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COMBUSTION, EXPLOSION, AND SHOCK WAVES

Oxidation and Combustion Mechanisms of Paraffin Hydrocarbons: Transfer from C_1–C_7 to C_8H_{18}, C_9H_{20}, and $C_{10}H_{22}$

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Abstract—At the present time, detailed kinetic mechanisms (DKMs) for higher hydrocarbons, which include hundreds of particles and thousands of reactions, are proposed. These DKMs have a number of undoubted advantages because they aspire to description of a wide class of phenomena. However, their application, e.g., for modeling of turbulent combustion, is difficult due to their extreme inconvenience. In addition, they are limited to a certain degree and cannot be considered to be comprehensive. As an alternative to such DKMs, we construct no maximum mechanism in this work, but an optimum mechanism of high- and low-temperature oxidation and combustion of normal paraffin hydrocarbons. This mechanism, in accordance with the previously proposed algorithm, contains only general processes that govern the reaction rate and the formation of basic intermediate and final products. A such mechanism has the status of an nonempirical DKM because all parts, including elementary reactions, have kinetic substantiation. The mechanism itself has two features: (i) Reactions of so-called double addition of oxygen (first, to the alkyl radical, then to the isomerized form of the formed peroxide radical) are lacking because the first addition is considered to be sufficient; (ii) Isomeric compounds and their derivative substances as intermediate particles are not considered, because this means of oxidation is slower than through molecules and radicals of the normal structure. The application of the algorithm results in sufficiently compact mechanisms that are important for modeling chemical processes with the participation of paraffin hydrocarbons C_n with large n. Previously, this was done for propane, n-butane, n-pentane, n-hexane, and n-heptane; in the present article, it was done for n-octane, n-nonane, and n-decane. The major feature of all the mechanisms is the appearance of stages, viz., cold and blue flames during low-temperature spontaneous ignition. The direct comparison of the calculation and experiment results is carried out.

Keywords: normal paraffin hydrocarbons, oxidation mechanism, combustion.
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Detailed kinetic mechanisms (DKMs) containing hundreds of particles and thousands of reactions have been proposed that take a variety of intermediate stable molecules and radicals in reactions of their oxidation and combustion into account. For example, work [1] for n-heptane presented a scheme containing 650 species and 2300 reactions; in [2, 3] a scheme with 715 species and 3872 reactions was proposed for n-decane. Such DKMs have a number of undoubted advantages because they aspire to the description of a wide class of phenomena. At the same time, their capabilities should be not overestimated. First, their application, e.g., for modeling turbulent combustion, is difficult in view of extreme inconvenience. Secondly, a simple calculation shows that when all possible isomers and all reactions between all species are taken into account (e.g., reactions of the formation and consumption of polyaromatic hydrocarbons, soot, fullerenes, etc. are taken into account), mechanism numbers become significantly greater than in [1–3]. Consequently, the known DKMs are to a certain degree limited and cannot be considered as comprehensive. Thirdly, none of the known DKMs predicts the formation of both cold and blue flames before spontaneous ignition, although the adequate description of low-temperature multistage oxidation of hydrocarbons [4] is one of the important requirements for such mechanisms. Fourthly, due to the lack of many necessary and verified data on thermochemistry and reaction rates, such DKMs are often insufficiently valid and exact.

Meanwhile, to solve particular problems, optimum rather than maximum mechanisms are of interest, in which only general processes governing the reaction rate and formation of basic intermediate and final products are taken into account. These mechanisms, even if they are rather compact, have the status of DKMs because all their elementary reactions are kinetically valid. Thus, for the modeling of oxidation and combustion of hydrocarbons, there is a need for the method of nonextensive construction of DKMs with the restriction of a variety of products and reactions, but with the conservation of the basic channels of the process and fundamentally important types of elementary actions.

The approach used in the present article is based on the great similarity in the phenomenology of oxidation of paraffin hydrocarbons [4, 5]. In [6] this approach was performed in the form of an algorithm for the automatic construction of DKMs, which, at a later time, were applied for the construction of mechanisms of oxidation and combustion of propane [7], n-butane [6], n-pentane [8], n-hexane [9], and n-heptane [10]. In this article, the algorithm in [6] is used for the construction of the mechanisms of oxidation and combustion of n-octane (C_8H_{18}), n-nonane (C_9H_{20}), and n-decane ($C_{10}H_{22}$). The algorithm contains the principle of the nonextensive construction of DKMs, which has two features that assume the following:

(i) Low-temperature branching is described by a group of reactions with one addition of oxygen.

(ii) Oxidation through isomers can be eliminated because this is slower than oxidation through nonisomerized reagents.

Let us emphasize that the mechanisms of oxidation of $C_{10}H_{22}$ have already been proposed in the literature (see, e.g. [2]). However, as mentioned above, in the description of multistage low-temperature spontaneous ignition they do not explain the existence of the blue flame that was repeatedly observed experimentally. The construction of the mechanism of oxidation of $C_{10}H_{22}$, which is based on the principle of nonextensiveness, is necessary and important for the following oxidation of more complex hydrocarbons C_n on the basis of the principle of DKMs. One of our requirements for such mechanisms is the appearance of staging in the form of cold and blue flames during low-temperature spontaneous ignition.

CONSTRUCTION OF THE MECHANISM

According to the algorithm in [6] for the development of the DKM of oxidation of hydrocarbon C_nH_{2n+2}, the basis is the mechanism of its analog in homologous series with a number n of carbon atoms that is smaller by a unit, i.e., $C_{(n-1)}H_{2(n-1)+2}$. This is also related to both reagents and to reactions. The preceding analog for n-octane C_8H_{18} in the homologous series is n-heptane. Therefore, the basis of the construction of the mechanism of oxidation and combustion of C_8 was taken as the mechanism of oxidation and combustion of C_1–C_7 [10]. This contains 81 species and 623 reactions. Nine new species and 140 new elementary acts were taken in the mechanism of n-octane in comparison with the mechanism of n-heptane; thus, the total number of the octane mechanism is 90 species and 763 reactions. The corresponding number for the nonane mechanism is 99 species and 915 reactions; for the decane mechanism it is 108 species and 1083 reactions.

The computer program [6] selects both new species (Table 1) and new reactions with their Arrhenius parameters (Table 2). Apart from new species, Table 1 lists the formation enthalpy ΔH°_{298}, the entropy S°_{298}, and the specific heat at constant pressure $c_p = c_0 + c_1T/10^3 + c_2T^2/10^6 + c_3T^3/10^9$.

It is well known that critical phenomena in chemical kinetics are reproduced only at a certain ratio of rates of different elementary acts. Therefore, during the modeling of such phenomena, the simple substitution of approximate values of governing rate constants does not always lead to the goal, i.e., there is a need for additional analysis and the selection of rate constants (this is valid in a theory-admissible range of values that do not exceed the experimental error).

The appearance of the cold and blue flame during low-temperature spontaneous ignition of paraffin hydrocarbons is one of the striking examples of such critical phenomena. For the above reason, it was necessary to correct the obtained DKMs as applied to a limited number of reactions, i.e., reactions of hydrocarbons with hydroperoxide radicals and reactions of alkyl radical with molecular oxygen.

VERIFICATION OF MECHANISM

Experiments on the Spontaneous Ignition of Gas Mixtures

The obtained DKM was verified using literature data related to spontaneous ignition of mixtures of $C_{10}H_{22}$ with air. The appropriate experiments on n-C_8H_{12} and n-C_9H_{20} were not found in the literature. As in [6], we applied a standard kinetic program.

Figure 1, as an example, presents typical calculated time dependences of temperature during the spontaneous ignition of an n-decane–air mixture, which are characteristic for low and high initial temperatures. The first stepped increase for the relatively low initial temperature $T_0 = 588$ K at $t \sim 1.27$ s is related to the appearance of the cool flame. The blue flame (clearly visible in Fig. 2 with a change of the scale) then appears after a lapse of about 0.28 s; the hot flame then appears at approximately 1.57 s and the temperature increases to 2500 K and higher.

The stages of spontaneous ignition, i.e. stepwise appearance of cold, blue, and hot flames, occur as follows. The acceleration of the reaction in the cool flame is the consequence of branching during decomposition of alkyl hydroperoxide (here, alkyl hydroperoxide $C_{10}H_{21}O_2H$) with the formation of hydroxyl and oxyradical. The appearance of the blue flame is the consequence of branching because of the decomposition of hydrogen peroxide H_2O_2. This is clearly evident in Fig. 2 from the calculated kinetic curves for peroxide and the two peaks in the concentration of hydroxyl. A such division of stages by pressure recording in

Table 1. Reagents of mechanism of oxidation and combustion of n-octane, n-nonane, and n-decane

Species no.	Formula	$\Delta H^{\circ}_{f\,298}$ cal/mol	S^{0}_{298} cal/mol K	c_0	c_1	c_2	c_3
84	C_8H_{18}	–0.495E+05	0.112E+03	0.825E+00	0.180E+03	–0.981E+02	0.208E+02
85	C_8H_{17}	–0.126E+04	0.116E+03	0.246E+01	0.171E+03	–0.959E+02	0.232E+02
86	$C_8H_{17}O_2$	–0.289E+05	0.134E+03	0.329E+01	0.196E+03	–0.117E+03	0.319E+02
87	$C_8H_{17}O_2H$	–0.646E+05	0.133E+03	0.297E+01	0.199E+03	–0.117E+03	0.313E+02
88	$C_8H_{17}O$	-0.311E+05	0.125E+03	0.572E+00	0.195E+03	–0.119E+03	0.340E+02
89	$C_7H_{15}CHO$	–0.698E+05	0.120E+03	0.115E+02	0.130E+03	–0.187E+02	–0.325E+02
90	$C_7H_{15}CO$	–0.346E+05	0.121E+03	0.115E+02	0.130E+03	–0.187E+02	–0.325E+02
91	C_8H_{16}	–0.197E+05	0.111E+03	0.276E+01	0.163E+03	–0.879E+02	0.184E+02
92	C_8H_{15}	0.243E+05	0.110E+03	0.337E+01	0.149E+03	–0.767E+02	0.152E+02
93	C_9H_{20}	–0.544E+05	0.121E+03	0.122E+01	0.201E+03	–0.110E+03	0.234E+02
94	C_9H_{19}	–0.619E+04	0.125E+03	0.285E+01	0.192E+03	–0.107E+03	0.258E+02
95	$C_9H_{19}O_2$	–0.338E+05	0.143E+03	0.368E+01	0.218E+03	–0.129E+03	0.345E+02
96	$C_9H_{19}O_2H$	–0.695E+05	0.142E+03	0.336E+01	0.220E+03	–0.129E+03	0.339E+02
97	$C_9H_{19}O$	–0.360E+05	0.134E+03	0.967E+00	0.217E+03	–0.131E+03	0.366E+02
98	$C_8H_{17}CHO$	–0.747E+05	0.130E+03	0.119E+02	0.152E+03	–0.307E+02	–0.299E+02
99	$C_8H_{17}CO$	–0.395E+05	0.131E+03	0.119E+02	0.152E+03	–0.307E+02	–0.295E+02
100	C_9H_{18}	–0.247E+05	0.121E+03	0.315E+01	0.184E+03	–0.999E+02	0.209E+02
101	C_9H_{17}	0.194E+05	0.120E+03	0.376E+01	0.170E+03	–0.887E+02	0.178E+02
102	$C_{10}H_{22}$	–0.593E+05	0.131E+03	0.161E+01	0.222E+03	–0.122E+03	0.260E+02
103	$C_{10}H_{21}$	–0.111E+05	0.135E+03	0.325E+01	0.213E+03	–0.119E+03	0.284E+02
104	$C_{10}H_{21}O_2$	–0.388E+05	0.153E+03	0.408E+01	0.239E+03	–0.141E+03	0.371E+02
105	$C_{10}H_{21}O_2H$	–0.745E+05	0.152E+03	0.376E+01	0.242E+03	–0.141E+03	0.365E+03
106	$C_{10}H_{21}O$	–0.410E+05	0.144E+03	0.136E+01	0.238E+03	–0.143E+03	0.392E+02
107	$C_9H_{19}CHO$	–0.797E+05	0.139E+03	0.123E+02	0.173E+03	–0.426E+02	–0.273E+02
108	$C_9H_{19}CO$	–0.445E+05	0.140E+03	0.123E+02	0.173E+03	–0.426E+02	–0.273E+02
109	$C_{10}H_2O$	–0.296E+05	0.130E+03	0.355E+01	0.205E+03	–0.111E+03	0.235E+02
110	$C_{10}H_{19}$	0.144E+05	0.129E+03	0.416E+01	0.192E+03	–0.100E+03	0.204E+02

experiments cannot occur because of temperature nonuniformity and multiple not spots, while it occurs in reality. The stages result in the phenomenon of the negative temperature coefficient (NTC) of the reaction rate; the total spontaneous ignition lags at a higher initial temperature are then greater than at a low temperature. This effect is clearly seen in Fig. 1.

