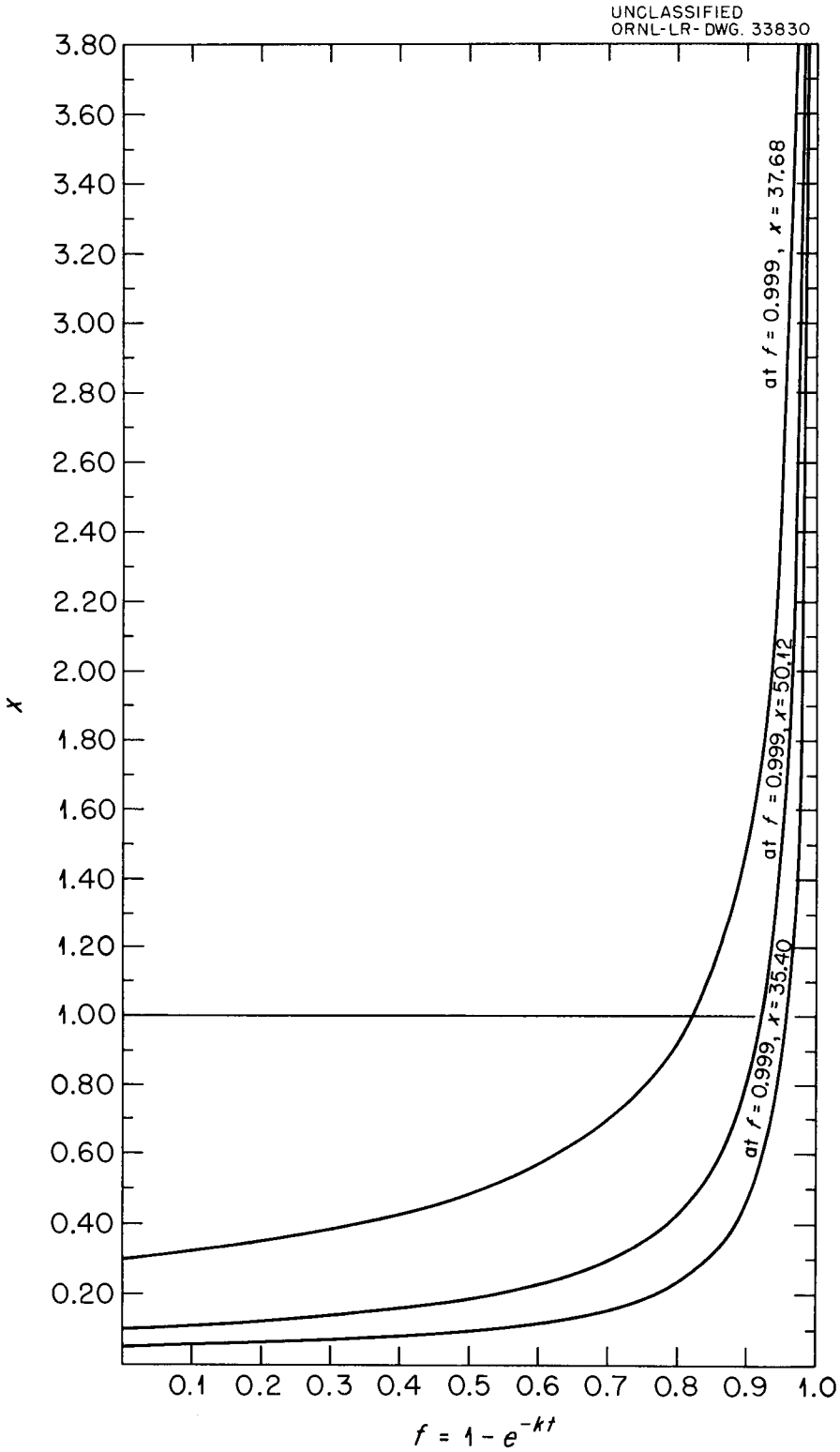
UNCLASSIFIED
ORNL-LR-DWG. 33830
3.80
3.60
3.40
3.20
3.00
2.80
2.60
2.40
2.20
2.00
1.80
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
x
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
f = 1 - e^-kt
at f = 0.999, x = 37.68
at f = 0.999, x = 50.12
at f = 0.999, x = 35.40

