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THEORETICAL NITRIC OXIDE PRODUCTION INCIDENTAL TO AUTOIGNITION AND COMBUSTION OF SEVERAL FUELS HOMOGENEOUSLY DISPERSED IN AIR UNDER SOME TYPICAL HYPERSONIC FLIGHT CONDITIONS

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16. Abstract
A reaction package of 100 chemical reactions and attendant reaction rate constants has been defined for the autoignition and combustion of four carbonaceous fuels, CH_4, CH_3OH, C_2H_6, and C_2H_5OH. Definition of the package was made primarily by means of comparison between trial calculations and experimental data for the autoignition of CH_4. Autoignition and combustion of each of these four fuels was calculated under three sets of conditions realistic for hypersonic flight applications, for comparison to hydrogen fuel, particularly with respect to formation of nitric oxide. Results showed that, for all of the fuels including hydrogen, if NO production is a significant problem, compromise must be made between approaching equilibrium heat release and approaching equilibrium NO concentration. Preliminary design studies would be required to effect choice of the best carbonaceous candidate. The reaction package satisfies the requirement for one critical tool.

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SUMMARY

A reaction package of 100 chemical reactions and attendant reaction rate constants has been defined for the combustion in air of four carbonaceous fuels, CH_4, CH_3OH, C_2H_6, and C_2H_5OH. Definition of the package was made primarily by means of comparison between trial calculations and experimental data for the autoignition of CH_4. There was then some expansion made to deal with either CH_3OH or C_2H_5OH as the fuel, and then limited inspection of trials with C_2H_6 to assure that the reaction package was also suitable in this case. These latter steps, in the absence of comparable experimental data, were validated by monitoring the instantaneous mole fractions and net reaction rates and by ensuring that no values were markedly improbable, but rather that they showed reasonable consistency both internally and in appropriate comparisons with the CH_4 results.

This package of 100 reactions was used to calculate the autoignition and combustion of each of the four carbonaceous fuels under three sets of conditions realistic for hypersonic flight applications. That portion of the package limited to H-O-N chemistry was used similarly to make such calculations for H_2 as the fuel. These calculations were carried on until essential attainment of chemical equilibrium. The primary interest of the calculations was the production of NO. Results showed that combustion, in terms of heat release, was practically completed at times substantially before the concentration of NO reached its equilibrium value. Nevertheless, at times sufficiently short for trivial concentrations of NO to have arisen, the temperatures developed were substantially below the equilibrium values. Therefore, if NO production is a significant problem, compromise must be made between approaching equilibrium heat release and approaching equilibrium NO concentration, and

specific calculations would be required for specific operating conditions of interest.

The specificity of results beclouds comparisons among the fuels considered. The most outstanding distinction is imposed by autoignition time at low initial temperature, where CH_4 has an unacceptably long ignition delay for flight application. However, piloting of the flame might overcome this limitation. Choice of an alternative to H_2 would depend upon preliminary design studies, taking into account all of the design and performance distinctions between the several candidates. The results presented in this report can provide some guidance for devising the steps of such analysis, and the reaction package can satisfy the requirement for one critical tool.

INTRODUCTION

This report is concerned with selected portions of a large problem. The large problem is this: what environmental significance is there to the production of nitric oxide by airbreathing aerospace engines, what production of NO will result from operation of such engines, and how can such production be estimated in advance? No attempt will be made here to assess the environmental significance of NO production. This problem is widely recognized as being important, is under study, and is at present unresolved. For background information, the reader may wish to seek out references 1-4. With this first problem unresolved, there is thus interest in the others. Much of the analytical work done to date on the production of NO in engines has been concerned with abnormally high concentrations resulting from nonuniform fuel distributions leading to abnormally high temperatures. These, of course, are cases where the overall fuel quantity is appreciably less than stoichiometric. Depending on the fuel identity and the engine operating conditions, the need for such nonuniformity of fuel distribution, or the feasibility of avoiding it, may be lesser or greater. When the overall fuel quantity is approximately stoichiometric, nonuniform distribution can lead only to abnormally low temperatures, in either fuel-lean or fuel-rich regions, so that emphasis is upon uniform distribution in anticipating or interpreting NO production, as well as in designing for engine performance optimization. The interest of this report is limited to hypersonic flight applications, with fuel proportions approaching stoichiometric, and thus only uniform fuel distributions, leading inherently to high equilibrium combustion temperatures, will be considered. Thus the problem of the degree of NO formation is only partially addressed, for different fuels at a few different operating conditions pertinent to hypersonic flight, where initial and final temperatures are high, and times for reaction are short. The final problem, how can NO production be estimated in advance, is really the essence of the report's appendix. By dealing with this problem in detail in the appendix, and delivering from it a suitable calculational approach, the main text is reserved for application of this approach and interpretation of the results obtained. References 5-13 are concerned with data aspects of this approach, and are noted here so as to validate presentation of a uniform reference list.

The objective of the work being reported was the comparison to hydrogen of a number of other fuels, especially as regards their likelihood of producing significant nitric oxide during the combustion process. Of course, it is recognized that the formation of nitric oxide is dependent upon the rate of the reaction $O + N_2 = N + NO$, which in turn is dependent on the temperature and on the concentrations of O and N_2. If there were no room for controversy over the reaction data packages employed in calculations, reporting such work would be straightforward, centering around discussion of temperature and atomic oxygen concentration as affected by fuel type, initial conditions, and progress of reaction. However, there is much room for controversy over the reaction chemistry, and one objective in reporting becomes directed to a substantiation of the reaction chemistry employed. At the outset of preparation of this report, and with this thought in mind, it was determined to create a principal report and an appendix. The appendix serves as accompanying reference, for those interested chiefly in the principal text. For those interested in the combustion chemistry of the various fuels other than hydrogen, the appendix is the principal material.

PRESENTATION AND DISCUSSION OF RESULTS

A useful reference condition for the kinetic formation of nitric oxide in an airbreathing engine is the case of pure hot air dissociating. In this case the attainment of high temperature is immediate, by definition, and indeed represents somewhat of an overshoot because the ensuing dissociation is endothermic. Also, the concentration of O_2, and so potentially of O, is maximum. At least this is true in comparison to a hydrocarbon fuel, where any oxygen which becomes bound to carbon as CO is virtually inert to any other reaction, such as NO formation.

If creation of nitric oxide is considered to be an environmental problem, then an upper limit to the acceptable flight Mach number for an airbreather might be imposed by the engine inlet static temperature. Note that such a limit would much more likely be imposed in practice by simple structural considerations. Figure 1 presents the time histories of NO formation in pure air at 1 atm elevated to starting static tempertures of 2500, 2750, 3000, 3250, and 3500 K. Suppose (to read the graph conveniently) that a mole fraction of 0.01 is the upper limit set for NO, and that the appropriate reaction time is 1 millisecond. Then the starting temperatures of 3250 and 3500 K are too great. Actually, if NO is considered to be a serious problem, then the maximum tolerable mole fraction will be much less than 0.01, such that the scale of figure 1 is inappropriate for interpolating among the lines of assigned starting temperature. A graph to be introduced subsequently (fig. 4) would be appropriate to this problem.

When attention is directed to the actual static temperature that may apply to the air leaving the engine inlet and entering the combustor, one recognizes that even 2500 K is extreme, and would correspond to a hypothetical situation far into the hypersonic flight regime. However, figure 1 is useful because a temperature of 2500 K may very well be encountered during the progress of combustion in a hypersonic engine and a temperature of 2750 K may perhaps be attained, depending upon what flight Mach number is chosen and what degree of diffusion is prescribed for the inlet air and what fuel stoichiometry is imposed. In other words, figure 1 is sufficient to show that there may be a real problem with NO formation in a hypersonic engine. Furthermore, the close spacing of the several lines indicates that there is little temperature tolerance. Beyond the point that is just suitable, things become rapidly worse and worse.

Comparisons to figure 1 are two others, figures 2 and 3. The first shows temperature history as dissociation proceeds, and the second plots NO mole fraction against temperature. These figures are counterparts of figures to be shown subsequently for combustion cases. The endothermicity of the dissociation process is emphasized by figure 3. The endothermicity is due primarily to the dissociation of O_2 to O, rather than to the formation of

NO. This explains the fact that the NO concentration maximizes for the higher initial temperatures, as shown by figure 1. At the outset, the dissociation of O_2 is rapid, and since the formation of NO becomes even more rapid, a high concentration of NO is rapidly formed, up to a value close to partial equilibrium. However, the dissociation of O_2 continues toward its own equilibrium point, reducing the system temperature and thus revising the partial equilibrium point for NO, which then adjusts downward in its concentration in order to compensate. This intermediate maximization of NO would not, of course, be expected in a combustion case, where only NO formation itself is endothermic, and the continuing combustion process continues to be exothermic as final equilibrium is approached.

Figure 4 is a replot of figure 1 using a logarithmic scale for the ordinate. This scale is labelled "incremental time," and the time at the end of the first integration increment of the calculation has been subtracted from the total elapsed time. Whereas the time of the first integration increment was around 10^{-14} second, in all of the dissociating air calculations, the subtraction is completely immaterial as regards figure 4. However, the same type of ordinate has significance for the presentation of combustion results, as will be discussed later.

Figure 4 depicts exponential growth of NO concentration with time until equilibrium is approached. The growth is of second order. It does not seem at first glance that this can be explained simply, because the growth depends upon all three of the following reactions:

$$O_2 + M = O + O + M$$

$$O + N_2 = N + NO$$

$$N + O_2 = O + NO$$

and the relative rates of the second and third reactions, contrasted with the first, change markedly as the buildup of O concentration proceeds. On the other hand, to the extent that temperature is constant, so that the reaction rate constants are constant, one may consider that the growth of NO is proportional to the concentration of atomic oxygen and to the elapsed time, and the concentration of atomic oxygen itself is proportional to the elapsed time, leading to a net dependency of NO upon the second power of the elapsed time. From the above, figure 4 provides the basis of a viewpoint that there might be expected, in a combustion case, an exponential growth of NO upon establishment of a developing concentration of atomic oxygen.

Figure 4 is convenient to read in terms of time to reach a given concentration of NO. If this is set at one part per million (log = -6.0), one finds times ranging from 2 microseconds to 0.3 millisecond, for the assigned temperature range represented. In other words, in this temperature range one might expect a problem with NO formation simply in the diffusing inlet air. By inference, one would expect no such problem with the air static temperature held below 2000 K, thus directing attention to the combustion zone is such a case.

In choosing initial temperatures for the combustion calculations, probably a number of subjective factors were involved. However, at this point it seems sufficient to cite only two factors. The minimum temperature considered was 1100 K, which is about the lower practical limit for autoignition of hydrogen at 1 atm under supersonic flow conditions.

The other temperature considered was 1500 K, which does lead to combustion temperatures upwards of 2500 K and is about as high as the designer wishes to go from a structural standpoint. It was decided to perform calculations with stoichiometric proportions of fuel and air at both of these temperatures, and then to consider the effect of stoichiometry by running calculations at 1500 K with only 2/3 the stoichiometric amount of fuel. This would reduce the equilibrium combustion temperature somewhat, but make available much more O_2, and presumably much more O, for production of NO upon attainment of the high temperature.

Since the activation energy term of the reaction rate constant expression decreases substantially with temperature decrease when the activation energy is high and the temperature is low, the definition of a proper reaction scheme ought to be performed at the lowest temperature of interest. Otherwise, a reaction that appears competitive at a higher temperature may prove noncompetitive at a lower one, and the need may exist, but be neither satisfied nor perceived, for an alternative reaction which would prove competitive at the lower temperature. In other words, screening to the least extensive but suitable reaction scheme needs to be done at the lowest temperature of interest. Thus the screening calculations, to define a suitable package of 100 reactions for the combustion of each of the fuels of interest, were performed with initial temperature of 1100 K , and, as has been noted, stoichiometric fuel in air at 1 atm assigned pressure. The screening calculations are discussed in the appendix. All of the combustion results to be discussed here were obtained with the final package of 100 reactions.

Figures 5-7 present the mole fraction of NO as a function of time, using a normal scale for NO and a logarithmic scale for time. Figure 5 applies to 1100 K initial temperature, figure 6 to 1500 K with stoichiometric fuel, and figure 7 to 1500 K with 2/3 stoichiometric fuel. (The same order will be used below for comparable sets of three figures each.) The calculations were continued until essential equilibrium was achieved. Clearly, on any figure there is not a great difference in the equilibrium concentration of NO. It is interesting to make some individual comparisons. Hydrogen yields a higher equilibrium temperature in each case. Where there is plenty of oxygen (fig. 7), H_2 produces the most NO. However, where free oxygen depends upon dissociation at stoichiometric proportions, the greater tendency of CO_2 to dissociate, contrasted with water, tends to offset the temperature advantage of H_2 as the fuel. The competitive aspect is lesser at lower temperature (fig. 5), with less overall dissociation, and greater as the carbon to hydrogen ratio of the fuel increases (e.g., C_2H_6 versus CH_4 in figure 6).

Figures 8-10 show the development of combustion temperature with time, again using a normal scale for the ordinate and a logarithmic one for the abscissa. Here the temperature advantage of H_2 is obvious, and a small advantage to the alkane over the related alcohol can be discerned. The most notable feature of these figures is the pronounced difference in autoignition time between CH_4 on the one hand and the four other fuels on the other hand; one does not require an exact definition of autoignition time to see this, for the different locations of the nearly vertical portions of the curves make it obvious. The stoichiometry has very little effect upon the autoignition, as shown by comparison of figures 9 (St.) and 10 (2/3 St.). Comparing figures 8 (1100 K) and 9 (1500 K), one finds the expected sort of improvement with temperature rise; the longer the autoignition time at 1100 K, the greater the effective activation energy has been, and thus the greater the relative improvement with increase of temperature to 1500 K. The long autoignition time of CH_4 is the problem not only of the delay per se, but also of the increased opportunity for degradation of the fuel by pyrolysis to adverse intermediates, the most extreme of which is particulate solid carbon. However, piloting of flame for ignition of CH_4 gives promise for application, and the figures have more significance in implying the need for such piloting than in declaring a basic unsuitability of CH_4.

Recognizing that a log scale of time is being used, one can readily see, except for CH_4, that much less time is required to react substantially to equilibrium temperature than to react virtually to it. Thus, it is of interest to graph the mole fraction of NO versus the temperature in order to see what compromise in NO formation might be effected by a compromise in temperature. (Such graphs are presented as figs. 11-13.) If NO is to be held to a level that is negligible for the scale of these graphs, the temperature must be held to 2200 K by devising incomplete residence time for the combustion process. (Subsequent graphs show that if NO is to be held to no more than one part per million, the temperature must be held to somewhere around 2000 K, depending on particular conditions.) Clearly, limiting the temperature by 50 K to less than the equilibrium value would mean a marked decrease in the NO concentration below the equilibrium value but fractionally so and not by orders of magnitude.

The whole issue comes down to the question of the tolerable level of NO production, at present of nebulous definition. Even after the tolerable level is defined, particular engine operating conditions will influence strongly the extent of NO production. The essential message of this report should be that NO appears copiously above 2200 K, as the final stage of the combustion process occurs, which stage encompasses substantially the recombination of molecular fragments. Depending upon how much one is willing (and able, in fixed geometry with variable operating conditions) to cut short the combustion process, one can cut short the equilibrium production of NO.

As possible aids to a first evaluation of the problem once the tolerable level of NO production has been specified, figures 14-19 have been prepared. The retionale goes back to figure 4. In figure 4 the induction time for the development of experimental growth of NO was the time of the first integration increment of calculation. For the combustion calculations, an apparent induction time for an ensuing period of exponential growth of NO was sought by trial and error. Graphs such as figure 14 were prepared, using different assigned values of the NO induction time for each plot. In each case (i.e., for each fuel at each operating condition) that time was finally chosen which led most nearly to a straight-line portion of the plot at lower NO concentrations or shorter times; these various times provided the basis for the final graphs, figures 14-16. (A pattern was sought in the corresponding "cut-off" temperatures, but none was found.)

As figures 14-16 show, the result in every case is an exponential power for influence of time on NO concentration somewhat greater, or much greater, than the power of two shown by figure 4. With the same NO induction times assigned, the companion graphs of the temperature versus incremental time, figures 17-19, were prepared. Since no "law" has been revealed by the preparation of these figures, they serve chiefly to provide an expanded scale for depiction of NO growth as equilibrium is approached. By deciding what temperature below the equilibrium value is acceptable, one can read the logarithm of the incremental time required kinetically to achieve that temperature. For example, on figure 17 suppose that a temperature 100 K below the equilibrium value is considered acceptable, amounting to 2620 K instead of 2720 K. The abscissa value for H_2 is then -3.29. On figure 14 with abscissa of -3.29 one finds an ordinate value for H_2 of 3.05, corresponding to a mole fraction of about 0.0009 for NO.

In the design-point operation of a supersonic-combustion ramjet, the combustion temperature level may be controlled by initiating expansion before combustion is complete. Thus some temperature decrement may be reasonable. With the sample value of 100 K retained, the following results have been obtained from appropriate pairs of graphs, indicating some advantage to CH_3OH in competition with the other fuels:

Fuel	1100 K	1500 K, St.	1500 K, 2/3 St.
H_2	0.0009	0.0017	0.0012
CH_4	0.0005	0.0013	0.0007
CH_3OH	0.0004	0.0009	0.0006
C_2H_6	0.0007	0.0015	0.0009
C_2H_5OH	0.0005	0.0013	0.0008

These same pairs of graphs have been used in reverse order to determine the temperature corresponding to attainment of one part per million of NO. Among the five fuels and the three selected operating conditions, this temperature ranged from 1950 to 2050 K, amounting to a severe compromise below the equilibrium combustion temperature if the stringent limitation of one ppm of NO were applied. Thus it seems that, on the one hand, toleration of more than one ppm of NO would be required, whereas on the other, a temperature compromise of about 100 K would be required to hold the NO concentration to about one part per thousand.

The final presentation of the basic output data of the calculations is made in figures 20-22, which were conceived as a result of the application of figures 14-19 just discussed. It might seem that these final three figures would suffice in themselves; figures 20-22 yield duplicate readings for NO concentrations at 100 K below the equilibrium combustion temperature, as they ought to. However, it has been felt worthwhile to provide the information on incremental time contained in figures 14-19, for possible use in considering performance with piloted ignition. Nevertheless, figures 20-22 will prove convenient to employ where the time factor is of secondary interest.

In bringing this main text to completion, it seems appropriate to make some remarks about the comparative performance of the various fuel candidates, as the purpose of the work was to investigate such comparison. However, definitive conclusions were not reached. The fundamental differences in propulsion performance between hydrogen and the carbonaceous fuels would seem to exert much greater leverage of selection between hydrogen or one of the others than the rather trivial differences calculated in NO production, either kinetically or with chemical equilibrium. With the set of four carbonaceous candidates, the following general distinctions again would seem to be more significant than relative tendency to form NO under comparable conditions:

(1) CH_4 requires cryogenic storage, and has extreme autoignition delay at low temperature, implying need for piloting of flame;

(2) C_2H_6 requires either cryogenic or pressurized storage, and has the greatest tendency to yield particulate carbon among the four fuels considered;

(3) CO_3OH is already half oxidizer by weight, and while this does not greatly influence the stoichiometric combustion temperature attainable, it has severe effect on the fuel requirements in

gravimetric terms (but the volumetric heating value of liquid CH_3OH is approximately the same as that of cryogenic liquid CH_4);

(4) C_2H_5OH represents some sort of compromise from the standpoints of gravimetric heating value, density, storability, thermal stability (e.g., tendency to form particulate carbon in the combustor), and autoignition delay, but is probably the least attractive of the four candidates at present from the economic standpoint.

With all of the marked distinctions prevailing among the fuels considered, the calculated production of NO is seen to be but a small piece of the overall problem. Perhaps selected operating conditions might be such as to dictate preference for one fuel over another on the basis of tendency to exceed or not to exceed a limit for NO concentration. It is more likely than one would wish to be able to calculate the kinetic progress of the combustion process, and the kinetic production of NO as subsidiary information. Then the provision by this report of a detailed reaction package designed for use with any of the four selected fuels may be its most significant contribution.

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TABLE 1
PACKAGE OF 250 REACTIONS FOR OXIDATION OF ALKANES CH4-C7H16

	REACTION EQUATIONS						RATE CONSTANT DATA				
1	H2	+M	+	=H	+H	+M	9.976243E+19	-1.260488E+00	1.053737E+05	HO.	1
2	O2	+M	+	=O	+O	+M	6.389865E+20	-1.645428E+00	1.204503E+05	HO.	2
3	OH	+M	+	=O	+H	+M	6.758609E+19	-1.264565E+00	1.032301E+05	HO.	4
4	H2O	+M	+	=H	+OH	+M	2.108870E+27	-3.199173E+00	1.213838E+05	HO.	7
5	HO2	+M	+	=H	+O2	+M	2.400000E+15	0.	4.590000E+04	HO.	10
6	HO2	+M	+	=O	+OH	+M	1.227389E+12	5.000000E-01	6.626380E+04	HO.	12
7	H2	+O2	+	=OH	+OH	+	2.500000E+14	0.	6.700000E+04	HO.	3
8	H	+O2	+	=O	+OH	+	2.240000E+14	0.	1.680000E+04	HO.	5
9	O	+H2	+	=H	+OH	+	1.740000E+13	0.	9.450000E+03	HO.	6
10	H	+H2O	+	=OH	+H2	+	8.410000E+13	0.	2.010000E+04	HO.	8
11	O	+H2O	+	=OH	+OH	+	5.750000E+13	0.	1.800000E+04	HO.	9
12	H2	+O2	+	=H	+HO2	+	9.749874E+11	5.000000E-01	5.778610E+04	HO.	11
13	OH	+O2	+	=O	+HO2	+	3.712735E+11	6.357610E-01	5.531791E+04	HO.	13
14	OH	+OH	+	=H	+HO2	+	1.683908E+11	5.000000E-01	4.206055E+04	HO.	14
15	O	+H2O	+	=H	+HO2	+	5.822703E+11	5.000000E-01	5.696670E+04	HO.	15
16	OH	+H2O	+	=HO2	+H2	+	1.237191E+12	2.108070E-01	7.911243E+04	HO.	16
17	O2	+H2O	+	=OH	+HO2	+	1.899763E+11	5.000000E-01	7.212030E+04	HO.	17
18	H	+CO2	+	=OH	+CO	+	5.600000E+13	0.	2.350000E+04	1.	3
19	HO2	+CO	+	=OH	+CO2	+	7.700000E+10	5.000000E-01	0.	1.	4
20	O	+CO	+	=C	+O2	+	2.116311E+12	5.000000E-01	1.390171E+05	2.	1

TABLE 1. - CONTINUED.

	REACTION EQUATIONS						RATE CONSTANT DATA				
21	H	+CO2	+	=O	+HCO	+	2.600000E+12	5.000000E-01	5.870000E+04	3.	1
22	OH	+CO2	+	=O2	+HCO	+	7.200000E+10	5.000000E-01	8.190000E+04	3.	3
23	H	+HCO	+	=H2	+CO	+	5.000000E+11	5.000000E-01	4.000000E+03	3.	5
24	HCO	+M	+	=H	+CO	+M	1.000000E+15	0.	2.300000E+04	3.	6
25	O	+HCO	+	=OH	+CO	+	5.000000E+11	5.000000E-01	4.000000E+03	3.	7
26	OH	+HCO	+	=CO	+H2O	+	3.000000E+10	5.000000E-01	6.000000E+03	3.	8
27	HO2	+CO	+	=O2	+HCO	+	7.700000E+10	5.000000E-01	2.540000E+04	3.	9
28	OH	+CO	+	=CH	+O2	+	7.098324E+11	5.000000E-01	1.619796E+05	4.	1
29	O	+HCO	+	=CH	+O2	+	7.106977E+11	5.000000E-01	8.653890E+04	4.	2
30	HCO	+CO	+	=CH	+CO2	+	1.010355E+11	5.000000E-01	8.209300E+04	4.	3
31	H2	+HCO	+	=H	+HCHO	+	6.667766E+10	5.000000E-01	3.425755E+04	5.	1
32	OH	+HCO	+	=O	+HCHO	+	1.535023E+10	5.000000E-01	3.284792E+04	5.	2
33	HCO	+H2O	+	=OH	+HCHO	+	1.222396E+10	5.000000E-01	4.501285E+04	5.	3
34	H	+HCO	+	=CH2	+O	+	1.377158E+12	5.000000E-01	1.039299E+05	6.	1
35	OH	+HCO	+	=CH2	+O2	+	4.535500E+10	5.000000E-01	8.876630E+04	6.	3
36	CH	+OH	+	=CH2	+O	+	7.062861E+10	5.000000E-01	1.317055E+04	6.	5
37	O	+HCHO	+	=CH2	+O2	+	2.147872E+11	5.000000E-01	6.030240E+04	6.	7
38	HO2	+HCHO	+	=O2	+CH2OH	+	2.627709E+09	5.000000E-01	1.549833E+04	7.	1
39	H	+HCHO	+	=O	+CH3	+	4.201262E+11	5.000000E-01	6.924640E+04	8.	1
40	H2	+HCHO	+	=CH3	+OH	+	3.414275E+10	5.000000E-01	7.112590E+04	8.	2

TABLE 1. - CONTINUED.

	REACTION EQUATIONS						RATE CONSTANT DATA				
41	O	+CH3	+	=CH2	+OH	+	2.145985E+11	5.000000E-01	1.616470E+04	8.	3
42	CH2	+H2O	+	=CH3	+OH	+	2.200686E+10	5.000000E-01	1.900022E+04	8.	4
43	H	+CH2OH	+	=CH3	+OH	+	4.270118E+10	5.000000E-01	1.751170E+04	8.	5
44	OH	+CH2OH	+	=O	+CH3OH	+	1.810799E+09	5.000000E-01	2.092967E+04	9.	1
45	CH2OH	+H2O	+	=OH	+CH3OH	+	1.440900E+10	5.000000E-01	3.309460E+04	9.	2
46	O	+CH3OH	+	=CH3	+HO2	+	2.179380E+10	5.000000E-01	3.863410E+04	9.	4
47	CH4	+	+	=H	+CH3	+	4.394323E+17	-6.089130E-01	1.083358E+05	10.	1
48	CH3	+H2	+	=H	+CH4	+	2.311698E+09	5.000000E-01	1.267142E+04	10.	2
49	O	+CH4	+	=CH3	+OH	+	2.149499E+10	5.000000E-01	1.173820E+04	10.	3
50	CH3	+H2O	+	=OH	+CH4	+	4.998376E+09	5.000000E-01	2.342672E+04	10.	4
51	HCO	+CH4	+	=CH3	+HCHO	+	2.603697E+10	5.000000E-01	3.308612E+04	10.	6
52	CH4	+HCHO	+	=CH3	+CH2OH	+	2.619601E+10	5.000000E-01	6.154840E+04	10.	7
53	OH	+CH4	+	=H	+CH3OH	+	1.762802E+09	5.000000E-01	1.515617E+04	10.	8
54	CH2OH	+CH4	+	=CH3	+CH3OH	+	2.635561E+10	5.000000E-01	2.116787E+04	10.	9
55	CO	+CO	+	=C2	+O2	+	8.054442E+11	5.000000E-01	2.551744E+05	11.	1
56	C	+CO	+	=C2	+O	+	2.667882E+12	5.000000E-01	1.161573E+05	11.	2
57	HCO	+CO	+	=C2H	+O2	+	2.423974E+11	5.000000E-01	1.478417E+05	12.	1
58	CH	+CO	+	=C2H	+O	+	7.815618E+11	5.000000E-01	6.130280E+04	12.	2
59	C2H	+O	+	=C2	+OH	+	7.897215E+11	5.000000E-01	3.541900E+04	12.	3
60	C2H	+OH	+	=C2	+H2O	+	9.359400E+10	5.000000E-01	2.325407E+04	12.	4

TABLE 1. - CONTINUED.

	REACTION EQUATIONS						RATE CONSTANT DATA				
61	O	+C2H2	+	=CH	+HCO	+	2.377935E+11	5.000000E-01	2.626195E+04	13.	1
62	C2H2	+	+	=C2H	+H	+	7.783707E+17	-7.049160E-01	1.138829E+05	13.	3
63	C2H2	+H	+	=C2H	+H2	+	4.643078E+11	5.000000E-01	1.424890E+04	13.	4
64	O	+C2H2	+	=C2H	+OH	+	2.377935E+11	5.000000E-01	1.565852E+04	13.	5
65	C2H	+H2O	+	=C2H2	+OH	+	2.396886E+10	5.000000E-01	1.950640E+04	13.	6
66	C2H2	+CH3	+	=C2H	+CH4	+	5.018279E+09	5.000000E-01	1.542033E+04	13.	7
67	C2H3	+	+	=C2H2	+H	+	1.425486E+13	1.608430E-01	4.100172E+04	14.	3
68	C2H4	+OH	+	=CH2	+CH2OH	+	1.104438E+10	5.000000E-01	5.014230E+04	15.	1
69	C2H4	+H2	+	=CH3	+CH3	+	3.850738E+10	5.000000E-01	5.381780E+04	15.	2
70	C2H4	+	+	=C2H3	+H	+	4.359407E+16	-6.443150E-01	1.092024E+05	15.	3
71	C2H3	+H2	+	=H	+C2H4	+	5.666014E+09	5.000000E-01	1.209535E+04	15.	4
72	CH3	+C2H4	+	=C2H3	+CH4	+	1.566002E+10	5.000000E-01	1.207608E+04	15.	5
73	C2H3	+C2H2	+	=C2H	+C2H4	+	9.626454E+09	5.000000E-01	1.484425E+04	15.	6
74	CH2	+HCHO	+	=O	+C2H4	+	9.697242E+09	5.000000E-01	1.981637E+04	15.	7
75	CH3	+HCHO	+	=C2H4	+OH	+	2.245000E+10	5.000000E-01	2.448107E+04	15.	8
76	C2H3	+H2O	+	=C2H4	+OH	+	1.020706E+10	5.000000E-01	2.285065E+04	15.	9
77	O	+C2H4	+	=C2H3	+OH	+	2.396887E+10	5.000000E-01	1.231428E+04	15.	10
78	C2H5	+	+	=H	+C2H4	+	9.969550E+14	-4.639780E-01	4.047757E+04	16.	1
79	CH3	+CH4	+	=C2H5	+H2	+	2.203170E+10	5.000000E-01	2.134795E+04	16.	2
80	C2H4	+HO2	+	=C2H5	+O2	+	8.024782E+09	5.000000E-01	1.954832E+04	16.	3

TABLE 1. - CONTINUED.

	REACTION EQUATIONS						RATE CONSTANT DATA				
81	C2H3	+C2H4	+	=C2H2	+C2H5	+	1.290002E+10	5.000000E-01	1.456202E+04	16.	4
82	C2H6	+	+	=CH3	+CH3	+	4.893779E+23	-2.272211E+00	9.531851E+04	17.	1
83	CH3	+CH4	+	=H	+C2H6	+	1.180116E+10	5.000000E-01	2.809915E+04	17.	2
84	C2H5	+H2	+	=H	+C2H6	+	2.086489E+10	5.000000E-01	1.825120E+04	17.	3
85	C2H5	+OH	+	=O	+C2H6	+	4.644379E+09	5.000000E-01	1.684157E+04	17.	4
86	C2H5	+H2O	+	=OH	+C2H6	+	2.427573E+10	5.000000E-01	2.900650E+04	17.	5
87	C2H5	+CH4	+	=CH3	+C2H6	+	2.906356E+10	5.000000E-01	1.707977E+04	17.	6
88	C2H2	+C2H5	+	=C2H	+C2H6	+	2.985656E+10	5.000000E-01	2.100010E+04	17.	7
89	C2H2	+HCHO	+	=C3H2	+H2O	+	2.707892E+10	5.000000E-01	2.945635E+04	19.	1
90	C3H3	+H2	+	=C2H	+CH4	+	1.103028E+10	5.000000E-01	2.360162E+04	20.	1
91	C3H3	+CH4	+	=C2H2	+C2H5	+	3.131609E+10	5.000000E-01	2.952925E+04	20.	2
92	C3H3	+CH4	+	=C2H	+C2H6	+	3.131609E+10	5.000000E-01	3.902935E+04	20.	3
93	C3H2	+OH	+	=C3H3	+O	+	7.842213E+09	5.000000E-01	2.654185E+04	20.	4
94	C3H2	+H2O	+	=C3H3	+OH	+	2.619431E+10	5.000000E-01	3.870678E+04	20.	5
95	C2H	+CH2OH	+	=O	+C3H4	+	2.719647E+10	5.000000E-01	2.298760E+04	21.	1
96	C3H4	+	+	=C2H	+CH3	+	1.968081E+20	-1.508230E+00	1.052549E+05	21.	2
97	C2H	+CH4	+	=H	+C3H4	+	2.872277E+10	5.000000E-01	1.721410E+04	21.	3
98	C2H2	+CH3	+	=H	+C3H4	+	6.121556E+09	5.000000E-01	2.113442E+04	21.	4
99	C3H4	+	+	=C3H3	+H	+	4.337609E+16	-6.969340E-01	8.658383E+04	21.	6
100	C3H3	+H2	+	=H	+C3H4	+	1.345530E+10	5.000000E-01	2.931572E+04	21.	7

TABLE 1. - CONTINUED.

	REACTION EQUATIONS						RATE CONSTANT DATA				
101	C3H3	+OH	+	=O	+C3H4	+	2.777048E+09	5.000000E-01	2.790610E+04	21.	8
102	C3H3	+H2O	+	=C3H4	+OH	+	2.200756E+10	5.000000E-01	4.007102E+04	21.	9
103	C3H3	+CH4	+	=C3H4	+CH3	+	3.131609E+10	5.000000E-01	2.814430E+04	21.	10
104	C3H5	+	+	=C2H2	+CH3	+	3.325344E+17	-1.571363E+00	5.712418E+04	22.	1
105	C3H5	+H2	+	=C2H3	+CH4	+	1.060092E+08	5.000000E-01	1.771367E+04	22.	5
106	C3H5	+H2	+	=CH3	+C2H4	+	1.973335E+08	5.000000E-01	1.713760E+04	22.	6
107	C3H5	+H2O	+	=C2H4	+CH2OH	+	9.295746E+06	5.000000E-01	2.188120E+04	22.	7
108	C3H5	+CH4	+	=C2H3	+C2H6	+	4.102427E+08	5.000000E-01	3.314140E+04	22.	8
109	C3H5	+	+	=H	+C3H4	+	4.908251E+13	-7.673710E-01	6.574881E+04	22.	9
110	C3H4	+OH	+	=O	+C3H5	+	2.636578E+10	5.000000E-01	4.373440E+04	22.	10
111	C3H5	+O2	+	=C3H4	+HO2	+	2.001573E+08	5.000000E-01	2.119037E+04	22.	12
112	C2H3	+CH3OH	+	=OH	+C3H6	+	2.722622E+10	5.000000E-01	1.952582E+04	23.	1
113	C2H3	+CH4	+	=H	+C3H6	+	2.888147E+10	5.000000E-01	2.318200E+04	23.	2
114	C2H4	+CH2OH	+	=OH	+C3H6	+	2.713073E+10	5.000000E-01	2.976977E+04	23.	3
115	CH3	+C2H4	+	=H	+C3H6	+	1.993981E+10	5.000000E-01	2.375807E+04	23.	4
116	C2H5	+C2H4	+	=CH3	+C3H6	+	2.981576E+10	5.000000E-01	1.273870E+04	23.	5
117	CH3	+C3H6	+	=C2H3	+C2H6	+	1.146856E+10	5.000000E-01	1.641715E+04	23.	6
118	C3H5	+H2	+	=H	+C3H6	+	1.349809E+08	5.000000E-01	2.939567E+04	23.	8
119	C3H5	+OH	+	=O	+C3H6	+	2.757950E+07	5.000000E-01	2.798605E+04	23.	9
120	C3H5	+H2O	+	=OH	+C3H6	+	2.184587E+08	5.000000E-01	4.015097E+04	23.	10

TABLE 1. - CONTINUED.

	REACTION EQUATIONS						RATE CONSTANT DATA				
121	C3H5	+CH4	+	=CH3	+C3H6	+	1.143486E+09	5.000000E-01	2.822425E+04	23.	12
122	C2H2	+C3H5	+	=C2H	+C3H6	+	1.974813E+08	5.000000E-01	3.214457E+04	23.	13
123	C3H5	+C2H4	+	=C2H3	+C3H6	+	6.087564E+08	5.000000E-01	2.880032E+04	23.	14
124	C3H7	+	+	=CH3	+C2H4	+	5.820454E+20	-1.836060E+00	2.880521E+04	24.	1
125	CH3	+C2H6	+	=C3H7	+H2	+	2.890416E+10	5.000000E-01	1.908543E+04	24.	6
126	C2H5	+CH4	+	=H	+C3H8	+	2.906356E+10	5.000000E-01	3.206042E+04	25.	1
127	CH3	+C2H6	+	=H	+C3H8	+	1.307818E+10	5.000000E-01	2.648065E+04	25.	2
128	C2H5	+C2H6	+	=CH3	+C3H8	+	2.981050E+10	5.000000E-01	1.546128E+04	25.	3
129	C3H7	+H2	+	=H	+C3H8	+	2.121774E+10	5.000000E-01	1.889522E+04	25.	5
130	C3H7	+H2O	+	=OH	+C3H8	+	2.667845E+10	5.000000E-01	2.965052E+04	25.	7
131	C3H7	+CH4	+	=CH3	+C3H8	+	3.175763E+10	5.000000E-01	1.772380E+04	25.	8
132	C3H7	+C2H4	+	=C2H3	+C3H8	+	3.134790E+10	5.000000E-01	1.829988E+04	25.	9
133	C3H5	+C2H6	+	=C2H3	+C3H8	+	3.935539E+08	5.000000E-01	3.152290E+04	25.	12
134	C2H2	+C3H7	+	=C2H	+C3H8	+	3.061387E+10	5.000000E-01	2.164412E+04	25.	13
135	C3H8	+	+	=C2H5	+CH3	+	4.484202E+23	-2.449698E+00	9.101247E+04	XTRA	1
136	C4H	+H2	+	=C2H	+C2H2	+	5.075372E+10	5.000000E-01	2.144747E+04	27.	1
137	C4H2	+H	+	=C2H	+C2H2	+	6.519694E+10	5.000000E-01	1.188813E+04	28.	2
138	C4H2	+	+	=C4H	+H	+	6.626220E+15	-4.430310E-01	9.603632E+04	28.	7
139	C4H	+H2	+	=C4H2	+H	+	1.115565E+10	5.000000E-01	2.105935E+04	28.	8
140	C4H	+H2O	+	=C4H2	+OH	+	1.728147E+10	5.000000E-01	3.181465E+04	28.	18

TABLE 1.-- CONTINUED.

	REACTION EQUATIONS						RATE CONSTANT DATA				
141	C4H3	+	+	=C2H	+C2H2	+	1.392122E+16	-6.256500E-01	5.940110E+04	29.	1
142	C4H3	+H2	+	=C2H3	+C2H2	+	5.176236E+10	5.000000E-01	1.960997E+04	29.	3
143	C4H3	+CH4	+	=C2H2	+C3H5	+	3.365351E+10	5.000000E-01	1.339630E+04	29.	4
144	C4H3	+	+	=C4H2	+H	+	5.104610E+13	-1.647750E-01	5.691810E+04	29.	7
145	C4H8	+	+	=C3H5	+CH3	+	9.278239E+21	-1.232907E+00	7.584027E+04	31.	3
146	C3H5	+CH3OH	+	=OH	+C4H8	+	8.349596E+08	5.000000E-01	3.447632E+04	31.	4
147	C3H6	+CH2OH	+	=OH	+C4H8	+	2.847250E+10	5.000000E-01	2.741995E+04	31.	5
148	CH3	+C3H6	+	=H	+C4H8	+	2.231384E+09	5.000000E-01	2.140825E+04	31.	6
149	C2H5	+C4H8	+	=C3H7	+C3H6	+	3.283870E+10	5.000000E-01	1.592838E+04	31.	9
150	C4H9	+	+	=C2H5	+C2H4	+	2.226393E+16	-6.667180E-01	2.343171E+04	32.	1
151	C4H9	+	+	=CH3	+C3H6	+	7.857412E+16	-5.530180E-01	2.436842E+04	32.	3
152	CH3	+C3H8	+	=C4H9	+H2	+	3.381792E+09	5.000000E-01	1.387600E+04	32.	8
153	C4H10	+	+	=C2H5	+C2H5	+	3.326753E+16	-6.183720E-01	8.374956E+04	33.	1
154	C2H5	+C2H6	+	=H	+C4H10	+	1.140515E+10	5.000000E-01	2.373070E+04	33.	2
155	C4H10	+	+	=CH3	+C3H7	+	5.458504E+17	-7.002010E-01	8.867925E+04	33.	3
156	C3H7	+CH4	+	=H	+C4H10	+	1.046553E+10	5.000000E-01	2.599322E+04	33.	4
157	CH3	+C3H8	+	=H	+C4H10	+	1.894700E+09	5.000000E-01	1.976942E+04	33.	7
158	CH3	+C4H10	+	=C2H5	+C3H8	+	3.489281E+10	5.000000E-01	1.424995E+04	33.	8
159	C4H9	+H2	+	=H	+C4H10	+	3.017739E+10	5.000000E-01	1.739342E+04	33.	10
160	C4H9	+OH	+	=O	+C4H10	+	5.757581E+09	5.000000E-01	1.598380E+04	33.	11

TABLE 1. - CONTINUED.

	REACTION EQUATIONS						RATE CONSTANT DATA				
161	C4H9	+H2O	+	=OH	+C4H10	+	2.896813E+10	5.000000E-01	2.814872E+04	33.	12
162	C2H5	+C4H8	+	=C2H3	+C4H10	+	3.283870E+10	5.000000E-01	1.873960E+04	33.	17
163	C5H10	+	+	=C3H5	+C2H5	+	2.542027E+17	-3.446400E-02	6.754323E+04	34.	1
164	CH3	+C5H10	+	=C2H3	+C4H10	+	3.717782E+10	5.000000E-01	1.794407E+04	34.	11
165	C5H11	+	+	=C2H5	+C3H6	+	1.841685E+12	6.608500E-01	1.757461E+04	35.	1
166	C5H11	+	+	=C3H7	+C2H4	+	8.388000E+12	4.676450E-01	2.155841E+04	35.	3
167	C5H11	+	+	=CH3	+C4H8	+	1.095777E+15	-3.759400E-02	2.038258E+04	35.	4
168	C5H11	+CH4	+	=C2H5	+C4H10	+	3.676159E+10	5.000000E-01	1.659887E+04	35.	6
169	C5H12	+	+	=C2H5	+C3H7	+	2.440374E+10	1.177278E+00	7.997781E+04	36.	1
170	C3H7	+C2H6	+	=H	+C5H12	+	1.394737E+09	5.000000E-01	1.853777E+04	36.	2
171	C2H5	+C3H8	+	=H	+C5H12	+	1.671950E+09	5.000000E-01	1.789375E+04	36.	3
172	C4H9	+CH4	+	=H	+C5H12	+	1.506166E+10	5.000000E-01	2.536570E+04	36.	5
173	C5H12	+	+	=CH3	+C4H9	+	7.205752E+14	8.708000E-03	8.534736E+04	36.	6
174	CH3	+C4H10	+	=H	+C5H12	+	2.220110E+09	5.000000E-01	2.064370E+04	36.	10
175	OH	+C5H11	+	=O	+C5H12	+	7.648566E+09	5.000000E-01	1.448500E+04	36.	13
176	C5H11	+H2O	+	=OH	+C5H12	+	3.112922E+10	5.000000E-01	2.664992E+04	36.	14
177	C5H11	+H2	+	=H	+C5H12	+	4.177680E+10	5.000000E-01	1.589462E+04	36.	15
178	C3H7	+C4H8	+	=C2H3	+C5H12	+	7.375838E+09	5.000000E-01	1.354668E+04	36.	20
179	C2H5	+C5H10	+	=C2H3	+C5H12	+	3.447530E+10	5.000000E-01	1.606840E+04	36.	21
180	C3H7	+C3H6	+	=H	+C6H12	+	1.497982E+08	5.000000E-01	2.014225E+04	37.	2

TABLE 1. - CONTINUED.

	REACTION EQUATIONS						RATE CONSTANT DATA				
181	C4H9	+C2H4	+	=H	+C6H12	+	2.282483E+09	5.000000E-01	2.262910E+04	37.	10
182	CH3	+C5H10	+	=H	+C6H12	+	1.919299E+09	5.000000E-01	2.377510E+04	37.	11
183	CH3	+C6H12	+	=C2H3	+C5H12	+	3.956116E+10	5.000000E-01	1.481268E+04	37.	12
184	C6H13	+	+	=C3H7	+C3H6	+	3.246704E+10	1.218871E+00	1.610265E+04	38.	1
185	C6H13	+	+	=C2H5	+C4H8	+	1.191232E+12	6.007480E-01	1.398660E+04	38.	2
186	C6H13	+	+	=C4H9	+C2H4	+	2.721748E+14	-6.377900E-02	2.053798E+04	38.	4
187	C6H13	+	+	=CH3	+C5H10	+	4.784720E+16	-5.968470E-01	2.228086E+04	38.	6
188	C6H14	+	+	=C3H7	+C3H7	+	4.105054E+08	1.561694E+00	7.834562E+04	39.	1
189	C3H7	+C3H8	+	=H	+C6H14	+	3.198478E+09	5.000000E-01	1.712560E+04	39.	2
190	C6H14	+	+	=C2H5	+C4H9	+	7.436416E+11	4.740120E-01	7.878875E+04	39.	3
191	C4H9	+C2H6	+	=H	+C6H14	+	3.140022E+10	5.000000E-01	2.233503E+04	39.	4
192	C2H5	+C4H10	+	=H	+C6H14	+	3.064686E+10	5.000000E-01	2.319280E+04	39.	6
193	CH3	+C6H14	+	=C3H7	+C4H10	+	2.416608E+10	5.000000E-01	1.414383E+04	39.	7
194	C6H14	+	+	=CH3	+C5H11	+	3.540539E+16	-7.407060E-01	8.558671E+04	39.	9
195	C5H11	+CH4	+	=H	+C6H14	+	3.676159E+10	5.000000E-01	2.829167E+04	39.	10
196	CH3	+C5H12	+	=H	+C6H14	+	3.741239E+10	5.000000E-01	2.506847E+04	39.	14
197	C6H13	+H2	+	=H	+C6H14	+	6.602916E+10	5.000000E-01	1.672262E+04	39.	17
198	OH	+C6H13	+	=O	+C6H14	+	3.338173E+10	5.000000E-01	1.531300E+04	39.	18
199	C6H13	+H2O	+	=OH	+C6H14	+	3.317412E+10	5.000000E-01	2.747792E+04	39.	19
200	C4H9	+C4H8	+	=C2H3	+C6H14	+	3.346622E+10	5.000000E-01	1.734393E+04	39.	24

TABLE 1. - CONTINUED.

	REACTION EQUATIONS						RATE CONSTANT DATA				
201	C3H7	+C5H10	+	=C2H3	+C6H14	+	3.400663E+10	5.000000E-01	1.530025E+04	39.	25
202	C2H5	+C6H12	+	=C2H3	+C6H14	+	3.608355E+10	5.000000E-01	1.736178E+04	39.	26
203	C7H14	+	+	=C3H5	+C4H9	+	5.226418E+18	-3.320750E-01	6.394014E+04	40.	2
204	C3H6	+C6H13	+	=C2H5	+C7H14	+	1.013534E+10	5.000000E-01	1.368790E+04	40.	11
205	C2H5	+C5H10	+	=H	+C7H14	+	1.123069E+10	5.000000E-01	2.843620E+04	40.	12
206	CH3	+C7H14	+	=C2H3	+C6H14	+	4.182059E+10	5.000000E-01	1.270068E+04	40.	13
207	C7H15	+	+	=C3H7	+C4H8	+	6.796747E+08	1.466832E+00	8.570490E+03	41.	1
208	C7H15	+	+	=C4H9	+C3H6	+	3.413548E+10	9.953390E-01	1.113766E+04	41.	3
209	C7H15	+	+	=C2H5	+C5H10	+	1.680189E+12	3.495900E-01	1.194011E+04	41.	4
210	C7H15	+	+	=C2H4	+C5H11	+	4.529115E+14	-3.315560E-01	1.699279E+04	41.	6
211	C7H15	+	+	=CH3	+C6H12	+	1.983107E+15	-4.597530E-01	1.863232E+04	41.	8
212	C7H15	+CH4	+	=C2H5	+C6H14	+	4.123649E+10	5.000000E-01	1.226373E+04	41.	11
213	C7H16	+	+	=C3H7	+C4H9	+	8.637022E+08	1.555830E+00	7.362382E+04	42.	1
214	C4H9	+C3H8	+	=H	+C7H16	+	1.789341E+09	5.000000E-01	2.065637E+04	42.	2
215	C3H7	+C4H10	+	=H	+C7H16	+	1.456852E+09	5.000000E-01	2.215817E+04	42.	3
216	C4H9	+C4H10	+	=CH3	+C7H16	+	2.948212E+10	5.000000E-01	1.238695E+04	42.	4
217	C7H16	+	+	=C2H5	+C5H11	+	2.505969E+12	4.225950E-01	7.549383E+04	42.	5
218	C5H11	+C2H6	+	=H	+C7H16	+	1.689757E+10	5.000000E-01	2.499452E+04	42.	6
219	CH3	+C7H16	+	=C5H11	+C3H8	+	4.100864E+10	5.000000E-01	1.298613E+04	42.	7
220	C5H11	+C4H10	+	=C2H5	+C7H16	+	3.421759E+10	5.000000E-01	1.276382E+04	42.	8

TABLE 1. - CONTINUED.

	REACTION EQUATIONS						RATE CONSTANT DATA				
221	C2H5	+C5H12	+	=H	+C7H16	+	1.338986E+10	5.000000E-01	2.735110E+04	42.	9
222	C3H7	+C5H12	+	=CH3	+C7H16	+	2.302497E+10	5.000000E-01	1.301447E+04	42.	10
223	C4H9	+C5H12	+	=C2H5	+C7H16	+	3.375433E+10	5.000000E-01	1.426262E+04	42.	11
224	C7H16	+	+	=CH3	+C6H13	+	2.518369E+15	-2.161860E-01	8.189083E+04	42.	12
225	C6H13	+CH4	+	=H	+C7H16	+	3.905724E+10	5.000000E-01	2.885320E+04	42.	13
226	C6H13	+C2H6	+	=CH3	+C7H16	+	3.594859E+10	5.000000E-01	1.225405E+04	42.	14
227	C3H6	+C6H13	+	=C2H3	+C7H16	+	2.962812E+10	5.000000E-01	1.717120E+04	42.	15
228	C2H5	+C7H16	+	=C6H13	+C3H8	+	3.778748E+10	5.000000E-01	1.470723E+04	42.	16
229	CH3	+C6H14	+	=H	+C7H16	+	1.069099E+09	5.000000E-01	2.480200E+04	42.	17
230	C2H5	+C6H14	+	=CH3	+C7H16	+	1.326577E+10	5.000000E-01	1.378262E+04	42.	18
231	C2H5	+C7H16	+	=C3H7	+C6H14	+	3.778748E+10	5.000000E-01	1.253463E+04	42.	19
232	C2H4	+C7H15	+	=C2H3	+C7H16	+	3.797430E+10	5.000000E-01	1.512243E+04	42.	22
233	H2	+C7H15	+	=H	+C7H16	+	1.772140E+10	5.000000E-01	1.571777E+04	42.	23
234	C7H15	+CH4	+	=CH3	+C7H16	+	4.123649E+10	5.000000E-01	1.454635E+04	42.	24
235	C2H5	+C7H16	+	=C7H15	+C2H6	+	3.778748E+10	5.000000E-01	1.403343E+04	42.	25
236	C3H5	+C7H16	+	=C3H6	+C7H15	+	4.416400E+08	5.000000E-01	2.517790E+04	42.	26
237	HCO	+CO	+	=O	+C2HO	+	2.423974E+11	5.000000E-01	1.538883E+05	50.	1
238	HCO	+HCO	+	=C2HO	+OH	+	2.431088E+10	5.000000E-01	7.844760E+04	50.	2
239	CH	+CO2	+	=O	+C2HO	+	2.799644E+11	5.000000E-01	7.179530E+04	50.	3
240	HCO	+HCHO	+	=C2HO	+H2O	+	2.438496E+10	5.000000E-01	3.682285E+04	50.	4

TABLE 1. - CONCLUDED.

	REACTION EQUATIONS						RATE CONSTANT DATA				
241	CH2	+CO	+	=C2HO	+H	+	2.619181E+11	5.000000E-01	4.995840E+04	50.	5
242	CH2	+CO2	+	=C2HO	+OH	+	2.764567E+10	5.000000E-01	6.956790E+04	50.	6
243	C3H3	+OH	+	=C2HO	+CH3	+	2.626423E+10	5.000000E-01	1.559245E+04	50.	7
244	C2H	+C2HO	+	=C4H2	+O	+	1.411918E+09	5.000000E-01	1.379110E+04	50.	9
245	C2H2	+C2HO	+	=C4H2	+OH	+	8.485286E+09	5.000000E-01	1.794962E+04	50.	10
246	CH3CO	+	+	=CH3	+CO	+	2.480040E+19	-1.566075E+00	1.659003E+04	52.	2
247	CH3CO	+	+	=C2H2	+OH	+	9.839954E+12	2.256700E-01	6.845635E+04	52.	3
248	C2H	+	+	=H	+C2*	+	2.296555E-03	5.866230E-01	-6.203459E+04	C*.	4
249	C3H3	+	+	=CH3	+C2*	+	1.306384E-01	-2.243270E-01	-4.336523E+04	C*.	11
250	CO	+CO	+	=C2*	+O2	+	3.705159E-03	5.000000E-01	5.991280E+04	C*.	6

TABLE 2
PACKAGE OF 100 REACTIONS FOR OXIDATION OF CH4, CH3OH, AND C2H5OH

	REACTION EQUATIONS						RATE CONSTANT DATA				
1	H2	+M	+	=H	+H	+M	9.976243E+19	-1.260488E+00	1.053737E+05	HO.	1
2	O2	+M	+	=O	+O	+M	6.389865E+20	-1.645428E+00	1.204503E+05	HO.	2
3	OH	+M	+	=O	+H	+M	6.758609E+19	-1.264565E+00	1.032301E+05	HO.	4
4	H2O	+M	+	=H	+OH	+M	2.108870E+27	-3.199173E+00	1.213838E+05	HO.	7
5	HO2	+M	+	=H	+O2	+M	2.400000E+15	0.	4.590000E+04	HO.	10
6	H2O2	+M	+	=OH	+OH	+M	7.800000E+16	0.	4.550000E+04	HO.	18
7	H	+O2	+	=O	+OH	+	2.240000E+14	0.	1.680000E+04	HO.	5
8	O	+H2	+	=H	+OH	+	1.740000E+13	0.	9.450000E+03	HO.	6
9	H	+H2O	+	=OH	+H2	+	8.410000E+13	0.	2.010000E+04	HO.	8
10	O	+H2O	+	=OH	+OH	+	5.750000E+13	0.	1.800000E+04	HO.	9
11	H2	+O2	+	=H	+HO2	+	9.749874E+11	5.000000E-01	5.778610E+04	HO.	11
12	OH	+O2	+	=O	+HO2	+	3.712735E+11	6.357610E-01	5.531791E+04	HO.	13
13	OH	+OH	+	=H	+HO2	+	1.683908E+11	5.000000E-01	4.206055E+04	HO.	14
14	OH	+H2O	+	=H	+H2O2	+	5.600000E+13	0.	7.790000E+04	HO.	19
15	HO2	+H2	+	=H	+H2O2	+	9.600000E+12	0.	2.400000E+04	HO.	20
16	O	+N2	+	=N	+NO	+	1.360000E+14	0.	7.540000E+04	NO.	1
17	O	+NO	+	=N	+O2	+	1.550000E+09	1.000000E+00	3.864000E+04	NO.	2
18	N	+OH	+	=H	+NO	+	5.000000E+11	5.000000E-01	5.000000E+03	NO.	3
19	CO2	+M	+	=O	+CO	+M	2.700000E+32	-4.500000E+00	1.275550E+05	1.	2
20	H	+CO2	+	=OH	+CO	+	5.600000E+13	0.	2.350000E+04	1.	3

TABLE 2. - CONTINUED.

	REACTION EQUATIONS						RATE CONSTANT DATA				
21	HCO	+M	+	=H	+CO	+M	1.000000E+15	0.	2.300000E+04	3.	6
22	H	+CO2	+	=O	+HCO	+	1.587573E+12	5.000000E-01	9.506290E+04	3.	1
23	H2	+CO	+	=H	+HCO	+	1.103555E+12	5.000000E-01	7.730750E+04	3.	5
24	OH	+CO	+	=O	+HCO	+	7.098324E+11	5.000000E-01	7.539880E+04	3.	7
25	CO	+H2O	+	=OH	+HCO	+	2.142333E+11	5.000000E-01	9.170250E+04	3.	8
26	HO2	+CO	+	=O2	+HCO	+	2.167440E+11	5.000000E-01	2.616595E+04	3.	9
27	CO	+H2O2	+	=HO2	+HCO	+	2.183350E+10	5.000000E-01	5.871250E+04	3.	10
28	H2	+HCO	+	=H	+HCHO	+	6.667766E+10	5.000000E-01	3.425755E+04	5.	1
29	OH	+HCO	+	=O	+HCHO	+	1.535023E+10	5.000000E-01	3.284792E+04	5.	2
30	HCO	+H2O	+	=OH	+HCHO	+	1.222396E+10	5.000000E-01	4.501285E+04	5.	3
31	HCHO	+	+	=H	+HCO	+	5.127526E+12	7.359910E-01	7.492603E+04	5.	4
32	HCO	+H2O2	+	=HO2	+HCHO	+	2.110503E+09	5.000000E-01	2.030177E+04	5.	5
33	O2	+HCHO	+	=HO2	+HCO	+	2.164724E+10	5.000000E-01	3.206665E+04	5.	6
34	H	+HCO	+	=CH2	+O	+	1.295424E+12	5.000000E-01	1.039426E+05	6.	1
35	O	+HCHO	+	=CH2	+O2	+	2.147872E+11	5.000000E-01	6.030240E+04	6.	7
36	HO2	+HCHO	+	=O2	+CH2OH	+	1.048331E+09	5.000000E-01	1.550853E+04	7.	1
37	CH2OH	+	+	=H	+HCHO	+	1.918474E+07	1.859993E+00	3.405550E+04	7.	3
38	HCO	+H2O	+	=O	+CH2OH	+	1.186111E+09	5.000000E-01	1.059146E+05	7.	4
39	H2	+HCHO	+	=H	+CH2OH	+	6.254432E+09	5.000000E-01	6.309760E+04	7.	5
40	HCHO	+H2O	+	=OH	+CH2OH	+	9.391612E+09	5.000000E-01	7.749260E+04	7.	6

TABLE 2. - CONTINUED.

	REACTION EQUATIONS						RATE CONSTANT DATA				
41	HCHO	+H2O2	+	=HO2	+CH2OH	+	1.151497E+09	5.000000E-01	4.487695E+04	7.	7
42	OH	+HCHO	+	=O	+CH2OH	+	1.493763E+09	5.000000E-01	6.118890E+04	7.	8
43	H	+HCHO	+	=O	+CH3	+	4.201262E+11	5.000000E-01	6.924640E+04	8.	1
44	H	+CH2OH	+	=CH3	+OH	+	8.540236E+10	5.000000E-01	1.755265E+04	8.	5
45	CH3	+O2	+	=O	+CH2OH	+	1.116270E+09	5.000000E-01	1.686100E+04	8.	6
46	OH	+CH2OH	+	=O	+CH3OH	+	8.301155E+08	5.000000E-01	2.089825E+04	9.	1
47	CH2OH	+H2O	+	=OH	+CH3OH	+	5.217154E+09	5.000000E-01	3.312602E+04	9.	2
48	CH3	+H2O	+	=H	+CH3OH	+	6.650271E+07	5.000000E-01	2.707337E+04	9.	3
49	CH3OH	+	+	=H	+CH2OH	+	5.742335E+03	2.606363E+00	8.046134E+04	9.	5
50	H2	+CH2OH	+	=H	+CH3OH	+	3.505536E+09	5.000000E-01	2.232977E+04	9.	6
51	CH2OH	+H2O2	+	=HO2	+CH3OH	+	6.372953E+08	5.000000E-01	8.383520E+03	9.	7
52	CH3OH	+	+	=CH3	+OH	+	1.519648E+02	3.396359E+00	8.394671E+04	9.	8
53	OH	+CH4	+	=H	+CH3OH	+	2.090216E+08	5.000000E-01	1.511522E+04	9.	9
54	CH2OH	+CH4	+	=CH3	+CH3OH	+	1.999222E+10	5.000000E-01	2.116787E+04	9.	10
55	CH4	+	+	=H	+CH3	+	4.394323E+17	-6.089130E-01	1.083358E+05	10.	1
56	CH3	+H2	+	=H	+CH4	+	2.311698E+09	5.000000E-01	1.267142E+04	10.	2
57	O	+CH4	+	=CH3	+OH	+	2.149499E+10	5.000000E-01	1.173820E+04	10.	3
58	CH3	+H2O	+	=OH	+CH4	+	4.998376E+09	5.000000E-01	2.342672E+04	10.	4
59	O2	+CH4	+	=CH3	+HO2	+	2.315458E+10	5.000000E-01	5.621730E+04	10.	5
60	HCO	+CH4	+	=CH3	+HCHO	+	2.603697E+10	5.000000E-01	3.308612E+04	10.	6

TABLE 2. - CONTINUED.

	REACTION EQUATIONS						RATE CONSTANT DATA				
61	HO2	+CH4	+	=CH3	+H2O2	+	2.339375E+10	5.000000E-01	2.273882E+04	10.	10
62	HCO	+CO	+	=C2H	+O2	+	2.423974E+11	5.000000E-01	1.478417E+05	12.	1
63	C2H2	+	+	=C2H	+H	+	7.783707E+17	-7.049160E-01	1.138829E+05	13.	3
64	C2H2	+H	+	=C2H	+H2	+	4.643078E+11	5.000000E-01	1.424390E+04	13.	4
65	O	+C2H2	+	=C2H	+OH	+	2.377935E+11	5.000000E-01	1.565852E+04	13.	5
66	C2H	+H2O	+	=C2H2	+OH	+	2.396886E+10	5.000000E-01	1.950640E+04	13.	6
67	C2H2	+CH3	+	=C2H	+CH4	+	5.018279E+09	5.000000E-01	1.542033E+04	13.	7
68	C2H3	+	+	=C2H2	+H	+	1.425486E+13	1.608430E-01	4.100172E+04	14.	3
69	C2H3	+H2	+	=H	+C2H4	+	5.666014E+09	5.000000E-01	1.209535E+04	15.	4
70	CH3	+C2H4	+	=C2H3	+CH4	+	1.566002E+10	5.000000E-01	1.207608E+04	15.	5
71	CH2	+HCHO	+	=O	+C2H4	+	9.697242E+09	5.000000E-01	1.981637E+04	15.	7
72	C2H3	+H2O	+	=C2H4	+OH	+	1.020706E+10	5.000000E-01	2.285065E+04	15.	9
73	C2H5	+	+	=H	+C2H4	+	9.969550E+14	-4.639780E-01	4.047757E+04	16.	1
74	CH3	+CH4	+	=C2H5	+H2	+	2.203170E+10	5.000000E-01	2.134795E+04	16.	2
75	C2H6	+	+	=CH3	+CH3	+	4.893779E+23	-2.272211E+00	9.531851E+04	17.	1
76	CH3	+CH4	+	=H	+C2H6	+	1.180116E+10	5.000000E-01	2.809915E+04	17.	2
77	C2H5	+H2	+	=H	+C2H6	+	2.086489E+10	5.000000E-01	1.825120E+04	17.	3
78	C2H5	+OH	+	=O	+C2H6	+	4.644379E+09	5.000000E-01	1.684157E+04	17.	4
79	C2H5	+H2O	+	=OH	+C2H6	+	2.427573E+10	5.000000E-01	2.900650E+04	17.	5
80	C2H5	+CH4	+	=CH3	+C2H6	+	2.906356E+10	5.000000E-01	1.707977E+04	17.	6

TABLE 2. - CONCLUDED.

	REACTION EQUATIONS						RATE CONSTANT DATA				
81	CH3	+CH2OH	+	=O	+C2H6	+	7.345105E+09	5.000000E-01	3.387265E+04	17.	9
82	CH3	+CH3OH	+	=OH	+C2H6	+	2.669389E+10	5.000000E-01	2.447440E+04	17.	10
83	HCO	+CH2OH	+	=O	+CH3CHO+		8.308835E+09	5.000000E-01	4.404550E+04	18.	1
84	CH3CHO+		+	=CH3	+HCO	+	5.092062E+12	5.558380E-01	6.812229E+04	18.	2
85	HCO	+CH4	+	=H	+CH3CHO+		7.784111E+09	5.000000E-01	3.826247E+04	18.	3
86	C2H4OH+		+	=CH3	+HCHO	+	3.678929E+08	1.546829E+00	2.615509E+04	18.	5
87	C2H4OH+		+	=H	+CH3CHO+		1.440074E+07	1.726982E+00	3.295883E+04	18.	6
88	C2H4OH+		+	=C2H4	+OH	+	3.069210E+05	2.317707E+00	3.977859E+04	18.	7
89	CH2OH	+CH2OH	+	=O	+C2H5OH+		7.409123E+09	5.000000E-01	3.524035E+04	19.	1
90	C2H5OH+		+	=CH3	+CH2OH	+	7.748735E+05	2.304652E+00	7.031304E+04	19.	2
91	CH2OH	+CH3OH	+	=OH	+C2H5OH+		2.466308E+10	5.000000E-01	2.584210E+04	19.	3
92	CH3	+CH3OH	+	=H	+C2H5OH+		2.754353E+09	5.000000E-01	1.978945E+04	19.	4
93	CH2OH	+CH4	+	=H	+C2H5OH+		2.062855E+09	5.000000E-01	2.945732E+04	19.	5
94	C2H5	+H2O	+	=H	+C2H5OH+		4.874434E+07	5.000000E-01	2.435297E+04	19.	6
95	CH2OH	+C2H6	+	=CH3	+C2H5OH+		1.733996E+09	5.000000E-01	1.286770E+04	19.	7
96	H2	+C2H4OH+		=H	+C2H5OH+		5.696268E+09	5.000000E-01	2.403520E+04	19.	8
97	C2H4OH	+H2O	+	=OH	+C2H5OH+		7.631990E+09	5.000000E-01	3.483145E+04	19.	9
98	OH	+C2H4OH+		=O	+C2H5OH+		1.219903E+09	5.000000E-01	2.260367E+04	19.	10
99	CH4	+C2H4OH+		=CH3	+C2H5OH+		2.898471E+10	5.000000E-01	2.287330E+04	19.	11
100	OH	+C2H6	+	=H	+C2H5OH+		2.031918E+07	5.000000E-01	6.815050E+03	19.	12

TABLE 3

COMPARISON OF EXPERIMENTAL AND CALCULATED AUTOIGNITION INDUCTION TIMES FOR CH4

SKINNER IDENTIFICATION AND CONDITIONS	TEMPERATURE, K	EXPERIMENTAL TIME, MILLISECONDS	SKINNER CALCULATION, MILLISECONDS	BAHN CALCULATION, MILLISECONDS
SERIES 1C, 10 ATM,	1600	0.3	0.325	0.348
3.5 MOLE PERCENT CH4,	1800	0.059	0.055	0.067
7.0 MOLE PERCENT O2,	2000	0.015	0.015	0.020
89.5 MOLE PERCENT AR				
SERIES 2A, 10 ATM,	1600	1.1	0.99	0.836(0.676)
2.12 MOLE PERCENT CH4,	1800	0.2	0.19	0.176
2.12 MOLE PERCENT O2,	2000	0.054	0.047	0.041(0.039)
95.76 MOLE PERCENT AR				
SERIES 2C, 10 ATM,	1400	-	-	4.261(3.618)
6.7 MOLE PERCENT CH4,	1600	0.43	0.303	0.321
6.7 MOLE PERCENT O2,	1800	0.083	0.051	0.053
86.6 MOLE PERCENT AR	2000	0.021	0.014	0.018

TABLE 4

COMPARISON OF EXPERIMENTAL AND CALCULATED INTERMEDIATE PRODUCT MOLE FRACTIONS DURING AUTOIGNITION OF CH_4

CONDITIONS. SERIES 2C, 1400 K INITIAL TEMPERATURE, AFTER 0.7 MILLISECONDS.

SPECIES	EXPERIMENTAL VALUE	SKINNER VALUE	BAHN VALUE
H_2	0.00009	0.00028	0.00003
H_2O	-	0.00037	0.00013
CO	-	0.00028	0.00001
C_2H_4	0.00002	-	0.00003
C_2H_6	0.00013	0.00006	0.00006

TABLE 5
SUMMARY RESULTS OF REACTION CALCULATIONS FOR ALL 100 REACTIONS

REACTION	RATE-AVG.	RATE-DIFF.	FUEL	TEMP.-AVG.	TEMP.-DIFF.	FUEL
1	3.208	1.895	5	2073.1	582.4	5
2	1.477	.975	5	1918.7	428.0	5
3	3.157	1.472	5	2059.6	568.9	5
4	3.262	1.261	5	2073.3	550.8	5
5	3.844	1.214	5	1849.5	525.5	5
6	2.831	.875	5	1891.3	690.3	1
7	5.124	.948	5	1802.0	456.5	5
8	4.146	1.792	5	1714.7	438.2	4
9	4.780	1.524	5	1748.2	795.3	4
10	4.280	.150	2	1952.6	607.1	5
11	3.263	1.247	5	1662.2	567.1	4
12	3.748	.610	4	1533.5	209.5	5
13	3.652	1.161	5	1799.7	475.7	5
14	2.737	.944	5	2005.1	314.3	1
15	1.489	.956	5	2005.8	317.1	4
16	1.787	.351	5	2556.9	90.8	5
17	1.371	.179	5	2560.0	87.8	5
18	1.575	.434	5	2560.0	87.8	5
19	3.073	.498	4	1838.6	472.5	4
20	4.651	.248	3	1940.9	205.5	1
21	4.665	.159	3	1911.4	321.9	1
22	1.814	.516	3	1789.2	405.1	4
23	2.958	.556	3	1948.7	359.1	1
24	3.521	.507	3	1789.2	405.1	4
25	2.175	.405	3	1911.4	321.9	1
26	3.668	.564	4	1556.2	114.5	4
27	.277	1.119	4	1424.0	169.5	4
28	3.957	1.031	4	1603.1	61.5	1
29	3.941	.791	4	1586.5	45.0	1
30	3.565	.687	4	1556.8	36.6	4
31	4.580	.029	2	2095.0	234.3	3
32	1.486	1.202	4	1267.4	191.5	4
33	.829	.389	4	1575.9	52.0	1
34	1.823	.529	2	1955.6	298.0	3
35	2.209	1.004	3	1808.4	397.2	3
36	.684	1.354	4	1325.2	218.2	3
37	4.287	.654	3	1713.8	346.8	4
38	.191	1.420	4	1534.7	76.0	3
39	-.018	1.673	4	1510.6	115.7	3
40	.043	1.356	4	1487.1	106.3	4

TABLE 5. - CONTINUED.

REACTION	RATE-AVG.	RATE-DIFF.	FUEL	TEMP.-AVG.	TEMP.-DIFF.	FUEL
41	-.688	2.225	4	1244.9	214.0	4
42	.057	1.429	4	1520.3	73.1	4
43	4.484	.096	3	2181.2	32.2	1
44	2.356	.050	4	2225.0	49.2	2
45	2.183	.172	3	2122.1	83.5	3
46	3.216	.951	3	1839.6	171.9	4
47	3.671	.897	3	1826.1	202.6	3
48	3.095	1.188	3	1877.7	195.6	2
49	3.495	.049	4	2144.7	84.9	3
50	3.306	1.128	3	1903.5	169.8	2
51	.660	1.655	3	1433.9	322.4	4
52	3.704	.178	1	2056.4	282.1	2
53	2.243	1.383	3	1787.2	210.3	4
54	2.422	.478	3	1771.2	438.0	3
55	4.827	.131	3	1933.7	291.5	4
56	4.300	.131	3	2171.6	191.0	3
57	4.068	.044	4	2033.1	189.6	1
58	4.733	.008	2	2129.3	69.5	3
59	.667	.518	1	1497.2	635.3	4
60	2.351	.397	1	1412.2	137.7	3
61	.233	.342	3	1714.4	248.1	1
62	2.851	.692	3	1972.3	281.3	3
63	2.666	.342	2	2254.6	41.7	3
64	2.743	.376	2	2132.0	206.5	2
65	2.495	.664	3	1964.5	289.1	3
66	2.347	.579	3	1988.5	265.2	3
67	.307	.742	3	1934.1	319.5	3
68	3.012	.668	2	1887.7	196.8	1
69	2.087	.476	2	1836.3	417.3	3
70	1.302	.880	3	1936.3	317.3	3
71	2.385	.774	3	1831.2	422.5	3
72	2.631	.578	3	1831.2	422.5	3
73	3.305	.896	3	1609.7	34.3	4
74	2.556	.248	3	2122.1	83.5	3
75	3.362	.652	2	1867.9	337.7	3
76	3.055	.714	3	1627.8	16.1	4
77	2.613	.716	3	1627.8	16.1	4
78	2.584	.937	3	1627.8	16.1	4
79	2.989	.995	3	1598.5	35.7	2
80	1.375	1.627	3	1497.1	72.4	4

TABLE 5. - CONCLUDED.

REACTION	RATE-AVG.	RATE-DIFF.	FUEL	TEMP.-AVG.	TEMP.-DIFF.	FUEL
81	3.041	.937	3	1627.8	16.1	4
82	1.968	1.202	3	1687.1	173.6	3
83	1.232	.850	4	1475.3	80.4	3
84	1.908	.492	3	1553.7	220.5	3
85	1.052	1.149	4	1458.7	87.5	4
86	3.424	1.105	3	1627.4	103.5	1
87	1.887	.485	3	1585.5	190.7	3
88	3.291	.971	3	1664.0	35.0	2
89	1.316	2.725	1	1583.6	63.8	3
90	1.488	2.290	1	1631.7	524.6	3
91	.258	2.690	1	1579.2	64.8	4
92	1.313	2.128	1	1833.7	292.1	1
93	.581	2.870	1	1579.2	64.8	4
94	-.109	2.880	1	1526.5	91.7	4
95	-.827	2.968	1	1428.9	164.6	4
96	.554	2.847	1	1579.2	64.8	4
97	1.035	2.719	1	1526.5	91.7	4
98	.514	2.718	1	1583.6	63.8	3
99	.096	2.785	1	1438.7	154.8	4
100	.290	1.599	3	1582.1	58.2	1

TABLE 6
RANKED RATES (MAXIMUM VALUE IN LOGARITHMIC FORM AS ADJUSTED) FOR EACH FUEL AND ALL 100 REACTIONS

REACTION	RATE-AVG.	FUEL	RATE	FUEL	RATE	FUEL	RATE	FUEL	RATE	FUEL	RATE
1	3.208	5	5.104	3	2.932	2	2.719	4	2.662	1	2.625
2	1.477	5	2.452	3	1.577	1	1.206	2	1.145	4	1.004
3	3.157	5	4.629	3	3.105	2	2.749	1	2.655	4	2.649
4	3.262	5	4.523	3	3.180	2	2.890	4	2.864	1	2.853
5	3.844	5	5.058	3	3.917	1	3.619	2	3.349	4	3.275
6	2.831	5	3.706	3	2.996	1	2.544	4	2.519	2	2.389
7	5.124	5	6.072	3	5.031	1	4.895	2	4.824	4	4.798
8	4.146	5	5.938	3	4.209	1	3.920	2	3.398	4	3.267
9	4.780	5	6.304	3	4.793	1	4.560	4	4.291	2	3.952
10	4.280	3	4.412	5	4.406	1	4.322	4	4.131	2	4.130
11	3.263	5	4.509	3	3.341	1	3.217	2	2.674	4	2.571
12	3.748	5	4.258	3	3.919	1	3.871	2	3.555	4	3.138
13	3.652	5	4.813	3	3.737	1	3.576	2	3.095	4	3.037
14	2.737	5	3.681	3	2.975	2	2.357	1	2.356	4	2.318
15	1.489	5	2.445	3	1.734	2	1.110	1	1.093	4	1.065
16	1.787	5	2.138	2	1.802	1	1.695	4	1.694	3	1.607
17	1.371	5	1.550	2	1.437	1	1.334	4	1.313	3	1.222
18	1.575	5	2.008	2	1.557	4	1.486	1	1.447	3	1.376
19	3.073	3	3.441	1	3.368	2	2.908	4	2.575		
20	4.651	3	4.899	1	4.748	2	4.548	4	4.410		
21	4.665	3	4.825	1	4.665	2	4.599	4	4.573		
22	1.814	3	2.329	1	2.056	2	1.547	4	1.322		
23	2.958	3	3.514	1	3.043	2	2.667	4	2.607		
24	3.521	3	4.028	1	3.735	2	3.246	4	3.075		
25	2.175	3	2.579	1	2.290	2	1.925	4	1.904		
26	3.668	3	4.019	1	3.988	2	3.559	4	3.104		
27	.277	3	1.055	1	.982	2	-.087	4	-.843		
28	3.957	3	4.692	1	4.464	2	3.746	4	2.926		
29	3.941	3	4.456	1	4.325	2	3.832	4	3.150		
30	3.565	3	4.007	1	3.942	2	3.434	4	2.878		
31	4.580	2	4.609	4	4.591	3	4.564	1	4.556		
32	1.486	1	2.526	3	2.077	2	1.057	4	.284		
33	.829	1	1.061	3	.992	2	.824	4	.440		
34	1.823	2	2.352	1	2.170	3	1.402	4	1.368		
35	2.209	2	2.937	1	2.506	4	2.188	3	1.205		
36	.684	3	1.800	1	1.264	2	.342	4	-.670		
37	4.287	3	4.941	1	4.523	2	3.850	4	3.836		
38	.191	3	1.273	1	.877	2	-.158	4	-1.229		
39	-.018	3	1.267	1	.831	2	-.479	4	-1.691		
40	.043	3	1.099	1	.741	2	-.356	4	-1.313		

TABLE 6. - CONTINUED.

REACTION	RATE-AVG.	FUEL	RATE	FUEL	RATE	FUEL	RATE	FUEL	RATE
41	-.688	3	.857	1	.552	2	-1.248	4	-2.914
42	.057	3	1.148	1	.747	2	-.297	4	-1.372
43	4.484	2	4.547	4	4.517	1	4.482	3	4.387
44	2.356	4	2.407	3	2.351	1	2.350	2	2.318
45	2.183	4	2.285	2	2.219	1	2.217	3	2.010
46	3.216	3	4.167	1	3.051	2	2.842	4	2.803
47	3.671	3	4.568	1	3.419	4	3.400	2	3.298
48	3.095	3	4.283	1	2.979	4	2.566	2	2.553
49	3.495	4	3.543	2	3.484	3	3.477	1	3.476
50	3.306	3	4.434	1	3.132	4	2.833	2	2.823
51	.660	3	2.315	1	.662	2	-.141	4	-.195
52	3.704	3	3.865	4	3.819	2	3.608	1	3.527
53	2.243	3	3.626	1	2.267	2	1.642	4	1.437
54	2.422	3	2.899	4	2.468	2	2.210	1	2.110
55	4.827	3	4.959	4	4.895	1	4.757	2	4.699
56	4.300	3	4.431	2	4.288	4	4.255	1	4.225
57	4.068	2	4.099	3	4.087	1	4.062	4	4.024
58	4.733	4	4.741	3	4.733	1	4.732	2	4.724
59	.667	1	1.186	3	.570	2	.487	4	.426
60	2.351	1	2.748	2	2.404	3	2.267	4	1.984
61	.233	1	.383	4	.357	2	.301	3	-.110
62	2.851	2	3.444	4	2.972	1	2.829	3	2.160
63	2.666	2	3.008	1	2.763	4	2.524	3	2.368
64	2.743	2	3.119	1	2.805	4	2.654	3	2.395
65	2.495	2	3.098	4	2.543	1	2.507	3	1.831
66	2.347	2	2.878	4	2.485	1	2.258	3	1.768
67	.307	2	.861	4	.404	1	.398	3	-.435
68	3.012	2	3.680	4	2.920	1	2.918	3	2.529
69	2.087	2	2.563	1	2.382	3	1.745	4	1.660
70	1.302	2	2.058	4	1.609	1	1.119	3	.422
71	2.385	2	3.031	1	2.664	4	2.234	3	1.610
72	2.631	2	3.168	1	2.751	4	2.550	3	2.053
73	3.305	2	3.924	1	3.546	4	3.341	3	2.409
74	2.556	4	2.702	2	2.617	1	2.598	3	2.308
75	3.362	2	4.013	1	3.279	4	3.200	3	2.955
76	3.055	2	3.658	1	3.392	4	2.830	3	2.341
77	2.613	2	3.215	1	2.947	4	2.395	3	1.898
78	2.584	2	3.284	1	2.812	4	2.592	3	1.647
79	2.989	2	3.672	1	3.164	4	3.127	3	1.995
80	1.375	2	2.364	4	1.943	1	1.445	3	-.252

TABLE 6.-CONCLUDED.