Figures 3 and 4 present comparisons of calculated and measured spontaneous ignition lags for various initial temperatures and pressures. In all cases, the mixture composition is stoichiometric (1.33% $C_{10}H_{22}$—air) and the initial pressures P_0 are 1, 12, and 50 atm. The points on the graphs correspond to the experimental data of work [3] for pressures of 12 and 50 atm, experimental data of work [11] for pressures of 13 and 80 atm, experimental data of [12] for a pressure of 1 atm, and experimental data of [13, 14] for pressures of 10 and 40 atm and the curves correspond to calcu-

Table 2. Mechanism of oxidation and combustion of n-octane, n-nonane, and n-decane

No.	Reaction	*A*, l, mol, s	*E/R*, K
	n-Decane		
1	$C_{10}H_{22} + O_2 = C_{10}H_{21} + HO_2$	0.400E+10	0.239E+05
2	$C_{10}H_{22} + OH = C_{10}H_{21} + H_2O$	0.630E+10	0.600E+03
3	$C_{10}H_{22} + H = C_{10}H_{21} + H_2$	0.930E+11	0.403E+04
4	$C_{10}H_{22} + O = C_{10}H_{21} + OH$	0.506E+12	0.483E+04
5	$C_{10}H_{22} + HO_2 = C_{10}H_{21} + H_2O_2$	0.600E+09	0.856E+04
6	$C_{10}H_{20} + H = C_{10}H_{21}$	0.189E+10	0.315E+03
7	$C_{10}H_{21} + O_2 = C_{10}H_{20} + HO_2$	0.300E+11	0.700E+04
8	$C_{10}H_{21} + OH = C_{10}H_{20} + H_2O$	0.600E+10	0.000E+00
9	$C_{10}H_{22} = H + C_{10}H_{21}$	0.359E+14	0.376E+05
10	$C_{10}H_{22} = CH_3 + C_9H_{19}$	0.404E+16	0.421E+05
11	$C_{10}H_{22} = C_2H_5 + C_8H_{17}$	0.195E+17	0.428E+05
12	$C_{10}H_{22} = C_3H_7 + C_7H_{15}$	0.158E+17	0.428E+05
13	$C_{10}H_{22} = C_4H_9 + C_6H_{13}$	0.158E+17	0.428E+05
14	$C_{10}H_{22} = C_5H_{11} + C_5H_{11}$	0.158E+17	0.428E+05
15	$C_{10}H_{21} + H = C_{10}H_{20} + H_2$	0.600E+10	0.000E+00
16	$C_{10}H_{21} + CH_3 = C_{10}H_{20} + CH_4$	0.351E+09	−0.106E+03
17	$C_{10}H_{21} + C_2H_5 = C_{10}H_{20} + C_2H_6$	0.158E+11	0.466E+03
18	$C_{10}H_{21} + C_3H_7 = C_{10}H_{20} + C_3H_8$	0.138E+09	0.488E+03
19	$C_{10}H_{21} + C_4H_9 = C_{10}H_{20} + C_4H_{10}$	0.138E+09	0.488E+03
20	$C_{10}H_{21} + C_5H_{11} = C_{10}H_{20} + C_5H_{12}$	0.138E+09	0.488E+03
21	$C_{10}H_{21} + C_6H_{13} = C_{10}H_{20} + C_6H_{14}$	0.138E+09	0.488E+03
22	$C_{10}H_{21} + C_7H_{15} = C_{10}H_{20} + C_7H_{16}$	0.138E+09	0.488E+03
23	$C_{10}H_{21} + C_8H_{17} = C_{10}H_{20} + C_8H_{18}$	0.138E+09	0.488E+03
24	$C_{10}H_{21} + C_9H_{19} = C_{10}H_{20} + C_9H_{20}$	0.203E+10	0.243E+03
25	$C_{10}H_{21} + O = C_{10}H_{20} + OH$	0.200E+12	0.000E+00
26	$C_{10}H_{21} + O_2 = C_{10}H_{21}O_2$	0.398E+08	−0.500E+03
27	$C_{10}H_{22} + CH_3O_2 = C_{10}H_{21} + CH_3O_2H$	0.245E+11	0.650E+04
28	$C_{10}H_{22} + C_2H_5O_2 = C_{10}H_{21} + C_2H_5O_2H$	0.245E+11	0.650E+04
29	$C_{10}H_{22} + C_3H_7O_2 = C_{10}H_{21} + C_3H_7O_2H$	0.245E+11	0.650E+04
30	$C_{10}H_{22} + C_4H_9O_2 = C_{10}H_{21} + C_4H_{10}O_2$	0.245E+11	0.650E+04
31	$C_{10}H_{22} + C_5H_{11}O_2 = C_{10}H_{21} + C_5H_{12}O_2$	0.245E+11	0.650E+04
32	$C_{10}H_{22} + C_6H_{13}O_2 = C_{10}H_{21} + C_6H_{14}O_2$	0.245E+11	0.650E+04
33	$C_{10}H_{22} + C_7H_{15}O_2 = C_{10}H_{21} + C_7H_{16}O_2$	0.245E+11	0.650E+04
34	$C_{10}H_{22} + C_8H_{17}O_2 = C_{10}H_{21} + C_8H_{18}O_2$	0.245E+11	0.650E+04
35	$C_{10}H_{22} + C_9H_{19}O_2 = C_{10}H_{21} + C_9H_{20}O_2$	0.245E+11	0.650E+04
36	$C_{10}H_{22} + C_{10}H_{21}O_2 = C_{10}H_{21} + C_{10}H_{22}O_2$	0.245E+11	0.650E+04
37	$C_{10}H_{22}O_2 = C_{10}H_{21}O + OH$	0.500E+16	0.200E+05
38	$C_{10}H_{21}O = H_2CO + C_9H_{19}$	0.159E+15	0.797E+04
39	$C_{10}H_{21}O = CH_3CHO + C_8H_{17}$	0.314E+15	0.113E+05
40	$C_{10}H_{21}O = C_2H_5CHO + C_7H_{15}$	0.305E+15	0.103E+05
41	$C_{10}H_{21}O = C_4H_8O + C_6H_{13}$	0.304E+15	0.103E+05
42	$C_{10}H_{21}O = C_5H_{10}O + C_5H_{11}$	0.304E+15	0.103E+05
43	$C_{10}H_{21}O = C_6H_{12}O + C_4H_9$	0.304E+15	0.103E+05
44	$C_{10}H_{21}O = C_7H_{14}O + C_3H_7$	0.303E+15	0.103E+05
45	$C_{10}H_{21}O = C_8H_{16}O + C_2H_5$	0.374E+15	0.103E+05
46	$C_{10}H_{21}O = C_9H_{18}O + CH_3$	0.775E+14	0.108E+05
47	$C_{10}H_{21}O = C_{10}H_{20}O + H$	0.688E+12	0.626E+04
48	$C_{10}H_{21}O_2 + H = C_{10}H_{21}O + OH$	0.236E+11	−0.161E+04
49	$C_{10}H_{21}O_2 + CH_3 = C_{10}H_{21}O + CH_3O$	0.364E+09	−0.166E+03
50	$C_{10}H_{21}O_2 + C_2H_5 = C_{10}H_{21}O + C_2H_5O$	0.827E+09	−0.649E+03
51	$C_{10}H_{21}O_2 + C_3H_7 = C_{10}H_{21}O + C_3H_7O$	0.630E+09	0.000E+00
52	$C_{10}H_{21}O_2 + C_4H_9 = C_{10}H_{21}O + C_4H_9O$	0.630E+09	0.000E+00

Table 2. (Contd.)