Figure 4

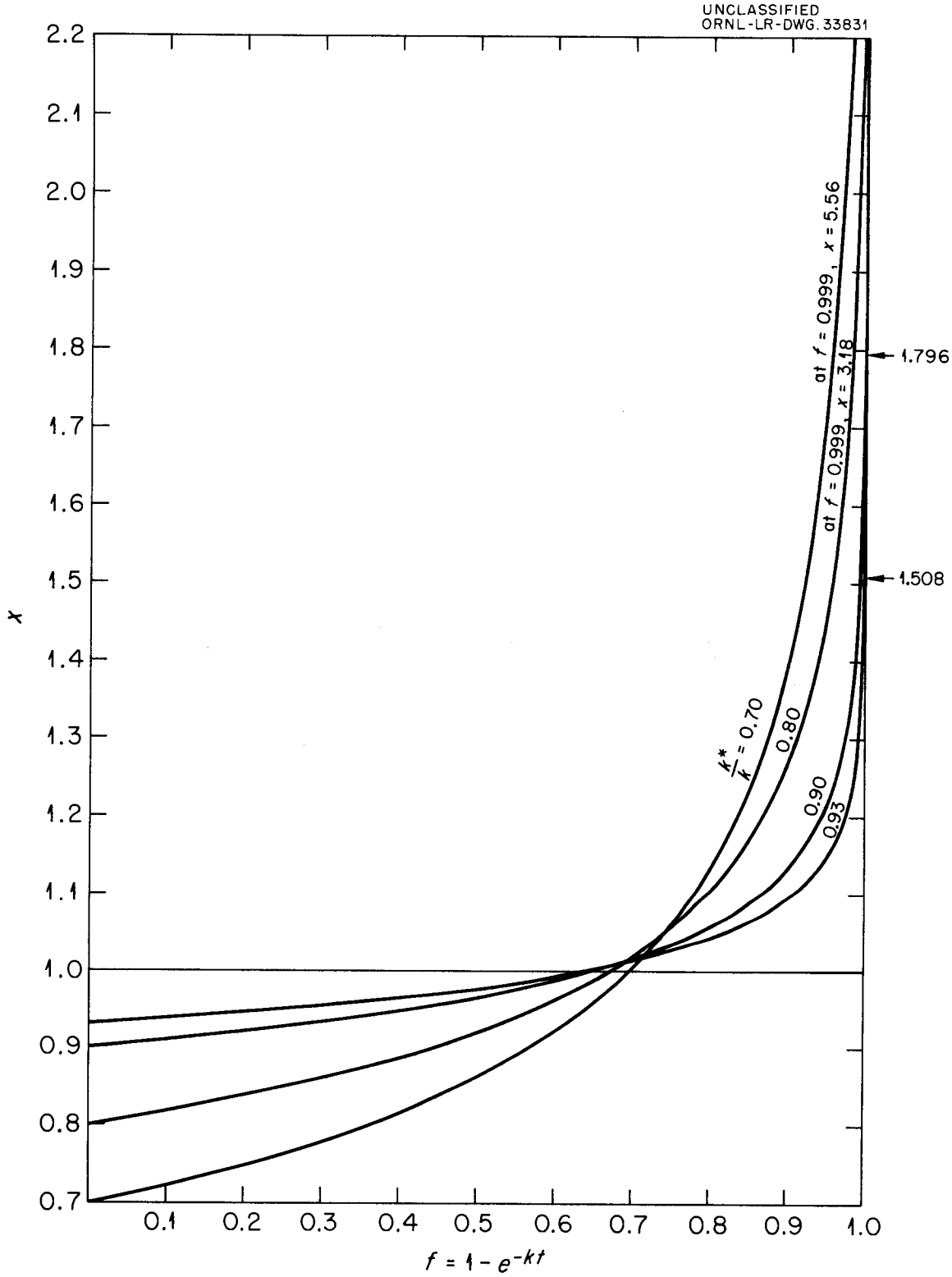
UNCLASSIFIED
ORNL-LR-DWG. 33831
2.2
2.1
2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
x
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
f = 1 - e^-kt
at f = 0.999, x = 5.56
at f = 0.999, x = 3.18
1.796
1.508
k*/k = 0.70
0.80
0.90
0.93

Figure 5

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