REACTION	RATE-AVG.	FUEL	RATE	FUEL	RATE	FUEL	RATE	FUEL	RATE
81	3.041	2	3.741	1	3.268	4	3.050	3	2.104
82	1.968	2	2.720	1	2.194	4	2.192	3	.766
83	1.232	1	1.952	2	1.336	3	1.258	4	.382
84	1.908	1	2.293	2	2.243	4	1.678	3	1.416
85	1.052	1	1.974	3	1.303	2	1.027	4	-.097
86	3.424	1	4.097	2	3.951	4	3.328	3	2.319
87	1.887	2	2.260	1	2.206	4	1.680	3	1.402
88	3.291	2	3.958	1	3.548	4	3.337	3	2.320
89	1.316	1	4.041	3	.926	2	.492	4	-.196
90	1.488	1	3.778	4	.800	2	.754	3	.622
91	.258	1	2.948	3	-.266	2	-.566	4	-1.085
92	1.313	1	3.440	4	.796	2	.552	3	.462
93	.581	1	3.451	3	.395	2	-.351	4	-1.170
94	-.109	1	2.771	3	-.270	2	-1.048	4	-1.889
95	-.827	1	2.041	2	-1.667	3	-1.709	4	-1.974
96	.554	1	3.401	3	.343	2	-.357	4	-1.171
97	1.035	1	3.753	3	.599	2	.172	4	-.386
98	.514	1	3.232	3	.114	2	-.302	4	-.988
99	.096	1	2.881	2	-.609	3	-.819	4	-1.068
100	.290	1	1.752	2	.631	4	.084	3	-1.310

TABLE 7
RANKED TEMPERATURES CORRESPONDING TO RATE DATA OF TABLE 6

REACTION	TEMP.-AVG.	FUEL	TEMP.	FUEL	TEMP.	FUEL	TEMP.	FUEL	TEMP.	FUEL	TEMP.
1	2073.1	4	2341.3	2	2338.8	1	2334.0	3	1860.7	5	1490.7
2	1918.7	4	2271.8	2	2235.2	3	1860.7	1	1735.4	5	1490.7
3	2059.6	4	2319.3	2	2315.3	1	2311.9	3	1860.7	5	1490.7
4	2073.3	4	2331.9	2	2330.2	1	2321.2	3	1860.7	5	1522.4
5	1849.5	4	2247.4	2	2235.2	3	1770.6	1	1670.3	5	1323.9
6	1891.3	2	2330.2	4	2225.2	3	1860.7	5	1839.4	1	1201.1
7	1802.0	2	2175.8	4	2132.5	3	1686.1	1	1670.3	5	1345.5
8	1714.7	4	2152.9	2	1774.3	3	1686.1	1	1614.8	5	1345.5
9	1748.2	4	2543.6	2	1687.0	3	1623.6	1	1541.6	5	1345.5
10	1952.6	4	2543.6	3	2059.8	2	1970.4	1	1843.5	5	1345.5
11	1662.2	4	2229.3	3	1686.1	2	1629.0	1	1466.3	5	1300.3
12	1533.5	4	1670.7	2	1629.0	1	1523.9	3	1519.8	5	1323.9
13	1799.7	2	2235.2	4	2229.3	3	1686.1	1	1523.9	5	1323.9
14	2005.1	4	2319.3	2	2315.3	3	1860.7	5	1839.4	1	1690.8
15	2005.8	4	2322.9	2	2315.3	3	1860.7	5	1839.4	1	1690.8
16	2556.9	5	2647.7	2	2549.7	1	2547.2	4	2528.3	3	2511.7
17	2560.0	5	2647.7	2	2549.7	1	2547.2	4	2543.6	3	2511.7
18	2560.0	5	2647.7	2	2549.7	1	2547.2	4	2543.6	3	2511.7
19	1838.6	4	2311.1	2	1687.0	3	1686.1	1	1670.3		
20	1940.9	4	2094.2	2	2073.3	3	1860.7	1	1735.4		
21	1911.4	4	2194.3	2	2175.8	3	1686.1	1	1589.6		
22	1789.2	4	2194.3	2	1687.0	3	1686.1	1	1589.6		
23	1948.7	2	2235.2	4	2225.2	3	1744.7	1	1589.6		
24	1789.2	4	2194.3	2	1687.0	3	1686.1	1	1589.6		
25	1911.4	4	2194.3	2	2175.8	3	1686.1	1	1589.6		
26	1556.2	4	1670.7	2	1629.0	1	1466.3	3	1458.7		
27	1424.0	4	1593.4	2	1493.8	1	1334.3	3	1274.4		
28	1603.1	2	1629.0	3	1623.6	4	1618.2	1	1541.6		
29	1586.5	3	1623.6	4	1618.2	2	1562.8	1	1541.6		
30	1556.8	4	1593.4	2	1562.8	3	1547.0	1	1523.9		
31	2095.0	4	2194.3	2	2175.8	1	2149.0	3	1860.7		
32	1267.4	4	1458.9	2	1288.5	3	1172.7	1	1149.6		
33	1575.9	3	1623.6	4	1593.4	2	1562.8	1	1523.9		
34	1955.6	3	2253.6	4	2132.5	2	1745.6	1	1690.8		
35	1808.4	3	2205.7	2	1687.0	4	1670.7	1	1670.3		
36	1325.2	4	1501.5	2	1358.1	1	1334.3	3	1107.1		
37	1713.8	4	2060.6	2	1629.0	1	1589.6	3	1576.2		
38	1534.7	4	1593.4	2	1562.8	1	1523.9	3	1458.7		
39	1510.6	4	1618.2	2	1562.8	1	1466.3	3	1394.8		
40	1487.1	4	1593.4	2	1493.8	1	1466.3	3	1394.8		

TABLE 7. - CONTINUED.

REACTION	TEMP.-AVG.	FUEL	TEMP.	FUEL	TEMP.	FUEL	TEMP.	FUEL	TEMP.
41	1244.9	4	1458.9	2	1233.4	1	1149.6	3	1137.5
42	1520.3	4	1593.4	2	1562.8	1	1466.3	3	1458.7
43	2181.2	3	2205.7	4	2194.3	2	2175.8	1	2149.0
44	2225.0	3	2253.6	1	2245.6	4	2225.2	2	2175.8
45	2122.1	3	2205.7	1	2149.0	2	2073.3	4	2060.6
46	1839.6	4	2011.5	2	1925.6	1	1735.4	3	1686.1
47	1826.1	4	1975.1	2	1970.4	1	1735.4	3	1623.6
48	1877.7	2	2073.3	4	2060.6	1	1690.8	3	1686.1
49	2144.7	4	2194.3	2	2175.8	1	2149.0	3	2059.8
50	1903.5	2	2073.3	4	2060.6	3	1744.7	1	1735.4
51	1433.9	4	1756.3	2	1562.8	1	1243.7	3	1172.7
52	2056.4	1	2245.6	4	2225.2	3	1980.7	2	1774.3
53	1787.2	4	1997.4	2	1774.3	1	1690.8	3	1686.1
54	1771.2	1	2046.1	4	1931.2	2	1774.3	3	1333.2
55	1933.7	4	2225.2	3	2005.7	1	1758.1	2	1745.6
56	2171.6	1	2245.6	2	2235.2	4	2225.2	3	1980.7
57	2033.1	2	2175.8	4	2132.5	3	1980.7	1	1843.5
58	2129.3	2	2175.8	1	2149.0	4	2132.5	3	2059.8
59	1497.2	4	2132.5	2	1429.9	3	1225.4	1	1201.1
60	1412.2	4	1546.2	2	1493.8	1	1334.3	3	1274.4
61	1714.4	3	1860.7	2	1774.3	4	1756.3	1	1466.3
62	1972.3	3	2253.6	4	1975.1	2	1856.6	1	1804.1
63	2254.6	3	2296.3	1	2261.8	2	2235.2	4	2225.2
64	2132.0	3	2296.3	1	2245.6	4	2060.6	2	1925.6
65	1964.5	3	2253.6	4	1975.1	2	1825.4	1	1804.1
66	1988.5	3	2253.6	4	1931.2	2	1925.6	1	1843.5
67	1934.1	3	2253.6	2	1925.6	1	1843.5	4	1713.7
68	1887.7	3	2005.7	4	1997.4	2	1856.6	1	1690.8
69	1836.3	3	2253.6	4	1713.7	1	1690.8	2	1687.0
70	1936.3	3	2253.6	1	2149.0	4	1713.7	2	1629.0
71	1831.2	3	2253.6	4	1713.7	2	1687.0	1	1670.3
72	1831.2	3	2253.6	4	1713.7	2	1687.0	1	1670.3
73	1609.7	4	1643.9	2	1629.0	1	1589.6	3	1576.2
74	2122.1	3	2205.7	1	2149.0	2	2073.3	4	2060.6
75	1867.9	3	2205.7	2	1774.3	4	1756.3	1	1735.4
76	1627.8	4	1643.9	2	1629.0	3	1623.6	1	1614.8
77	1627.8	4	1643.9	2	1629.0	3	1623.6	1	1614.8
78	1627.8	4	1643.9	2	1629.0	3	1623.6	1	1614.8
79	1598.5	3	1623.6	4	1618.2	1	1589.6	2	1562.8
80	1497.1	4	1569.4	2	1493.8	1	1466.3	3	1458.7

TABLE 7. - CONDLUDED.

REACTION	TEMP.-AVG.	FUEL	TEMP.	FUEL	TEMP.	FUEL	TEMP.	FUEL	TEMP.
81	1627.8	4	1643.9	2	1629.0	3	1623.6	1	1614.8
82	1687.1	3	1860.7	4	1643.9	2	1629.0	1	1614.8
83	1475.3	4	1546.2	2	1493.8	1	1466.3	3	1394.8
84	1553.7	2	1687.0	4	1670.7	1	1523.9	3	1333.2
85	1458.7	4	1546.2	2	1493.8	1	1399.8	3	1394.8
86	1627.4	3	1686.1	4	1670.7	2	1629.0	1	1523.9
87	1585.5	2	1687.0	4	1670.7	1	1589.6	3	1394.8
88	1664.0	3	1686.1	4	1670.7	1	1670.3	2	1629.0
89	1583.6	4	1643.9	2	1629.0	1	1541.6	3	1519.8
90	1631.7	4	1975.1	2	1774.3	1	1670.3	3	1107.1
91	1579.2	4	1643.9	2	1629.0	1	1523.9	3	1519.8
92	1833.7	2	2073.3	4	1975.1	3	1744.7	1	1541.6
93	1579.2	4	1643.9	2	1629.0	1	1523.9	3	1519.8
94	1526.5	4	1618.2	2	1562.8	1	1466.3	3	1458.7
95	1428.9	4	1593.4	2	1562.8	1	1284.7	3	1274.4
96	1579.2	4	1643.9	2	1629.0	1	1523.9	3	1519.8
97	1526.5	4	1618.2	2	1562.8	1	1466.3	3	1458.7
98	1583.6	4	1643.9	2	1629.0	1	1541.6	3	1519.8
99	1438.7	4	1593.4	2	1493.8	1	1334.3	3	1333.2
100	1582.1	3	1623.6	4	1618.2	2	1562.8	1	1523.9

TABLE 8
MAXIMUM CONCENTRATIONS OF CERTAIN CHEMICAL SPECIES FOR EACH FUEL, IN RANKED ORDER

SPECIES	FUEL	MAX. PPM	FUEL	MAX. PPM	FUEL	MAX. PPM	FUEL	MAX. PPM	FUEL	MAX. PPM
H	5	106046.2	2	13270.6	4	12452.3	3	12109.6	1	11858.4
OH	5	27492.9	3	17767.6	1	16698.4	4	16631.2	2	16559.1
HO2	1	1048.3	3	459.1	2	142.8	5	115.4	4	46.9
H2	5	295278.4	3	19875.7	4	18685.8	1	16949.8	2	16876.9
H2O2	1	1254.8	3	332.6	2	27.8	5	3.7	4	1.6
N	5	1.5	2	.7	1	.5	4	.5	3	.5
NO	5	6943.8	2	5565.5	1	4874.5	4	4676.4	3	4261.6
O	5	23509.4	3	11590.2	2	9607.5	1	8541.6	4	8132.4
CO	1	46416.4	2	45162.3	3	42286.5	4	37678.2		
HCO	3	135.7	1	121.0	2	42.1	4	14.3		
HCHO	1	8833.5	3	6736.7	2	1816.5	4	592.1		
CH3	4	2679.6	1	2342.1	2	2325.3	3	1796.2		
CH2OH	3	27.4	1	6.2	2	.8	4	.1		
CH4	4	94793.8	2	38136.8	1	36077.8	3	18831.4		
CH3OH	3	122550.5	1	3224.1	4	3118.8	2	2451.8		
C2H2	2	1798.5	4	962.2	1	277.6	3	25.8		
C2H4	2	4722.0	4	1358.5	1	956.3	3	36.9		
C2H6	2	56476.6	4	7940.9	1	4163.5	3	214.4		

TABLE 9

REACTIONS EMPLOYED BY CHINITZ, BOWMAN, OR SKINNER

NUMBER	REACTION	CODE	CHINITZ	BOWMAN	SKINNER
1	$H_2 + M = H + H + M$	HO. 1	C		S
2	$O_2 + M = O + O + M$	HO. 2	C		S
4	$H_2O + M = H + OH + M$	HO. 7		B	S
5	$HO_2 + M = H + O_2 + M$	HO.10			S
6	$H_2O_2 + M = OH + OH + M$	HO.18			S
7	$H + O_2 = O + OH$	HO. 5	C	B	S
8	$O + H_2 = H + OH$	HO. 6	C	B	S
9	$H + H_2O = OH + H_2$	HO. 8	C	B	S
10	$O + H_2O = OH + OH$	HO. 9	C	B	S
11	$H_2 + O_2 = H + HO_2$	HO.11			S
15	$HO_2 + H_2 = H + H_2O_2$	HO.20			S
19	$CO_2 + M = O + CO + M$	1. 2			S
20	$H + CO_2 = OH + CO$	1. 3	C	B	S
21	$HCO + M = H + CO + M$	3. 6		B	
25	$CO + H_2O = OH + HCO$	3. 8	C	B	
26	$HO_2 + CO = O_2 + HCO$	3. 9	C*		
30	$HCO + H_2O = OH + HCHO$	5. 3	C		
32	$HCO + H_2O_2 = HO_2 + HCHO$	5. 5	C*		
33	$O_2 + HCHO = HO_2 + HCO$	5. 6	C*		
55	$CH_4 = H + CH_3$	10. 1		B**	S**
56	$CH_3 + H_2 = H + CH_4$	10. 2		B	S
57	$O + CH_4 = CH_3 + OH$	10. 3	C	B	S
58	$CH_3 + H_2O = OH + CH_4$	10. 4	C	B	S
59	$O_2 + CH_4 = CH_3 + HO_2$	10. 5	C*		S
61	$HO_2 + CH_4 = CH_3 + H_2O_2$	10.10	C*		S
75	$C_2H_6 = CH_3 + CH_3$	17. 1			S
43	$H + HCHO = O + CH_3$	8. 1			
-	$H_2 + HCO = O + CH_3$	-		B	
45	$CH_3 + O_2 = O + CH_2OH$	8. 6			
-	$CH_3 + O_2 = HCO + H_2O$	-		B	
-	$CH_3 + O_2 = OH + H_2 + CO$	-			S
-	$CH_3 + O_2 = OH + HCHO$	-	C		
-	$CHO_3 + M = O_2 + HCO + M$	-	C*		
-	$CHO_3 + CH_2O = OH + CO + CO + H_2O$	-	C*		

* TABULATED BY CHINITZ FROM HIS REFERENCE SOURCES, BUT NOT USED BY HIM

** BIMOLECULAR DISSOCIATION/TERMOLECULAR RECOMBINATION

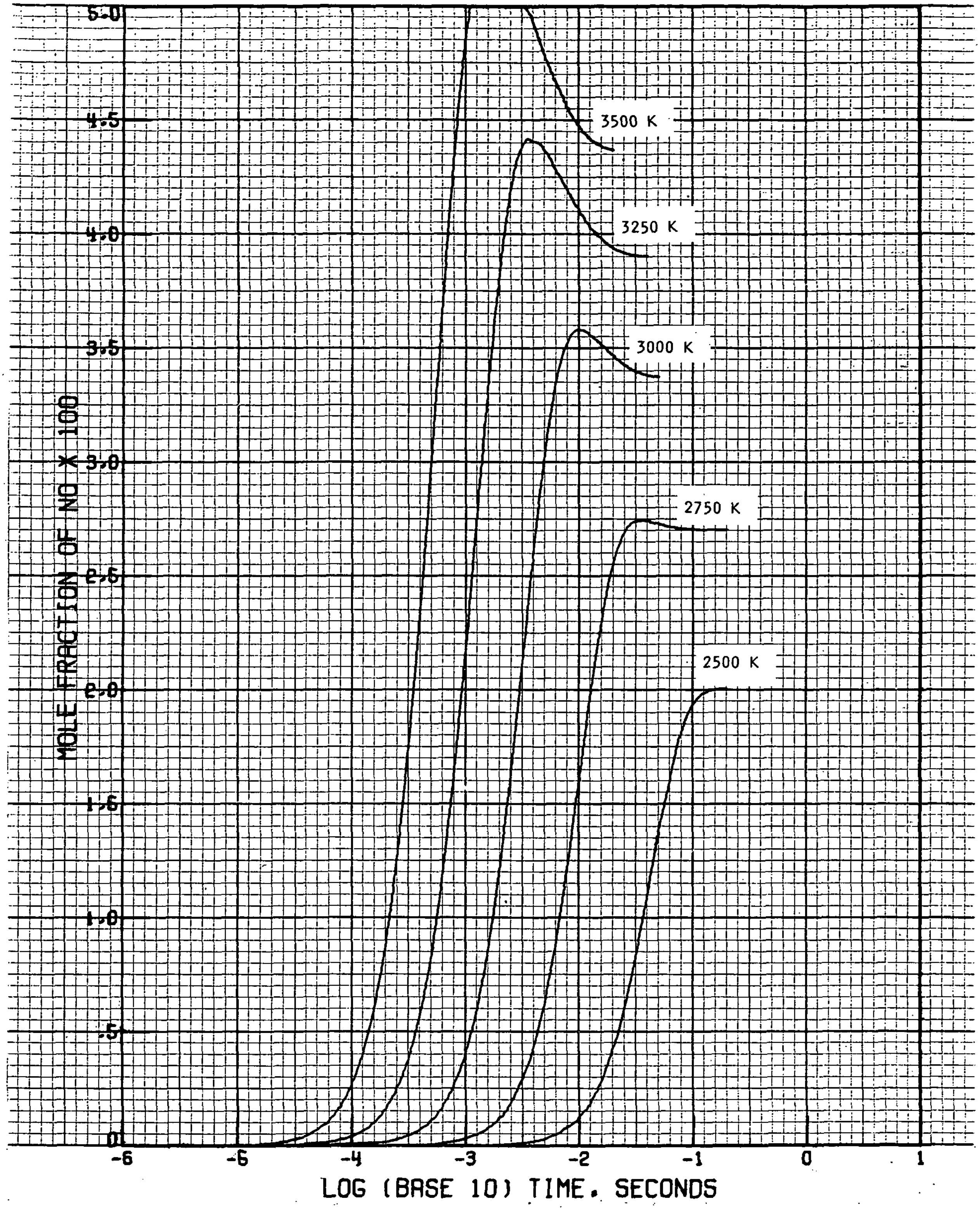

Figure 1. - NO Concentration as a function of time in air heated instantaneously to temperature shown and dissociating kinetically thereafter.

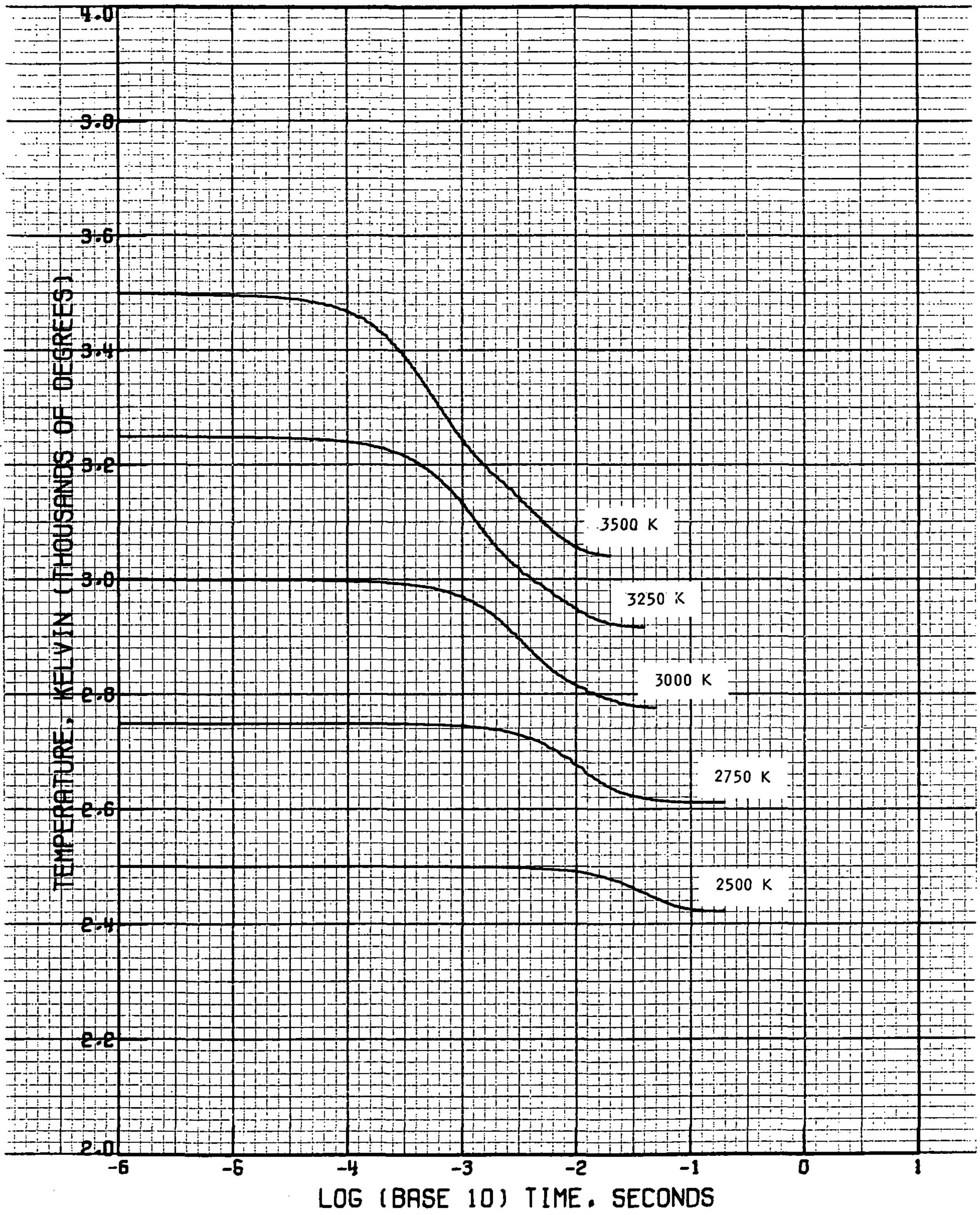

Figure 2. - Temperature as a function of time in air heated instantaneously to temperature shown and dissociating kinetically thereafter.

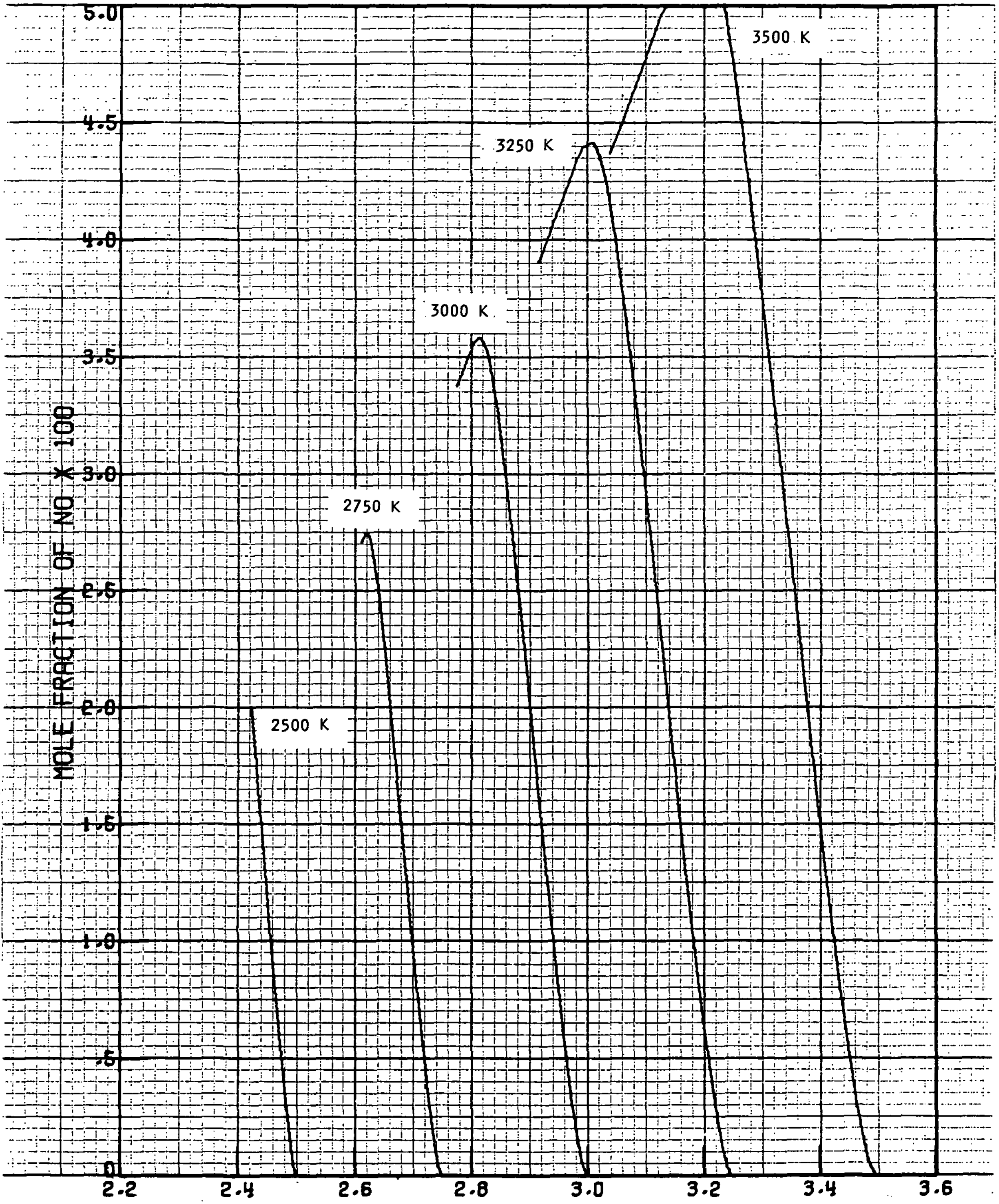

Figure 3. - NO Concentration as a function of temperature in air heated instantaneously to temperature shown and dissociating kinetically thereafter.

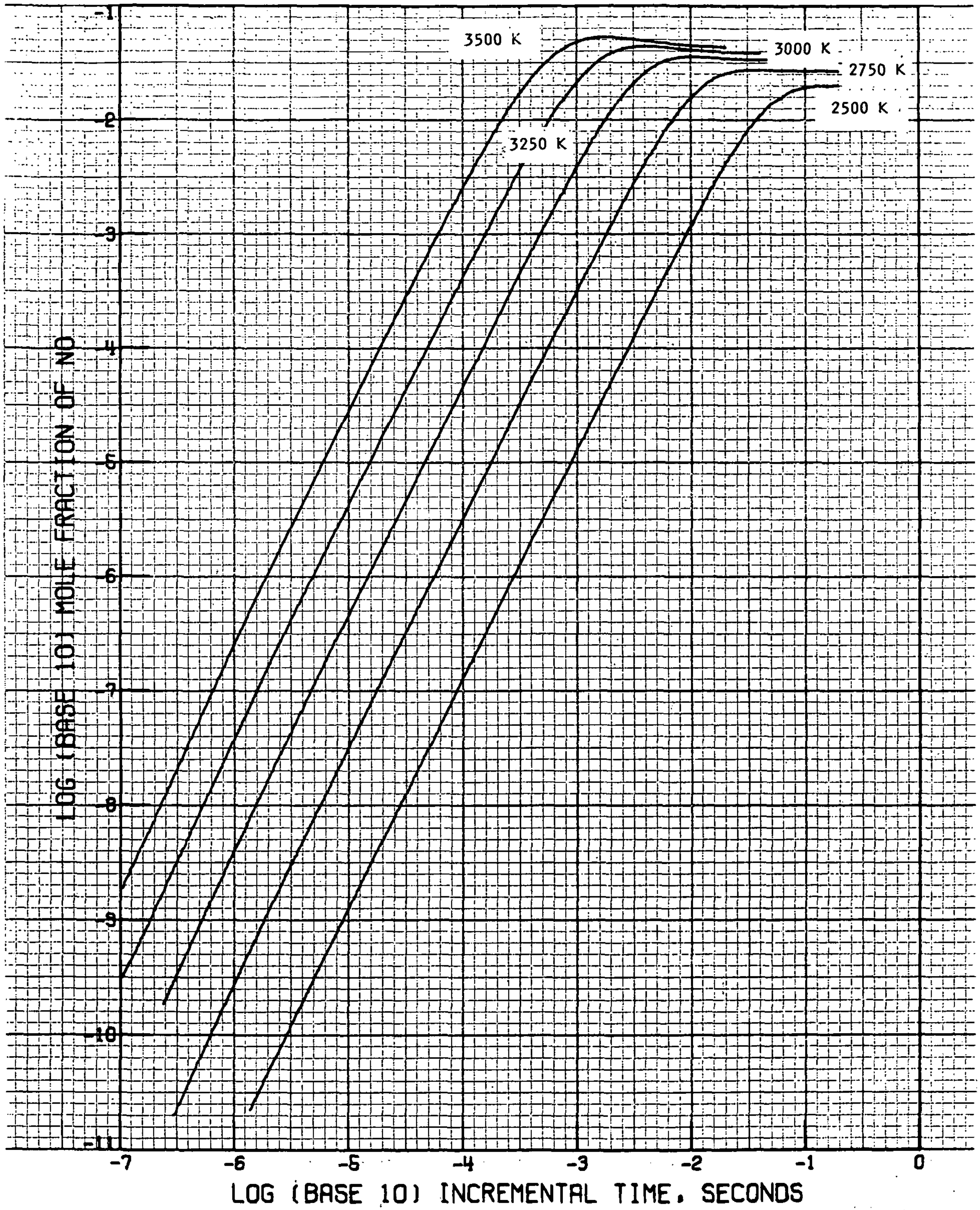

Figure 4. - NO Concentration (logarithmic representation) as a function of time in air heated instantaneously to temperature shown and dissociating kinetically thereafter.

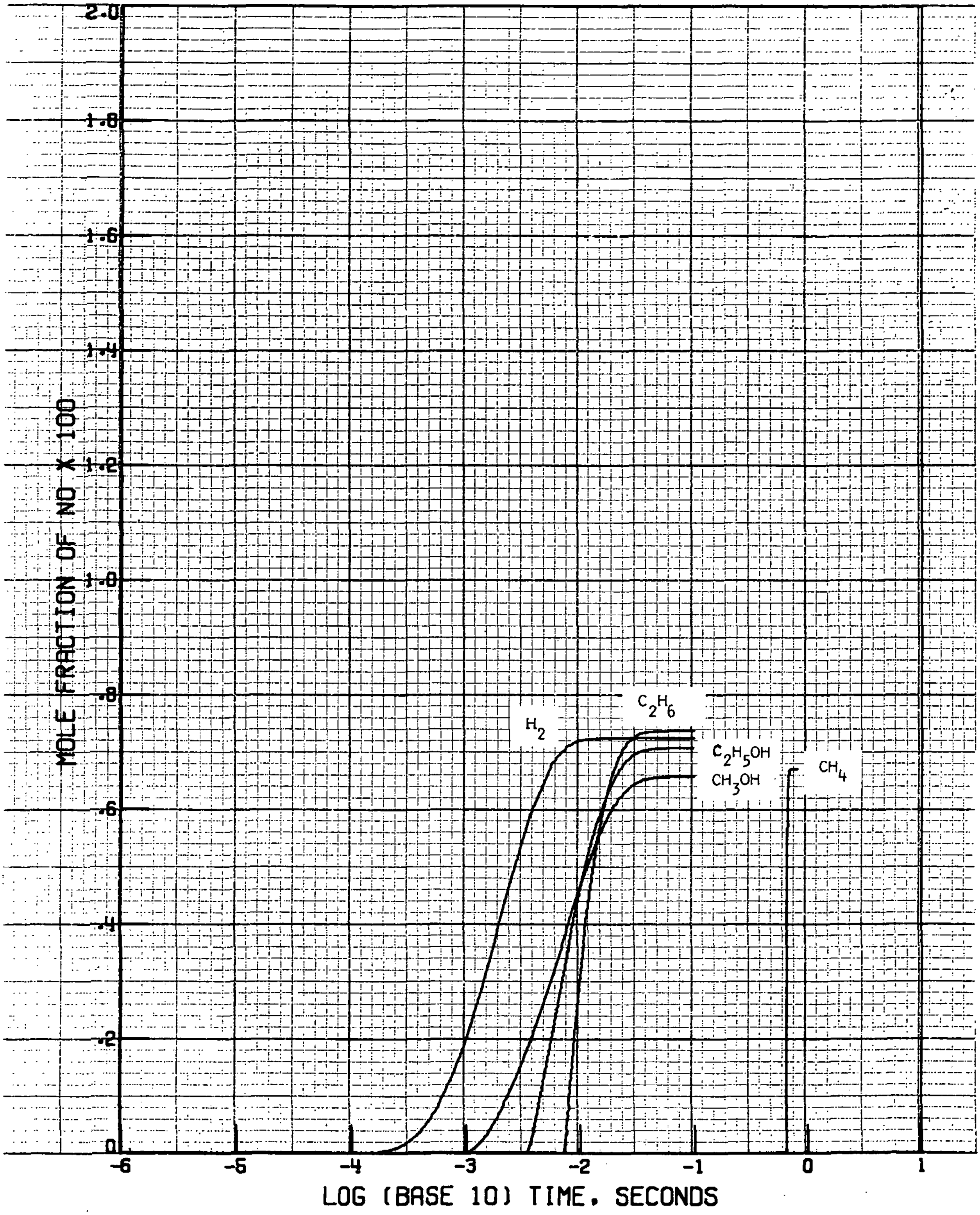

Figure 5. - NO Concentration as a function of time in combustion products of several fuels each dispersed stoichiometrically in air at 1100 K initially and reacting spontaneously at 1 atm.

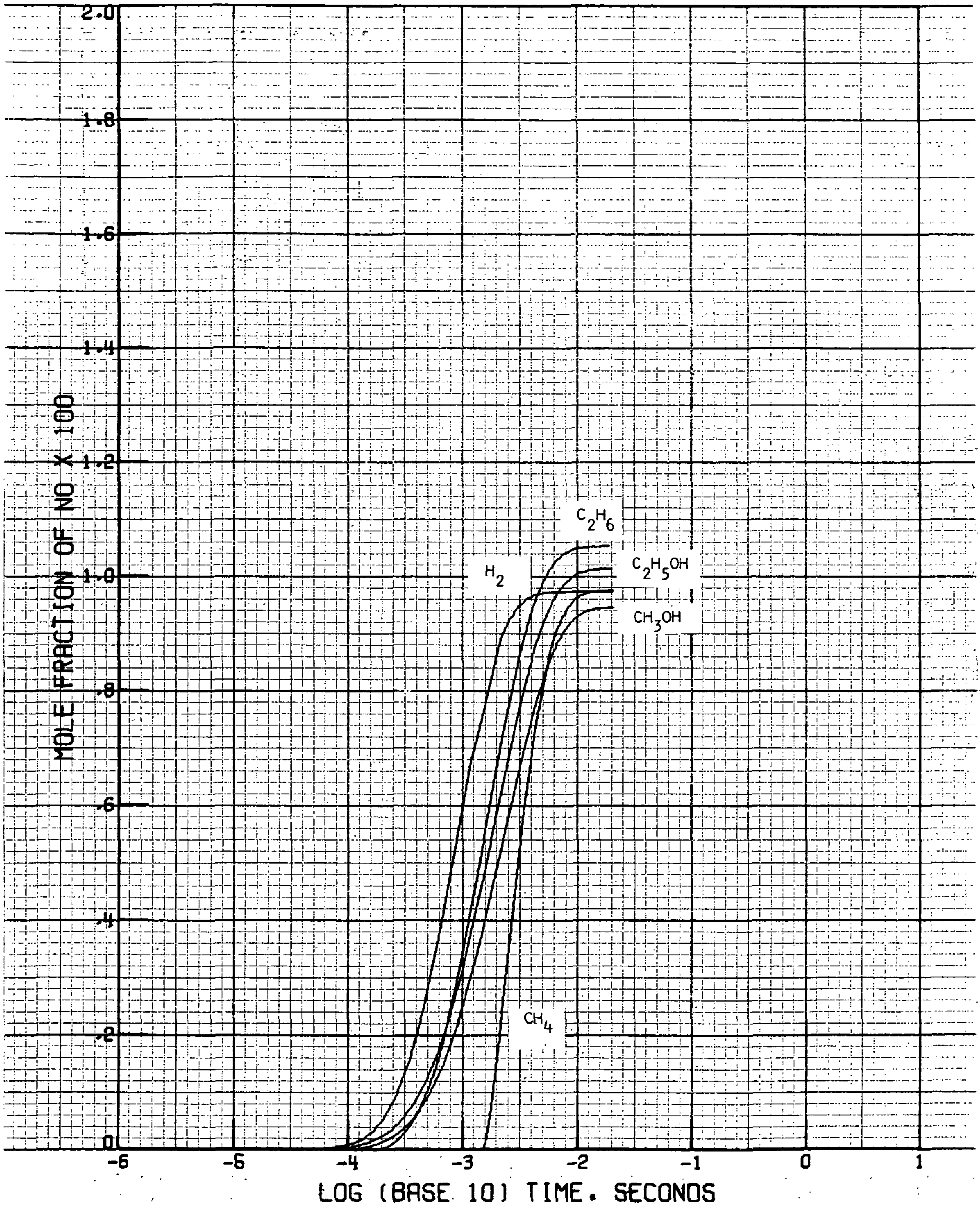

Figure 6. - NO Concentration as a function of time in combustion products of several fuels each dispersed stoichiometeically in air at 1500 K initially and reacting spontaneously at 1 atm.

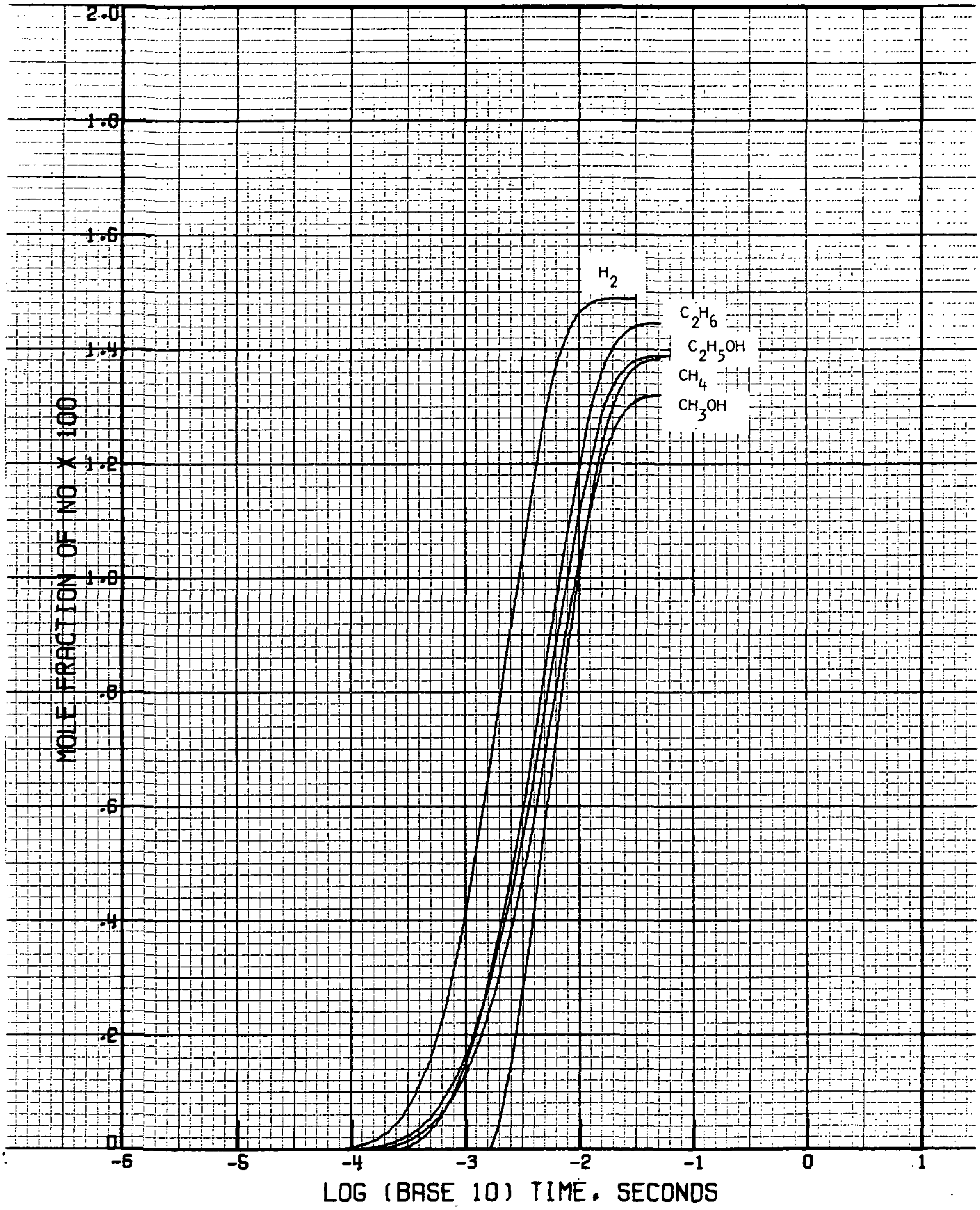

Figure 7. - NO Concentration as a function of time in combustion products of several fuels each dispersed in 2/3 of stoichiometric amount in air at 1500 K initially and reacting spontaneously at 1 atm.

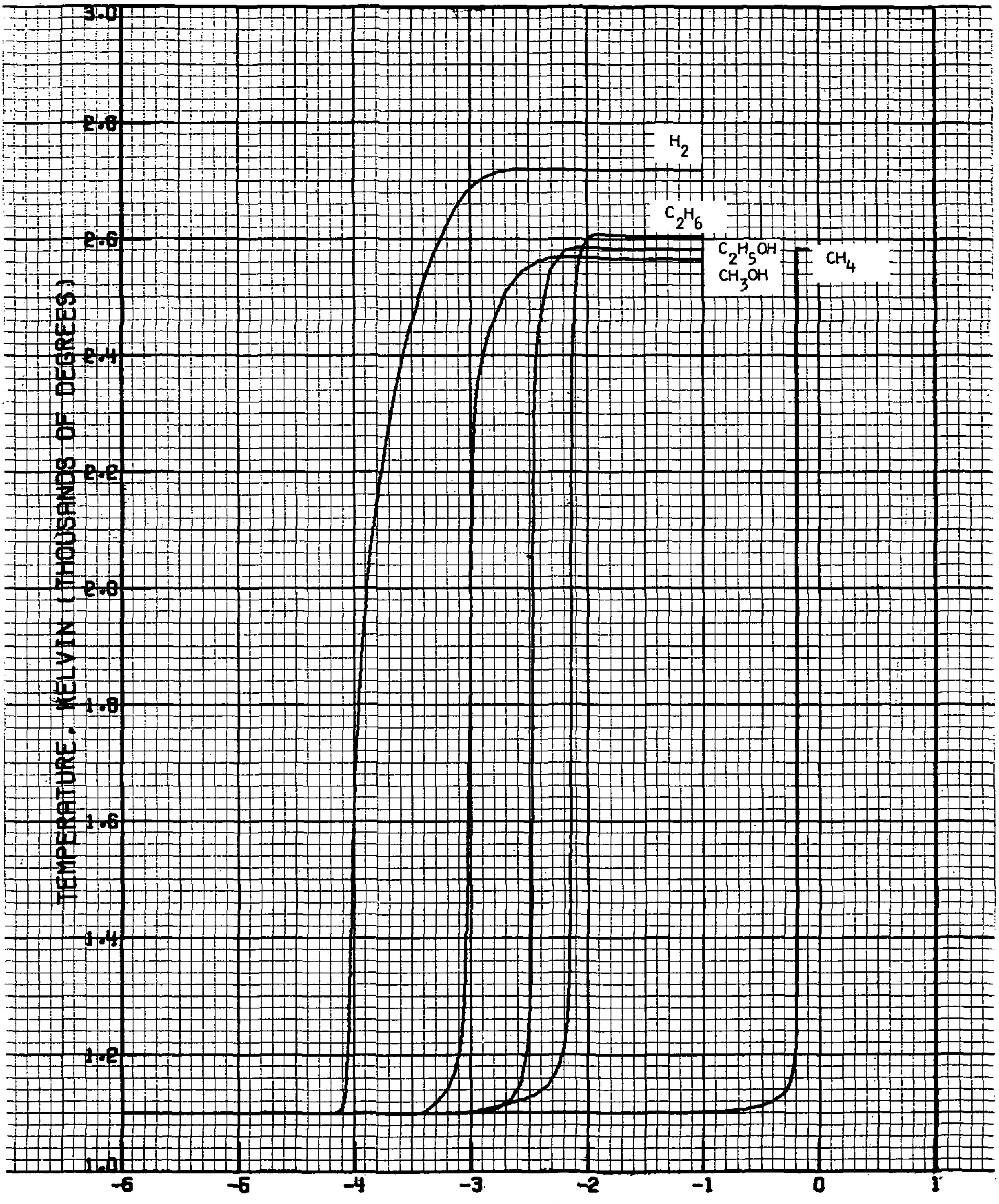

Figure 8. - Temperature as a function of time in combustion products of several fuels each dispersed stoichiometrically in air at 1100 K initially and reacting spontaneously at 1 atm.

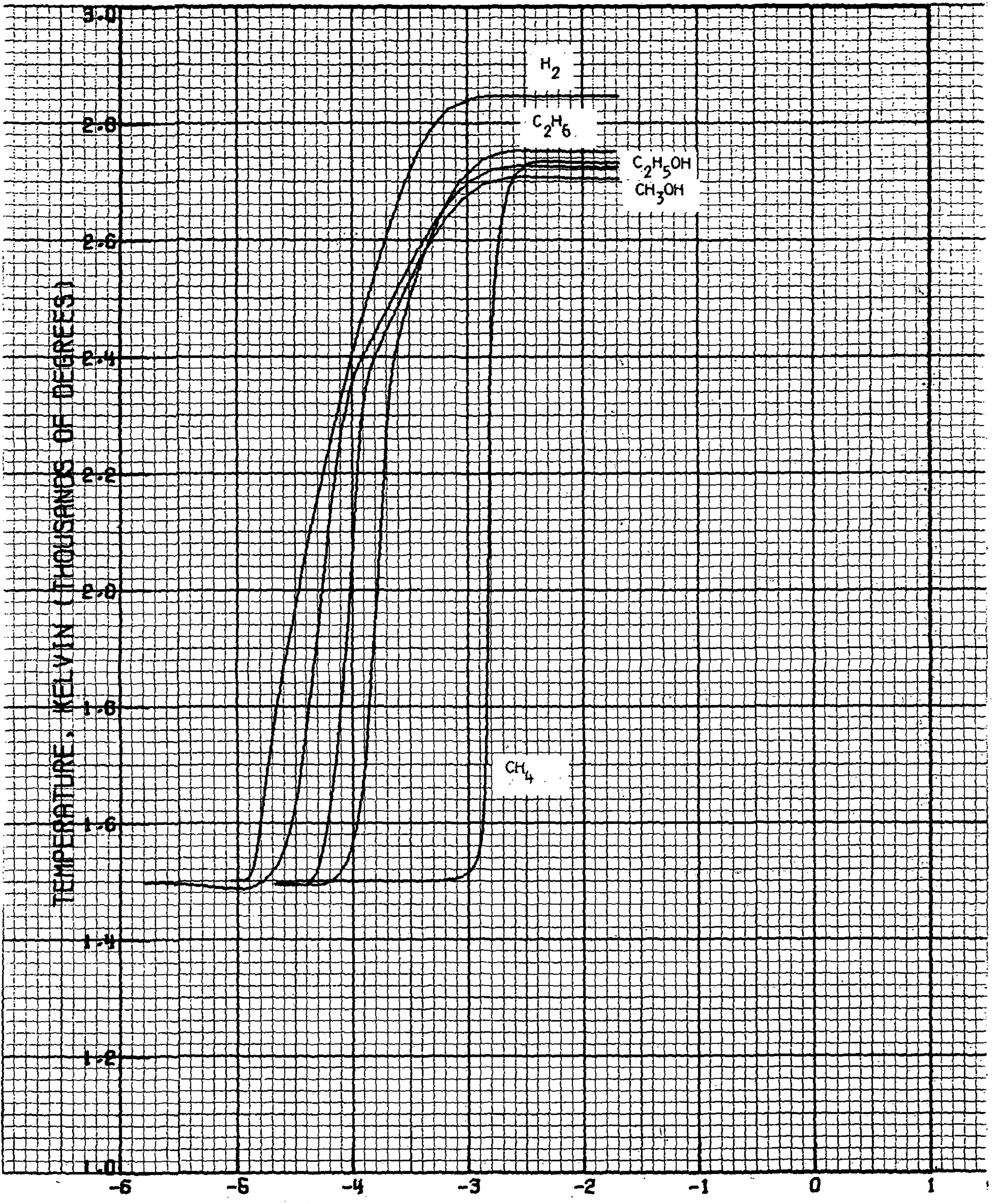

Figure 9. - Temperature as a function of time in combustion products of several fuels each dispersed stoichiometrically in air at 1500 K initially and reacting spontaneously at 1 atm.

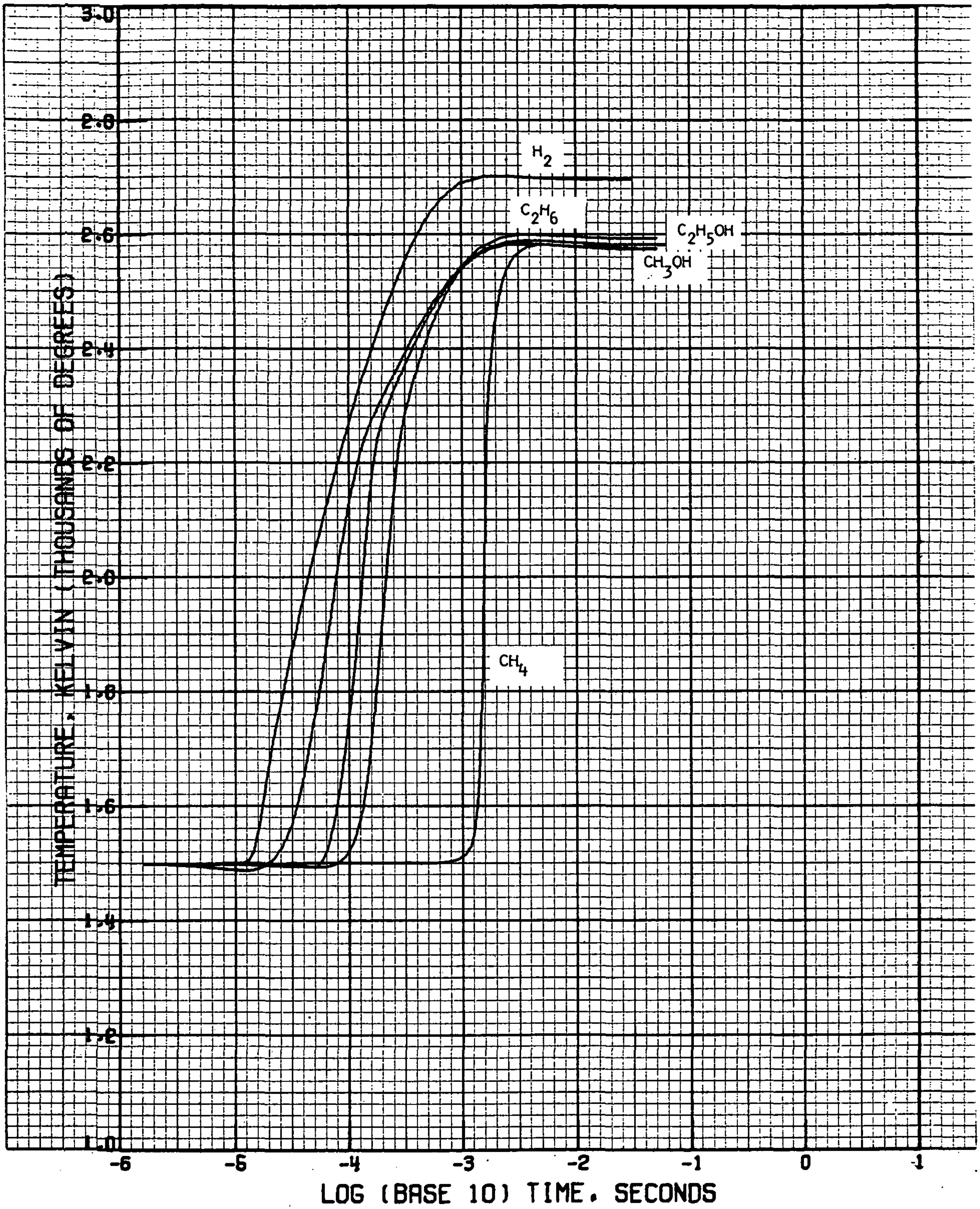

Figure 10. - Temperature as a function of time in combustion products of several fuels each dispersed in 2/3 of stoichiometric amount in air at 1500 K initially and reacting spontaneously at 1 atm.

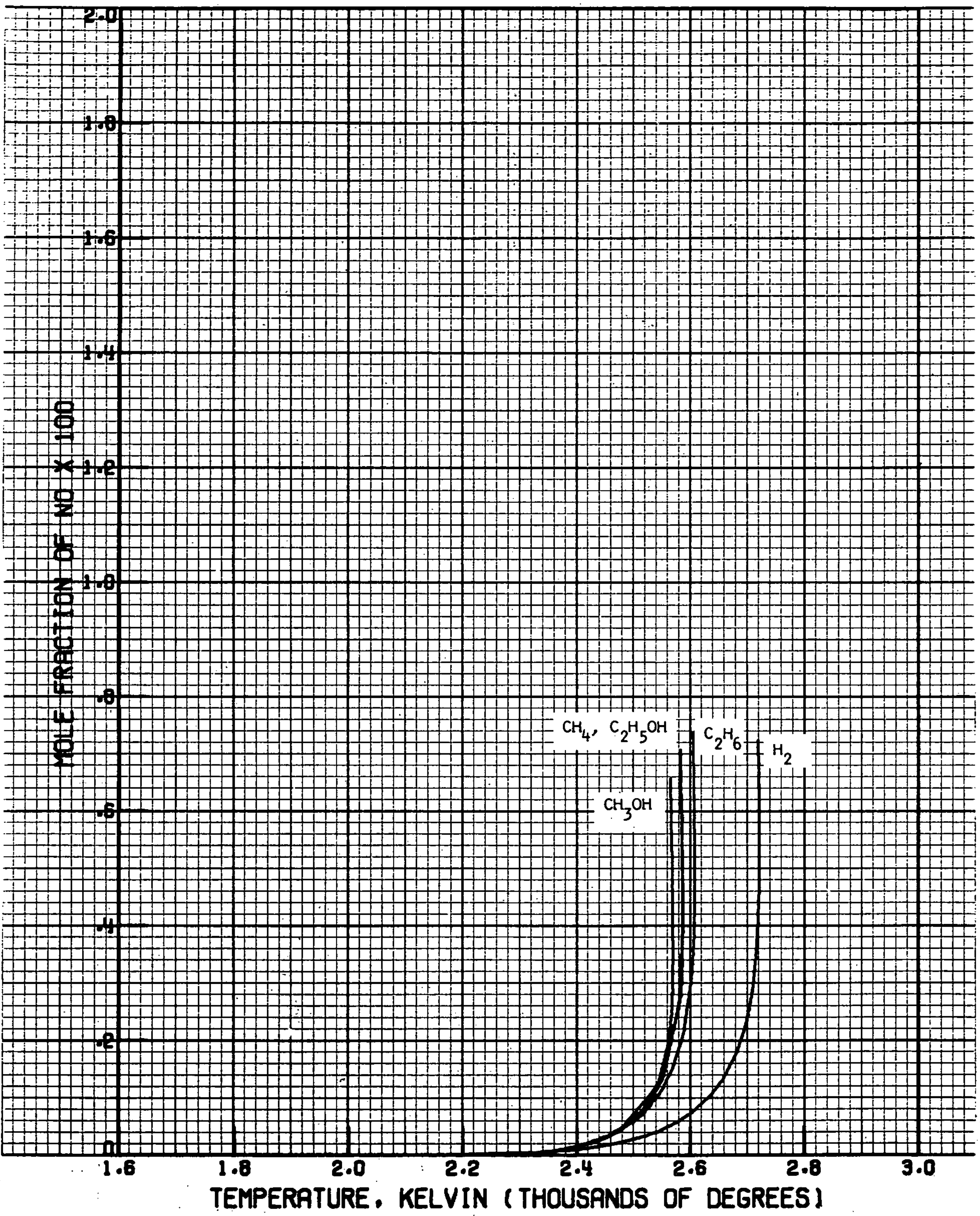

Figure 11. - NO Concentration as a function of temperature in combustion products of several fuels each dispersed stoichiometrically in air at 1100 K initially and reacting spontaneously at 1 atm.

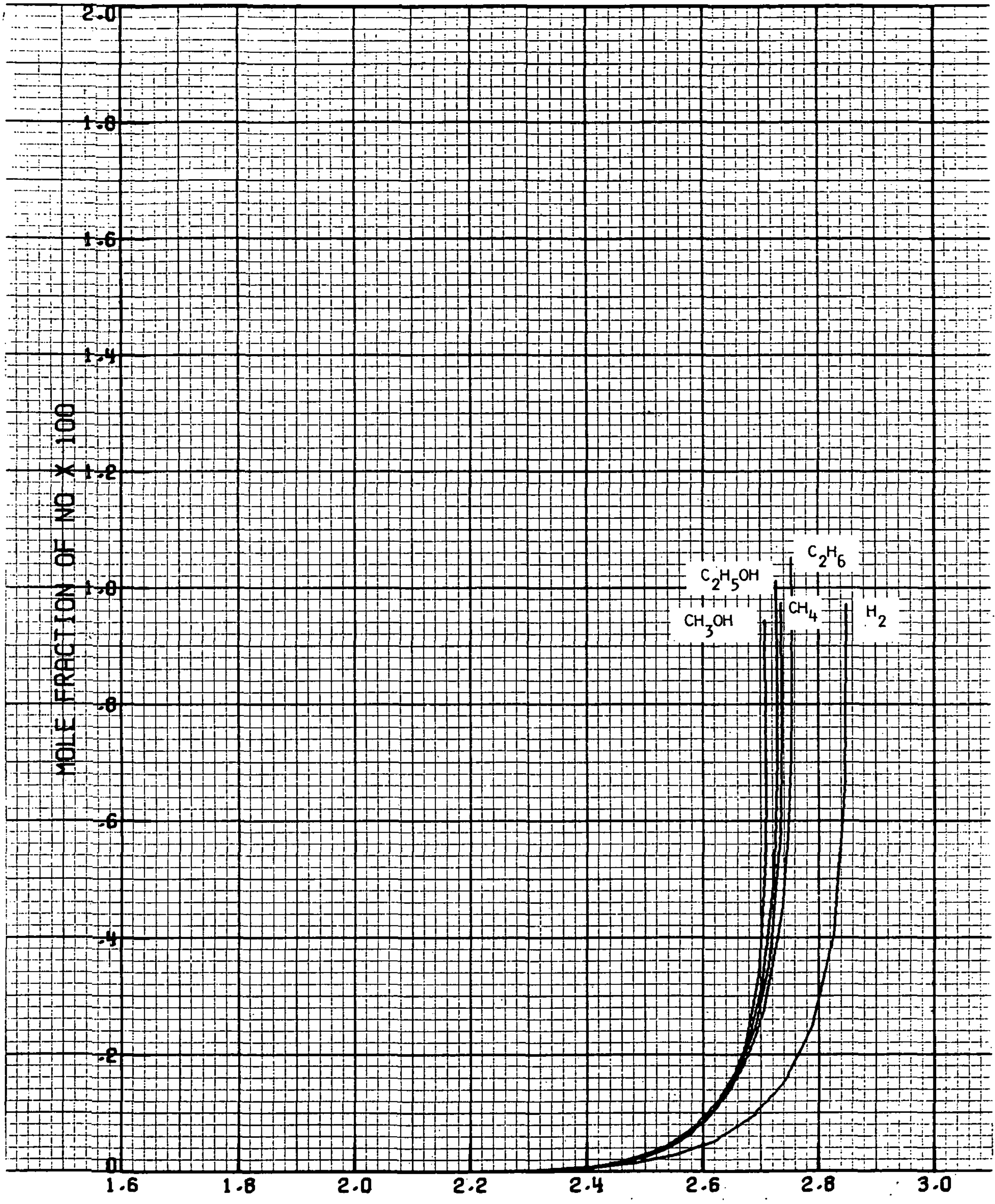

Figure 12. - NO Concentration as a function of temperature in combustion products of several fuels each dispersed stoichiometrically in air at 1500 K initially and reacting spontaneously at 1 atm.

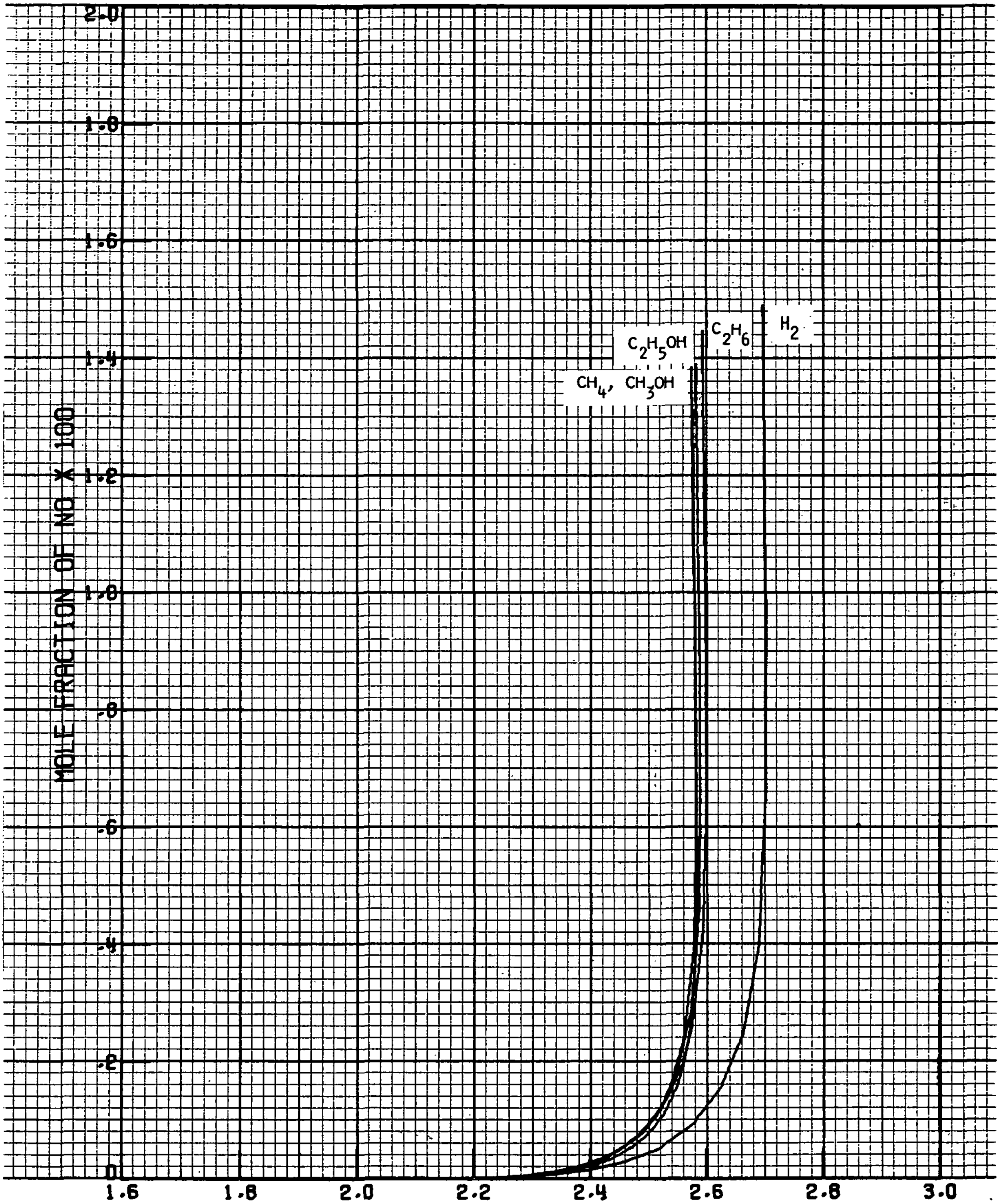

Figure 13. - NO Concentration as a function of temperature in combustion products of several fuels each dispersed in 2/3 of stoichiometric amount in air at 1500 K initially and reacting spontaneously at 1 atm.

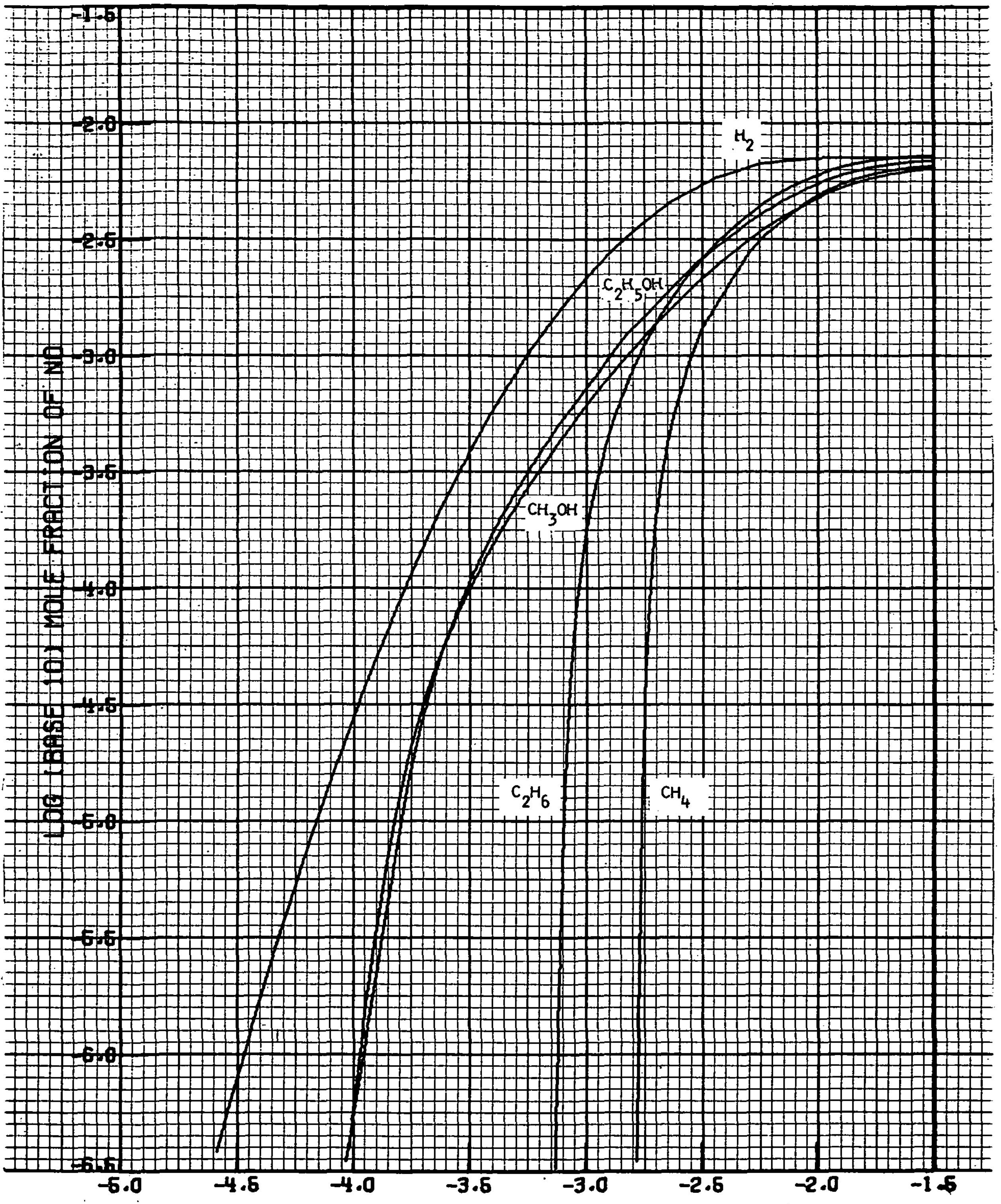

Figure 14. - NO Concentration (logarithmic representation) as a function of incremental time after induction in combustion products of several fuels each dispersed stoichiometrically in air at 1100 K initially and reacting spontaneously at 1 atm.

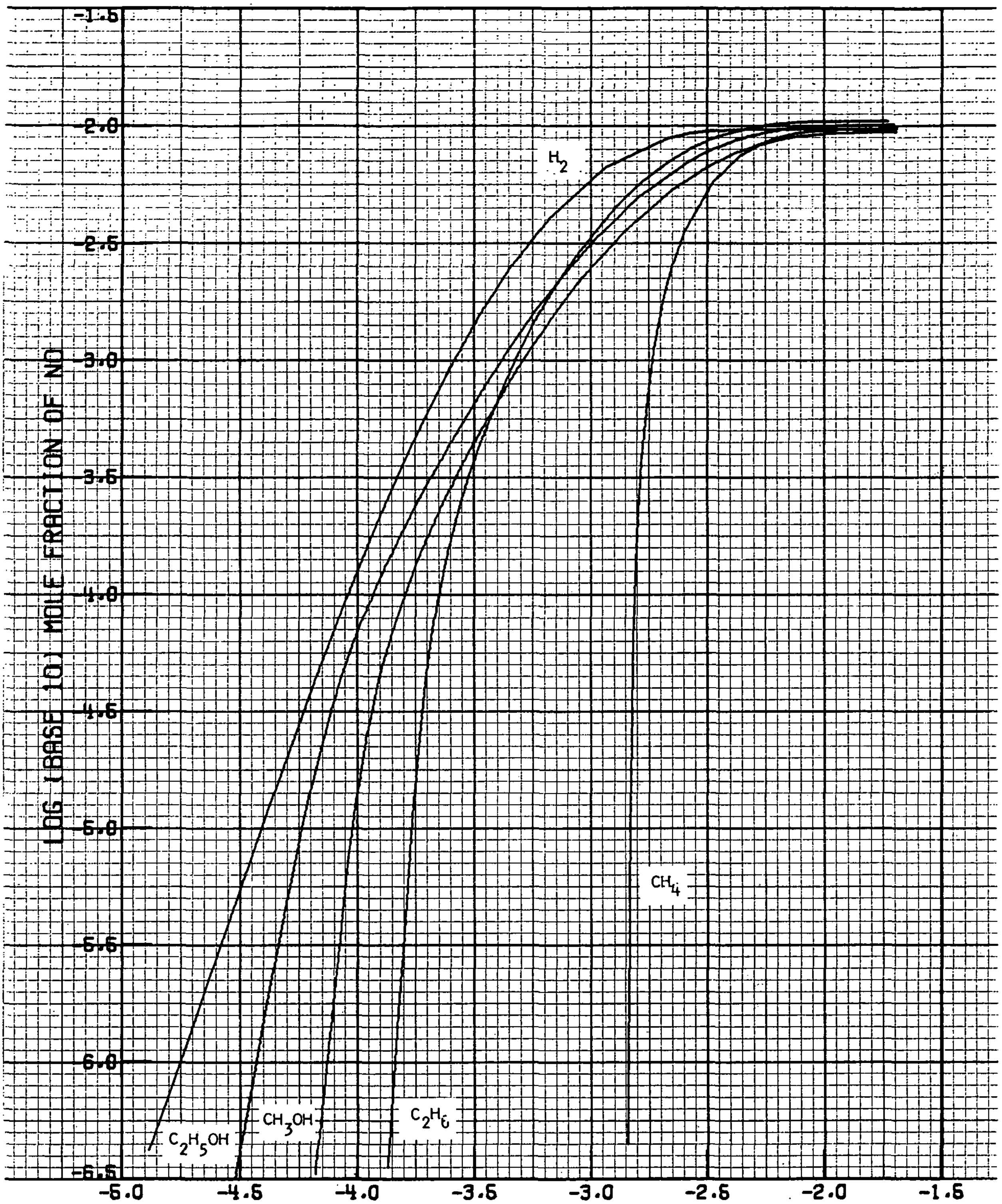

Figure 15. - NO Concentration (logarithmic representation) as a function of incremental time after induction in combustion products of several fuels each dispersed stoichiometrically in air at 1500 K initially and reacting spontaneously at 1 atm.

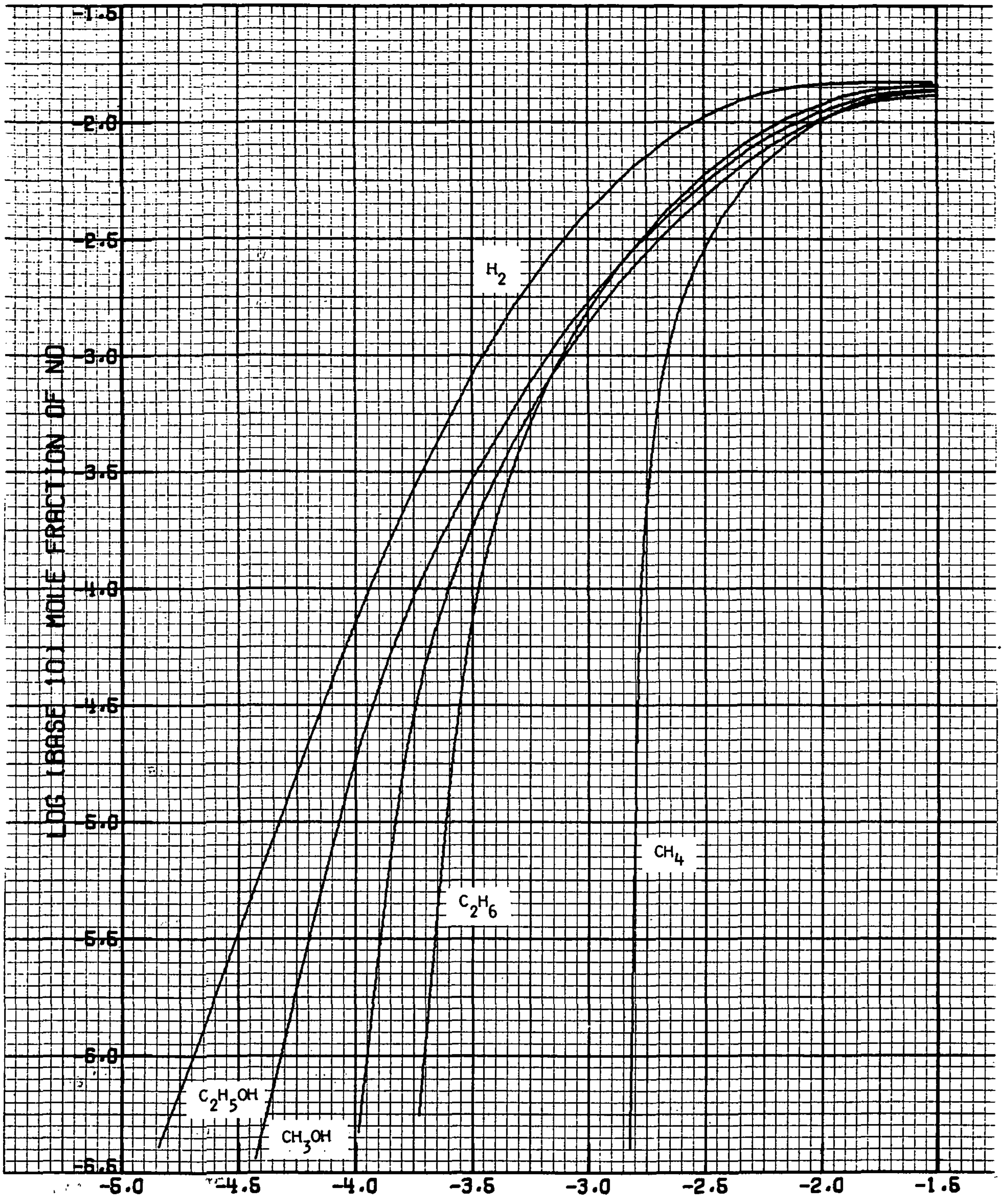

Figure 16. - NO Concentration (Logarithmic representation) as a function of incremental time after induction in combustion products of several fuels each dispersed in 2/3 of stoichiometric amount in air at 1500 K initially and reacting spontaneously at 1 atm.

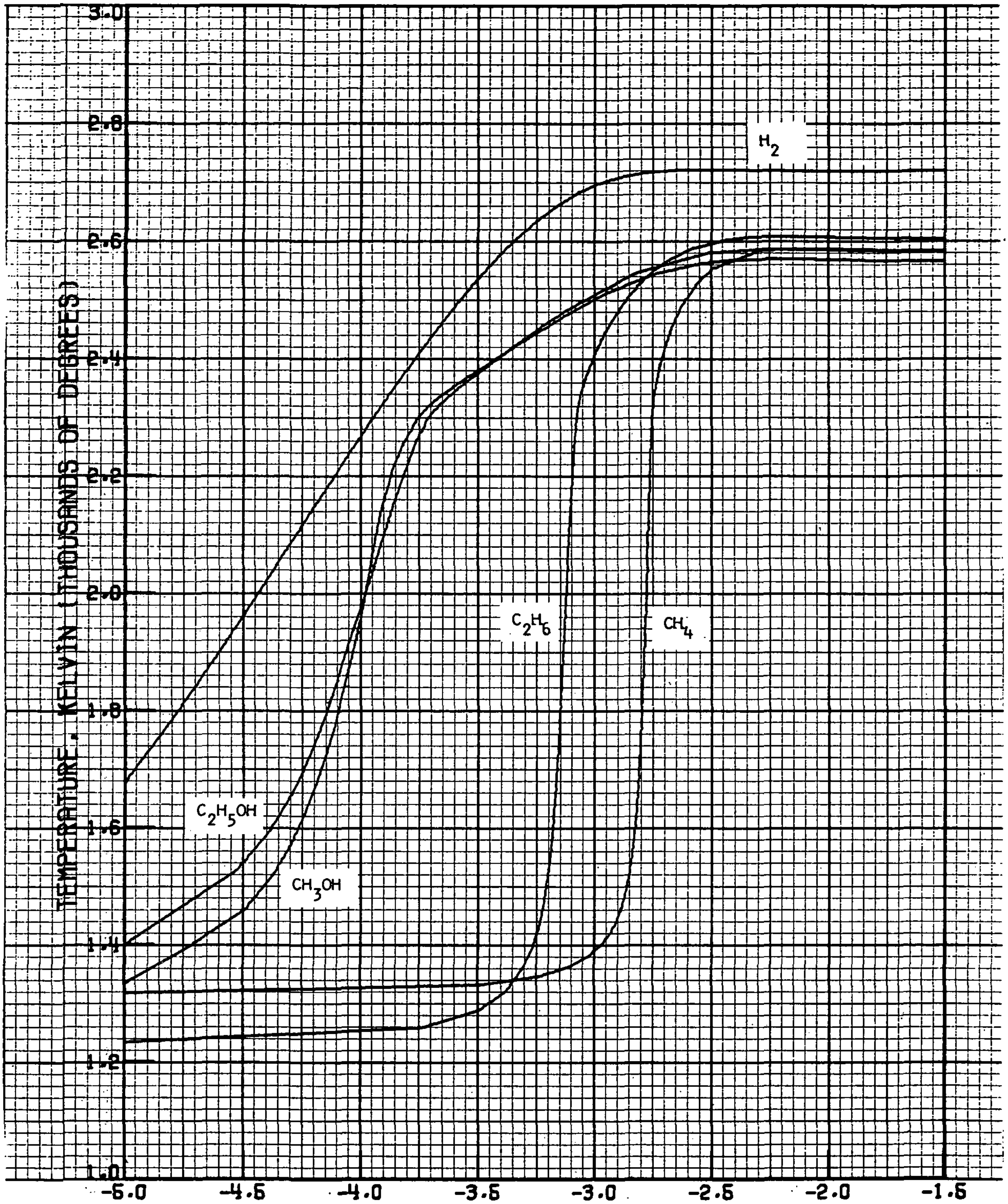

Figure 17. - Temperature as a function of incremental time after induction in combustion products of several fuels each dispersed stoichiometrically in air at 1100 K initially and reacting spontaneously at 1 atm.