No.	Reaction	*A*, l, mol, s	*E/R*, K
53	$C_{10}H_{21}O_2 + C_5H_{11} = C_{10}H_{21}O + C_5H_{11}O$	0.630E+09	0.000E+00
54	$C_{10}H_{21}O_2 + C_6H_{13} = C_{10}H_{21}O + C_6H_{13}O$	0.629E+09	0.000E+00
55	$C_{10}H_{21}O_2 + C_7H_{15} = C_{10}H_{21}O + C_7H_{15}O$	0.627E+09	0.000E+00
56	$C_{10}H_{21}O_2 + C_8H_{17} = C_{10}H_{21}O + C_8H_{17}O$	0.627E+09	0.000E+00
57	$C_{10}H_{21}O_2 + C_9H_{19} = C_{10}H_{21}O + C_9H_{19}O$	0.365E+09	0.156E+04
58	$C_{10}H_{21}O_2 + C_{10}H_{21} = C_{10}H_{21}O + C_{10}H_{21}O$	0.365E+09	0.156E+04
59	$C_{10}H_{21}O_2 + H_2CO = C_{10}H_{22}O_2 + HCO$	0.320E+09	0.564E+04
60	$C_{10}H_{21}O_2 + CH_3CHO = C_{10}H_{22}O_2 + CH_3CO$	0.315E+09	0.560E+04
61	$C_{10}H_{21}O_2 + C_2H_5CHO = Ñ_{10}H_{22}O_2 + C_2H_5CO$	0.315E+09	0.554E+04
62	$C_{10}H_{21}O_2 + C_4H_8O = C_{10}H_{22}O_2 + C_4H_7O$	0.315E+09	0.554E+04
63	$C_{10}H_{21}O_2 + C_5H_{10}O = C_{10}H_{22}O_2 + C_5H_9O$	0.315E+09	0.554E+04
64	$C_{10}H_{21}O_2 + C_6H_{12}O = C_{10}H_{22}O_2 + C_6H_{11}O$	0.315E+09	0.554E+04
65	$C_{10}H_{21}O_2 + C_7H_{14}O = C_{10}H_{22}O_2 + C_7H_{13}O$	0.315E+09	0.554E+04
66	$C_{10}H_{21}O_2 + C_8H_{16}O = C_{10}H_{22}O_2 + C_8H_{15}O$	0.315E+09	0.554E+04
67	$C_{10}H_{21}O_2 + C_9H_{18}O = C_{10}H_{22}O_2 + C_9H_{17}O$	0.315E+09	0.554E+04
68	$C_{10}H_{21}O_2 + C_{10}H_{20}O = C_{10}H_{22}O_2 + C_{10}H_{19}O$	0.619E+11	0.289E+04
69	$C_{10}H_{21} + HO_2 = C_{10}H_{21}O + OH$	0.298E+11	0.000E+00
70	$C_{10}H_{21} + O_2 = C_{10}H_{20}O + OH$	0.398E+10	0.900E+04
71	$C_{10}H_{21} + C_2H_5 = C_{10}H_{22} + C_2H_4$	0.625E+09	0.335E+03
72	$C_{10}H_{21} + C_3H_7 = C_{10}H_{22} + C_3H_6$	0.190E+10	0.000E+00
73	$C_{10}H_{21} + C_4H_9 = C_{10}H_{22} + C_4H_8$	0.190E+10	0.000E+00
74	$C_{10}H_{21} + C_5H_{11} = C_{10}H_{22} + C_5H_{10}$	0.190E+10	0.000E+00
75	$C_{10}H_{21} + C_6H_{13} = C_{10}H_{22} + C_6H_{12}$	0.190E+10	0.000E+00
76	$C_{10}H_{21} + C_7H_{15} = C_{10}H_{22} + C_7H_{14}$	0.190E+10	0.000E+00
77	$C_{10}H_{21} + C_8H_{17} = C_{10}H_{22} + C_8H_{16}$	0.190E+10	0.000E+00
78	$C_{10}H_{21} + C_9H_{19} = C_{10}H_{22} + C_9H_{18}$	0.190E+10	0.000E+00
79	$C_{10}H_{21} + C_{10}H_{21} = C_{10}H_{22} + C_{10}H_{20}$	0.190E+10	0.000E+00
80	$C_{10}H_{21} + O_2 = H_2CO + C_9H_{19}O$	0.368E+09	0.565E+04
81	$C_{10}H_{21} + O_2 = CH_3CHO + C_8H_{17}O$	0.725E+09	0.454E+04
82	$C_{10}H_{21} + O_2 = C_2H_5CHO + C_7H_{15}O$	0.703E+09	0.446E+04
83	$C_{10}H_{21} + O_2 = C_4H_8O + C_6H_{13}O$	0.705E+09	0.446E+04
84	$C_{10}H_{21} + O_2 = C_5H_{10}O + C_5H_{11}O$	0.706E+09	0.446E+04
85	$C_{10}H_{21} + O_2 = C_6H_{12}O + C_4H_9O$	0.705E+09	0.446E+04
86	$C_{10}H_{21} + O_2 = C_7H_{14}O + C_3H_7O$	0.703E+09	0.446E+04
87	$C_{10}H_{21} + O_2 = C_8H_{16}O + C_2H_5O$	0.114E+10	0.382E+04
88	$C_{10}H_{21} + O_2 = C_9H_{18}O + CH_3O$	0.104E+09	0.453E+04
89	$C_{10}H_{21} + OH = CH_3 + C_9H_{19}O$	0.184E+11	–0.194E+04
90	$C_{10}H_{21} + OH = C_2H_5 + C_8H_{17}O$	0.888E+11	0.417E+03
91	$C_{10}H_{21} + OH = C_3H_7 + C_7H_{15}O$	0.719E+11	0.413E+03
92	$C_{10}H_{21} + OH = C_4H_9 + C_6H_{13}O$	0.720E+11	0.413E+03
93	$C_{10}H_{21} + OH = C_5H_{11} + C_5H_{11}O$	0.721E+11	0.413E+03
94	$C_{10}H_{21} + OH = C_6H_{13} + C_4H_9O$	0.721E+11	0.413E+03
95	$C_{10}H_{21} + OH = C_7H_{15} + C_3H_7O$	0.722E+11	0.413E+03
96	$C_{10}H_{21} + OH = C_8H_{17} + C_2H_5O$	0.117E+12	–0.232E+03
97	$C_{10}H_{21} + OH = C_9H_{19} + CH_3O$	0.107E+11	0.480E+03
98	$C_{10}H_{21} + H = CH_3 + C_9H_{19}$	0.388E+11	0.546E+03
99	$C_{10}H_{21} + H = C_2H_5 + C_8H_{17}$	0.187E+12	0.318E+03
100	$C_{10}H_{21} + H = C_3H_7 + C_7H_{15}$	0.152E+12	0.314E+03
101	$C_{10}H_{21} + H = C_4H_9 + C_6H_{13}$	0.151E+12	0.314E+03
102	$C_{10}H_{21} + H = C_5H_{11} + C_5H_{11}$	0.151E+12	0.314E+03
103	$C_{10}H_{21} + H = CH_2 + C_9H_{20}$	0.423E+08	0.302E+04
104	$C_{10}H_{21} + H = C_2H_4 + C_8H_{18}$	0.723E+07	–0.641E+04

Table 2. (Contd.)

No.	Reaction	*A*, l, mol, s	*E/R*, K
105	$C_{10}H_{21} + H = C_3H_6 + C_7H_{16}$	0.178E+08	–0.675E+04
106	$C_{10}H_{21} + H = C_4H_8 + C_6H_{14}$	0.178E+08	–0.675E+04
107	$C_{10}H_{21} + H = C_5H_{10} + C_5H_{12}$	0.178E+08	–0.675E+04
108	$C_{10}H_{21} + H = C_6H_{12} + C_4H_{10}$	0.178E+08	–0.675E+04
109	$C_{10}H_{21} + H = C_7H_{14} + C_3H_8$	0.178E+08	–0.675E+04
110	$C_{10}H_{21} + H = C_8H_{16} + C_2H_6$	0.252E+10	–0.677E+04
111	$C_{10}H_{21} + H = C_9H_{18} + CH_4$	0.116E+08	–0.711E+04
112	$C_{10}H_{21} + O = H + C_{10}H_{20}O$	0.699E+09	0.565E+03
113	$C_{10}H_{21} + O = \tilde{N}H_3 + C_9H_{18}O$	0.787E+11	–0.952E+03
114	$C_{10}H_{21} + O = C_2H_5 + C_8H_{16}O$	0.380E+12	–0.118E+04
115	$C_{10}H_{21} + O = C_3H_7 + C_7H_{14}O$	0.308E+12	–0.118E+04
116	$C_{10}H_{21} + O = C_4H_9 + C_6H_{12}O$	0.308E+12	–0.118E+04
117	$C_{10}H_{21} + O = C_5H_{11} + C_5H_{10}O$	0.309E+12	–0.118E+04
118	$C_{10}H_{21} + O = C_6H_{13} + C_4H_8O$	0.309E+12	–0.118E+04
119	$C_{10}H_{21} + O = C_7H_{15} + C_2H_5CHO$	0.309E+12	–0.118E+04
120	$C_{10}H_{21} + O = C_8H_{17} + CH_3CHO$	0.319E+12	–0.111E+04
121	$C_{10}H_{21} + O = C_9H_{19} + H_2CO$	0.162E+12	–0.352E+01
122	$C_{10}H_{19}O + HO_2 = C_{10}H_{20}O + O_2$	0.530E+08	0.000E+00
123	$C_{10}H_{20}O + OH = C_{10}H_{19}O + H_2O$	0.100E+11	0.000E+00
124	$C_{10}H_{20}O + H = C_{10}H_{19}O + H_2$	0.140E+11	0.165E+04
125	$C_{10}H_{20}O + O = C_{10}H_{19}O + OH$	0.568E+10	0.780E+03
126	$C_{10}H_{20}O + HO_2 = C_{10}H_{19}O + H_2O_2$	0.600E+09	0.500E+04
127	$C_9H_{19} + HCO = C_{10}H_{20}O$	0.222E+11	0.352E+01
128	$C_9H_{19} + CO = C_{10}H_{19}O$	0.186E+09	0.242E+04
129	$C_{10}H_{19}O + H = C_9H_{19} + HCO$	0.487E+10	0.240E+04
130	$C_{10}H_{19}O + O = C_9H_{19}O + CO$	0.369E+10	0.646E+03
131	$C_{10}H_{20} + OH = C_{10}H_{19} + H_2O$	0.900E+11	0.325E+04
132	$C_{10}H_{19} + H_2 = C_{10}H_{20} + H$	0.853E+11	0.533E+04
133	$C_{10}H_{19} + O_2 = C_8H_{17}O_2 + C_2H_2$	0.241E+11	0.396E+04
134	$C_{10}H_{20} + HCO = C_{10}H_{19} + H_2CO$	0.600E+11	0.900E+04
135	$C_{10}H_{20} + CH_3 = C_{10}H_{19} + CH_4$	0.107E+09	0.268E+04
136	$C_{10}H_{20} + C_2H_5 = C_{10}H_{19} + C_2H_6$	0.481E+10	0.325E+04
137	$C_{10}H_{20} + C_3H_7 = C_{10}H_{19} + C_3H_8$	0.420E+08	0.328E+04
138	$C_{10}H_{20} + C_4H_9 = C_{10}H_{19} + C_4H_{10}$	0.420E+08	0.328E+04
139	$C_{10}H_{20} + C_5H_{11} = C_{10}H_{19} + C_5H_{12}$	0.420E+08	0.328E+04
140	$C_{10}H_{20} + C_6H_{13} = C_{10}H_{19} + C_6H_{14}$	0.420E+08	0.328E+04
141	$C_{10}H_{20} + C_7H_{15} = C_{10}H_{19} + C_7H_{16}$	0.420E+08	0.328E+04
142	$C_{10}H_{20} + C_8H_{17} = C_{10}H_{19} + C_8H_{18}$	0.420E+08	0.328E+04
143	$C_{10}H_{20} + C_9H_{19} = C_{10}H_{19} + C_9H_{20}$	0.420E+08	0.328E+04
144	$C_8H_{17} + C_2H_2 = C_{10}H_{19}$	0.141E+10	0.143E+04
145	$C_{10}H_{20} = C_2H_3 + C_8H_{17}$	0.390E+14	0.379E+05
146	$C_{10}H_{20} = C_3H_5 + C_7H_{15}$	0.113E+14	0.446E+05
147	$C_{10}H_{20} = C_4H_7 + C_6H_{13}$	0.113E+14	0.446E+05
148	$C_{10}H_{20} = C_5H_9 + C_5H_{11}$	0.113E+14	0.446E+05
149	$C_{10}H_{20} = C_6H_{11} + C_4H_9$	0.113E+14	0.446E+05
150	$C_{10}H_{20} = C_7H_{13} + C_3H_7$	0.113E+14	0.446E+05
151	$C_{10}H_{20} = C_8H_{15} + C_2H_5$	0.140E+14	0.446E+05
152	$C_{10}H_{20} = C_9H_{17} + CH_3$	0.289E+13	0.439E+05
153	$C_{10}H_{20} + O_2 = C_{10}H_{19} + HO_2$	0.600E+11	0.236E+05
154	$C_{10}H_{20} + O = C_9H_{19} + HCO$	0.404E+10	0.226E+03
155	$C_{10}H_{19} + OH = C_9H_{19} + HCO$	0.485E+10	–0.352E+01
156	$C_{10}H_{19} + H = C_8H_{18} + C_2H_2$	0.918E+10	0.362E+03

Table 2. (Contd.)

No.	Reaction	*A*, l, mol, s	*E/R*, K
157	$C_{10}H_{19} + O = C_9H_{19} + CO$	0.485E+10	–0.352E+01
158	$C_{10}H_{19} + O = C_8H_{17}O + C_2H_2$	0.403E+11	–0.662E+02
159	$CH_3 + C_9H_{19} = C_{10}H_{20} + H_2$	0.248E+14	0.191E+05
160	$C_2H_5 + C_8H_{17} = C_{10}H_{20} + H_2$	0.512E+13	0.193E+05
161	$C_3H_7 + C_7H_{15} = C_{10}H_{20} + H_2$	0.633E+13	0.193E+05
162	$C_4H_9 + C_6H_{13} = C_{10}H_{20} + H_2$	0.634E+13	0.193E+05
163	$C_5H_{11} + C_5H_{11} = C_{10}H_{20} + H_2$	0.634E+13	0.193E+05
164	$C_6H_{13} + C_4H_9 = C_{10}H_{20} + H_2$	0.634E+13	0.193E+05
165	$C_7H_{15} + C_3H_7 = C_{10}H_{20} + H_2$	0.633E+13	0.193E+05
166	$C_8H_{17} + C_2H_5 = C_{10}H_{20} + H_2$	0.512E+13	0.193E+05
167	$C_{10}H_{20} + H + H = CH_3 + C_9H_{19}$	0.356E+10	–0.414E+04
168	$C_{10}H_{20} + H + H = C_2H_5 + C_8H_{17}$	0.172E+11	–0.437E+04
169	$C_{10}H_{20} + H + H = C_3H_7 + C_7H_{15}$	0.139E+11	–0.438E+04
170	$C_{10}H_{20} + H + H = C_4H_9 + C_6H_{13}$	0.139E+11	–0.438E+04
171	$C_{10}H_{20} + H + H = C_5H_{11} + C_5H_{11}$	0.139E+11	–0.438E+04
172	$C_{10}H_{20} + H + H = C_6H_{13} + C_4H_9$	0.139E+11	–0.438E+04
173	$C_{10}H_{20} + H + H = C_7H_{15} + C_3H_7$	0.139E+11	–0.438E+04
174	$C_{10}H_{20} + H + H = C_8H_{17} + C_2H_5$	0.172E+11	–0.437E+04
	n-Nonane		
1	$C_9H_20 + O_2 = C_9H_{19} + HO_2$	0.400E+10	0.239E+05
2	$Ñ_9H_{20} + OH = C_9H_{19} + H_20$	0.630E+10	0.600E+03
3	$C_9H_{20} + H = C_9H_{19} + H_2$	0.930E+11	0.403E+04
4	$C_9H_{20} + O = C_9H_{19} + OH$	0.506E+12	0.483E+04
5	$C_9H_{20} + HO_2 = C_9H_{19} + H_2O_2$	0.600E+09	0.856E+04
6	$C_9H_{18} + H = C_9H_{19}$	0.189E+10	0.315E+03
7	$C_9H_{19} + O_2 = C_9H_{18} + HO_2$	0.300E+11	0.700E+04
8	$C_9H_{19} + OH = C_9H_{18} + H_2O$	0.600E+10	0.000E+00
9	$C_9H_{20} = H + C_9H_{19}$	0.359E+14	0.376E+05
10	$C_9H_{20} = CH_3 + C_8H_{17}$	0.404E+16	0.421E+05
11	$C_9H_{20} = C_2H_5 + C_7H_{15}$	0.195E+17	0.428E+05
12	$C_9H_{20} = C_3H_7 + C_6H_{13}$	0.157E+17	0.428E+05
13	$C_9H_{20} = C_4H_9 + C_5H_{11}$	0.157E+17	0.428E+05
14	$C_9H_{19} + H = C_9H_{18} + H_2$	0.600E+10	0.000E+00
15	$C_9H_{19} + CH_3 = C_9H_{18} + CH_4$	0.351E+09	–0.106E+03
16	$C_9H_{19} + C_2H_5 = C_9H_{18} + C_2H_6$	0.158E+11	0.466E+03
17	$C_9H_{19} + C_3H_7 = C_9H_{18} + C_3H_8$	0.138E+09	0.488E+03
18	$C_9H_{19} + C_4H_9 = C_9H_{18} + C_4H_{10}$	0.138E+09	0.488E+03
19	$C_9H_{19} + C_5H_{11} = C_9H_{18} + C_5H_{12}$	0.138E+09	0.488E+03
20	$C_9H_{19} + C_6H_{13} = C_9H_{18} + C_6H_{14}$	0.138E+09	0.488E+03
21	$C_9H_{19} + C_7H_{15} = C_9H_{18} + C_7H_{16}$	0.138E+09	0.488E+03
22	$C_9H_{19} + C_8H_{17} = C_9H_{18} + C_8H_{18}$	0.138E+09	0.488E+03
23	$C_9H_{19} + O = C_9H_{18} + OH$	0.200E+12	0.000E+00
24	$C_9H_{19} + O_2 = C_9H_{19}O_2$	0.398E+08	–0.500E+03
25	$C_9H_{20} + CH_3O_2 = C_9H_{19} + CH_3O_2H$	0.207E+11	0.650E+04
26	$C_9H_{20} + C_2H_5O_2 = C_9H_{19} + C_2H_5O_2H$	0.207E+11	0.650E+04
27	$C_9H_{20} + C_3H_7O_2 = C_9H_{19} + C_3H_7O_2H$	0.207E+11	0.650E+04
28	$C_9H_{20} + C_4H_9O_2 = C_9H_{19} + C_4H_{10}O_2$	0.207E+11	0.650E+04
29	$C_9H_{20} + C_5H_{11}O_2 = C_9H_{19} + C_5H_{12}O_2$	0.207E+11	0.650E+04
30	$C_9H_{20} + C_6H_{13}O_2 = C_9H_{19} + C_6H_{14}O_2$	0.207E+11	0.650E+04
31	$C_9H_{20} + C_7H_{15}O_2 = C_9H_{19} + C_7H_{16}O_2$	0.207E+11	0.650E+04
32	$C_9H_{20} + C_8H_{17}O_2 = C_9H_{19} + C_8H_{18}O_2$	0.207E+11	0.650E+04
33	$C_9H_{20} + C_9H_{19}O_2 = C_9H_{19} + C_9H_{20}O_2$	0.207E+11	0.650E+04

Table 2. (Contd.)

No.	Reaction	*A*, l, mol, s	*E/R*, K
34	$C_9H_{20}O_2 = C_9H_{19}O + OH$	0.500E+16	0.200E+05
35	$C_9H_{19}O = H_2CO + C_8H_{17}$	0.159E+15	0.797E+04
36	$C_9H_{19}O = CH_3CHO + C_7H_{15}$	0.314E+15	0.113E+05
37	$C_9H_{19}O = C_2H_5CHO + C_6H_{13}$	0.303E+15	0.103E+05
38	$C_9H_{19}O = C_4H_8O + C_5H_{11}$	0.303E+15	0.103E+05
39	$C_9H_{19}O = C_5H_{10}O + C_4H_9$	0.303E+15	0.103E+05
40	$C_9H_{19}O = C_6H_{12}O + \tilde{N}_3H_7$	0.303E+15	0.103E+05
41	$C_9H_{19}O = C_7H_{14}O + C_2H_5$	0.374E+15	0.103E+05
42	$C_9H_{19}O = C_8H_{16}O + CH_3$	0.775E+14	0.108E+05
43	$C_9H_{19}O = C_9H_{18}O + H$	0.688E+12	0.626E+04
44	$C_9H_{19}O_2 + H = C_9H_{19}O + OH$	0.236E+11	–0.161E+04
45	$C_9H_{19}O_2 + CH_3 = C_9H_{19}O + CH_3O$	0.364E+09	–0.166E+03
46	$C_9H_{19}O_2 + C_2H_5 = C_9H_{19}O + C_2H_5O$	0.827E+09	–0.649E+03
47	$C_9H_{19}O_2 + C_3H_7 = C_9H_{19}O + C_3H_7O$	0.630E+09	0.000E+00
48	$C_9H_{19}O_2 + C_4H_9 = C_9H_{19}O + C_4H_9O$	0.630E+09	0.000E+00
49	$C_9H_{19}O_2 + C_5H_{11} = C_9H_{19}O + C_5H_{11}O$	0.630E+09	0.000E+00
50	$C_9H_{19}O_2 + C_6H_{13} = C_9H_{19}O + C_6H_{13}O$	0.629E+09	0.000E+00
51	$C_9H_{19}O_2 + C_7H_{15} = C_9H_{19}O + C_7H_{15}O$	0.627E+09	0.000E+00
52	$C_9H_{19}O_2 + C_8H_{17} = \tilde{N}_9H_{19}O + C_8H_{17}O$	0.627E+09	0.000E+00
53	$C_9H_{19}O_2 + C_9H_{19} = C_9H_{19}O + C_9H_{19}O$	0.365E+09	0.156E+04
54	$C_9H_{19}O_2 + H_2CO = C_9H_{20}O_2 + HCO$	0.320E+09	0.564E+04
55	$C_9H_{19}O_2 + CH_3CHO = C_9H_{20}O_2 + CH_3CO$	0.315E+09	0.560E+04
56	$C_9H_{19}O_2 + C_2H_5CHO = C_9H_{20}O_2 + C_2H_5CO$	0.315E+09	0.554E+04
57	$C_9H_{19}O_2 + C_4H_8O = C_9H_{20}O_2 + C_4H_7O$	0.315E+09	0.554E+04
58	$C_9H_{19}O_2 + C_5H_{10}O = C_9H_{20}O_2 + C_5H_9O$	0.315E+09	0.554E+04
59	$C_9H_{19}O_2 + C_6H_{12}O = C_9H_{20}O_2 + C_6H_{11}O$	0.315E+09	0.554E+04
60	$C_9H_{19}O_2 + C_7H_{14}O = C_9H_{20}O_2 + C_7H_{13}O$	0.315E+09	0.554E+04
61	$C_9H_{19}O_2 + C_8H_{16}O = C_9H_{20}O_2 + C_8H_{15}O$	0.315E+09	0.554E+04
62	$C_9H_{19}O_2 + C_9H_{18}O = C_9H_{20}O_2 + C_9H_{17}O$	0.315E+09	0.554E+04
63	$C_9H_{19} + HO_2 = C_9H_{19}O + OH$	0.298E+11	0.000E+00
64	$C_9H_{19} + O_2 = C_9H_{18}O + OH$	0.398E+10	0.900E+04
65	$C_9H_{19} + C_2H_5 = C_9H_{20} + C_2H_4$	0.625E+09	0.335E+03
66	$C_9H_{19} + C_3H_7 = C_9H_{20} + C_3H_6$	0.190E+10	0.000E+00
67	$C_9H_{19} + C_4H_9 = C_9H_{20} + C_4H_8$	0.190E+10	0.000E+00
68	$C_9H_{19} + C_5H_{11} = C_9H_{20} + C_5H_{10}$	0.190E+10	0.000E+00
69	$C_9H_{19} + C_6H_{13} = C_9H_{20} + C_6H_{12}$	0.190E+10	0.000E+00
70	$C_9H_{19} + C_7H_{15} = C_9H_{20} + C_7H_{14}$	0.190E+10	0.000E+00
71	$C_9H_{19} + C_8H_{17} = C_9H_{20} + C_8H_{16}$	0.190E+10	0.000E+00
72	$C_9H_{19} + C_9H_{19} = C_9H_{20} + C_9H_{18}$	0.190E+10	0.000E+00
73	$C_9H_{19} + O_2 = H_2CO + C_8H_{17}O$	0.368E+09	0.565E+04
74	$C_9H_{19} + O_2 = CH_3CHO + C_7H_{15}O$	0.725E+09	0.454E+04
75	$C_9H_{19} + O_2 = C_2H_5CHO + C_6H_{13}O$	0.703E+09	0.446E+04
76	$C_9H_{19} + O_2 = C_4H_8O + C_5H_{11}O$	0.704E+09	0.446E+04
77	$C_9H_{19} + O_2 = C_5H_{10}O + C_4H_9O$	0.704E+09	0.446E+04
78	$C_9H_{19} + O_2 = C_6H_{12}O + C_3H_7O$	0.703E+09	0.446E+04
79	$C_9H_{19} + O_2 = C_7H_{14}O + C_2H_5O$	0.114E+10	0.382E+04
80	$C_9H_{19} + O_2 = C_8H_{16}O + CH_3O$	0.104E+09	0.453E+04
81	$C_9H_{19} + OH = CH_3 + C_8H_{17}O$	0.184E+11	–0.194E+04
82	$C_9H_{19} + OH = C_2H_5 + C_7H_{15}O$	0.888E+11	0.417E+03
83	$C_9H_{19} + OH = C_3H_7 + C_6H_{13}O$	0.719E+11	0.413E+03
84	$C_9H_{19} + OH = C_4H_9 + C_5H_{11}O$	0.719E+11	0.413E+03
85	$C_9H_{19} + OH = C_5H_{11} + C_4H_9O$	0.719E+11	0.413E+03

Table 2. (Contd.)