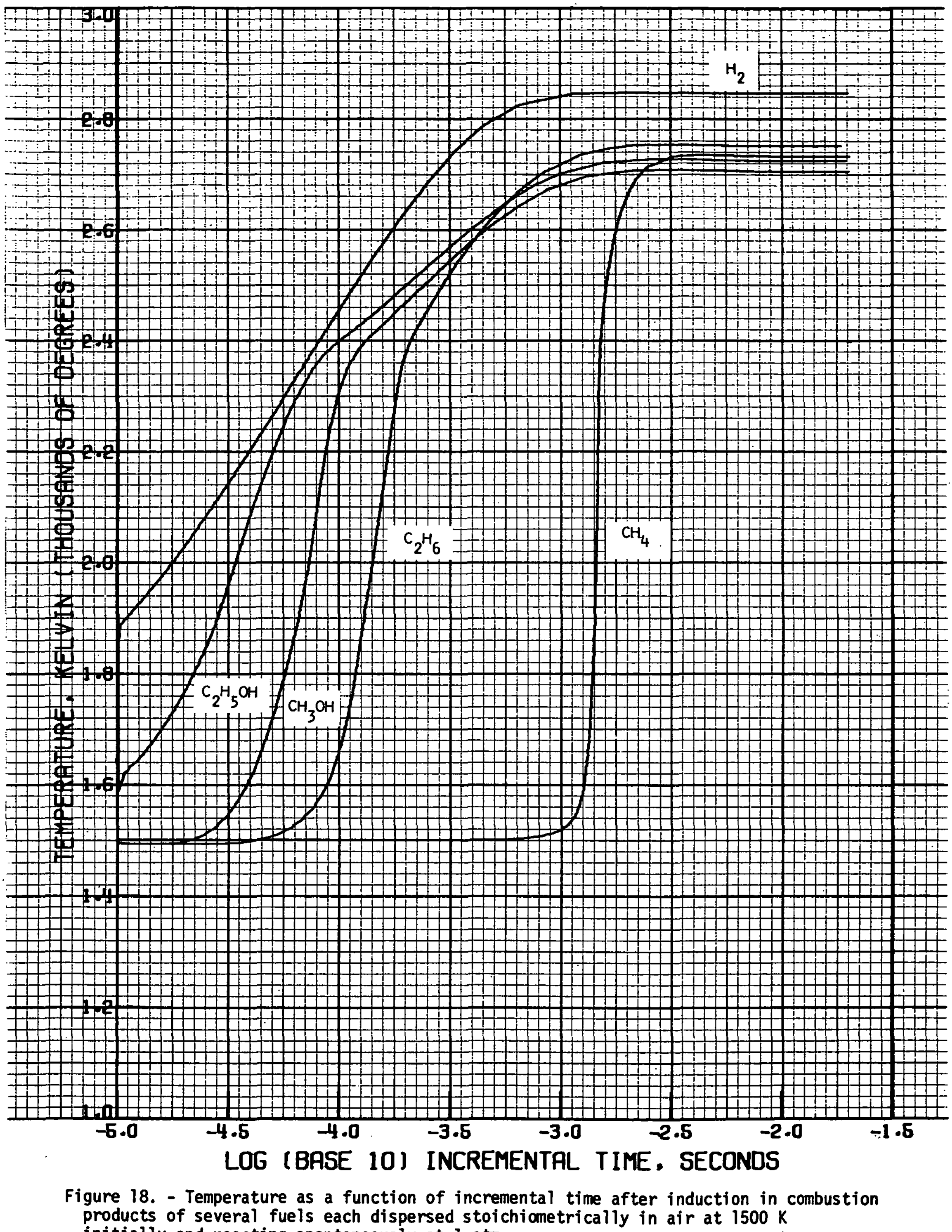

Figure 18. - Temperature as a function of incremental time after induction in combustion products of several fuels each dispersed stoichiometrically in air at 1500 K initially and reacting spontaneously at 1 atm.

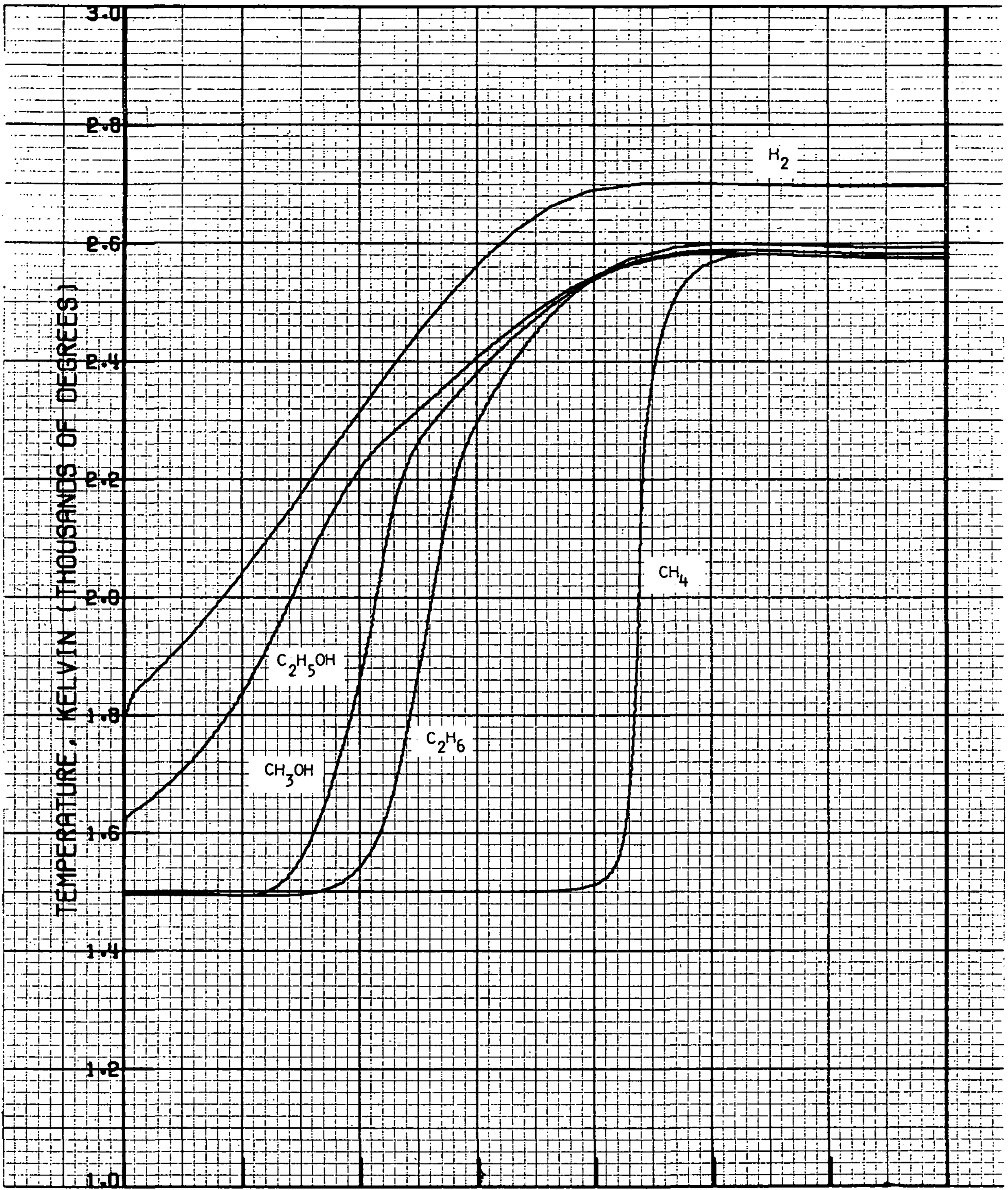

Figure 19. - Temperature as a function of incremental time after induction in combustion products of several fuels each dispersed in 2/3 of stoichiometric amount in air at 1500 K initially and reacting spontaneously at 1 atm.

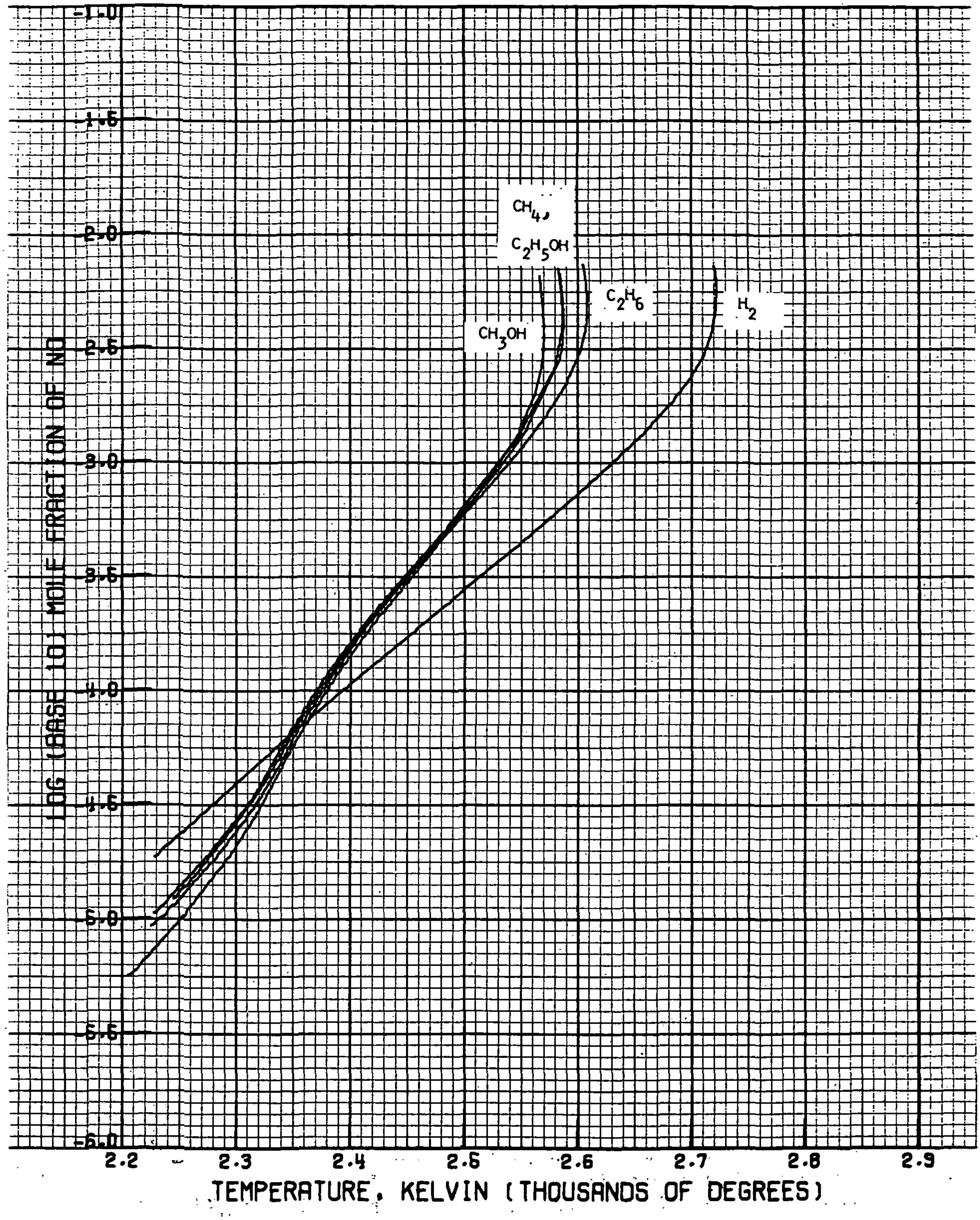

Figure 20. - NO Concentration (logarithmic representation) as a function of temperature in combustion products of several fuels each dispersed stoichiometrically in air at 1100 K initially and reacting spontaneously at 1 atm.

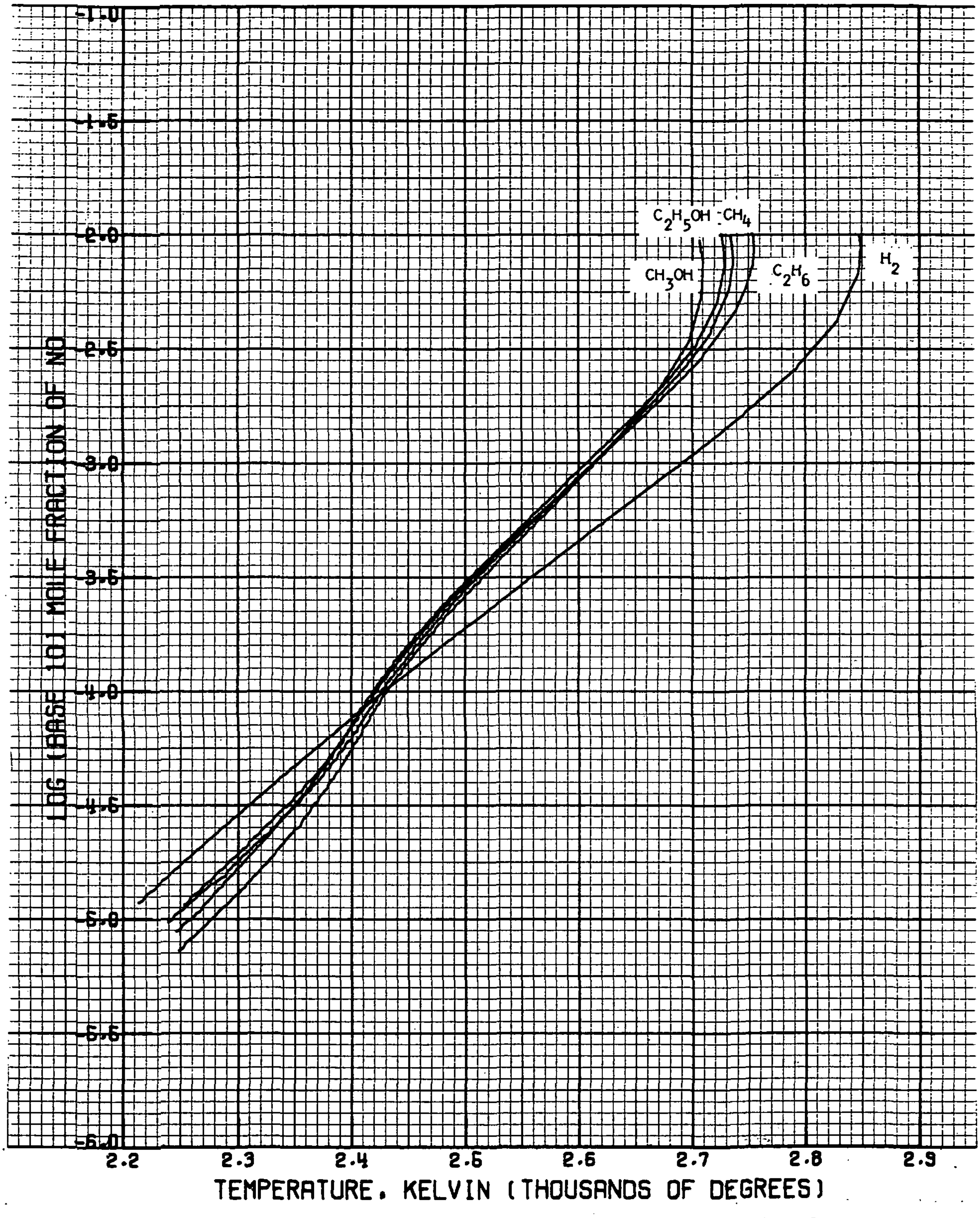

Figure 21. - NO Concentration (logarithmic representation) as a function of temperature in combustion products of several fuels each dispersed stoichiometrically in air at 1500 K initially and reacting spontaneously at 1 atm.

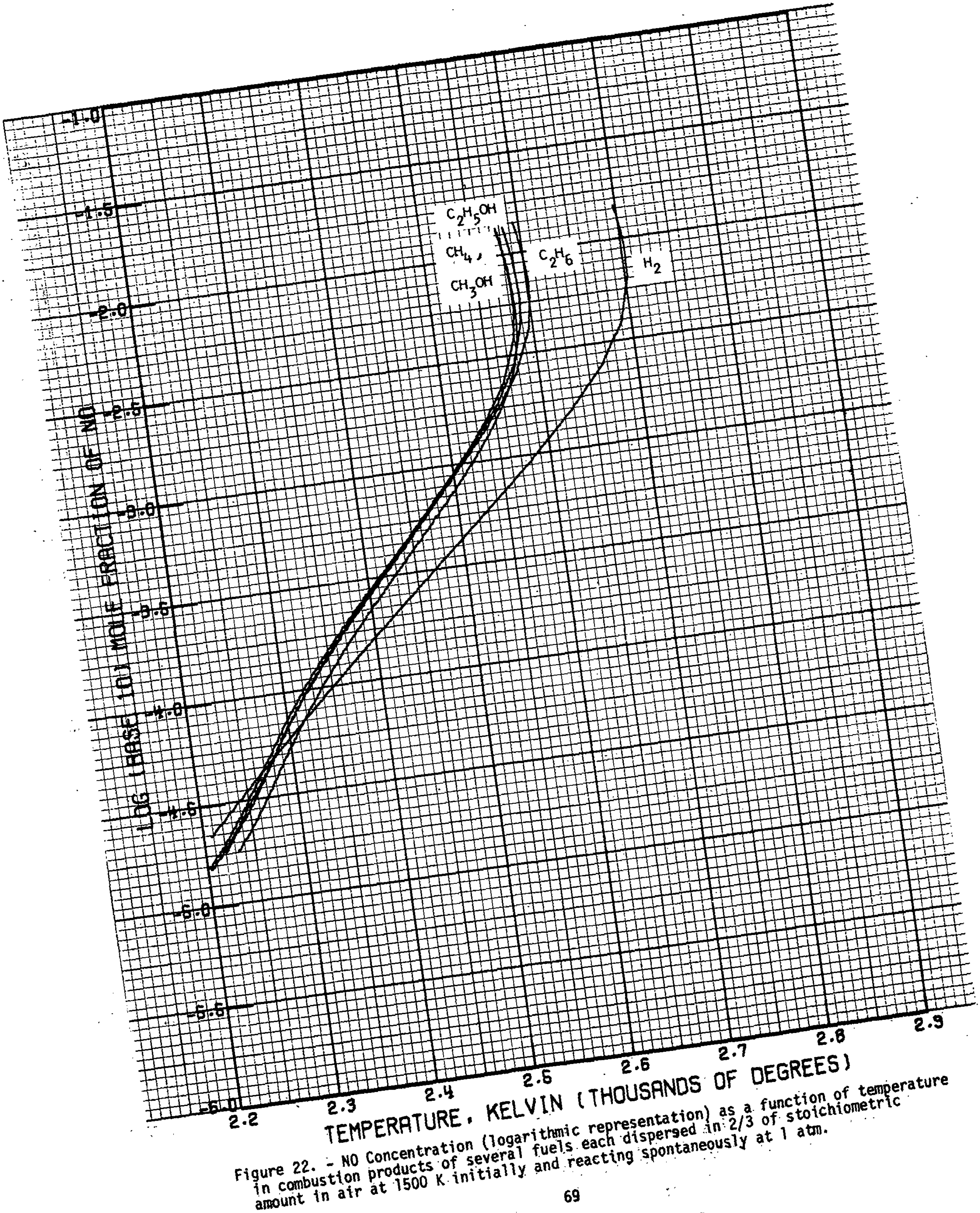

Figure 22. - NO Concentration (logarithmic representation) as a function of temperature in combustion products of several fuels each dispersed in 2/3 of stoichiometric amount in air at 1500 K initially and reacting spontaneously at 1 atm.

APPENDIX

Selection of a Package of One Hundred Reactions and Rate Constants for the Combustion of CH_4, CH_3OH, C_2H_6, and C_2H_5OH

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INTRODUCTION

The calculation of change of composition with time in a complex chemical system is a formidable problem. The problem is simplified if the temperature is held constant, which may be quite appropriate in chemical processing. However, this simplification is precluded in a customary combustion process, and the next simplest specification is adiabacity. With a homogeneous mixture, constant pressure, and constant enthalpy, one may consider reaction in either a system at rest or a control volume flowing at constant velocity. The important problem elements then are the pertinent physicochemical properties, mathematical techniques for solution of chemical changes, computers of size and speed to employ the mathematical techniques at reasonable cost, and suitable display and interpretation of results. All of these problem elements have acted in the past to inhibit progress. While all become more tractable with passage of time, it is important to recognize how they reinforced one another in the past to dictate approximate approaches. As the difficulties now become tractable, such approximate approaches become indefensible, no matter how astute they were under previous circumstances and no matter how much underlying exposition they provided for the general field of finite chemical kinetics. Ultimately, so much may be learned in the field that approximate approaches can be defined with assurance that the approximations are justified, not simply with hope and trust that they are; such a time is not yet here.

To move from the abstract to the specific, present computational capability will permit practical solutions to be obtained for hundreds of reactions among at least half a hundred chemical species. This represents significant accomplishment in both hardware and software areas. Reliable physicochemical properties are in short supply when measured against this computational facility, but estimates can be made, especially for members of families of chemical species when part of the desired information is in hand. Within the range of application of such partially validated properties, the biggest remaining stumbling block may be the human difficulty in extracting the significant results from a time-dependent calculation.

Contrast this kinetic situation with the case of equilibrium chemical calculations. In a complex system there is a step-by-step approach toward arriving at the answer. However, if the answer is equilibrium chemistry, the intermediate steps have no physical significance, only mathematical significance, and there is nothing for the engineer to learn about his chemical system by examining the intermediate computational steps. In the case of reaction chemical calculations, much along the way may be at least as meaningful as the final values. Furthermore, this is all dependent information, in that the computer program necessarily controls the integration step size internally. Thus, one must devise special controls merely to sample the intermediate data in a revealing manner, most likely after generating and inspecting the solution. This leads either to voluminous output (printout or punched cards) or appreciable utilization of computer tapes for storage, perhaps long-term storage. Nevertheless, while the burden on the engineer now to comprehend and elucidate what he has attained may be greater even than the burden in the past to devise tractable approximations, there really is no justification for ignoring the burden. One is not entitled to protest simply, "Well, that is what the computer says," unless the reaction data fed to the computer comprise a standardized tool. And that latter possibility has very rarely been realized as yet.

The purpose of this appendix, as almost a report in itself, is to present substantiation for the reaction data package employed for the substantive calculations of this report. There is a general tendency to question rates while accepting reaction schemes of record. Of course, in the limit it may be said that every conceivable reaction is valid as long as the assigned rate is appropriate; if the unlikeliest reactions are assigned rate constants slow enough to represent minimal likelihood, both concept and application are satisfied. It is an easy step from there to say that omitting a reaction from consideration is done on the basis of assigning a rate constant so slow as to make the reaction insignificant. However, this approach is acceptable only if the assignment of such a rate constant is deliberate. It is not defensible to exclude the reaction on some other basis and then to claim that assignment of effectively zero rate would obviously have precluded it from participation in the reaction scheme. However, this seems to be the line of argument implied frequently, especially when alternative reaction paths are reduced to just one favored path --whether really favored in nature, or only favored in the perspective and prejudice of the investigation.

A secondary path under one set of conditions may very likely become the primary path under other conditions. The following text will recount the selection of a set of 100 reactions for the combustion of CH_4, CH_3OH, C_2H_6, and C_2H_5OH. Even with the restrictions to be discussed, especially restriction to reasonably high temperature, it appears that the set is not really complete. Yet every one of the hundred reactions proved nearly enough competitive with the rest for at least one of the fuels, at some point in the progress of reaction, to warrant its incorporation in the reaction scheme, and the very great majority of them meet this criterion for at least three of the four fuels. This number of 100 reactions is so much greater than others have customarily assigned to date for such combustion kinetics as to influence the structure and scope of this report. It is certainly not claimed that this set of 100 reactions is a definitive solution. It is claimed that the set is closer to a definitive solution than previous sets, and that both experimenters and analysts should be guided by its details and by its inferences.

PRIOR EFFORT

Development by the author of pyrolysis and oxidation reaction data packages for hydrocarbons was initiated at The Marquardt Company in 1967. An early stage of accomplishment was reported in Reference 5, and an application was reported in Reference 6. Further exploratory work was done later at Langley Research Center in preparation for just the sort of study with which the main text of this report is concerned. The aim of the latter, unpublished effort was to assemble a reaction data package suitable for any one of a series of alkanes; the outcome actually was two such packages, one for combustion and one for pyrolysis. Computer storage requirements for representation and manipulation of species concentrations truncated the series at C_8H_{18} for pyrolysis and at C_7H_{16} for oxidation. The number of reactions provided for was 250, and, of course, allowance for important oxidation reactions in the oxidation package caused these to supplant some of the pyrolysis reactions out of the total of 250 comprising the entire pyrolysis package. The oxidation package is reproduced here as Table 1; discussion of the ingredient format is reserved until later.

It is perhaps important to note that these reaction packages did provide output data which were consistent for the family of alkanes considered. There were enough reactions for attack on any designated starting species, all within the prescribed limit of 250. Limitation to fewer, closely related alkanes would have permitted either fewer reactions to be employed, or a finer representation of the reaction chemistry to be made. However, it is also important to note that the lower alkanes, such as the lowest, CH_4, tend to produce higher alkanes as intermediate products, and the higher alkanes, such as C_7H_{16}, tend to produce lower ones as intermediate products. Pertinent to the present work is an earlier calculation for oxidation of C_2H_6, using the oxidation package of 250 reactions. Nontrivial mole fractions of C_3H_8, C_3H_6, C_3H_5, C_3H_4, C_3H_3, and C_3H_2 were calculated, as well as C_2H_4, C_2H_2, and C_2H. That reaction scheme also provided for creation and consumption of solid carbon (according to rate constants approximated by separate analysis and adapted to the requisite format of the general kinetics computer program, FINEK).

These earlier calculations were made with a very few rate constants extracted from the literature, but almost all estimated in a systematic manner in the absence of any literature values. It was an appreciable effort to advance to the stage of internally consistent results which displayed reaction time versus starting temperature generally consistent with natural experience. The attainments provided a starting point for further work which would seek to relate results to specific experimental information.

It has been stated earlier that a computer at present can handle hundreds of reactions among upwards of 50 chemical species. However, running times are rather long, and so the earlier pyrolysis and oxidation runs were made piecemeal, with several restarts. In the present work it was deemed desirable to restrict the problem to 100 reactions among 30 species, so as to yield a reasonable computer storage requirement and reasonable running times. Reactions permitting the formation of solid carbon (or, of course, its consumption) were arbitrarily excluded. In all respects except direct interest in solid carbon, this is a minor distortion in a normal combustion case. Earlier work at the Marquardt Company on the formation of solid cargon had demonstrated the importance of CH_3CO and C_4H_2 in the reaction scheme; allowance for formation and consumption of these species provides alternate reaction paths so that inordinate formation of solid carbon does not occur. (Reference 7 deals with part of this work.) With C_4H_2 able to be omitted, another species, C_2HO, involved in its consumption, also could be omitted. Thus, 7 species (CH_3CO, C_2HO, C_2, solid C_2, CH, C, and solid C) which earlier had been considered, were omitted in assembling the reaction package of present interest, besides the arbitrary exclusion of all C_3, C_4, C_5, C_6, and C_7, species. It should be noted here, as well as being restated later, that exclusion of C_3 species would have most significance for C_2H_6, among the fuels being considered. This is so because the C_3 species form essentially from C_2H_6, among the fuels considered, and the prior formation of C_2H_6 from one of the other fuels is a necessary step, of limited scope, in such an alternative case.

Five species not incorporated in the general treatment of alkanes were added for the present work, N and NO obviously for the direct purpose of the study, and the other three (CH_3CHO, C_2H_4OH, and C_2H_5OH) to deal with one of the chosen fuels, C_2H_5OH. Early in the work at the Marquardt Company, C_2H_5OH had been provided for as a combustion intermediate but had been found to appear in only trivial amounts. Its presence as the fuel, of course, constituted an entirely different matter.

Tabulated below are the distinctions in species considered, between the earlier and present work:

Omitted from earlier work but included in present.	Omitted from present work
N	Solid carbon as C
NO	C
CH_3CHO	CH
C_2H_4OH	Solid carbon as C_2
C_2H_5OH	C_2
	C_2HO
	CH_3CO
	C_3 species, etc.

These distinctions are noted here so as to institute a measure of restriction on the general applicability of the reaction package used in the present work. The earlier package is still considered more fundamental, but subject to certain amplification to increase its scope (as the five new species attest) and to certain revision of reactions and rates (as will be discussed).

DEFINITION OF REACTION PACKAGE

When a great many changes have been made on a trial-and-error basis in moving from one model to another, a faithfully detailed record of the sequence of trials may provide a less satisfactory exposition of the situation than a cursory treatment. The present situation has involved evolution of two models, and also merger of the two, and would be extremely complicated to record in detail. Thus a cursory treatment will be employed. One evolution was the progression from the earlier alkane oxidation data package (suitable for alkanes up to C_7H_{16}) to a more restricted package, one which nevertheless is also suitable for CH_3OH and C_2H_5OH. The other evolution was the progression from an earlier oxidation data package specific to CH_4 (and substantially consistent with the general alkane package) to a refined package which is in substantial agreement with reported experimental data. The ensuing discussion will include a report on the adjustment of the CH_4 package for reconciliation with experimental data. All of the rest of the evolutionary changes made in arriving at the reaction package which has been applied to the NO problem are immaterial taken one by one.

The reaction package finally decided upon for the output calculations is recorded in Table 2, which has the same format as Table 1. The 100 reactions are serially numbered, as assembled, along the left margin; these numbers are used subsequently for indexing. The permanently assigned reaction numbers appear along the right margin. (Reaction 19.1 in Table 1 is not the same as Reaction 19.1 in Table 2.) Across the line between the two reaction numbers appear the reaction and its assigned rate constant coefficients, A, b, and E in the equation

$$k_f = AT^b e^{\frac{-E}{RT}}$$

with R = 1.98726, T in degrees Kelvin, and k_f in either cm^3/mole-sec for a unimolecular reaction or cm^6/$mole^2$-sec for a bimolecular reaction. The first six reactions in Table 2 are bimolecular dissociations/termolecular recombinations of the hydrogen/oxygen system, and the termolecular third body is designated by M (as in subsequent reactions of this type). In the past, specific third-body efficiency factors had been assigned to these first reactions (and were actually used in conjunction with the earlier package shown in Table 1); however, all such factors were set to unity for the present work as a simplification in comparing to certain other calculations.

The experimental data employed as benchmarks for adjustment of the CH_4 reaction package appear in Reference 8. Early efforts benefitted from comparison with theoretical calculations reported in the reference, and considerable assistance was afforded by correspondence with Dr. Gordon B. Skinner, the first-named author. Skinner expressed 23 reactions in the reference, but in the terminology of this report there were 21; the extra two represented the only two instances of imposition of a third-body efficiency factor other than unity (with H_2O as a particular third body in two recombinations). Skinner represented the third body otherwise as argon, and assigned reaction rate constants accordingly. This was the basis for the assignment of third-body efficiencies all of unity, referenced to argon as the standard, in the present work.

Skinner introduced one particular reaction with an arbitrary rate constant and adjusted the originally selected rate constants for several others, so as to achieve generally satisfactory reconciliation between the data available to him and the calculations he made. He compared ignition induction times under various conditions at initial temperatures of 1600, 1800, and

2000 K. His calculational determination of this time was the point of maximization of the rate of temperture rise, and the same criterion was, of course, used for the comparative calculations of this report, made at some of the assigned conditions which he studied. For the conditions considered, such maximizations were found at points of very substantial temperature elevation There is no argument made here against the criterion, a simple and useful one, but in common parlance the points were well above what might have been anticipated as "ignition" temperatures.

Skinner also compared calculated and experimental product distributions for reactions initiated at temperatures ranging downward from 1600 K and then quenched. A certain one of these was also calculated for comparison in the presently reported work; the quantity of pertinent experimental data available was quite limited.

Starting with an initial reaction package for CH_4, revisions of both participating reactions and assigned rate constants were made seeking reconciliation with the corresponding experimental data. The first efforts dealt with the autoignition times, and the following efforts with the intermediate product distributions. As noted, Skinner's own calculational results served as a sort of monitor on the work, especially in depicting something of the degree of consistency that might be achieved.

The particular objective was to define a reaction set consistent with general rules, and to assign rate constants consistent with general rules, so that these rules might be extended to other fuels with some confidence. The rate constants for the restricted hydrogen/oxygen/nitrogen component system (18 reactions) were held inviolate, and also those for three reactions of CO where literature data were available. For all the rest of the reactions considered, the progress of work led ultimately to doubling of the assigned rate constant, as compared to initial estimation according to the method reported in Reference 9. This was the only adjustment made in rate constants, and whereas it was made consistently, the desire to adhere to general rules was sustained. (Note that the coefficients A in Table 2 reflect this doubling, made by the computer program immediately after the data are read in; the data cards read in were not themselves adjusted.) The great scope of the work of adjustment thus dealt with addition or subtraction of particular reactions, addition to permit an alternate reaction path and deletion to forestall an alternate path because second attention to an important reaction decided it to be sterically improbable.

(The indicated doubling of rates, and especially the deletion of sterically improbable reactions, are the principal modifications to be made if one were going back to the original reaction package of Table 1 to adapt it to other application. Of course, a line-by-line comparison between Table 1 and Table 2 would be necessary to ensure improving the former by adding all of the experience of the latter. Documentation toward this end was not a part of the work reported here, and thus in its absence it can only be emphasized that one would need to reinvestigate the deletions made from Table 1, through C_2H_6 as the highest species, i.e., through Reaction 17.7, in evolving Table 2. Some of these deletions were for triviality, which might not prevail under other conditions, while some were for steric considerations of general significance, where a sterically improbable reaction falsely exhibited an important influence.)

Table 3 records the experimental and calculated ignition induction times. The results of the present study differ from the experimental values a little more, generally, than do Skinner's results, but the biggest percentage deviations are Skinner's in Series 2C. For these calculations, the evolving reaction package for CH_4 was used. It did not contain the 28 reactions involving CH_3OH, CH_3CHO, C_2H_4OH, and C_2H_5OH which are in the full reaction package of Table 2. Also, it did not contain the three reactions for production of NO. The package contained 72 reactions, so that with the addition of the above 28 plus 3, three relatively minor reactions had to be removed in finalizing on 100 reactions in Table 2. Those removed were:

10.7 $CH_4 + HCHO = CH_3 + CH_2OH$;
16.5 $CH_2 + CH_2OH = O + C_2H_5$;
16.6 $CH_3 + CH_2OH = C_2H_5 + OH$.

After the final package of 100 reactions had been defined, three of the points of Table 3 were recalculated. These results are the parenthetical numbers appended to Table 3. The changes were noticeable, but tolerable. Taking the changes into account, one might wonder whether the doubling of most of the reaction rate constants was really appropriate, but this point was not pursued in calculation, and there is further discussion below. All in all, the final package of 100 reactions (with the doubling) was deemed reasonably to represent the real situation for autoignition of CH_4.

The other comparison with experiment was that made for concentrations of intermediate species. This constituted the most demanding restraint in evolving the final reaction package, despite the fact that there are very few data of this kind to work with. Comparative values are recorded in Table 4. (Bahn's results were repeated by the full set of 100 reactions;

i.e., they correspond to both induction times recorded for Series 2C at 1400 K in Table 3.) Substantially, of course, the meaningful comparisons are between a calculated value and the corresponding experimental value, and not between Skinner's and Bahn's results. For H_2, Bahn's value is one-third as great as the experimental number, while Skinner's is three times as great. For C_2H_6, both calculated values are half of the experimental number. For C_2H_4, Skinner computed no participation in the reaction scheme, whereas Bahn computed a value close to the experimental number, depicted either as within 0.00001 mole fraction, or differing by a factor of 1.5. If Skinner's results are taken as a criterion of the degree of agreement that may be hoped for, Bahn's results are favorable ones. It bears reiterating that many trial revisions of the reaction package were required to achieve this degree of agreement with the experimental data.

Because of interactions in a complex chemical system, one cannot expect certainty in the effect upon the overall reaction time of a general adjustment of the rates. However, a trial calculation was made at 1400 K with the CH_4 package of 72 reactions wherein the rates for the final 54 reactions were not doubled. The computed autoignition time was 7.765 milliseconds, nearly twice the time shown in Table 3 obtained with doubling. Quite naturally, the mole fractions of intermediate products at 0.7 milliseconds were much less than those shown in Table 4. This emphasizes the difficulty in adjusting a reaction package for reconciliation with experiment: one requires consistency of relative values of mole fractions, one to another, and of absolute values related to the intermediate time of concern, and also consistency in the much longer autoignition times. It is unfortunate that there is not an experimental autoignition time available for Skinner's

Series 1C point initially at 1400 K. Extrapolation to 1400 K of his three points at 1600, 1800, and 2000 K, plotted as logarithm of time versus reciprocal of temperature, predicts an autoignition time of 2.6 milliseconds, which is not greatly different than the value of 3.6 milliseconds calculated with the package of 100 reactions and given parenthetically in Table 3. This situation argues for the adjustment (i.e., doubling) of the rates.

The degree of reconciliation between calculation and experiment that has been attainted for CH_4 is certainly not all that one would desire. Doubtless there are further complications to the overall reaction beyond those expressed by the package of 100 reactions. For example, 17 of the 28 reactions added for CH_3OH, CH_3CHO, C_2H_4OH, and C_2H_5OH proved of some significance for the oxidation of CH_4, whereas it had not been envisioned that any of them would do so. This point is discussed further below.

At this stage of the discussion, the following claims are made:

(1) a package of 100 reactions has been composed which provides results more or less consistent with experimental data for CH_4;

(2) the package encompasses the reactions deemed sterically acceptable (there is discussion on this point subsequently), and found by trial and error to be prominent in the oxidation of CH_3OH or C_2H_5OH;

(3) the package provides for oxidation of C_2H_6, but with fewer participating species and fewer reactions directly involving C_2H_6 than had previously been arrived at in defining the earlier, larger package of Table 1;

(4) general rules were followed in composing the present package, and no species nor reaction (and rate) has been included which, so far as

is known or can be foretold, would offend if the package were applied to other operating conditions, or would offend if the package were incorporated into a larger package to deal with other fuels.

The importance of single reactions being absent or present in the reaction package is emphasized by various autoignition times calculated for Skinner's Series 1C point at 1400 K. A package of 61 reactions yielded a time of 28.3 milliseconds. Addition of Reaction 8.1,

$H + HCHO = O + CH_3$,

reduced the time to 13.7 milliseconds. Then the further addition of Reaction 5.4,

$HCHO = H + HCO$,

reduced it to 7.2 milliseconds. One more addition,of Reaction 16.2,

$CH_3 + CH_4 = C_2H_5 + H_2$,

reduced the time to 4.2 milliseconds. Then the addition of 11 more reactions, and the removal of three, served only to increase the time by the slightest amount, to 4.3 milliseconds. The reactions removed were three trivial ones involving HO_2 in the limited hydrogen/oxygen system. Three of those added were the three finally removed in arriving at the package of 100, namely 10.7, 16.5, and 16.6. The others added were important to the distribution of intermediate products (as reported in Table 4), and thus perhaps important to the autoignition time under other conditions, despite their lack of influence on the time for this particular operating point. For the record, these eight reactions were 3.1, 3.10, 7.1, 7.4, 7.5, 7.6, 7.7, and 7.8; their identities may be read in Table 2.

One other comparison ought to be reported for the record. This was a calculation made with a revised rate constant for Reaction 10.1. Dr. Skinner kindly provided information which permitted evaluation of the rate constant for the unimolecular decomposition of CH_4 at specified temperature and pressure, dependent upon excitation by bimolecular collisions. The undoubled/doubled pre-exponential factors for Reaction 10.1 per Table 2 stood approximately in the following relationship to the corresponding value for 1400 K and 10 atm implied by Skinner's information:

A undoubled: Skinner: A doubled = 0.8:1:1.6.

The standard pre-exponential factor thus was divided by (approximately) 1.6 and the point was recalculated with the package of 100 reactions. The resulting autoignition time turned out to be 3.483 milliseconds, slightly less than the reference value appearing parenthetically in Table 3. This result is significant on two counts: (1) slowing this one reaction actually speeded the overall reaction rate, and (2) for the chosen operating point of the calculation, the unimolecular rate constant predicted from general rules came very close to the value actually imposed by a fundamental treatment of some particular data acquired and analyzed by Skinner. (It should be noted that, since Skinner's treatment has a temperature dependence, aligning the pre-exponential factors at 1400 K means some ensuing misalignment with rising temperature, but this is a situation of little importance for a process dominated by a nearly isothermal induction.)

DISCUSSION

The remainder of this appendix is concerned with reporting and discussing the importance of all of the 100 reactions of the final reaction package of Table 2. It should be noted that the results may suffer from limitations of data on chemical thermodynamic properties. On this point, the reader is referred to Reference 10. The data used are believed to be the best available, and any recommendations for improvement have been invited in Reference 10, so this potential problem will now be tabled in the present discussion.

It is believed that none of the reactions in Table 2 is sterically improbable, i.e., none would have a frequency factor orders of magnitude less than might otherwise be estimated without configurational difficulties. It is also believed that the estimated rate constants for the reactions are approximately valid. As has been stated earlier, all 100 reactions are calculated to be of significance to at least one of the fuels considered, somewhere during its course of combustion. This claim, which will be substantiated below,* should lead either to marked expansion of perspective for this sort of calculation, or else to specific refutations of estimated rate constants or chemical thermodynamic data used here.

Each reaction has been graphed from punched cards prepared during the calculation, all to the same scales. Numbering of the 100 graphs is identical to the numbering of the reactions in Table 2. Table 5 helps to read and interpret the graphs, as will be discussed below. For easy reference, the five fuels are numbered as follows: 1 is C_2H_5OH, 2 is C_2H_6, 3 is CH_3OH, 4 is CH_4, and 5 is H_2. The "rates" used to graph and tabulate results are logarithmic representations of net rates, whether net in the reaction direction implied in Table 2 (the endothermic direction) or in the reverse

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* See the point where treatment of reactions 41, 61, and 67 is made.

direction. The rates are all artificially increased by a factor of 100 (i.e., logarithm plus 2) over the values output by the calculations, so as to simplify the scale range of the figures; "rates" falling below the ordinate base of the graphs simply were not punched onto output cards.

For the abscissa, "progress of reaction," a convenient pictorial representation was devised. The maximum number of "rate" values output for any of the 100 reactions was used in fixing the basic increment of the scale. The logarithm of this number was divided into the scale length of 7 inches, and this provided the scale increment per unit (logarithm of number of values) for this fuel. Thus each fuel, with a different maximum number of reaction rate values, had its own increment. Then for any reaction, the logarithm of the number of values for that reaction dictated the total distance to be graphed along the abscissa. A reaction prominent during almost all of the calculation thus would extend over very nearly all of the abscissa. The total distance used was divided equally among the number of values to be graphed. As a hypothetical example, assume 100 values as the maximum of any reaction for fuel 1, so the scale increment would be 7.0/log(100) = 7./2. = 3.5. Now assume a reaction with 10 output values, so the scale length used for this reaction would be 3.5 x log(10) = 3.5 x 1. = 3.5; with 10 values, the increment per value would be 3.5/10 = 0.35, so each value would plot another 0.35 inches from the axis. In this way, the reactions with few values were displayed reasonably well across the graph, yet the reader can appreciate that these reactions were prominent over only a limited portion of the overall progress of reaction.

It is emphasized that these graphs have been prepared for simple display of the reactions, not for numerical interpretation. Over the full progress of oxidation of the fuel, some reactions dictate very small step sizes in the calculation, while others predominate where the tolerable step size is large. Thus there is no ready means of selecting appropriate abscissa scales for individual reactions, but also no need to do so for the approach selected. The reader should only keep in mind that the graphs are all left-adjusted, and that a vertical termination of the plot on the right-hand side implies that the reaction was still of significance when the calculation was terminated.

A few of the graphs exhibit pronounced fluctuations. This is attributable to relaxed tolerances in the convergence of calculational increments. Suitable solutions can be obtained from Program FINEK with some "bouncing around" of the concentrations of some intermediate species; if produced in excess in one increment, they are consumed in excess in the next, and the net effect is tolerable despite the appearance of gross instability.

As stated earlier, Table 5 provides a key to interpreting the graphs in terms of the individual fuels, by recording the maximum "rate" for each fuel, for each reaction. By noting the peaks of the four or five plots on a graph (fewer plots if the "rate" as shown by Table 5 never achieved zero value), and the ranked "rates" in the table, one can see which plot applies to which fuel. This has been felt to suffice, rather than crowded labelling on each graph. Futhermore, examination in detail of the graphs is left to the reader, in preference to tedious discussion of them singly. Collectively they show the importance of all 100 reactions.

Two other tables supplement Table 5. The first, Table 6, presents the average, for the four or five fuels, of the maximum "rates" for the given reaction, and the average of the corresponding temperatures. It also shows the individual values, as differences, which differ most from the averages, and identifies the fuels concerned. Table 7 presents the ranked temperatures corresponding to maximum "rates" for each fuel, for each reaction. For the first 18 reactions, where H_2 is involved in the comparison, H_2 provides the highest "rate" in every case except one, and in most cases at the lowest temperature, demonstrating some of its singular characteristics as a fuel. The average values, maximum "rate" or corresponding temperature, also appear in the appropriate ranking table, as well as in Table 5.

Principal interest in these tables, aside from keying to the graphs, is the magnitude of the maximum "rates" and the general temperature level at which maximization occurs. Of course, the decision to truncate even outputting of rate data at an adjusted level of unity (log = 0) is arbitrary, but is based on long experience in screening down inordinate numbers of combustion or pyrolysis reactions to manageable packages. This cutoff point is generally somewhat conservative, but not always so. The exception is the case where reaction initiation depends upon one or a few reactions which thereafter never amount to much; furthermore, this "dependence" may mean either enhancement or inhibition. In screening out reactions, one must ensure that the induction period is examined carefully. This is why it is important to consider the temperature as well as the maximum rate. Of the two reactions with lowest maximum rates, 41 and 61, the first one peaks for CH_3OH (fuel 3) at one of the lowest temperatures encountered in Table 7, i.e., at 1137.5 K, and thus is presumably of significance for this fuel, at least. The second does similarly for C_2H_5OH (fuel 1), peaking at 1466.3 K. Others of the slowest 10 or 12 reactions involve species (HO_2, CH_2OH) of limited thermal stability, so that they would be expected to increase in importance with any reduction of assigned initial temperature. Consequently, it is reaction 67 which would be the first candidate for excision if one wished further to reduce the size of the reaction package, yet its maximum rate is within a factor of about 10^4 of the fastest reaction of all (55, the unimolecular decomposition of CH_4) in the carbonaceous system. Thus it is claimed that all 100 reactions are significant for at least one of the fuels considered.

Generally speaking, the reactions (83-100) introduced to permit assignment of C_2H_5OH as the fuel proved unimportant to the oxidation of CH_3OH or CH_4. However, there were significant exceptions, especially reactions 84, 86, 87, and 88. Inspection of the reactions reveals that the combination of 86 and 88 provides a means of progression of C_2H_4 and OH to CH_3 and HCHO, via C_2H_4OH, while 84 and 87 together permit the transformation of C_2H_4OH to H, CH_3, and HCO, via CH_3CHO. These are good examples of how complicated the overall oxidation scheme may be.

It bears repeating at this point that the use of the package of 100 reactions to calculate oxidation of C_2H_6 has been an approximation. One can appreciate that various C_3 species (all of which are excluded) might have provided alternate reaction paths even if no significant concentrations arose. There are in Table 1, 47 reactions of C_3 species without allowing for any C_4 species, etc., and for a more definitive treatment of C_2H_6 one would wish to examine the significance of these 47 reactions added to the basic package of 100. The only calculational result which can be presented here by way of comparison applies to reaction initiated at 1500 K with either the 250 reactions of Table 1 or the 100 reactions (but with rates not doubled) of Table 2. (Thus, identical reactions did have identical rates in the two calculations.) The calculated ignition time was 0.48 millisecond with the package of 250 reactions and 0.26 millisecond with the package of 100. From this it would seem that other contributions of alternate reaction paths, acquired in treating CH_3OH and C_2H_5OH as particular fuels or in bringing the treatment of CH_4 into alignment with experimental data, were more important than paths lost in excising C_3 species. (For comparison with the above autoignition times at 1500 K, it may be noted that the standardized package of 100 reactions, with most of the rates doubled, yielded a corresponding value of 0.17 millisecond.)

It is very well known that the autoignition of hydrogen depends upon a chain-branching reaction process, wherein one free radical, H, produces two, O and OH, by its reaction with O_2, and likewise O with H_2 yields H and OH. What happens in the case of hydrocarbons is less well known, but there have been analyses for methane, at least, showing that chain-branching, while present, is not predominant early in the reaction process. This is confirmed by the present results. The critical initiating reaction for methane is the unimolecular decomposition of CH_4 to H and CH_3. Chain-branching proceeds by attack of H on O_2, but initially the O and OH formed serve only to propagate the chain, and not to branch it further. Later there is additional chain-branching when CH_3 attacks O_2, but for a considerable period it remains to the decomposition of CH_4 essentially to develop the reaction mechanism. The situation is very similar in the case of ethane, where the critical initiating reaction is the unimolecular decomposition of C_2H_6 to two CH_3 fragments. Atomic hydrogen arises when CH_3 withdraws H from C_2H_6, producing CH_4 and C_2H_5, and

C_2H_5 then decomposes to H and C_2H_4. Because the dissociation energy of C_2H_6 is considerably less than that of CH_4, the autoignition of C_2H_6 occurs much more expeditiously than that of CH_4 at given temperature.

The two alcohols appear to come much closer to exemplifying chain-branching than do the two alkanes. As before, the critical initiating reactions are shown by the calculations to be unimolecular dissociations. In the case of C_2H_5OH, the immediate dissociation products are CH_2OH and CH_3, but CH_2OH itself dissociates to H and HCHO. In the case of CH_3OH, the two alternative decompositions, to OH and CH_3 or to CH_2OH and H, were both found to be prominent. Again, of course, CH_2OH directly yields H and HCHO. It is this decomposition of CH_2OH and then the subsequent destruction of HCHO which seem to be most responsible for rapid development of chain-branching, not only as the CH_2OH arises from the unimolecular decompositions, but also as it is formed (instead of CH_3) in what would otherwise be simple chain-propagating steps. To clarify this, compare $H + CH_4 = H_2 + CH_3$ and $H + CH_3OH = H_2 + CH_2OH$. The former is indeed a chain-propagating step, but the latter, considering the ensuing transformation of CH_2OH to H and HCHO, and the consumption of HCHO to yield more free radicals, is effectively a chain-branching step. In the case of CH_3OH as the fuel, this secondary formation (i.e., secondary in the sense of not being the critical initiating reaction) of CH_2OH is very extensive. In the case of C_2H_5OH as the fuel, the chain-propagating steps yield both CH_2OH and C_2H_4OH. The latter dissociates rapidly to CH_3 and HCHO. Since some CH_3 formed means less H formed, the direct chain-branching of $H + O_2$ does not occur as readily in the case of C_2H_5OH. Thus it is that CH_3OH, with a higher activation energy for its critical initiating reaction, manages to overtake C_2H_5OH in the development of autoignition, or so it would appear. It should be pointed out here that what has been calculated, and what has been deduced from the calculations, emphasize the importance of the assigned thermochemistry for C_2H_4OH and CH_2OH. If substantial changes were ordered in the thermochemistry, substantial changes in activation energies, and thus in reaction rate constants, would be expected, affecting not only the preceding exposition but some of the results in the main text. It can only be repeated here that the thermochemistry represents present "best estimates." While the significance of the selected 100 reactions has been demonstrated, and assurance has been given that these have survived screening operations to remove less prominent reactions, one significant loop-closing step has not been taken. This would be the trial insertion of sterically rejected reactions into the reaction package, to determine their apparent contributions. Those found to overwhelm the generally satisfactory package would be finally rejected as sterically "impossible," and those influencing the results unnoticeably would be assigned to the "trivial" list. In between, some might be found which had significant but not overwhelming effect, and these would deserve a search for any validation (and rate assignment) in the literature.

An example is afforded by Reference 11, brought to attention by another paper just published while this report was being written. For the reaction of O with C_2H_4, the following reactions can be envisioned:

15.7 $O + C_2H_4 = CH_2 + HCHO$, exothermic by 8 kcal;

15.10 $O + C_2H_4 = C_2H_3 + OH$, endothermic by 4 kcal;

15.11 $O + C_2H_4 = CH_3 + HCO$, exothermic by 40 kcal;

The writer has long considered the last reaction to be sterically improbable, and it does not appear in Table 1 and did not otherwise participate in the calculations leading to Table 2. Yet Reference 11 (which does not mention the second reaction, incidentally), presents experimental results to show that the last reaction does occur and the first ostensibly does not (but the fairer statement might be that the last is very much favored over the first). An explanation would be that some sort of intermediate, unstable C_2H_4O species is formed which then decomposes into the products favored by free energy considerations, CH_3 and HCO. The actual existence in nature of a stable C_2H_4O species, ethylene oxide, might tend to support this explanation.

In this particular case, since either pair of products considered by Reference 11 is formed exothermically, there probably would be only little effect on the overall results for the fuels considered if the last reaction were substituted for the first (which is reaction 71 in Table 2), with the rate constant coefficients assigned for the last reaction according to the standard technique, of course. The expected consequence would be some increase in chain-branching, since CH_2 was computed to lead to HCO and HCHO and then to their decomposition fragments, whereas CH_3 was found principally to engage in simple chain propagation.

If C_2H_4 were the fuel, this change in the reaction package suggested by Reference 11 could be quite important. Thus it is well to recognize that there may be comparable situations which are of more importance to the particular fuels of interest here. On the other hand, it also should be noted that this suggested change applies to attack by a free radical on a double bond. None of the fuels of present interest has a double bond (or triple bond). C_2H_2 is the only other multiply-bonded intermediate species encountered, and its peak concentration is only a fraction of the peak for C_2H_4, both encountered with C_2H_6 as the fuel.

In summary on this point, the particular substitution of reaction 15.11 for reaction 15.7 suggested by Reference 11 apparently would have most influence on the calculations for C_2H_6 (for which the least definitive work was done in creating the package of 100 reactions), presumably would not be very important even for C_2H_6, but does imply that some other changes in the reaction package may be in order, especially some additions involving reactions previously classified as sterically unlikely. This having been concluded, substitution of 15.11 for 15.7 was made and the autoignition of stoichiometric C_2H_6 initially at 1500 K was calculated. The resulting autoignition time was 0.15 millisecond, as compared to the value of 0.17 millisecond obtained with the standard package of 100 reactions.

There are 18 maximum reaction "rates" for CH_4 in Table 5 which fall below the cut-off value of zero adopted for the figures. As a test case, these 18 reactions were removed and the calculation for stoichiometric CH_4 initially at 1500 K was repeated. The calculated autoignition times were virtually identical for the two runs, as one would certainly expect. Significantly, no species was reduced to inactivity by elimination of the 18 reactions, so computer running time was not noticeably affected by the modification.

Figures 101-118 of the Appendix comprise a set of graphs showing the instantaneous concentrations of important intermediate (or initial) species during the progress of combustion for stoichiometric fuel in air at 1 atm and initially at 1100 K. These species concentrations, along with those of other initial species and the final stable species, of course, enter into the evaluation of the net reaction rates. These graphs clearly demonstrate that there is no easy basis for inferring the approximate time histories of intermediate species; if one has interest in such histories, he requires direct access to them.

Allied to figures 101-118, Table 8 records the maximum concentrations of the various species encountered anywhere during the progress of reaction, for the five fuels each initially at 1100 K. Recall that fuel 1 is C_2H_5OH; fuel 2 is C_2H_6; fuel 3 is CH_3OH; fuel 4 is CH_4; and fuel 5 is H_2. Fuel 5 is extraordinary in its formation of H, OH, and O according to the chain-branching reactions $H + O_2 = O + OH$ and $O + H_2 = H + OH$ which are, of course, accentuated not only because of the prevalence of H_2, but also because it has few other ways to react (of which $OH + H_2 = H + H_2O$ is the most prominent). Among the other four fuels, the maximum concentrations of H, OH, and O are grossly the same, with the largest deviation being that of O in the case of CH_3OH. Also, the intermediate levels of H_2 maximize at grossly the same level in the case of the other four fuels. The concentrations of N and NO attained are discussed in the main text.

Insofar as HO_2 and H_2O_2 are concerned, there are marked differences in the individual maximum concentrations. This seems to imply that the package of 100 reactions is perhaps unbalanced in its treatment of HO_2 and H_2O_2. This would be a circumstance that might noticeably affect the relative accuracy of solutions for the different fuels at initial temperatures below 1100 K where these two species have greater thermal stability. However, while a definite inbalance is discernible when the reaction package is examined in detail, this does not seem to account for the discrepancies in HO_2 and H_2O_2 concentrations. Eleven reactions might be added;

3 of O_2 abstraction of H from C_2H_5OH, C_2H_6, and CH_3OH
(complementing $O_2 + CH_4$);

3 more for O_2 abstraction of H from C_2H_4OH, C_2H_5, and CH_3
(complementing $O_2 + CH_2OH$),

2 for HO_2 abstraction of H from C_2H_5OH and C_2H_6
(complementing HO_2 + CH_3OH and HO_2 + CH_4), and
3 more for HO_2 abstraction of H from C_2H_4OH, C_2H_5, and CH_3
(complementing HO_2 + CH_2OH).

The permitted O_2 abstraction of H from CH_4 might be expected to lead to substantial HO_2, relative to the other carbonaceous fuels for which the equivalent reaction was not permitted, but instead it led to the smallest amount of HO_2 recorded in Table 8. Principally, the results in Table 8 seem to reflect the formation of HO_2 from the simpler reaction species, H, OH, H_2, O_2, HCO, and HCHO, by reactions equally available to each fuel, so that it is the particular, differing, intermediate concentrations of these simpler species which dictate the particular results; the same may be said as well for H_2O_2 formation.

Inspection of the entries in Table 8 for the carbonaceous species reinforces the conclusion drawn relative to HO_2 and H_2O_2, namely that there are inherent characteristics of the fuels that result in dissimilar reaction paths. Some of the species show general consistency, however; these are CO, CH_3, and CH_3OH (except as itself the fuel). The quantities of CH_4 formed are high, grossly 4 mole percent (of reacting mixture) by both C_2H_5OH and C_2H_6, and 2 mole percent by CH_3OH. Very different amounts of C_3H_6 are formed, depending on the starting material. A general pattern of C_2H_6 degradation to C_2H_4 and C_2H_2 is exhibited. The two alcohols exhibit much greater production of CH_2OH, HCHO, and HCO than the two alkanes. All in all, the evidence of Table 8 seems consistent with chain-branching being most rapid in the case of CH3OH; the pyrolysis reactions yielding CH_3, CH_4, C_2H_6, C_2H_4, and C_2H_2 are suppressed to lesser or greater degree, while the oxidation intermediates, CH_2OH, HCHO, and HCO are enhanced. The only anomaly is that HCHO reaches a higher value with C_2H_5OH as the fuel, as between the two alcohols. Otherwise, not only does CH_3OH seemingly exhibit the greatest chain-branching, but also C_2H_5OH seemingly exhibits the next greatest.

It seems appropriate that there be included herein the identification of the reactions used by others to calculate the oxidation of CH_4. The contrast with the total of 82 reactions, shown by Table 6 to be significant for CH_4, is great. Table 9 presents the pertinent information. Given first are the reactions from Table 2 to which some consideration was given by at least one of three authors. Chinitz (Ref. 12) assembled reactions from three sources, and then used only a portion for his calculations, as noted. Skinner (Ref. 8) as mentioned elsewhere, gave separate identification to reactions HO.1 and HO.4 with H_2O as the third body. Both Skinner and Bowman (Ref. 13) treated CH_4 dissociation as bimolecular.

The final eight entries in the table show disparities. Reaction 8.1 in the present work, for $O + CH_3$, is paralleled by a different reaction of Bowman. Reaction 8.6 in the present work, for $CH_3 + O_2$, has a different counterpart in each of the other three reaction schemes. The last two entries record reactions noted but rejected by Chinitz, and require no discussion.

Skinner's version of $CH_3 + O_2$ apparently was the key to his reconciliation between experiment and analysis, and the same may be true in Bowman's case, whereas Chinitz did not make such a reconciliation. Of all the reactions in Table 9 for which reaction rate constant data are not yet available, reaction 8.6 is the most critical for experimentation. In substantiating or modifying the "standard" package of 100 reactions, it would be most significant to know at least what products do actually ensue when CH_3 attacks O_2.


HO.1
$H_2 + M = H + H + M$
RATE OF REACTION
PROGRESS OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7

Figure A-1

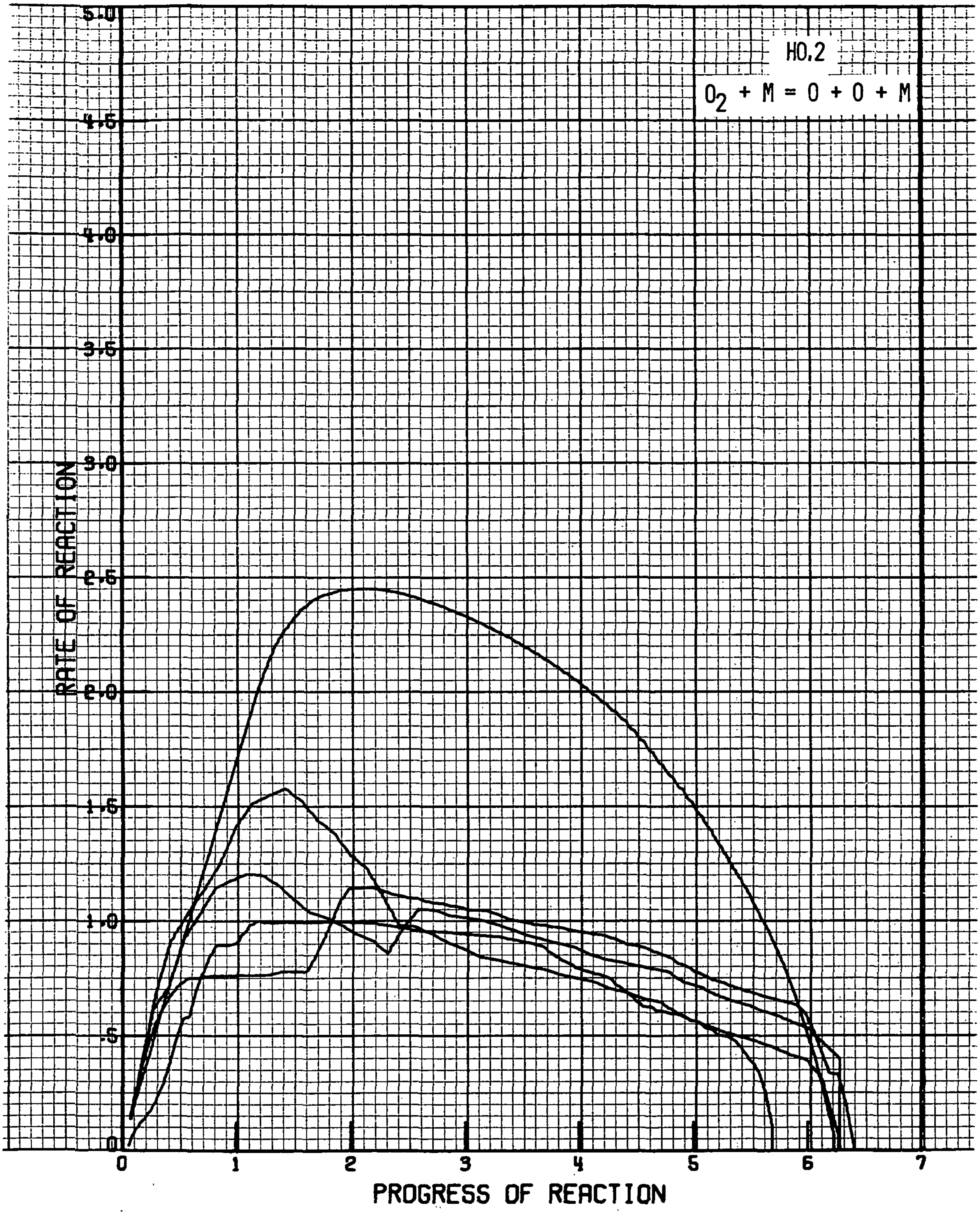

HO.2
$O_2 + M = O + O + M$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-2

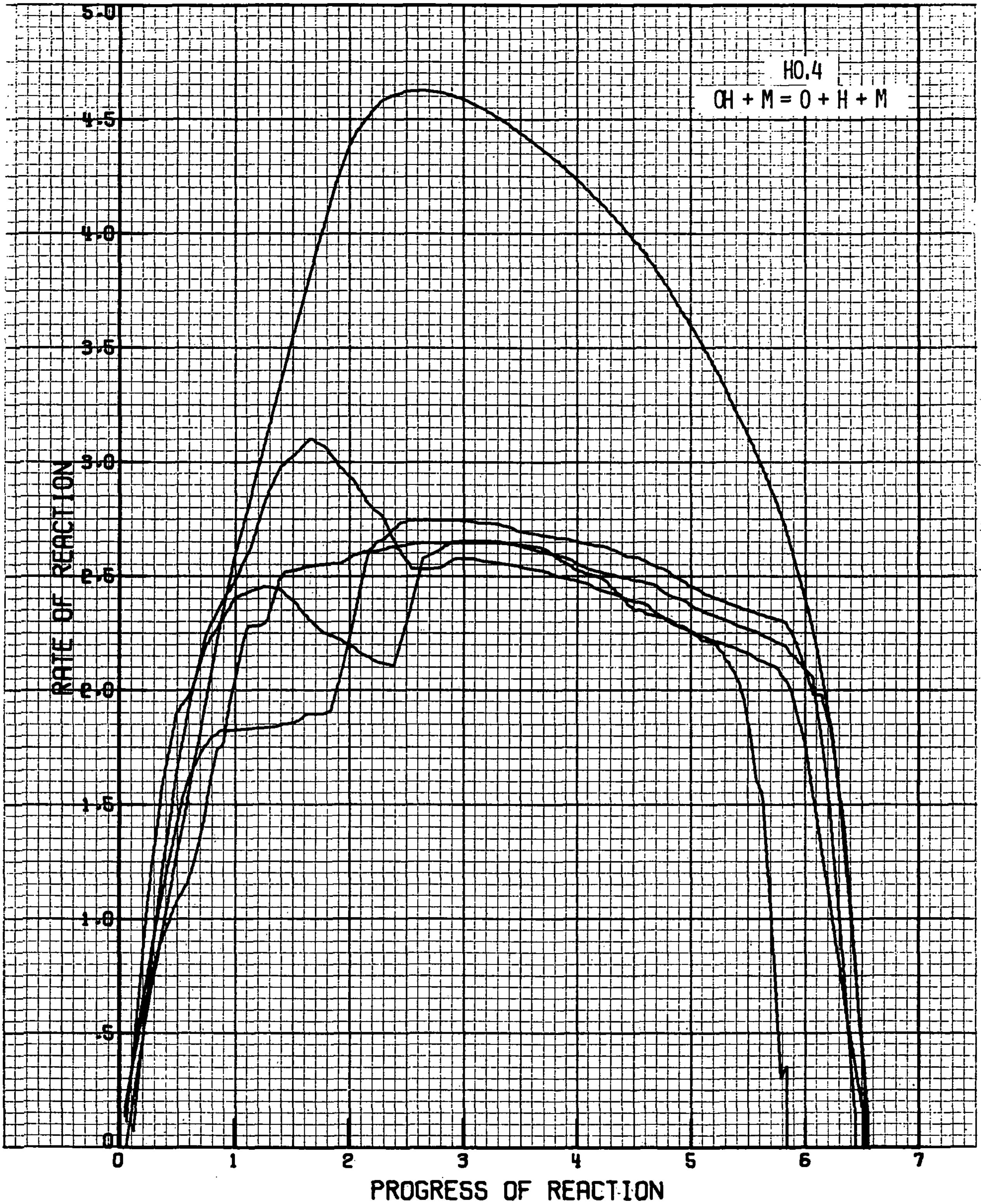

HO.4
OH + M = O + H + M
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-3

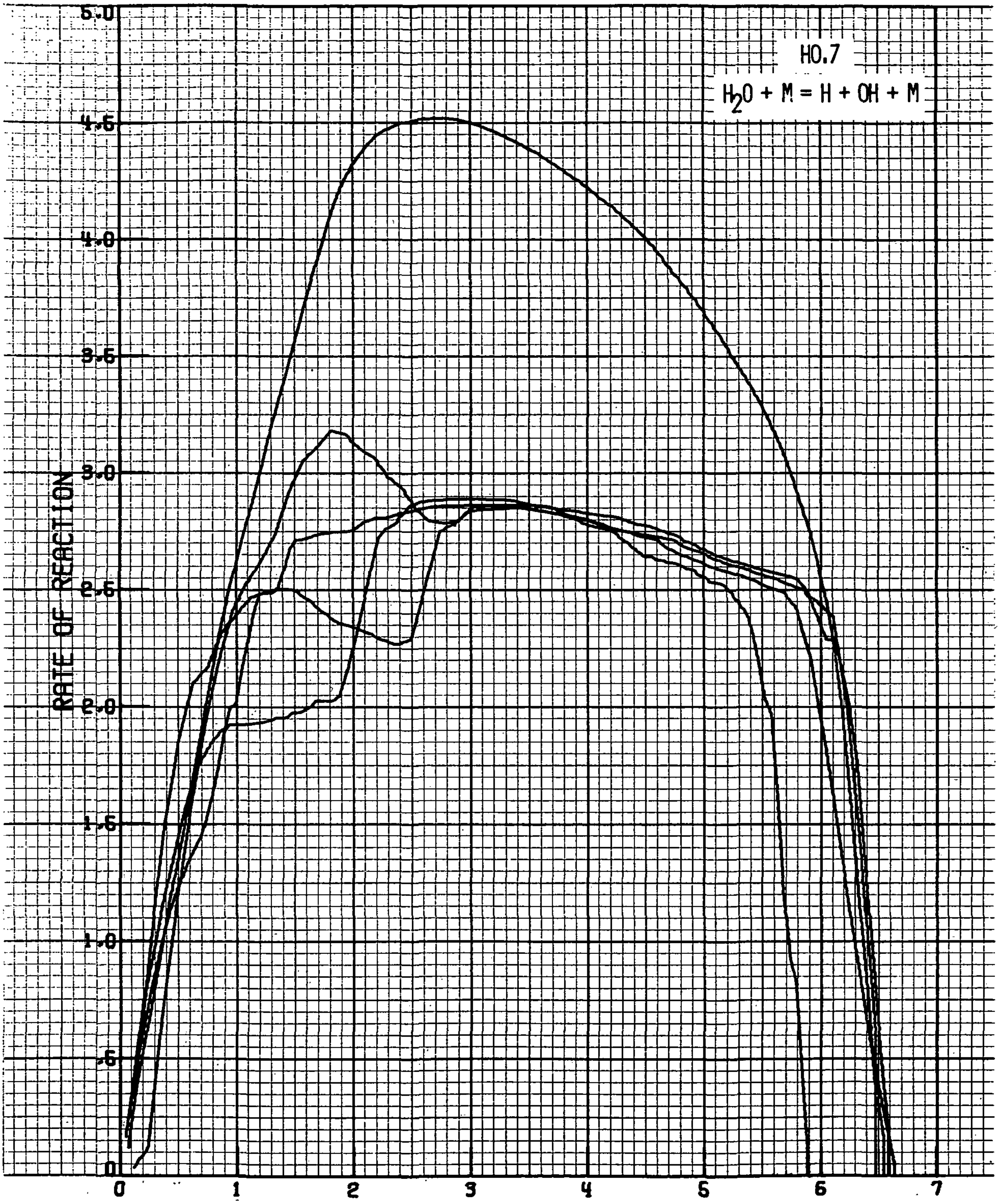
HO.7
$H_2O + M = H + OH + M$
RATE OF REACTION
PROGRESS OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7

Figure A-4.

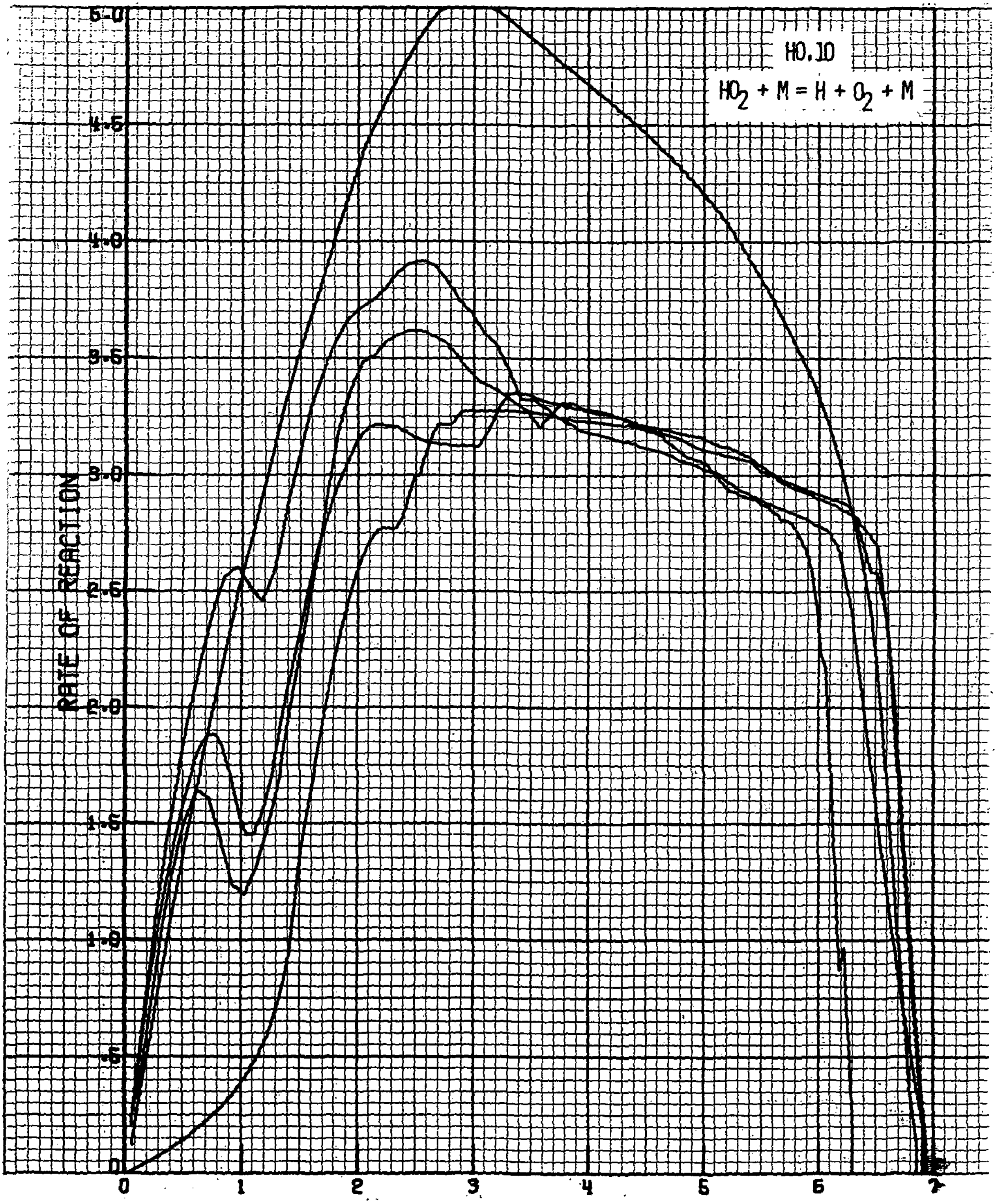
HO.10
$HO_2 + M = H + O_2 + M$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-5

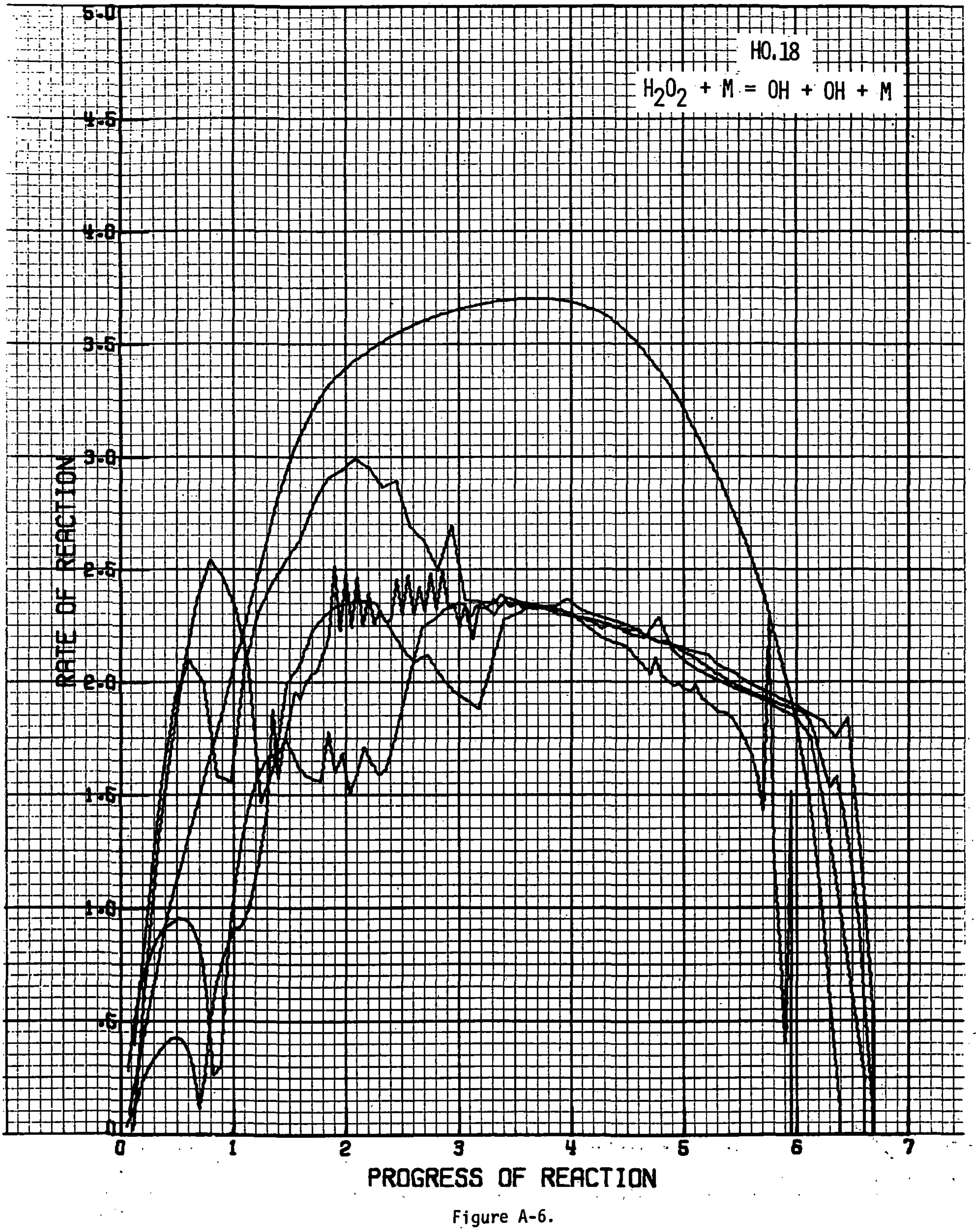

HO.18
$H_2O_2 + M = OH + OH + M$
RATE OF REACTION
PROGRESS OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7

Figure A-6.