No.	Reaction	*A*, l, mol, s	*E/R*, K
86	$C_9H_{19} + OH = C_6H_{13} + C_3H_7O$	0.719E+11	0.413E+03
87	$C_9H_{19} + OH = C_7H_{15} + C_2H_5O$	0.117E+12	–0.232E+03
88	$C_9H_{19} + OH = C_8H_{17} + CH_3O$	0.107E+11	0.480E+03
89	C_9H_{19} + H = ÑÍ$_3$ + C_8H_{17}	0.388E+11	0.546E+03
90	$C_9H_{19} + H = C_2H_5 + C_7H_{15}$	0.187E+12	0.318E+03
91	$C_9H_{19} + H = C_3H_7 + C_6H_{13}$	0.151E+12	0.314E+03
92	$C_9H_{19} + H = C_4H_9 + C_5H_{11}$	0.151E+12	0.314E+03
93	$C_9H_{19} + H = CH_2 + C_8H_{18}$	0.423E+08	0.302E+04
94	$C_9H_{19} + H = C_2H_4 + C_7H_{16}$	0.723E+07	–0.641E+04
95	$C_9H_{19} + H = C_3H_6 + C_6H_{14}$	0.177E+08	–0.675E+04
96	$C_9H_{19} + H = C_4H_8 + C_5H_{12}$	0.177E+08	–0.675E+04
97	$C_9H_{19} + H = C_5H_{10} + C_4H_{10}$	0.177E+08	–0.675E+04
98	$C_9H_{19} + H = C_6H_{12} + C_3H_8$	0.177E+08	–0.675E+04
99	$C_9H_{19} + H = C_7H_{14} + C_2H_6$	0.252E+10	–0.677E+04
100	$C_9H_{19} + H = C_8H_{16} + CH_4$	0.116E+08	–0.711E+04
101	$C_9H_{19} + O = H + C_9H_{18}O$	0.699E+09	0.565E+03
102	$C_9H_{19} + O = CH_3 + C_8H_{16}O$	0.787E+11	–0.952E+03
103	$C_9H_{19} + O = C_2H_5 + C_7H_{14}O$	0.380E+12	–0.118E+04
104	$C_9H_{19} + O = C_3H_7 + C_6H_{12}O$	0.308E+12	–0.118E+04
105	$C_9H_{19} + O = C_4H_9 + C_5H_{10}O$	0.308E+12	–0.118E+04
106	$C_9H_{19} + O = C_5H_{11} + C_4H_8O$	0.308E+12	–0.118E+04
107	$C_9H_{19} + O = C_6H_{13} + C_2H_5CHO$	0.308E+12	–0.118E+04
108	$C_9H_{19} + O = C_7H_{15} + CH_3CHO$	0.319E+12	–0.111E+04
109	$C_9H_{19} + O = C_8H_{17} + H_2CO$	0.162E+12	–0.352E+01
110	$C_9H_{17}O + HO_2 = C_9H_{18}O + O_2$	0.530E+08	0.000E+00
111	$C_9H_{18}O + OH = C_9H_{17}O + H_2O$	0.100E+11	0.000E+00
112	$C_9H_{18}O + H = C_9H_{17}O + H_2$	0.140E+11	0.165E+04
113	$C_9H_{18}O + O = C_9H_{17}O + OH$	0.568E+10	0.780E+03
114	$C_9H_{18}O + HO_2 = C_9H_{17}O + H_2O_2$	0.600E+09	0.500E+04
115	$C_8H_{17} + HCO = C_9H_{18}O$	0.222E+11	0.352E+01
116	$C_8H_{17} + CO = C_9H_{17}O$	0.186E+09	0.242E+04
117	$C_9H_{17}O + H = C_8H_{17} + HCO$	0.487E+10	0.240E+04
118	$C_9H_{17}O + O = C_8H_{17}O + CO$	0.369E+10	0.646E+03
119	$C_9H_{18} + OH = C_9H_{17} + H_2O$	0.900E+11	0.325E+04
120	$C_9H_{17} + H_2 = C_9H_{18} + H$	0.853E+11	0.533E+04
121	$C_9H_{17} + O_2 = C_7H_{15}O_2 + C_2H$	0.241E+11	0.396E+04
122	$C_9H_{18} + HCO = C_9H_{17} + H_2CO$	0.600E+11	0.900E+04
123	$C_9H_{18} + CH_3 = C_9H_{17} + CH_4$	0.107E+09	0.268E+04
124	$C_9H_{18} + C_2H_5 = C_9H_{17} + C_2H_6$	0.481E+10	0.325E+04
125	$C_9H_{18} + C_3H_7 = C_9H_{17} + C_3H_8$	0.420E+08	0.328E+04
126	$C_9H_{18} + C_4H_9 = C_9H_{17} + C_4H_{10}$	0.420E+08	0.328E+04
127	$C_9H_{18} + C_5H_{11} = C_9H_{17} + C_5H_{12}$	0.420E+08	0.328E+04
128	$C_9H_{18} + C_6H_{13} = C_9H_{17} + C_6H_{14}$	0.420E+08	0.328E+04
129	$C_9H_{18} + C_7H_{15} = C_9H_{17} + C_7H_{16}$	0.420E+08	0.328E+04
130	$C_9H_{18} + C_8H_{17} = C_9H_{17} + C_8H_{18}$	0.420E+08	0.328E+04
131	$C_7H_{15} + C_2H_2 = C_9H_{17}$	0.141E+10	0.143E+04
132	$C_9H_{18} = C_2H_3 + C_7H_{15}$	0.390E+14	0.379E+05
133	$C_9H_{18} = C_3H_5 + C_6H_{13}$	0.113E+14	0.446E+05
134	$C_9H_{18} = C_4H_7 + C_5H_{11}$	0.113E+14	0.446E+05
135	$C_9H_{18} = C_5H_9 + C_4H_9$	0.113E+14	0.446E+05
136	$C_9H_{18} = C_6H_{11} + C_3H_7$	0.113E+14	0.446E+05
137	$C_9H_{18} = C_7H_{13} + C_2H_5$	0.140E+14	0.446E+05

Table 2. (Contd.)

No.	Reaction	A, l, mol, s	E/R, K
138	$C_9H_{18} = C_8H_{15} + CH_3$	0.289E+13	0.439E+05
139	$C_9H_{18} + O_2 = C_9H_{17} + HO_2$	0.600E+11	0.236E+05
140	$C_9H_{18} + O = C_8H_{17} + HCO$	0.404E+10	0.226E+03
141	$C_9H_{17} + OH = C_8H_{17} + HCO$	0.485E+10	–0.352E+01
142	$C_9H_{17} + H = C_7H_{16} + C_2H_2$	0.918E+10	0.362E+03
143	$C_9H_{17} + O = C_8H_{17} + CO$	0.485E+10	–0.352E+01
144	$C_9H_{17} + O = C_7H_{15}O + C_2H_2$	0.403E+11	–0.662E+02
145	$CH_3 + C_8H_{17} = C_9H_{18} + H_2$	0.248E+14	0.191E+05
146	$C_2H_5 + C_7H_{15} = C_9H_{18} + H_2$	0.512E+13	0.193E+05
147	$C_3H_7 + C_6H_{13} = C_9H_{18} + H_2$	0.636E+13	0.193E+05
148	$C_4H_9 + C_5H_{11} = C_9H_{18} + H_2$	0.636E+13	0.193E+05
149	$C_5H_{11} + C_4H_9 = C_9H_{18} + H_2$	0.636E+13	0.193E+05
150	$C_6H_{13} + C_3H_7 = C_9H_{18} + H_2$	0.636E+13	0.193E+05
151	$C_7H_{15} + C_2H_5 = C_9H_{18} + H_2$	0.512E+13	0.193E+05
152	$C_9H_{18} + H + H = CH_3 + C_8H_{17}$	0.356E+10	–0.414E+04
153	$C_9H_{18} + H + H = C_2H_5 + C_7H_{15}$	0.172E+11	–0.437E+04
154	$C_9H_{18} + H + H = C_3H_7 + C_6H_{13}$	0.139E+11	–0.438E+04
155	$C_9H_{18} + H + H = C_4H_9 + C_5H_{11}$	0.139E+11	–0.438E+04
156	$C_9H_{18} + H + H = C_5H_{11} + C_4H_9$	0.139E+11	–0.438E+04
157	$C_9H_{18} + H + H = C_6H_{13} + C_3H_7$	0.139E+11	–0.438E+04
158	$C_9H_{18} + H + H = C_7H_{15} + C_2H_5$	0.172E+11	–0.437E+04
	n-Octane		
1	$C_8H_{18} + O_2 = C_8H_{17} + HO_2$	0.400E+10	0.239E+05
2	$C_8H_{18} + OH = C_8H_{17} + H_2O$	0.630E+10	0.600E+03
3	$C_8H + H = C_8H_{17} + H_2$	0.930E+11	0.403E+04
4	$C_8H_{18} + O = C_8H_{17} + OH$	0.371E+04	0.277E+04
5	$C_8H_{18} + HO_2 = C_8H_{17} + H_2O_2$	0.600E+09	0.856E+04
6	$C_8H_{16} + H = C_8H_{17}$	0.189E+10	0.315E+03
7	$C_8H_{17} + O_2 = C_8H_{16} + HO_2$	0.300E+11	0.700E+04
8	$C_8H_{17} + OH = C_8H_{16} + H_20$	0.600E+10	0.000E+00
9	$C_8H_{18} = H + C_8H_{17}$	0.359E+14	0.376E+05
10	$C_8H_{18} = CH_3 + C_7H_{15}$	0.404E+16	0.421E+05
11	$C_8H_{18} = C_2H_5 + C_6H_{13}$	0.194E+17	0.428E+05
12	$C_8H_{18} = C_3H_7 + C_5H_{11}$	0.157E+17	0.428E+05
13	$C_8H_{18} = C_4H_9 + C_4H_9$	0.157E+17	0.428E+05
14	$C_8H_{17} + H = C_8H_{16} + H_2$	0.600E+10	0.000E+00
15	$C_8H_{17} + CH_3 = C_8H_{16} + CH_4$	0.351E+09	–0.106E+03
16	$C_8H_{17} + C_2H_5 = C_8H_{16} + C_2H_6$	0.158E+11	0.466E+03
17	$C_8H_{17} + C_3H_7 = C_8H_{16} + C_3H_8$	0.138E+09	0.488E+03
18	$C_8H_{17} + C_4H_9 = C_8H_{16} + C_4H_{10}$	0.138E+09	0.488E+03
19	$C_8H_{17} + C_5H_{11} = C_8H_{16} + C_5H_{12}$	0.138E+09	0.488E+03
20	$C_8H_{17} + C_6H_{13} = C_8H_{16} + C_6H_{14}$	0.138E+09	0.488E+03
21	$C_8H_{17} + C_7H_{15} = C_8H_{16} + C_7H_{16}$	0.138E+09	0.488E+03
22	$C_8H_{17} + O = C_8H_{16} + OH$	0.200E+12	0.000E+00
23	$C_8H_{17} + O_2 = C_8H_{17}O_2$	0.398E+08	–0.500E+03
24	$C_8H_{18} + CH_3O_2 = C_8H_{17} + CH_3O_2H$	0.169E+11	0.630E+04
25	$C_8H_{18} + C_2H_5O_2 = C_8H_{17} + C_2H_5O_2H$	0.169E+11	0.630E+04
26	$C_8H_{18} + C_3H_7O_2 = C_8H_{17} + C_3H_7O_2H$	0.169E+11	0.630E+04
27	$C_8H_{18} + C_4H_9O_2 = C_8H_{17} + C_4H_{10}O_2$	0.169E+11	0.630E+04
28	$C_8H_{18} + C_5H_{11}O_2 = C_8H_{17} + C_5H_{12}O_2$	0.169E+11	0.630E+04
29	$C_8H_{18} + C_6H_{13}O_2 = C_8H_{17} + C_6H_{14}O_2$	0.169E+11	0.630E+04
30	$C_8H_{18} + C_7H_{15}O_2 = C_8H_{17} + C_7H_{16}O_2$	0.169E+11	0.630E+04

Table 2. (Contd.)

No.	Reaction	*A*, l, mol, s	*E/R*, K
31	$C_8H_{18} + C_8H_{17}O_2 = C_8H_{17} + C_8H_{18}O_2$	0.169E+11	0.630E+04
32	$C_8H_{18}O_2 = C_8H_{17}O + OH$	0.500E+16	0.200E+05
33	$C_8H_{17}O = H_2CO + C_7H_{15}$	0.159E+15	0.797E+04
34	$C_8H_{17}O = CH_3CHO + C_6H_{13}$	0.313E+15	0.113E+05
35	$C_8H_{17}O = C_2H_5CHO + C_5H_{11}$	0.303E+15	0.103E+05
36	$C_8H_{17}O = C_4H_8O + C_4H_9$	0.303E+15	0.103E+05
37	$C_8H_{17}O = C_5H_{10}O + C_3H_7$	0.303E+15	0.103E+05
38	$C_8H_{17}O = C_6H_{12}O + C_2H_5$	0.374E+15	0.103E+05
39	$C_8H_{17}O = C_7H_{14}O + CH_3$	0.775E+14	0.108E+05
40	$C_8H_{17}O = C_8H_{16}O + H$	0.688E+12	0.626E+04
41	$C_8H_{17}O_2 + H = C_8H_{17}O + OH$	0.236E+11	–0.161E+04
42	$C_8H_{17}O_2 + CH_3 = C_8H_{17}O + CH_3O$	0.364E+09	–0.166E+03
43	$C_8H_{17}O_2 + C_2H_5 = C_8H_{17}O + C_2H_5O$	0.827E+09	–0.649E+03
44	$C_8H_{17}O_2 + C_3H_7 = C_8H_{17}O + C_3H_7O$	0.630E+09	0.000E+00
45	$C_8H_{17}O_2 + C_4H_9 = C_8H_{17}O + C_4H_9O$	0.630E+09	0.000E+00
46	$C_8H_{17}O_2 + C_5H_{11} = C_8H_{17}O + C_5H_{11}O$	0.630E+09	0.000E+00
47	$C_8H_{17}O_2 + C_6H_{13} = C_8H_{17}O + C_6H_{13}O$	0.629E+09	0.000E+00
48	$C_8H_{17}O_2 + C_7H_{15} = C_8H_{17}O + Ñ_7Í_{15}O$	0.627E+09	0.000E+00
49	$C_8H_{17}O_2 + C_8H_{17} = C_8H_{17}O + C_8H_{17}O$	0.627E+09	0.000E+00
50	$C_8H_{17}O_2 + H_2CO = C_8H_{18}O_2 + HCO$	0.320E+09	0.564E+04
51	$C_8H_{17}O_2 + CH_3CHO = C_8H_{18}O_2 + CH_3CO$	0.315E+09	0.560E+04
52	$C_8H_{17}O_2 + C_2H_5CHO = C_8H_{18}O_2 + C_2H_5CO$	0.315E+09	0.554E+04
53	$C_8H_{17}O_2 + C_4H_8O = C_8H_{18}O_2 + C_4H_7O$	0.315E+09	0.554E+04
54	$C_8H_{17}O_2 + C_5H_{10}O = C_8H_{18}O_2 + C_5H_9O$	0.315E+09	0.554E+04
55	$C_8H_{17}O_2 + C_6H_{12}O = C_8H_{18}O_2 + C_6H_{11}O$	0.315E+09	0.554E+04
56	$C_8H_{17}O_2 + C_7H_{14}O = C_8H_{18}O_2 + C_7H_{13}O$	0.315E+09	0.554E+04
57	$C_8H_{17}O_2 + C_8H_{16}O = C_8H_{18}O_2 + C_8H_{15}O$	0.315E+09	0.554E+04
58	$C_8H_{17} + HO_2 = C_8H_{17}O + OH$	0.298E+11	0.000E+00
59	$C_8H_{17} + O_2 = C_8H_{16}O + OH$	0.398E+10	0.900E+04
60	$C_8H_{17} + C_2H_5 = C_8H_{18} + C_2H_4$	0.625E+09	0.335E+03
61	$C_8H_{17} + C_3H_7 = C_8H_{18} + C_3H_6$	0.190E+10	0.000E+00
62	$C_8H_{17} + C_4H_9 = C_8H_{18} + C_4H_8$	0.190E+10	0.000E+00
63	$C_8H_{17} + C_5H_{11} = C_8H_{18} + C_5H_{10}$	0.190E+10	0.000E+00
64	$C_8H_{17} + C_6H_{13} = C_8H_{18} + C_6H_{12}$	0.190E+10	0.000E+00
65	$C_8H_{17} + C_7H_{15} = C_8H_{18} + C_7H_{14}$	0.190E+10	0.000E+00
66	$C_8H_{17} + C_8H_{17} = C_8H_{18} + C_8H_{16}$	0.190E+10	0.000E+00
67	$C_8H_{17} + O_2 = H_2CO + C_7H_{15}O$	0.368E+09	0.565E+04
68	$C_8H_{17} + O_2 = CH_3CHO + C_6H_{13}O$	0.725E+09	0.454E+04
69	$C_8H_{17} + O_2 = C_2H_5CHO + C_5H_{11}O$	0.703E+09	0.446E+04
70	$C_8H_{17} + O_2 = C_4H_8O + C_4H_9O$	0.703E+09	0.446E+04
71	$C_8H_{17} + O_2 = C_5H_{10}O + C_3H_7O$	0.703E+09	0.446E+04
72	$C_8H_{17} + O_2 = C_6H_{12}O + C_2H_5O$	0.114E+10	0.382E+04
73	$C_8H_{17} + O_2 = C_7H_{14}O + CH_3O$	0.104E+09	0.453E+04
74	$C_8H_{17} + OH = CH_3 + C_7H_{15}O$	0.184E+11	–0.194E+04
75	$C_8H_{17} + OH = C_2H_5 + C_6H_{13}O$	0.888E+11	0.417E+03
76	$C_8H_{17} + OH = C_3H_7 + C_5H_{11}O$	0.718E+11	0.413E+03
77	$C_8H_{17} + OH = C_4H_9 + C_4H_9O$	0.718E+11	0.413E+03
78	$C_8H_{17} + OH = C_5H_{11} + C_3H_7O$	0.718E+11	0.413E+03
79	$C_8H_{17} + OH = C_6H_{13} + C_2H_5O$	0.117E+12	–0.232E+03
80	$C_8H_{17} + OH = C_7H_{15} + CH_3O$	0.107E+11	0.480E+03
81	$C_8H_{17} + H = CH_3 + C_7H_{15}$	0.388E+11	0.546E+03
82	$C_8H_{17} + H = C_2H_5 + C_6H_{13}$	0.187E+12	0.318E+03

Table 2. (Contd.)

No.	Reaction	*A*, l, mol, s	*E/R*, K
83	$C_8H_{17} + H = C_3H_7 + C5H_{11}$	0.151E+12	0.314E+03
84	$C_8H_{17} + H = C_4H_9 + C_4H_9$	0.151E+12	0.314E+03
85	$C_8H_{17} + H = CH_2 + C_7H_{16}$	0.423E+08	0.302E+04
86	$C_8H_{17} + H = C_2H_4 + C_6H_{14}$	0.721E+07	–0.641E+04
87	$C_8H_{17} + H = C_3H_6 + C_5H_{12}$	0.177E+08	–0.675E+04
88	$C_8H_{17} + H = C_4H_8 + C_4H_{10}$	0.177E+08	–0.675E+04
89	$C_8H_{17} + H = C_5H_{10} + C_3H_8$	0.177E+08	–0.675E+04
90	$C_8H_{17} + H = C_6H_{12} + C_2H_6$	0.251E+10	–0.677E+04
91	$C_8H_{17} + H = C_7H_{14} + CH_4$	0.116E+08	–0.711E+04
92	$C_8H_{17} + O = H + C_8H_{16}O$	0.699E+09	0.565E+03
93	$C_8H_{17} + O = CH_3 + C_7H_{14}O$	0.787E+11	–0.952E+03
94	$C_8H_{17} + O = C_2H_5 + C_6H_{12}O$	0.380E+12	–0.118E+04
95	$C_8H_{17} + O = C_3H_7 + C_5H_{10}O$	0.307E+12	–0.118E+04
96	$C_8H_{17} + O = C_4H_9 + C_4H_8O$	0.307E+12	–0.118E+04
97	$C_8H_{17} + O = C_5H_{11} + C_2H_5CHO$	0.307E+12	–0.118E+04
98	$C_8H_{17} + O = C_6H_{13} + CH_3CHO$	0.317E+12	–0.111E+04
99	$C_8H_{17} + O = C_7H_{15} + H_2CO$	0.162E+12	–0.352E+01
100	$C_8H_{15}O + HO_2 = C_8H_{16}O + O_2$	0.530E+08	0.000E+00
101	$C_8H_{16}O + OH = C_8H_{15}O + H_2O$	0.100E+11	0.000E+00
102	$C_8H_{16}O + H = C_8H_{15}O + H_2$	0.140E+11	0.165E+04
103	$C_8H_{16}O + O = C_8H_{15}O + OH$	0.568E+10	0.780E+03
104	$C_8H_{16}O + HO_2 = C_8H_{15}O + H_2O_2$	0.600E+09	0.500E+04
105	$C_7H_{15} + HCO = C_8H_{16}O$	0.222E+11	0.352E+01
106	$C_7H_{15} + CO = C_8H_{15}O$	0.186E+09	0.242E+04
107	$C_8H_{15}O + H = C_7H15 + HCO$	0.487E+10	0.240E+04
108	$C_8H_{15}O + O = C_7H_{15}O + CO$	0.369E+10	0.646E+03
109	$C_8H_{16} + OH = C_8H_{15} + H_2Î$	0.900E+11	0.325E+04
110	$C_8H_{15} + H_2 = C_8H_{16} + H$	0.853E+11	0.533E+04
111	$C_8H_{15} + O_2 = C_6H_{13}O_2 + C_2H_2$	0.241E+11	0.396E+04
112	$C_8H_{16} + HCO = C_8H_{15} + H_2CO$	0.600E+11	0.900E+04
113	$C_8H_{16} + CH_3 = C_8H_{15} + CH_4$	0.107E+09	0.268E+04
114	$C_8H_{16} + C_2H_5 = C_8H_{15} + C_2H_6$	0.481E+10	0.325E+04
115	$C_8H_{16} + C_3H_7 = C_8H_{15} + C_3H_8$	0.420E+08	0.328E+04
14	$C_8H_{17} + H = C_8H_{16} + H_2$	0.600E+10	0.000E+00
116	$C_8H_{16} + C_4H_9 = C_8H_{15} + C_4H_{10}$	0.420E+08	0.328E+04
117	$C_8H_{16} + C_5H_{11} = C_8H_{15} + C_5H_{12}$	0.420E+08	0.328E+04
118	$C_8H_{16} + C_6H_{13} = C_8H_{15} + C_6H_{14}$	0.420E+08	0.328E+04
119	$C_8H_{16} + C_7H_{15} = C_8H_{15} + C_7H_{16}$	0.420E+08	0.328E+04
120	$C_6H_{13} + C_2H_2 = C_8H_{15}$	0.141E+10	0.143E+04
121	$C_8H_{16} = C_2H_3 + C_6H_{13}$	0.389E+14	0.379E+05
122	$C_8H_{16} = C_3H_5 + C_5H_{11}$	0.112E+14	0.446E+05
123	$C_8H_{16} = C_4H_7 + C_4H_9$	0.112E+14	0.446E+05
124	$C_8H_{16} = C_5H_9 + C_3H_7$	0.112E+14	0.446E+05
125	$C_8H_{16} = C_6H_{11} + C_2H_5$	0.139E+14	0.446E+05
126	$C_8H_{16} = C_7H_{13} + CH_3$	0.289E+13	0.439E+05
127	$C_8H_{16} + O_2 = C_8H_{15} + HO_2$	0.600E+11	0.236E+05
128	$C_8H_{16} + O = C_7H_{15} + HCO$	0.404E+10	0.226E+03
129	$C_8H_{15} + OH = C_7H_{15} + HCO$	0.485E+10	–0.352E+01
130	$C_8H_{15} + H = C_6H_{14} + C_2H_2$	0.915E+10	0.362E+03
131	$C_8H_{15} + O = C_7H_{15} + CO$	0.485E+10	–0.352E+01
132	$C_8H_{15} + O = C_6H_{13}O + C_2H_2$	0.403E+11	–0.662E+02
133	$CH_3 + C_7H_{15} = C_8H_{16} + H_2$	0.248E+14	0.191E+05