5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
RATE OF REACTION
0
1
2
3
4
5
6
7
PROGRESS OF REACTION
HO.5
H + O2 = O + OH

Figure A-7

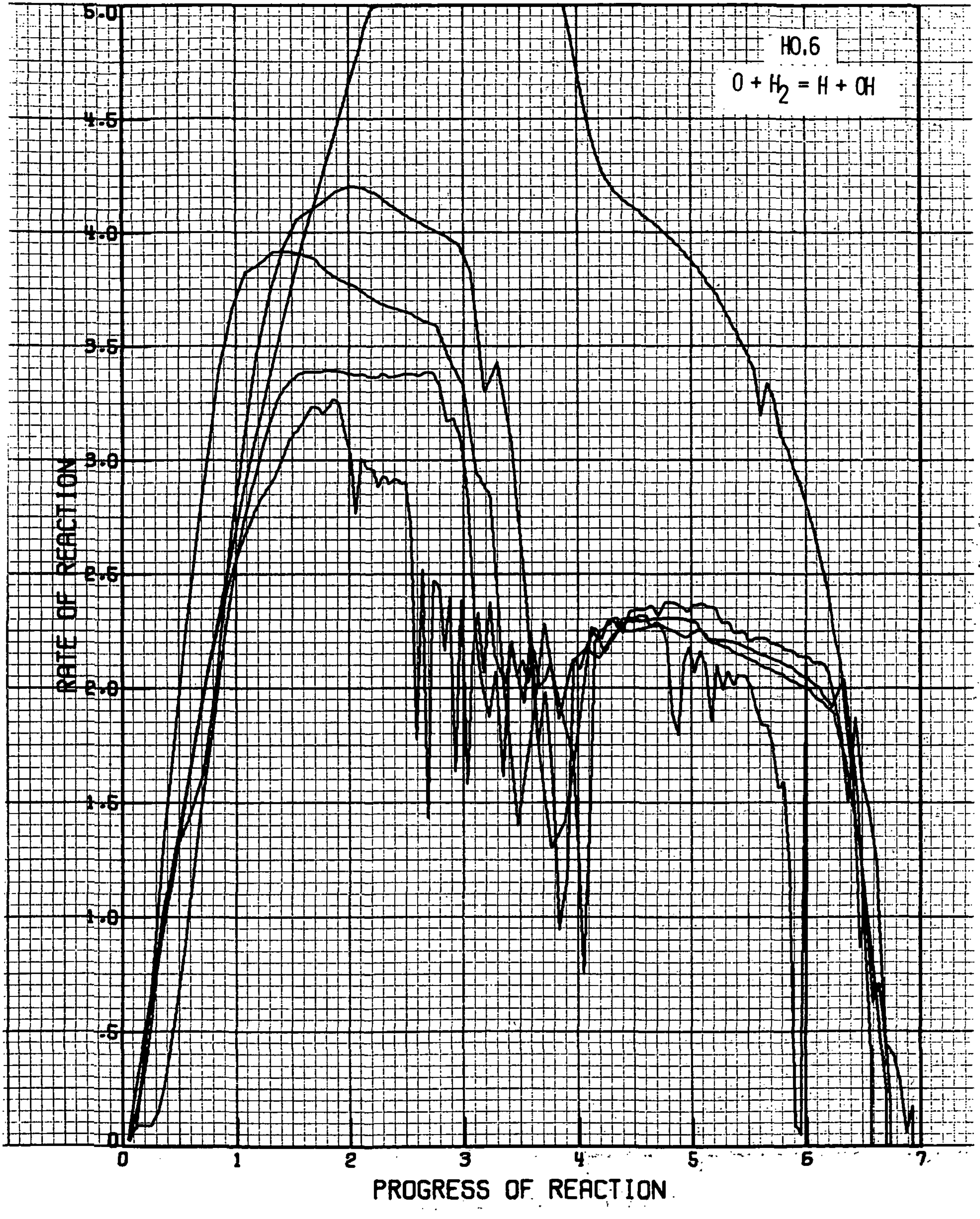

5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
RATE OF REACTION
0
1
2
3
4
5
6
7
PROGRESS OF REACTION
HO.6
$O + H_2 = H + OH$

Figure A-8

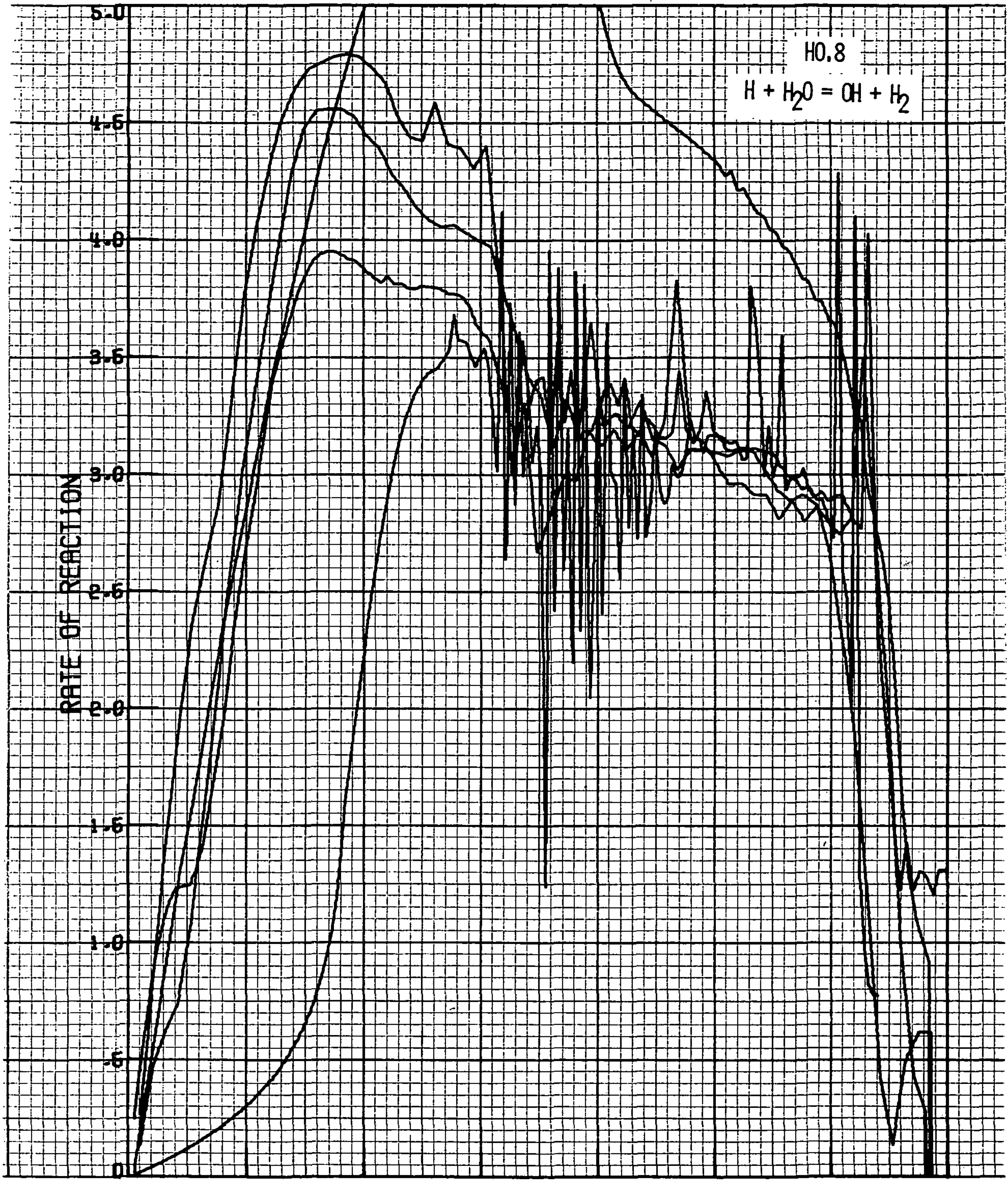

HO.8
H + H_2O = OH + H_2
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-9

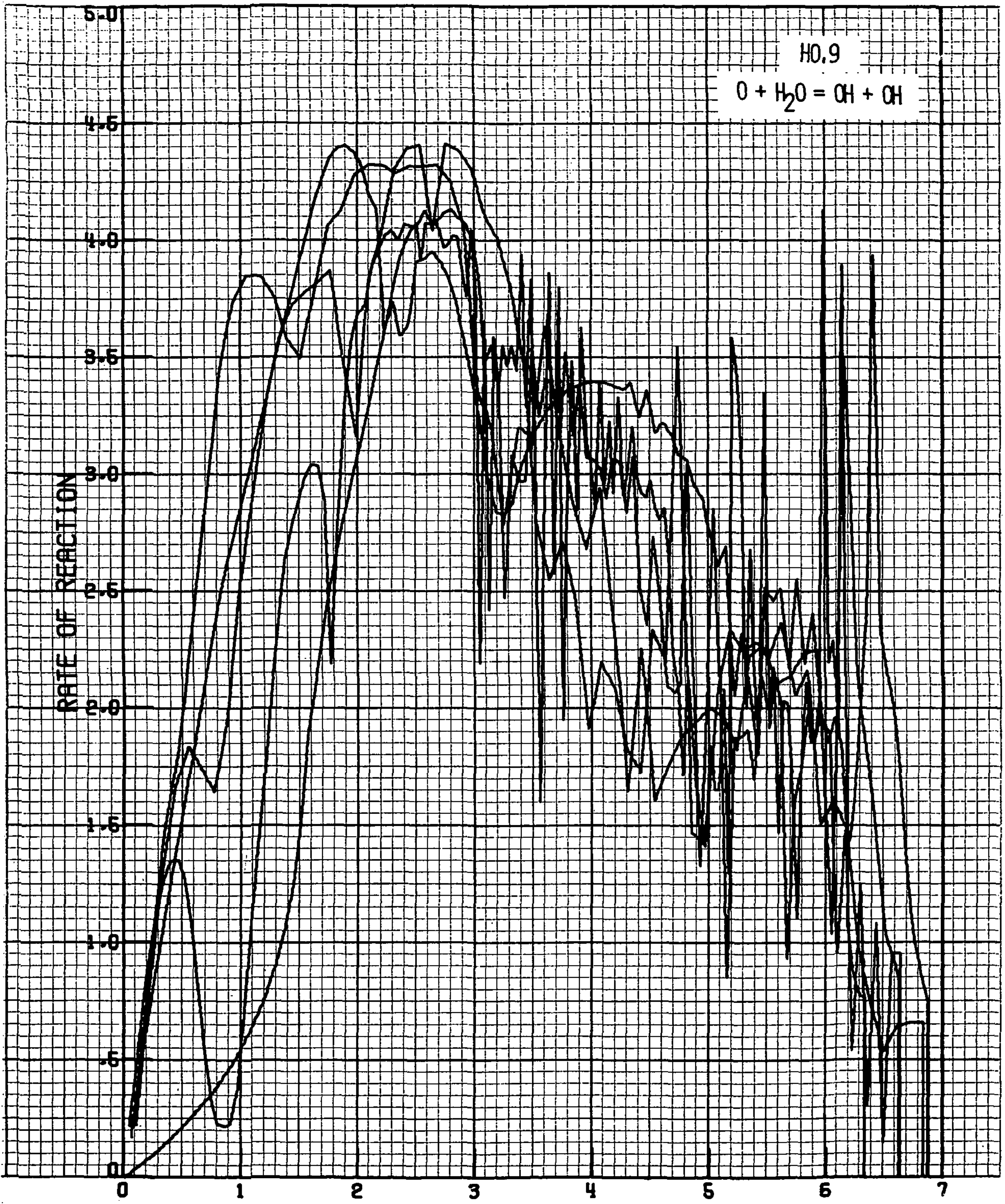

HO.9
$O + H_2O = OH + OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-10

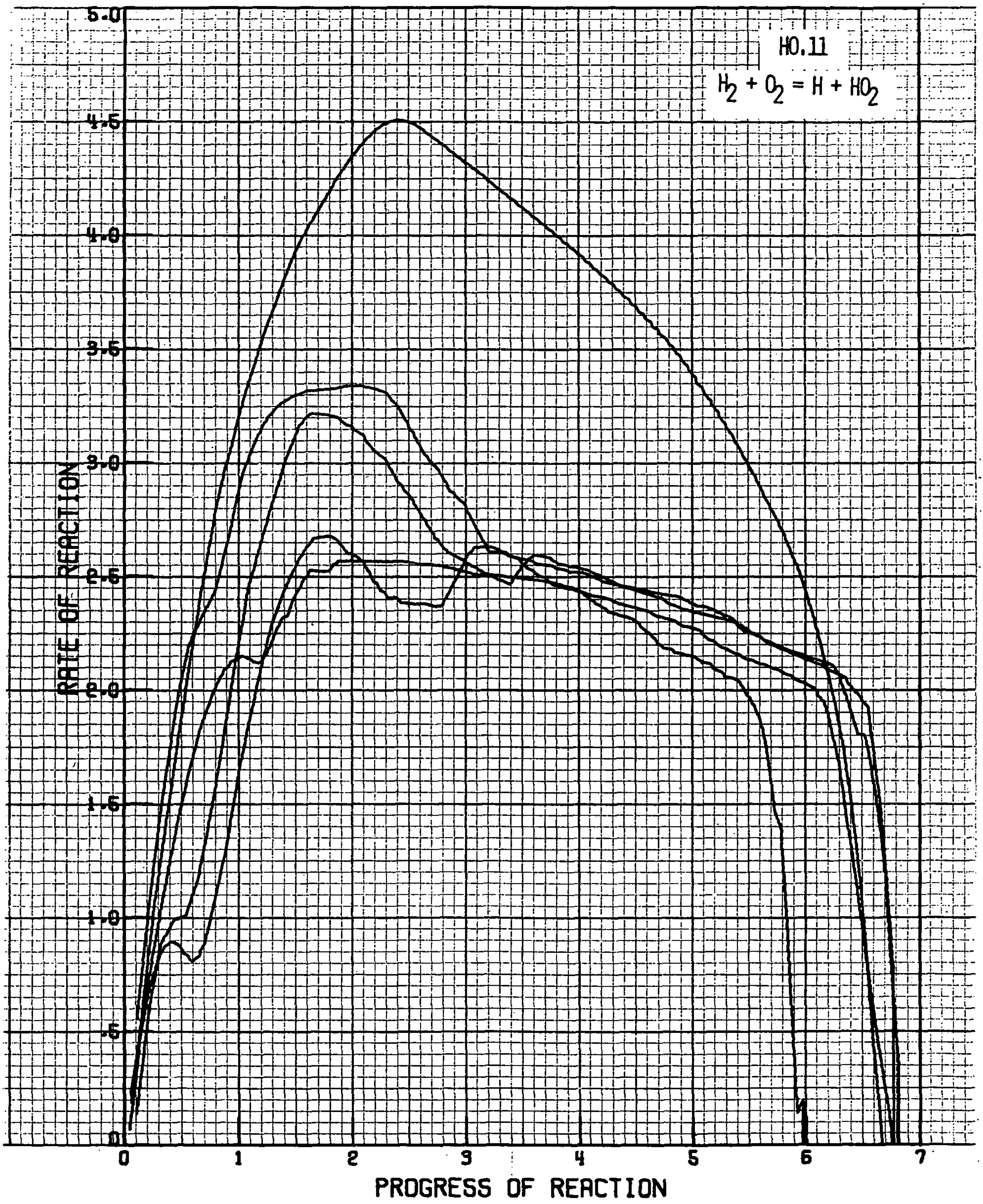

HO.11
$H_2 + O_2 = H + HO_2$
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
RATE OF REACTION
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-11

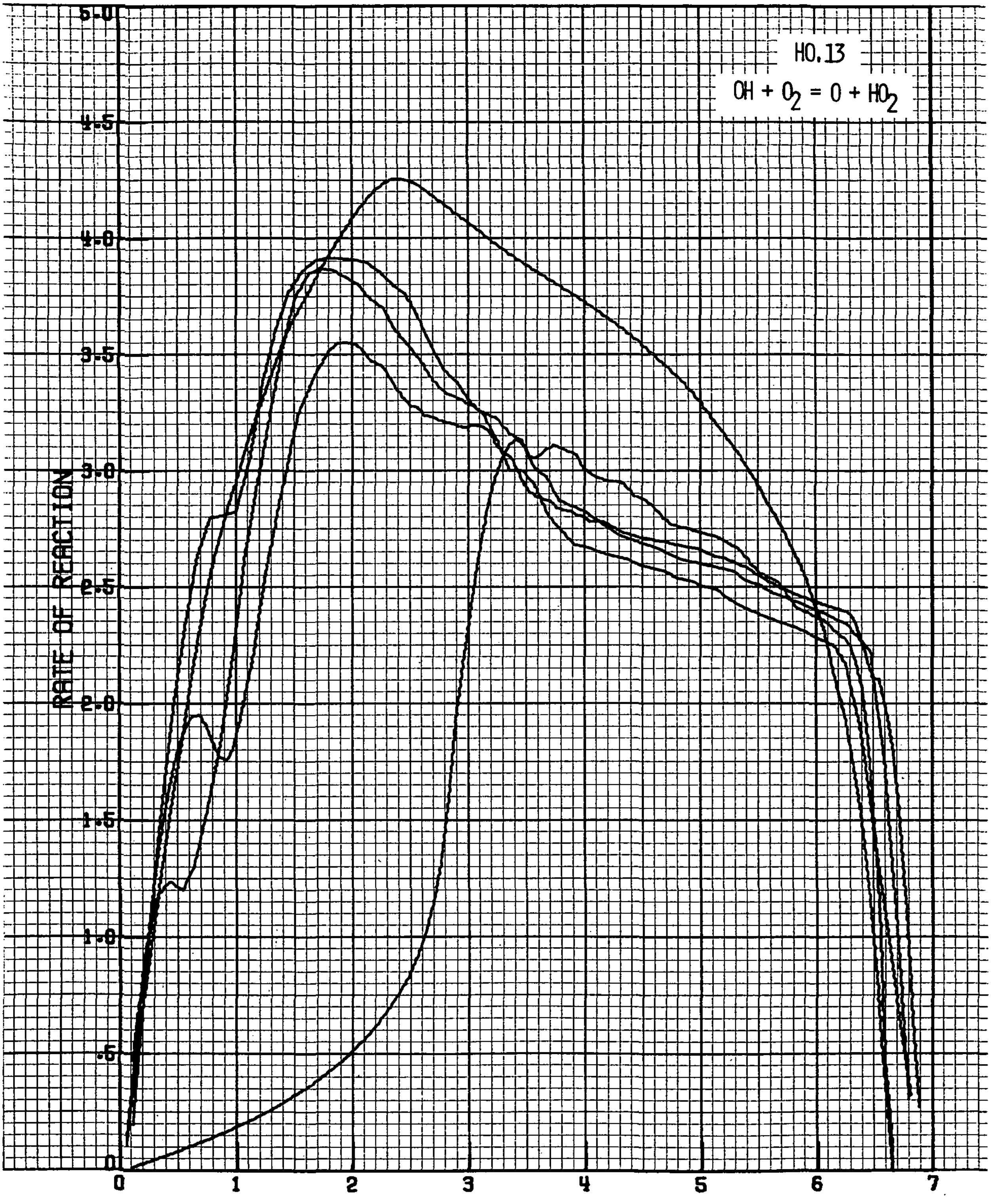

HO.13
$OH + O_2 = O + HO_2$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-12

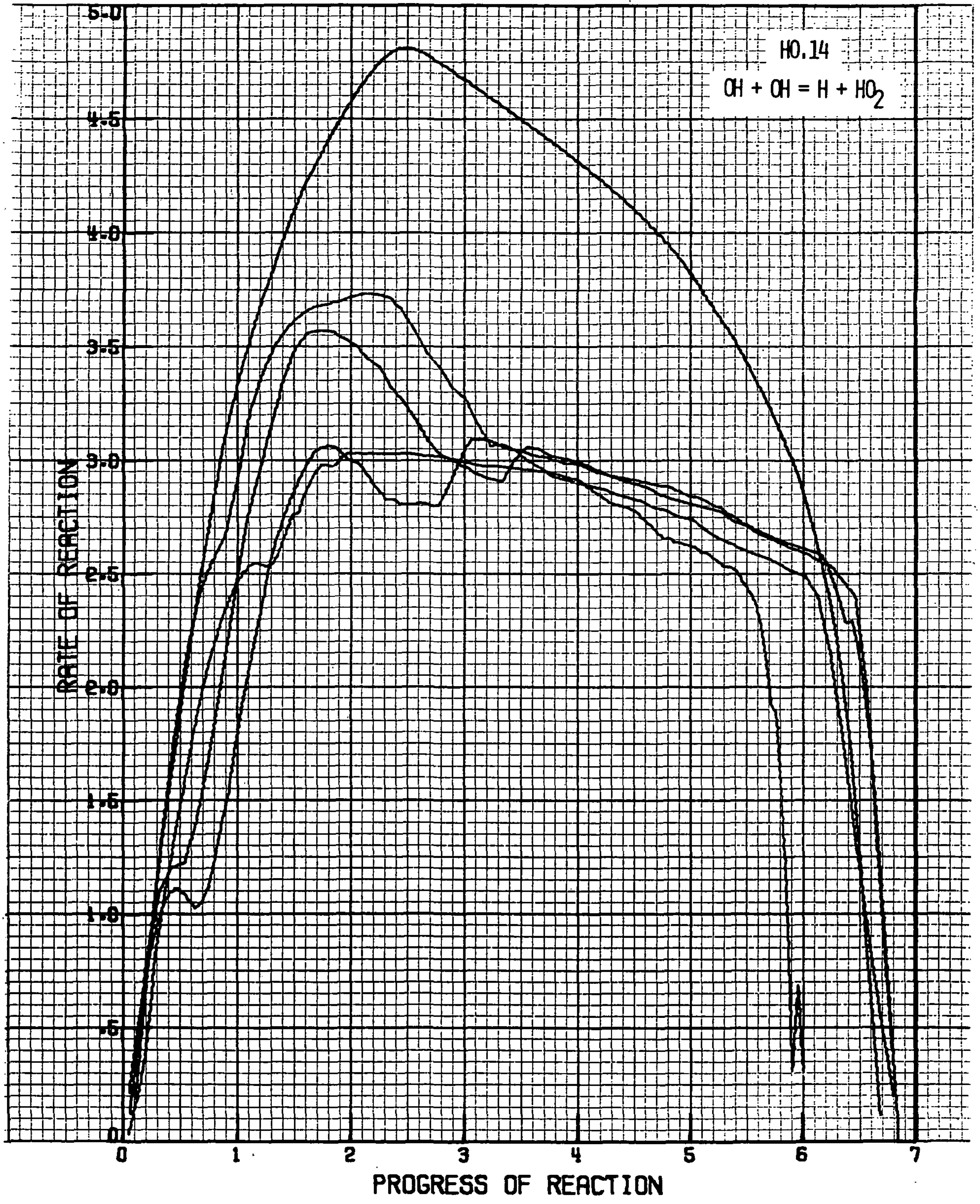

H0.14
OH + OH = H + HO$_2$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-13

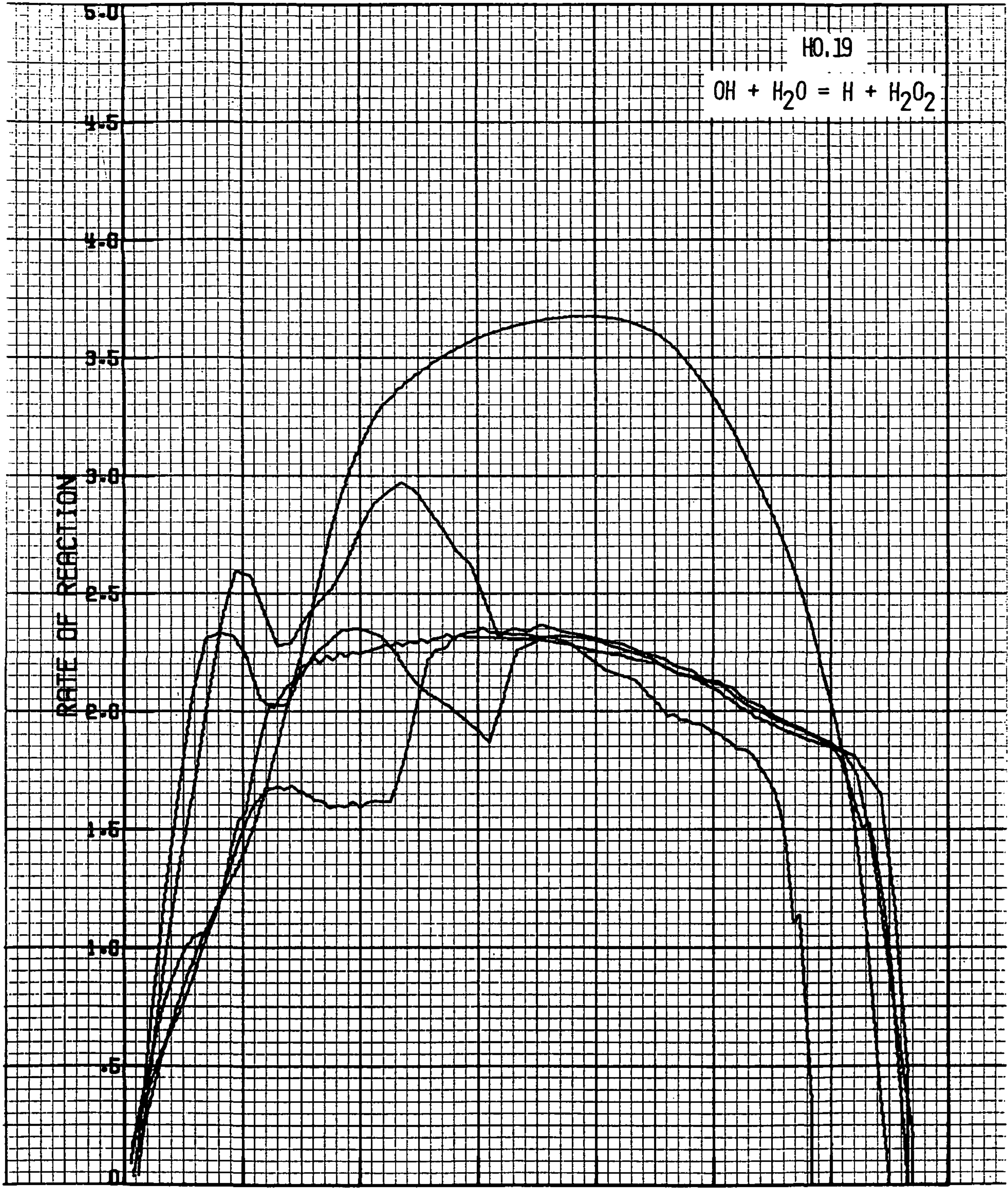

HO.19
OH + H_2O = H + H_2O_2
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-14

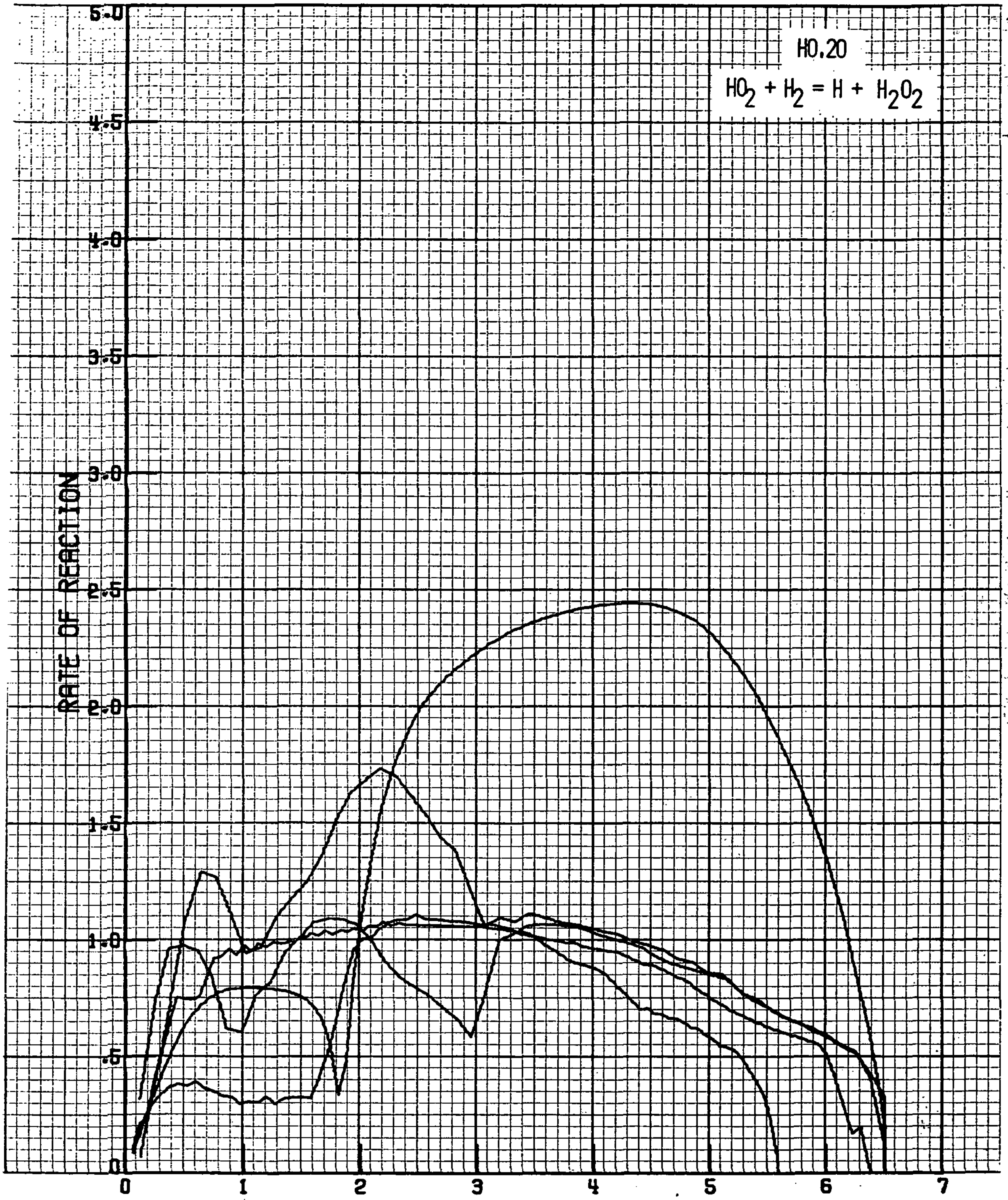

HO.20
$HO_2 + H_2 = H + H_2O_2$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-15

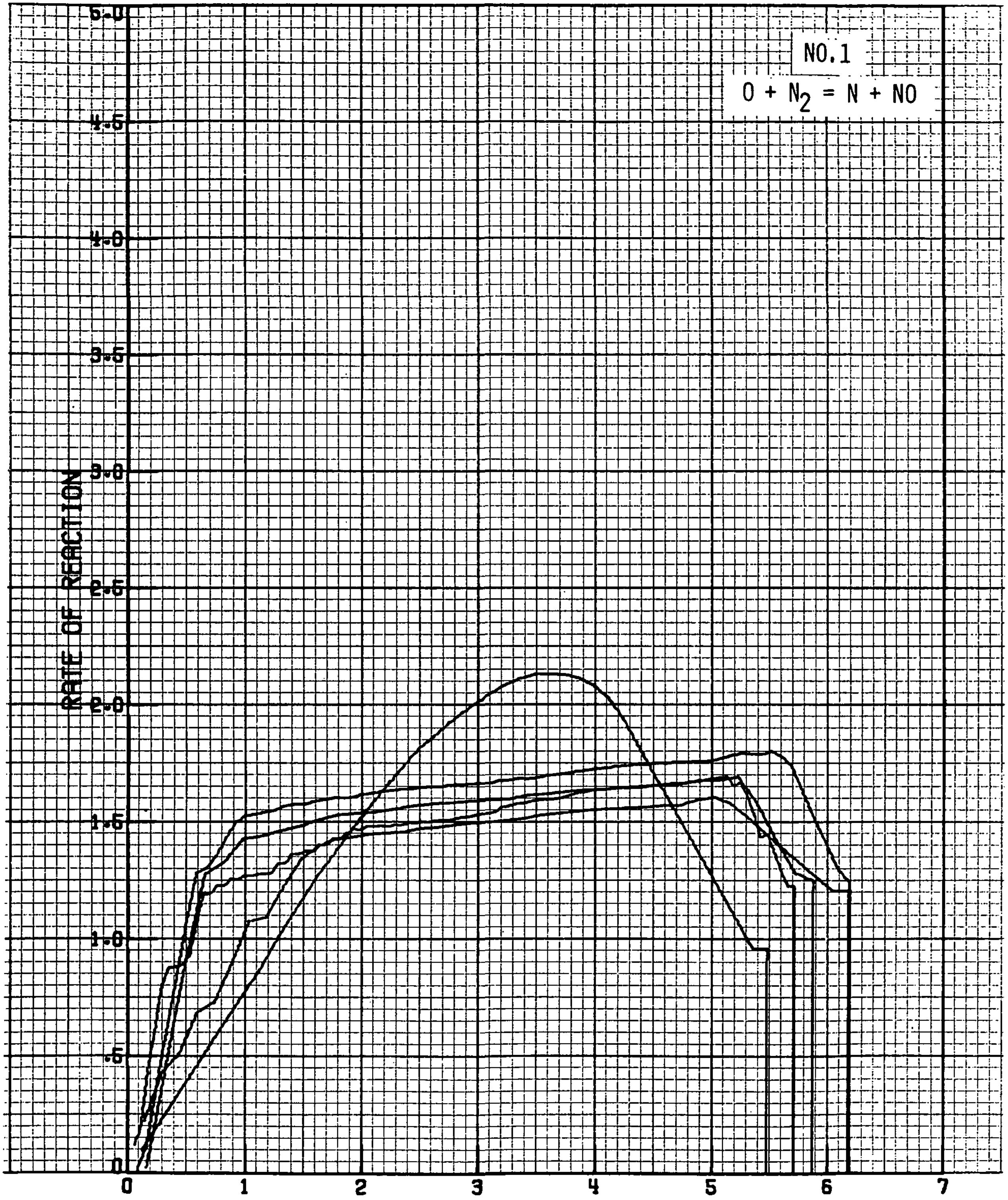

NO.1
$O + N_2 = N + NO$
RATE OF REACTION
0
.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-16

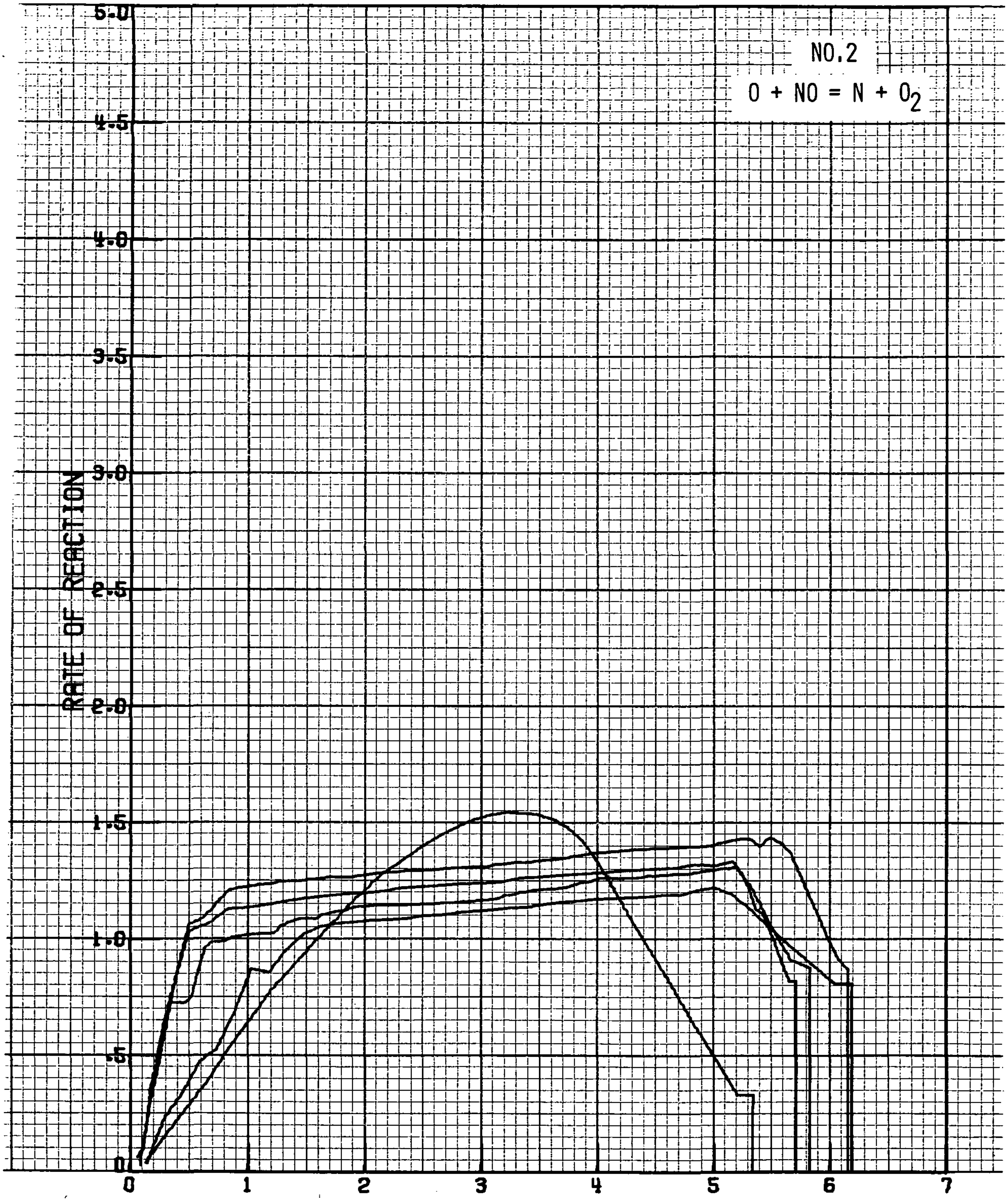

NO.2
0 + NO = N + O_2
RATE OF REACTION
PROGRESS OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7

Figure A-17

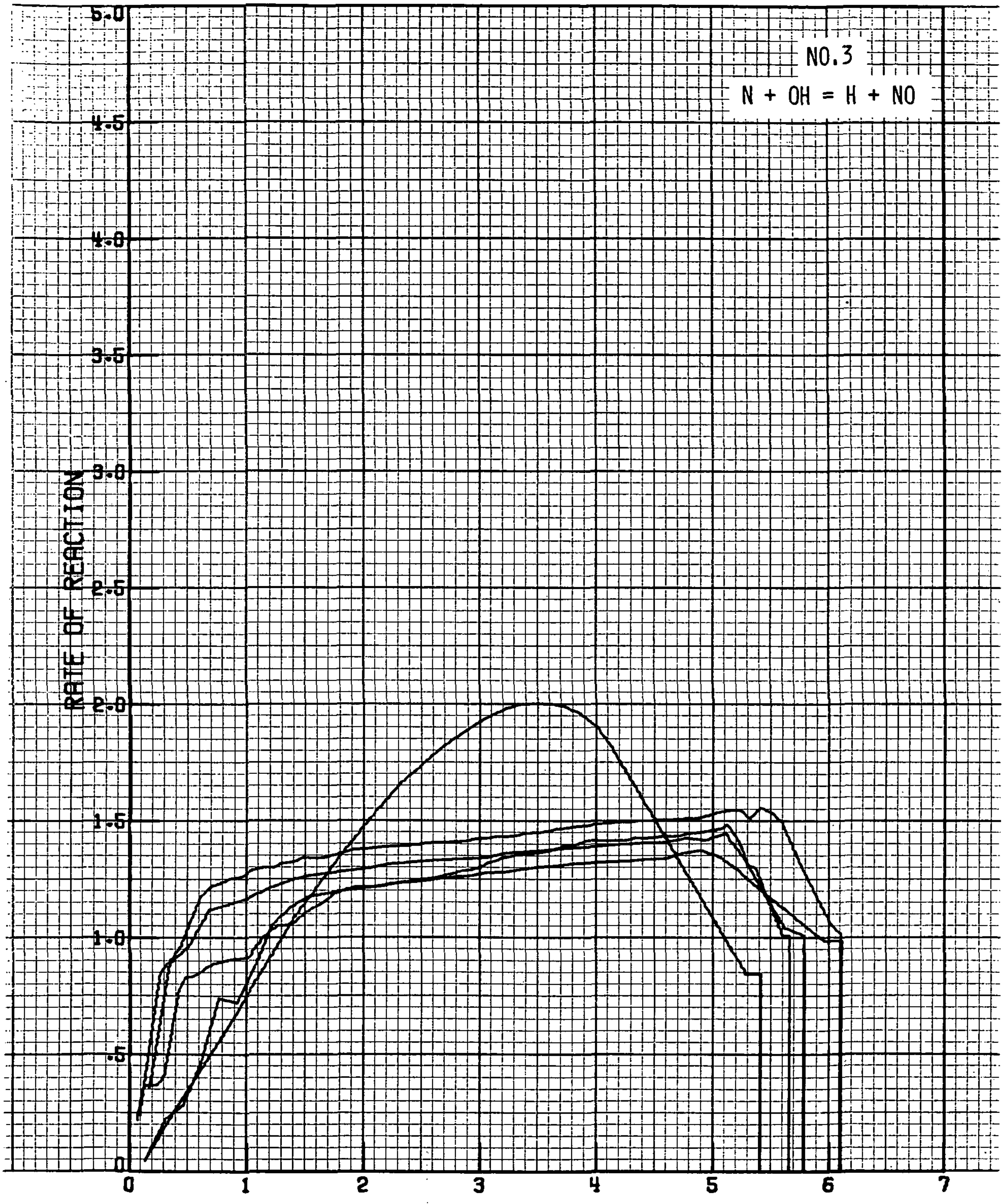

NO.3
N + OH = H + NO
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-18

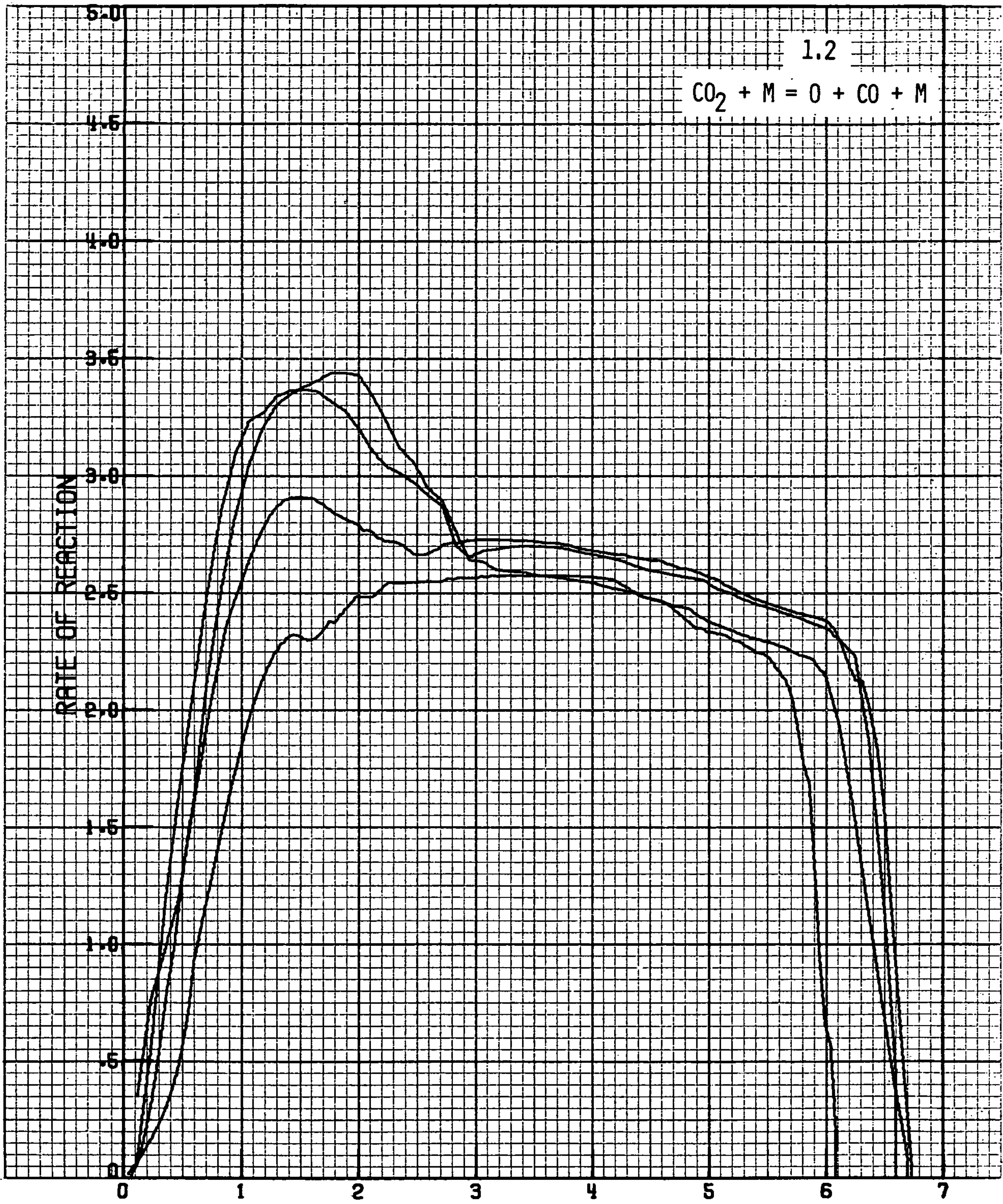

1.2
$CO_2 + M = O + CO + M$
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
RATE OF REACTION
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-19

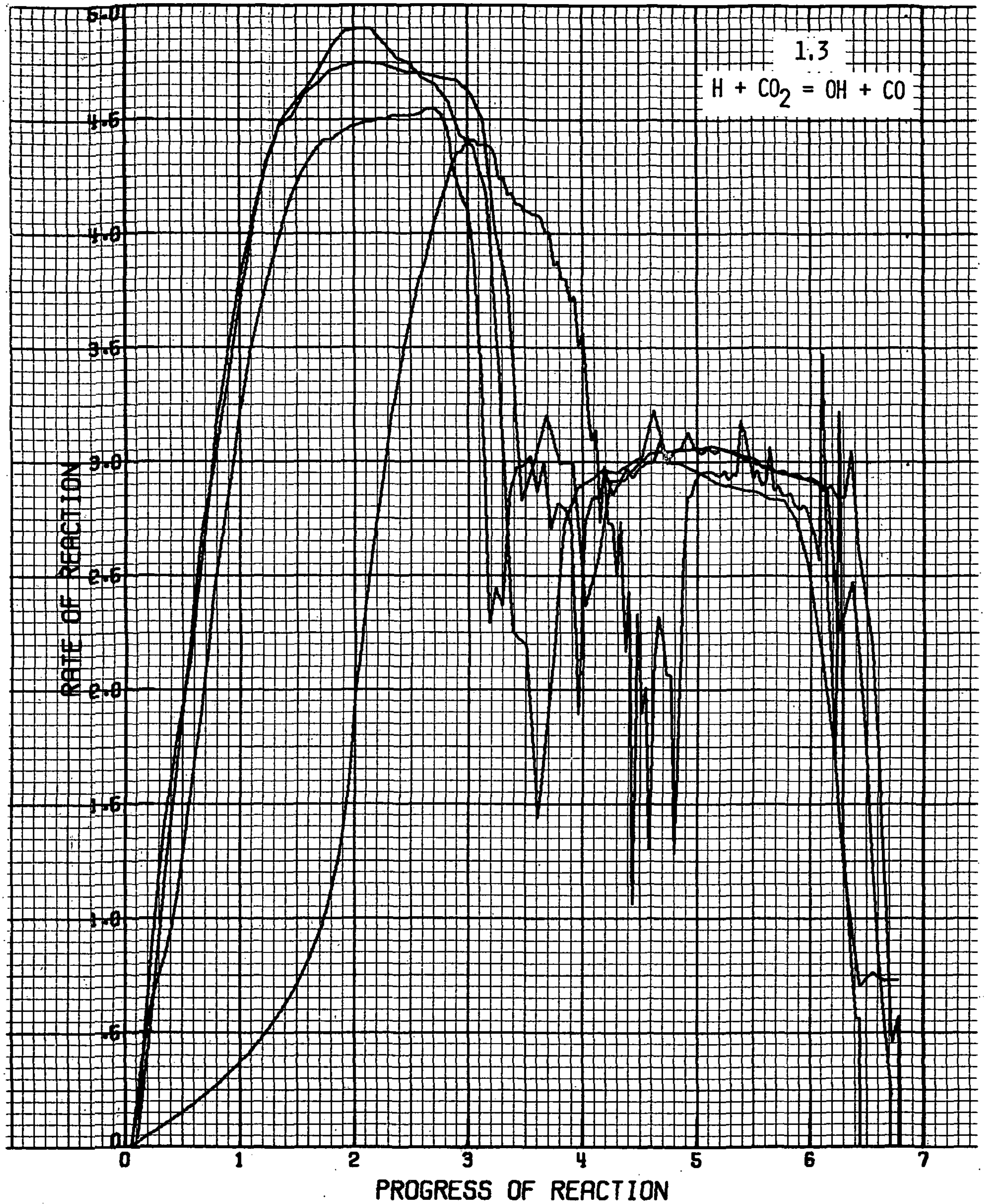

1.3
$H + CO_2 = OH + CO$
RATE OF REACTION
PROGRESS OF REACTION
5.0
4.6
4.0
3.6
3.0
2.6
2.0
1.6
1.0
.6
0
0
1
2
3
4
5
6
7

Figure A-20

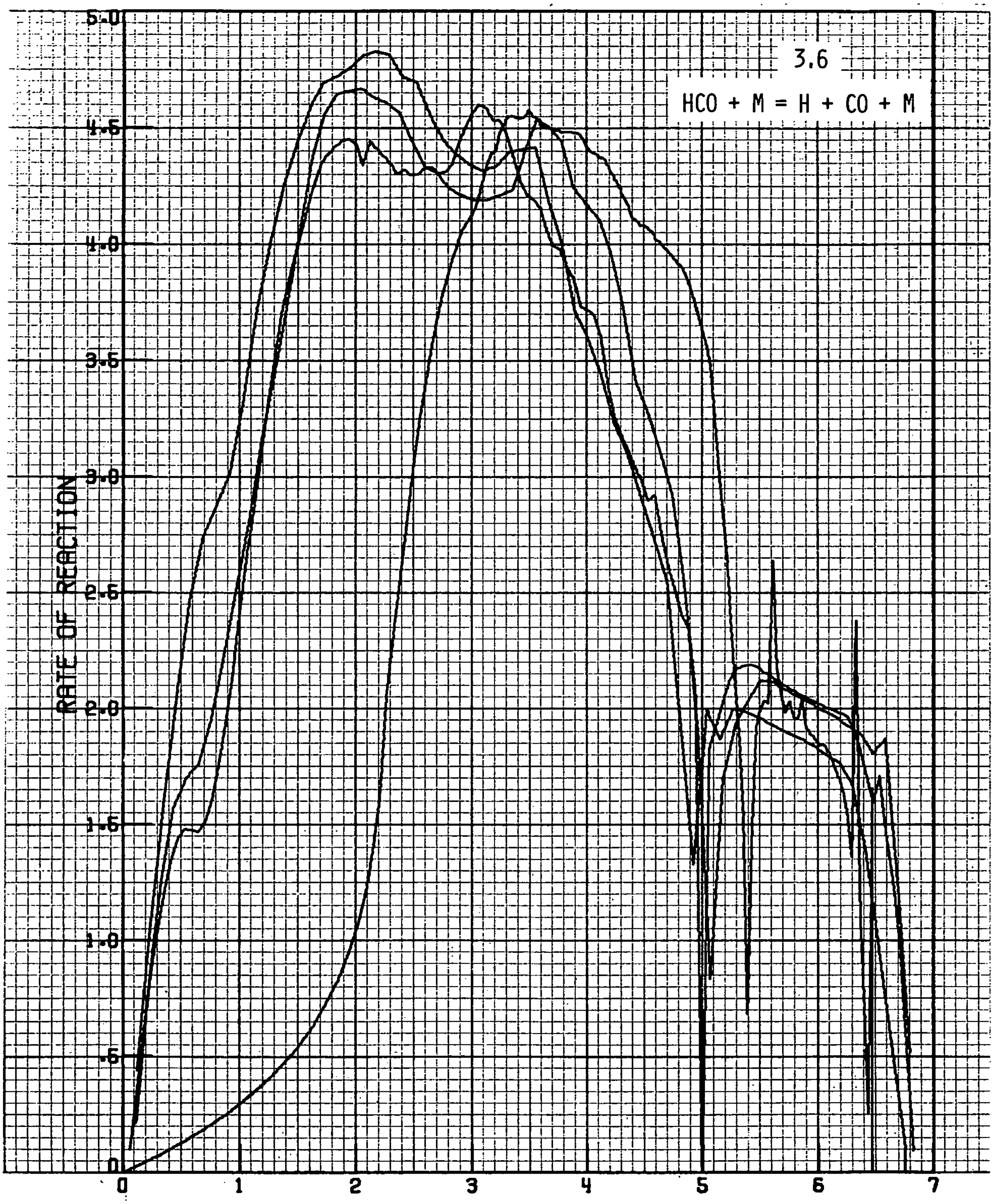

3.6
HCO + M = H + CO + M
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-21

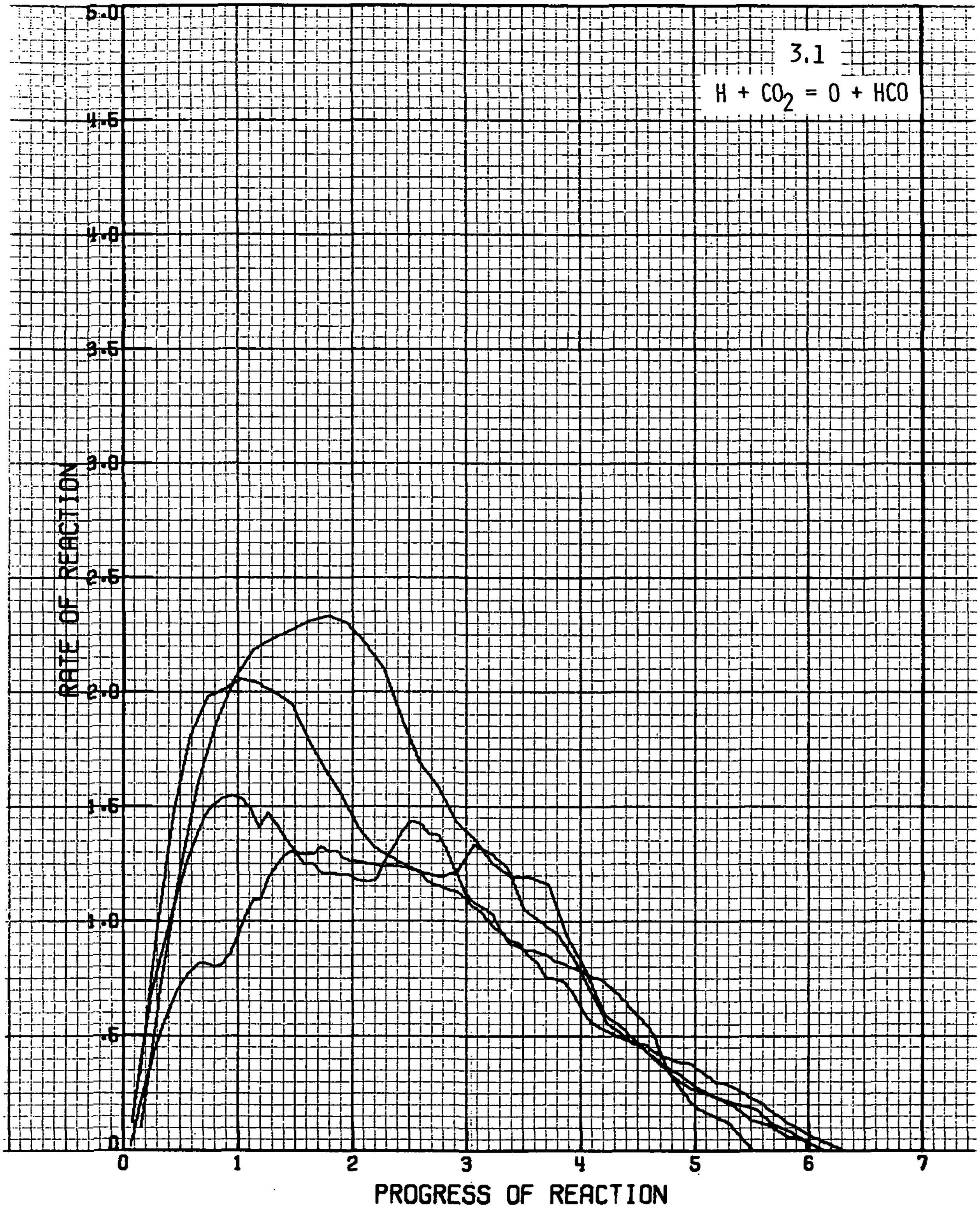

3.1
$H + CO_2 = 0 + HCO$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-22

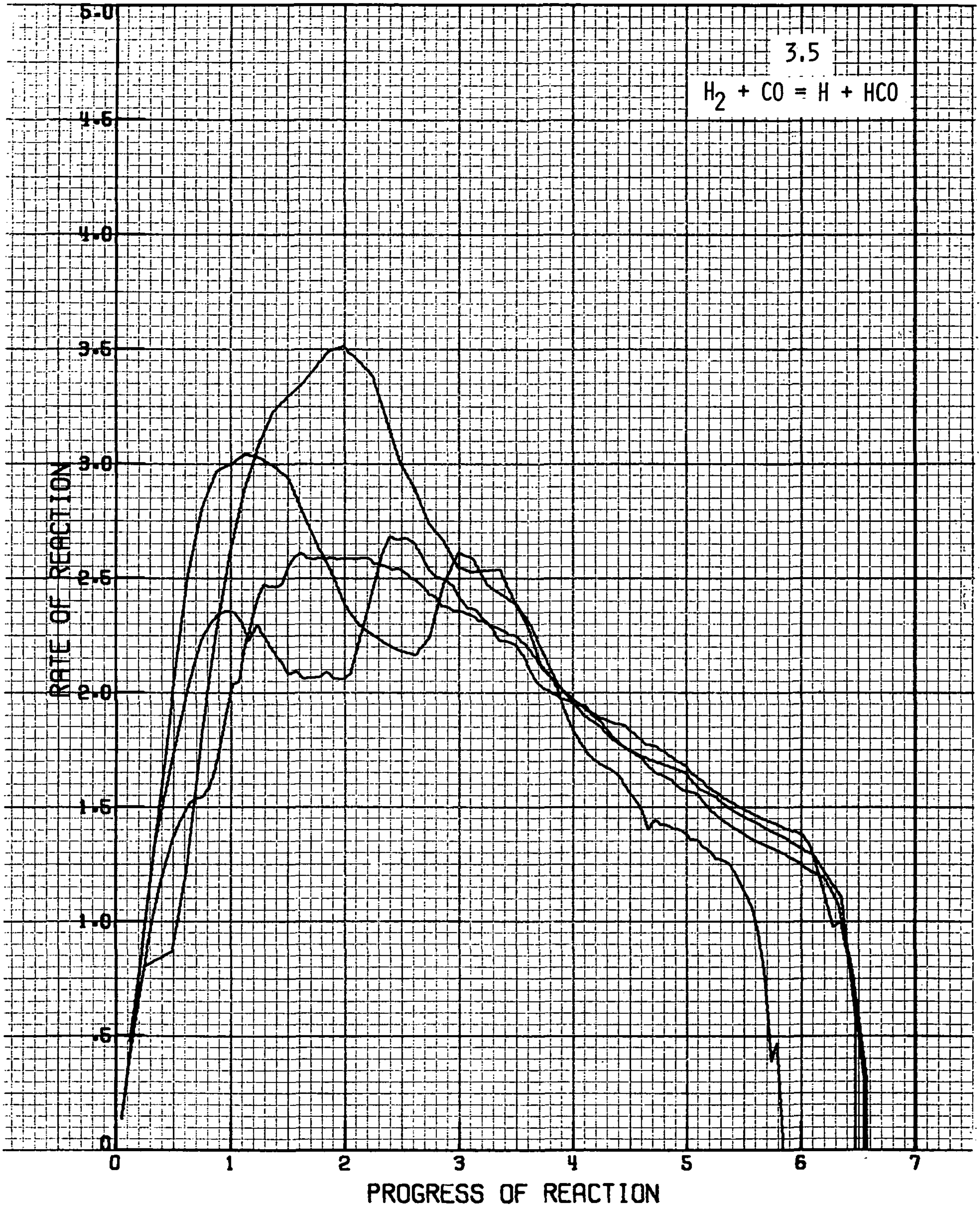

3.5
$H_2 + CO = H + HCO$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-23

3.7
OH + CO = O + HCO
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-24

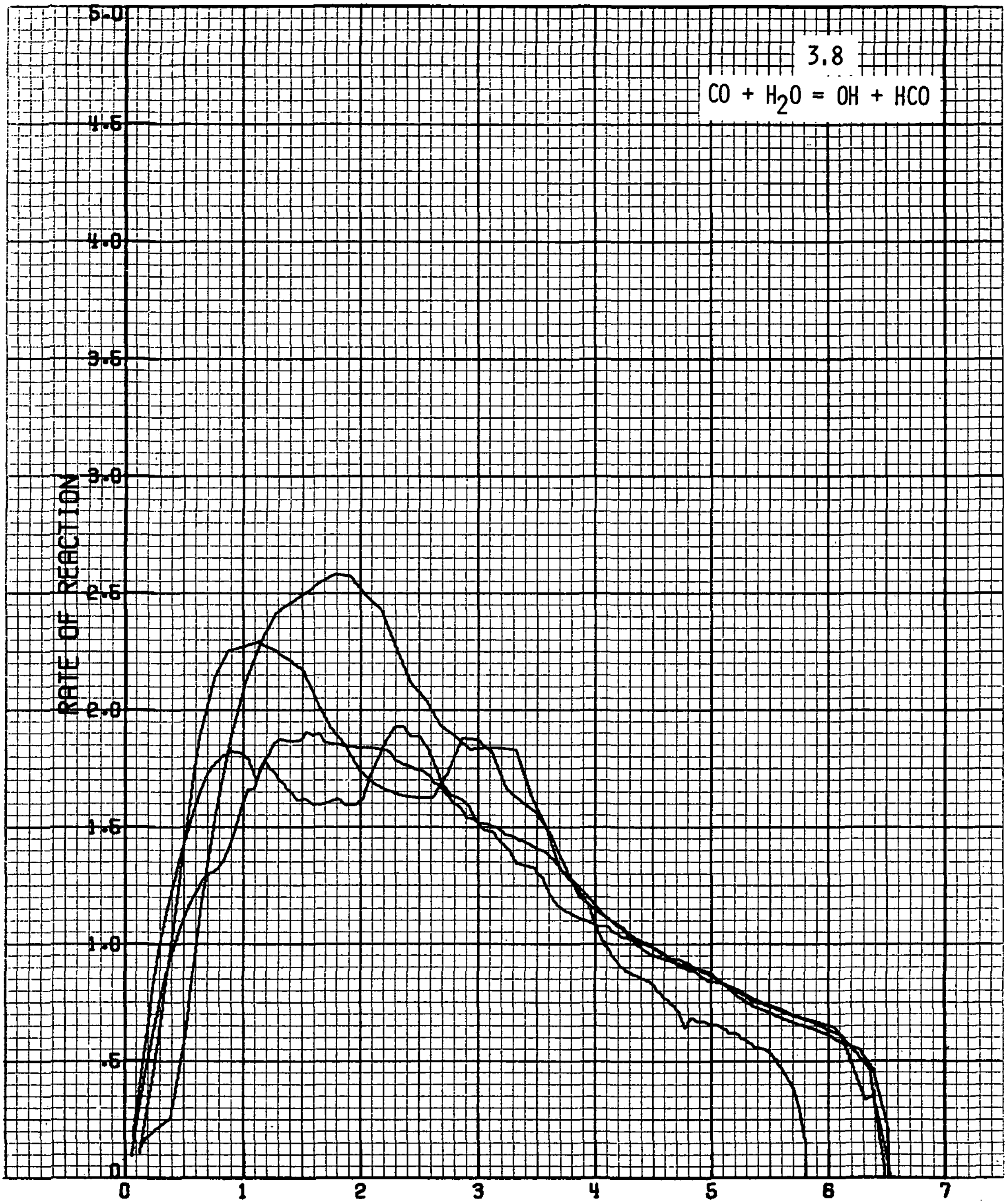

3.8
$CO + H_2O = OH + HCO$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-25

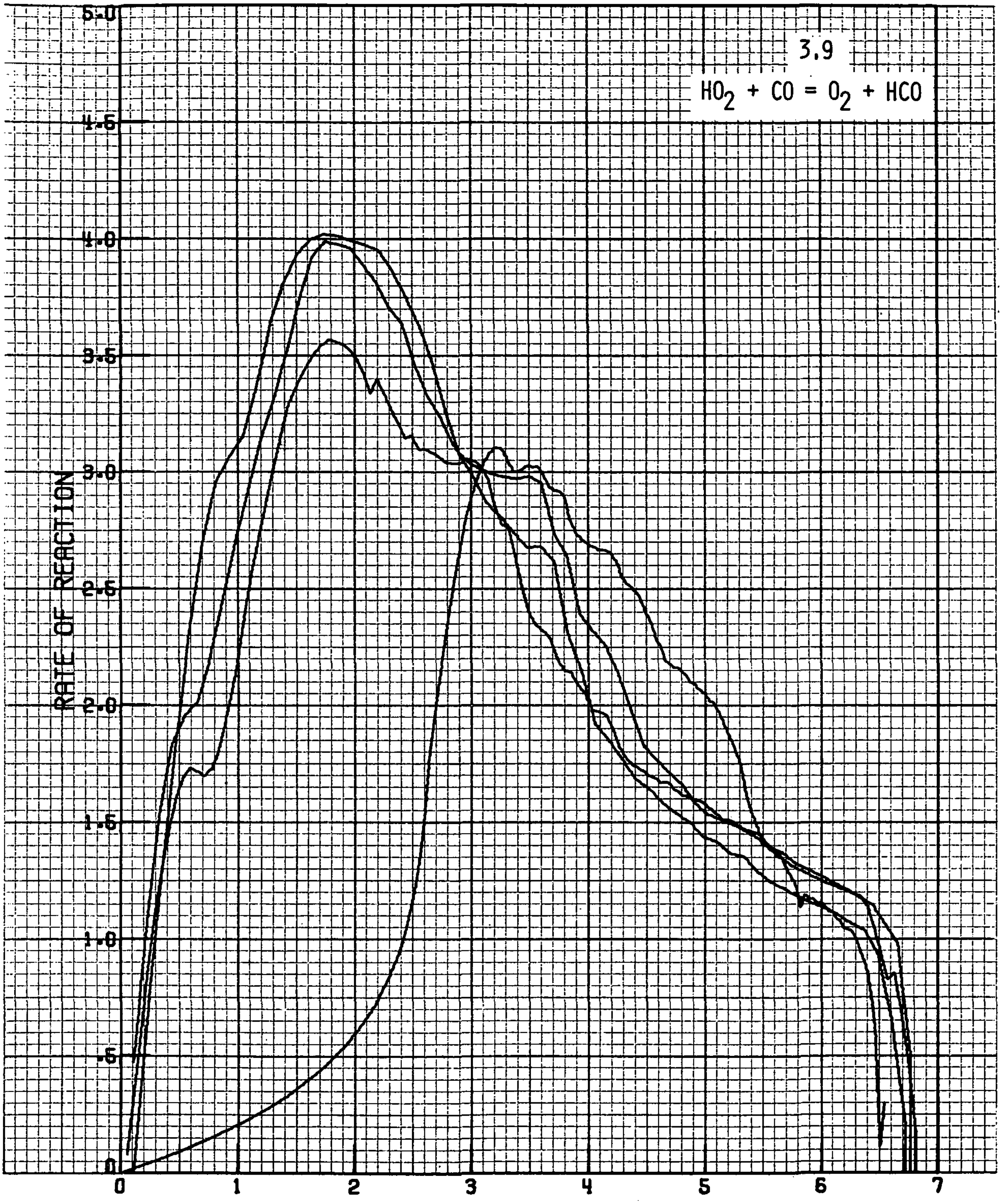

3.9
$HO_2 + CO = O_2 + HCO$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-26

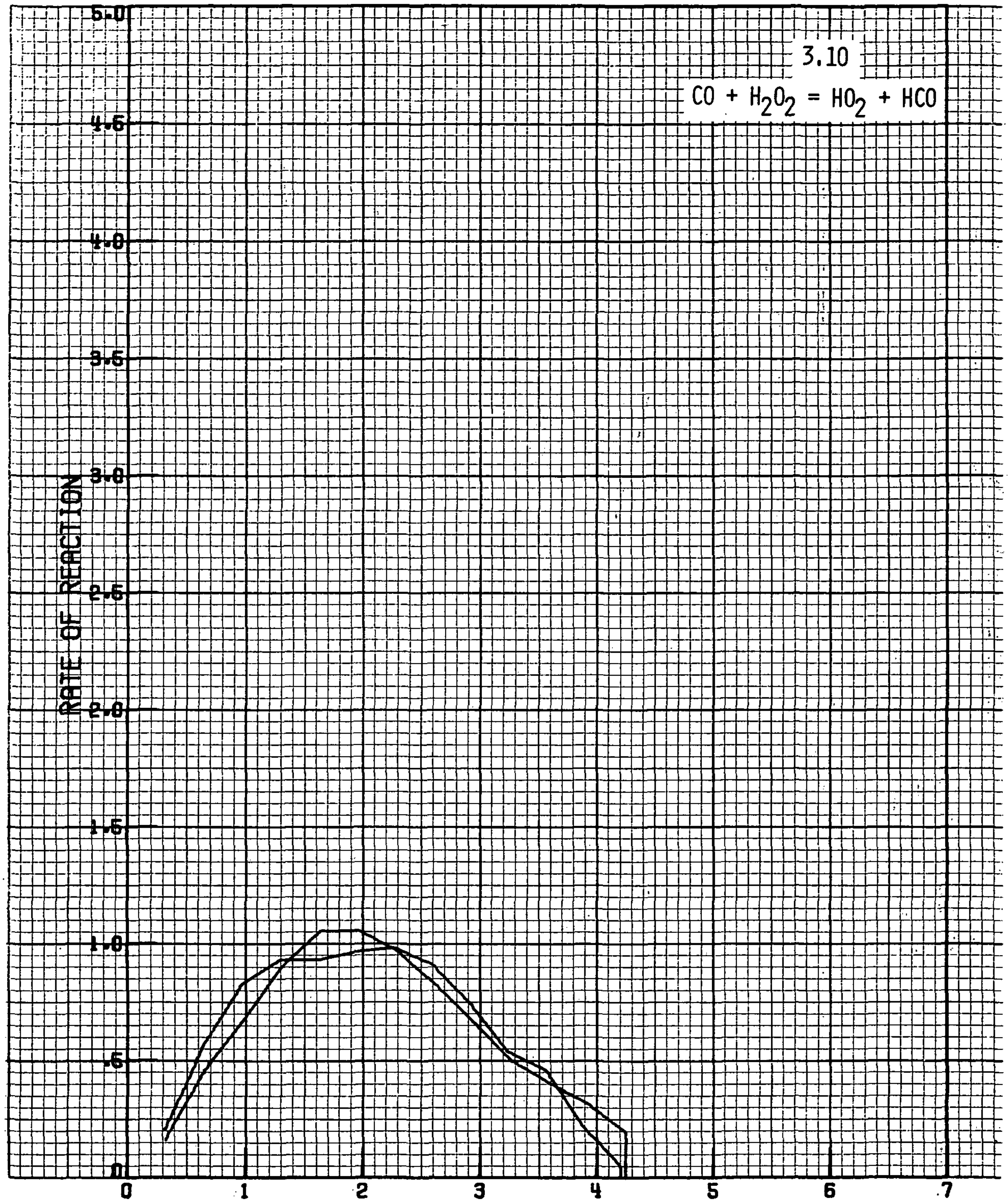

3.10
$CO + H_2O_2 = HO_2 + HCO$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-27

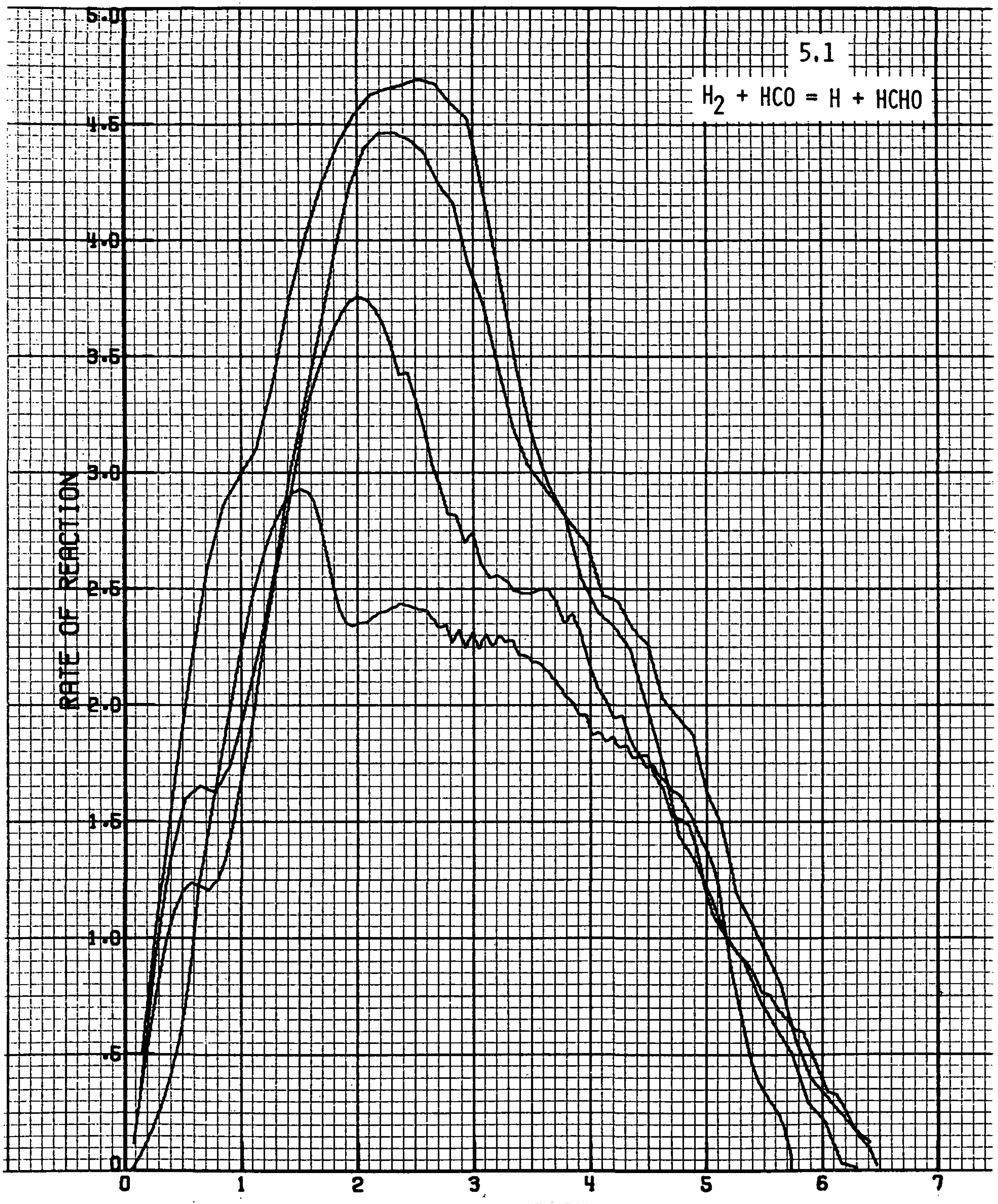

5.1
H_2 + HCO = H + HCHO
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-28

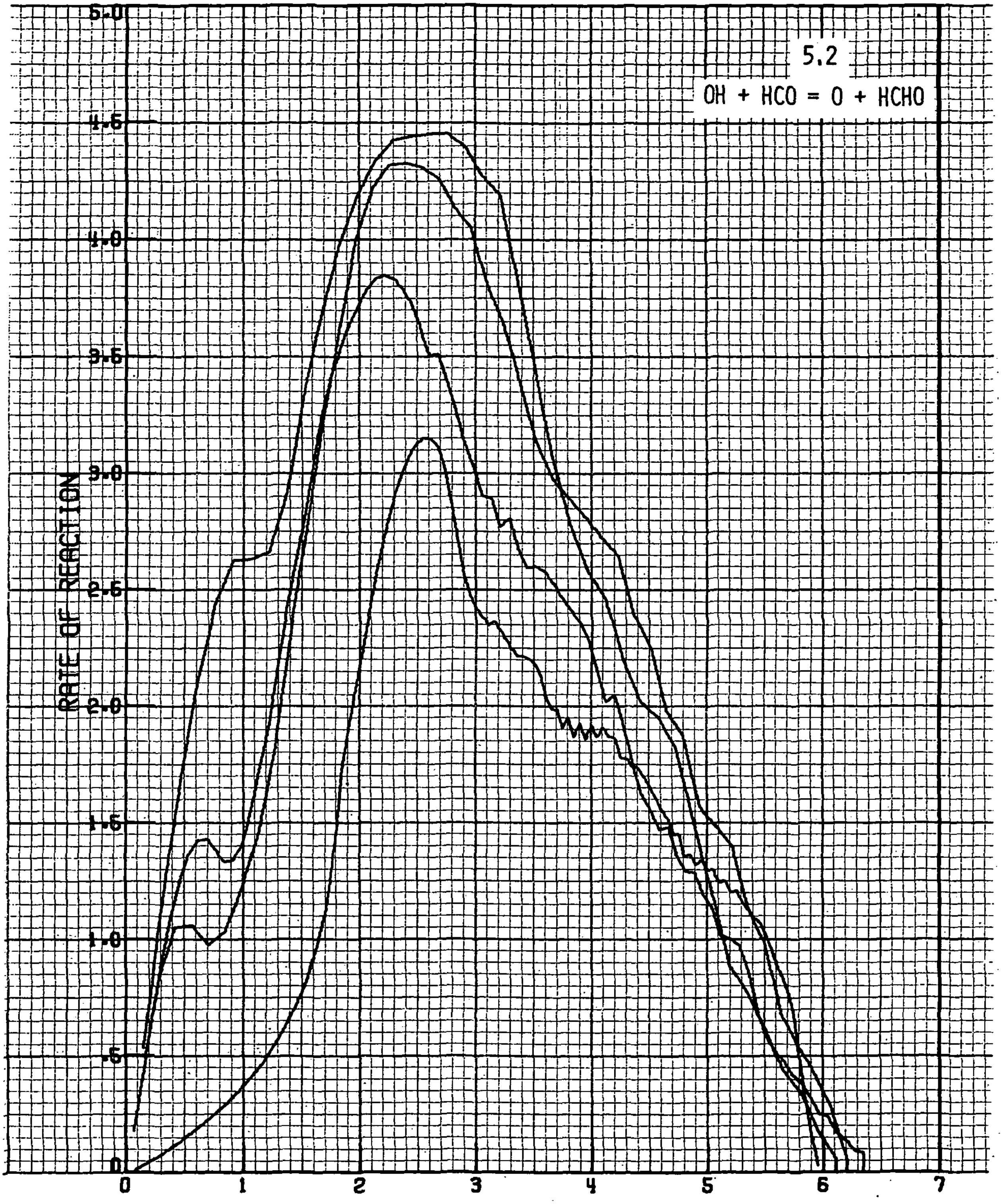

5.2
OH + HCO = O + HCHO
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-29

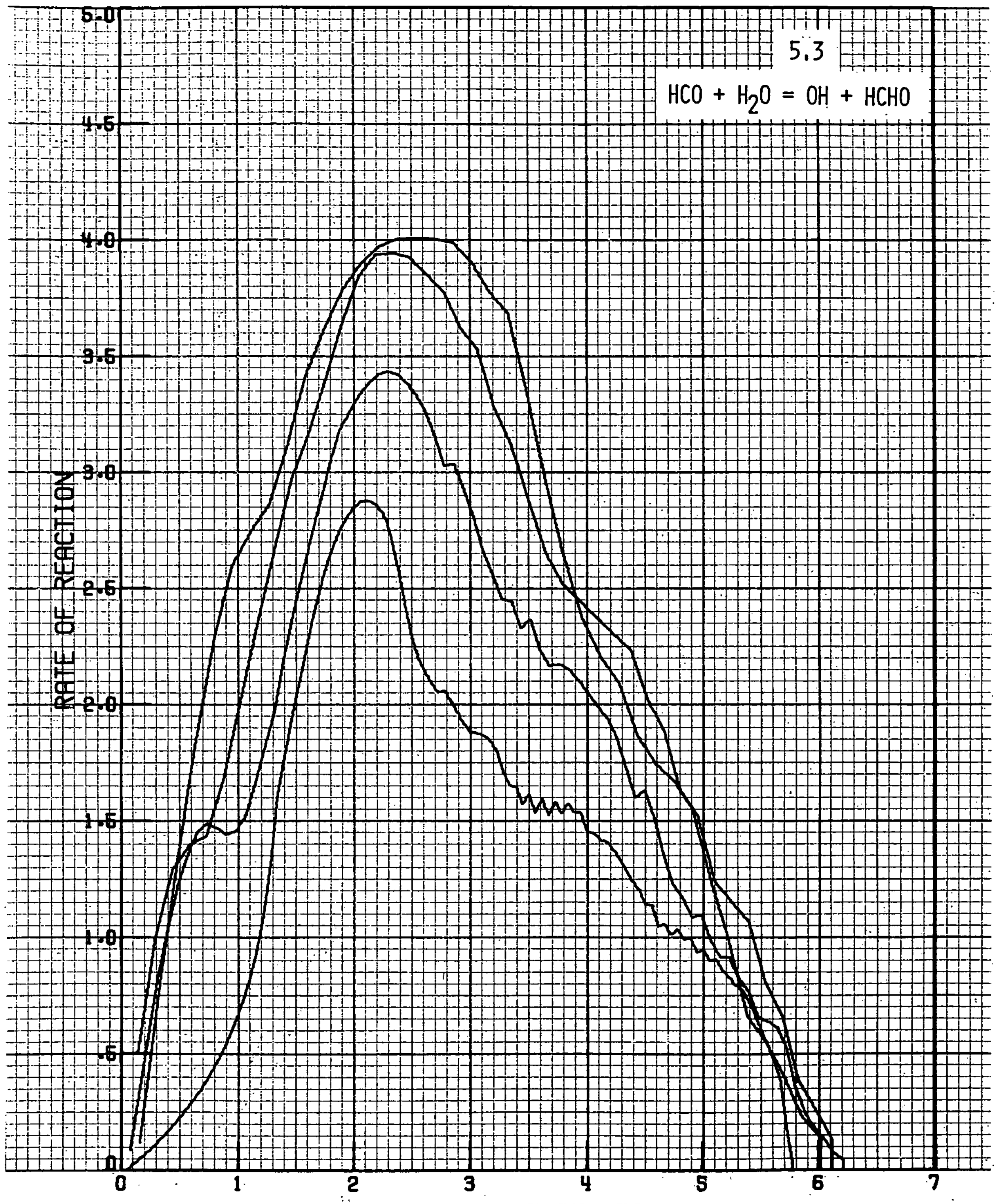

5.3
HCO + H_2O = OH + HCHO
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-30

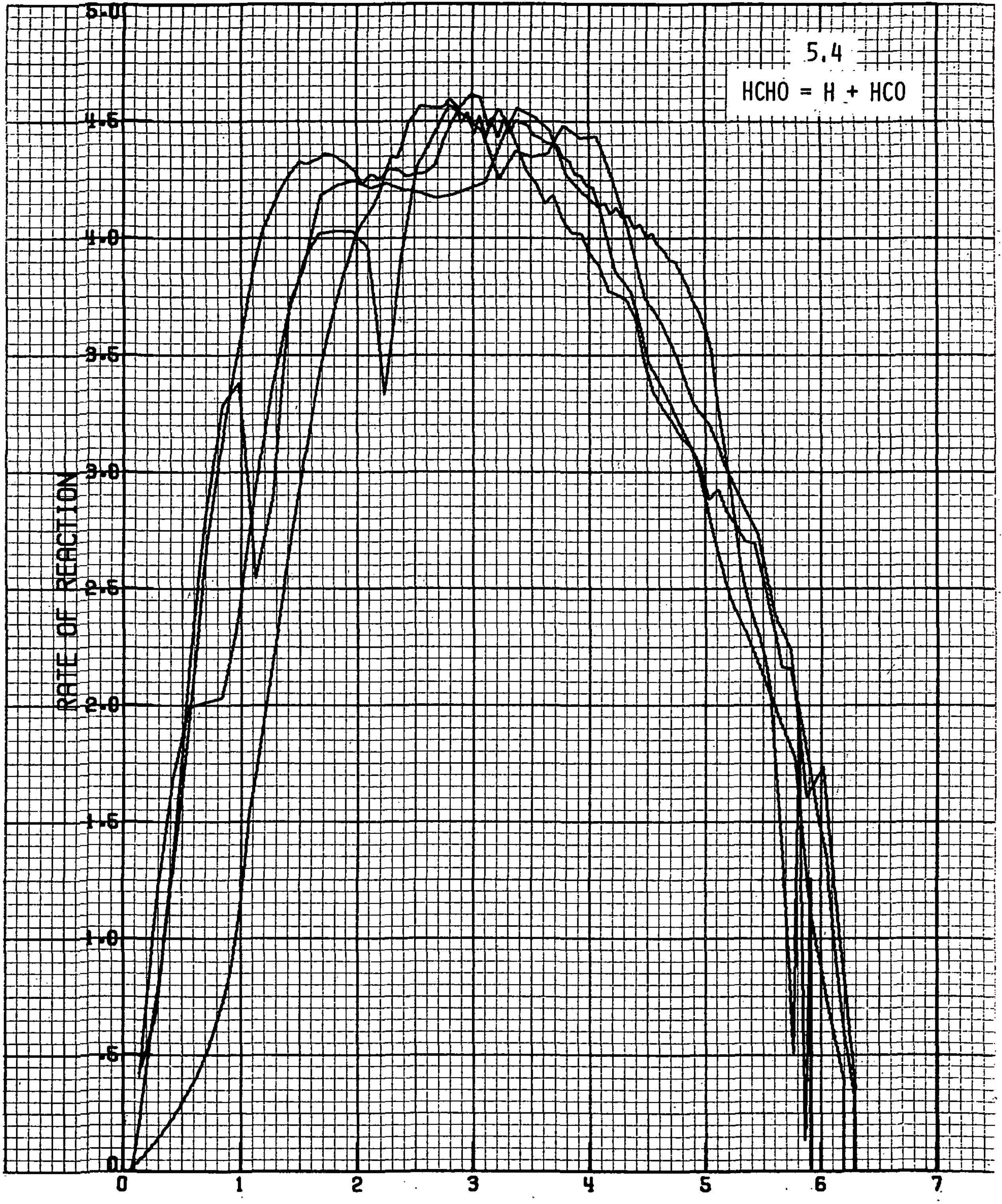

5.4
HCHO = H + HCO
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-31

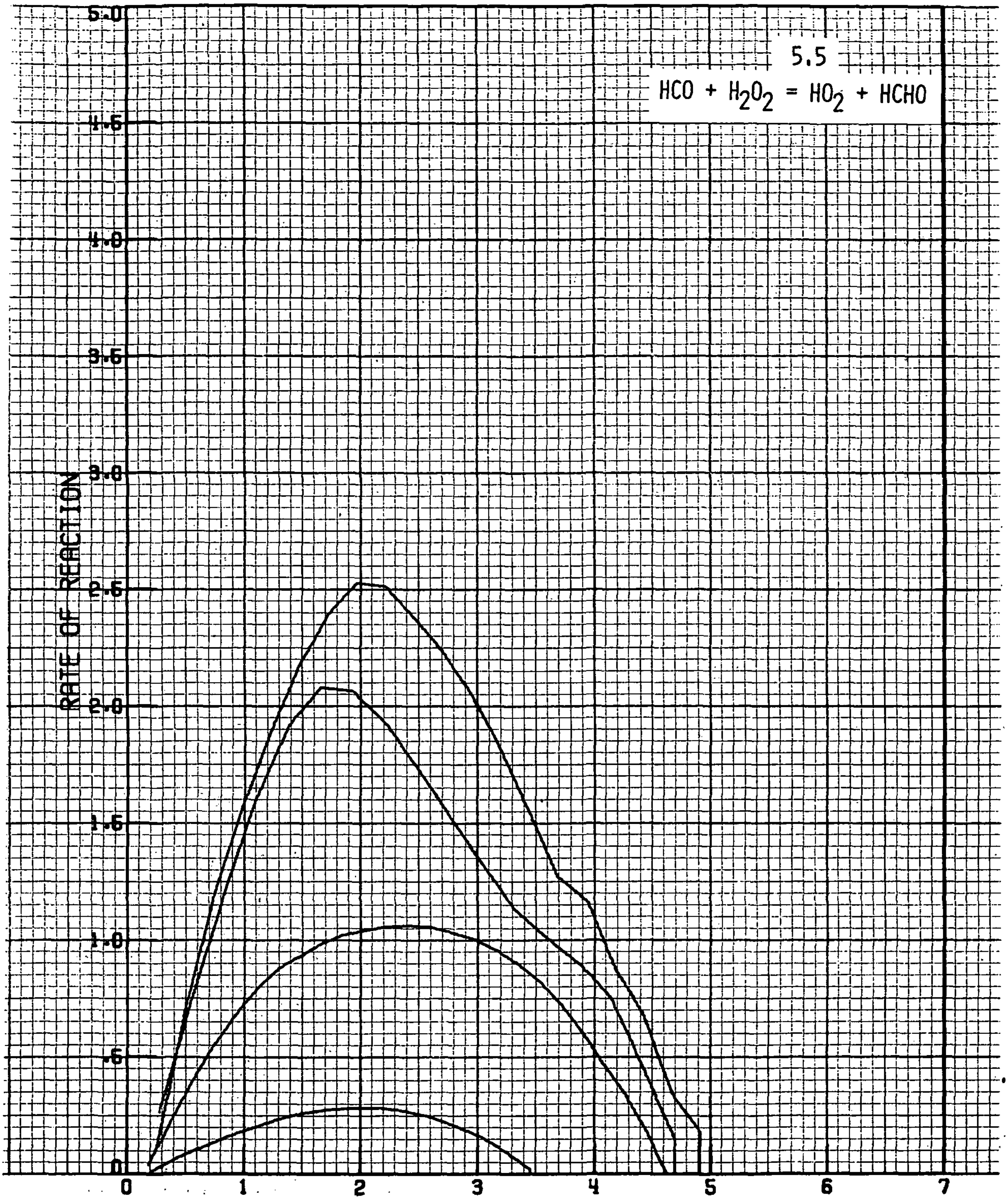

5.5
$HCO + H_2O_2 = HO_2 + HCHO$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-32