Table 2. (Contd.)

No.	Reaction	A, l, mol, s	E/R, K
134	$C_2H_5 + C_6H_{13} = C_8H_{16} + H_2$	0.514E+13	0.193E+05
135	$C_3H_7 + C_5H_{11} = C_8H_{16} + H_2$	0.637E+13	0.193E+05
136	$C_4H_9 + C_4H_9 = C_8H_{16} + H_2$	0.637E+13	0.193E+05
137	$C_5H_{11} + C_3H_7 = C_8H_{16} + H_2$	0.637E+13	0.193E+05
138	$C_6H_{13} + C_2H_5 = C_8H_{16} + H_2$	0.514E+13	0.193E+05
139	$C_8H_{16} + H + H = CH_3 + C_7H_{15}$	0.145E+07	–0.500E+04
140	$C_8H_{16} + H + H = C_2H_5 + C_6H_{13}$	0.700E+07	–0.523E+04
141	$C_8H_{16} + H + H = C_3H_7 + C_5H_{11}$	0.565E+07	–0.524E+04
142	$C_8H_{16} + H + H = C_4H_9 + C_4H_9$	0.565E+07	–0.524E+04
143	$C_8H_{16} + H + H = C_5H_{11} + C_3H_7$	0.565E+07	–0.524E+04
144	$C_8H_{16} + H + H = C_6H_{13} + C_2H_5$	0.700E+07	–0.523E+04

Note: Further, mechanism of oxidation and combustion of C_1–C_7 follows

lation results. Figure 5 presents the comparison of calculated spontaneous ignition lags for stoichiometric air mixtures of n-C_8H_{18}, n-C_9H_{20}, and n-$C_{10}H_{22}$ at equal initial temperatures and pressure $P_0 = 1$ atm. It is evident that as n increases, the spontaneous ignition lags shorten and in all cases the NTC of the reaction rate occurs. Such results are also obtained at higher pressures.

Experiments on Laminar Flame Propagation

Calculations for the determination of the laminar flame velocity u_n in air mixtures of all tree hydrocarbons at atmospheric pressures and different initial temperatures were also carried out. We used the procedure described in [15]. Comparison of the calculated u_n with the experimental data of works [16–19] is presented in Figs. 6–8.

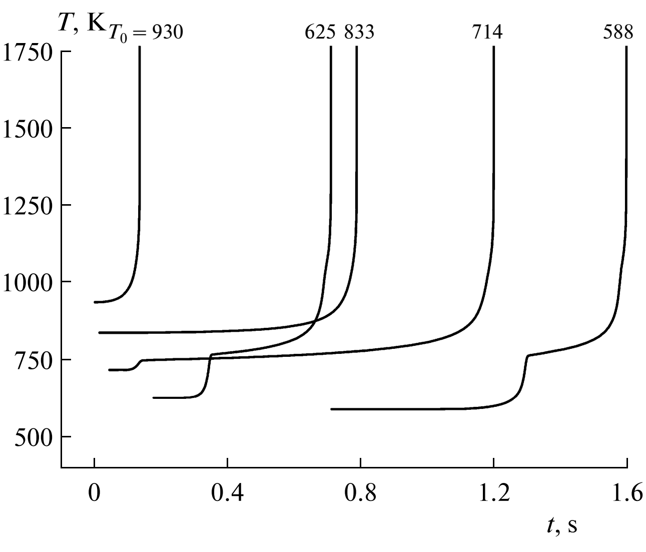

Fig. 1. Calculations of spontaneous ignition of stoichiometric n-decane–air mixture: time dependences of temperature. Initial temperatures $T_0 = 588$, 625, 714, 833, and 930 K, initial pressure $P_0 = 1$ atm.

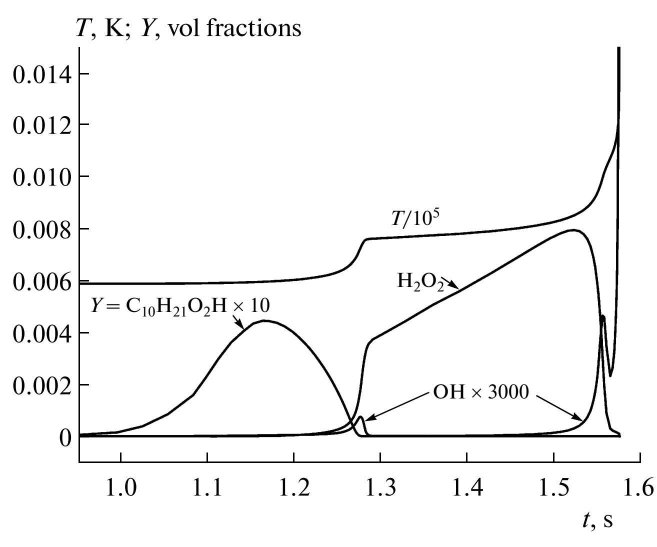

Fig. 2. Calculations of spontaneous ignition of stoichiometric n-decane–air mixture: time dependences of temperature, concentrations of peroxide and hydroxyl. Initial temperature $T_0 = 588$ K, initial pressure $P_0 = 1$ atm.

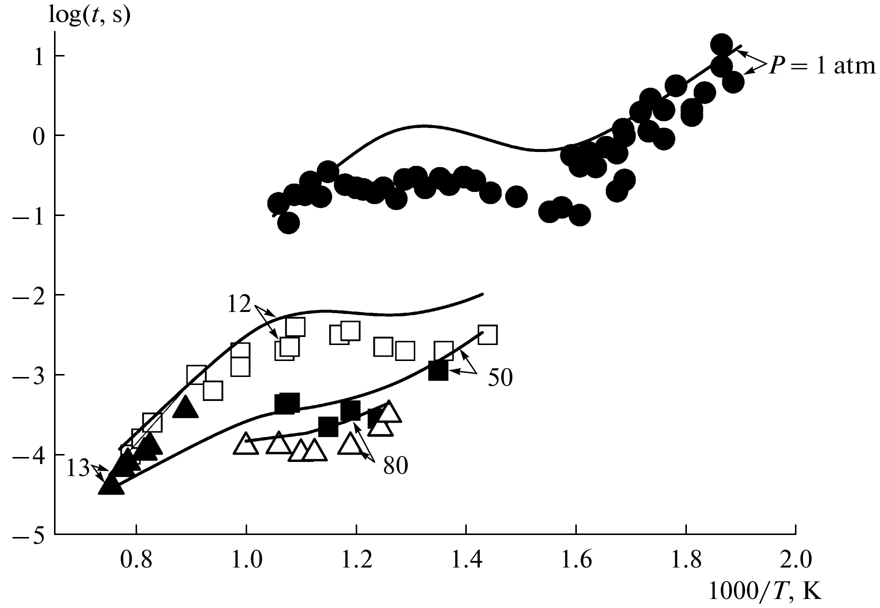

Fig. 3. Spontaneous ignition lags of stoichiometric n-decane–air mixture at different temperatures and pressures. Points are experiment [3, 11, 12]; curves, calculation.

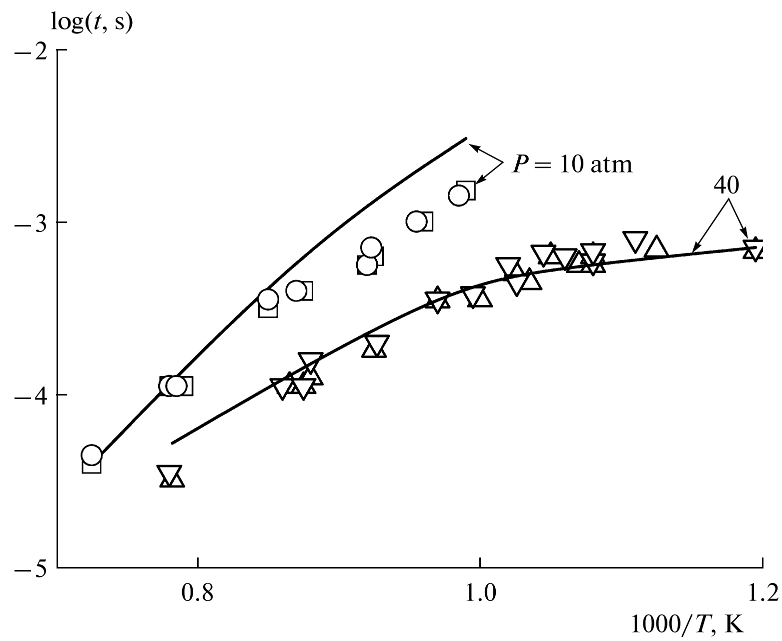

Fig. 4. Spontaneous ignition lags of stoichiometric n-decane–air mixture at different temperatures and pressures. Points are experiment [13, 14]; curves, calculation.