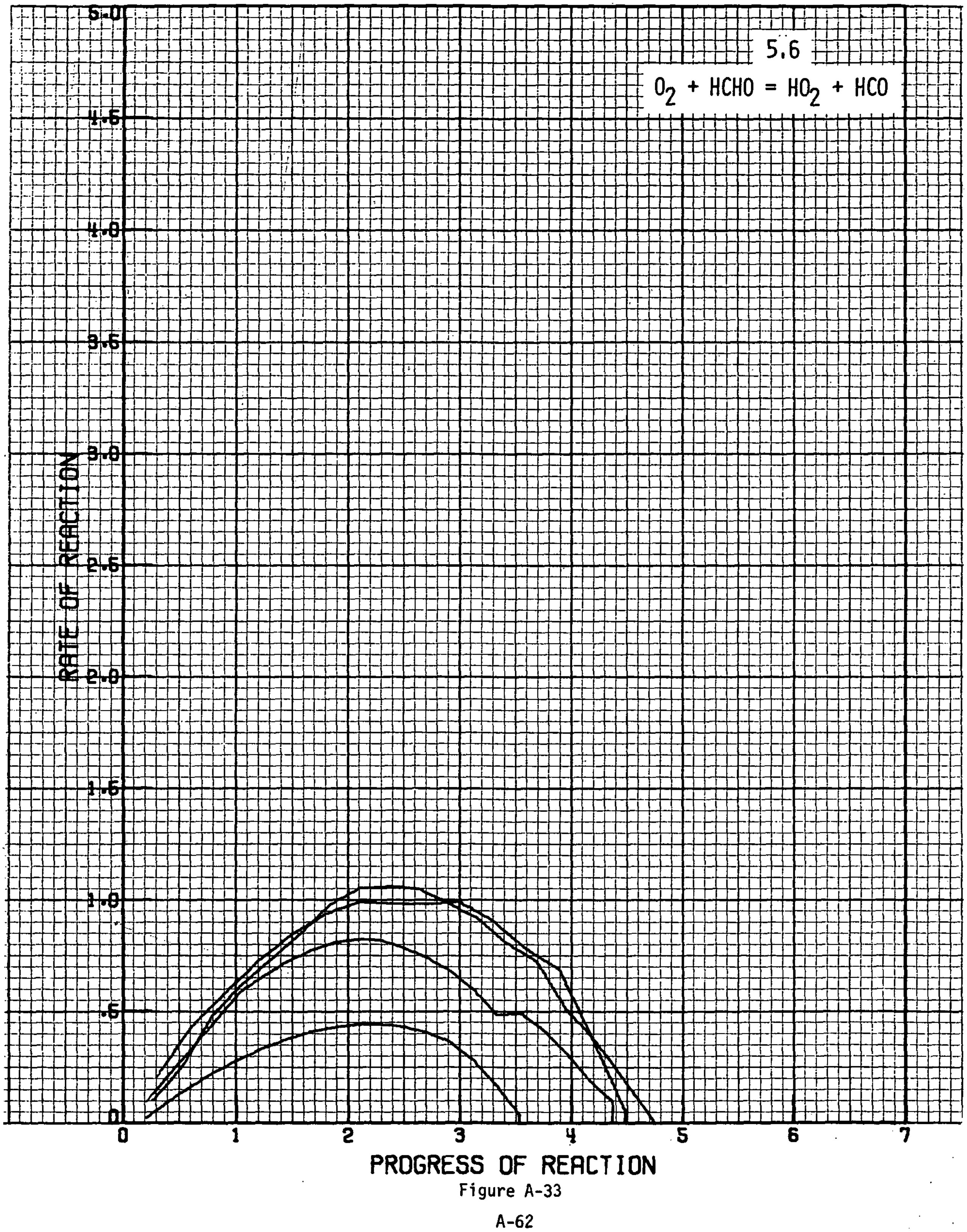

5.6
$O_2 + HCHO = HO_2 + HCO$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-33

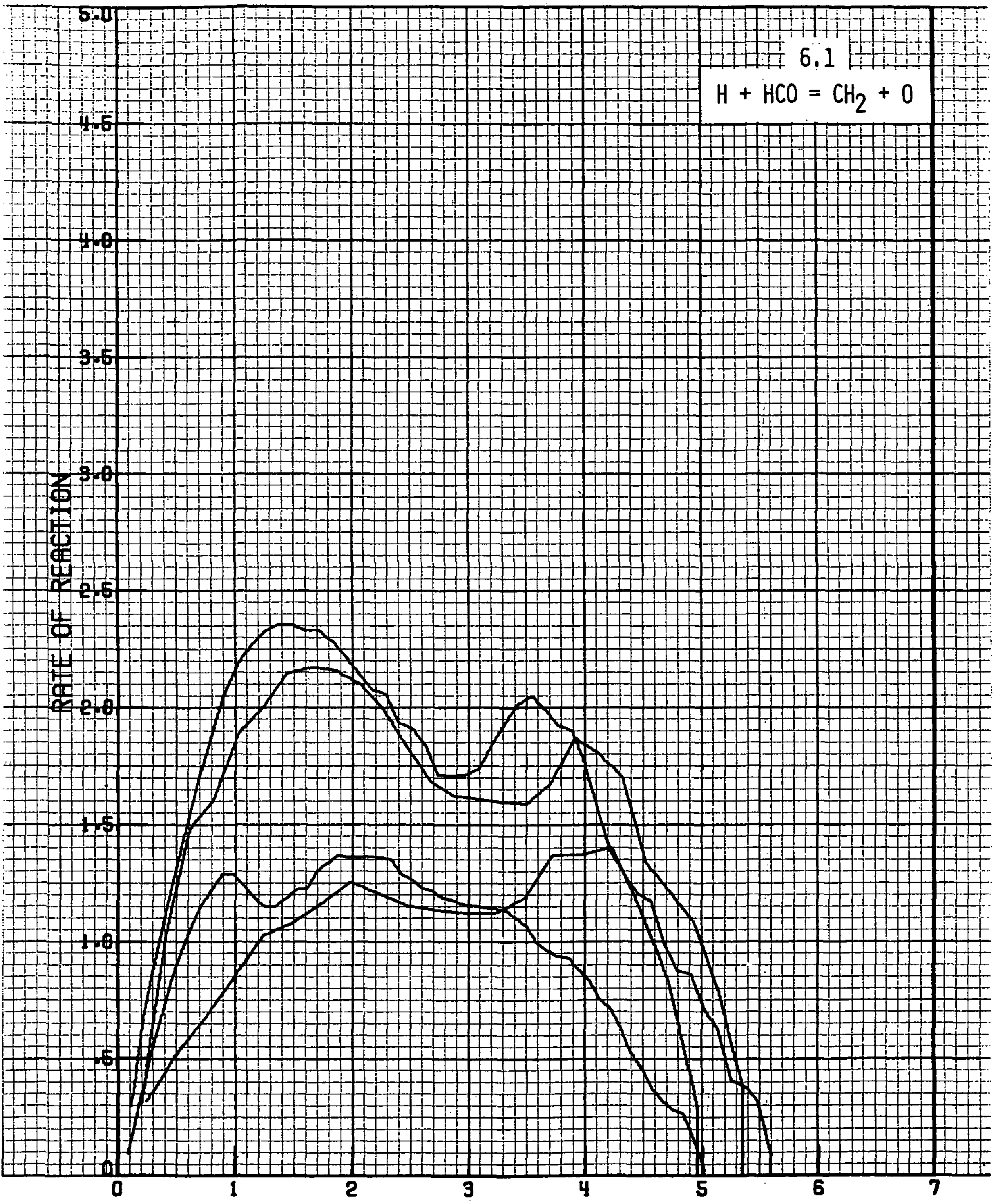

6.1
H + HCO = CH2 + O
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-34

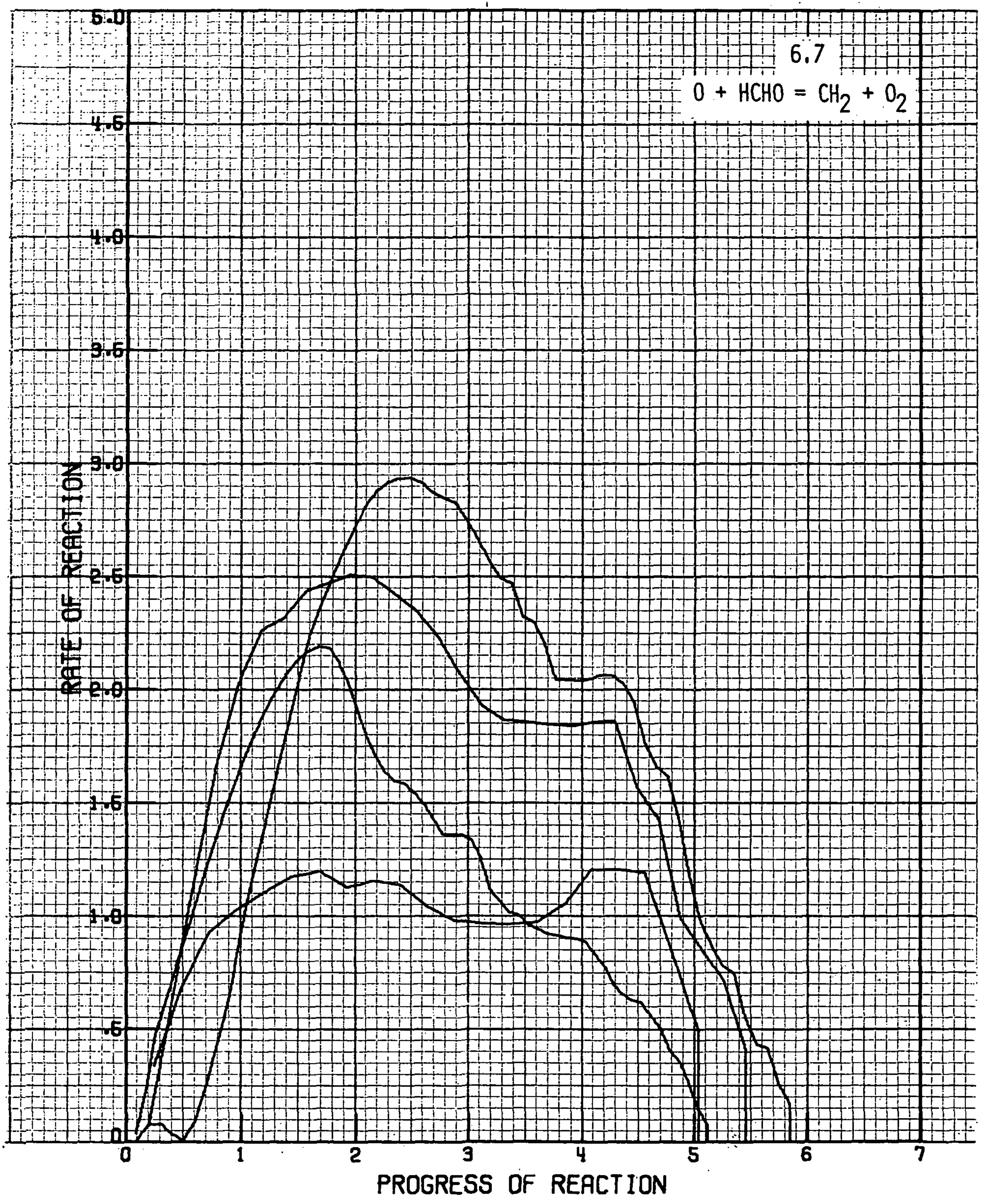

6.7
$O + HCHO = CH_2 + O_2$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
PROGRESS OF REACTION
0
1
2
3
4
5
6
7

Figure A-35

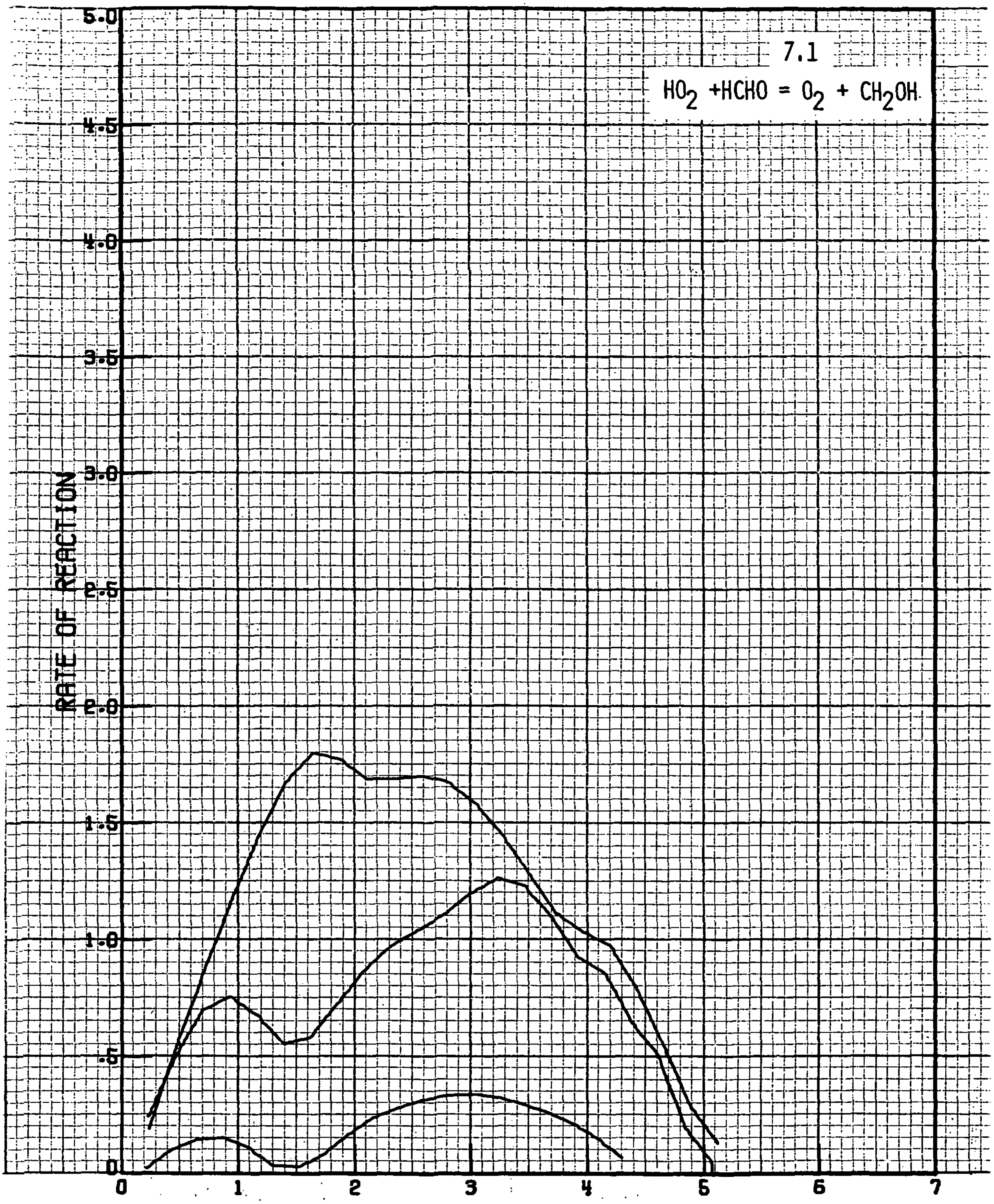

7.1
$HO_2 + HCHO = O_2 + CH_2OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-36

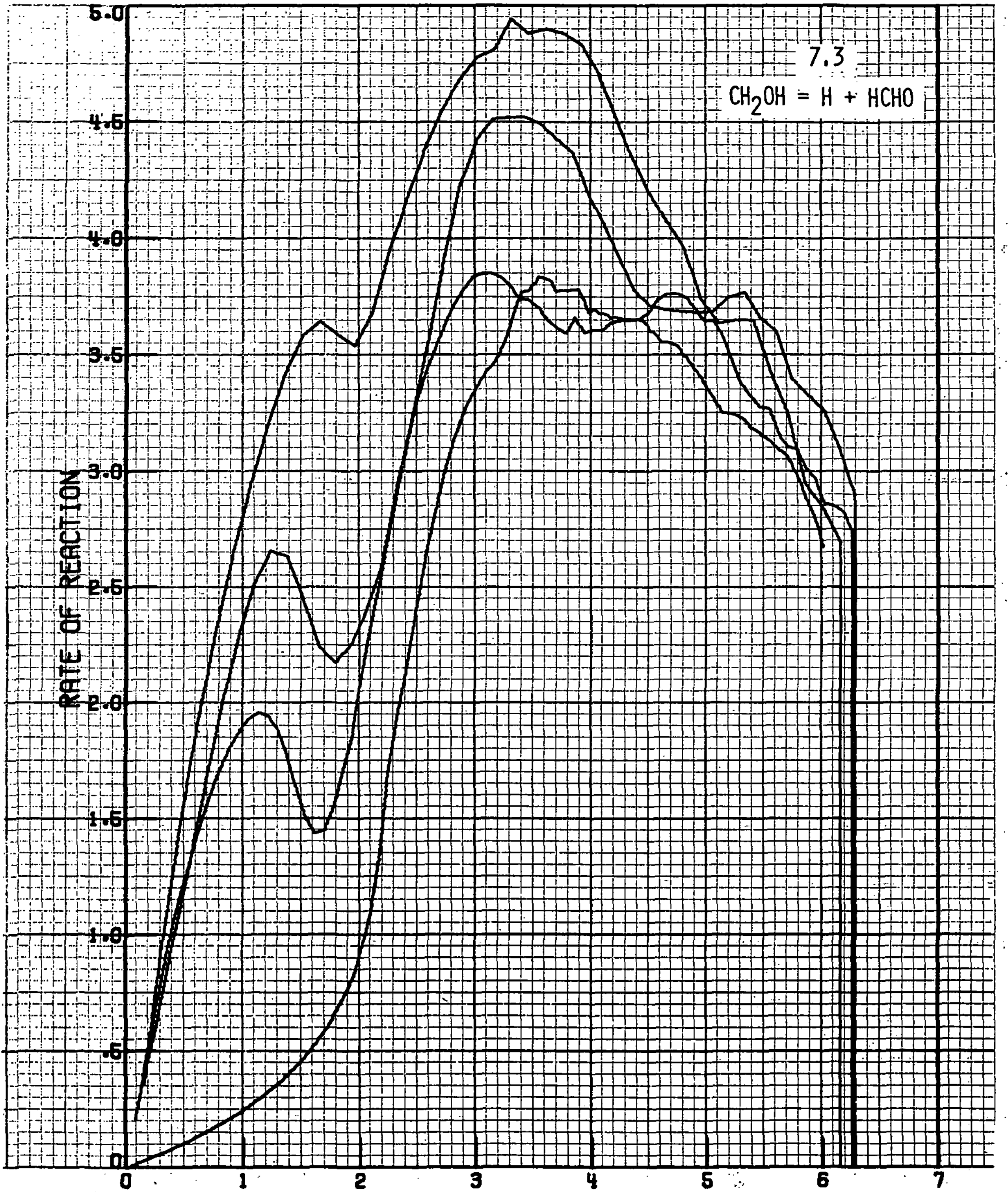

7.3
$CH_2OH = H + HCHO$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-37

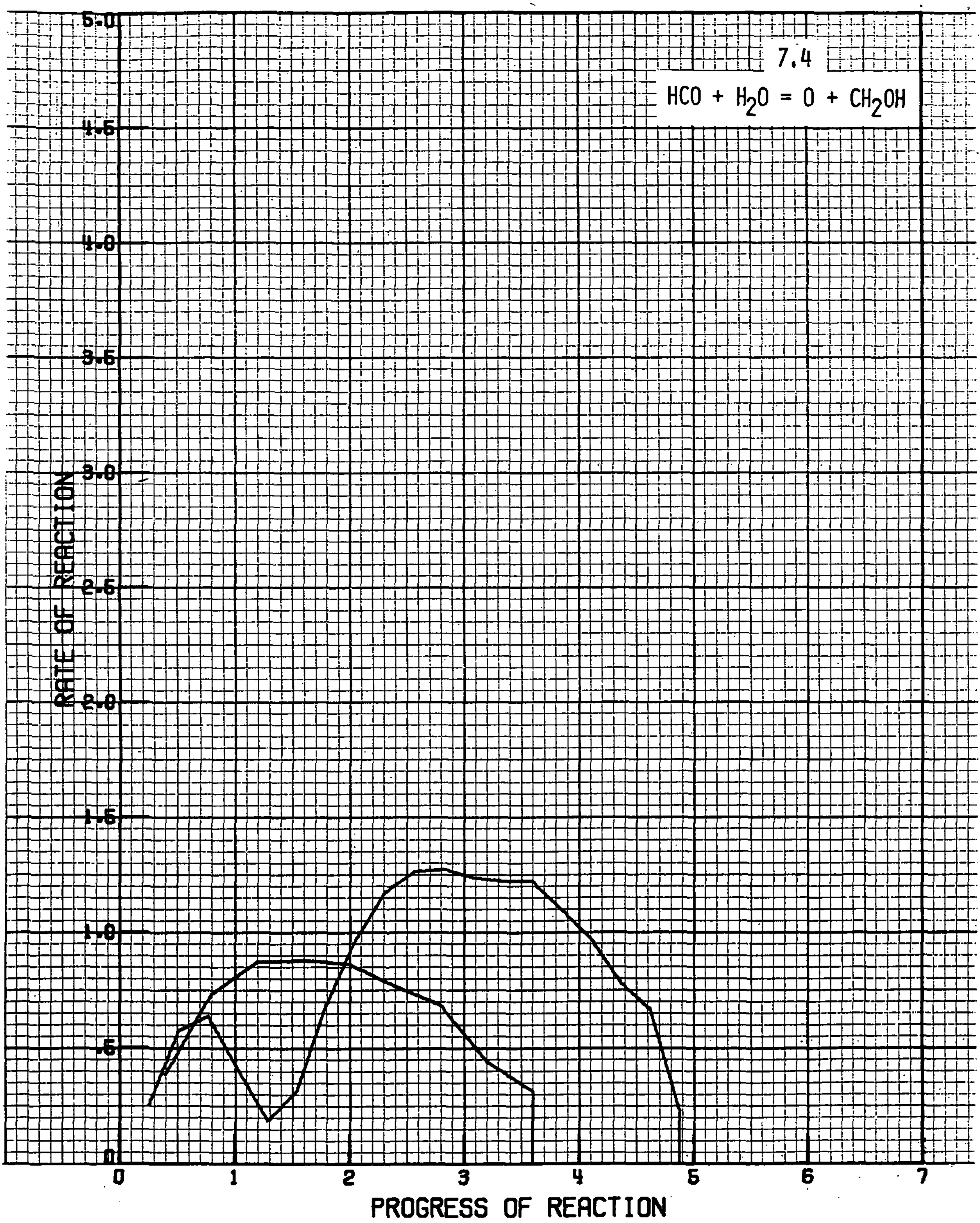

7.4
HCO + H2O = O + CH2OH
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-38

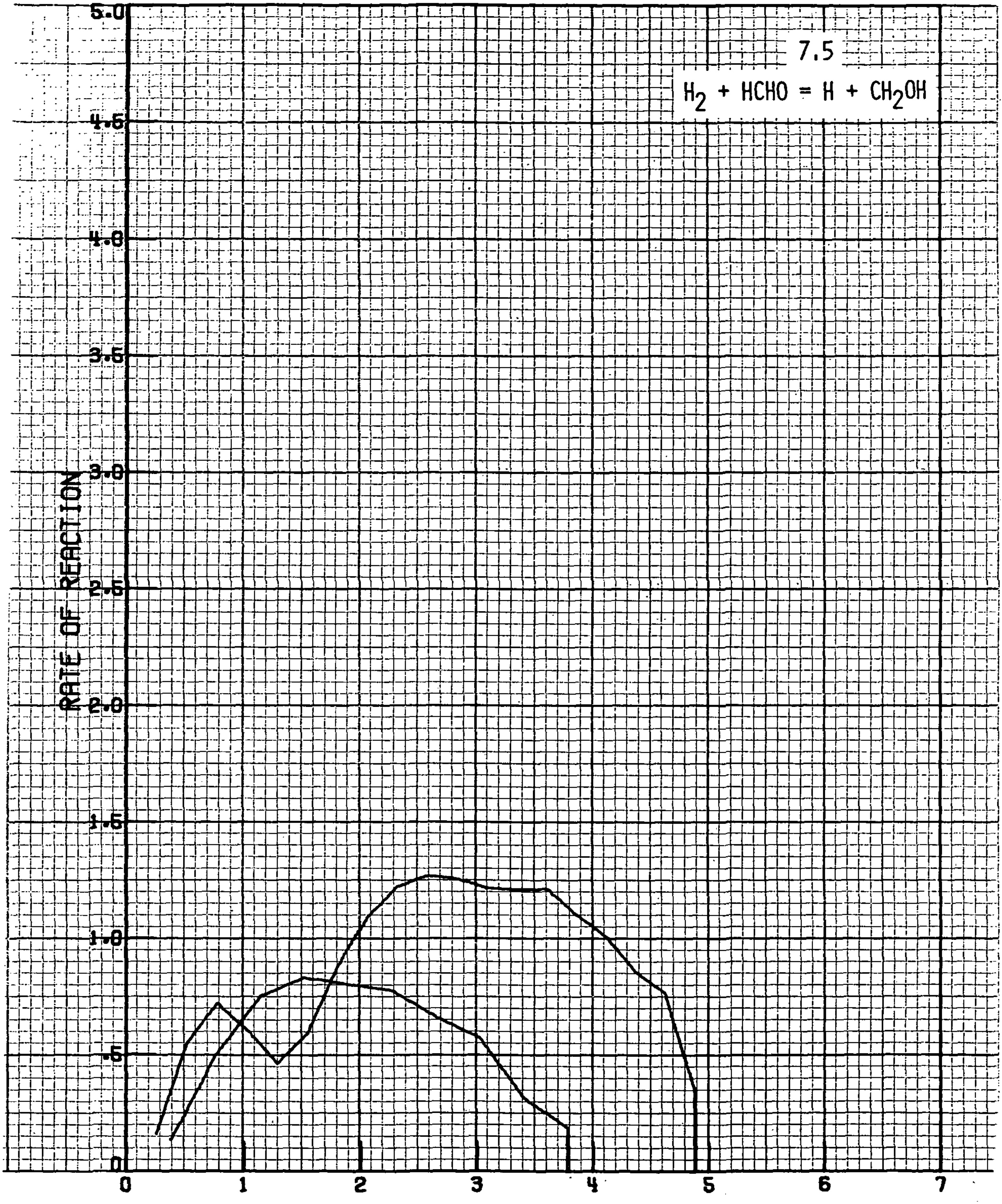

5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
RATE OF REACTION
0
1
2
3
4
5
6
7
PROGRESS OF REACTION
7.5
$H_2 + HCHO = H + CH_2OH$

Figure A-39

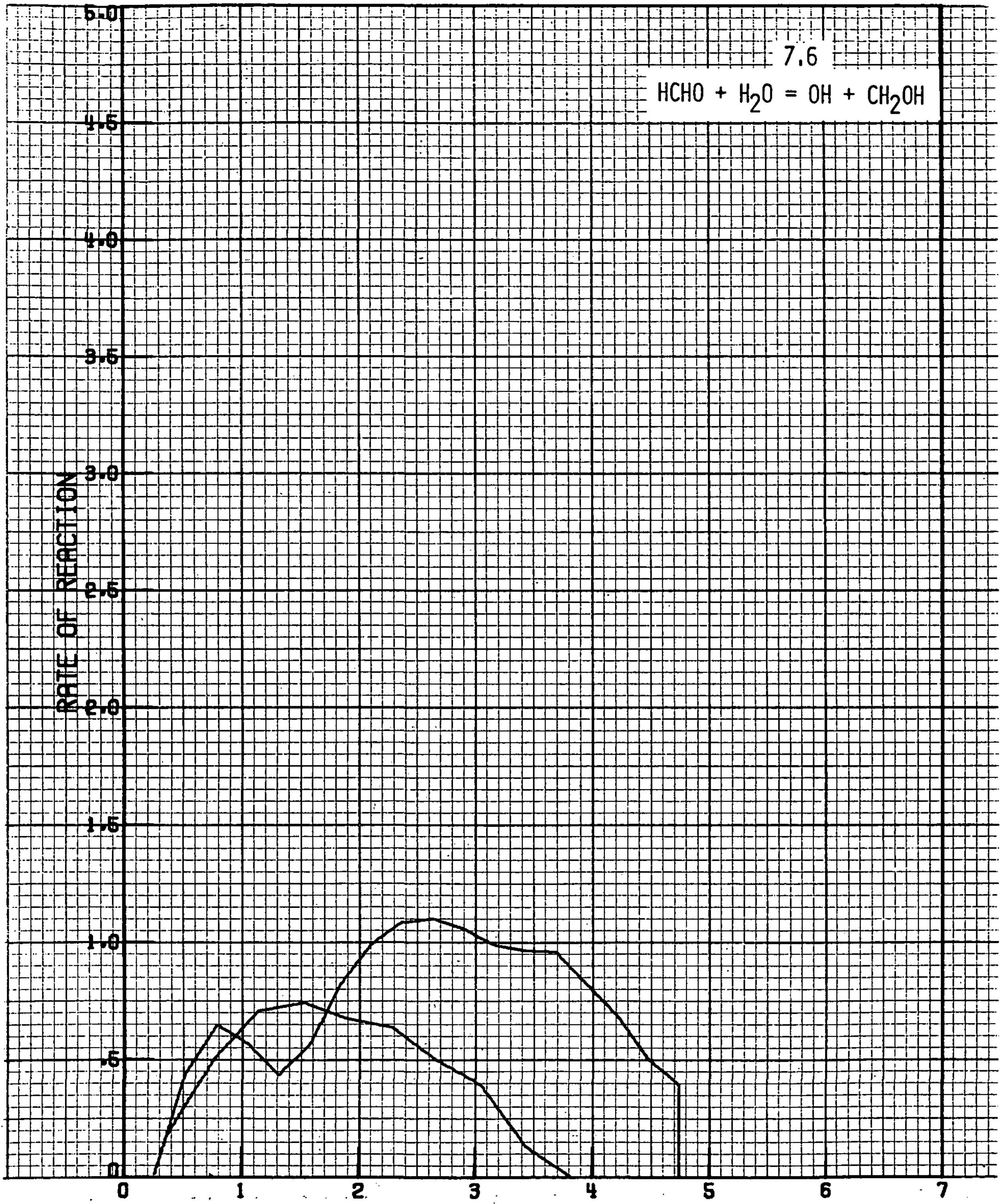

7.6
$HCHO + H_2O = OH + CH_2OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-40

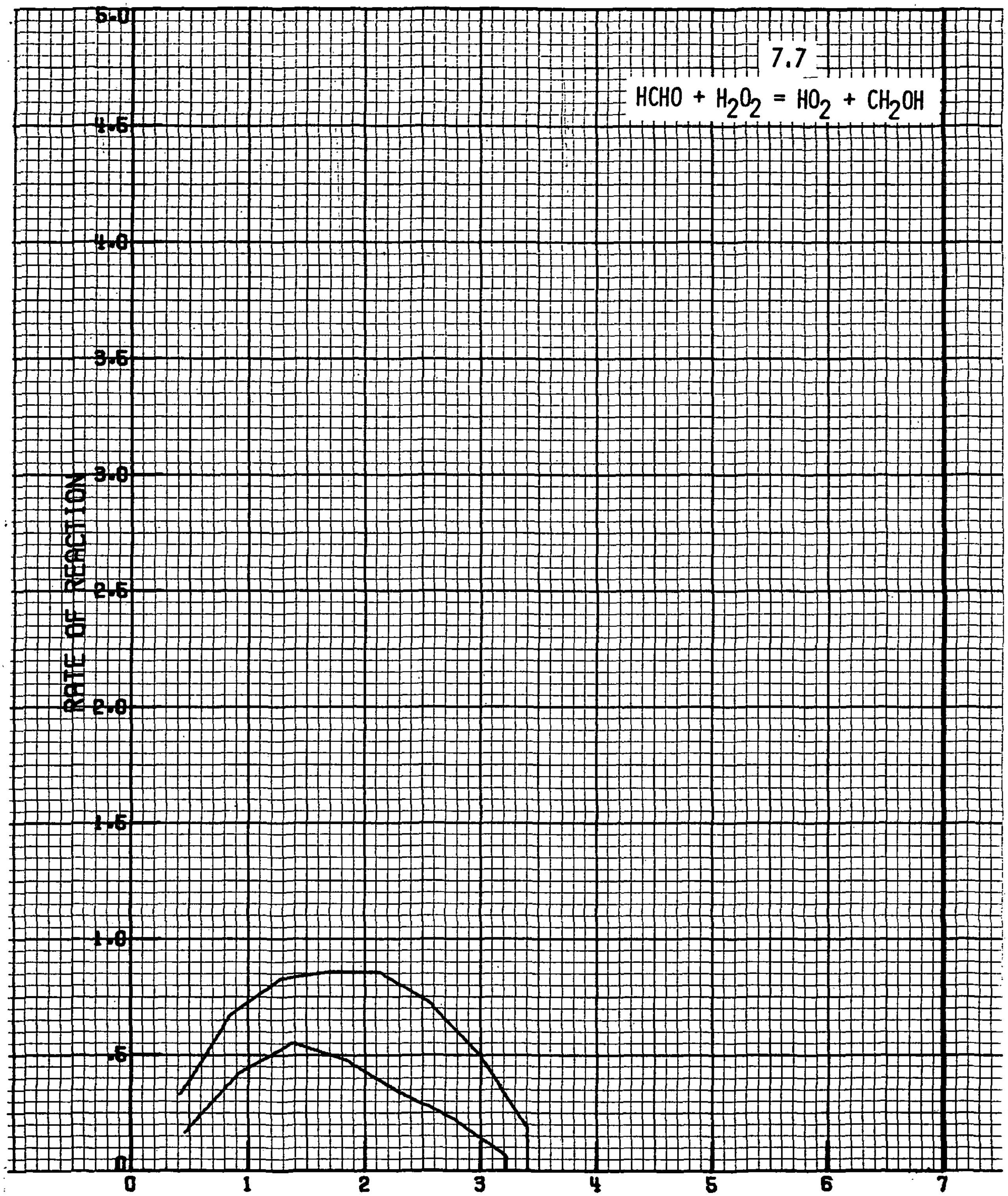

7.7
HCHO + H_2O_2 = HO_2 + CH_2OH
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-41

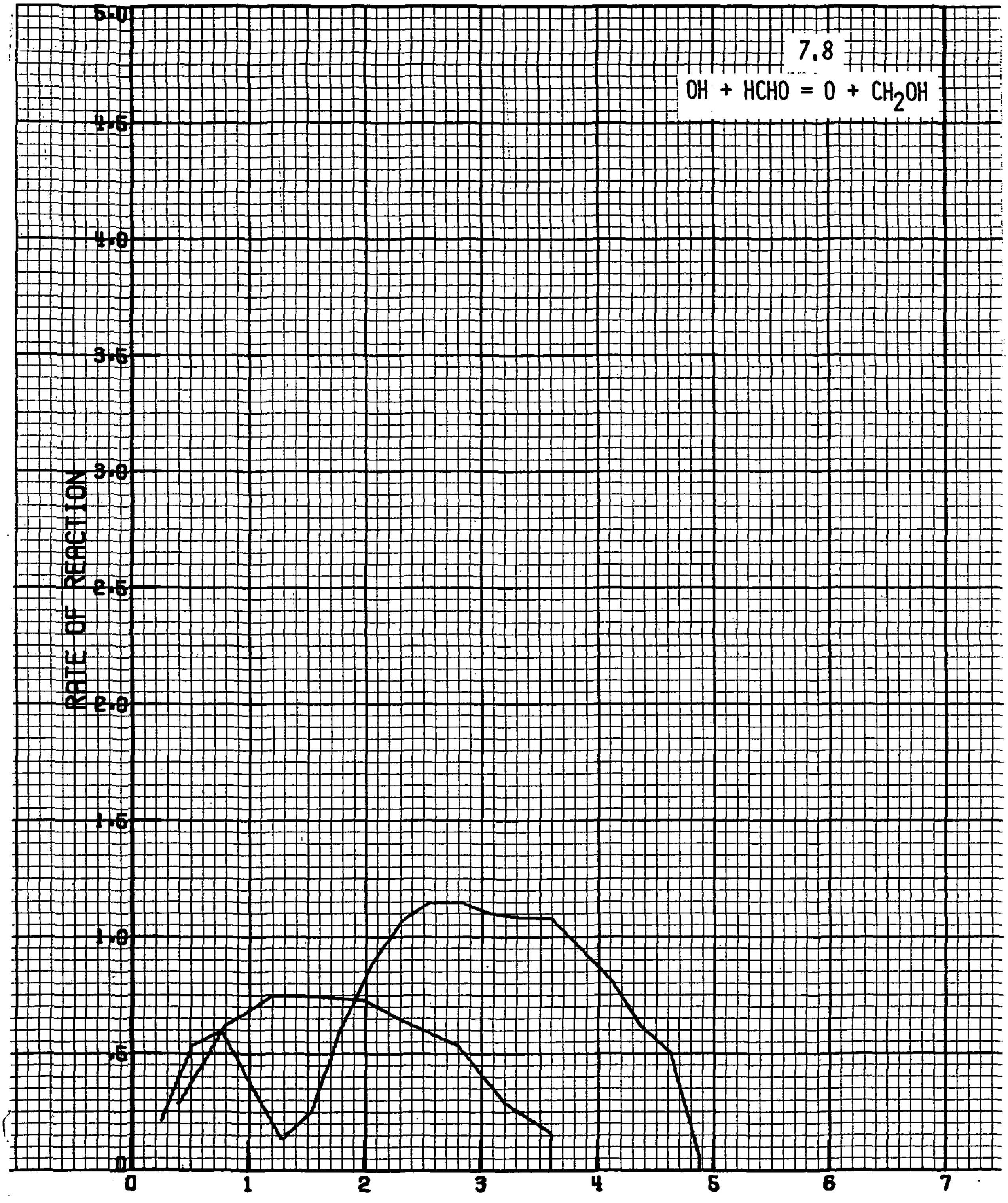

5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
RATE OF REACTION
0
1
2
3
4
5
6
7
PROGRESS OF REACTION
7.8
OH + HCHO = O + CH2OH

Figure A-42

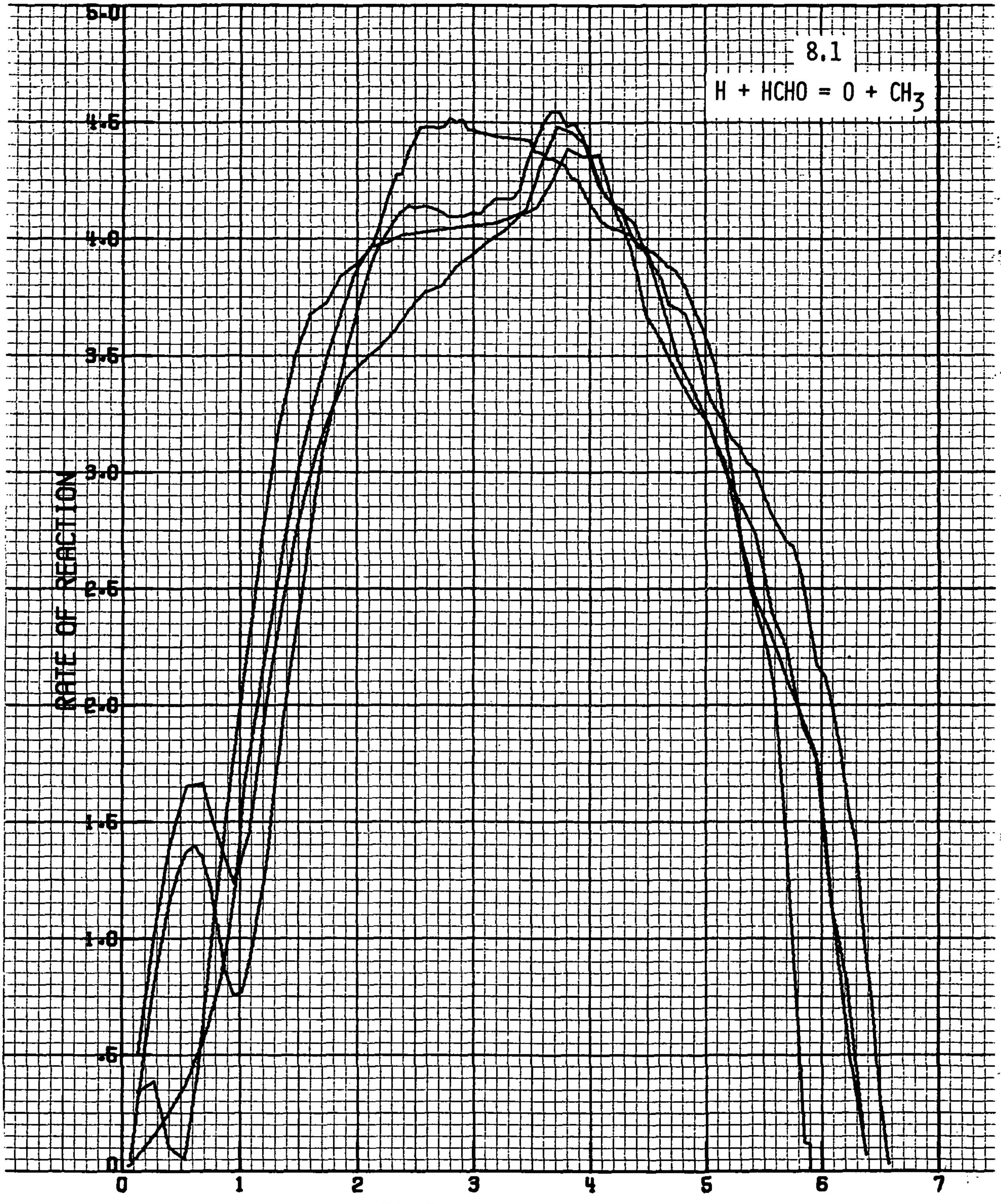

8.1
$H + HCHO = O + CH_3$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-43


8.5
H + CH_2OH = CH_3 + OH
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-44

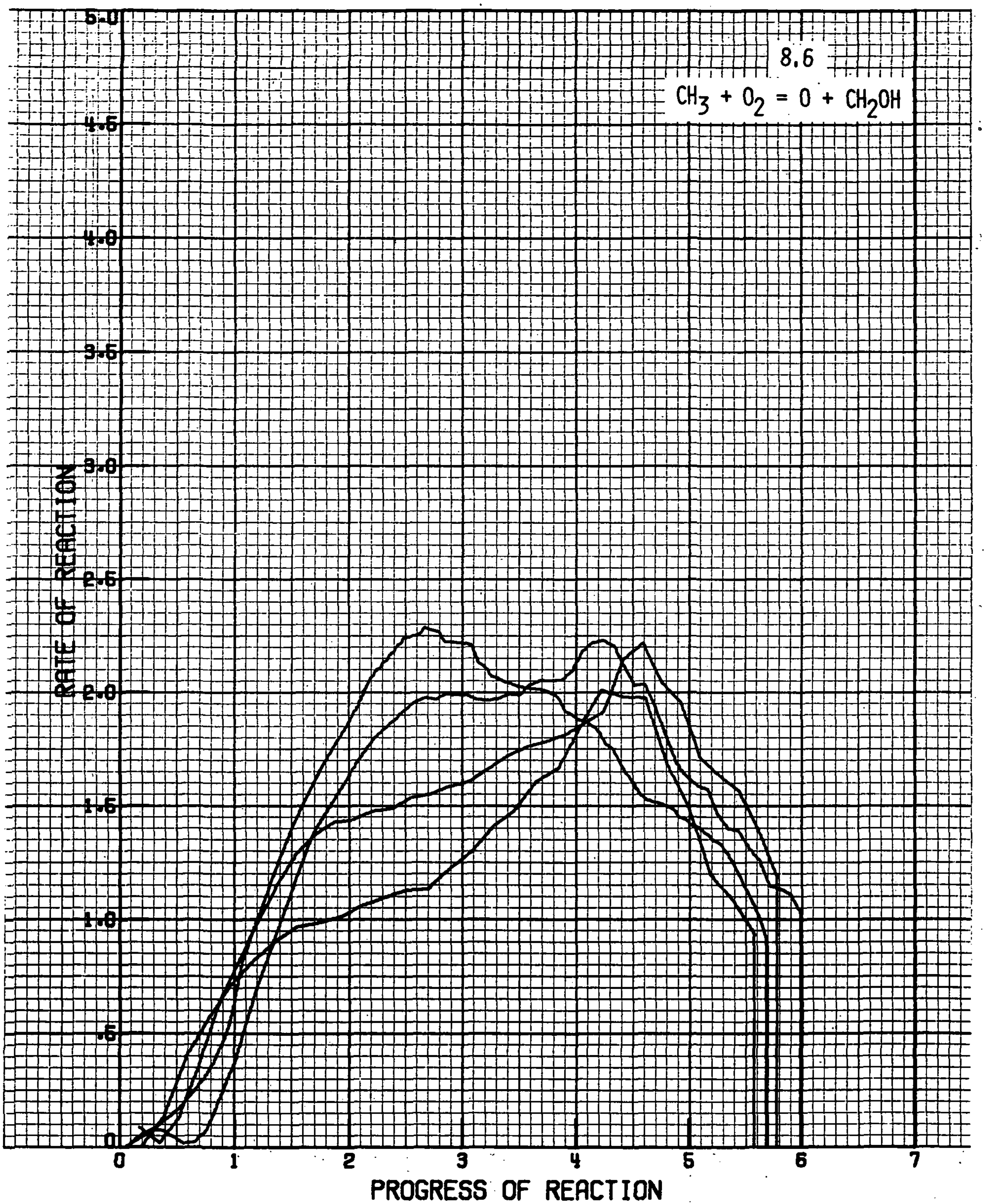

8.6
$CH_3 + O_2 = O + CH_2OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-45


9.1
OH + CH_2OH = O + CH_3OH
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-46

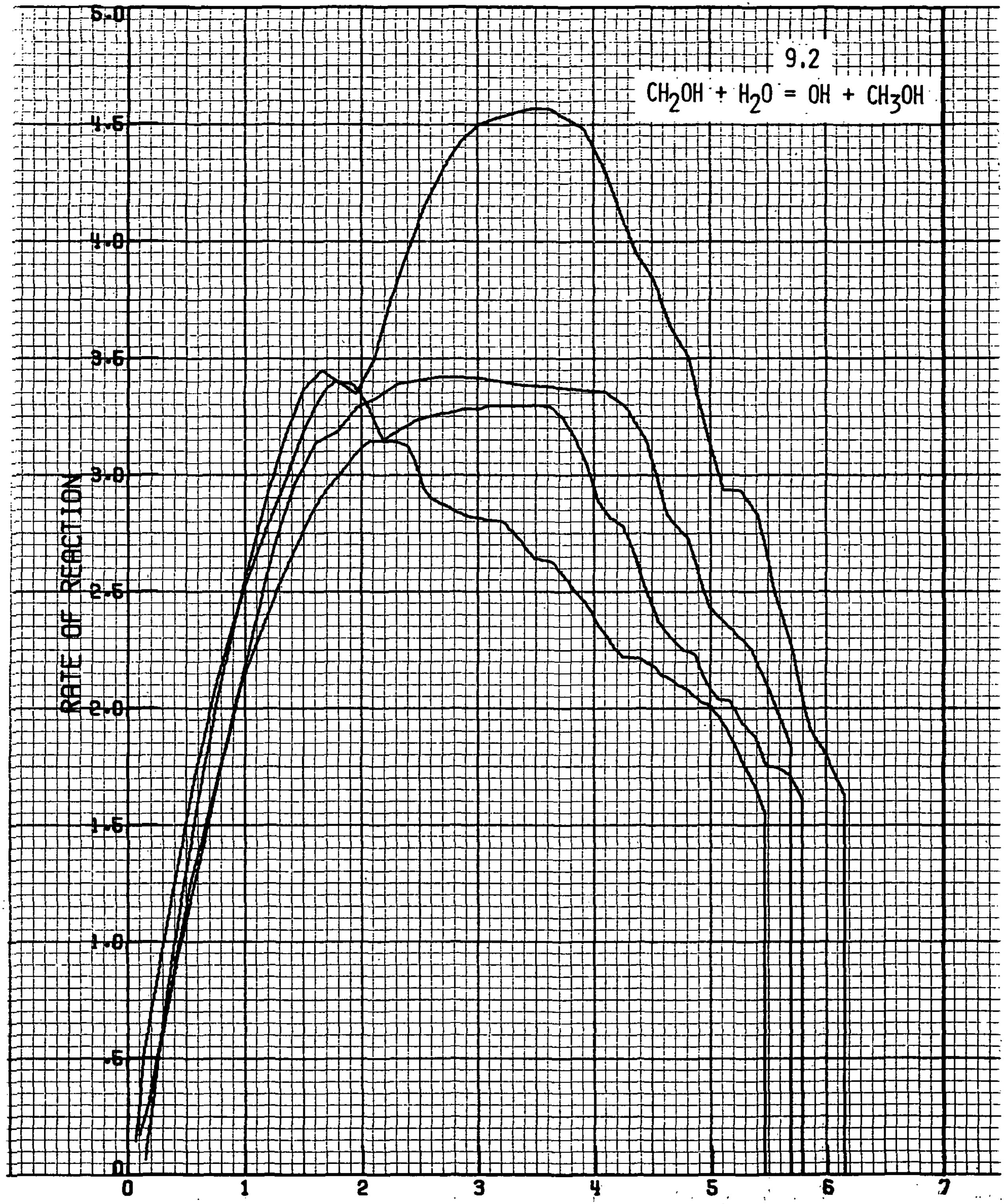

9.2
$CH_2OH + H_2O = OH + CH_3OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-47

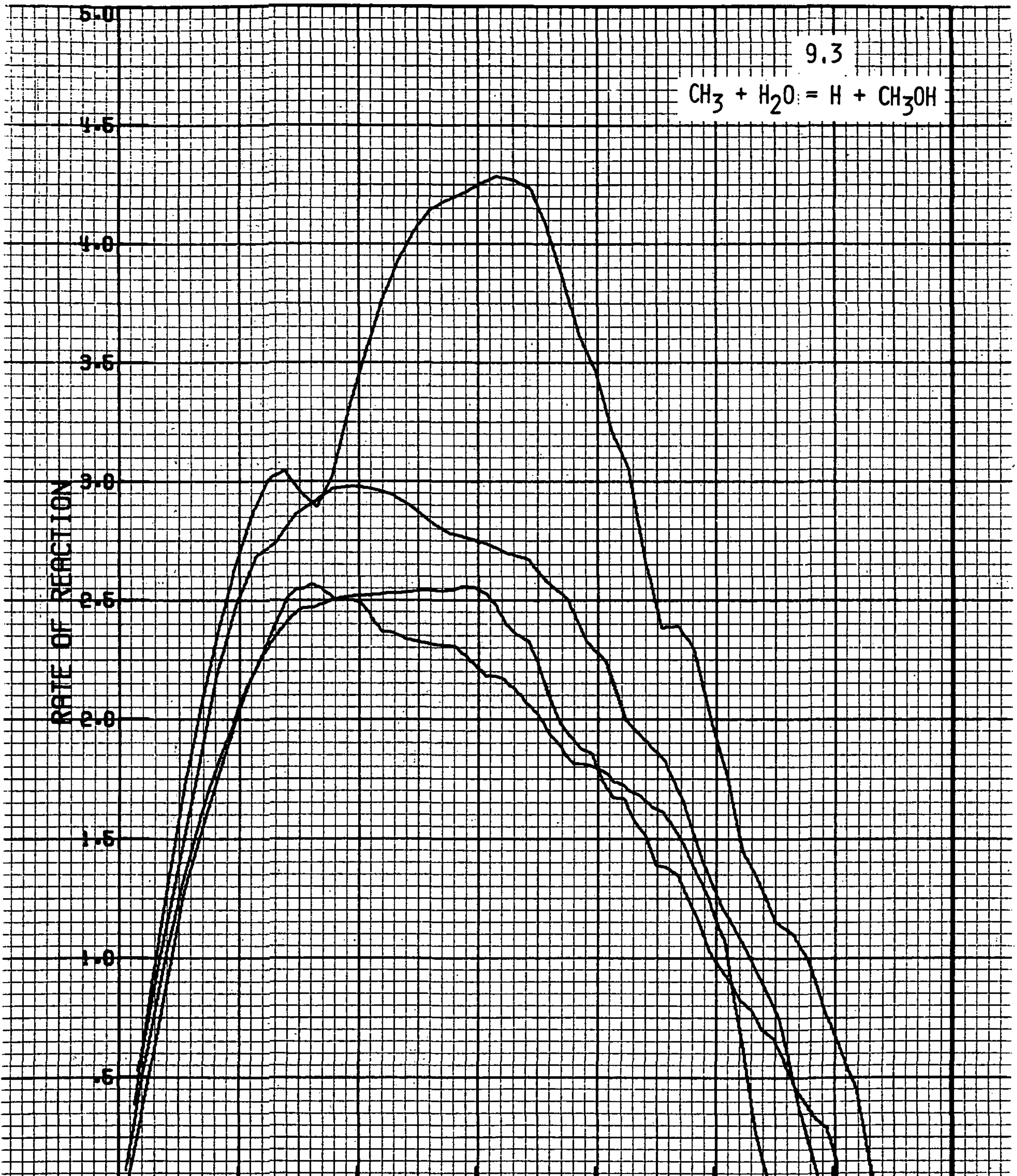

9.3
$CH_3 + H_2O = H + CH_3OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-48

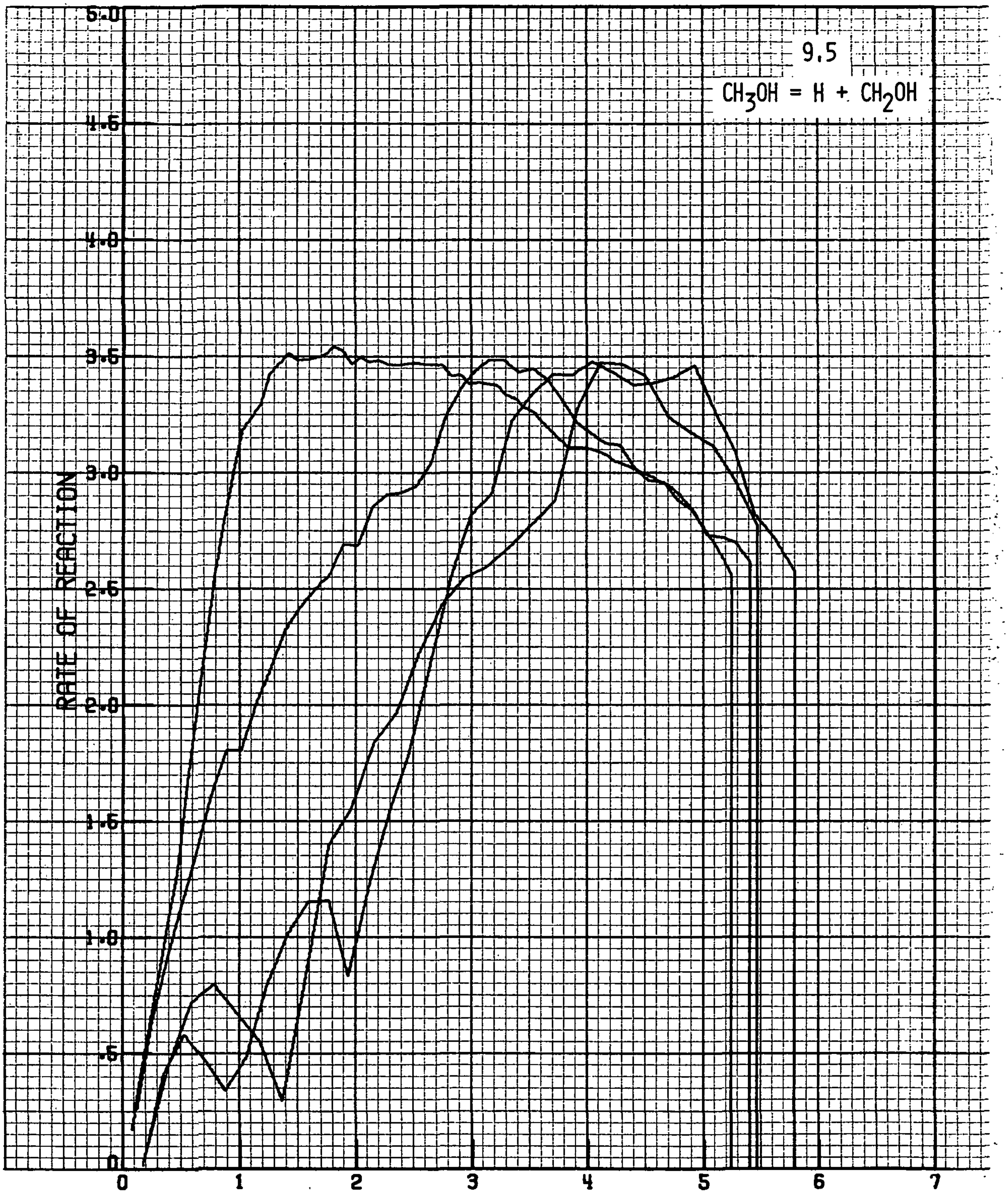

9.5
$CH_3OH = H + CH_2OH$
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
RATE OF REACTION
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-49

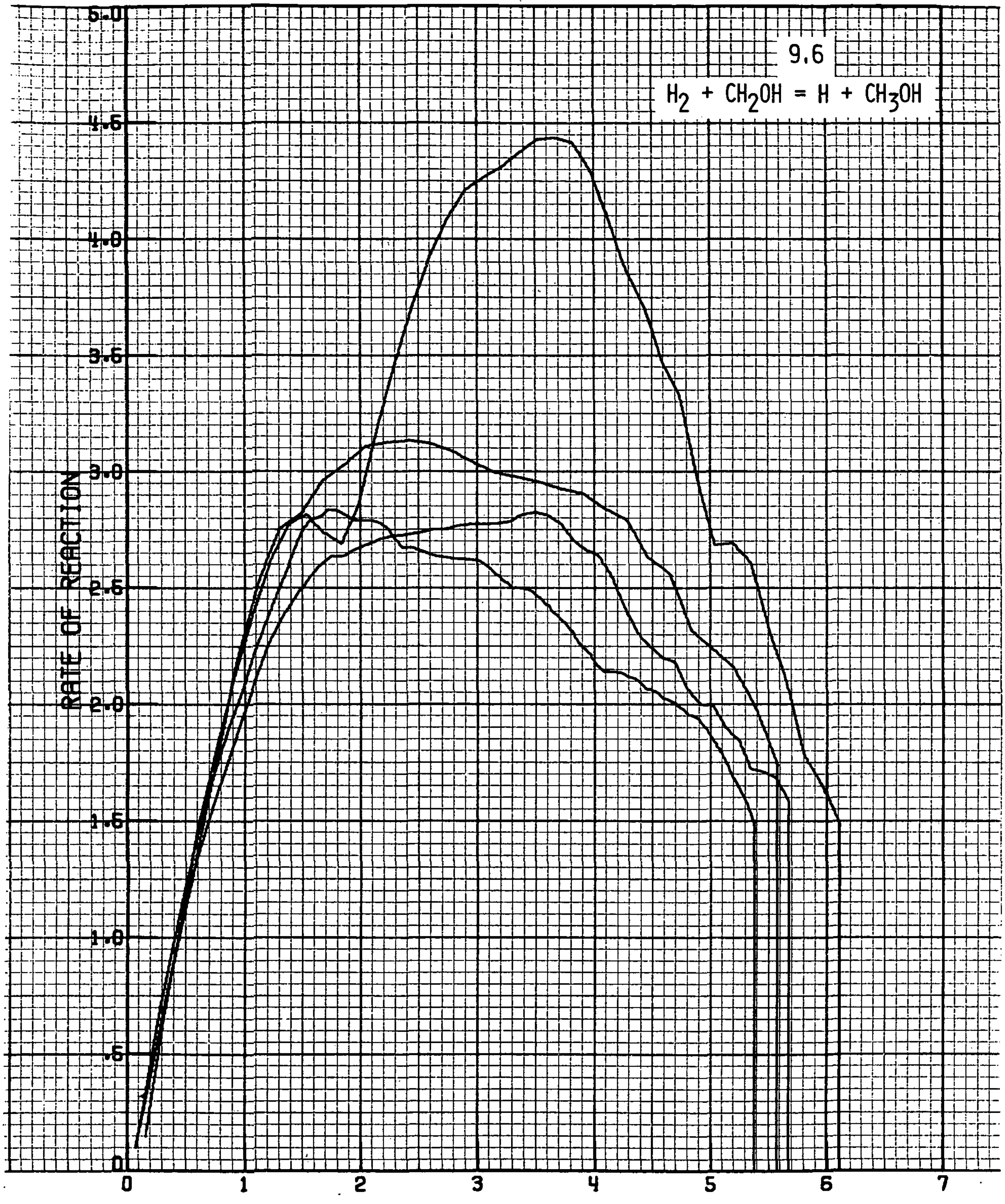

9.6
$H_2 + CH_2OH = H + CH_3OH$
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
RATE OF REACTION
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-50

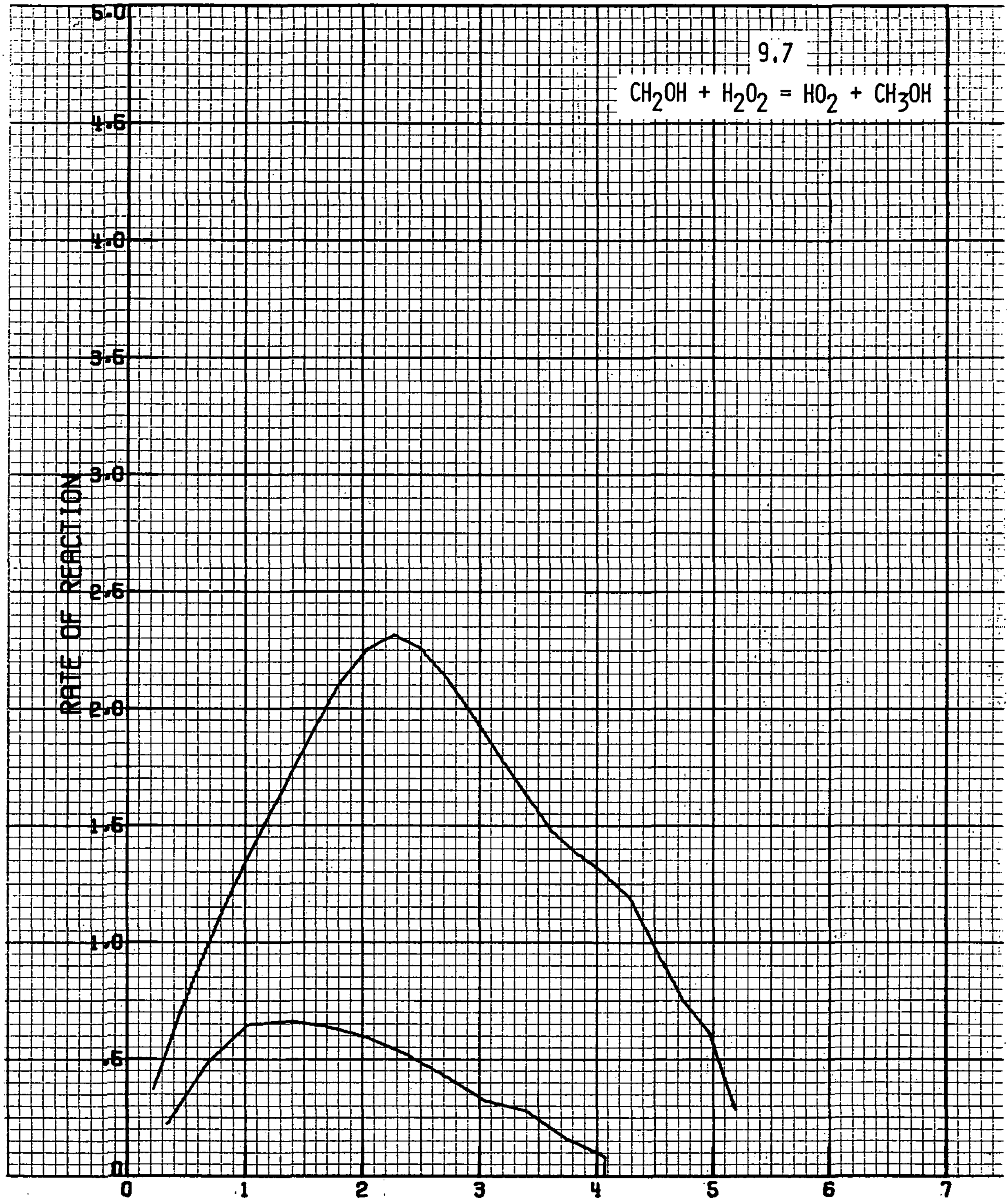

9.7
$CH_2OH + H_2O_2 = HO_2 + CH_3OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
PROGRESS OF REACTION
0
1
2
3
4
5
6
7

Figure A-51

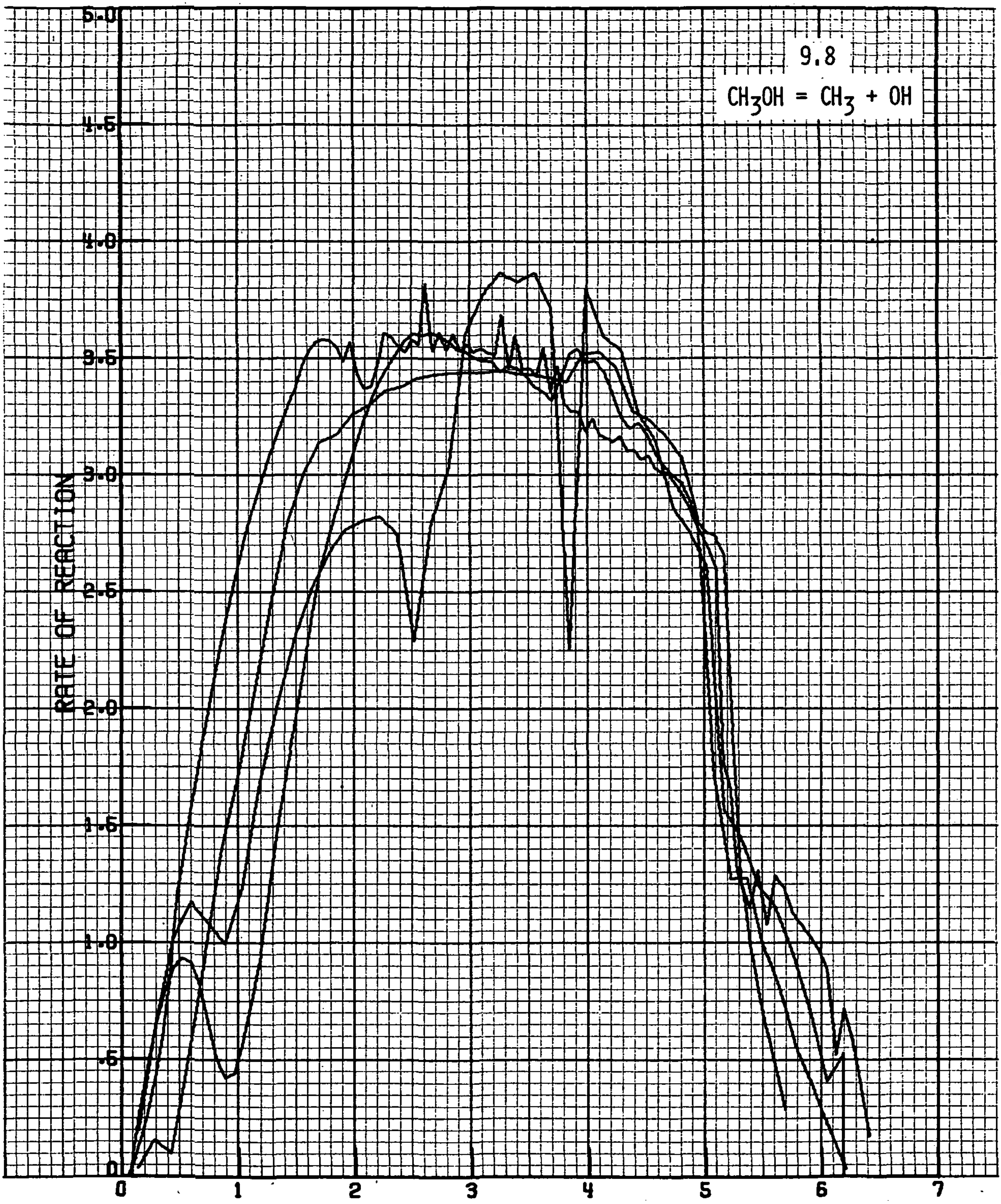

5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
RATE OF REACTION
0
1
2
3
4
5
6
7
PROGRESS OF REACTION
9.8
$CH_3OH = CH_3 + OH$

Figure A-52

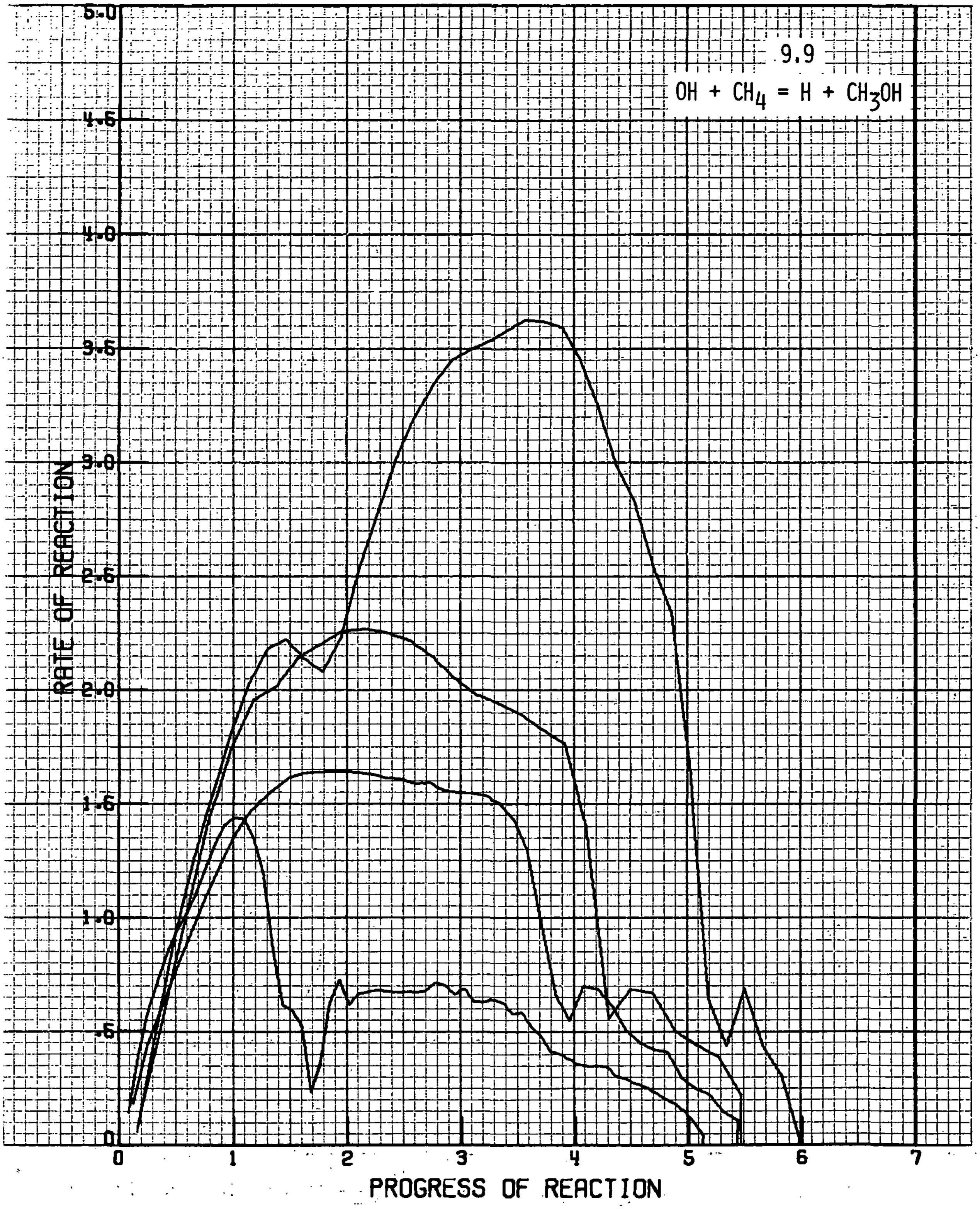

9.9
$OH + CH_4 = H + CH_3OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-53

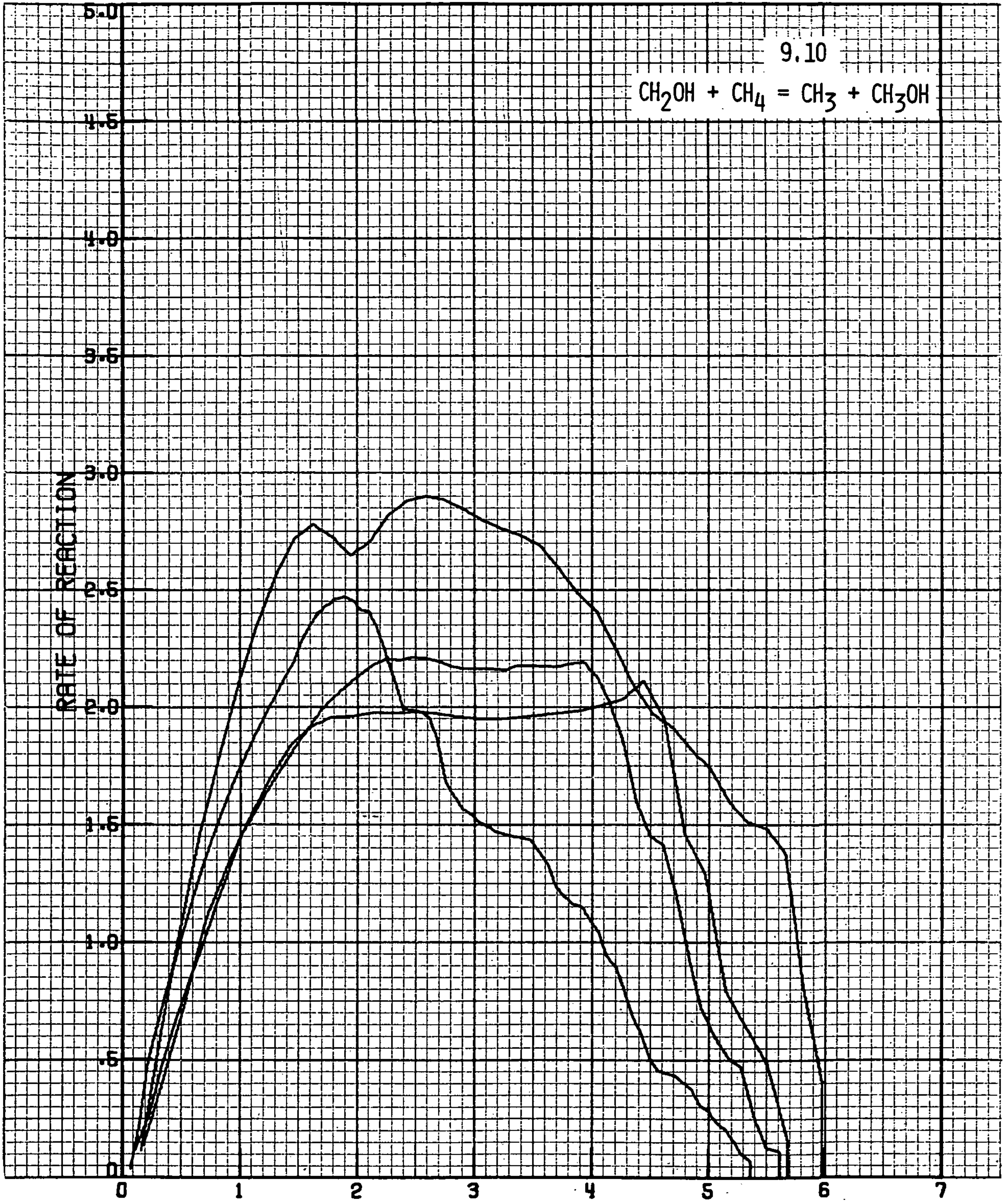

9.10
$CH_2OH + CH_4 = CH_3 + CH_3OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-54

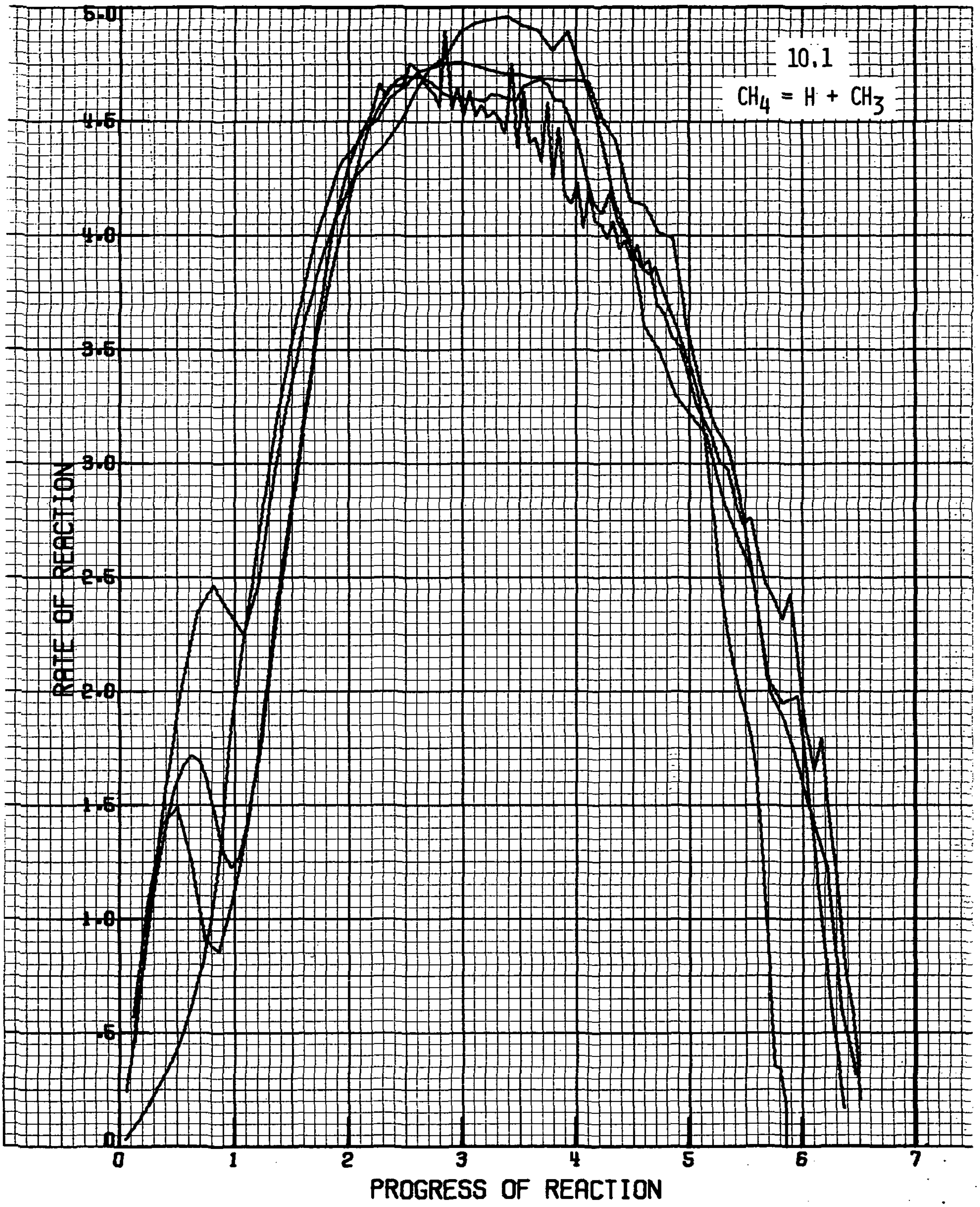

10.1
$CH_4 = H + CH_3$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-55

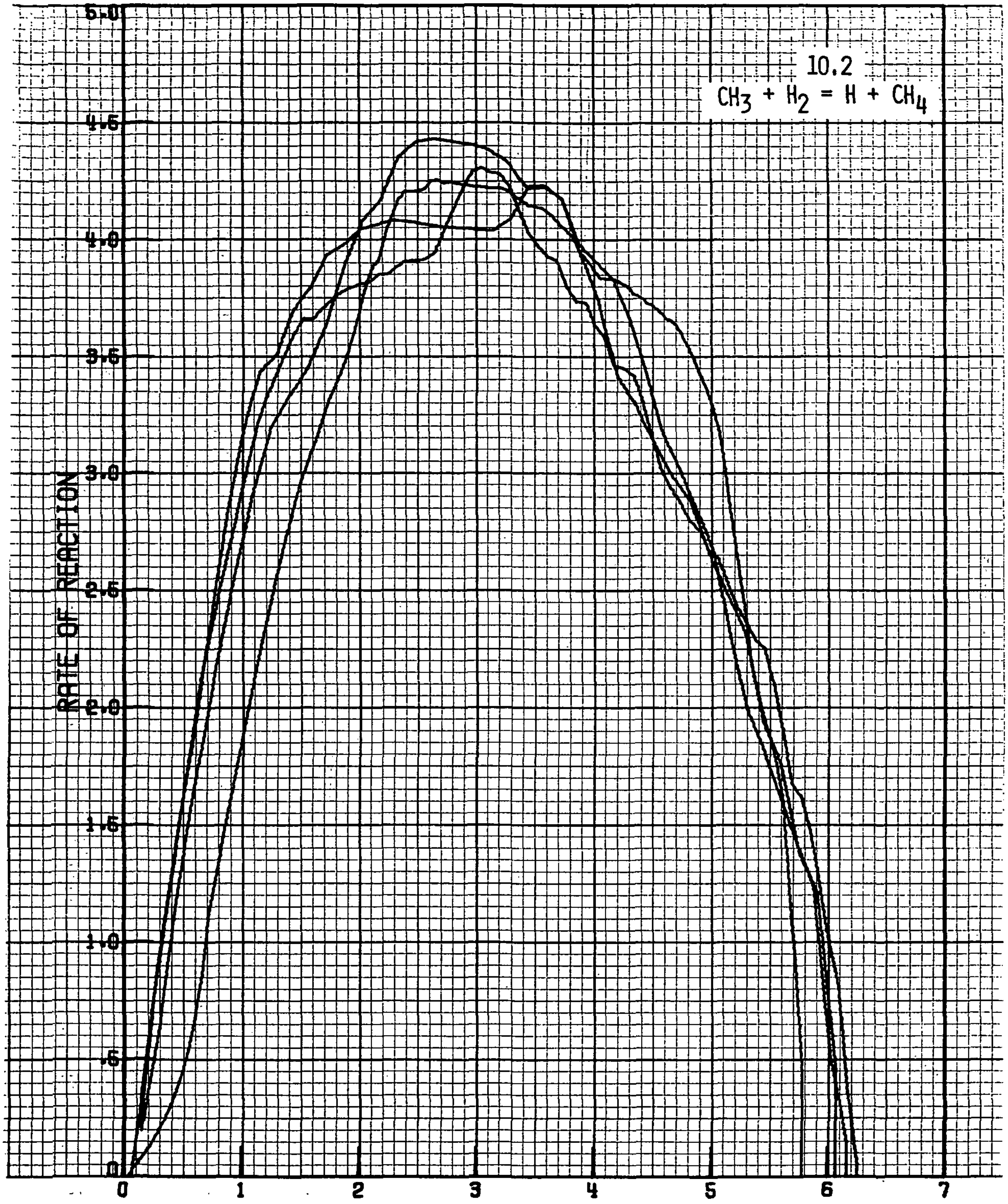

10.2
$CH_3 + H_2 = H + CH_4$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-56

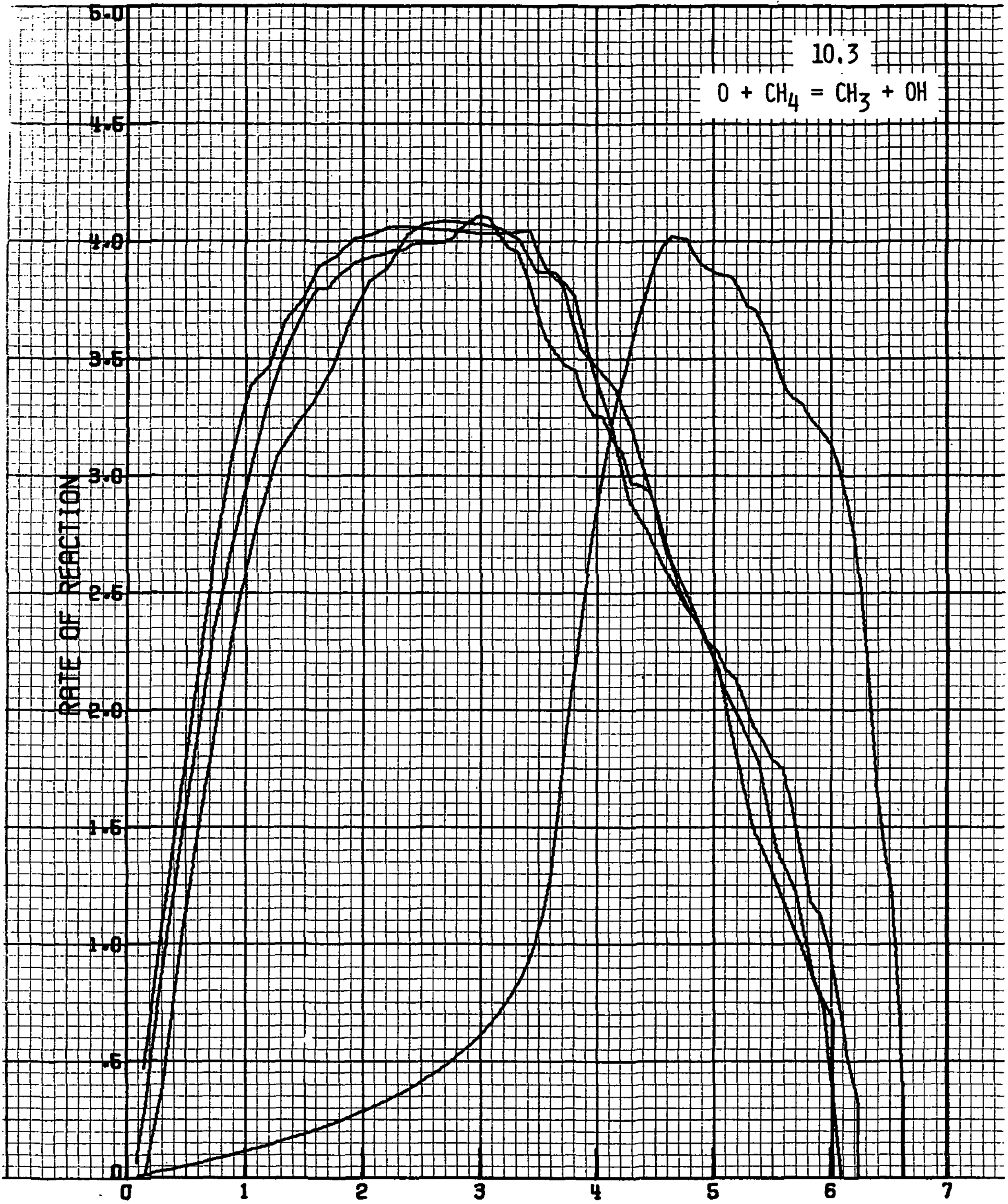

10.3
$O + CH_4 = CH_3 + OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-57

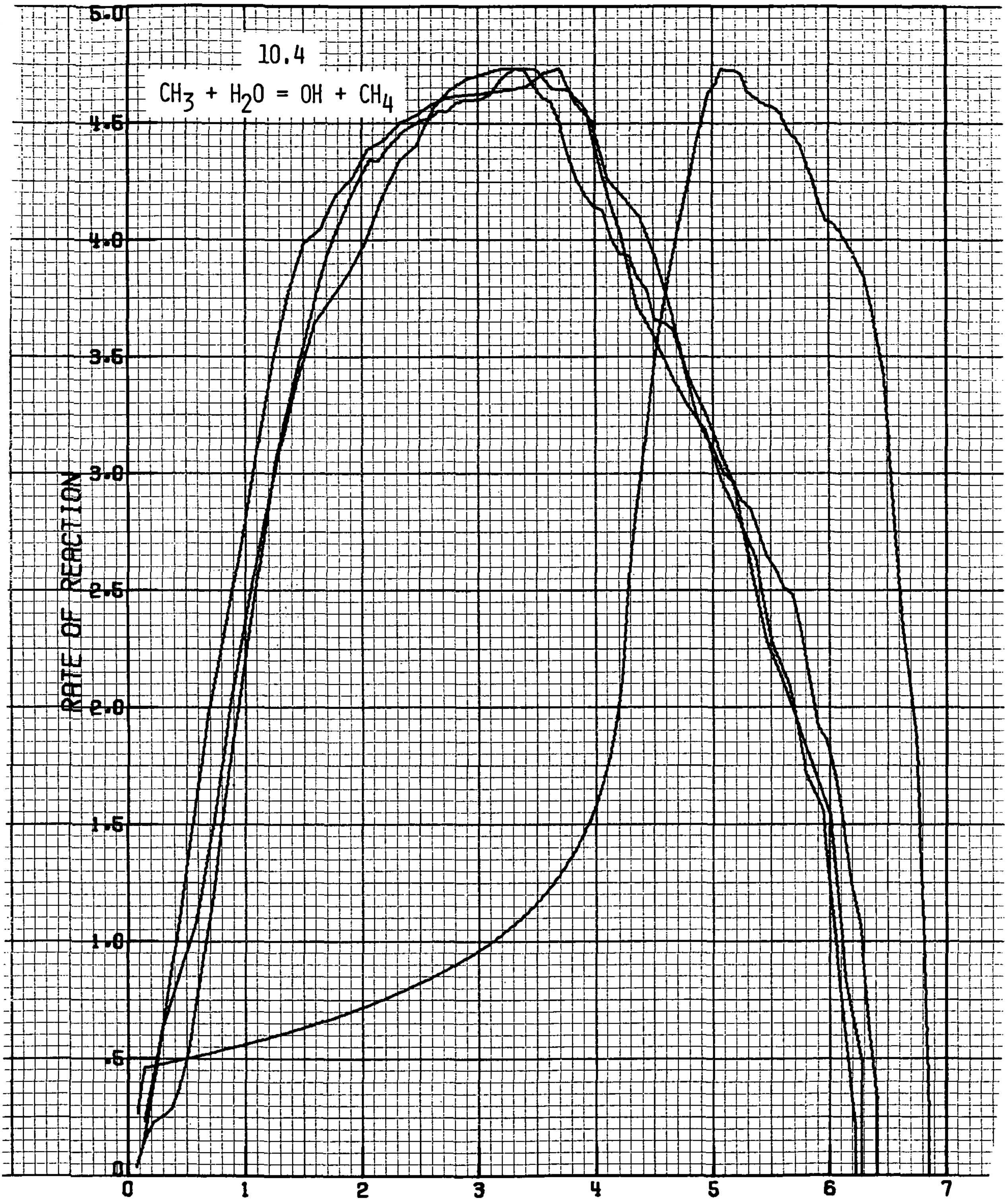
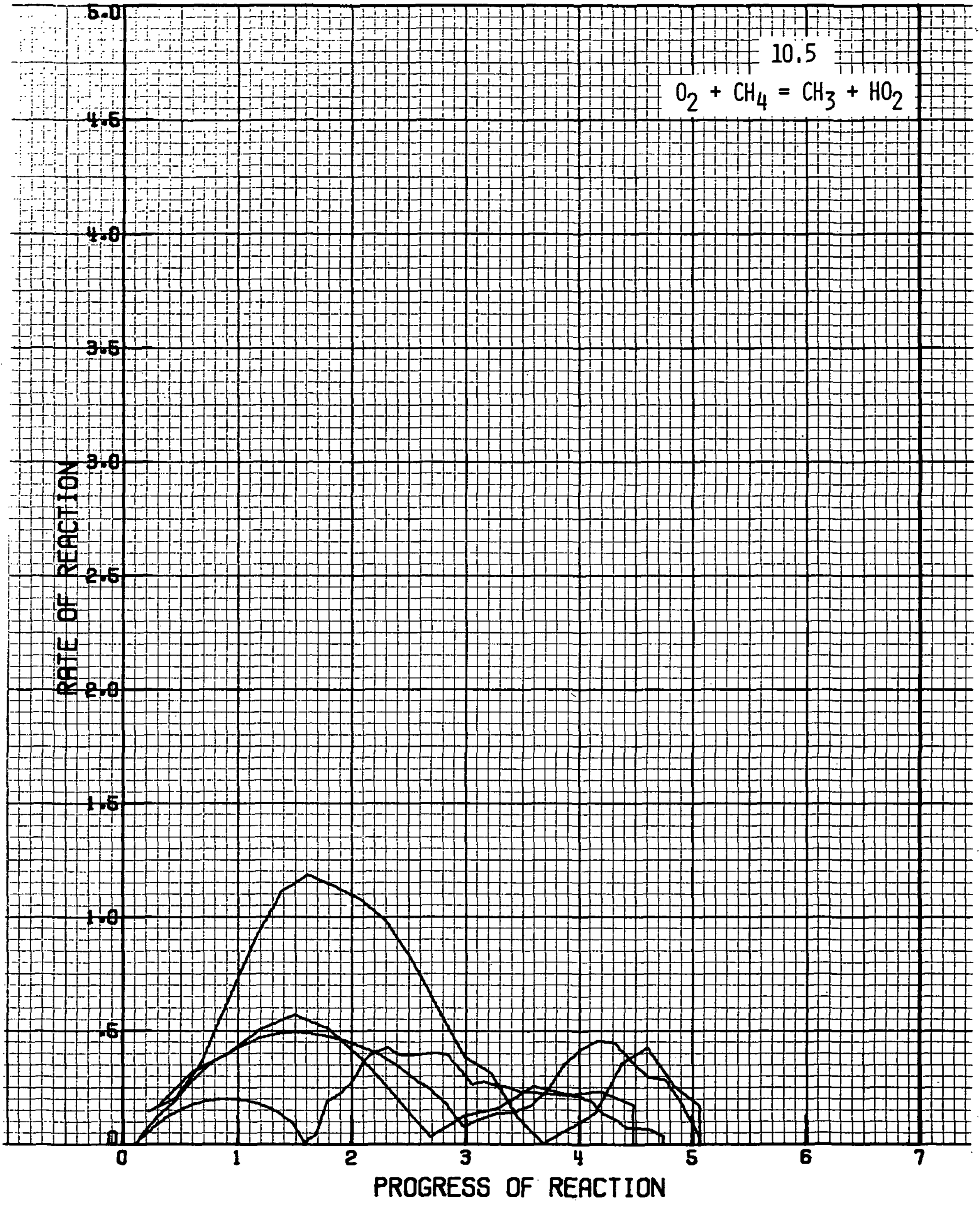

10.4
$CH_3 + H_2O = OH + CH_4$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-58



10.5
$O_2 + CH_4 = CH_3 + HO_2$
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
RATE OF REACTION
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-59

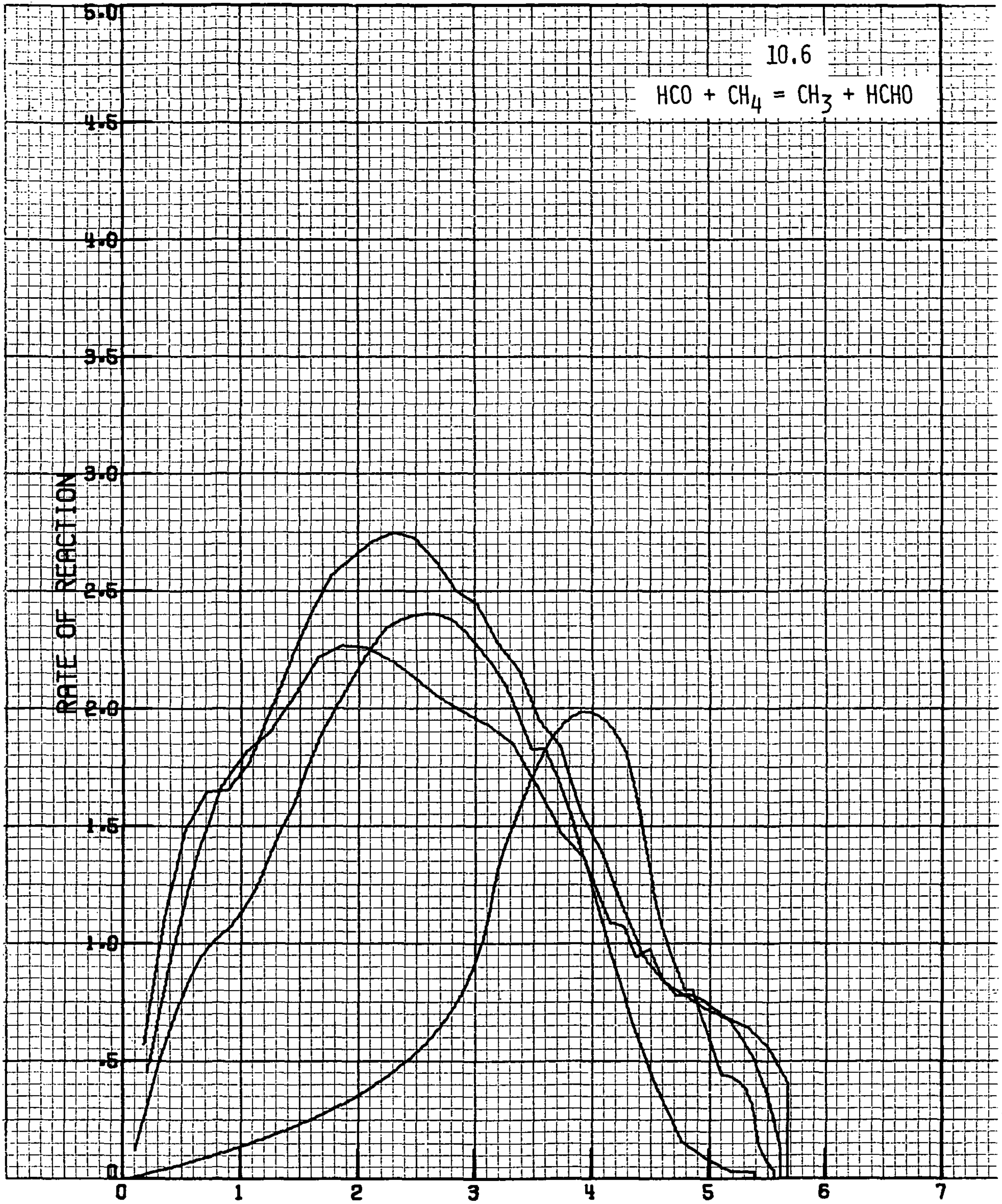

10.6
HCO + CH_4 = CH_3 + HCHO
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-60

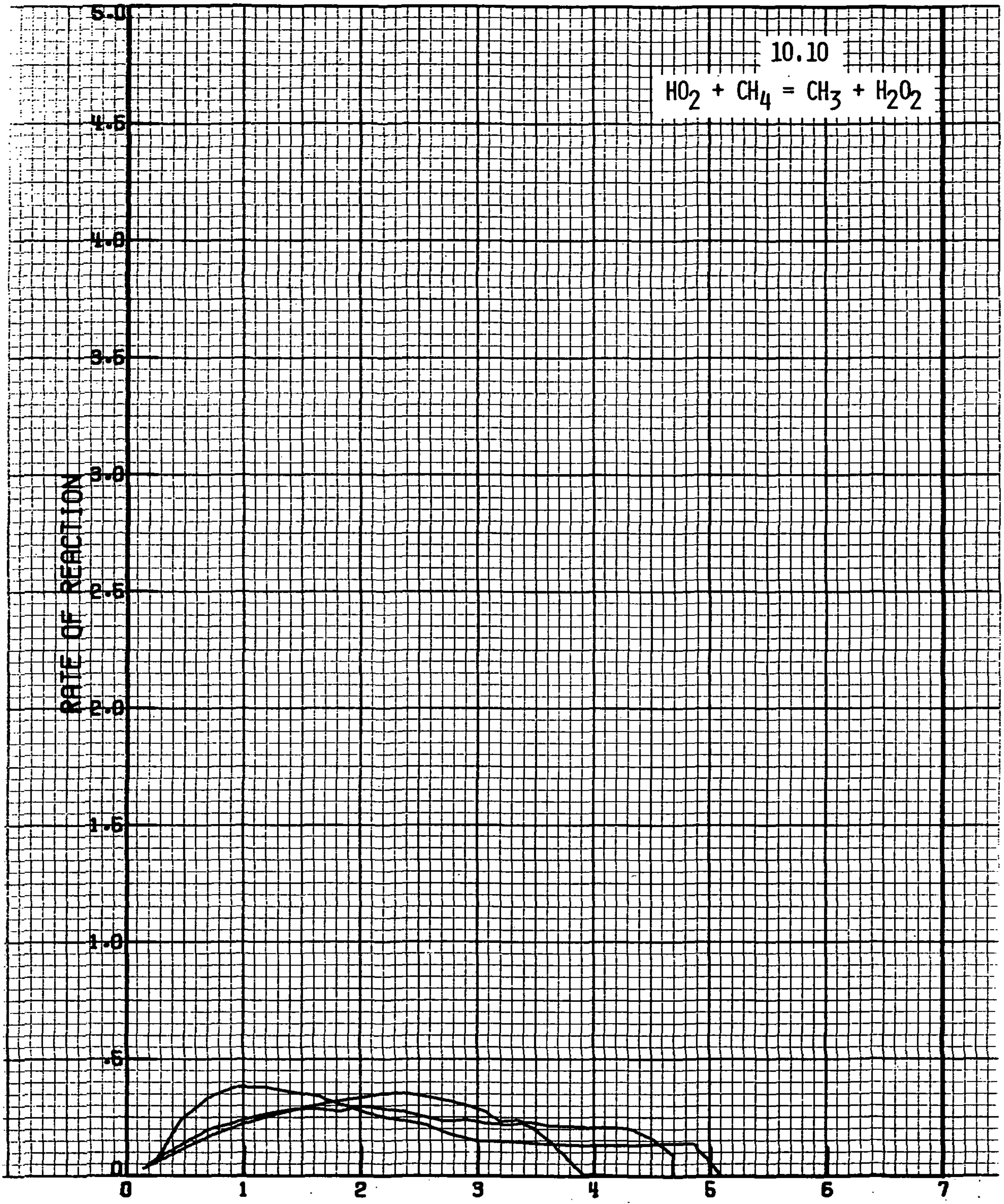

10.10
$HO_2 + CH_4 = CH_3 + H_2O_2$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-61

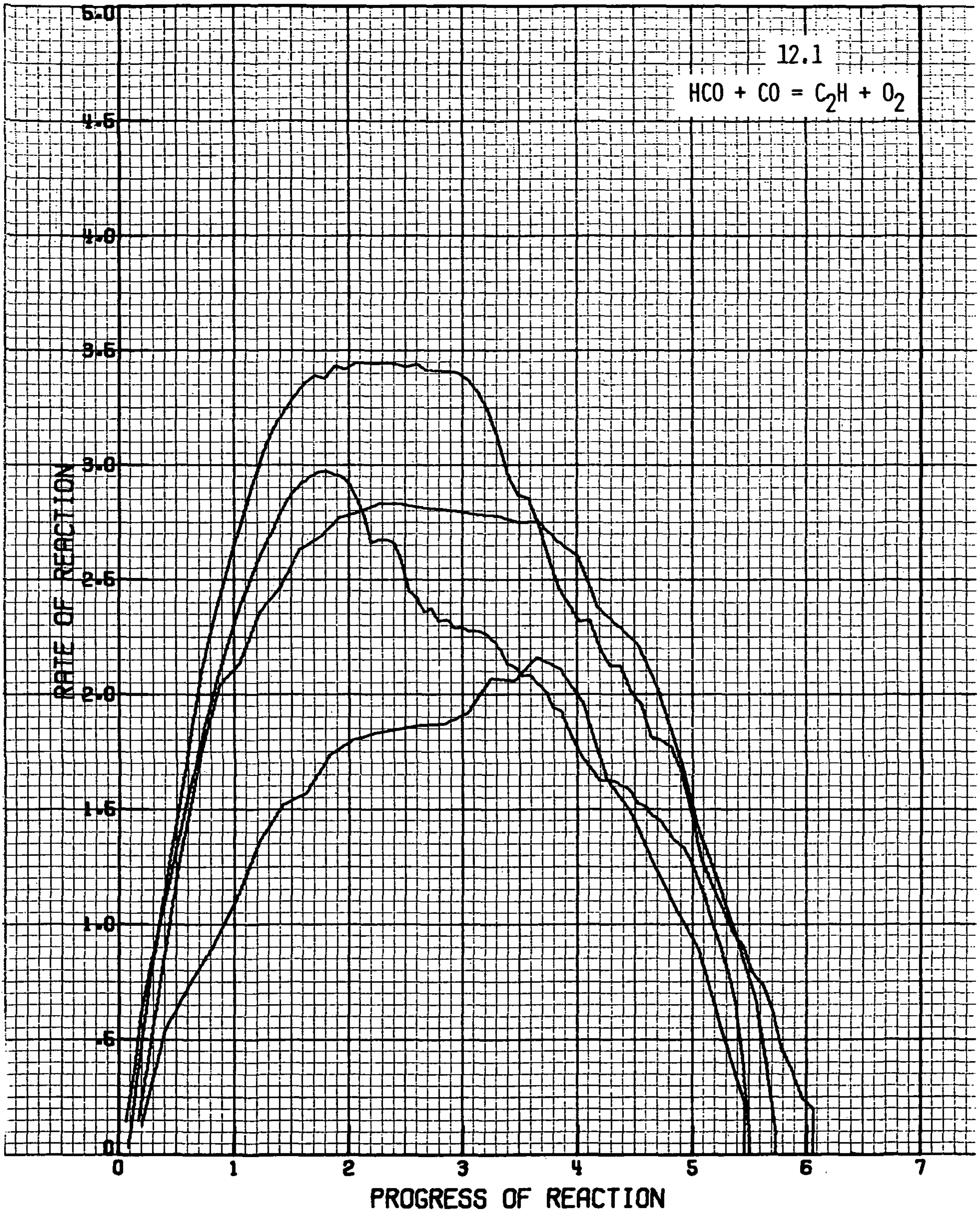
12.1
$HCO + CO = C_2H + O_2$
RATE OF REACTION
PROGRESS OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7

Figure A-62

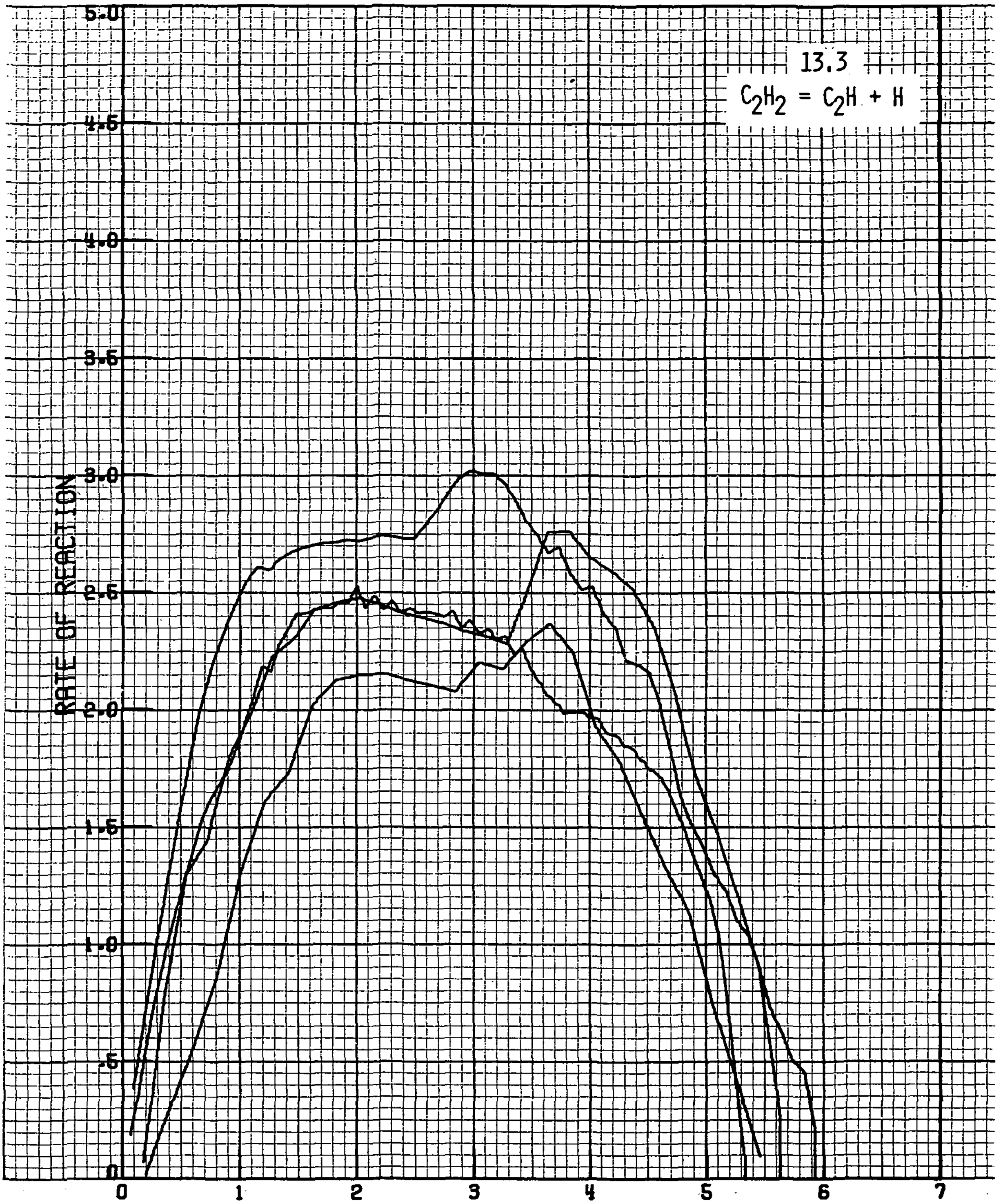

13.3
$C_2H_2 = C_2H + H$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-63

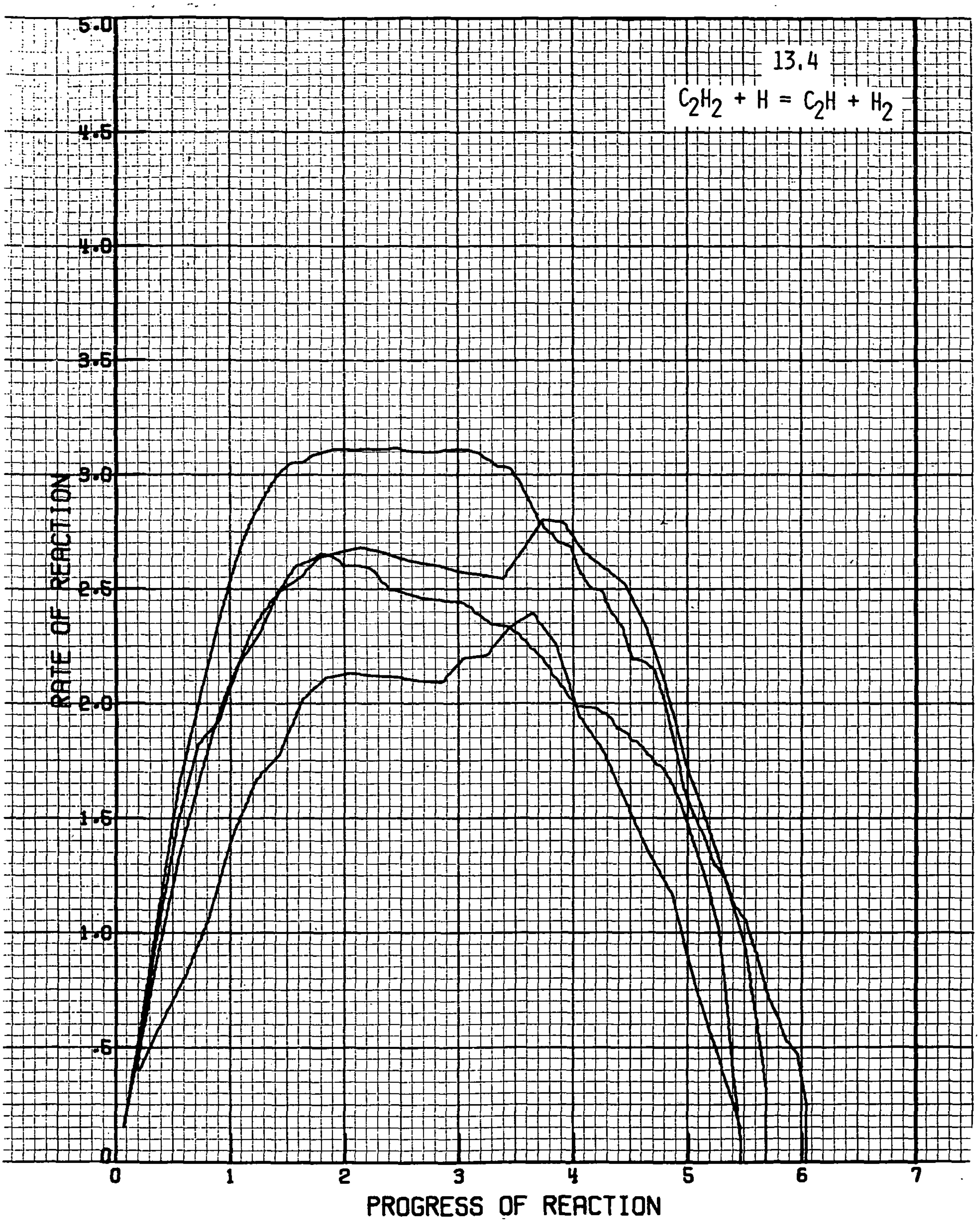

13.4
$C_2H_2 + H = C_2H + H_2$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-64

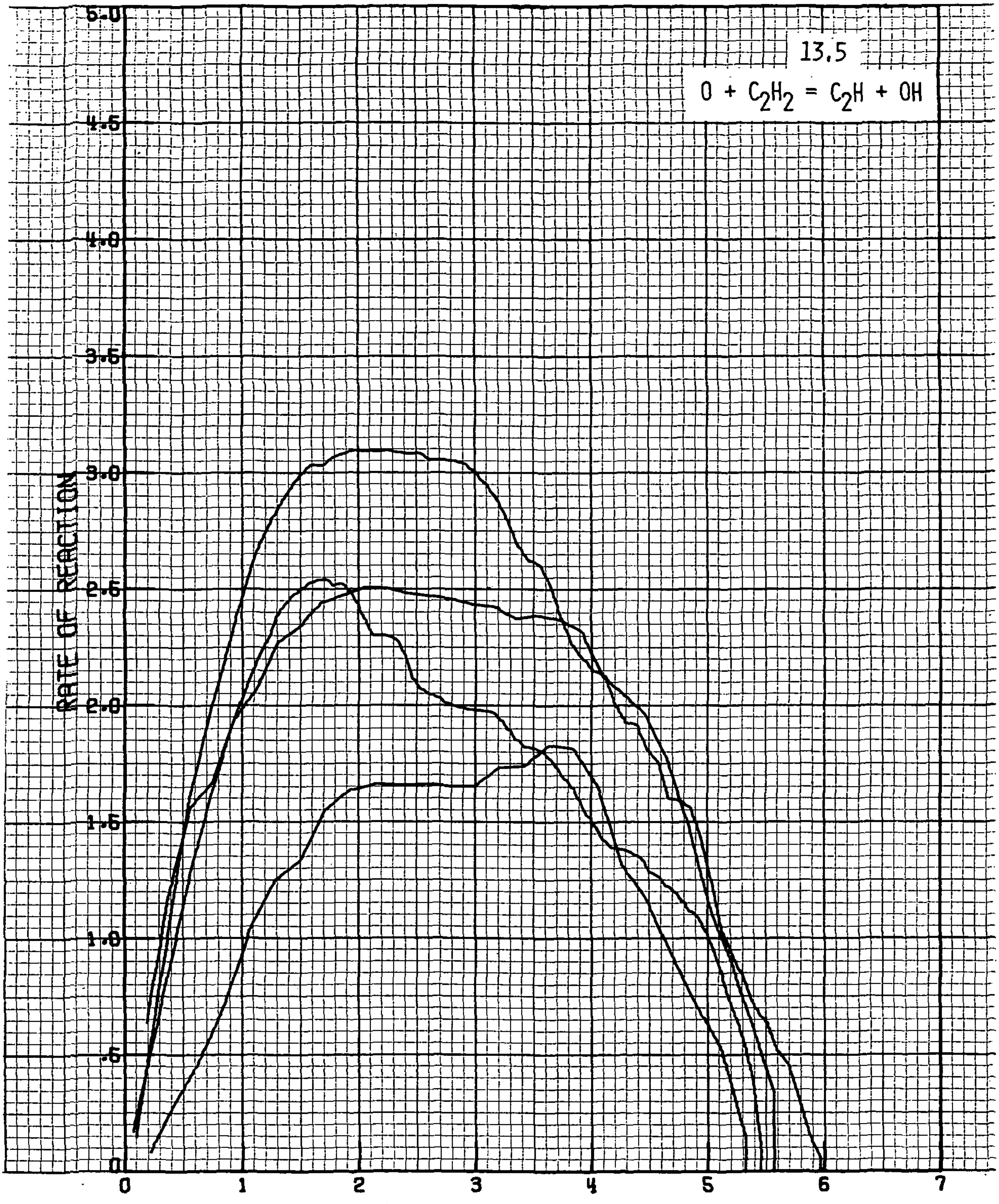

13.5
$O + C_2H_2 = C_2H + OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-65

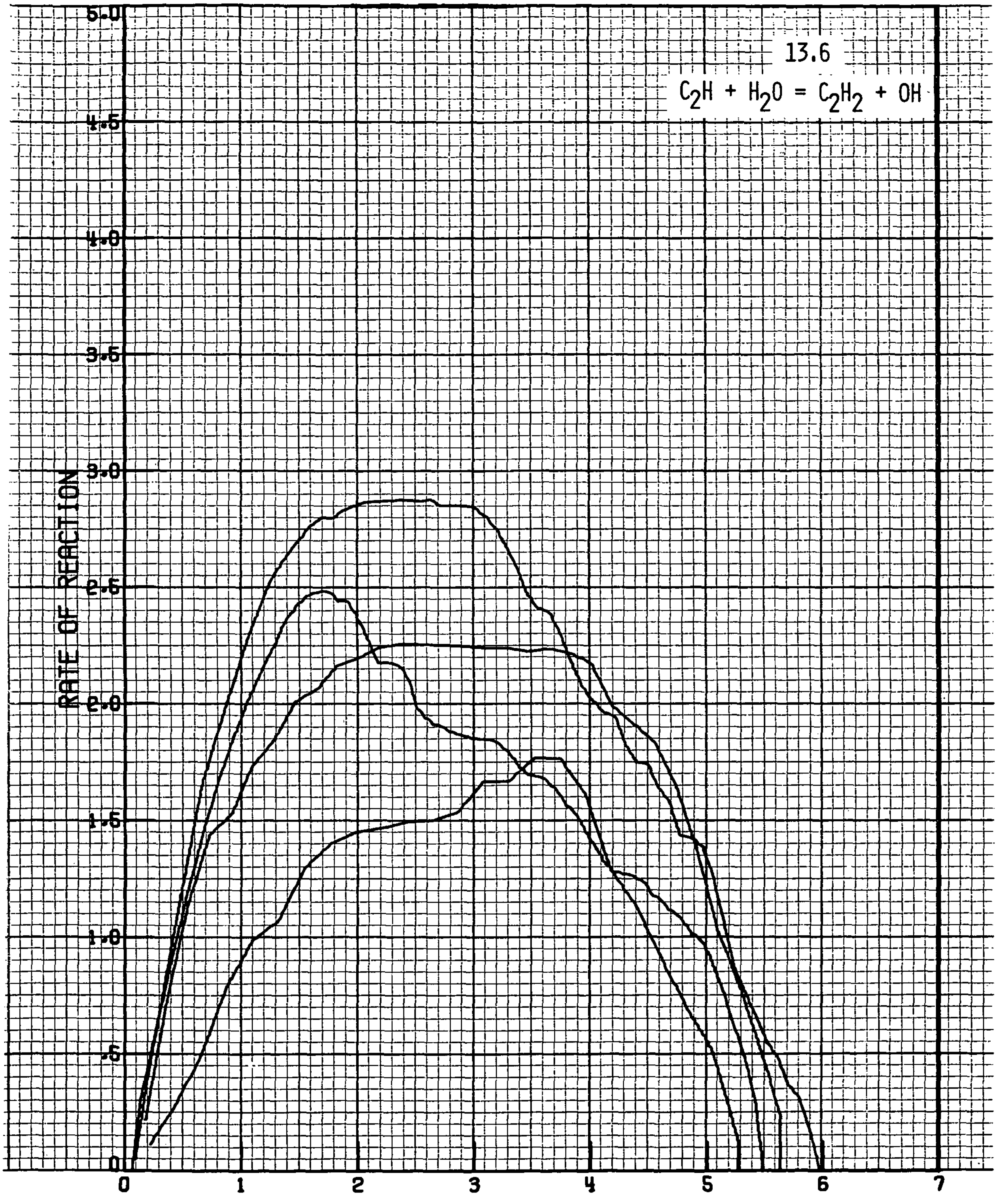
13.6
$C_2H + H_2O = C_2H_2 + OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-66

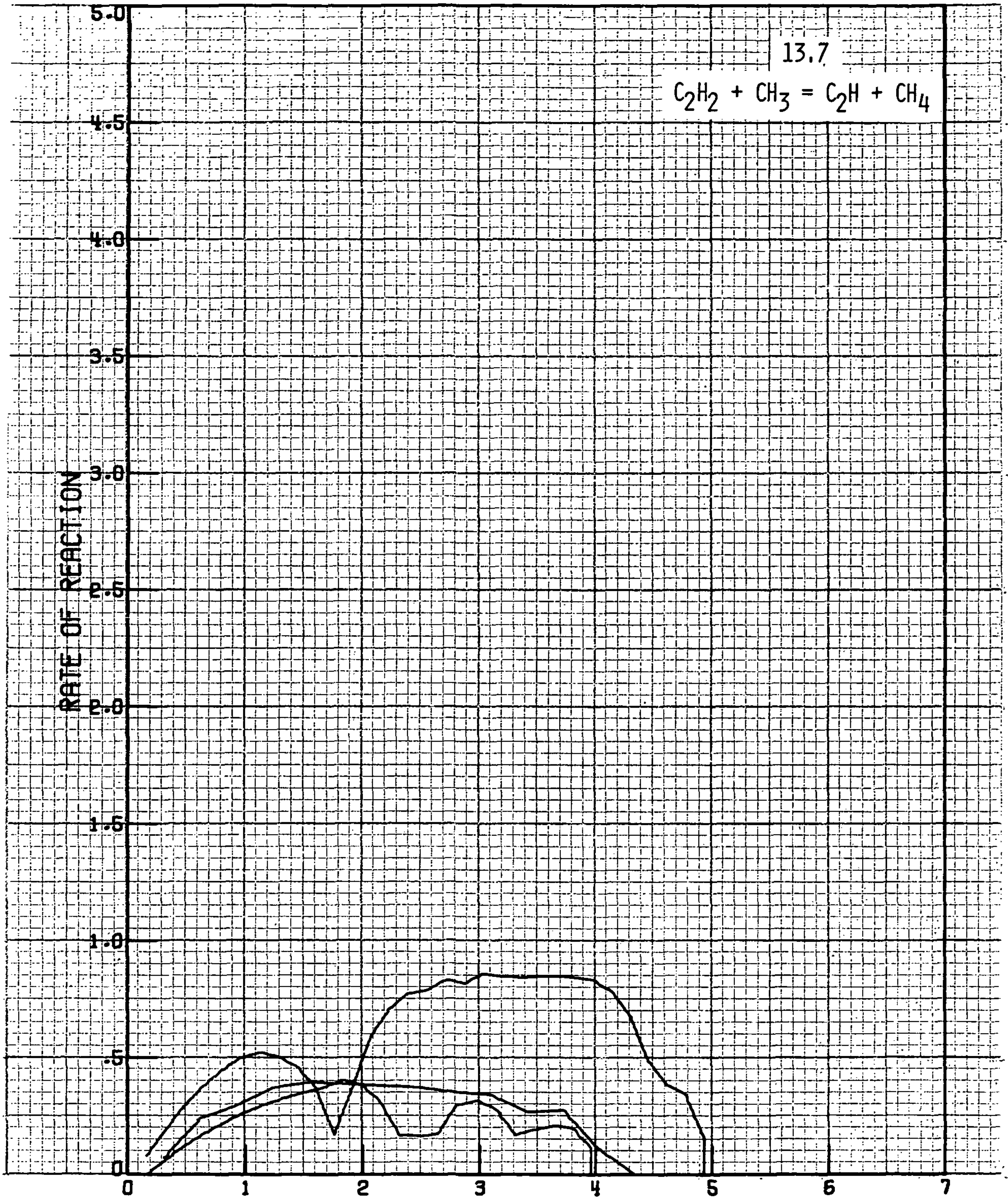

13.7
$C_2H_2 + CH_3 = C_2H + CH_4$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-67

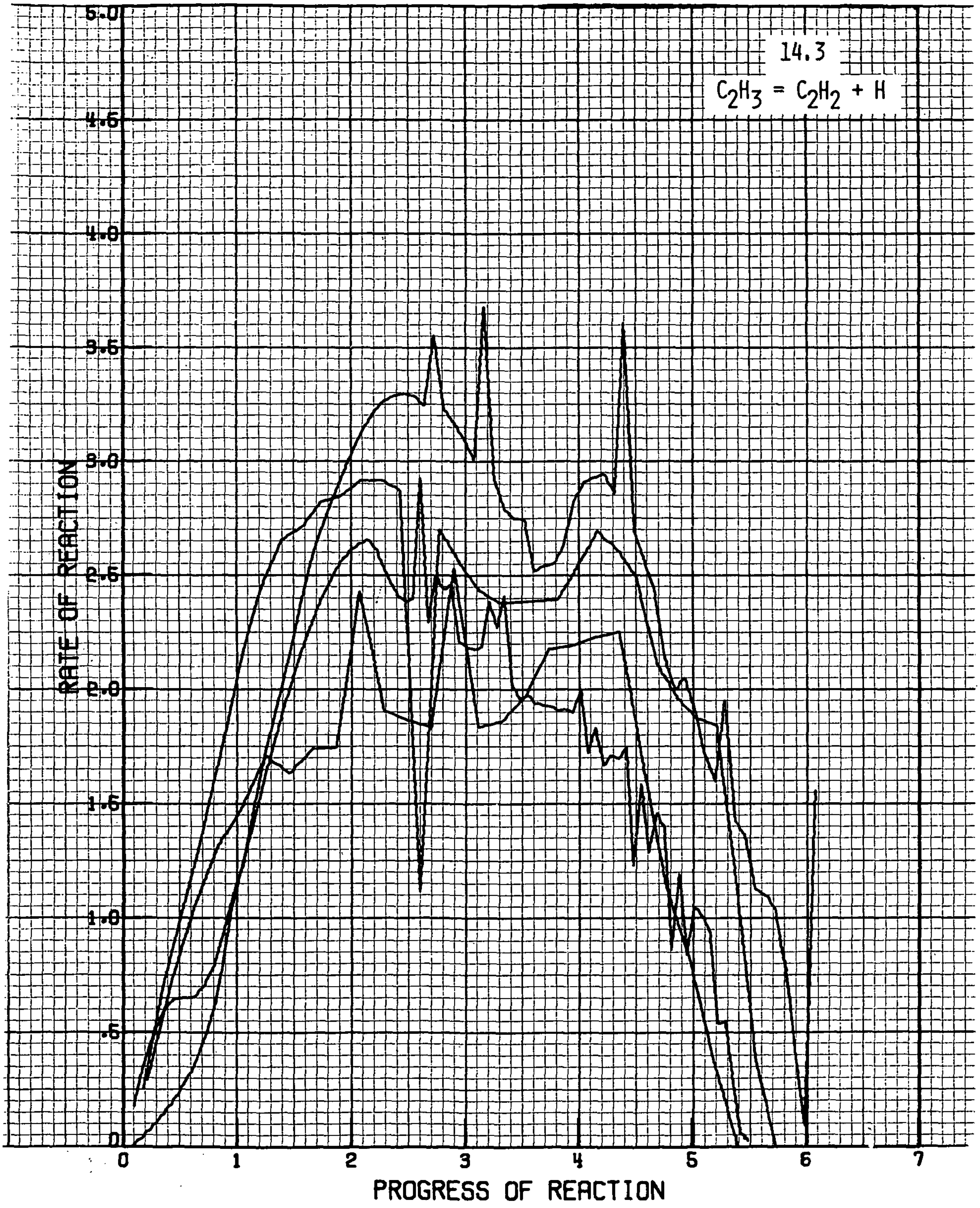

14.3
$C_2H_3 = C_2H_2 + H$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-68

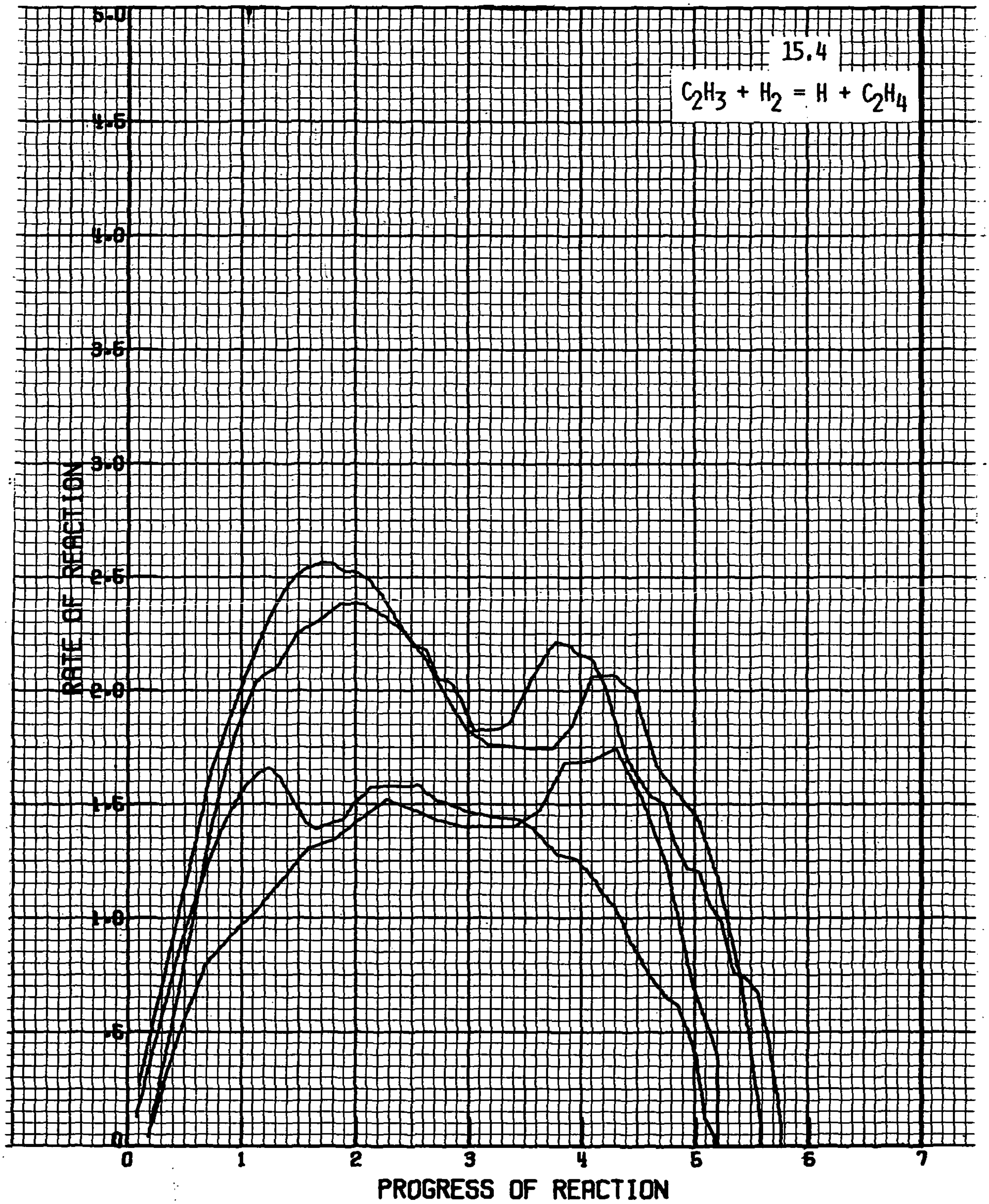

15.4
$C_2H_3 + H_2 = H + C_2H_4$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-69

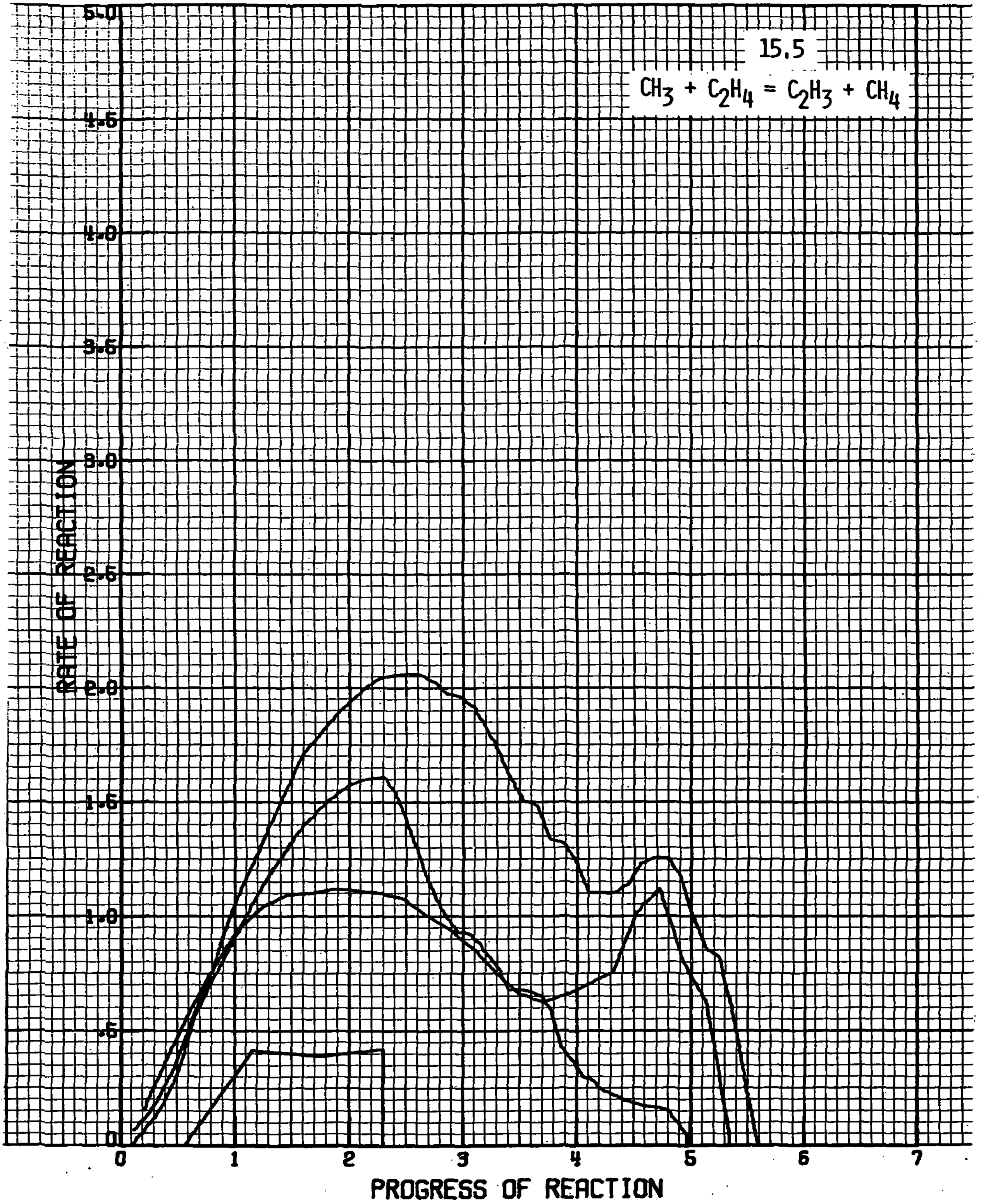

15.5
$CH_3 + C_2H_4 = C_2H_3 + CH_4$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-70

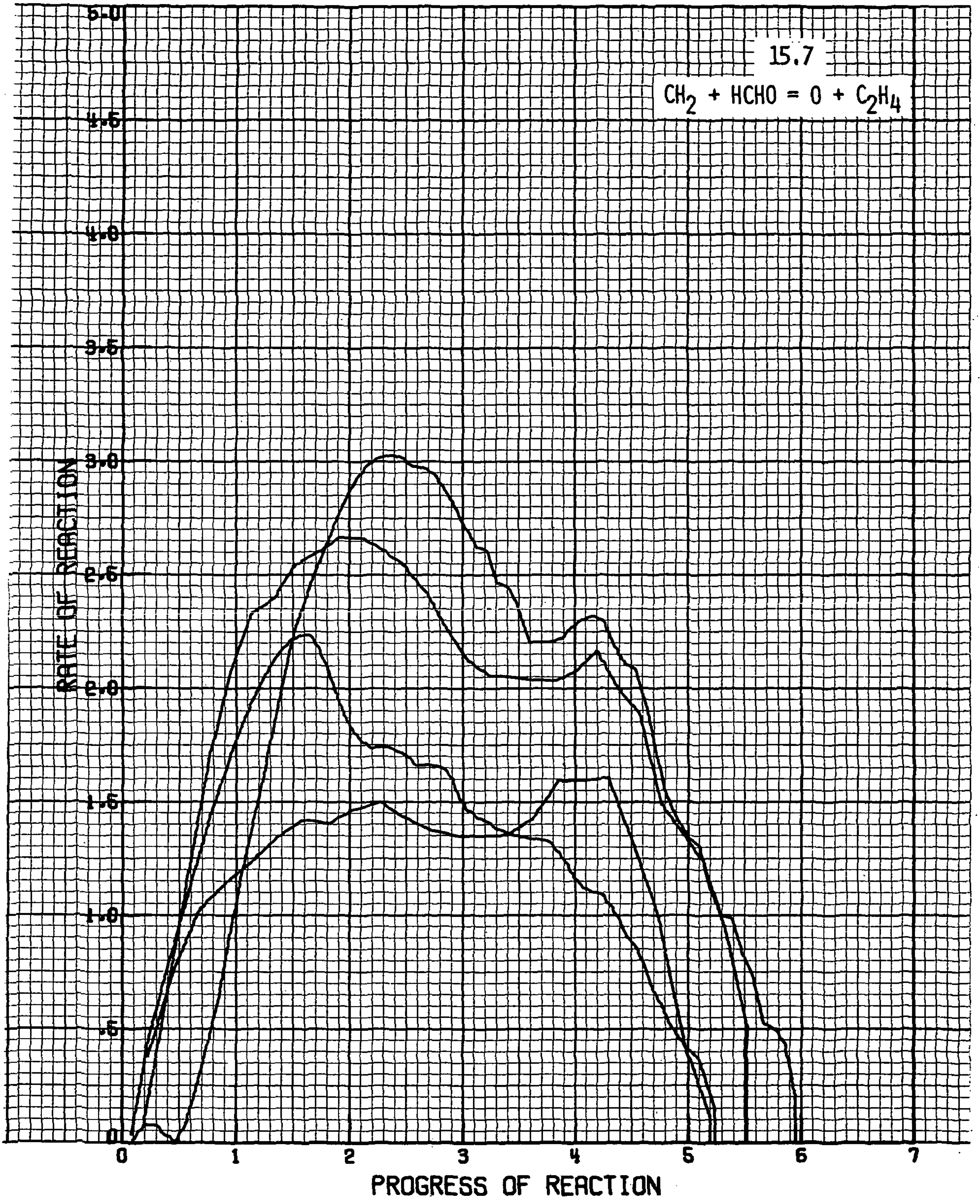

15.7
$CH_2 + HCHO = 0 + C_2H_4$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-71

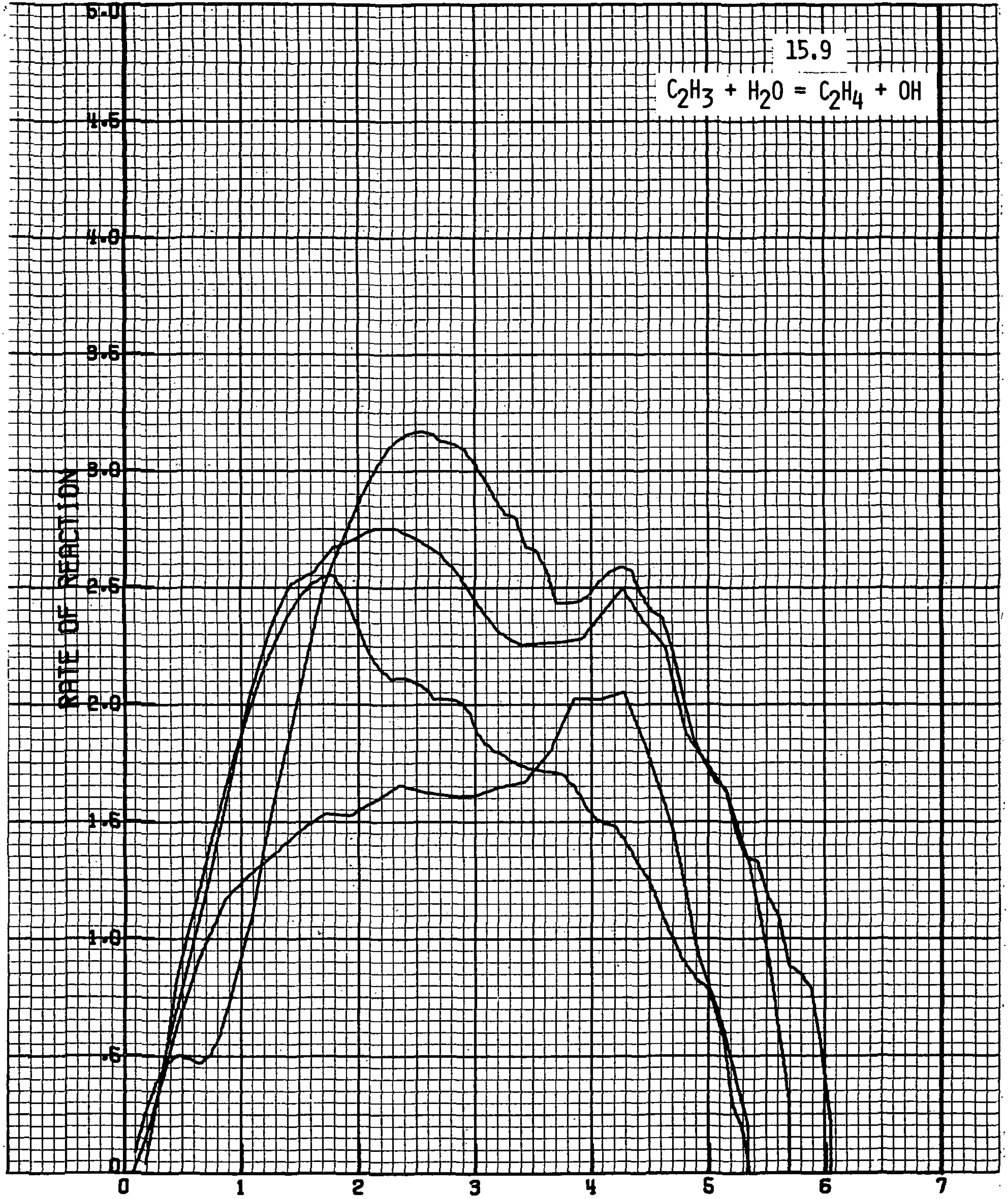
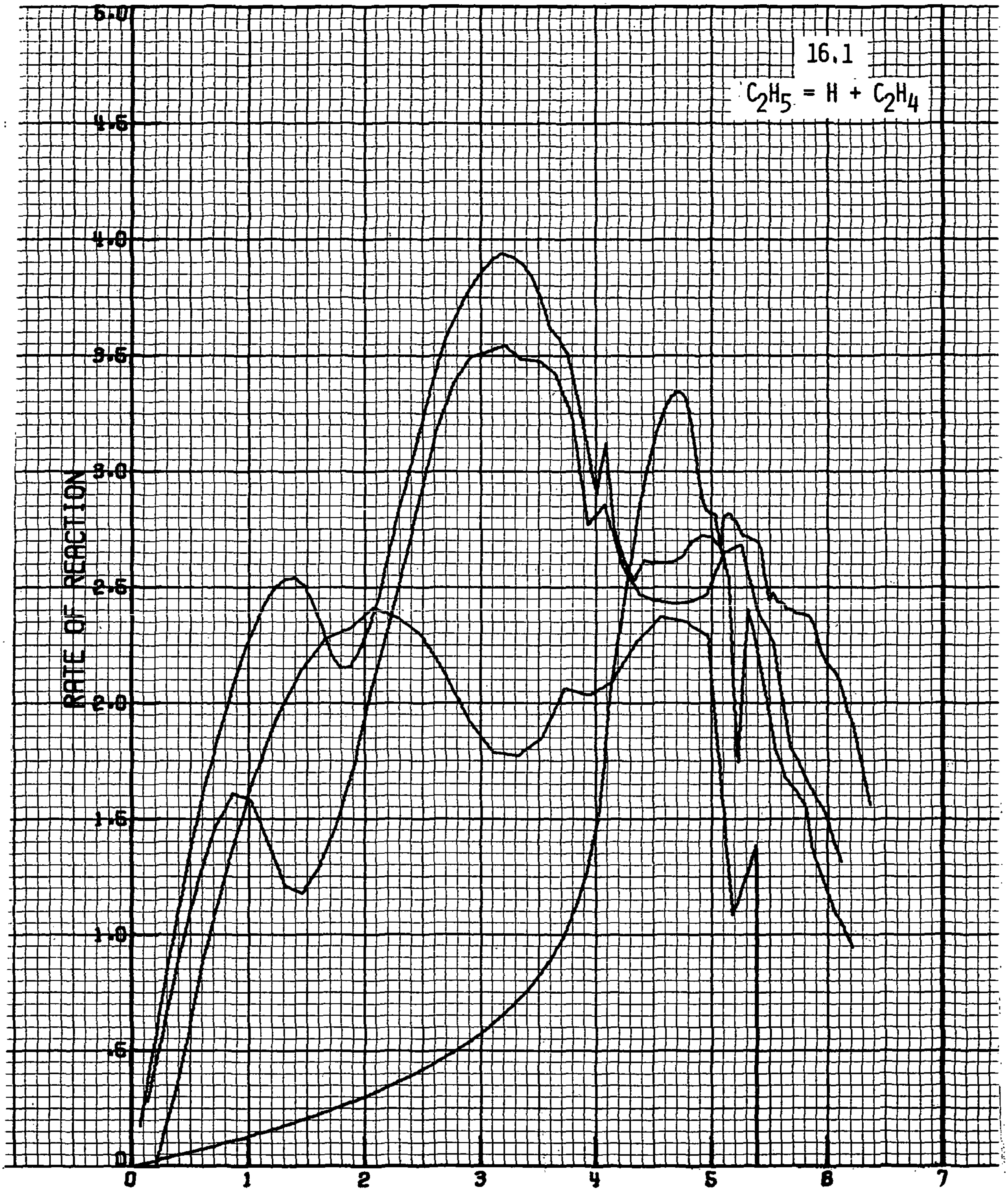

15.9
$C_2H_3 + H_2O = C_2H_4 + OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-72



16.1
$C_2H_5 = H + C_2H_4$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-73

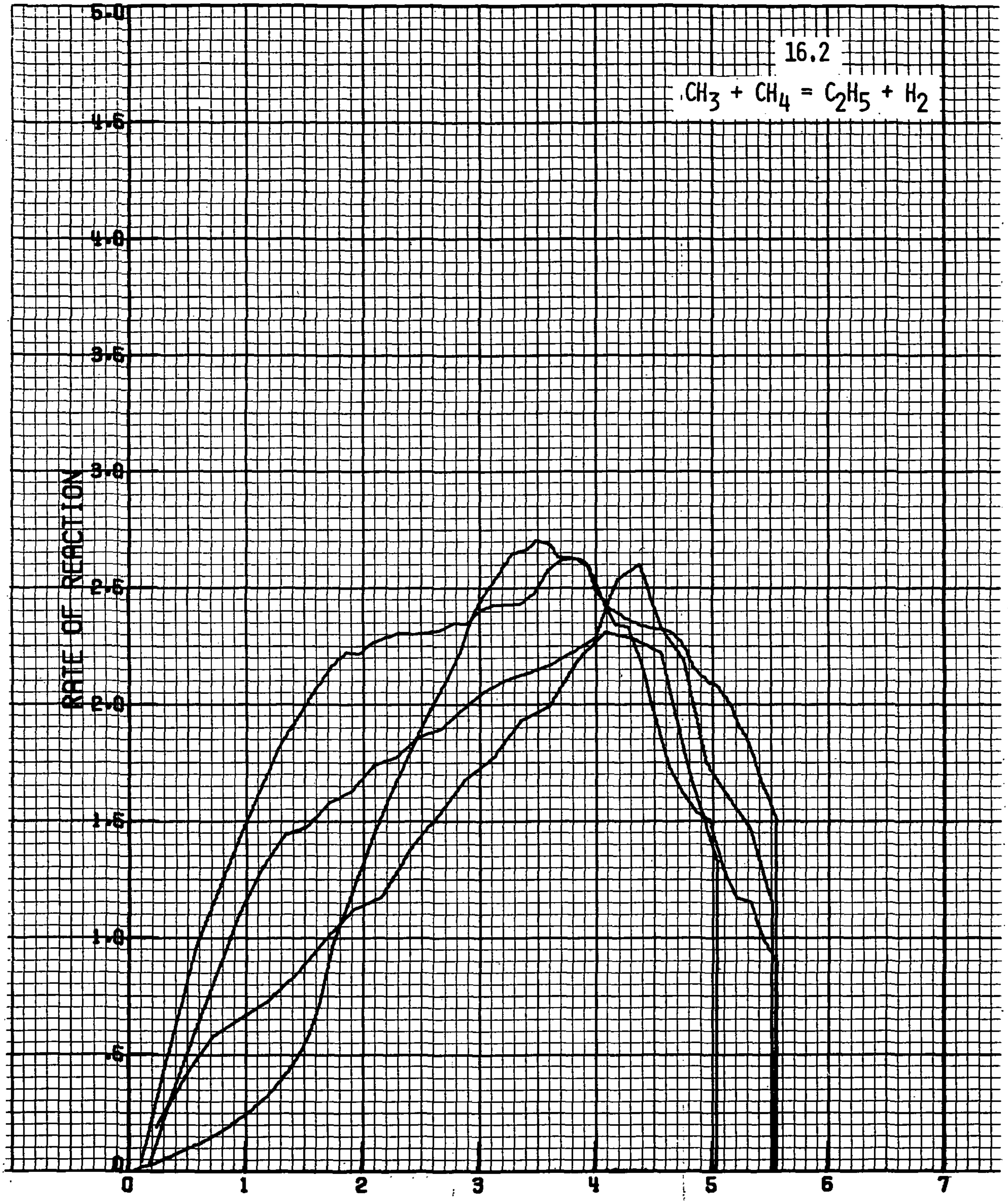

16.2
$CH_3 + CH_4 = C_2H_5 + H_2$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-74

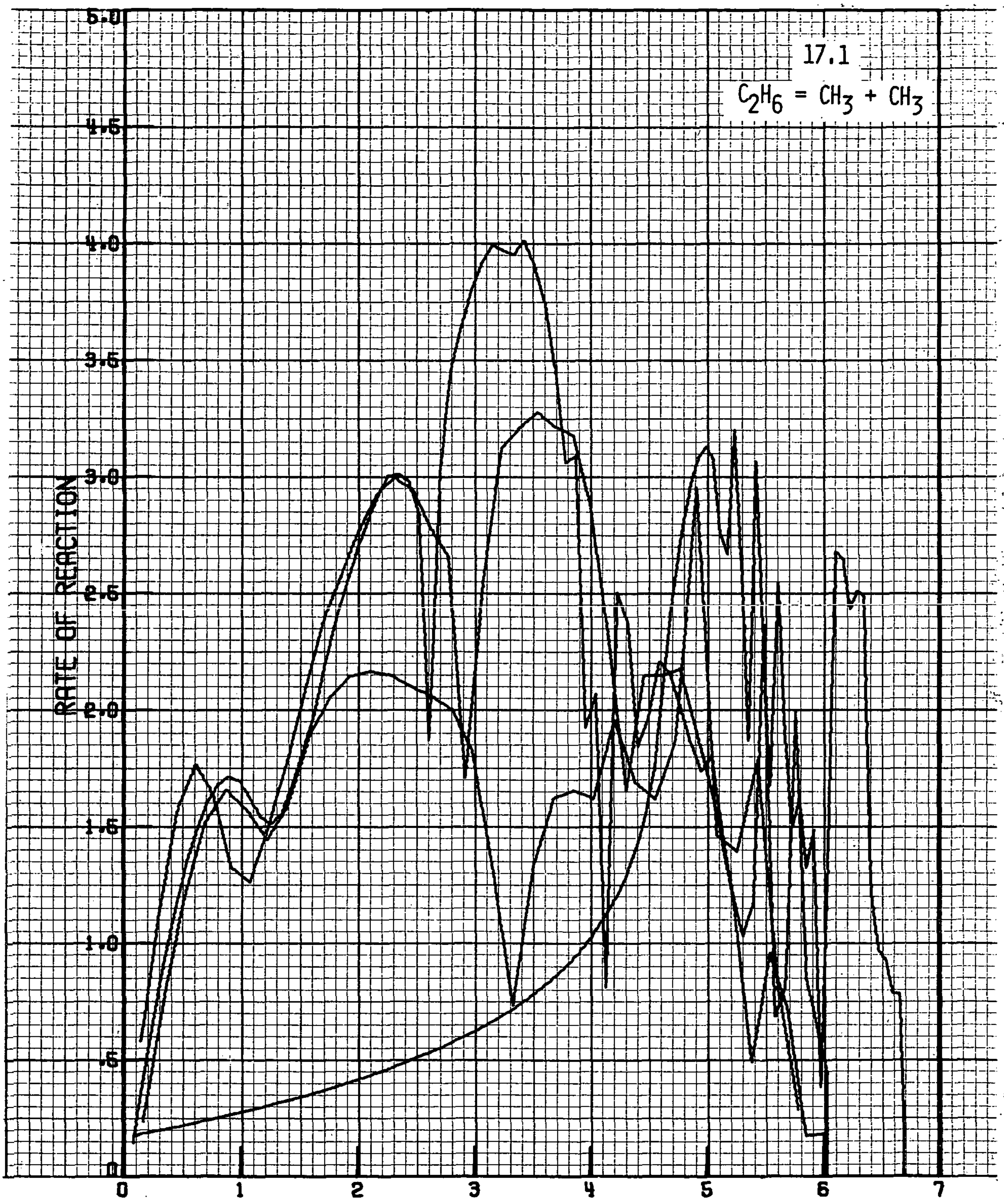

17.1
$C_2H_6 = CH_3 + CH_3$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-75