Experiment on the Spontaneous Ignition of Drops

The obtained DKM was also applied for the calculation of the spontaneous ignition and combustion of drops. The calculation basis is one-dimensional nonstationary equations of conservation of mass, chemical species, and energy for the gas and liquid phases with the conjugation of solutions on the spherical surface of the drop. The detailed description of the mathematical model and the calculation procedure are given in [20]. The air initial temperature T_0 around the drop was considered constant and the initial liquid temperature was taken as 293 K. The radius R of the calculation region was taken as sufficiently great in comparison with the initial drop radius r_0. Any selected R corresponded to the defined fuel–air equiv-

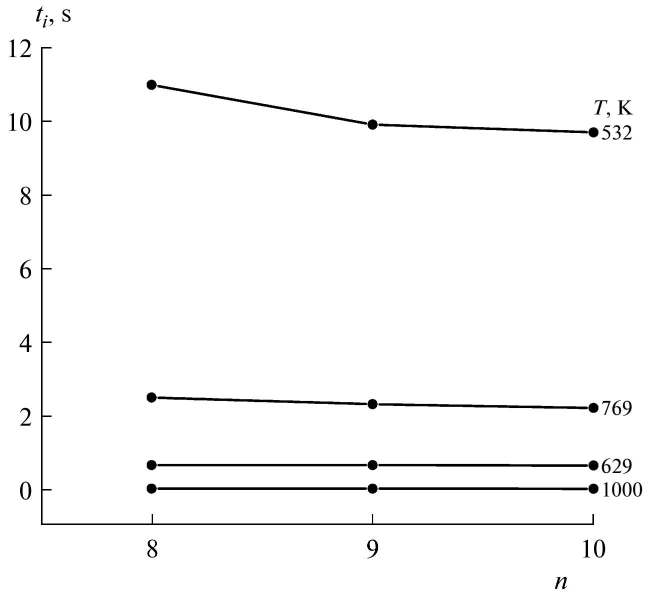

Fig. 5. Calculated spontaneous ignition lags of stoichiometric n-octane– ($n = 8$), n-nonane– ($n = 9$), and n-decane–air ($n = 10$) mixtures at different temperatures and atmospheric pressures.

alence ratio Φ in a homogeneous monodisperse drop-in-gas suspension [20]. After a lapse of the induction period in the gas, spontaneous ignition occurs at some distance from a drop center.

The problem was solved in a wide range of pressures, initial air temperatures, and initial compositions Φ of the mixture, both for single drops of different initial diameters and for homogeneous monodisperse drop-in-gas suspensions. It turned out that the stages in the calculations occurred in a such manner to that during the spontaneous ignition of the gas mixture. For example, Fig. 9 shows calculation results for a drop of n-decane with an initial diameter of 60 μm.

Cool flames during the spontaneous ignition of a spray of liquid drops were previously observed experimentally [21]. In [19] the total induction period t_s and the induction period t_1 of the cool flame were measured. In Fig. 10, comparison of the calculated and measured induction periods was carried out for a drop of n-decane with an initial diameter of 0.70 mm.

The so-called combustion rate constant k for the drop, which is included in the classical expression

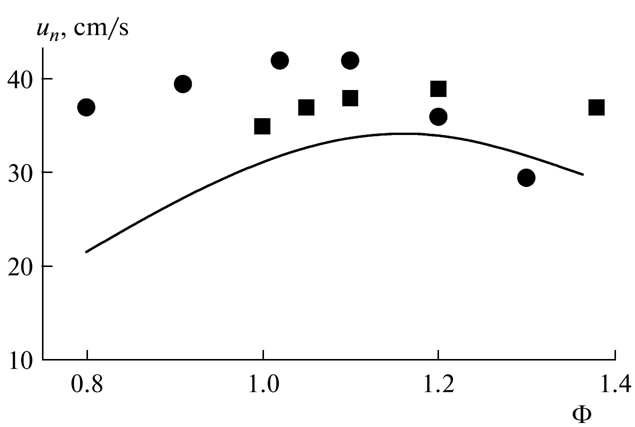

Fig. 6. Laminar flame velocity u_n as a function of composition Φ. N-octane–air mixture, atmospheric pressures, initial temperature $T_0 = 298$ K. Circles [16], squares [17] are experiments. Curve is calculation.

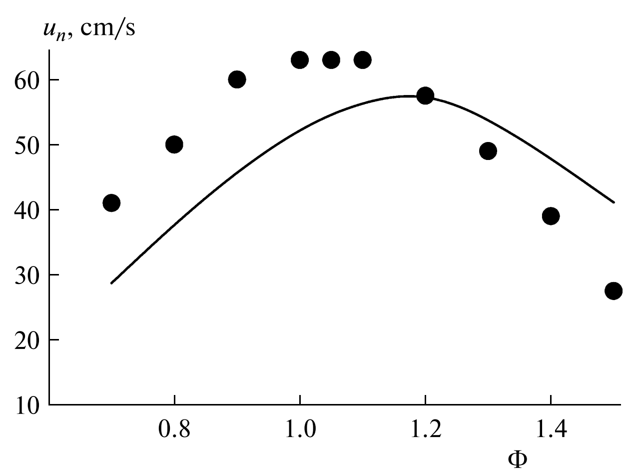

Fig. 7. Laminar flame velocity u_n as a function of composition Φ. N-nonane–air mixture, atmospheric pressures, initial temperature $T_0 = 403$ K. Points [18] are experiments; curve is calculation.

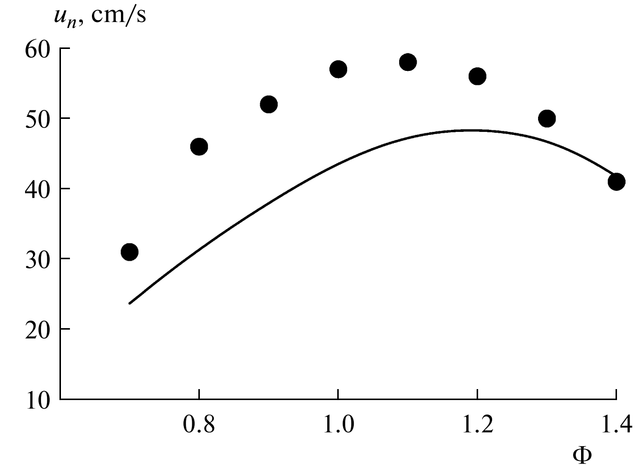

Fig. 8. Laminar flame velocity u_n as a function of composition Φ. N-decane–air mixture, atmospheric pressures, initial temperature T_0 = 360 K. Points [19] are experiments; curve is calculation.

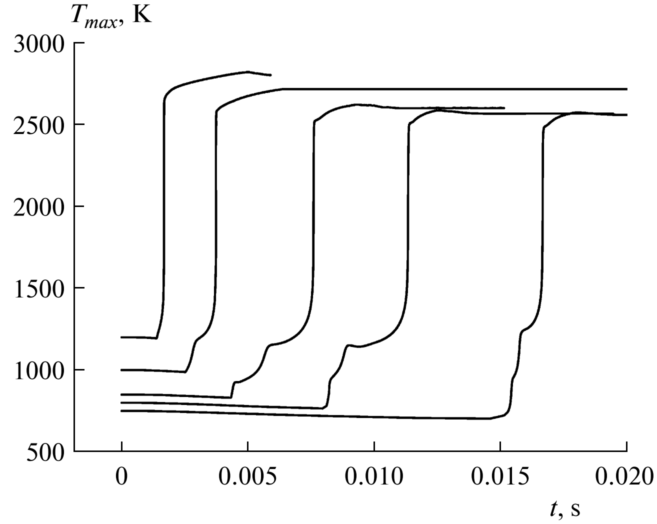

Fig. 9. Calculations of spontaneous ignition of stoichiometric n-decane drops–air mixtures: time dependences of temperature. Initial drop diameter of 60 μm, initial temperatures T_0 = 750, 800, 850, 1000, and 1200 K, initial pressure P_0 = 1 atm.

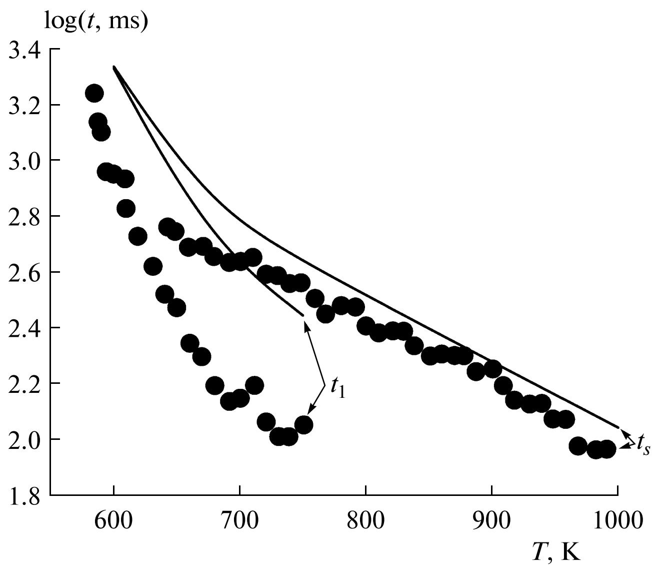

Fig. 10. Calculations of spontaneous ignition of drops of n-decane in air: spontaneous ignition lags as a function of initial temperature. Initial drop diameter of 0.70 mm, initial pressure P_0 = 1 atm. Points [22] are experiments; curves are calculation.

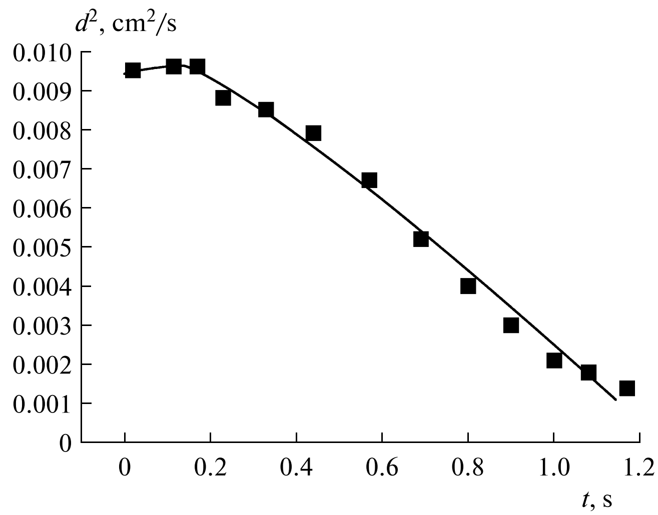

Fig. 11. Time dependence of n-decane drop diameter square d^2 at spontaneous ignition and combustion. Initial drop diameter of 0.91 mm, initial temperature T_0 = 1093 K, initial pressure P_0 = 1 atm. Points [22] are experiments; curve is calculation.

(known as the time dependence of the squared drop diameter)

$$d^2 = d_0^2 - kt,$$

where $d_0 = 2r_0$ is the initial drop diameter, can be determined by the regression rate of the square of the drop diameter.

Figure 11 presents a comparison of the calculated (line) and measured (points) time dependences of the drop squared diameter d^2 at spontaneous ignition of the drop of n-decane with an initial diameter of 0.91 mm. The spontaneous ignition lag corresponds to the time from the process origin ($t = 0$) to achieving the maximum d^2 (the increase in the drop diameter in this site is explained by the thermal expansion of the liquid). One can judge the drop burning rate k by the decrease in d^2 after achieving linearity (the straight segment of the line in Fig. 11). It is evident that the calculated drop burning rate coincides well with the measured value.

CONCLUSIONS

In the present work, new DKMs for the oxidation and combustion of n-octane, n-nonane, and n-decane were constructed. The major feature of the mechanisms is the appearance of the staging in the form of cold and blue flames at low-temperature spontaneous ignition. Calculations of spontaneous ignition and combustion of gas mixtures and drops of hydrocarbons in air were carried out in a wide range of initial conditions, as well as comparison of calculation results with experimental data. As a whole, satisfactory qualitative and quantitative argument of the results was obtained. Thus, one can discuss the appropriateness of the nonextensive principle used in the work for the construction of kinetic mechanisms with the goal of limitation of the variety of products and reactions, but with the conservation of the basic channels of the process and the principally important types of elementary acts.

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