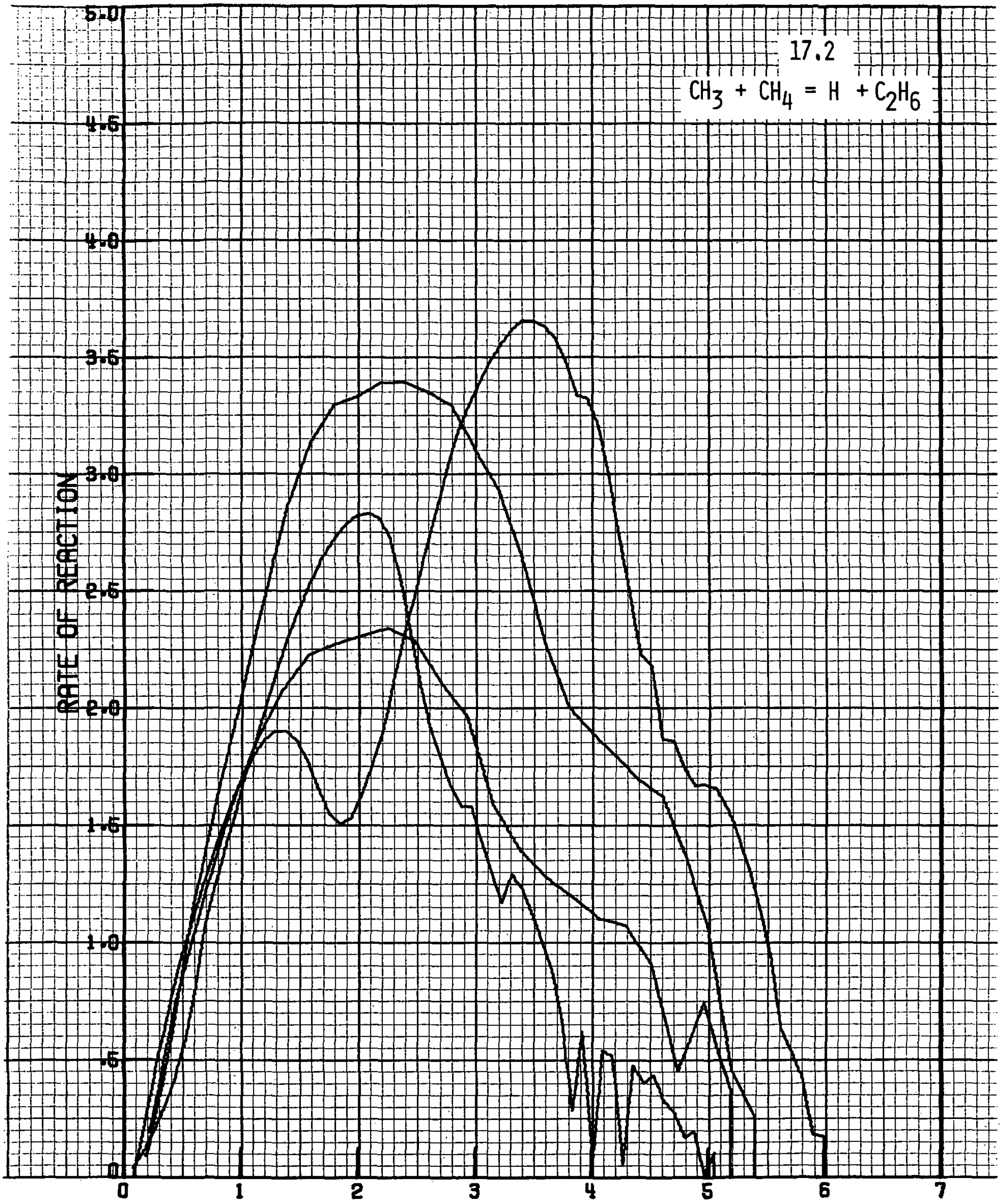
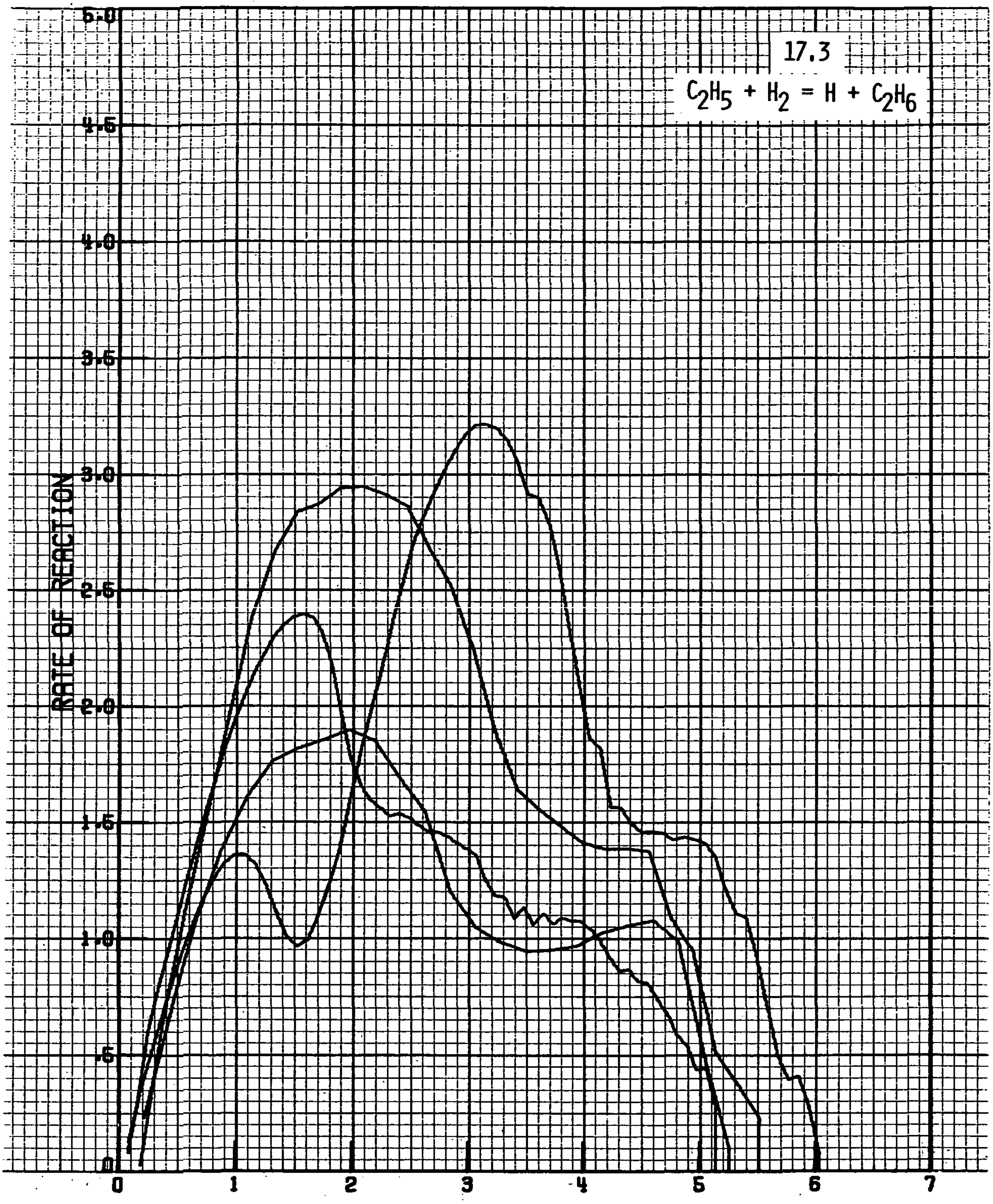

17.2
$CH_3 + CH_4 = H + C_2H_6$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-76



17.3
$C_2H_5 + H_2 = H + C_2H_6$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-77

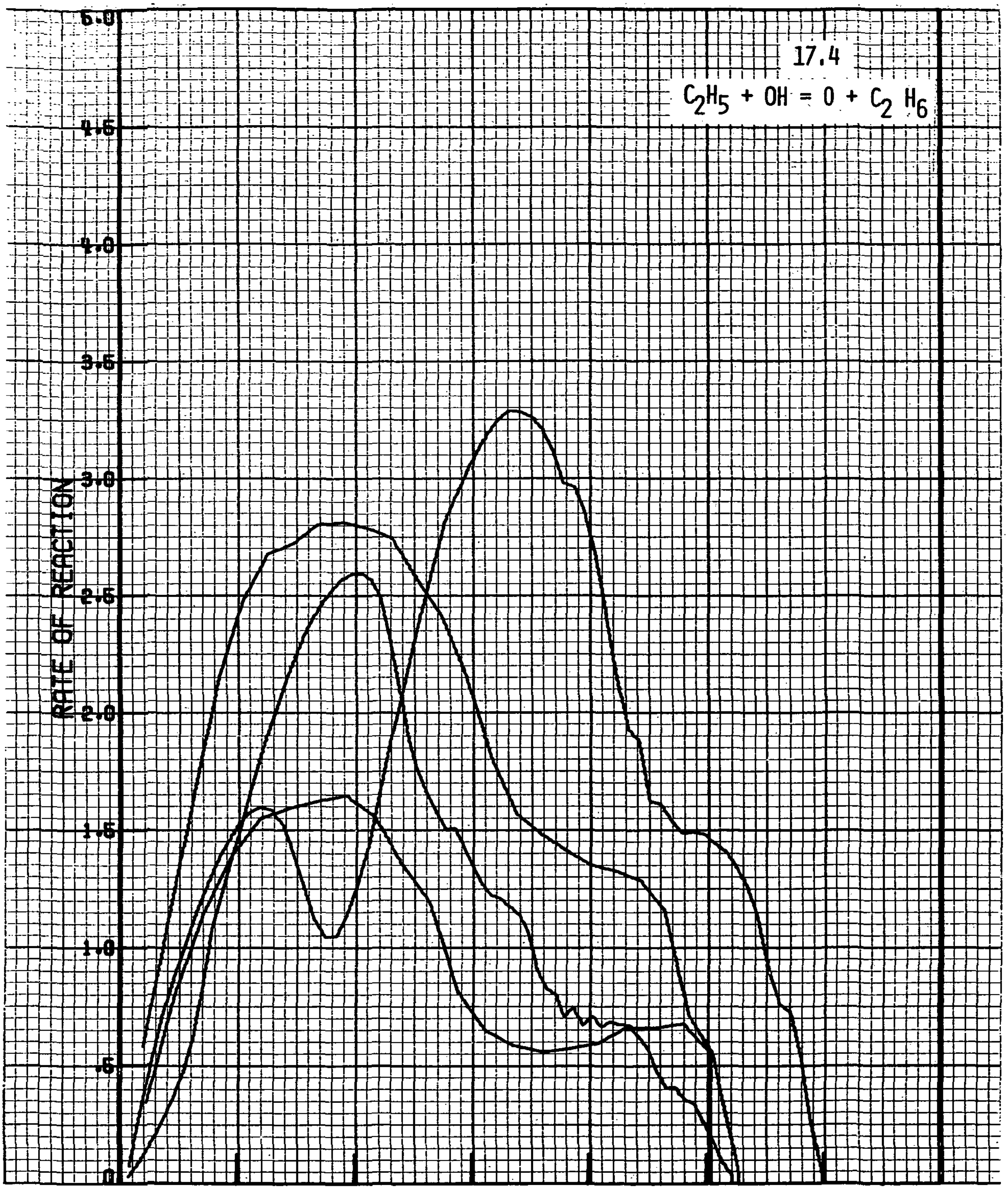

17.4
$C_2H_5 + OH = O + C_2H_6$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-78

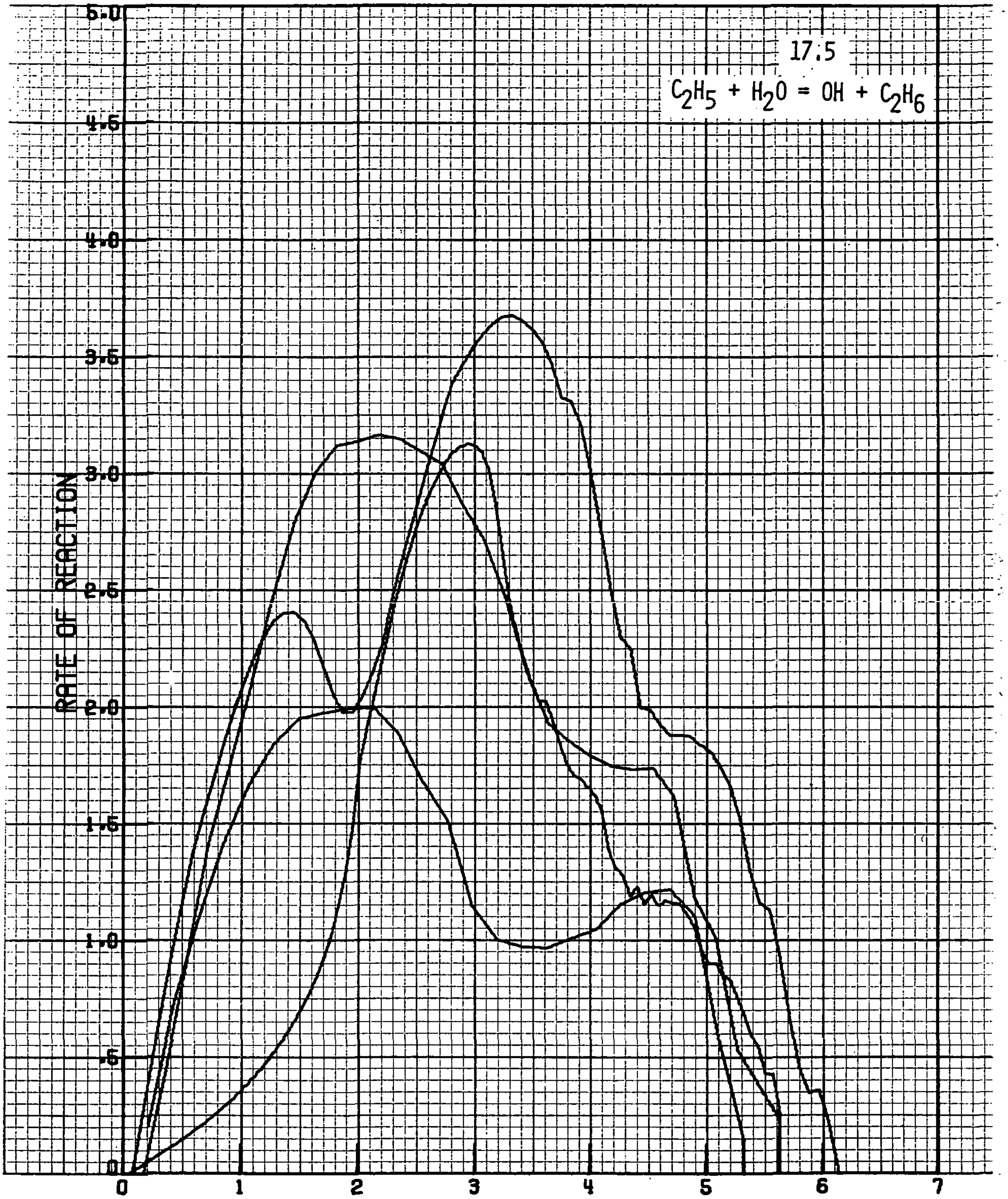

17.5
$C_2H_5 + H_2O = OH + C_2H_6$
RATE OF REACTION
PROGRESS OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7

Figure A-79

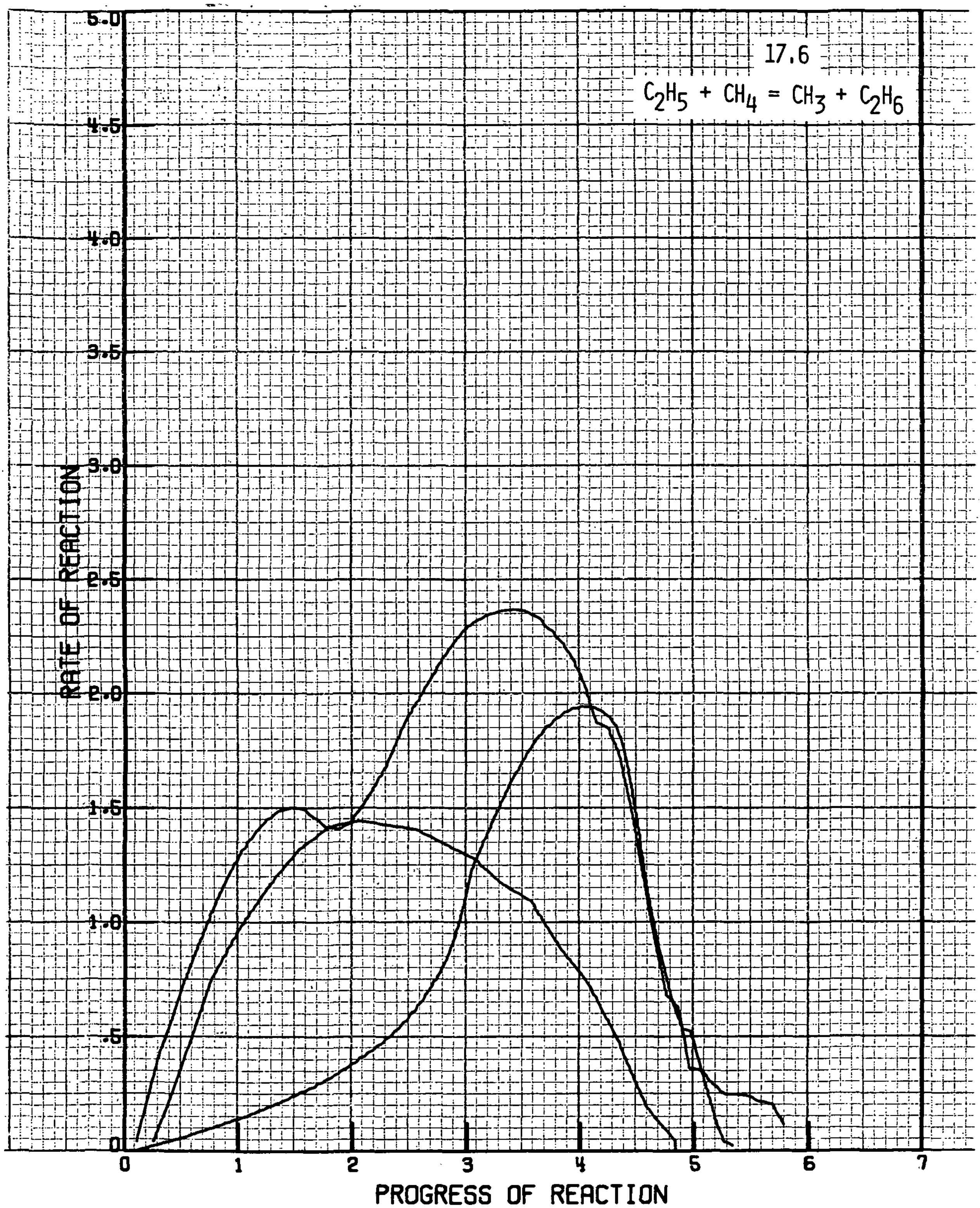

17.6
$C_2H_5 + CH_4 = CH_3 + C_2H_6$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-80

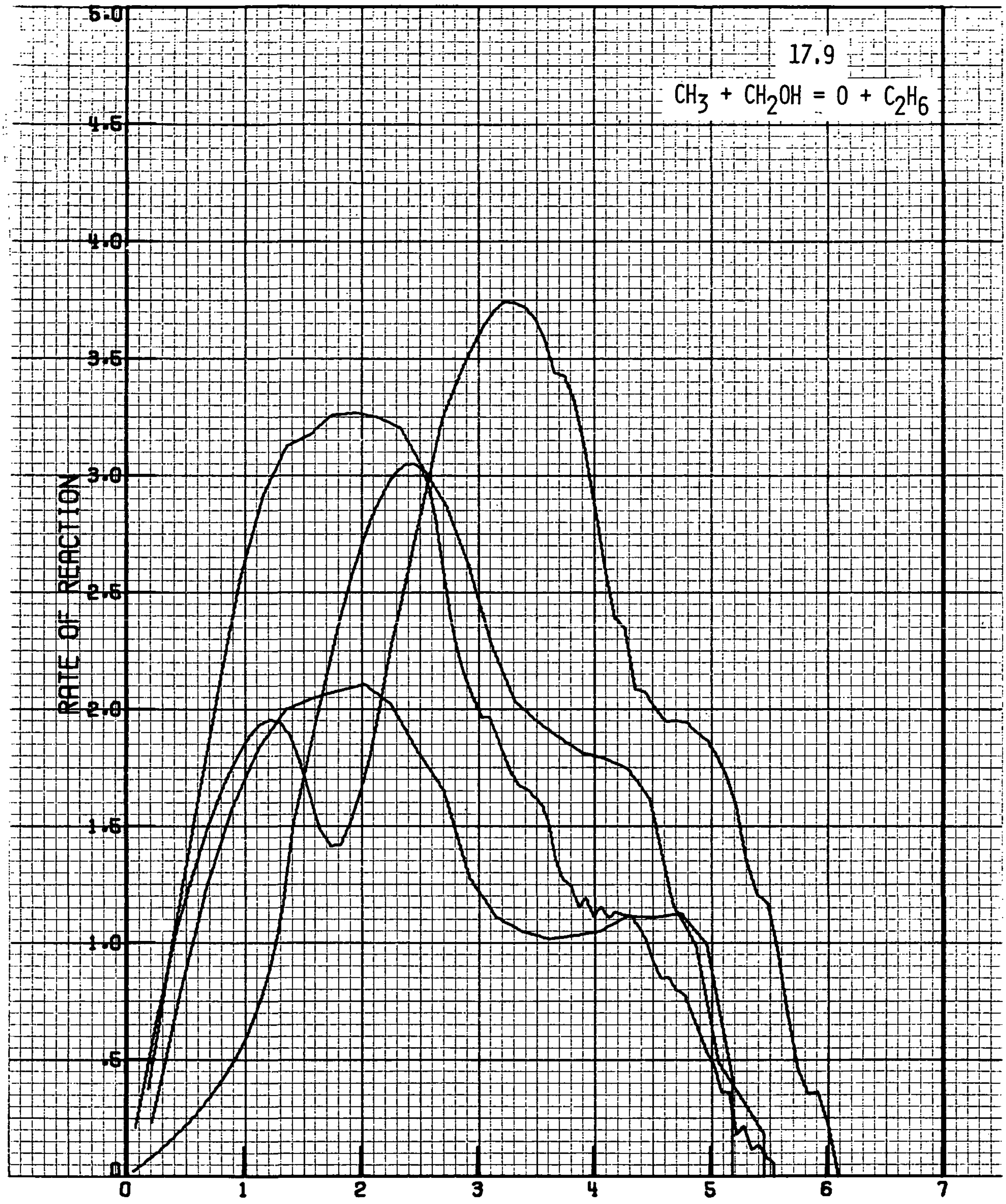

17.9
$CH_3 + CH_2OH = O + C_2H_6$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-81

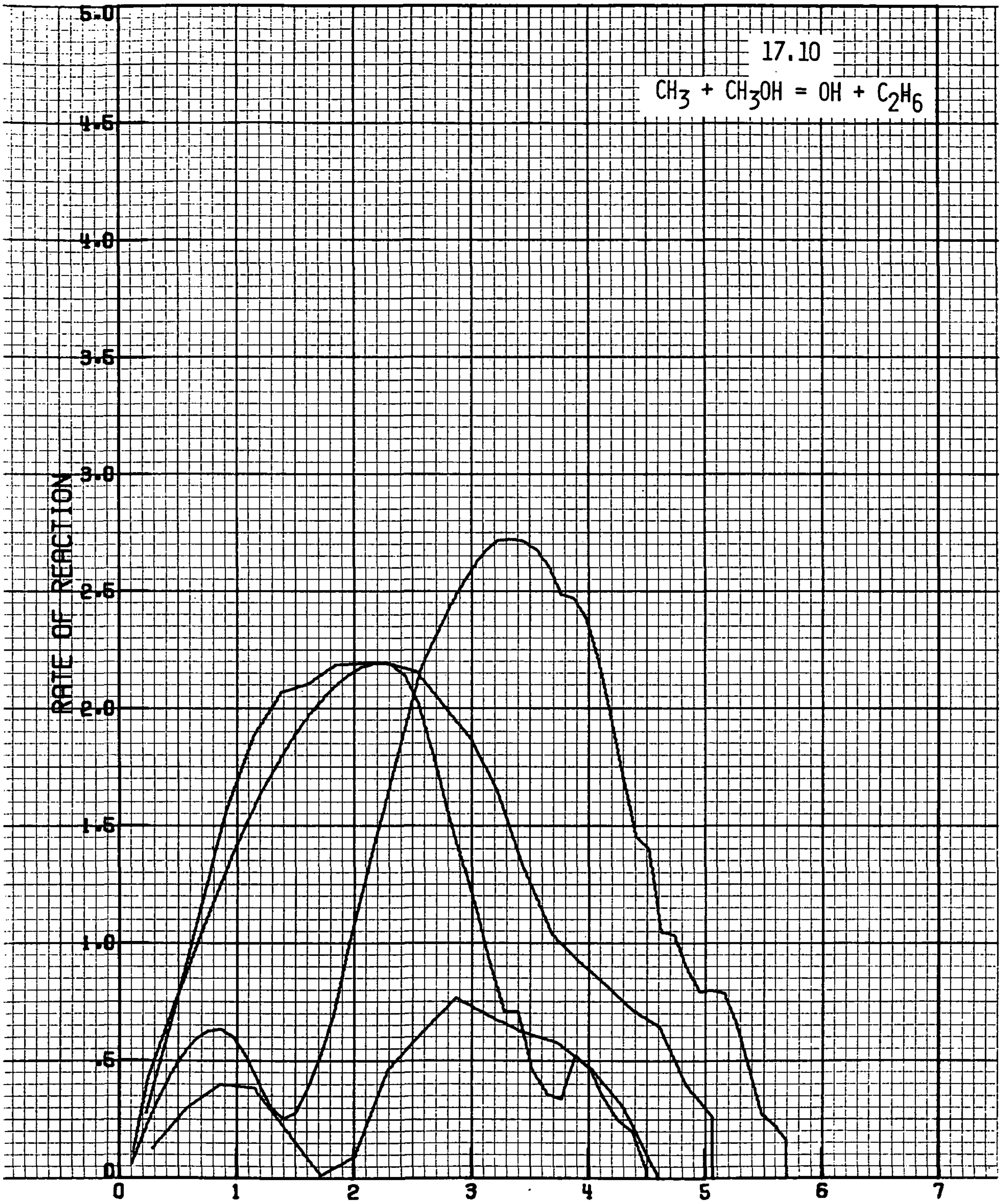

17.10
$CH_3 + CH_3OH = OH + C_2H_6$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-82

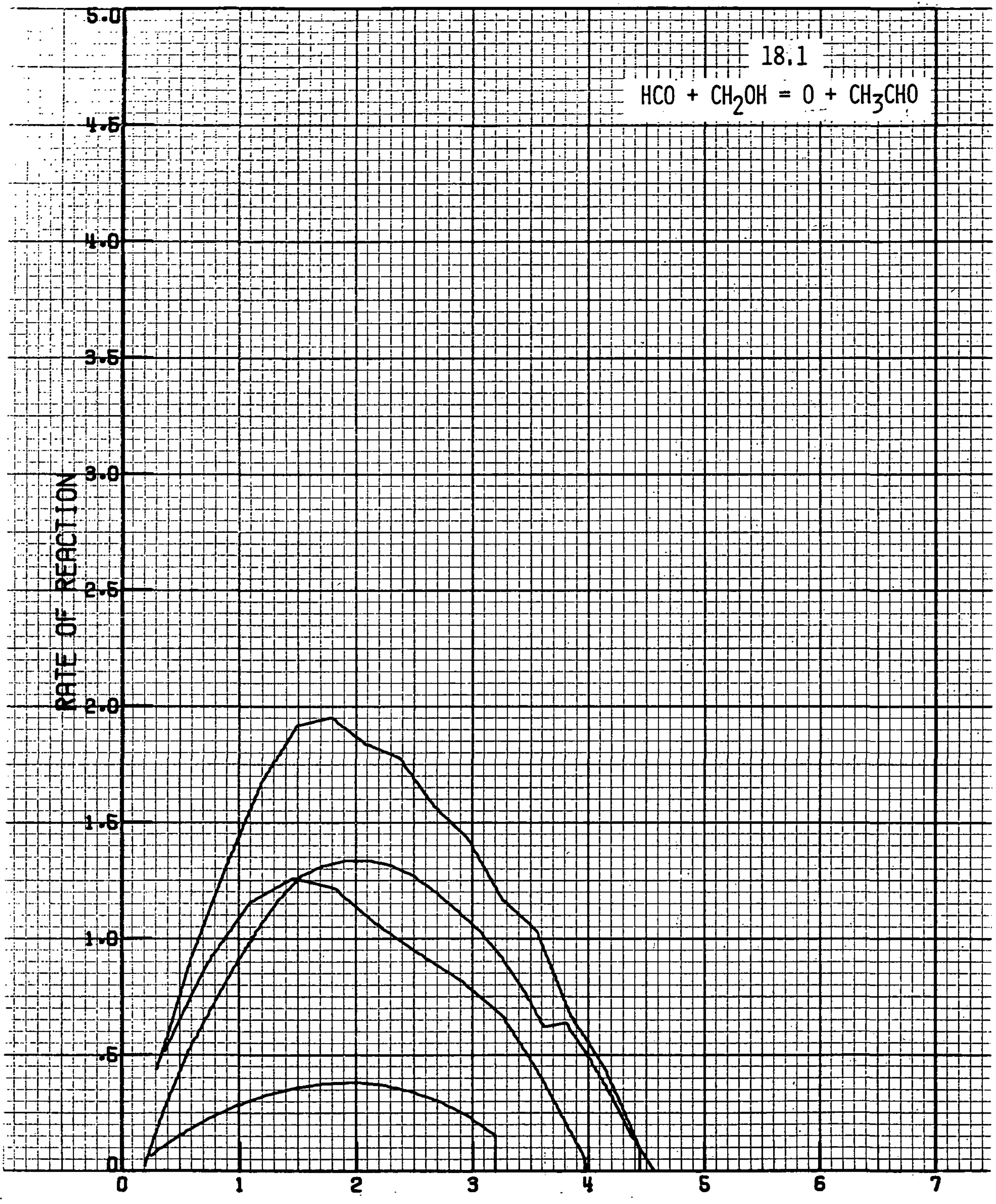
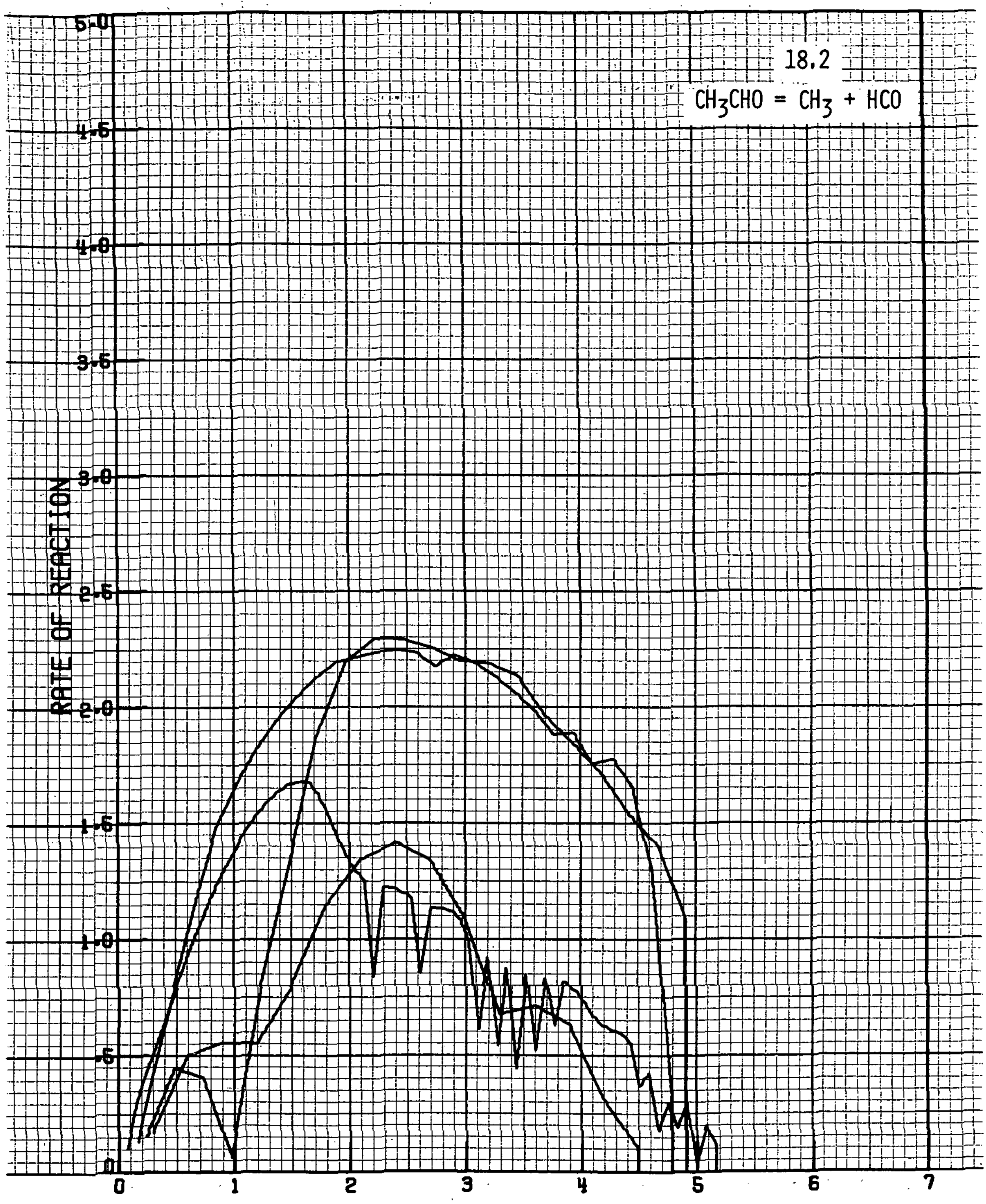

18.1
$HCO + CH_2OH = O + CH_3CHO$
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
RATE OF REACTION
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-83



18.2
$CH_3CHO = CH_3 + HCO$
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
RATE OF REACTION
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-84

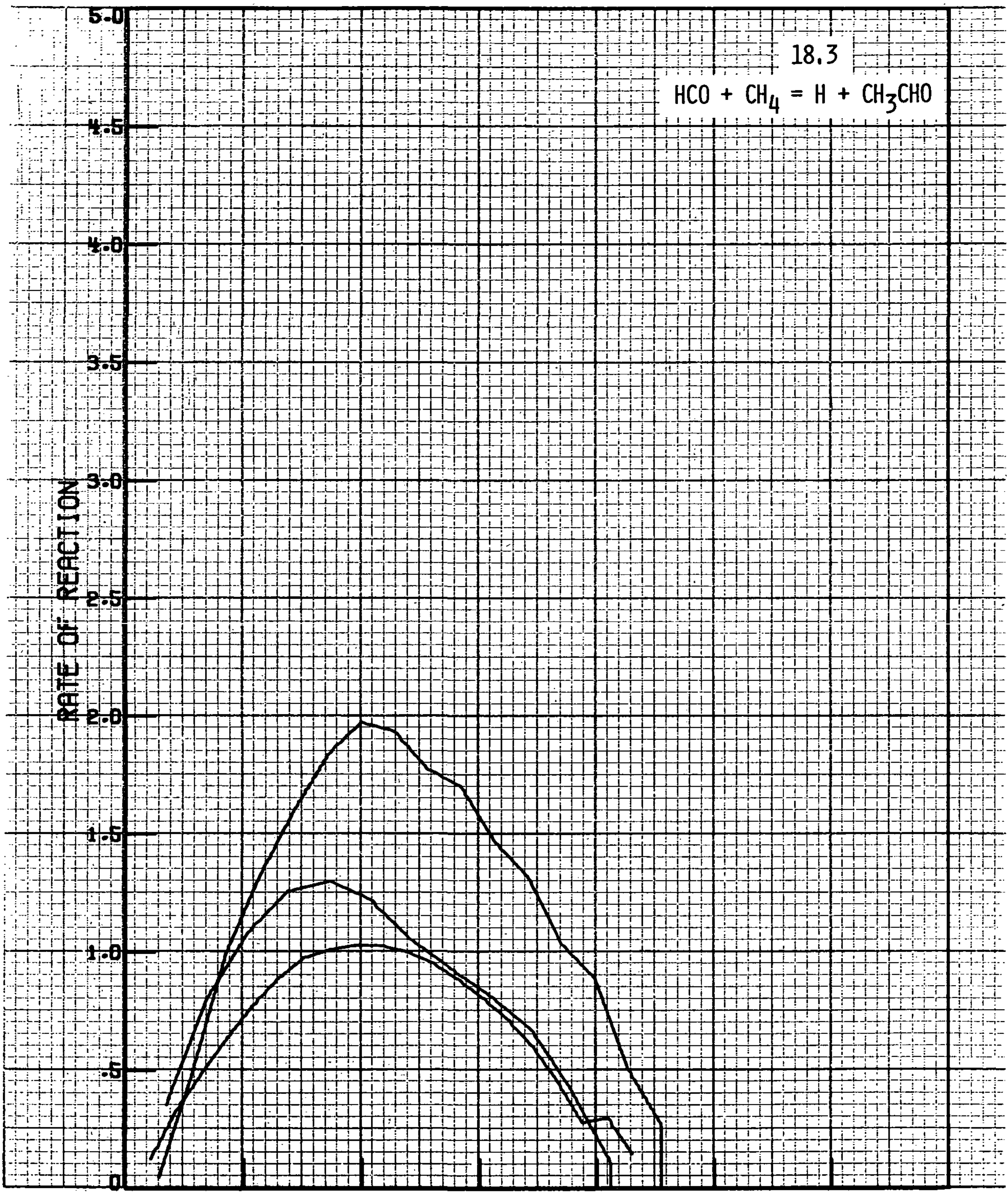

18.3
HCO + CH4 = H + CH3CHO
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-85

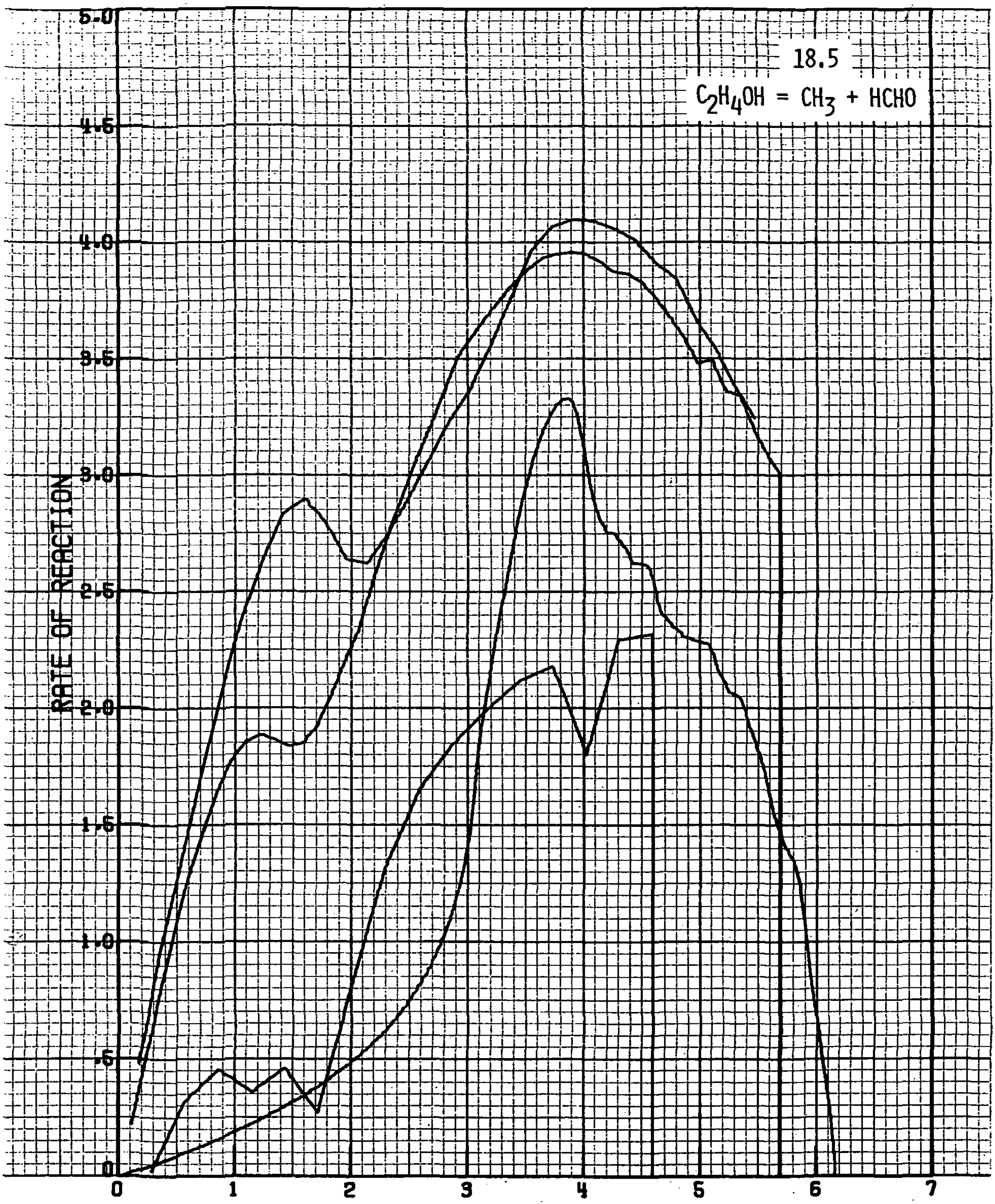

18.5
$C_2H_4OH = CH_3 + HCHO$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-86

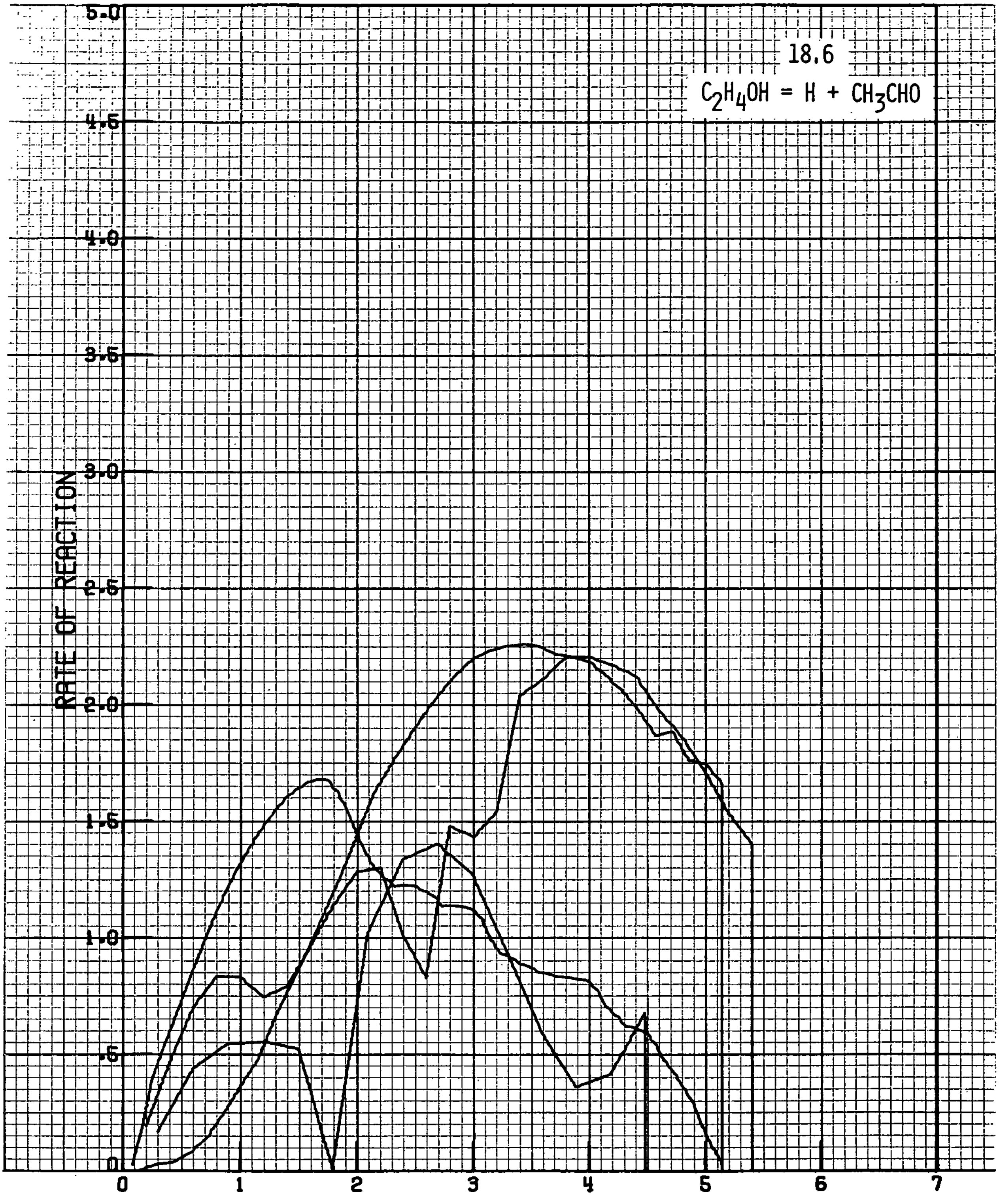

18.6
$C_2H_4OH = H + CH_3CHO$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-87

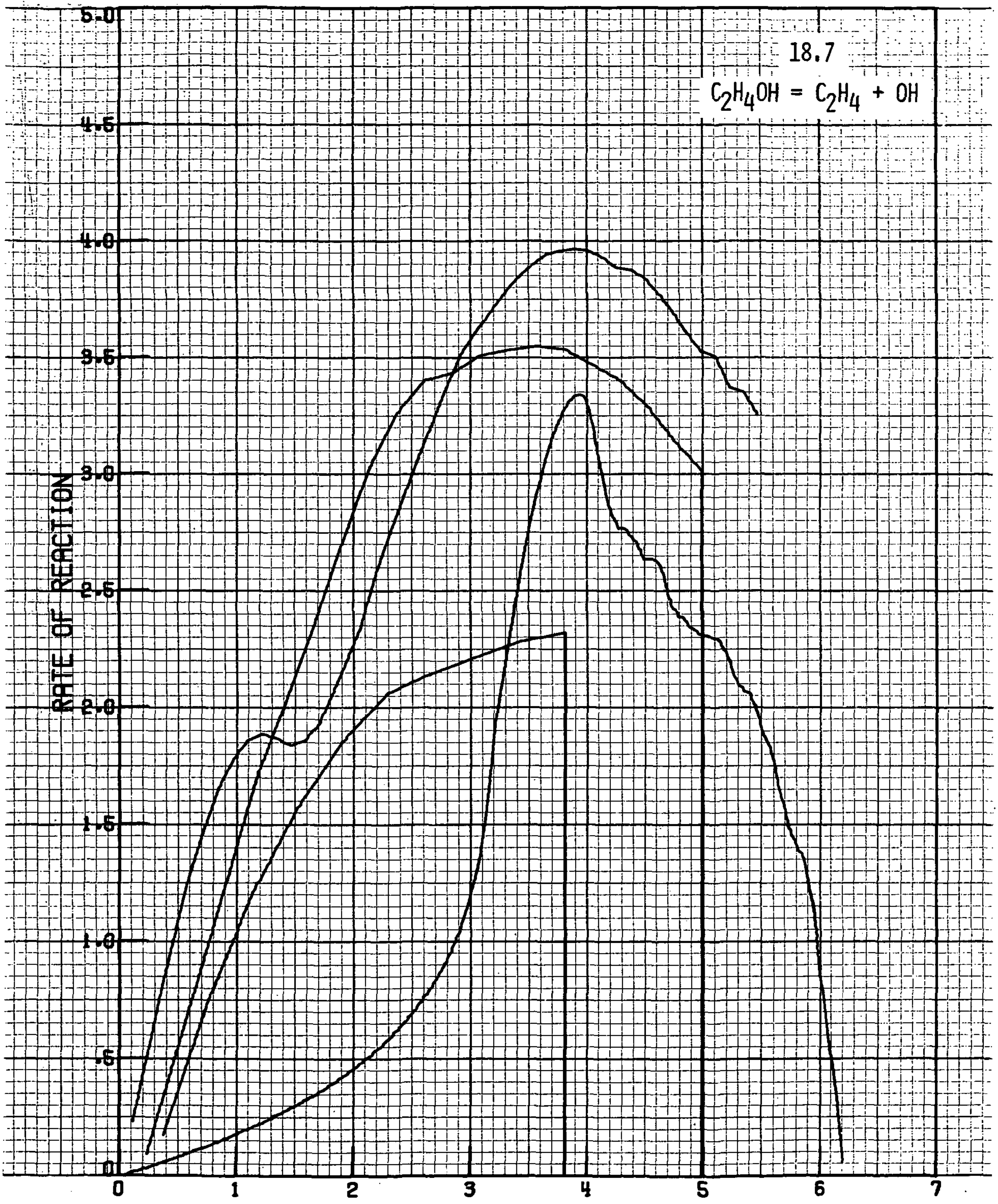

18.7
$C_2H_4OH = C_2H_4 + OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-88

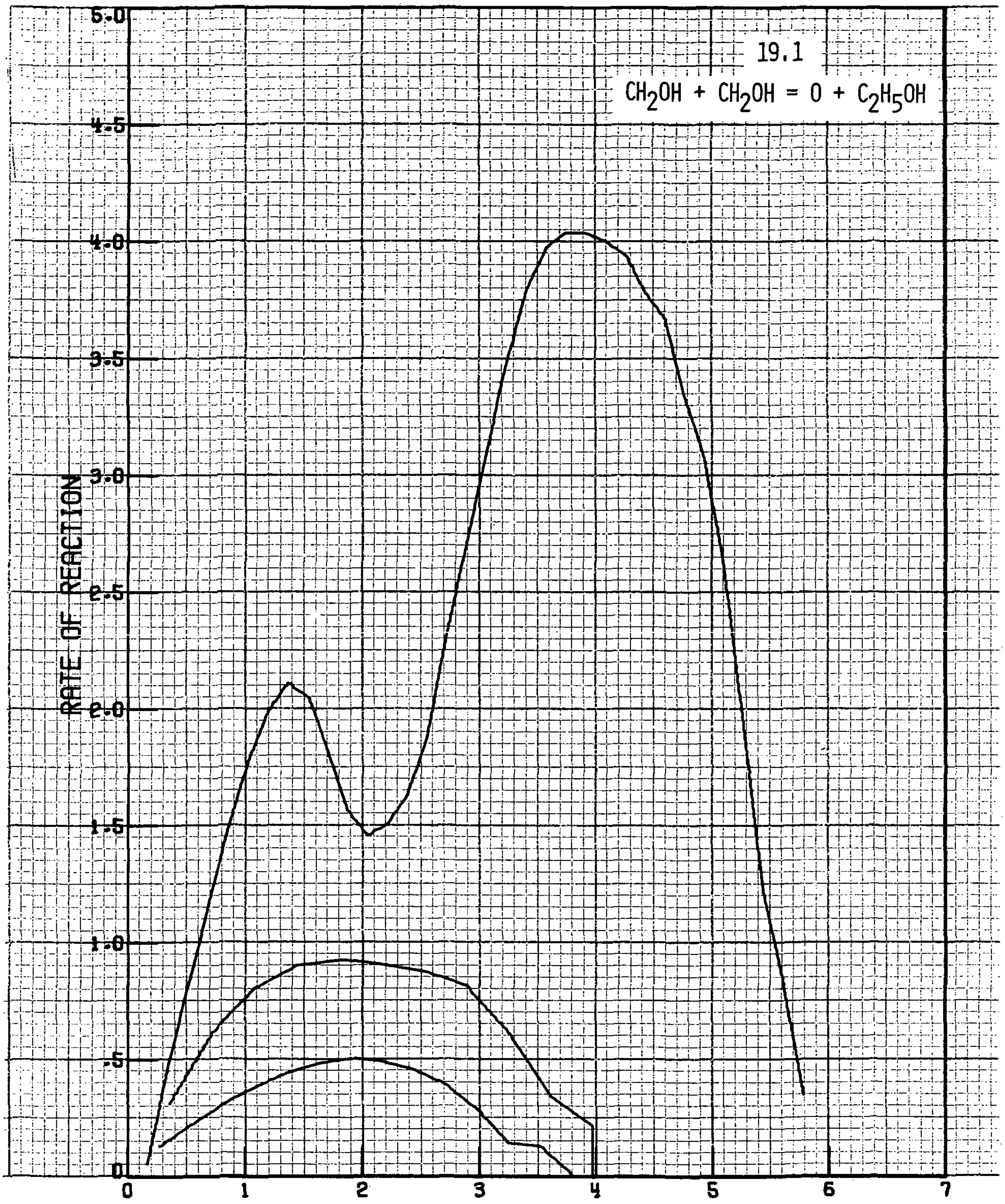

19.1
$CH_2OH + CH_2OH = O + C_2H_5OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-89

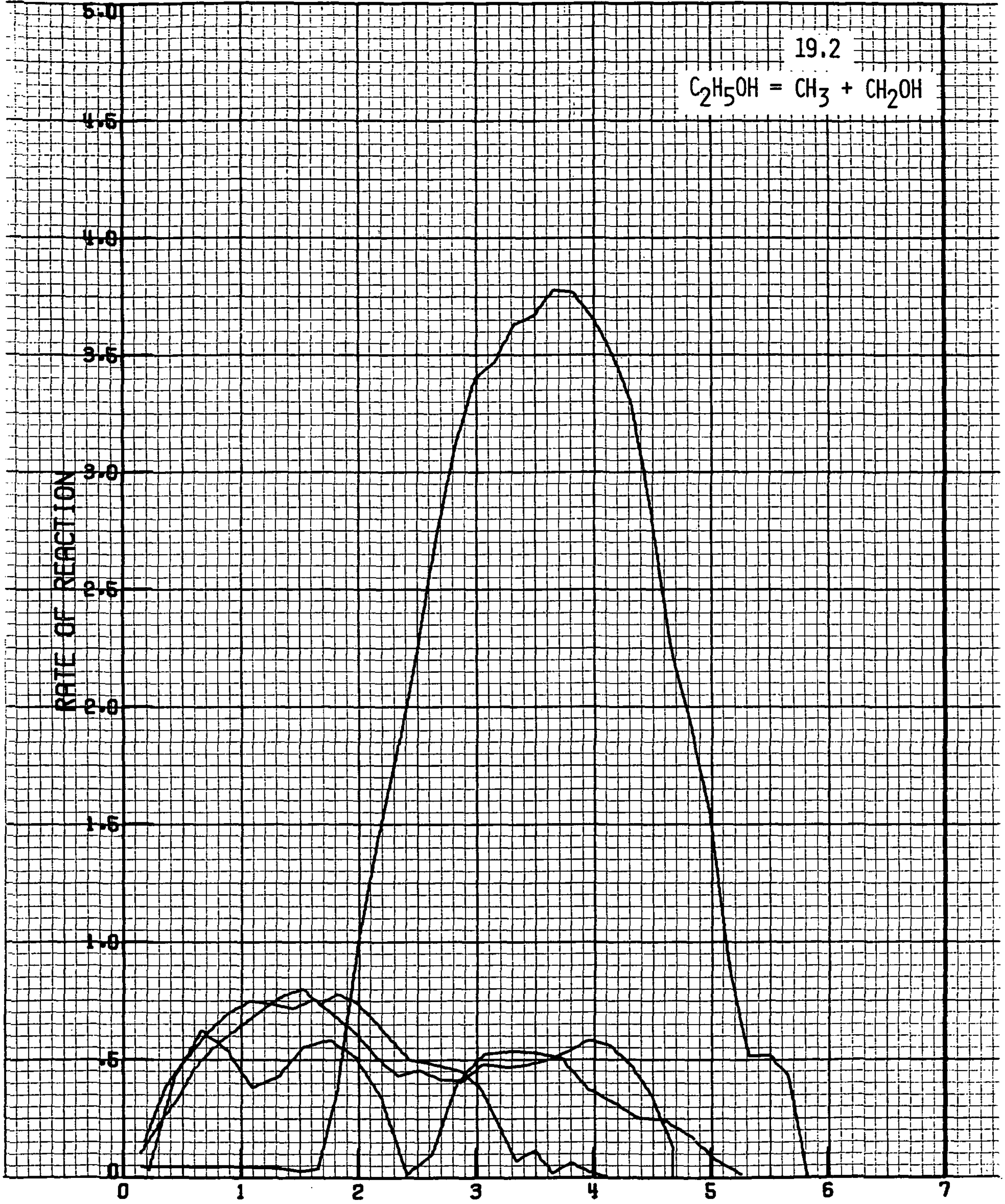

19.2
$C_2H_5OH = CH_3 + CH_2OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-90

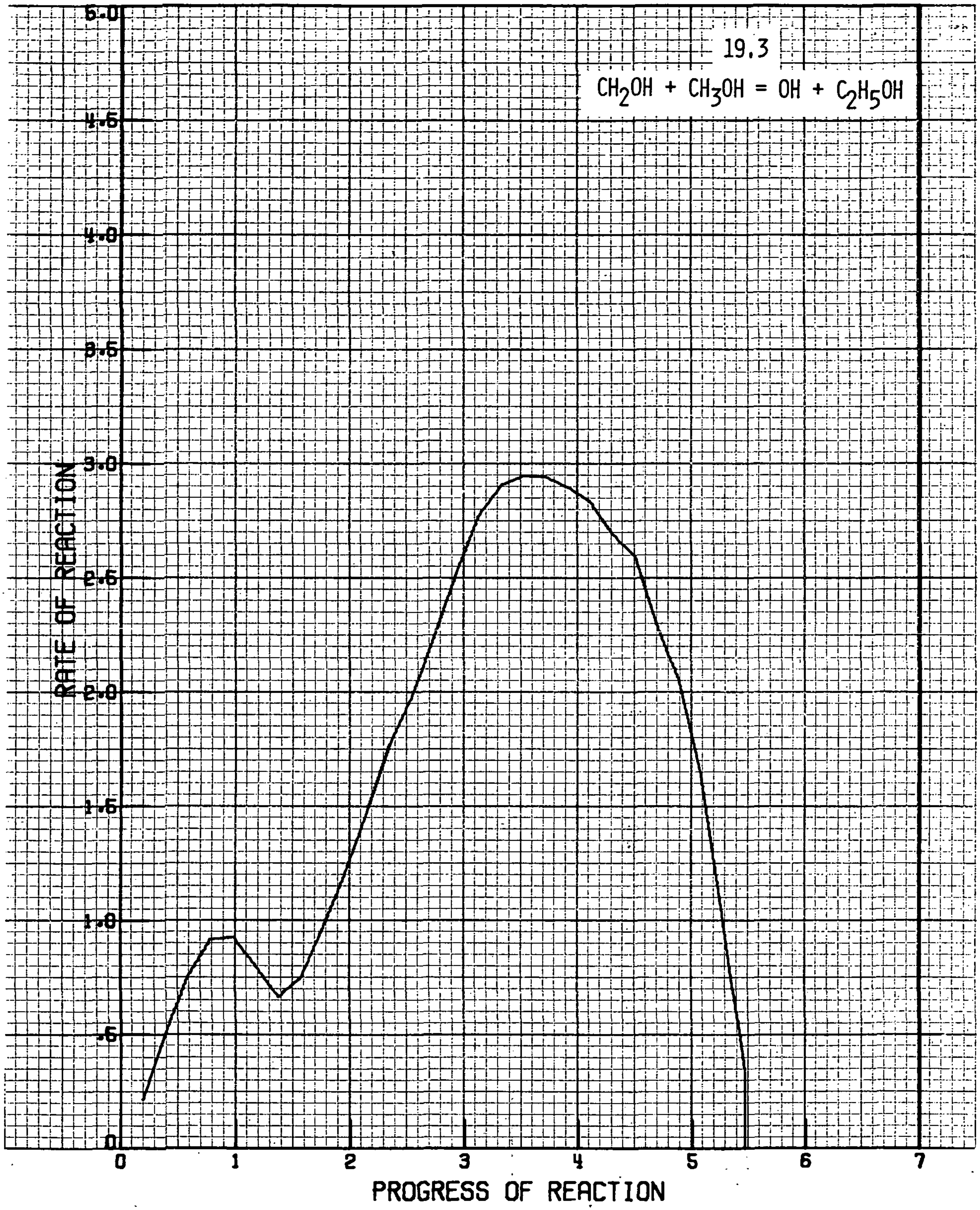

19.3
CH2OH + CH3OH = OH + C2H5OH
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
RATE OF REACTION
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-91

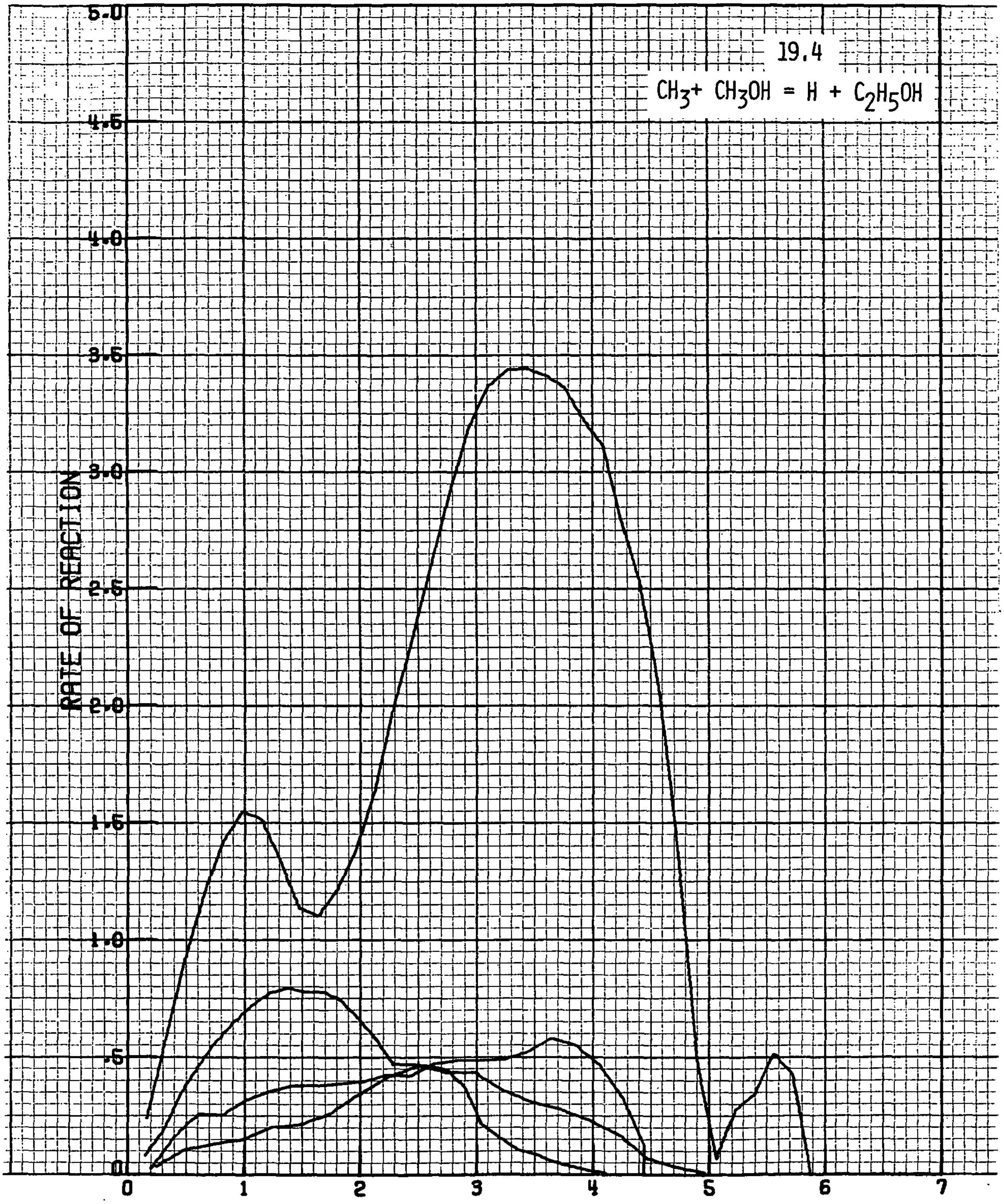

19.4
$CH_3 + CH_3OH = H + C_2H_5OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-92

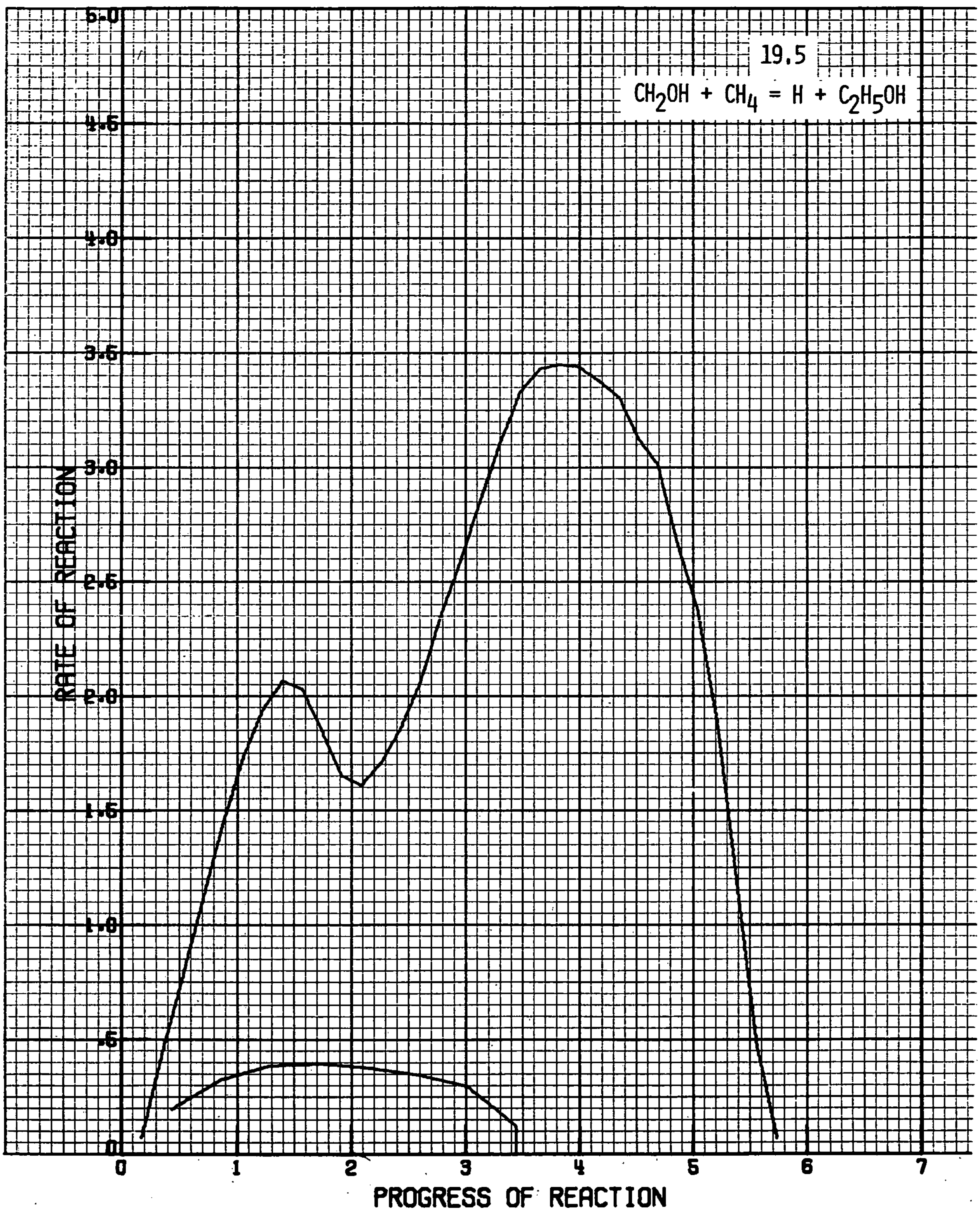

19.5
$CH_2OH + CH_4 = H + C_2H_5OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-93

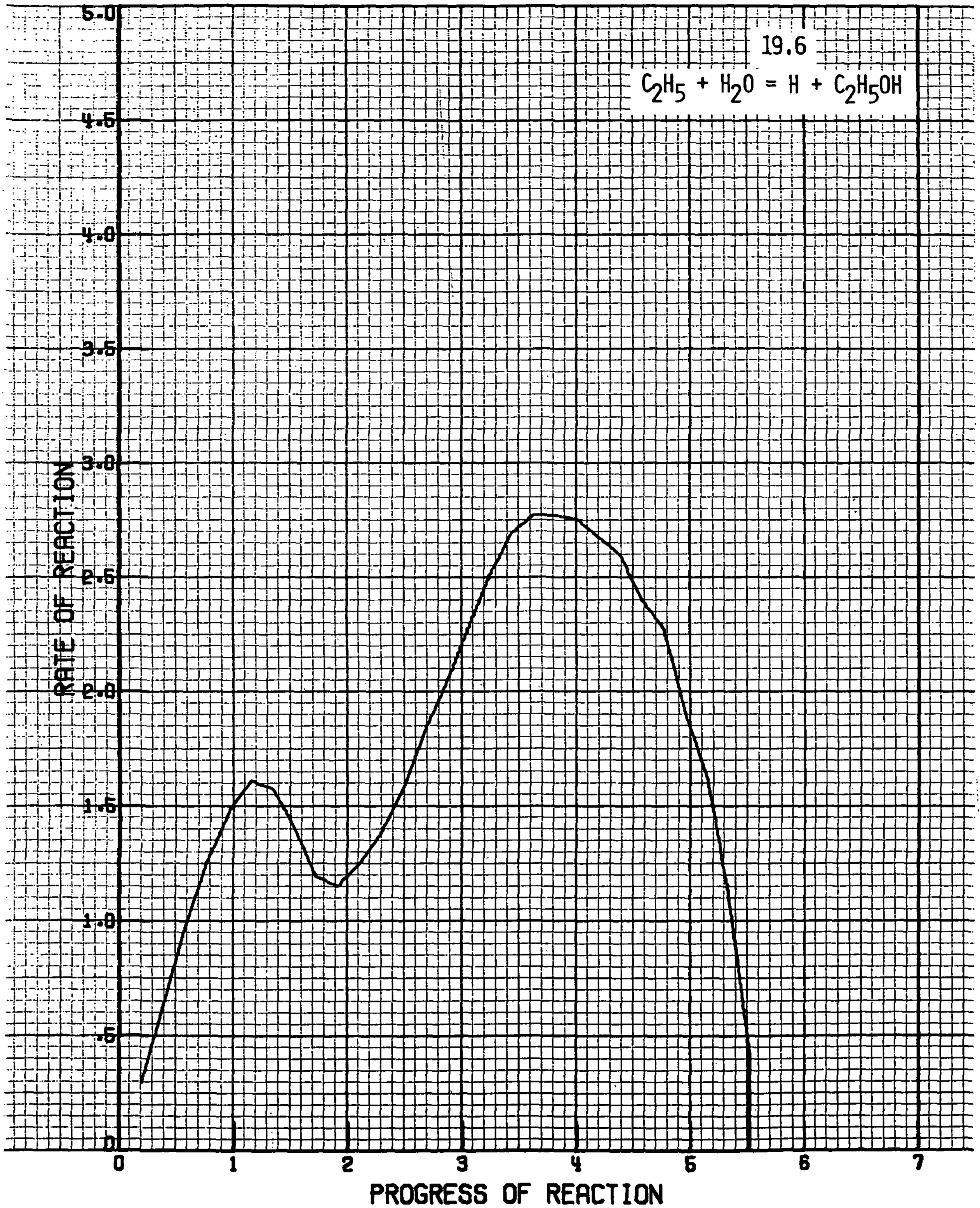
19.6
$C_2H_5 + H_2O = H + C_2H_5OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-94

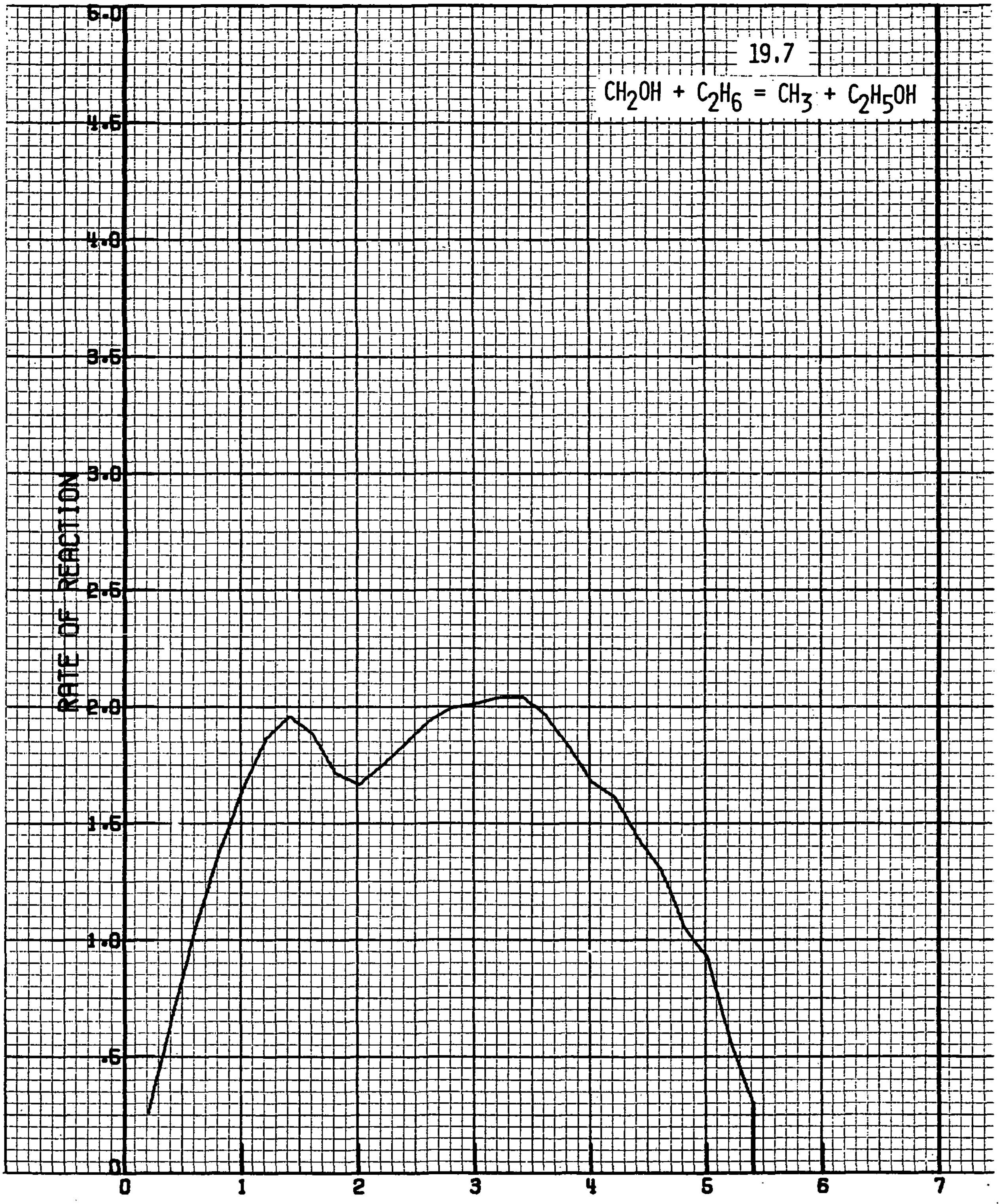

19.7
$CH_2OH + C_2H_6 = CH_3 + C_2H_5OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-95

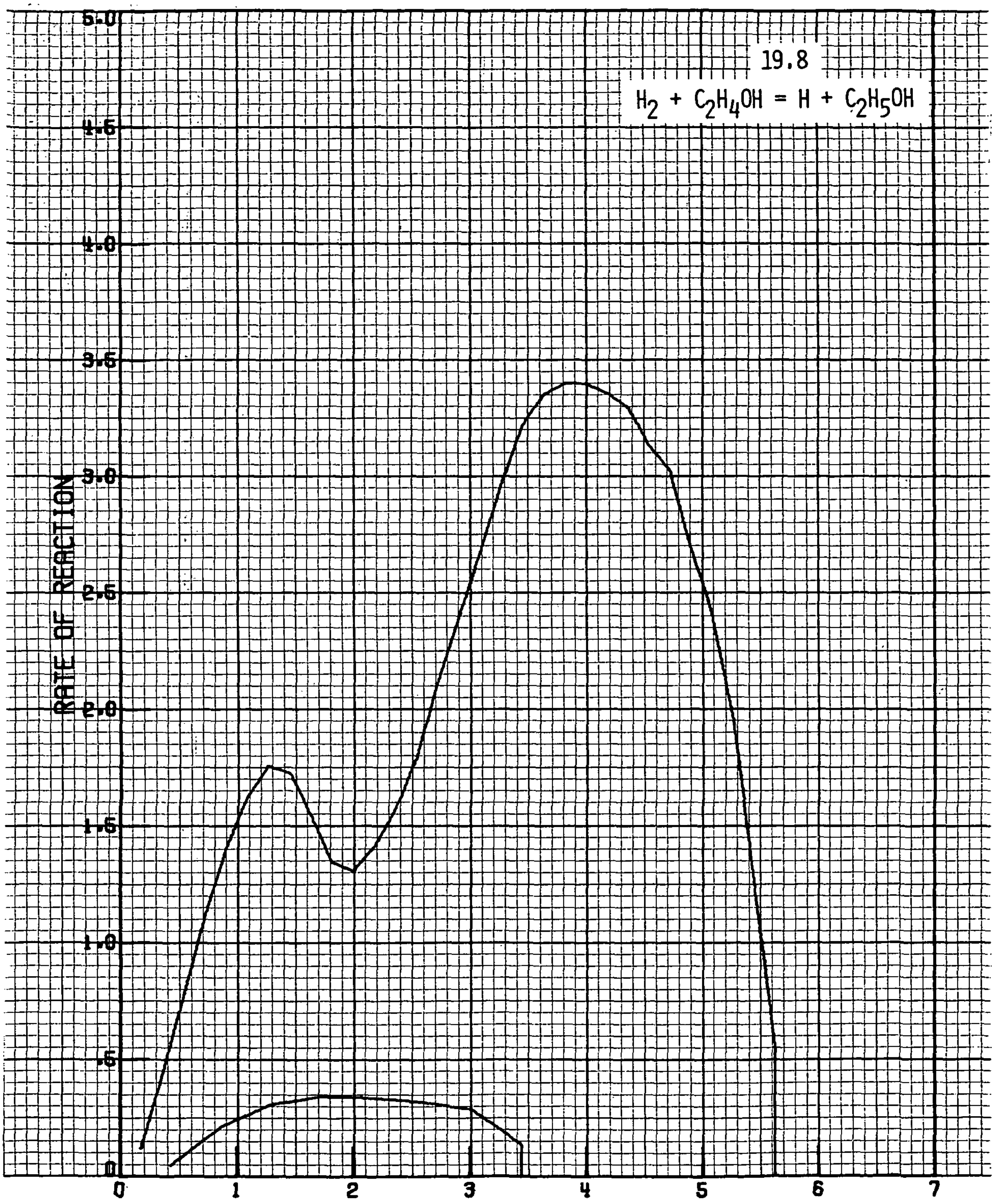

19.8
$H_2 + C_2H_4OH = H + C_2H_5OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-96

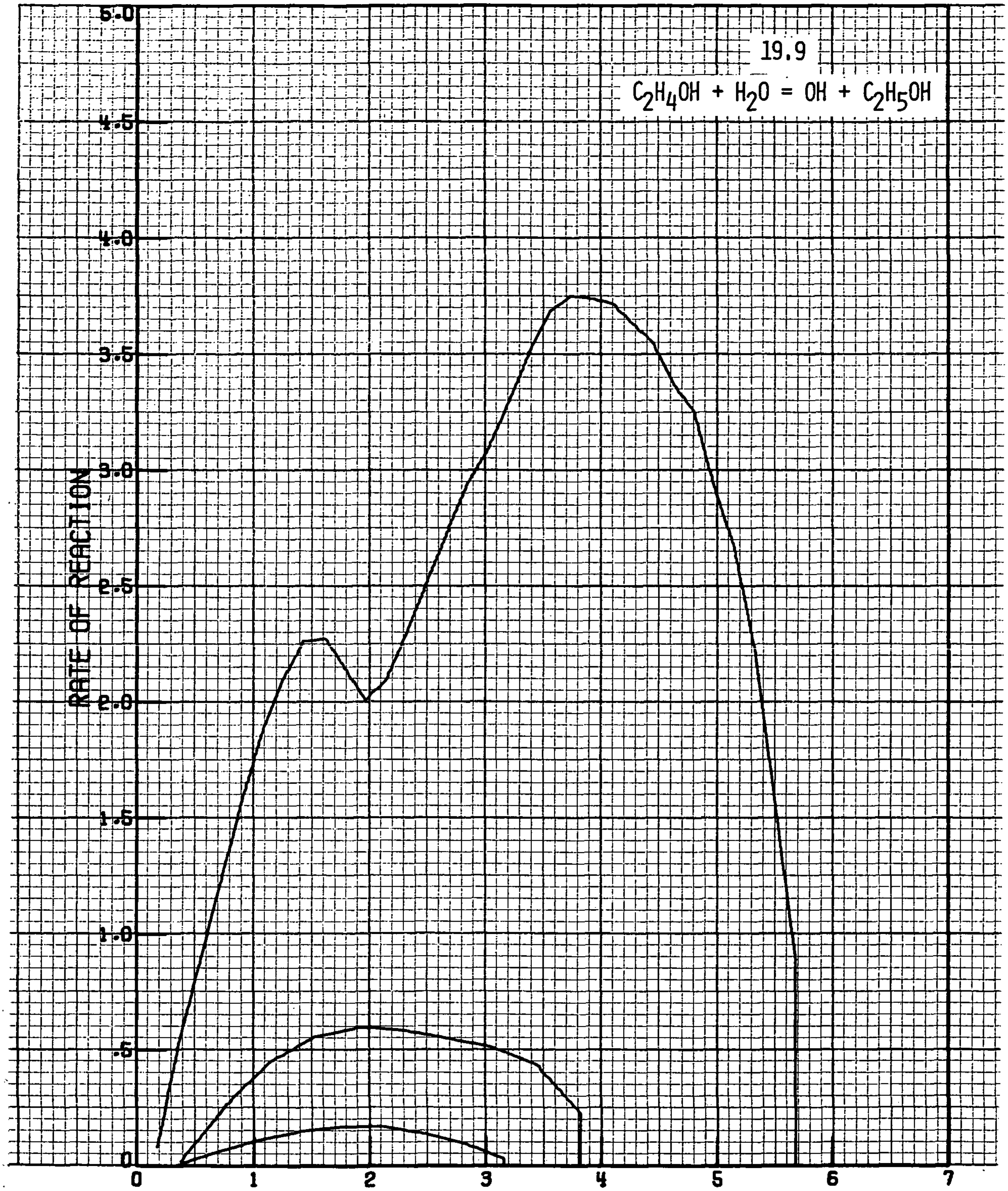

19.9
$C_2H_4OH + H_2O = OH + C_2H_5OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-97

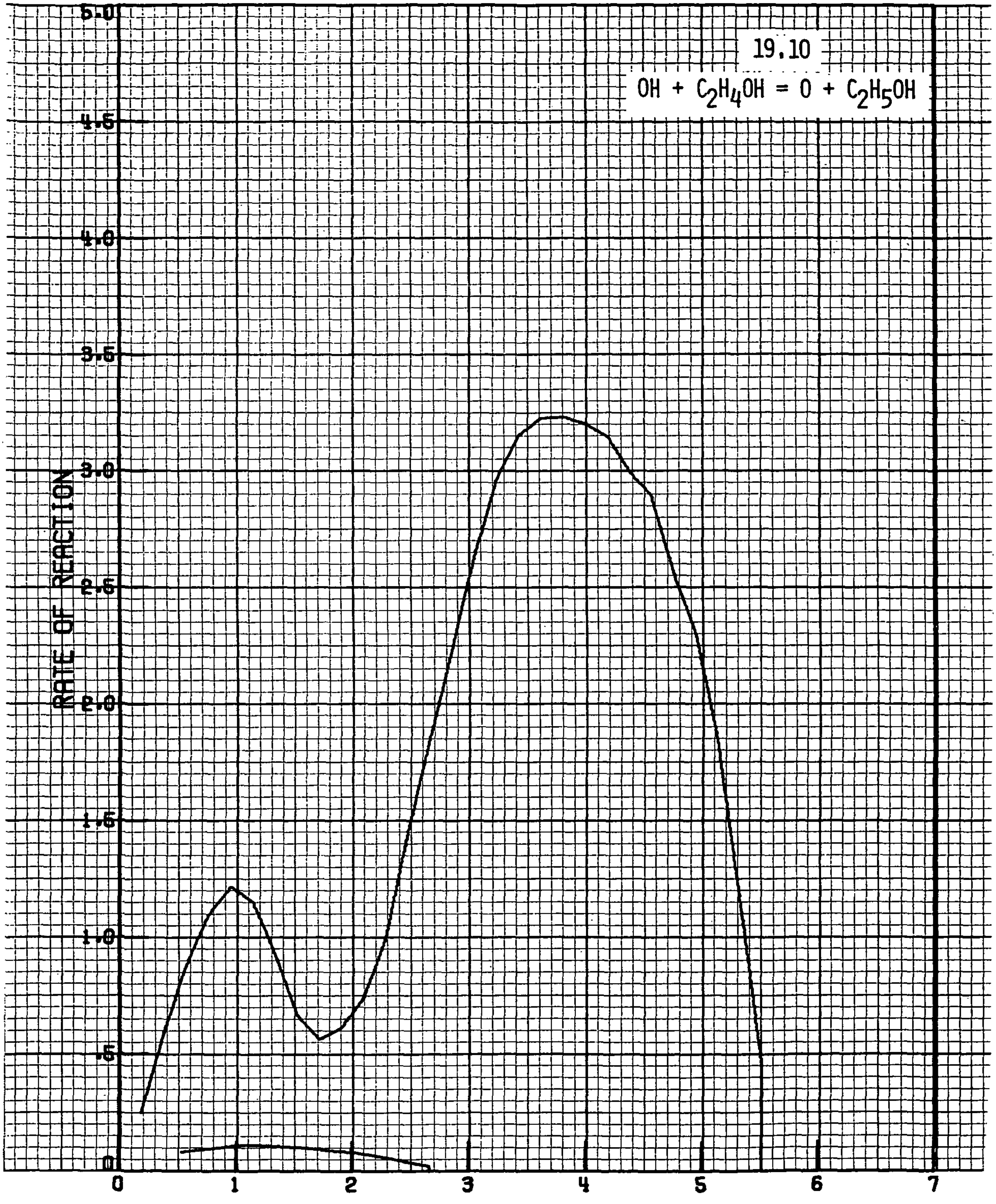
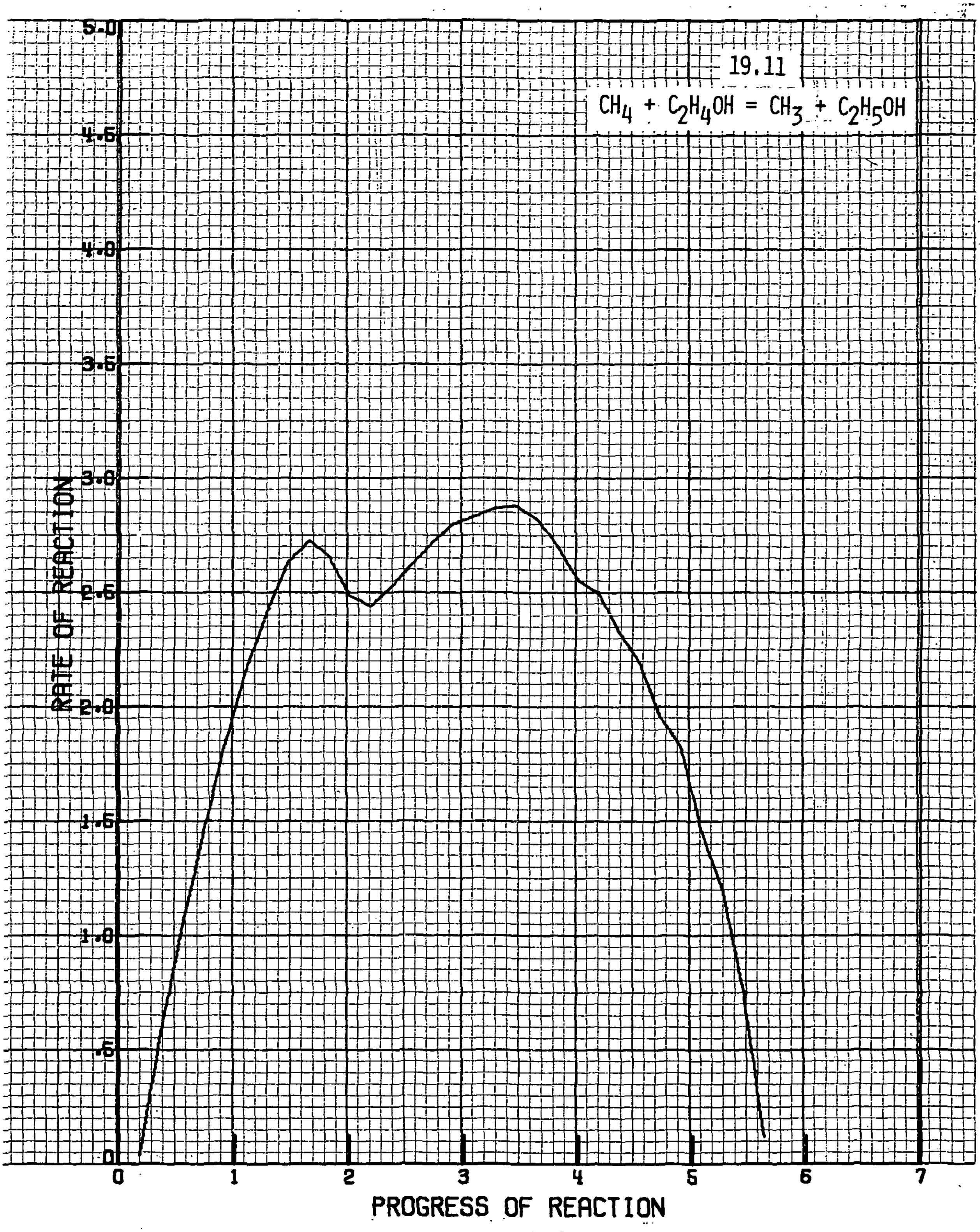

19.10
$OH + C_2H_4OH = O + C_2H_5OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-98



19.11
$CH_4 + C_2H_4OH = CH_3 + C_2H_5OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-99

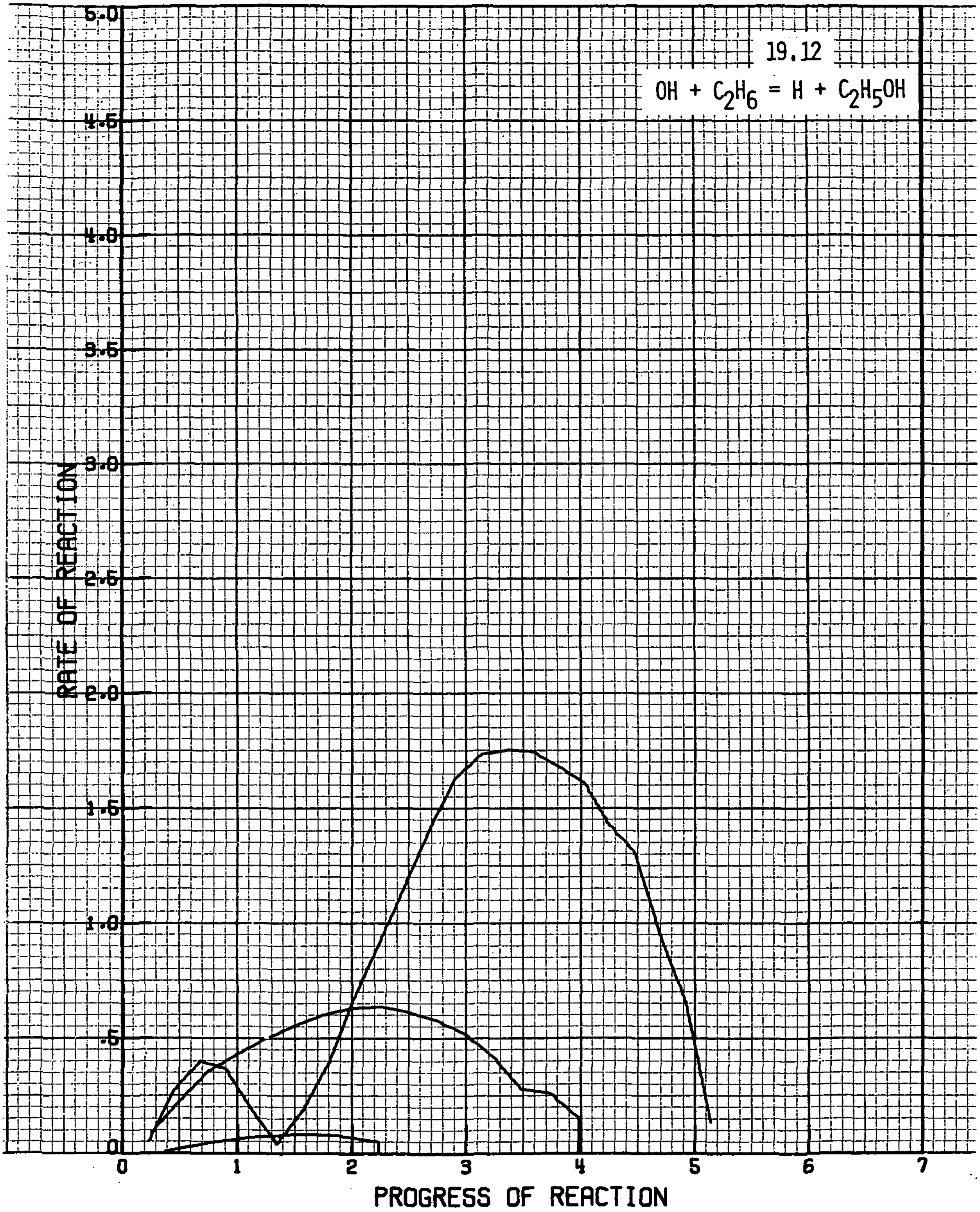

19.12
$OH + C_2H_6 = H + C_2H_5OH$
RATE OF REACTION
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0
0
1
2
3
4
5
6
7
PROGRESS OF REACTION

Figure A-100

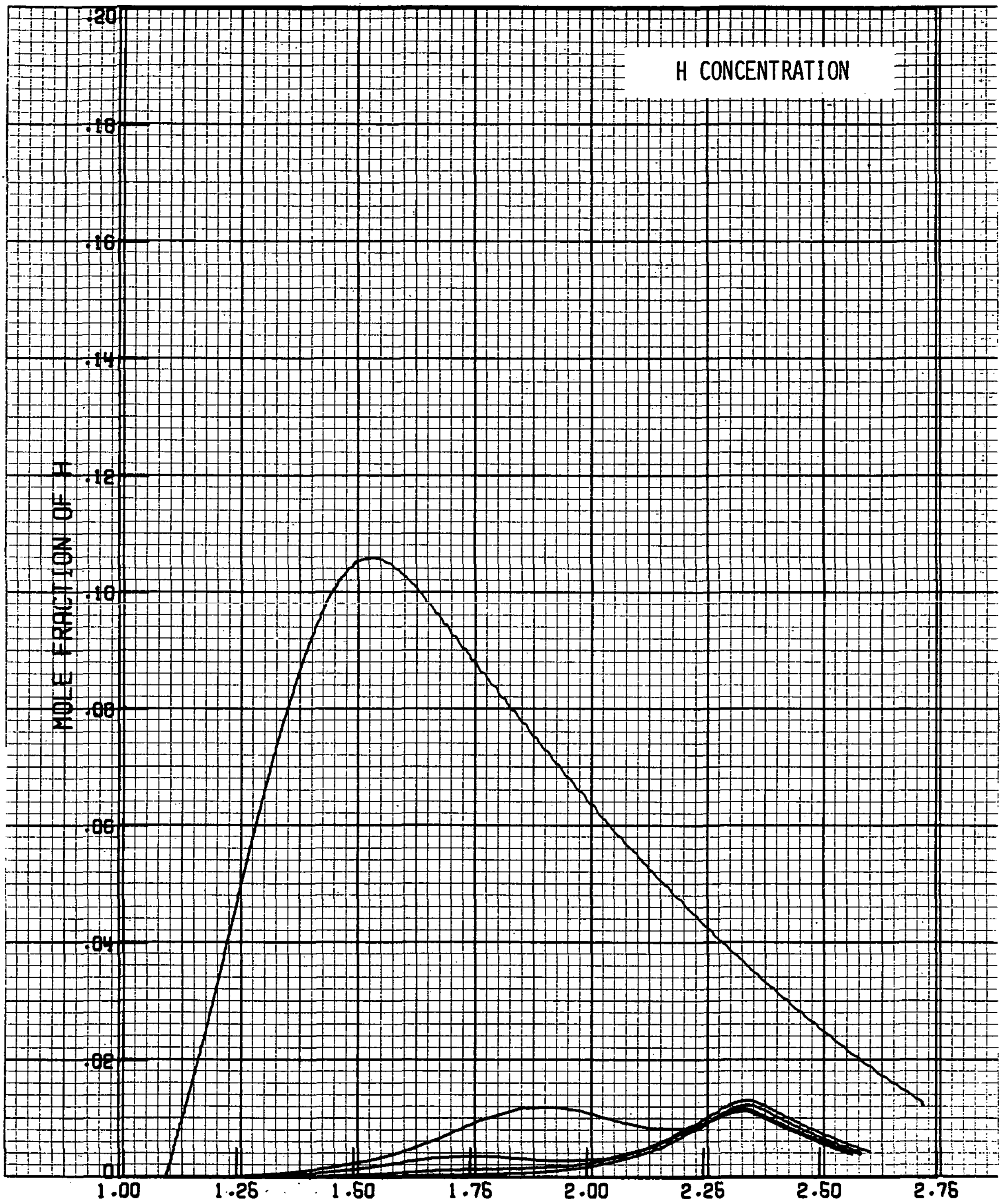

H CONCENTRATION
MOLE FRACTION OF H
.20
.18
.16
.14
.12
.10
.08
.06
.04
.02
0
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75
TEMPERATURE, KELVIN (THOUSANDS OF DEGREES)

Figure A-101

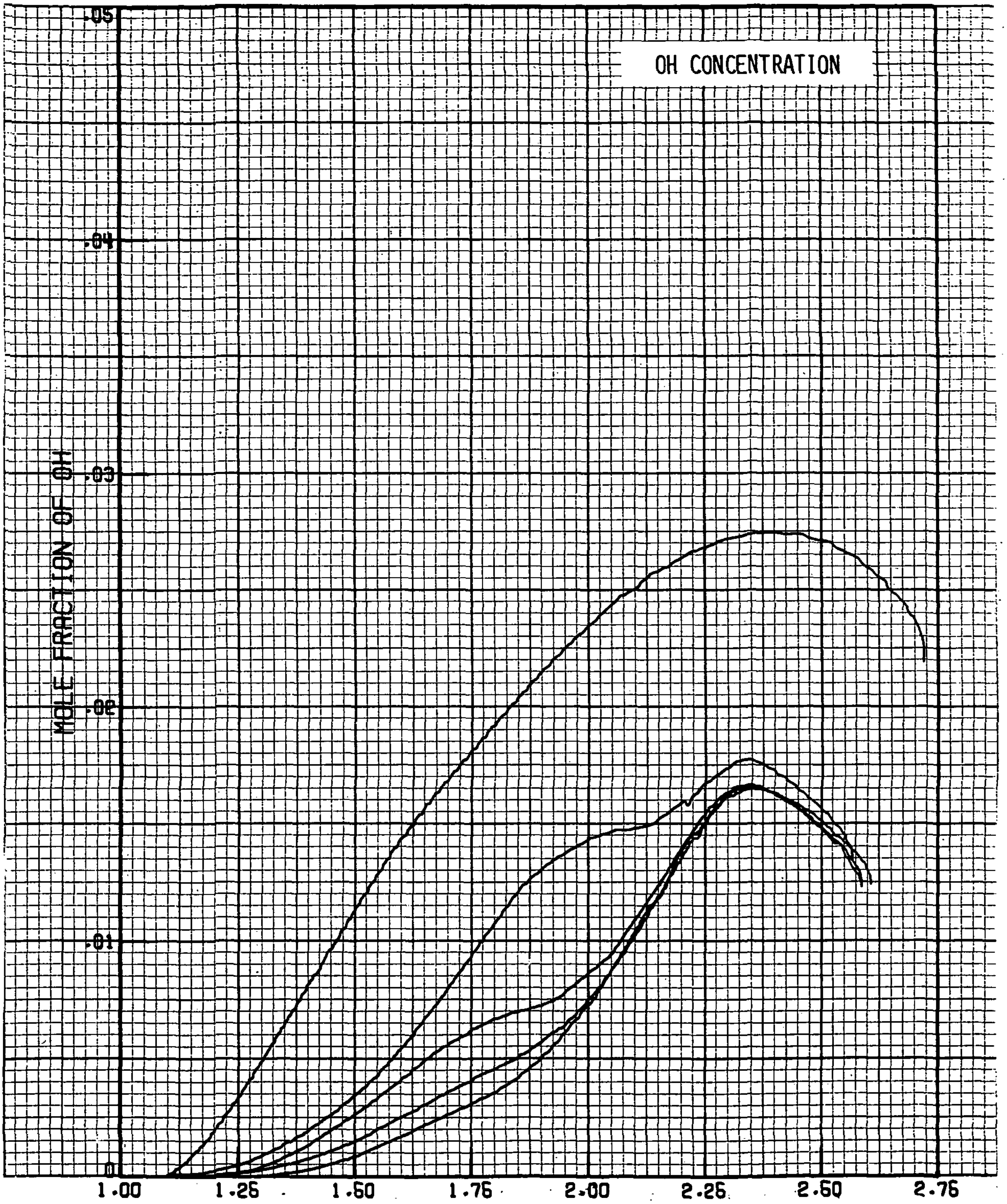
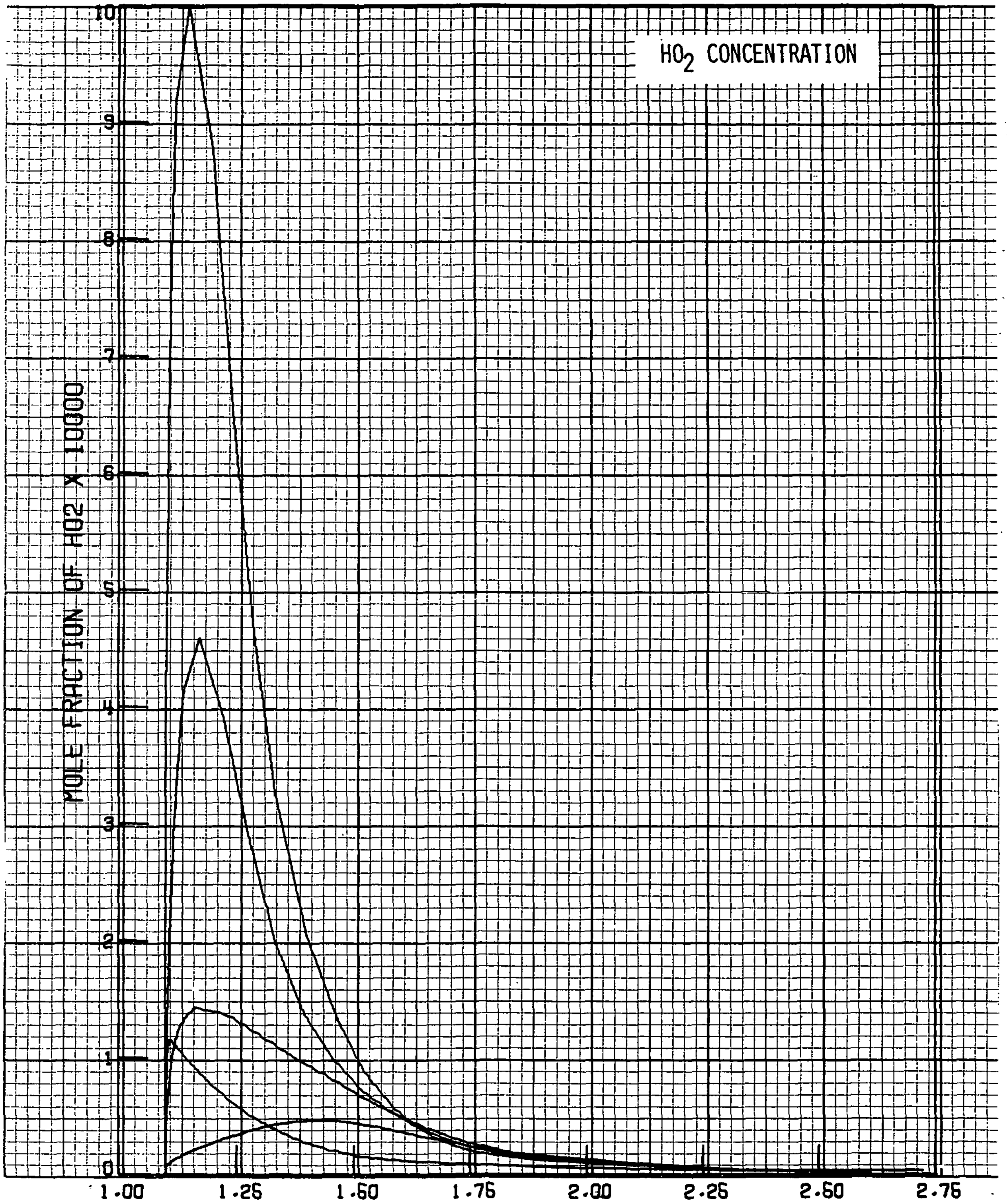

OH CONCENTRATION
MOLE FRACTION OF OH
.05
.04
.03
.02
.01
0
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75
TEMPERATURE, KELVIN (THOUSANDS OF DEGREES)

Figure A-102



HO_2 CONCENTRATION
MOLE FRACTION OF HO2 X 10000
10
9
8
7
6
5
4
3
2
1
0
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75
TEMPERATURE, KELVIN (THOUSANDS OF DEGREES)

Figure A-103

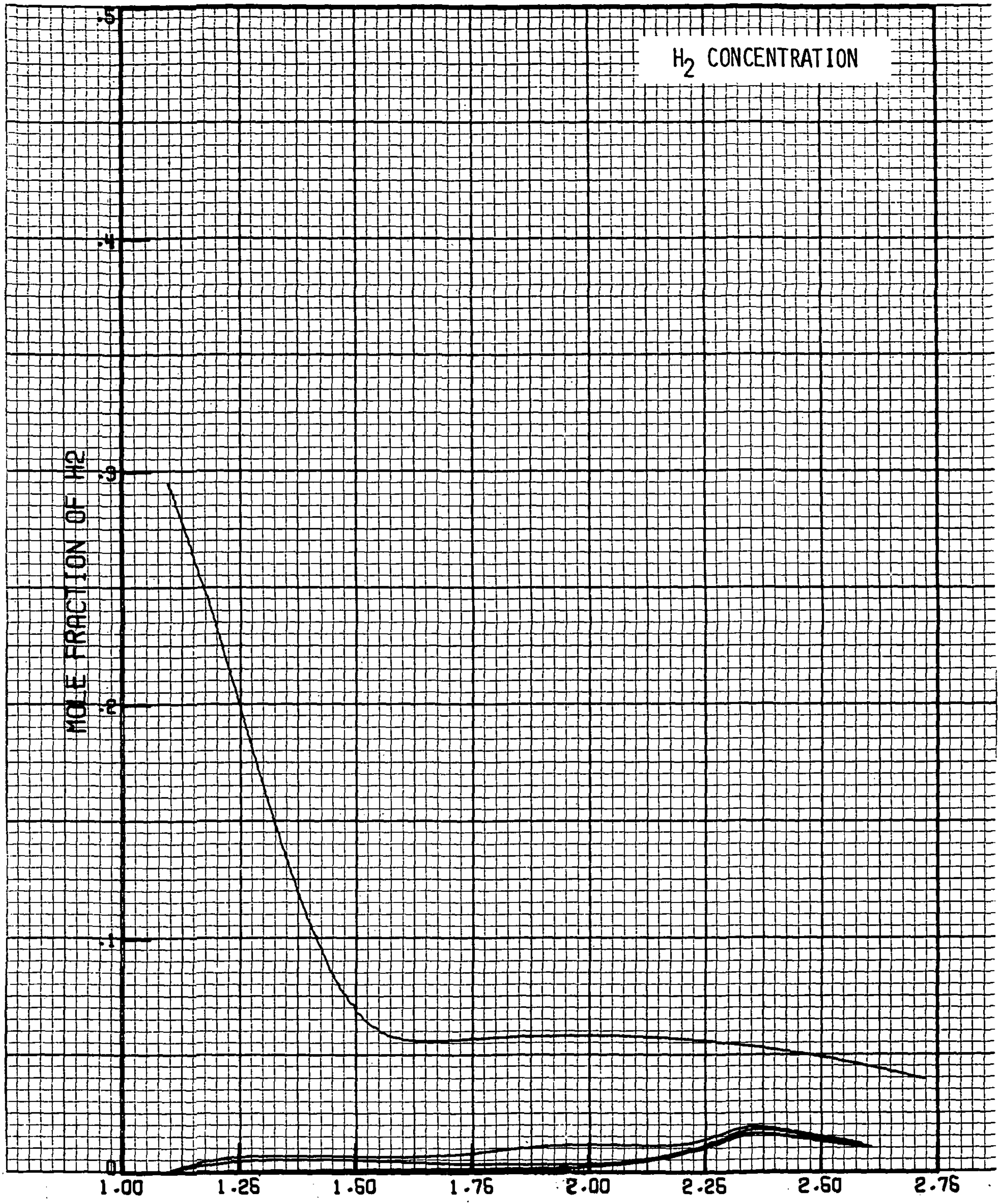

H$_2$ CONCENTRATION
MOLE FRACTION OF H2
.5
.4
.3
.2
.1
0
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75
TEMPERATURE, KELVIN (THOUSANDS OF DEGREES)

Figure A-104

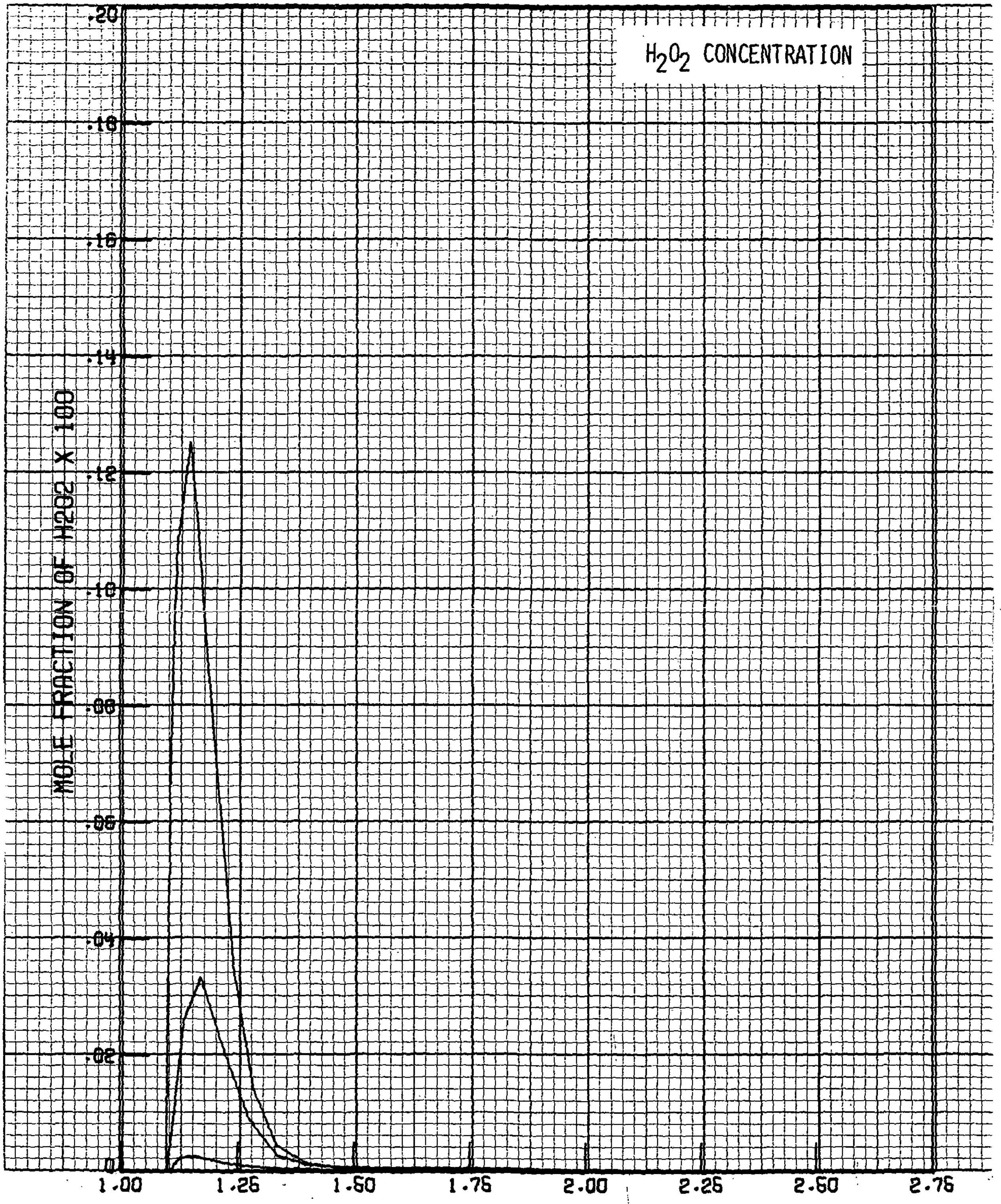

H$_2$O$_2$ CONCENTRATION
MOLE FRACTION OF H2O2 X 100
.20
.18
.16
.14
.12
.10
.08
.06
.04
.02
0
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75
TEMPERATURE, KELVIN (THOUSANDS OF DEGREES)

Figure A-105

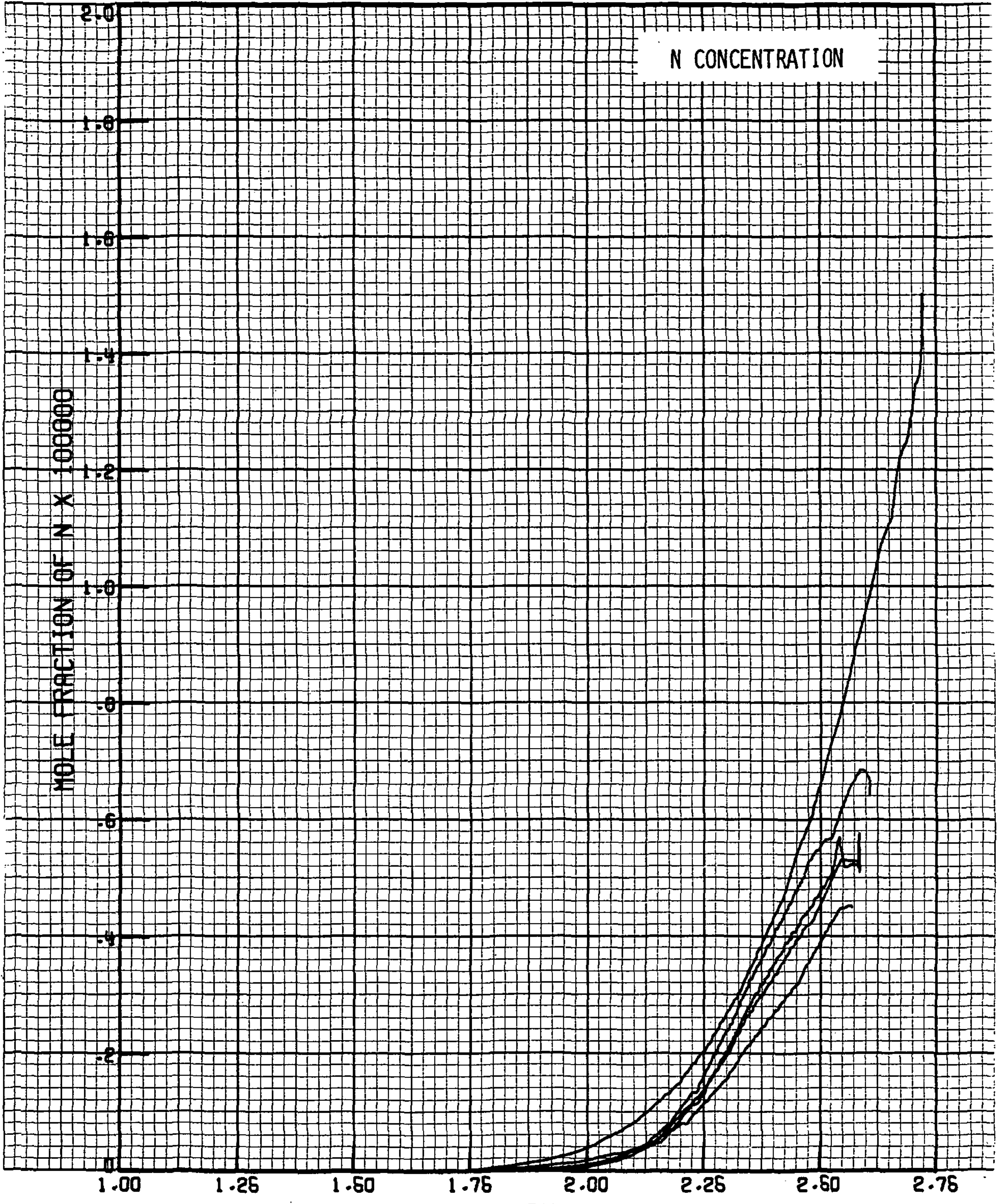

N CONCENTRATION
MOLE FRACTION OF N X 100000
2.0
1.8
1.6
1.4
1.2
1.0
.8
.6
.4
.2
0
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75
TEMPERATURE, KELVIN (THOUSANDS OF DEGREES)

Figure A-106

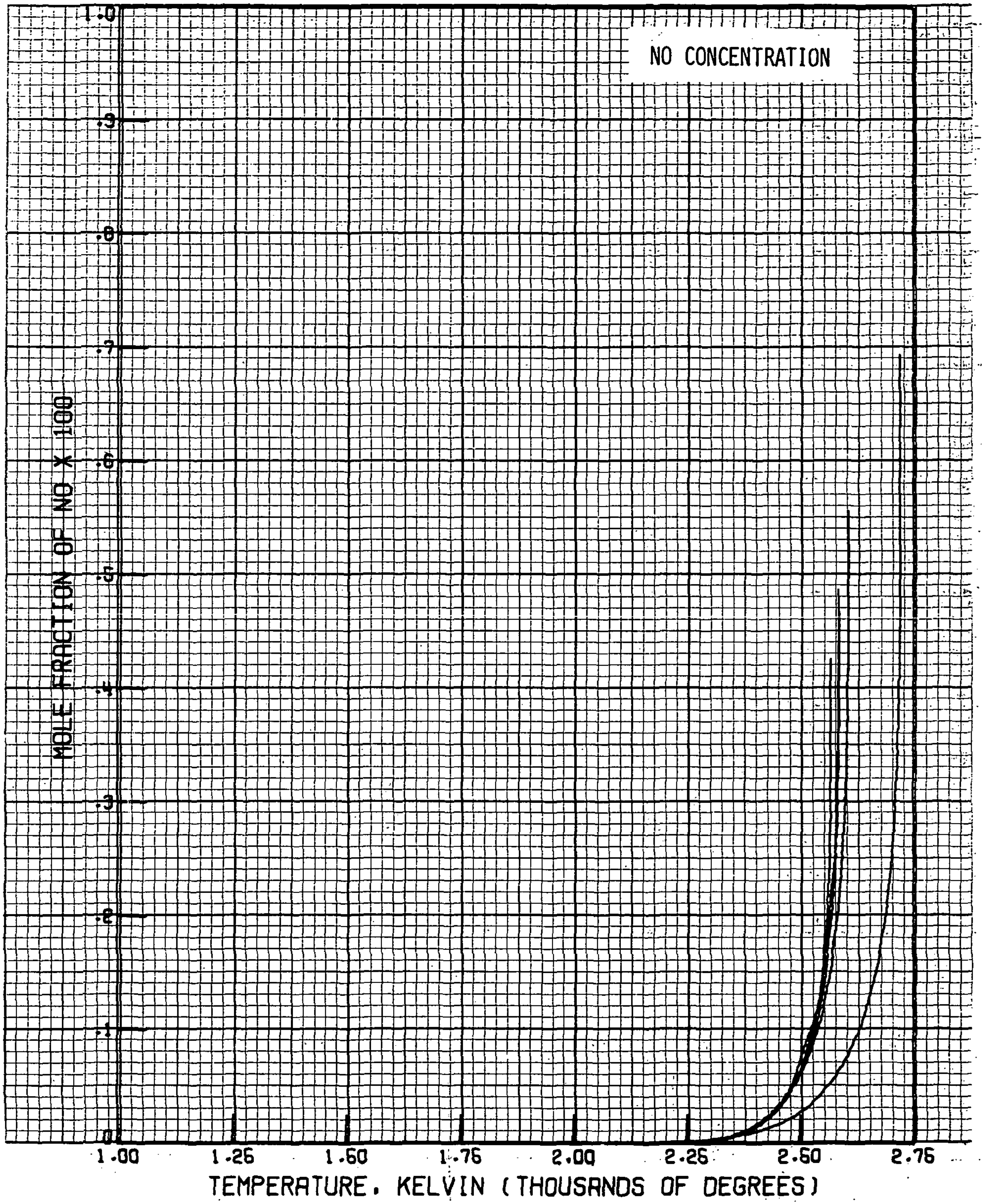

NO CONCENTRATION
MOLE FRACTION OF NO X 100
1.0
.9
.8
.7
.6
.5
.4
.3
.2
.1
0
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75
TEMPERATURE, KELVIN (THOUSANDS OF DEGREES)

Figure A-107

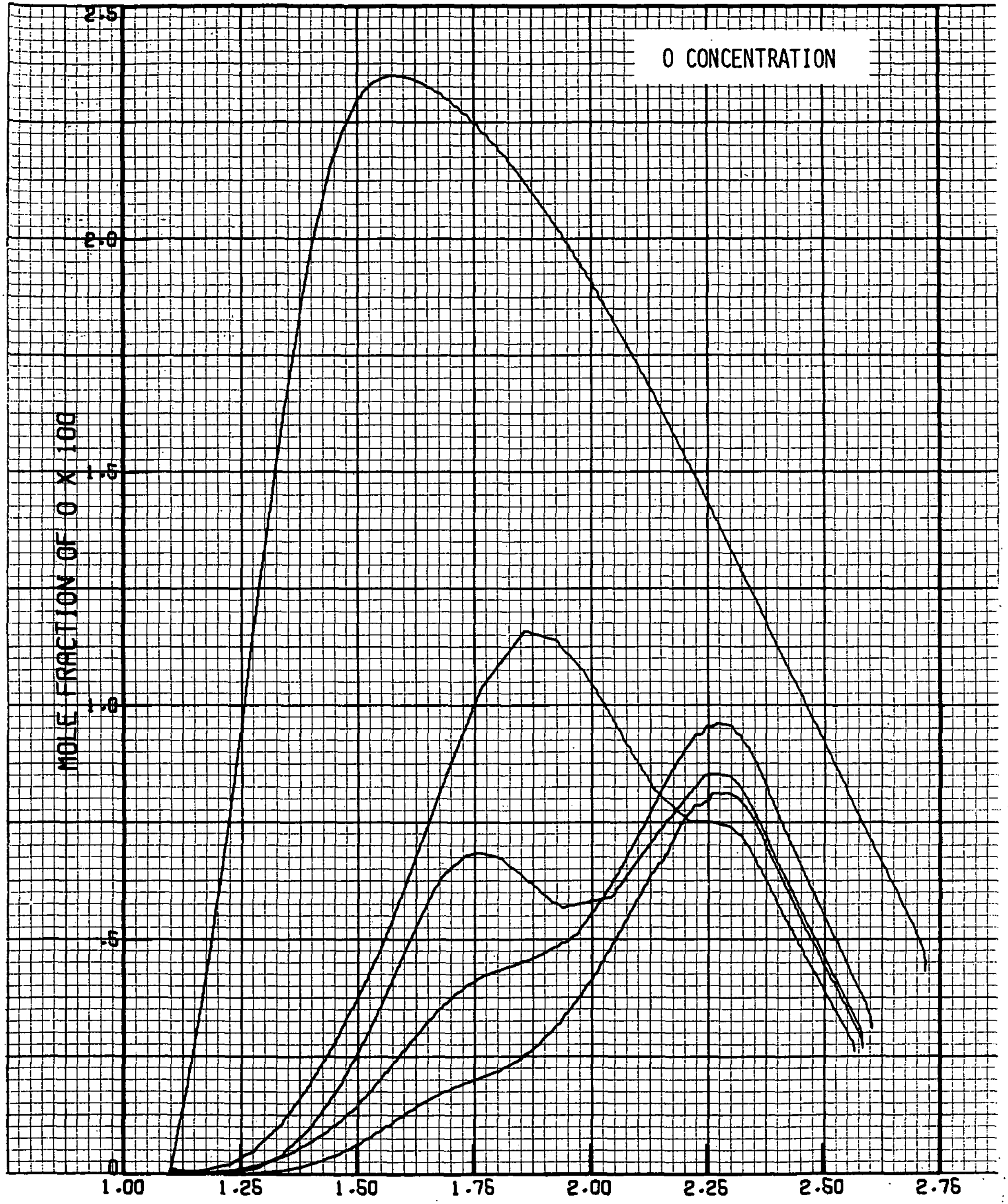

O CONCENTRATION
MOLE FRACTION OF O X 100
2.5
2.0
1.5
1.0
.5
0
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75
TEMPERATURE, KELVIN (THOUSANDS OF DEGREES)

Figure A-108

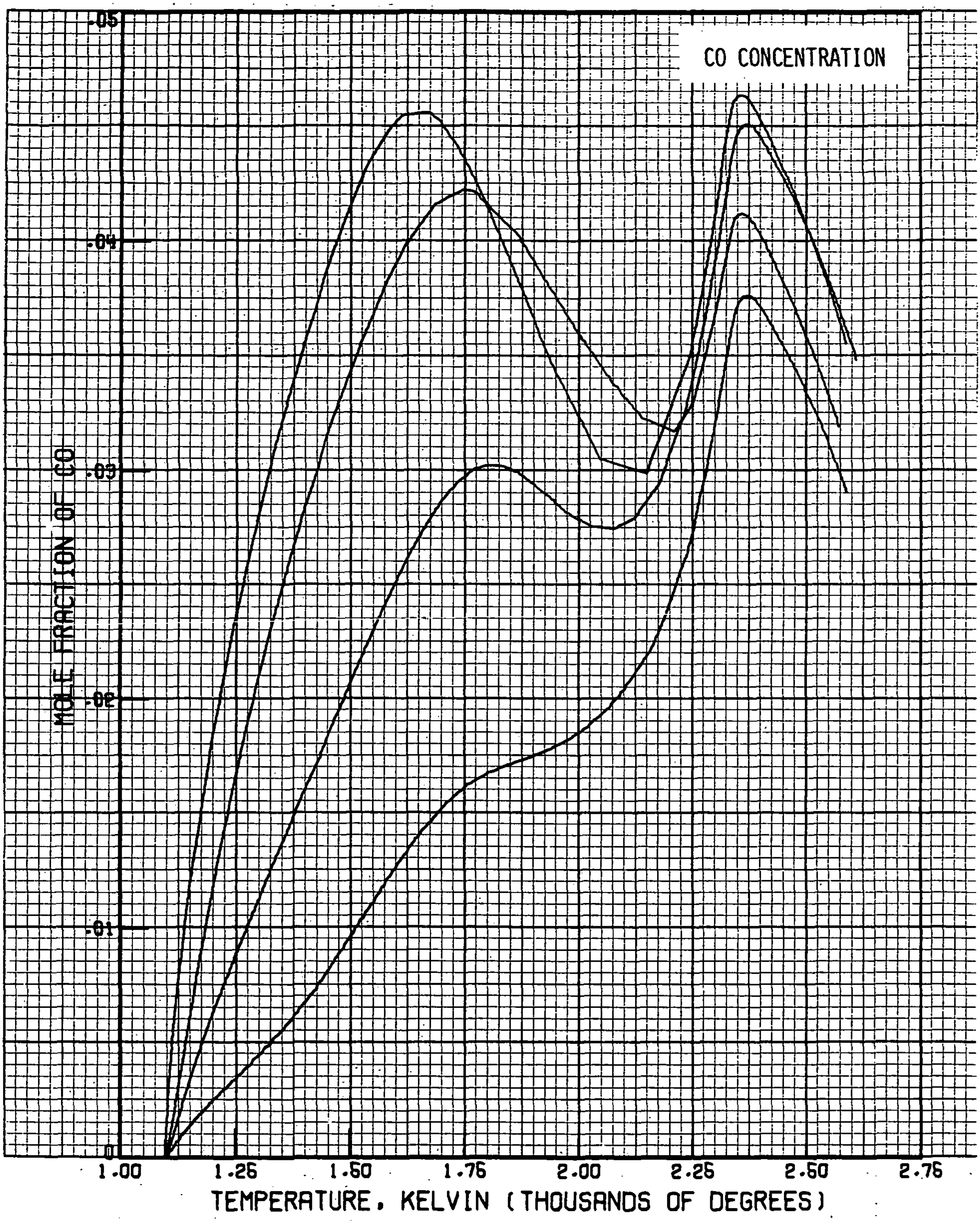

CO CONCENTRATION
.05
.04
.03
.02
.01
0
MOLE FRACTION OF CO
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75
TEMPERATURE, KELVIN (THOUSANDS OF DEGREES)

Figure A-109

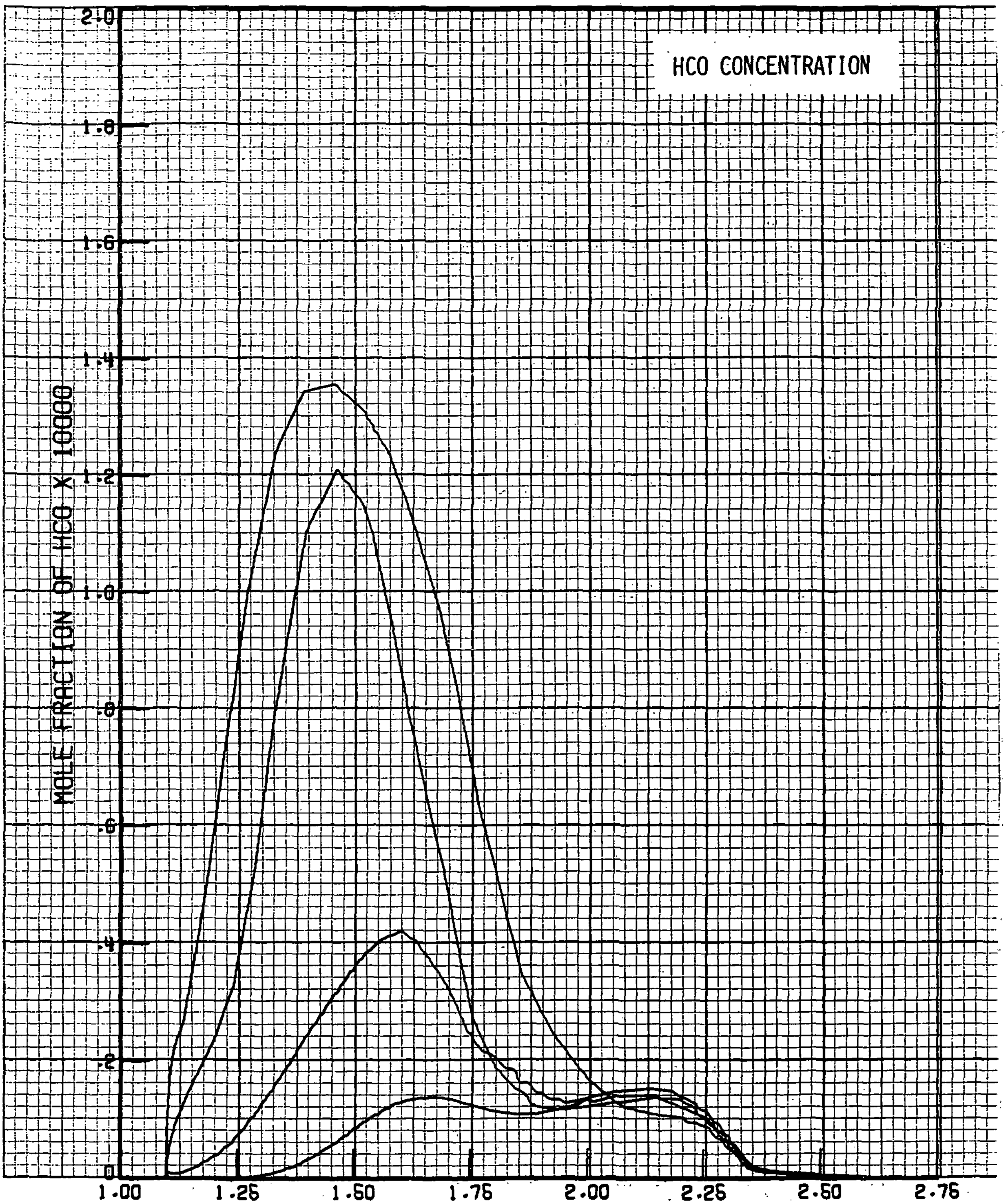

HCO CONCENTRATION
MOLE FRACTION OF HCO X 10000
2.0
1.8
1.6
1.4
1.2
1.0
.8
.6
.4
.2
0
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75
TEMPERATURE, KELVIN (THOUSANDS OF DEGREES)

Figure A-110

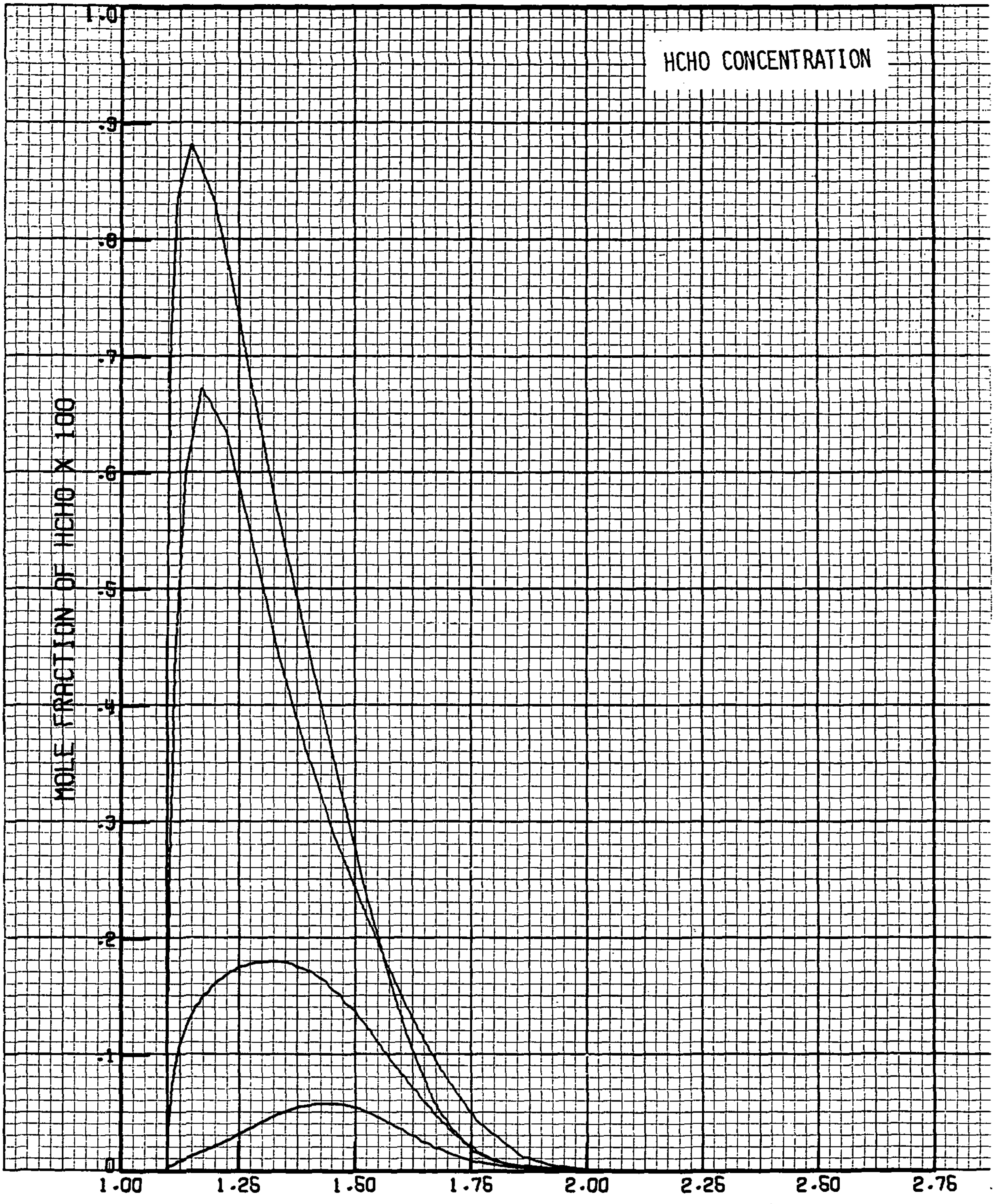

HCHO CONCENTRATION
MOLE FRACTION OF HCHO X 100
1.0
.9
.8
.7
.6
.5
.4
.3
.2
.1
0
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75
TEMPERATURE, KELVIN (THOUSANDS OF DEGREES)

Figure A-111

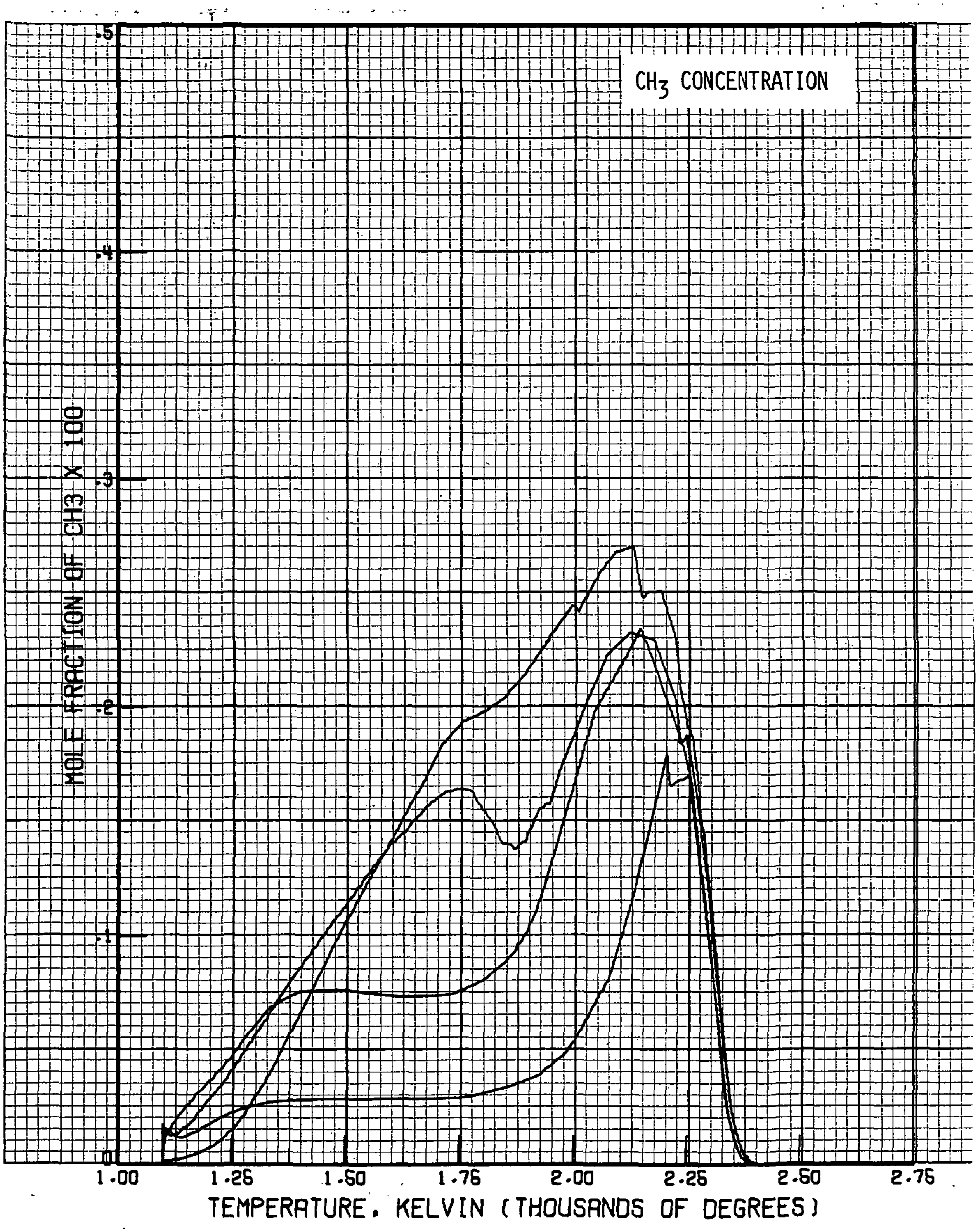

CH$_3$ CONCENTRATION
MOLE FRACTION OF CH3 X 100
.5
.4
.3
.2
.1
0
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75
TEMPERATURE, KELVIN (THOUSANDS OF DEGREES)

Figure A-112

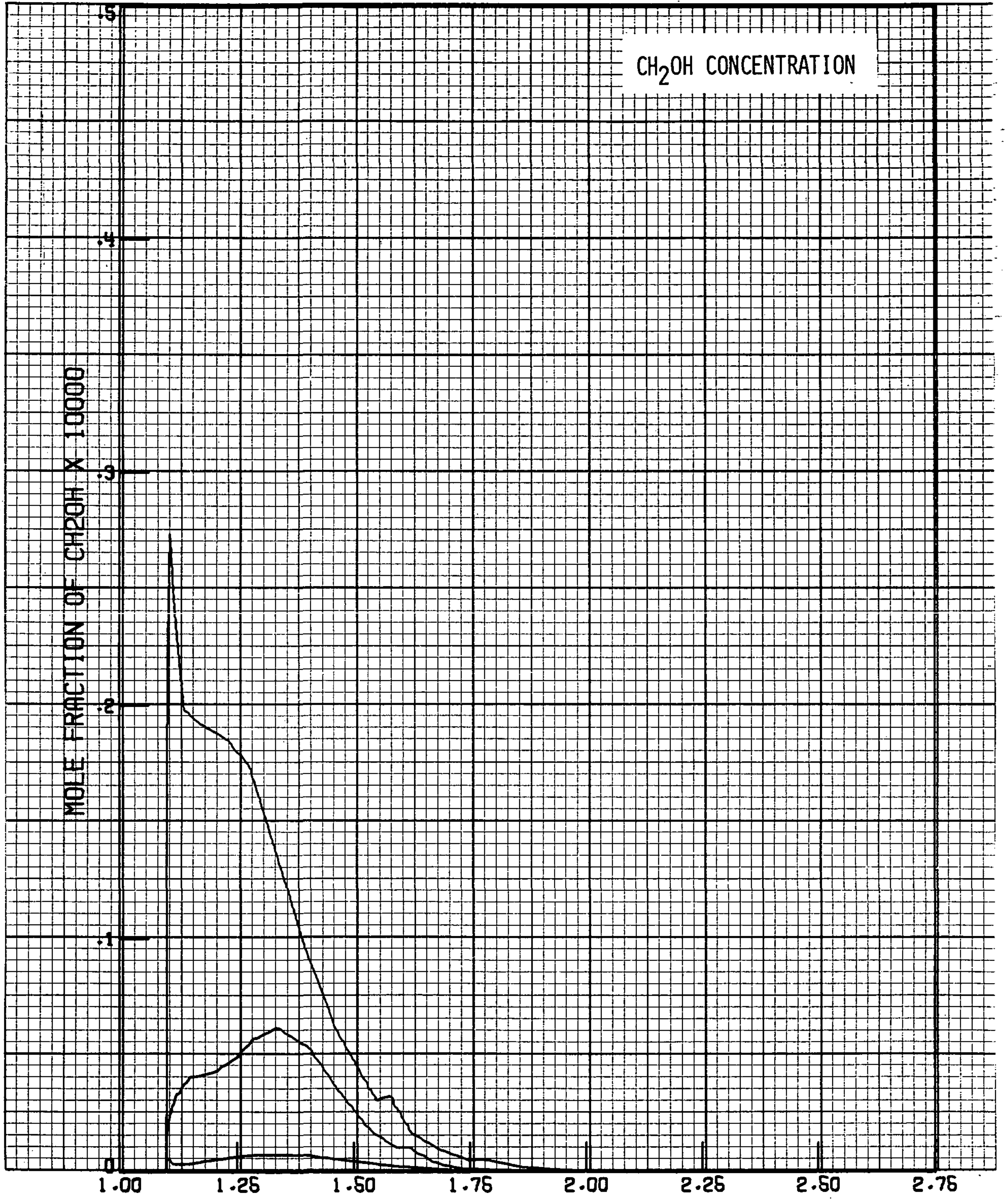

CH$_2$OH CONCENTRATION
MOLE FRACTION OF CH2OH X 10000
.5
.4
.3
.2
.1
0
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75
TEMPERATURE, KELVIN (THOUSANDS OF DEGREES)

Figure A-113

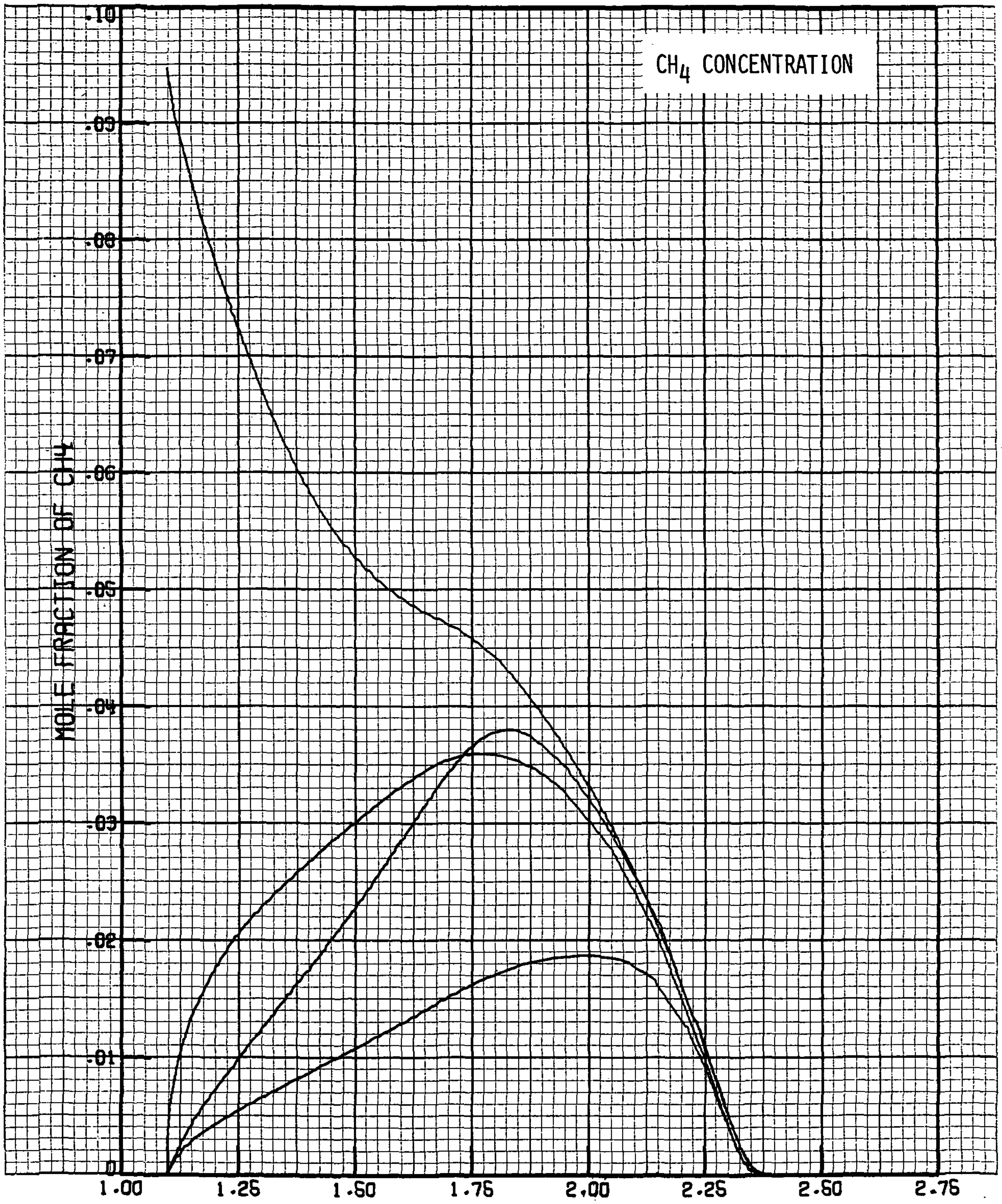

CH$_4$ CONCENTRATION
MOLE FRACTION OF CH4
.10
.09
.08
.07
.06
.05
.04
.03
.02
.01
0
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75
TEMPERATURE, KELVIN (THOUSANDS OF DEGREES)

Figure A-114

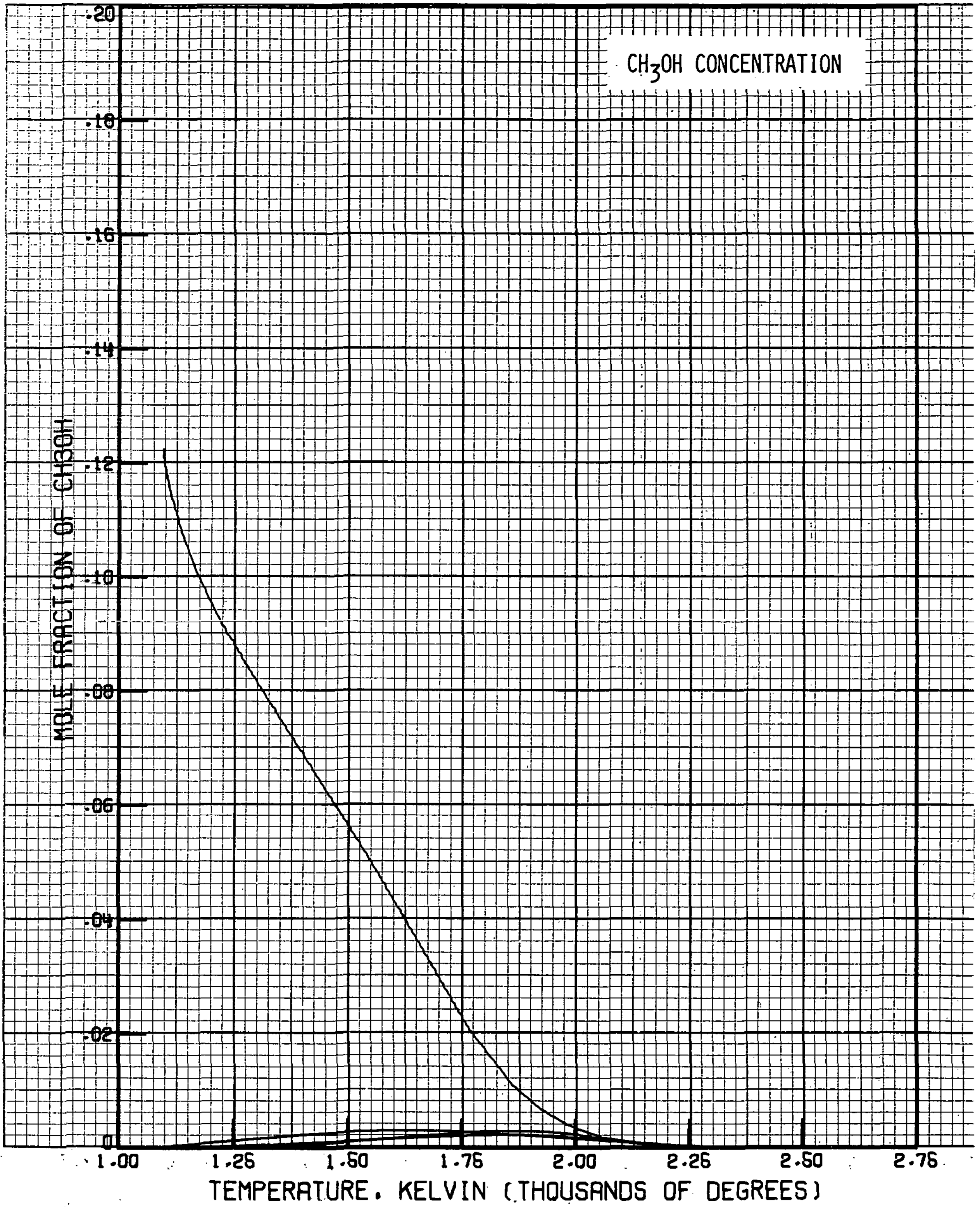

CH$_3$OH CONCENTRATION
MOLE FRACTION OF CH3OH
.20
.18
.16
.14
.12
.10
.08
.06
.04
.02
0
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75
TEMPERATURE, KELVIN (THOUSANDS OF DEGREES)

Figure A-115

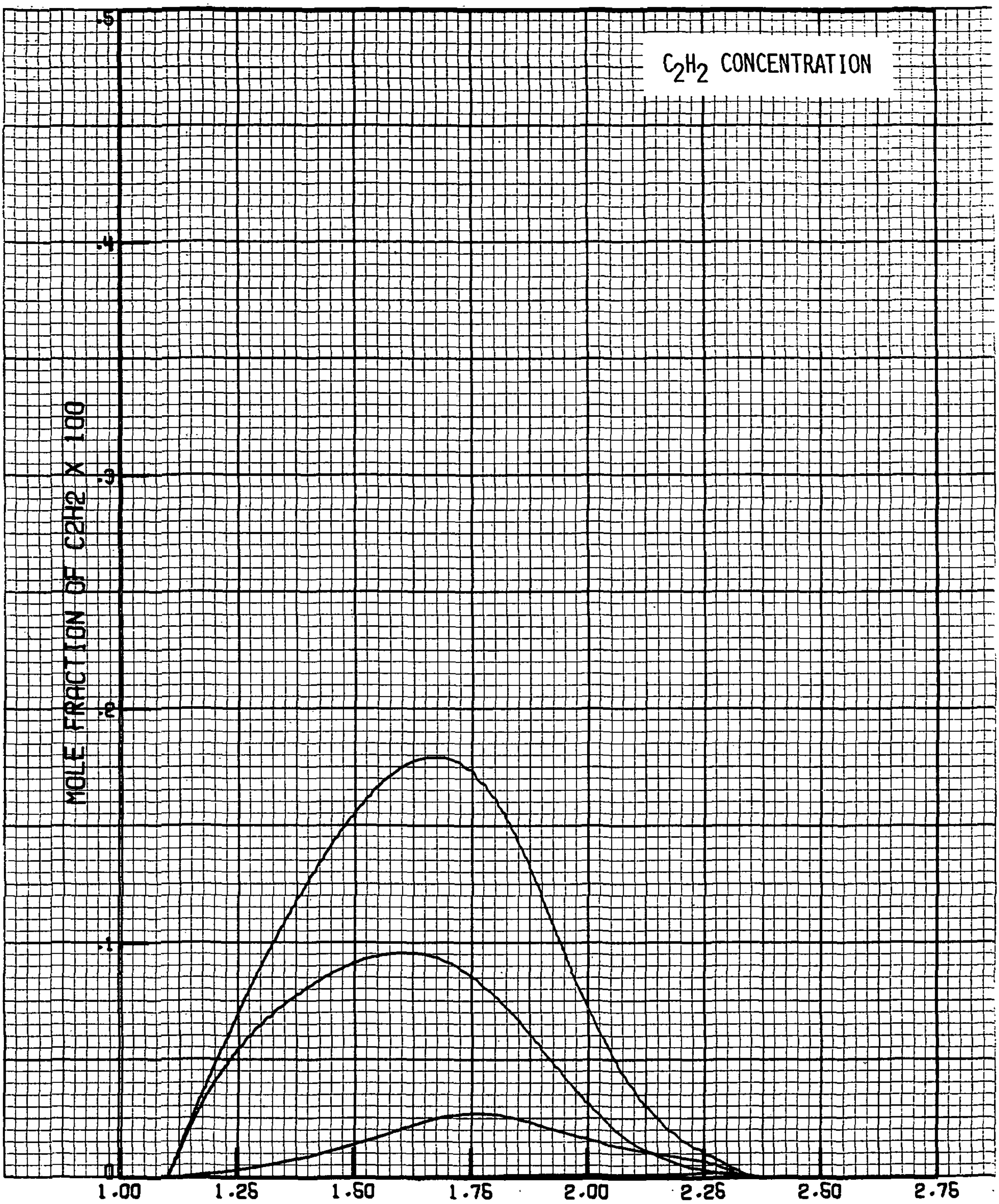

C$_2$H$_2$ CONCENTRATION
MOLE FRACTION OF C2H2 X 100
.5
.4
.3
.2
.1
0
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75
TEMPERATURE, KELVIN (THOUSANDS OF DEGREES)

Figure A-116

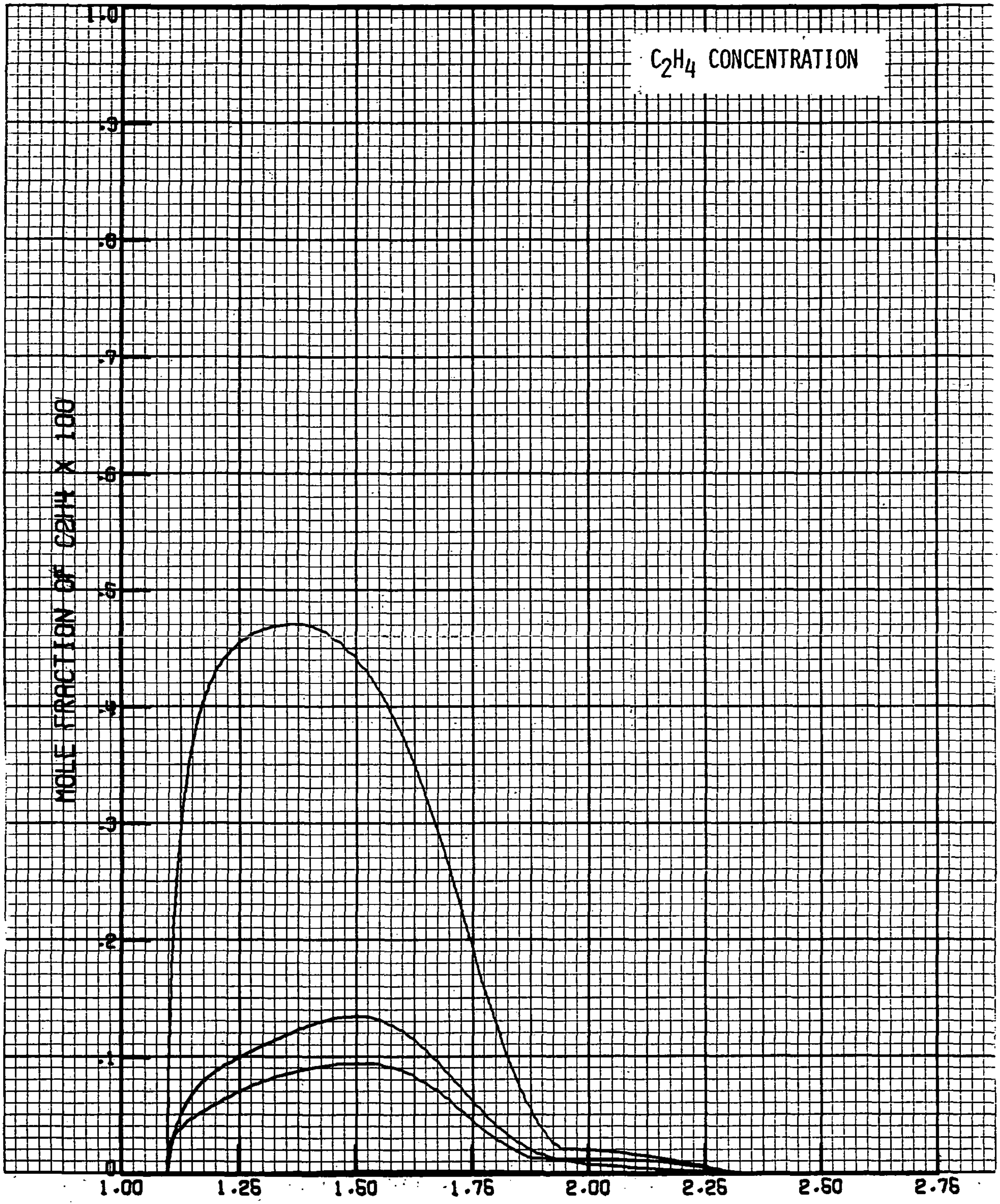

C$_2$H$_4$ CONCENTRATION
MOLE FRACTION OF C2H4 X 100
1.0
.9
.8
.7
.6
.5
.4
.3
.2
.1
0
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75
TEMPERATURE, KELVIN (THOUSANDS OF DEGREES)

Figure A-117

Figure A-118

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>
> —NATIONAL AERONAUTICS AND SPACE ACT OF 1958

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